Full wwPDB EM Validation Report ⓘ

Jul 20, 2025 – 02:13 PM JST

PDB ID	:	9VQQ / pdb_00009vqq
EMDB ID	:	EMD-65273
Title	:	Cryo-EM structure of drosophila TRPgamma determined in GDN, state 1
Deposited on	:	2025-07-05
Resolution	:	2.18 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

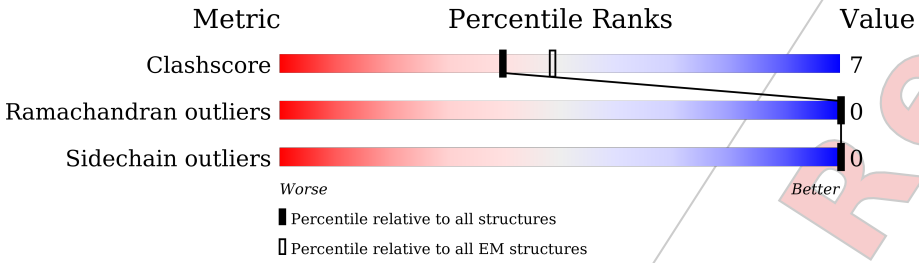
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.18 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1128	55% 7% 38%
1	B	1128	55% 7% 38%
1	C	1128	55% 7% 38%
1	D	1128	56% 6% 38%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 23664 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transient receptor potential-gamma protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	699	Total 5716	C 3691	N 966	O 1027	S 32	0	0
1	B	699	Total 5716	C 3691	N 966	O 1027	S 32	0	0
1	C	699	Total 5716	C 3691	N 966	O 1027	S 32	0	0
1	D	699	Total 5716	C 3691	N 966	O 1027	S 32	0	0

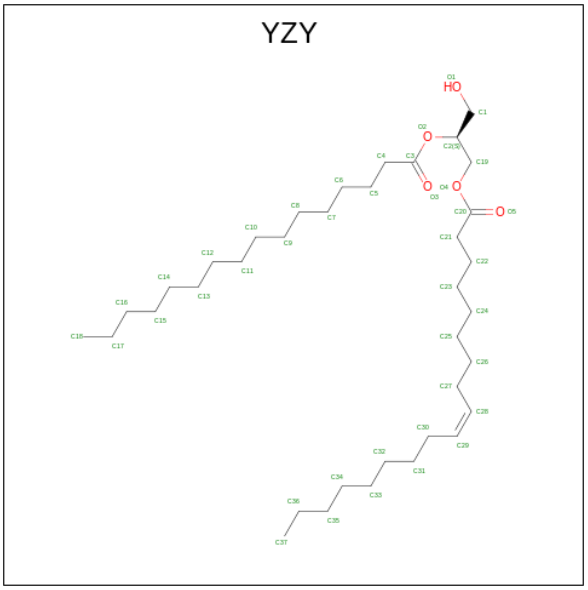
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	2	Total 2	Ca 2	0
2	B	2	Total 2	Ca 2	0
2	C	2	Total 2	Ca 2	0
2	D	2	Total 2	Ca 2	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

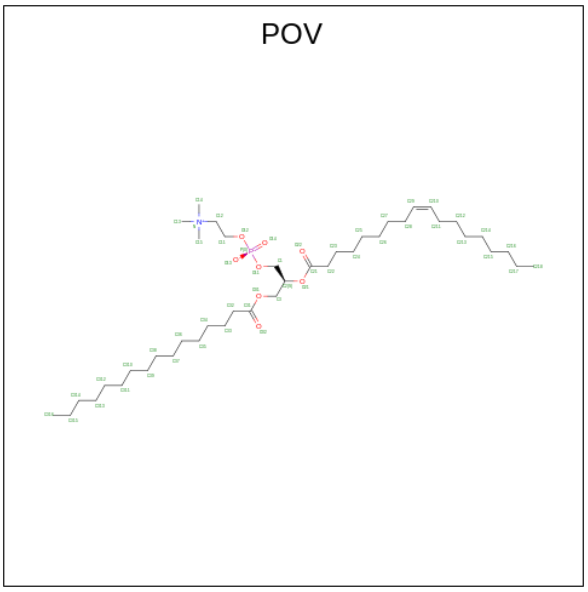
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total 1	Zn 1	0
3	B	1	Total 1	Zn 1	0
3	C	1	Total 1	Zn 1	0
3	D	1	Total 1	Zn 1	0

- Molecule 4 is (2S)-2-(hexadecanoyloxy)-3-hydroxypropyl (9Z)-octadec-9-enoate (CCD ID: YZY) (formula: $C_{37}H_{70}O_5$).



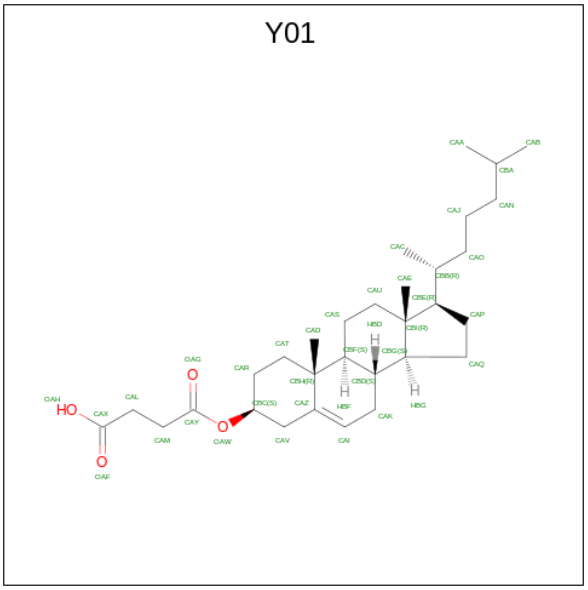
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C O 35 30 5	0
4	B	1	Total C O 35 30 5	0
4	C	1	Total C O 35 30 5	0
4	D	1	Total C O 35 30 5	0

- Molecule 5 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: $C_{42}H_{82}NO_8P$).



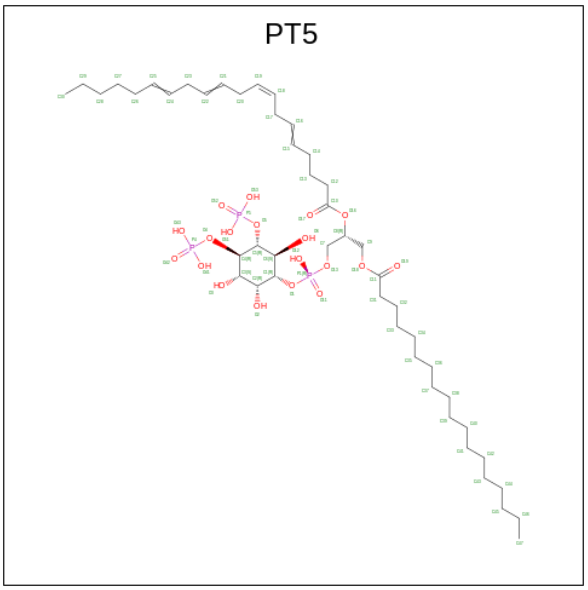
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	D	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 6 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total 35	C 31	O 4	0
6	B	1	Total 35	C 31	O 4	0
6	C	1	Total 35	C 31	O 4	0
6	D	1	Total 35	C 31	O 4	0

- Molecule 7 is [(2R)-1-octadecanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phospho ryl]oxy-propan-2-yl] (8Z)-icosa-5,8,11,14-tetraenoate (CCD ID: PT5) (formula: $C_{47}H_{85}O_{19}P_3$).



Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total 69	C 47	O 19	P 3	0
7	B	1	Total 69	C 47	O 19	P 3	0
7	C	1	Total 69	C 47	O 19	P 3	0
7	D	1	Total 69	C 47	O 19	P 3	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	A	6	Total 6	O 6	0

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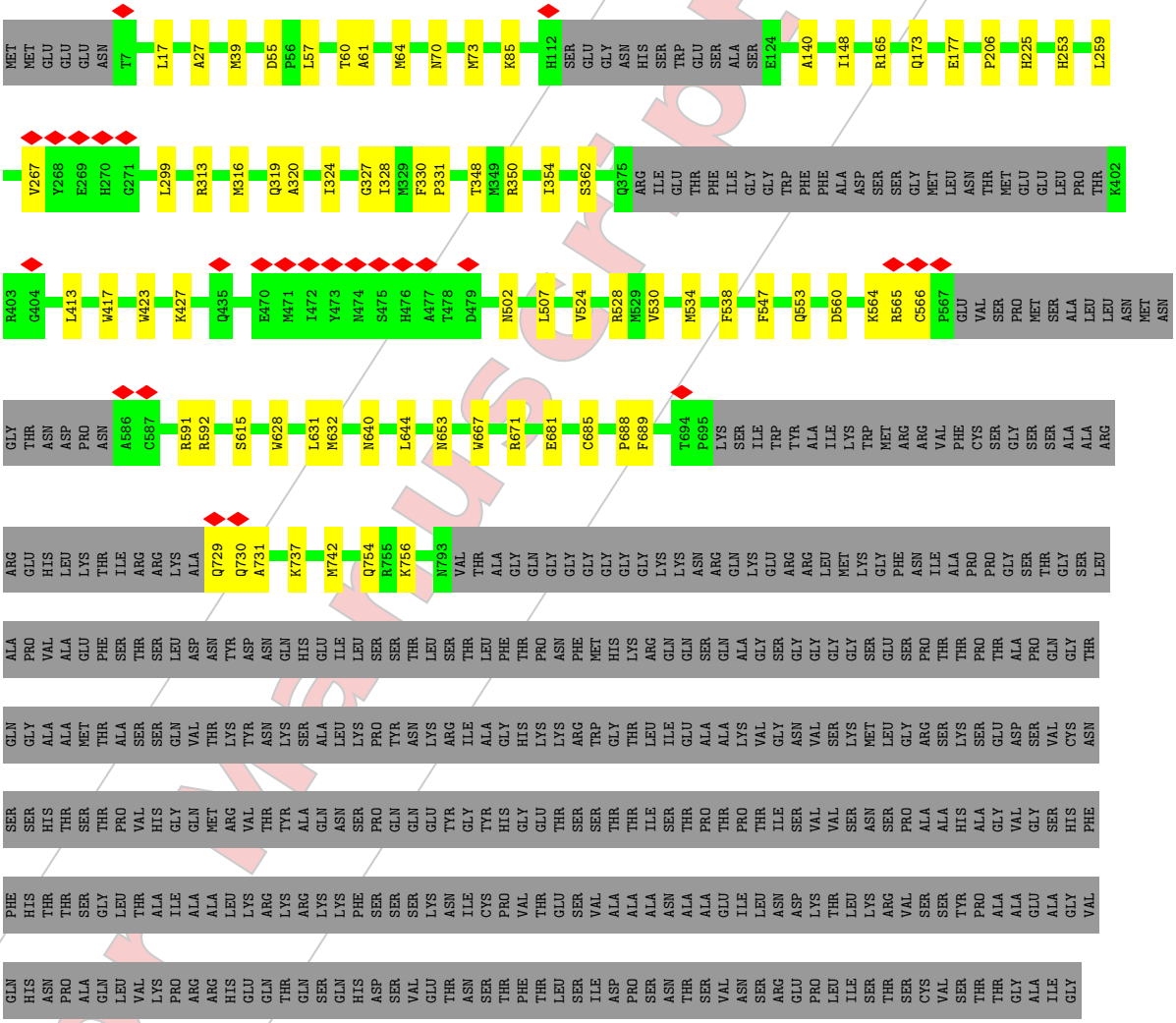
Mol	Chain	Residues	Atoms	AltConf
8	B	6	Total O 6 6	0
8	C	6	Total O 6 6	0
8	D	6	Total O 6 6	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Transient receptor potential-gamma protein

Chain A:

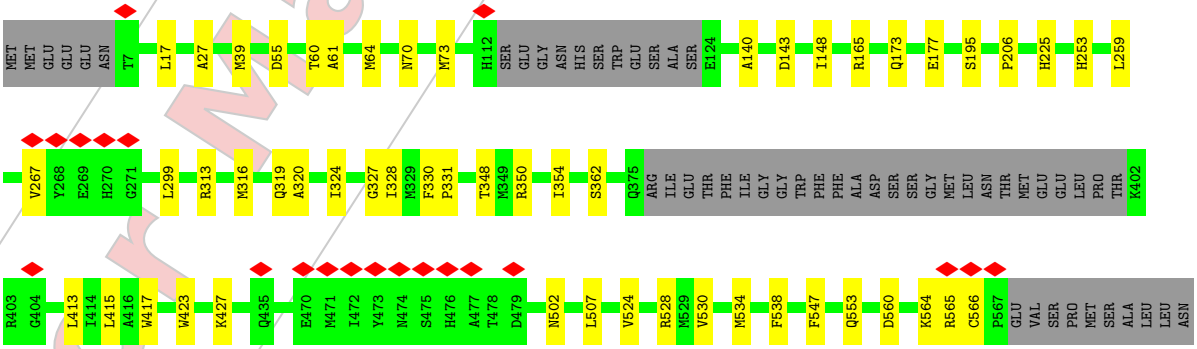


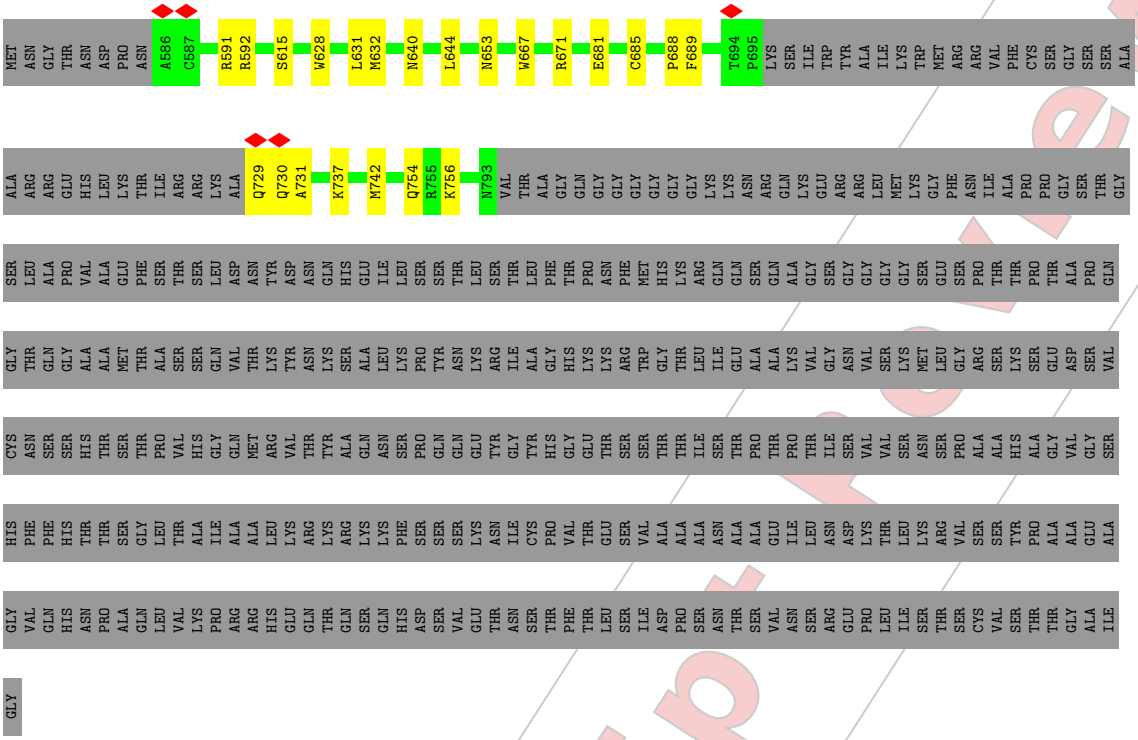
• Molecule 1: Transient receptor potential-gamma protein

Chain B:

• Molecule 1: Transient receptor potential-gamma protein

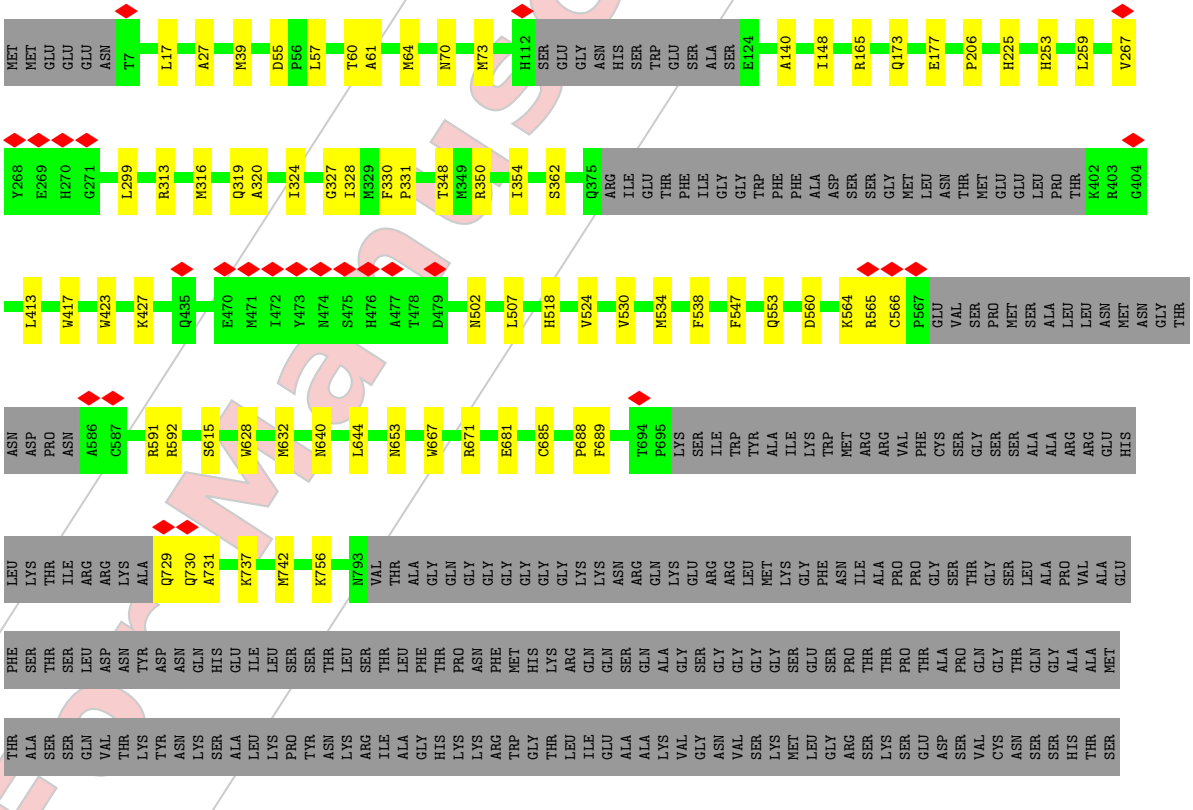
Chain C:





• Molecule 1: Transient receptor potential-gamma protein

Chain D:



THR PRO VAL HIS GLY GLN MET ARG VAL THR TYR ALA GLN ASN SER PRO GLN GLN GLU TYR GLY TYR HIS GLY GLU THR SER SER THR THR ILE SER THR PRO THR PRO THR ILE SER VAL VAL SER ASN SER PRO ALA ALA HIS ALA GLY VAL GLY SER HIS PHE PHE HIS THR THR SER

GLY LEU THR ALA ILE ALA ALA LEU LYS ARG LYS ARG LYS LYS PHE SER SER SER LYS ASN ILE CYS PRO VAL THR GLU SER VAL ALA ALA ALA ALA ASN ALA ALA ALA GLU ILE LEU ASN ASP LYS THR LEU LYS ARG VAL SER SER TYR PRO ALA ALA GLU ALA GLY VAL GLN HIS ASN PRO ALA

GLN LEU VAL LYS PRO ARG ARG HIS GLU GLN GLN THR GLN SER GLN HIS ASP SER VAL GLU THR ASN SER THR PHE THR LEU SER ILE ASP PRO SER ASN THR SER VAL ASN SER ARG GLU PRO LEU ILE SER THR SER CYS VAL SER THR THR GLY ALA ILE GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	633561	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	-1400	Depositor
Maximum defocus (nm)	-2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.331	Depositor
Minimum map value	-1.645	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.068	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, YZY, CA, PT5, POV, Y01

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.15	0/5848	0.29	0/7920
1	B	0.15	0/5848	0.29	0/7920
1	C	0.15	0/5848	0.29	0/7920
1	D	0.15	0/5848	0.29	0/7920
All	All	0.15	0/23392	0.29	0/31680

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5716	0	5706	88	0
1	B	5716	0	5706	88	0
1	C	5716	0	5706	84	0
1	D	5716	0	5706	82	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	35	0	53	1	0
4	B	35	0	53	1	0
4	C	35	0	53	1	0
4	D	35	0	53	1	0
5	A	52	0	82	15	0
5	B	52	0	82	16	0
5	C	52	0	82	15	0
5	D	52	0	82	16	0
6	A	35	0	49	8	0
6	B	35	0	49	10	0
6	C	35	0	49	8	0
6	D	35	0	49	9	0
7	A	69	0	80	5	0
7	B	69	0	80	5	0
7	C	69	0	80	4	0
7	D	69	0	80	4	0
8	A	6	0	0	0	0
8	B	6	0	0	0	0
8	C	6	0	0	0	0
8	D	6	0	0	0	0
All	All	23664	0	23880	329	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (329) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1205:POV:H15	1:D:225:HIS:CB	1.74	1.16
1:B:225:HIS:HB3	5:C:1205:POV:C15	1.75	1.16
1:C:225:HIS:HB3	5:D:1205:POV:C15	1.76	1.16
5:A:1205:POV:C15	1:D:225:HIS:HB3	1.76	1.15
1:B:225:HIS:CB	5:C:1205:POV:H15	1.76	1.15
1:C:225:HIS:CB	5:D:1205:POV:H15	1.76	1.14
1:A:225:HIS:HB3	5:B:1205:POV:C15	1.76	1.14
1:A:225:HIS:CB	5:B:1205:POV:H15	1.76	1.14
1:B:417:TRP:CZ3	1:B:688:PRO:HD3	1.83	1.14
1:D:417:TRP:CZ3	1:D:688:PRO:HD3	1.83	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:TRP:CZ3	1:A:688:PRO:HD3	1.83	1.13
1:A:417:TRP:CH2	1:A:688:PRO:HG3	1.84	1.12
1:B:417:TRP:CH2	1:B:688:PRO:HG3	1.84	1.12
1:C:417:TRP:CZ3	1:C:688:PRO:HD3	1.83	1.12
1:C:417:TRP:CH2	1:C:688:PRO:HG3	1.84	1.12
1:D:417:TRP:CH2	1:D:688:PRO:HG3	1.84	1.12
1:A:225:HIS:CB	5:B:1205:POV:C15	2.31	1.09
5:A:1205:POV:C15	1:D:225:HIS:CB	2.30	1.08
1:B:225:HIS:CB	5:C:1205:POV:C15	2.31	1.08
1:C:225:HIS:CB	5:D:1205:POV:C15	2.31	1.06
1:B:225:HIS:HB3	5:C:1205:POV:H15	1.05	1.04
1:A:225:HIS:HB3	5:B:1205:POV:H15	1.05	1.03
5:A:1205:POV:H15	1:D:225:HIS:HB3	1.04	1.01
1:C:225:HIS:HB3	5:D:1205:POV:H15	1.03	1.01
1:A:417:TRP:CE3	1:A:688:PRO:HD3	1.99	0.98
1:B:417:TRP:CE3	1:B:688:PRO:HD3	1.98	0.98
1:C:417:TRP:CE3	1:C:688:PRO:HD3	1.98	0.98
1:A:316:MET:HG3	5:A:1205:POV:H23A	1.46	0.98
1:D:316:MET:HG3	5:D:1205:POV:H23A	1.46	0.98
1:B:316:MET:HG3	5:B:1205:POV:H23A	1.46	0.97
1:D:417:TRP:CZ3	1:D:688:PRO:CD	2.48	0.97
1:D:417:TRP:CE3	1:D:688:PRO:HD3	1.98	0.97
1:A:417:TRP:CZ3	1:A:688:PRO:CD	2.48	0.96
1:C:417:TRP:CZ3	1:C:688:PRO:CD	2.48	0.96
1:C:316:MET:HG3	5:C:1205:POV:H23A	1.46	0.96
1:B:417:TRP:CZ3	1:B:688:PRO:CD	2.48	0.96
1:C:417:TRP:CZ3	1:C:688:PRO:HG3	2.01	0.95
1:D:417:TRP:CZ3	1:D:688:PRO:HG3	2.01	0.95
1:A:417:TRP:CZ3	1:A:688:PRO:HG3	2.01	0.95
1:B:417:TRP:CZ3	1:B:688:PRO:HG3	2.01	0.94
1:A:70:ASN:ND2	1:A:73:MET:HB2	1.84	0.93
1:C:70:ASN:ND2	1:C:73:MET:HB2	1.84	0.93
1:D:70:ASN:ND2	1:D:73:MET:HB2	1.84	0.93
1:B:70:ASN:ND2	1:B:73:MET:HB2	1.84	0.93
1:B:362:SER:HG	1:B:417:TRP:HZ3	0.95	0.92
1:C:362:SER:HG	1:C:417:TRP:HZ3	0.93	0.89
1:C:417:TRP:CZ3	1:C:688:PRO:CG	2.56	0.89
1:D:417:TRP:CZ3	1:D:688:PRO:CG	2.56	0.89
1:D:362:SER:HG	1:D:417:TRP:HZ3	0.93	0.89
1:A:417:TRP:CZ3	1:A:688:PRO:CG	2.56	0.89
1:A:362:SER:HG	1:A:417:TRP:HZ3	0.95	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:TRP:CZ3	1:B:688:PRO:CG	2.56	0.88
5:A:1205:POV:H15A	1:D:225:HIS:CG	2.15	0.81
1:B:225:HIS:CB	5:C:1205:POV:H15A	2.12	0.80
1:B:225:HIS:CG	5:C:1205:POV:H15A	2.16	0.80
1:A:225:HIS:CG	5:B:1205:POV:H15A	2.16	0.80
1:C:225:HIS:CG	5:D:1205:POV:H15A	2.16	0.80
1:A:225:HIS:CB	5:B:1205:POV:H15A	2.12	0.78
1:C:225:HIS:CB	5:D:1205:POV:H15A	2.13	0.78
5:A:1205:POV:H15A	1:D:225:HIS:CB	2.11	0.78
1:B:70:ASN:ND2	1:B:73:MET:CB	2.49	0.76
1:C:70:ASN:ND2	1:C:73:MET:CB	2.49	0.76
1:B:316:MET:CG	5:B:1205:POV:H23A	2.16	0.75
1:C:316:MET:CG	5:C:1205:POV:H23A	2.16	0.75
1:D:70:ASN:ND2	1:D:73:MET:CB	2.49	0.75
1:C:547:PHE:CZ	6:D:1206:Y01:HAC2	2.22	0.75
1:A:316:MET:CG	5:A:1205:POV:H23A	2.16	0.74
1:D:316:MET:CG	5:D:1205:POV:H23A	2.16	0.74
1:A:70:ASN:ND2	1:A:73:MET:CB	2.49	0.74
1:A:547:PHE:CZ	6:B:1206:Y01:HAC2	2.24	0.73
1:B:417:TRP:CH2	1:B:688:PRO:CG	2.70	0.73
1:B:547:PHE:CZ	6:C:1206:Y01:HAC2	2.24	0.72
1:C:653:ASN:HD22	1:D:653:ASN:ND2	1.87	0.72
6:A:1206:Y01:HAC2	1:D:547:PHE:CZ	2.25	0.72
1:A:653:ASN:ND2	1:D:653:ASN:HD22	1.87	0.72
5:A:1205:POV:C15	1:D:225:HIS:HB2	2.19	0.72
1:C:417:TRP:CH2	1:C:688:PRO:CG	2.70	0.71
1:B:316:MET:HG3	5:B:1205:POV:C23	2.20	0.71
1:A:70:ASN:HD22	1:A:73:MET:HB2	1.55	0.71
1:B:653:ASN:HD22	1:C:653:ASN:ND2	1.88	0.71
1:C:70:ASN:HD22	1:C:73:MET:HB2	1.55	0.71
1:C:547:PHE:CZ	6:D:1206:Y01:CAC	2.74	0.71
1:B:70:ASN:HD22	1:B:73:MET:HB2	1.55	0.70
1:C:316:MET:HG3	5:C:1205:POV:C23	2.20	0.70
1:A:362:SER:OG	1:A:417:TRP:HZ3	1.72	0.70
1:B:225:HIS:HB2	5:C:1205:POV:C15	2.20	0.70
1:A:653:ASN:HD22	1:B:653:ASN:ND2	1.88	0.70
1:D:362:SER:OG	1:D:417:TRP:HZ3	1.72	0.70
1:D:70:ASN:HD22	1:D:73:MET:HB2	1.55	0.70
1:C:225:HIS:HB2	5:D:1205:POV:C15	2.22	0.69
1:B:547:PHE:CZ	6:C:1206:Y01:CAC	2.76	0.69
1:A:547:PHE:CZ	6:B:1206:Y01:CAC	2.76	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:HIS:HB2	5:B:1205:POV:C15	2.21	0.69
1:B:362:SER:OG	1:B:417:TRP:HZ3	1.72	0.68
1:D:316:MET:HG3	5:D:1205:POV:C23	2.20	0.68
1:A:316:MET:HG3	5:A:1205:POV:C23	2.20	0.68
1:C:362:SER:OG	1:C:417:TRP:HZ3	1.72	0.68
1:C:547:PHE:HZ	6:D:1206:Y01:HAC2	1.58	0.68
1:B:547:PHE:HZ	6:C:1206:Y01:HAC2	1.60	0.67
6:A:1206:Y01:CAC	1:D:547:PHE:CZ	2.77	0.67
1:A:70:ASN:HD22	1:A:73:MET:CB	2.07	0.67
1:B:70:ASN:HD22	1:B:73:MET:CB	2.07	0.65
1:D:70:ASN:HD22	1:D:73:MET:CB	2.07	0.65
1:A:417:TRP:CH2	1:A:688:PRO:CG	2.70	0.65
1:C:70:ASN:HD22	1:C:73:MET:CB	2.07	0.65
6:A:1206:Y01:HAC2	1:D:547:PHE:HZ	1.60	0.65
1:B:592:ARG:HH11	1:B:615:SER:HB3	1.61	0.65
1:D:592:ARG:HH11	1:D:615:SER:HB3	1.61	0.64
1:A:592:ARG:HH11	1:A:615:SER:HB3	1.61	0.64
1:D:350:ARG:NH1	1:D:681:GLU:OE1	2.30	0.64
1:C:592:ARG:HH11	1:C:615:SER:HB3	1.61	0.64
1:D:328:ILE:HA	5:D:1205:POV:H31G	1.80	0.64
1:A:350:ARG:NH1	1:A:681:GLU:OE1	2.30	0.63
1:A:328:ILE:HA	5:A:1205:POV:H31G	1.80	0.63
1:B:328:ILE:HA	5:B:1205:POV:H31G	1.80	0.63
1:B:350:ARG:NH1	1:B:681:GLU:OE1	2.30	0.63
1:A:547:PHE:HZ	6:B:1206:Y01:HAC2	1.60	0.62
1:C:328:ILE:HA	5:C:1205:POV:H31G	1.80	0.62
1:C:350:ARG:NH1	1:C:681:GLU:OE1	2.30	0.61
1:C:206:PRO:HD2	1:C:742:MET:HG2	1.83	0.60
1:A:206:PRO:HD2	1:A:742:MET:HG2	1.83	0.60
1:B:206:PRO:HD2	1:B:742:MET:HG2	1.84	0.60
1:D:206:PRO:HD2	1:D:742:MET:HG2	1.83	0.60
1:D:685:CYS:SG	1:D:689:PHE:HB2	2.42	0.60
1:A:685:CYS:SG	1:A:689:PHE:HB2	2.42	0.60
1:C:685:CYS:SG	1:C:689:PHE:HB2	2.42	0.60
1:B:685:CYS:SG	1:B:689:PHE:HB2	2.42	0.59
1:D:417:TRP:CH2	1:D:688:PRO:CG	2.70	0.59
1:D:413:LEU:O	1:D:417:TRP:HD1	1.87	0.58
1:A:413:LEU:O	1:A:417:TRP:HD1	1.87	0.58
1:A:530:VAL:HG22	4:A:1204:YZY:H182	1.86	0.58
1:B:413:LEU:O	1:B:417:TRP:HD1	1.87	0.58
1:D:530:VAL:HG22	4:D:1204:YZY:H182	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:VAL:HG22	4:B:1204:YZY:H182	1.86	0.58
1:C:530:VAL:HG22	4:C:1204:YZY:H182	1.86	0.57
1:C:413:LEU:O	1:C:417:TRP:HD1	1.87	0.57
1:A:565:ARG:HH21	1:A:566:CYS:HB2	1.70	0.57
1:C:565:ARG:HH21	1:C:566:CYS:HB2	1.70	0.57
1:C:653:ASN:ND2	1:D:653:ASN:ND2	2.50	0.57
1:C:653:ASN:ND2	1:D:653:ASN:HD21	2.03	0.57
1:A:653:ASN:HD21	1:D:653:ASN:ND2	2.03	0.56
1:D:565:ARG:HH21	1:D:566:CYS:HB2	1.70	0.56
1:A:653:ASN:ND2	1:B:653:ASN:ND2	2.53	0.56
1:C:348:THR:HG22	1:C:354:ILE:HG21	1.88	0.56
1:D:348:THR:HG22	1:D:354:ILE:HG21	1.88	0.56
1:B:348:THR:HG22	1:B:354:ILE:HG21	1.88	0.56
1:A:348:THR:HG22	1:A:354:ILE:HG21	1.88	0.56
1:B:653:ASN:ND2	1:C:653:ASN:ND2	2.53	0.56
1:B:565:ARG:HH21	1:B:566:CYS:HB2	1.70	0.56
1:D:140:ALA:HA	1:D:148:ILE:HD11	1.89	0.55
1:A:653:ASN:ND2	1:D:653:ASN:ND2	2.52	0.55
1:A:140:ALA:HA	1:A:148:ILE:HD11	1.89	0.55
1:A:653:ASN:ND2	1:B:653:ASN:HD21	2.05	0.55
1:A:60:THR:O	1:A:64:MET:HG3	2.07	0.55
1:B:653:ASN:ND2	1:C:653:ASN:HD21	2.05	0.55
1:D:60:THR:O	1:D:64:MET:HG3	2.07	0.54
1:B:538:PHE:HB2	7:B:1207:PT5:H57	1.90	0.54
1:B:60:THR:O	1:B:64:MET:HG3	2.07	0.54
1:C:60:THR:O	1:C:64:MET:HG3	2.07	0.54
1:C:320:ALA:O	1:C:324:ILE:HG13	2.09	0.54
1:B:140:ALA:HA	1:B:148:ILE:HD11	1.89	0.53
1:A:538:PHE:HB2	7:A:1207:PT5:H57	1.90	0.53
1:C:140:ALA:HA	1:C:148:ILE:HD11	1.89	0.53
1:D:320:ALA:O	1:D:324:ILE:HG13	2.09	0.53
1:D:538:PHE:HB2	7:D:1207:PT5:H57	1.90	0.53
1:B:320:ALA:O	1:B:324:ILE:HG13	2.09	0.53
7:B:1207:PT5:H21	1:C:316:MET:HE1	1.91	0.53
1:D:560:ASP:OD2	1:D:564:LYS:NZ	2.41	0.53
1:A:225:HIS:HB2	5:B:1205:POV:H15	1.81	0.53
1:C:538:PHE:HB2	7:C:1207:PT5:H57	1.90	0.53
1:D:591:ARG:HG3	1:D:591:ARG:HH11	1.74	0.52
1:A:591:ARG:HG3	1:A:591:ARG:HH11	1.74	0.52
7:A:1207:PT5:H21	1:B:316:MET:HE1	1.91	0.52
1:A:320:ALA:O	1:A:324:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:591:ARG:HG3	1:C:591:ARG:HH11	1.74	0.52
1:B:591:ARG:HG3	1:B:591:ARG:HH11	1.73	0.52
1:B:560:ASP:OD2	1:B:564:LYS:NZ	2.41	0.52
1:C:560:ASP:OD2	1:C:564:LYS:NZ	2.41	0.51
1:D:507:LEU:CD1	6:D:1206:Y01:HAE2	2.41	0.51
1:A:507:LEU:CD1	6:A:1206:Y01:HAE2	2.41	0.51
1:A:316:MET:HE1	7:D:1207:PT5:H21	1.93	0.51
7:C:1207:PT5:H21	1:D:316:MET:HE1	1.93	0.51
1:A:327:GLY:HA3	5:A:1205:POV:H310	1.94	0.50
1:B:671:ARG:HH12	5:B:1205:POV:H14A	1.76	0.50
1:C:327:GLY:HA3	5:C:1205:POV:H310	1.94	0.50
1:C:671:ARG:HH12	5:C:1205:POV:H14A	1.76	0.50
1:D:327:GLY:HA3	5:D:1205:POV:H310	1.94	0.50
1:A:671:ARG:HH12	5:A:1205:POV:H14A	1.76	0.50
1:C:507:LEU:CD1	6:C:1206:Y01:HAE2	2.41	0.50
1:D:671:ARG:HH12	5:D:1205:POV:H14A	1.76	0.50
1:B:327:GLY:HA3	5:B:1205:POV:H310	1.94	0.50
1:C:507:LEU:HD13	6:C:1206:Y01:HAE1	1.94	0.50
1:B:507:LEU:HD13	6:B:1206:Y01:HAE1	1.95	0.49
7:C:1207:PT5:C12	1:D:316:MET:HE1	2.42	0.49
1:D:61:ALA:HA	1:D:64:MET:HE2	1.95	0.49
7:B:1207:PT5:C12	1:C:316:MET:HE1	2.41	0.49
1:C:61:ALA:HA	1:C:64:MET:HE2	1.95	0.49
1:A:507:LEU:HD13	6:A:1206:Y01:HAE1	1.95	0.49
1:B:61:ALA:HA	1:B:64:MET:HE2	1.95	0.49
1:D:507:LEU:HD13	6:D:1206:Y01:HAE1	1.94	0.49
1:A:560:ASP:OD2	1:A:564:LYS:NZ	2.41	0.49
1:B:507:LEU:CD1	6:B:1206:Y01:HAE2	2.41	0.49
7:A:1207:PT5:C12	1:B:316:MET:HE1	2.41	0.49
1:A:61:ALA:HA	1:A:64:MET:HE2	1.95	0.48
1:A:417:TRP:HZ3	1:A:688:PRO:CD	2.21	0.48
1:B:173:GLN:NE2	1:B:177:GLU:OE1	2.46	0.48
1:A:316:MET:HE1	7:D:1207:PT5:C12	2.44	0.47
1:B:417:TRP:HZ3	1:B:688:PRO:CD	2.21	0.47
1:C:165:ARG:HH21	1:D:313:ARG:HB3	1.80	0.47
1:C:756:LYS:HE3	1:C:756:LYS:HB2	1.68	0.47
1:A:756:LYS:HE3	1:A:756:LYS:HB2	1.68	0.47
1:C:413:LEU:O	1:C:417:TRP:CD1	2.67	0.47
1:C:729:GLN:HG3	1:C:731:ALA:H	1.80	0.47
1:D:413:LEU:O	1:D:417:TRP:CD1	2.67	0.47
1:A:413:LEU:O	1:A:417:TRP:CD1	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:GLN:HG2	1:D:57:LEU:HD13	1.97	0.47
6:A:1206:Y01:HAC3	6:A:1206:Y01:HAJ1	1.74	0.47
1:C:173:GLN:NE2	1:C:177:GLU:OE1	2.46	0.47
1:D:173:GLN:NE2	1:D:177:GLU:OE1	2.46	0.46
1:A:729:GLN:HG3	1:A:731:ALA:H	1.80	0.46
1:B:413:LEU:O	1:B:417:TRP:CD1	2.68	0.46
7:B:1207:PT5:H57	7:B:1207:PT5:H64	1.59	0.46
1:B:729:GLN:HG3	1:B:731:ALA:H	1.80	0.46
1:D:729:GLN:HG3	1:D:731:ALA:H	1.80	0.46
1:B:57:LEU:HD13	1:C:754:GLN:HG2	1.97	0.46
1:B:425:GLU:OE1	1:B:437:TYR:OH	2.29	0.45
1:A:57:LEU:HD13	1:B:754:GLN:HG2	1.98	0.45
1:C:267:VAL:HG21	1:C:730:GLN:HE21	1.81	0.45
1:D:507:LEU:CD1	6:D:1206:Y01:CAE	2.95	0.45
1:A:507:LEU:CD1	6:A:1206:Y01:CAE	2.95	0.45
1:B:267:VAL:HG21	1:B:730:GLN:HE21	1.81	0.45
1:A:640:ASN:HA	1:A:644:LEU:HB2	1.99	0.45
1:A:267:VAL:HG21	1:A:730:GLN:HE21	1.81	0.45
1:C:507:LEU:CD1	6:C:1206:Y01:CAE	2.95	0.45
7:D:1207:PT5:H57	7:D:1207:PT5:H64	1.59	0.45
1:B:507:LEU:CD1	6:B:1206:Y01:CAE	2.95	0.44
1:B:756:LYS:HB2	1:B:756:LYS:HE3	1.68	0.44
1:C:553:GLN:OE1	1:D:502:ASN:ND2	2.50	0.44
1:D:267:VAL:HG21	1:D:730:GLN:HE21	1.81	0.44
1:D:640:ASN:HA	1:D:644:LEU:HB2	1.99	0.44
1:A:173:GLN:NE2	1:A:177:GLU:OE1	2.46	0.44
7:B:1207:PT5:H76	7:B:1207:PT5:H70	1.67	0.44
1:D:628:TRP:CD1	1:D:632:MET:HE3	2.52	0.44
1:A:628:TRP:CD1	1:A:632:MET:HE3	2.52	0.44
7:A:1207:PT5:H76	7:A:1207:PT5:H70	1.67	0.44
1:C:628:TRP:CD1	1:C:632:MET:HE3	2.52	0.44
1:A:330:PHE:CD2	1:A:331:PRO:HD3	2.53	0.44
1:B:165:ARG:HH21	1:C:313:ARG:HB3	1.83	0.44
1:B:524:VAL:HG21	1:B:667:TRP:HA	2.00	0.44
1:B:628:TRP:CD1	1:B:632:MET:HE3	2.52	0.44
1:C:524:VAL:HG21	1:C:667:TRP:HA	2.00	0.44
1:A:165:ARG:HH21	1:B:313:ARG:HB3	1.83	0.44
6:D:1206:Y01:HAJ1	6:D:1206:Y01:HAC3	1.74	0.44
1:C:259:LEU:HD12	1:C:299:LEU:HD23	2.00	0.43
1:A:417:TRP:HZ3	1:A:688:PRO:HD3	1.69	0.43
1:B:330:PHE:CD2	1:B:331:PRO:HD3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:HIS:HE1	1:B:737:LYS:NZ	2.17	0.43
1:B:259:LEU:HD12	1:B:299:LEU:HD23	2.00	0.43
1:B:640:ASN:HA	1:B:644:LEU:HB2	1.99	0.43
1:D:253:HIS:HE1	1:D:737:LYS:NZ	2.17	0.43
1:C:253:HIS:HE1	1:C:737:LYS:NZ	2.17	0.43
1:B:85:LYS:HB2	1:B:85:LYS:HE2	1.86	0.43
1:A:313:ARG:HB3	1:D:165:ARG:HH21	1.83	0.43
1:C:225:HIS:CD2	5:D:1205:POV:H15A	2.51	0.43
1:A:259:LEU:HD12	1:A:299:LEU:HD23	2.00	0.43
1:C:330:PHE:CD2	1:C:331:PRO:HD3	2.53	0.43
1:B:17:LEU:HD11	1:B:55:ASP:HA	2.00	0.43
1:C:640:ASN:HA	1:C:644:LEU:HB2	1.99	0.43
1:D:330:PHE:CD2	1:D:331:PRO:HD3	2.53	0.43
1:A:316:MET:HA	1:A:319:GLN:HB2	2.01	0.43
1:D:259:LEU:HD12	1:D:299:LEU:HD23	2.00	0.43
1:A:524:VAL:HG21	1:A:667:TRP:HA	2.00	0.42
1:A:553:GLN:OE1	1:B:502:ASN:ND2	2.52	0.42
1:B:316:MET:HA	1:B:319:GLN:HB2	2.01	0.42
7:A:1207:PT5:H57	7:A:1207:PT5:H64	1.59	0.42
1:B:225:HIS:CD2	5:C:1205:POV:H15A	2.54	0.42
1:B:530:VAL:O	1:B:534:MET:HG2	2.20	0.42
1:D:524:VAL:HG21	1:D:667:TRP:HA	2.00	0.42
1:A:502:ASN:ND2	1:D:553:GLN:OE1	2.53	0.42
6:B:1206:Y01:HAE2	6:B:1206:Y01:HBB	1.91	0.42
1:D:756:LYS:HB2	1:D:756:LYS:HE3	1.68	0.42
1:A:253:HIS:HE1	1:A:737:LYS:NZ	2.17	0.42
1:C:143:ASP:OD1	1:C:195:SER:OG	2.30	0.42
1:A:85:LYS:HB2	1:A:85:LYS:HE2	1.86	0.42
1:C:225:HIS:HB2	5:D:1205:POV:H15	1.82	0.42
6:C:1206:Y01:HAE2	6:C:1206:Y01:HBB	1.91	0.42
1:D:17:LEU:HD11	1:D:55:ASP:HA	2.01	0.42
1:D:530:VAL:O	1:D:534:MET:HG2	2.19	0.42
1:C:415:LEU:HD23	1:C:415:LEU:HA	1.89	0.42
1:C:530:VAL:O	1:C:534:MET:HG2	2.19	0.42
1:D:70:ASN:ND2	1:D:73:MET:HB3	2.33	0.42
1:A:70:ASN:ND2	1:A:73:MET:HB3	2.33	0.42
1:D:417:TRP:HZ3	1:D:688:PRO:CD	2.21	0.42
1:C:631:LEU:HG	6:D:1206:Y01:HAB1	2.02	0.42
1:A:27:ALA:HB3	1:A:39:MET:HE1	2.02	0.42
1:A:530:VAL:O	1:A:534:MET:HG2	2.19	0.42
1:B:415:LEU:HD23	1:B:415:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:553:GLN:OE1	1:C:502:ASN:ND2	2.52	0.42
1:B:27:ALA:HB3	1:B:39:MET:HE1	2.02	0.41
1:C:316:MET:HA	1:C:319:GLN:HB2	2.01	0.41
1:D:27:ALA:HB3	1:D:39:MET:HE1	2.02	0.41
1:B:70:ASN:ND2	1:B:73:MET:HB3	2.33	0.41
6:B:1206:Y01:HAJ1	6:B:1206:Y01:HAC3	1.74	0.41
1:D:316:MET:HA	1:D:319:GLN:HB2	2.01	0.41
1:C:316:MET:SD	5:C:1205:POV:H23A	2.61	0.41
1:A:507:LEU:HD13	6:A:1206:Y01:CAE	2.51	0.41
1:D:316:MET:SD	5:D:1205:POV:H23A	2.61	0.41
1:A:17:LEU:HD11	1:A:55:ASP:HA	2.00	0.41
1:C:17:LEU:HD11	1:C:55:ASP:HA	2.00	0.41
1:D:507:LEU:HD13	6:D:1206:Y01:CAE	2.51	0.41
1:A:225:HIS:CD2	5:B:1205:POV:H15A	2.54	0.41
1:C:27:ALA:HB3	1:C:39:MET:HE1	2.02	0.41
1:A:316:MET:SD	5:A:1205:POV:H23A	2.61	0.41
1:A:423:TRP:NE1	1:A:427:LYS:HE3	2.36	0.41
1:B:631:LEU:HG	6:C:1206:Y01:HAB1	2.03	0.41
1:B:316:MET:SD	5:B:1205:POV:H23A	2.61	0.41
1:B:423:TRP:NE1	1:B:427:LYS:HE3	2.36	0.41
1:C:417:TRP:HZ3	1:C:688:PRO:CD	2.21	0.41
1:C:423:TRP:NE1	1:C:427:LYS:HE3	2.36	0.41
1:C:524:VAL:O	1:C:528:ARG:HG2	2.22	0.40
1:A:631:LEU:HG	6:B:1206:Y01:HAB1	2.03	0.40
1:B:417:TRP:HZ3	1:B:688:PRO:HD3	1.69	0.40
1:B:507:LEU:HD13	6:B:1206:Y01:CAE	2.51	0.40
1:B:591:ARG:HG3	1:B:591:ARG:NH1	2.37	0.40
7:C:1207:PT5:H17	1:D:518:HIS:CE1	2.57	0.40
1:D:423:TRP:NE1	1:D:427:LYS:HE3	2.36	0.40
1:A:524:VAL:O	1:A:528:ARG:HG2	2.22	0.40
1:A:644:LEU:HD23	1:A:644:LEU:HA	1.91	0.40
5:A:1205:POV:H15A	1:D:225:HIS:CD2	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	689/1128 (61%)	685 (99%)	4 (1%)	0	100	100
1	B	689/1128 (61%)	685 (99%)	4 (1%)	0	100	100
1	C	689/1128 (61%)	685 (99%)	4 (1%)	0	100	100
1	D	689/1128 (61%)	685 (99%)	4 (1%)	0	100	100
All	All	2756/4512 (61%)	2740 (99%)	16 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	629/985 (64%)	629 (100%)	0	100	100
1	B	629/985 (64%)	629 (100%)	0	100	100
1	C	629/985 (64%)	629 (100%)	0	100	100
1	D	629/985 (64%)	629 (100%)	0	100	100
All	All	2516/3940 (64%)	2516 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	50	ASN
1	A	70	ASN
1	A	253	HIS
1	A	428	GLN
1	A	502	ASN

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Mol	Chain	Res	Type
1	A	552	ASN
1	A	553	GLN
1	A	740	GLN
1	A	760	GLN
1	B	11	HIS
1	B	50	ASN
1	B	70	ASN
1	B	253	HIS
1	B	428	GLN
1	B	502	ASN
1	B	552	ASN
1	B	553	GLN
1	B	653	ASN
1	B	760	GLN
1	C	11	HIS
1	C	70	ASN
1	C	253	HIS
1	C	428	GLN
1	C	502	ASN
1	C	552	ASN
1	C	553	GLN
1	C	740	GLN
1	C	760	GLN
1	D	11	HIS
1	D	70	ASN
1	D	253	HIS
1	D	428	GLN
1	D	502	ASN
1	D	552	ASN
1	D	553	GLN
1	D	653	ASN
1	D	760	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 12 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	Y01	B	1206	-	38,38,38	0.55	0	57,57,57	1.12	5 (8%)
5	POV	D	1205	-	51,51,51	0.49	0	57,59,59	0.47	0
7	PT5	C	1207	-	69,69,69	1.21	6 (8%)	83,87,87	1.21	6 (7%)
5	POV	B	1205	-	51,51,51	0.49	0	57,59,59	0.47	0
6	Y01	A	1206	-	38,38,38	0.55	0	57,57,57	1.12	5 (8%)
7	PT5	A	1207	-	69,69,69	1.21	6 (8%)	83,87,87	1.21	6 (7%)
4	YZY	A	1204	-	34,34,41	0.93	4 (11%)	36,36,43	1.26	2 (5%)
6	Y01	C	1206	-	38,38,38	0.55	0	57,57,57	1.12	5 (8%)
4	YZY	B	1204	-	34,34,41	0.94	4 (11%)	36,36,43	1.26	2 (5%)
6	Y01	D	1206	-	38,38,38	0.55	0	57,57,57	1.12	5 (8%)
7	PT5	D	1207	-	69,69,69	1.21	6 (8%)	83,87,87	1.21	6 (7%)
5	POV	C	1205	-	51,51,51	0.49	0	57,59,59	0.47	0
5	POV	A	1205	-	51,51,51	0.49	0	57,59,59	0.47	0
4	YZY	C	1204	-	34,34,41	0.93	4 (11%)	36,36,43	1.26	2 (5%)
7	PT5	B	1207	-	69,69,69	1.21	6 (8%)	83,87,87	1.21	6 (7%)
4	YZY	D	1204	-	34,34,41	0.94	4 (11%)	36,36,43	1.26	2 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	Y01	B	1206	-	-	6/19/77/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	POV	D	1205	-	-	21/55/55/55	-
7	PT5	C	1207	-	-	34/66/90/90	0/1/1/1
5	POV	B	1205	-	-	21/55/55/55	-
6	Y01	A	1206	-	-	6/19/77/77	0/4/4/4
7	PT5	A	1207	-	-	34/66/90/90	0/1/1/1
4	YZY	A	1204	-	-	18/36/36/43	-
6	Y01	C	1206	-	-	6/19/77/77	0/4/4/4
4	YZY	B	1204	-	-	18/36/36/43	-
6	Y01	D	1206	-	-	6/19/77/77	0/4/4/4
7	PT5	D	1207	-	-	34/66/90/90	0/1/1/1
5	POV	C	1205	-	-	21/55/55/55	-
5	POV	A	1205	-	-	21/55/55/55	-
4	YZY	C	1204	-	-	18/36/36/43	-
7	PT5	B	1207	-	-	34/66/90/90	0/1/1/1
4	YZY	D	1204	-	-	18/36/36/43	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	1207	PT5	P5-O5	4.26	1.67	1.59
7	A	1207	PT5	P5-O5	4.25	1.67	1.59
7	C	1207	PT5	P5-O5	4.25	1.67	1.59
7	B	1207	PT5	P5-O5	4.21	1.67	1.59
7	A	1207	PT5	P4-O4	3.81	1.66	1.59
7	B	1207	PT5	P4-O4	3.81	1.66	1.59
7	C	1207	PT5	P4-O4	3.81	1.66	1.59
7	D	1207	PT5	P4-O4	3.79	1.66	1.59
7	A	1207	PT5	O18-C11	2.89	1.41	1.33
7	B	1207	PT5	O18-C11	2.89	1.41	1.33
7	C	1207	PT5	O18-C11	2.89	1.41	1.33
7	D	1207	PT5	O18-C11	2.88	1.41	1.33
7	A	1207	PT5	O16-C10	2.76	1.42	1.34
7	B	1207	PT5	O16-C10	2.76	1.42	1.34
7	C	1207	PT5	O16-C10	2.76	1.42	1.34
7	D	1207	PT5	O16-C10	2.74	1.42	1.34
7	D	1207	PT5	P1-O1	2.57	1.67	1.60
4	D	1204	YZY	O2-C2	-2.57	1.40	1.46
4	A	1204	YZY	O2-C2	-2.56	1.40	1.46
4	B	1204	YZY	O2-C2	-2.56	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1204	YZY	O2-C2	-2.56	1.40	1.46
7	A	1207	PT5	P1-O1	2.54	1.67	1.60
7	B	1207	PT5	P1-O1	2.53	1.67	1.60
7	C	1207	PT5	P1-O1	2.53	1.67	1.60
4	A	1204	YZY	O4-C20	2.33	1.40	1.33
4	B	1204	YZY	O4-C20	2.33	1.40	1.33
4	C	1204	YZY	O4-C20	2.33	1.40	1.33
7	B	1207	PT5	O16-C8	-2.33	1.40	1.46
7	D	1207	PT5	O16-C8	-2.31	1.40	1.46
4	D	1204	YZY	O4-C20	2.31	1.40	1.33
7	C	1207	PT5	O16-C8	-2.30	1.40	1.46
7	A	1207	PT5	O16-C8	-2.29	1.40	1.46
4	D	1204	YZY	O4-C19	-2.21	1.40	1.45
4	A	1204	YZY	O4-C19	-2.20	1.40	1.45
4	B	1204	YZY	O4-C19	-2.20	1.40	1.45
4	C	1204	YZY	O4-C19	-2.20	1.40	1.45
4	A	1204	YZY	O2-C3	2.11	1.40	1.34
4	B	1204	YZY	O2-C3	2.11	1.40	1.34
4	D	1204	YZY	O2-C3	2.11	1.40	1.34
4	C	1204	YZY	O2-C3	2.10	1.40	1.34

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	1207	PT5	C21-C20-C19	4.85	135.89	112.02
7	B	1207	PT5	C21-C20-C19	4.84	135.88	112.02
7	A	1207	PT5	C21-C20-C19	4.84	135.86	112.02
7	D	1207	PT5	C21-C20-C19	4.84	135.84	112.02
7	D	1207	PT5	O16-C10-C12	4.29	120.75	111.50
7	A	1207	PT5	O16-C10-C12	4.28	120.73	111.50
7	B	1207	PT5	O16-C10-C12	4.28	120.73	111.50
7	C	1207	PT5	O16-C10-C12	4.26	120.69	111.50
4	C	1204	YZY	O2-C3-C4	4.01	120.15	111.50
4	A	1204	YZY	O2-C3-C4	4.00	120.11	111.50
4	B	1204	YZY	O2-C3-C4	3.98	120.08	111.50
4	D	1204	YZY	O2-C3-C4	3.98	120.08	111.50
7	C	1207	PT5	C20-C19-C18	3.45	152.72	123.57
7	D	1207	PT5	C20-C19-C18	3.45	152.71	123.57
7	A	1207	PT5	C20-C19-C18	3.45	152.69	123.57
7	B	1207	PT5	C20-C19-C18	3.45	152.69	123.57
7	B	1207	PT5	C23-C22-C21	3.44	152.58	123.57
7	C	1207	PT5	C23-C22-C21	3.44	152.58	123.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	1207	PT5	C23-C22-C21	3.44	152.58	123.57
7	A	1207	PT5	C23-C22-C21	3.43	152.54	123.57
7	C	1207	PT5	C17-C16-C15	3.42	152.45	123.57
7	A	1207	PT5	C17-C16-C15	3.42	152.44	123.57
7	B	1207	PT5	C17-C16-C15	3.42	152.43	123.57
7	D	1207	PT5	C17-C16-C15	3.42	152.42	123.57
6	A	1206	Y01	CBC-CAV-CAZ	2.98	116.15	111.52
6	C	1206	Y01	CBC-CAV-CAZ	2.97	116.14	111.52
6	B	1206	Y01	CBC-CAV-CAZ	2.96	116.12	111.52
6	D	1206	Y01	CBC-CAV-CAZ	2.96	116.11	111.52
7	C	1207	PT5	O18-C11-C31	2.79	120.65	111.91
7	A	1207	PT5	O18-C11-C31	2.77	120.61	111.91
7	B	1207	PT5	O18-C11-C31	2.76	120.58	111.91
7	D	1207	PT5	O18-C11-C31	2.76	120.58	111.91
6	D	1206	Y01	CAR-CBC-CAV	2.68	114.98	110.99
6	B	1206	Y01	CAR-CBC-CAV	2.67	114.97	110.99
6	B	1206	Y01	CAV-CAZ-CAI	-2.66	116.77	120.61
6	A	1206	Y01	CAR-CBC-CAV	2.65	114.94	110.99
6	C	1206	Y01	CAV-CAZ-CAI	-2.65	116.78	120.61
6	C	1206	Y01	CAR-CBC-CAV	2.65	114.94	110.99
6	D	1206	Y01	CAV-CAZ-CAI	-2.64	116.80	120.61
6	A	1206	Y01	CAV-CAZ-CAI	-2.64	116.81	120.61
4	C	1204	YZY	O4-C20-C21	2.59	120.03	111.91
4	B	1204	YZY	O4-C20-C21	2.59	120.03	111.91
4	A	1204	YZY	O4-C20-C21	2.58	120.00	111.91
4	D	1204	YZY	O4-C20-C21	2.58	120.00	111.91
6	D	1206	Y01	CBG-CBI-CBE	2.30	102.80	100.07
6	A	1206	Y01	CBG-CBI-CBE	2.28	102.77	100.07
6	B	1206	Y01	CBG-CBI-CBE	2.28	102.77	100.07
6	C	1206	Y01	CBG-CBI-CBE	2.26	102.75	100.07
6	C	1206	Y01	CBH-CAZ-CAI	-2.03	119.80	122.90
6	A	1206	Y01	CBH-CAZ-CAI	-2.02	119.81	122.90
6	B	1206	Y01	CBH-CAZ-CAI	-2.02	119.81	122.90
6	D	1206	Y01	CBH-CAZ-CAI	-2.02	119.81	122.90

There are no chirality outliers.

All (316) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1204	YZY	O1-C1-C2-O2
4	A	1204	YZY	O1-C1-C2-C19
4	B	1204	YZY	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	B	1204	YZY	O1-C1-C2-C19
4	C	1204	YZY	O1-C1-C2-O2
4	C	1204	YZY	O1-C1-C2-C19
4	D	1204	YZY	O1-C1-C2-O2
4	D	1204	YZY	O1-C1-C2-C19
5	A	1205	POV	C1-O11-P-O14
5	A	1205	POV	C11-O12-P-O13
5	A	1205	POV	C11-O12-P-O14
5	A	1205	POV	O21-C2-C3-O31
5	B	1205	POV	C1-O11-P-O14
5	B	1205	POV	C11-O12-P-O13
5	B	1205	POV	C11-O12-P-O14
5	B	1205	POV	O21-C2-C3-O31
5	C	1205	POV	C1-O11-P-O14
5	C	1205	POV	C11-O12-P-O13
5	C	1205	POV	C11-O12-P-O14
5	C	1205	POV	O21-C2-C3-O31
5	D	1205	POV	C1-O11-P-O14
5	D	1205	POV	C11-O12-P-O13
5	D	1205	POV	C11-O12-P-O14
5	D	1205	POV	O21-C2-C3-O31
6	A	1206	Y01	CAR-CBC-OAW-CAY
6	B	1206	Y01	CAR-CBC-OAW-CAY
6	C	1206	Y01	CAR-CBC-OAW-CAY
6	D	1206	Y01	CAR-CBC-OAW-CAY
7	A	1207	PT5	C7-O13-P1-O12
7	A	1207	PT5	C7-O13-P1-O11
7	A	1207	PT5	C1-O1-P1-O12
7	A	1207	PT5	C6-C5-O5-P5
7	A	1207	PT5	C5-O5-P5-O53
7	A	1207	PT5	O17-C10-O16-C8
7	A	1207	PT5	C12-C10-O16-C8
7	B	1207	PT5	C7-O13-P1-O12
7	B	1207	PT5	C7-O13-P1-O11
7	B	1207	PT5	C1-O1-P1-O12
7	B	1207	PT5	C6-C5-O5-P5
7	B	1207	PT5	C5-O5-P5-O53
7	B	1207	PT5	O17-C10-O16-C8
7	B	1207	PT5	C12-C10-O16-C8
7	C	1207	PT5	C7-O13-P1-O12
7	C	1207	PT5	C7-O13-P1-O11
7	C	1207	PT5	C1-O1-P1-O12

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Mol	Chain	Res	Type	Atoms
7	C	1207	PT5	C6-C5-O5-P5
7	C	1207	PT5	C5-O5-P5-O53
7	C	1207	PT5	O17-C10-O16-C8
7	C	1207	PT5	C12-C10-O16-C8
7	D	1207	PT5	C7-O13-P1-O12
7	D	1207	PT5	C7-O13-P1-O11
7	D	1207	PT5	C1-O1-P1-O12
7	D	1207	PT5	C6-C5-O5-P5
7	D	1207	PT5	C5-O5-P5-O53
7	D	1207	PT5	O17-C10-O16-C8
7	D	1207	PT5	C12-C10-O16-C8
4	A	1204	YZY	C21-C20-O4-C19
4	B	1204	YZY	C21-C20-O4-C19
4	C	1204	YZY	C21-C20-O4-C19
4	D	1204	YZY	C21-C20-O4-C19
7	A	1207	PT5	C40-C41-C42-C43
7	B	1207	PT5	C40-C41-C42-C43
7	C	1207	PT5	C40-C41-C42-C43
7	D	1207	PT5	C40-C41-C42-C43
7	A	1207	PT5	C34-C35-C36-C37
7	B	1207	PT5	C34-C35-C36-C37
7	C	1207	PT5	C34-C35-C36-C37
7	D	1207	PT5	C34-C35-C36-C37
4	A	1204	YZY	O5-C20-O4-C19
4	B	1204	YZY	O5-C20-O4-C19
4	C	1204	YZY	O5-C20-O4-C19
4	D	1204	YZY	O5-C20-O4-C19
6	A	1206	Y01	CAM-CAY-OAW-CBC
6	B	1206	Y01	CAM-CAY-OAW-CBC
6	C	1206	Y01	CAM-CAY-OAW-CBC
6	D	1206	Y01	CAM-CAY-OAW-CBC
5	A	1205	POV	C11-O12-P-O11
5	B	1205	POV	C11-O12-P-O11
5	C	1205	POV	C11-O12-P-O11
5	D	1205	POV	C11-O12-P-O11
7	A	1207	PT5	C7-O13-P1-O1
7	B	1207	PT5	C7-O13-P1-O1
7	C	1207	PT5	C7-O13-P1-O1
7	D	1207	PT5	C7-O13-P1-O1
6	A	1206	Y01	OAG-CAY-OAW-CBC
6	B	1206	Y01	OAG-CAY-OAW-CBC
6	C	1206	Y01	OAG-CAY-OAW-CBC

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Mol	Chain	Res	Type	Atoms
6	D	1206	Y01	OAG-CAY-OAW-CBC
7	A	1207	PT5	C1-O1-P1-O13
7	B	1207	PT5	C1-O1-P1-O13
7	C	1207	PT5	C1-O1-P1-O13
7	D	1207	PT5	C1-O1-P1-O13
5	A	1205	POV	C23-C24-C25-C26
5	B	1205	POV	C23-C24-C25-C26
5	C	1205	POV	C39-C310-C311-C312
5	C	1205	POV	C23-C24-C25-C26
5	D	1205	POV	C23-C24-C25-C26
7	A	1207	PT5	C35-C36-C37-C38
7	B	1207	PT5	C35-C36-C37-C38
7	C	1207	PT5	C35-C36-C37-C38
7	D	1207	PT5	C35-C36-C37-C38
5	A	1205	POV	C39-C310-C311-C312
5	B	1205	POV	C39-C310-C311-C312
5	D	1205	POV	C39-C310-C311-C312
7	A	1207	PT5	C42-C43-C44-C45
7	B	1207	PT5	C42-C43-C44-C45
7	C	1207	PT5	C42-C43-C44-C45
7	D	1207	PT5	C42-C43-C44-C45
5	A	1205	POV	C36-C37-C38-C39
5	B	1205	POV	C36-C37-C38-C39
5	C	1205	POV	C36-C37-C38-C39
7	A	1207	PT5	C32-C33-C34-C35
7	B	1207	PT5	C32-C33-C34-C35
7	C	1207	PT5	C32-C33-C34-C35
7	D	1207	PT5	C32-C33-C34-C35
5	D	1205	POV	C36-C37-C38-C39
7	A	1207	PT5	C39-C40-C41-C42
7	B	1207	PT5	C39-C40-C41-C42
7	C	1207	PT5	C39-C40-C41-C42
7	D	1207	PT5	C39-C40-C41-C42
7	A	1207	PT5	C41-C42-C43-C44
7	B	1207	PT5	C41-C42-C43-C44
7	D	1207	PT5	C41-C42-C43-C44
7	C	1207	PT5	C41-C42-C43-C44
4	A	1204	YZY	C22-C23-C24-C25
4	B	1204	YZY	C22-C23-C24-C25
4	A	1204	YZY	C7-C8-C9-C10
4	B	1204	YZY	C7-C8-C9-C10
4	C	1204	YZY	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
4	C	1204	YZY	C22-C23-C24-C25
4	D	1204	YZY	C7-C8-C9-C10
4	D	1204	YZY	C22-C23-C24-C25
4	A	1204	YZY	C10-C11-C12-C13
4	B	1204	YZY	C10-C11-C12-C13
4	C	1204	YZY	C10-C11-C12-C13
4	D	1204	YZY	C10-C11-C12-C13
5	A	1205	POV	C210-C211-C212-C213
5	B	1205	POV	C210-C211-C212-C213
5	C	1205	POV	C210-C211-C212-C213
5	D	1205	POV	C210-C211-C212-C213
5	D	1205	POV	C35-C36-C37-C38
5	A	1205	POV	C35-C36-C37-C38
5	B	1205	POV	C35-C36-C37-C38
5	C	1205	POV	C35-C36-C37-C38
7	A	1207	PT5	C12-C13-C14-C15
7	B	1207	PT5	C12-C13-C14-C15
7	C	1207	PT5	C12-C13-C14-C15
7	D	1207	PT5	C12-C13-C14-C15
5	C	1205	POV	C34-C35-C36-C37
5	A	1205	POV	C34-C35-C36-C37
5	B	1205	POV	C34-C35-C36-C37
5	D	1205	POV	C34-C35-C36-C37
7	A	1207	PT5	C25-C26-C27-C28
7	B	1207	PT5	C25-C26-C27-C28
7	C	1207	PT5	C25-C26-C27-C28
7	D	1207	PT5	C25-C26-C27-C28
4	A	1204	YZY	C24-C25-C26-C27
4	D	1204	YZY	C24-C25-C26-C27
4	B	1204	YZY	C24-C25-C26-C27
4	C	1204	YZY	C24-C25-C26-C27
5	C	1205	POV	C32-C33-C34-C35
7	A	1207	PT5	C33-C34-C35-C36
5	A	1205	POV	C24-C25-C26-C27
5	A	1205	POV	C32-C33-C34-C35
5	B	1205	POV	C24-C25-C26-C27
5	B	1205	POV	C32-C33-C34-C35
5	C	1205	POV	C24-C25-C26-C27
5	D	1205	POV	C24-C25-C26-C27
5	D	1205	POV	C32-C33-C34-C35
7	B	1207	PT5	C33-C34-C35-C36
7	C	1207	PT5	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
7	D	1207	PT5	C33-C34-C35-C36
5	A	1205	POV	C1-C2-C3-O31
5	B	1205	POV	C1-C2-C3-O31
5	C	1205	POV	C1-C2-C3-O31
5	D	1205	POV	C1-C2-C3-O31
5	A	1205	POV	C213-C214-C215-C216
5	B	1205	POV	C213-C214-C215-C216
5	C	1205	POV	C213-C214-C215-C216
5	D	1205	POV	C213-C214-C215-C216
4	A	1204	YZY	C3-C4-C5-C6
4	B	1204	YZY	C3-C4-C5-C6
4	C	1204	YZY	C3-C4-C5-C6
4	D	1204	YZY	C3-C4-C5-C6
7	A	1207	PT5	C44-C45-C46-C47
7	C	1207	PT5	C44-C45-C46-C47
7	D	1207	PT5	C44-C45-C46-C47
7	B	1207	PT5	C44-C45-C46-C47
5	A	1205	POV	C2-C1-O11-P
5	B	1205	POV	C2-C1-O11-P
5	C	1205	POV	C2-C1-O11-P
5	D	1205	POV	C2-C1-O11-P
4	A	1204	YZY	O4-C19-C2-O2
4	B	1204	YZY	O4-C19-C2-O2
4	C	1204	YZY	O4-C19-C2-O2
4	D	1204	YZY	O4-C19-C2-O2
7	A	1207	PT5	C36-C37-C38-C39
7	B	1207	PT5	C36-C37-C38-C39
7	C	1207	PT5	C36-C37-C38-C39
7	D	1207	PT5	C36-C37-C38-C39
4	A	1204	YZY	C15-C16-C17-C18
4	B	1204	YZY	C15-C16-C17-C18
4	C	1204	YZY	C15-C16-C17-C18
4	D	1204	YZY	C15-C16-C17-C18
7	A	1207	PT5	C27-C28-C29-C30
7	B	1207	PT5	C27-C28-C29-C30
7	C	1207	PT5	C27-C28-C29-C30
7	D	1207	PT5	C27-C28-C29-C30
7	A	1207	PT5	C37-C38-C39-C40
7	B	1207	PT5	C37-C38-C39-C40
7	C	1207	PT5	C37-C38-C39-C40
7	D	1207	PT5	C37-C38-C39-C40
5	A	1205	POV	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	B	1205	POV	O11-C1-C2-C3
5	C	1205	POV	O11-C1-C2-C3
5	D	1205	POV	O11-C1-C2-C3
7	A	1207	PT5	C7-C8-C9-O18
7	B	1207	PT5	C7-C8-C9-O18
7	C	1207	PT5	C7-C8-C9-O18
7	D	1207	PT5	C7-C8-C9-O18
7	A	1207	PT5	C11-C31-C32-C33
7	C	1207	PT5	C11-C31-C32-C33
7	A	1207	PT5	C1-O1-P1-O11
7	B	1207	PT5	C1-O1-P1-O11
7	C	1207	PT5	C1-O1-P1-O11
7	D	1207	PT5	C1-O1-P1-O11
7	B	1207	PT5	C11-C31-C32-C33
7	A	1207	PT5	C16-C17-C18-C19
7	A	1207	PT5	C18-C19-C20-C21
7	B	1207	PT5	C16-C17-C18-C19
7	B	1207	PT5	C18-C19-C20-C21
7	C	1207	PT5	C16-C17-C18-C19
7	C	1207	PT5	C18-C19-C20-C21
7	D	1207	PT5	C16-C17-C18-C19
7	D	1207	PT5	C18-C19-C20-C21
7	D	1207	PT5	C11-C31-C32-C33
6	A	1206	Y01	CAN-CAJ-CAO-CBB
6	B	1206	Y01	CAN-CAJ-CAO-CBB
6	C	1206	Y01	CAN-CAJ-CAO-CBB
6	D	1206	Y01	CAN-CAJ-CAO-CBB
4	A	1204	YZY	C20-C21-C22-C23
4	B	1204	YZY	C20-C21-C22-C23
4	C	1204	YZY	C20-C21-C22-C23
4	D	1204	YZY	C20-C21-C22-C23
7	A	1207	PT5	C31-C32-C33-C34
7	B	1207	PT5	C31-C32-C33-C34
7	C	1207	PT5	C31-C32-C33-C34
7	D	1207	PT5	C31-C32-C33-C34
4	A	1204	YZY	C4-C5-C6-C7
4	B	1204	YZY	C4-C5-C6-C7
4	C	1204	YZY	C4-C5-C6-C7
4	D	1204	YZY	C4-C5-C6-C7
4	A	1204	YZY	C4-C3-O2-C2
4	B	1204	YZY	C4-C3-O2-C2
4	C	1204	YZY	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
4	D	1204	YZY	C4-C3-O2-C2
5	A	1205	POV	O11-C1-C2-O21
5	B	1205	POV	O11-C1-C2-O21
5	C	1205	POV	O11-C1-C2-O21
5	D	1205	POV	O11-C1-C2-O21
4	A	1204	YZY	O3-C3-O2-C2
4	B	1204	YZY	O3-C3-O2-C2
4	C	1204	YZY	O3-C3-O2-C2
4	D	1204	YZY	O3-C3-O2-C2
5	A	1205	POV	C1-O11-P-O12
5	B	1205	POV	C1-O11-P-O12
5	C	1205	POV	C1-O11-P-O12
5	D	1205	POV	C1-O11-P-O12
6	A	1206	Y01	CAJ-CAN-CBA-CAA
6	B	1206	Y01	CAJ-CAN-CBA-CAA
6	C	1206	Y01	CAJ-CAN-CBA-CAA
6	D	1206	Y01	CAJ-CAN-CBA-CAA
4	A	1204	YZY	O4-C19-C2-C1
4	B	1204	YZY	O4-C19-C2-C1
4	C	1204	YZY	O4-C19-C2-C1
4	D	1204	YZY	O4-C19-C2-C1
7	A	1207	PT5	C9-C8-O16-C10
7	B	1207	PT5	C9-C8-O16-C10
7	C	1207	PT5	C9-C8-O16-C10
7	D	1207	PT5	C9-C8-O16-C10
7	A	1207	PT5	O16-C8-C9-O18
7	B	1207	PT5	O16-C8-C9-O18
7	C	1207	PT5	O16-C8-C9-O18
7	D	1207	PT5	O16-C8-C9-O18
4	B	1204	YZY	C11-C12-C13-C14
4	D	1204	YZY	C11-C12-C13-C14
4	A	1204	YZY	C11-C12-C13-C14
4	C	1204	YZY	C11-C12-C13-C14
7	A	1207	PT5	C19-C20-C21-C22
7	A	1207	PT5	C21-C22-C23-C24
7	B	1207	PT5	C19-C20-C21-C22
7	B	1207	PT5	C21-C22-C23-C24
7	C	1207	PT5	C19-C20-C21-C22
7	C	1207	PT5	C21-C22-C23-C24
7	D	1207	PT5	C19-C20-C21-C22
7	D	1207	PT5	C21-C22-C23-C24
6	A	1206	Y01	CAC-CBB-CBE-CBI

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Mol	Chain	Res	Type	Atoms
6	B	1206	Y01	CAC-CBB-CBE-CBI
6	C	1206	Y01	CAC-CBB-CBE-CBI
6	D	1206	Y01	CAC-CBB-CBE-CBI
7	A	1207	PT5	C24-C25-C26-C27
7	B	1207	PT5	C24-C25-C26-C27
7	C	1207	PT5	C24-C25-C26-C27
7	D	1207	PT5	C24-C25-C26-C27
5	A	1205	POV	C32-C31-O31-C3
5	C	1205	POV	C32-C31-O31-C3
5	B	1205	POV	C32-C31-O31-C3
5	D	1205	POV	C32-C31-O31-C3
5	A	1205	POV	O32-C31-O31-C3
5	B	1205	POV	O32-C31-O31-C3
5	C	1205	POV	O32-C31-O31-C3
5	D	1205	POV	O32-C31-O31-C3
4	A	1204	YZY	C26-C27-C28-C29
4	B	1204	YZY	C26-C27-C28-C29
4	C	1204	YZY	C26-C27-C28-C29
4	D	1204	YZY	C26-C27-C28-C29

There are no ring outliers.

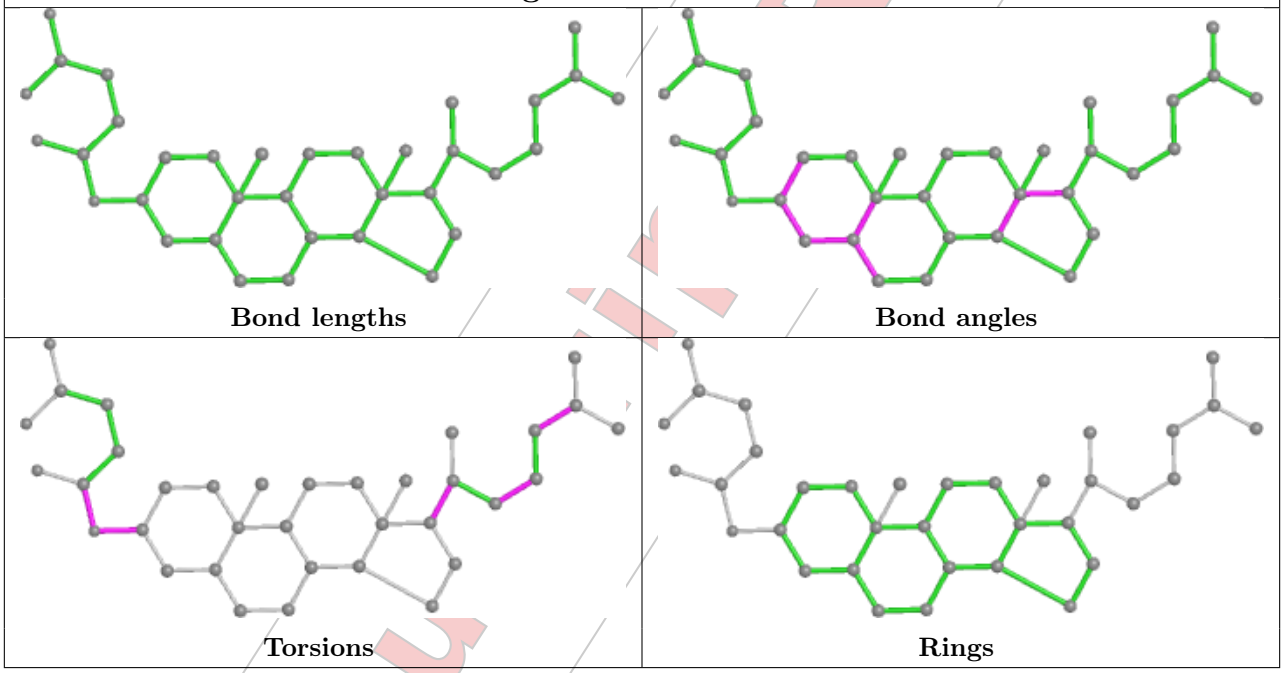
16 monomers are involved in 119 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1206	Y01	10	0
5	D	1205	POV	16	0
7	C	1207	PT5	4	0
5	B	1205	POV	16	0
6	A	1206	Y01	8	0
7	A	1207	PT5	5	0
4	A	1204	YZY	1	0
6	C	1206	Y01	8	0
4	B	1204	YZY	1	0
6	D	1206	Y01	9	0
7	D	1207	PT5	4	0
5	C	1205	POV	15	0
5	A	1205	POV	15	0
4	C	1204	YZY	1	0
7	B	1207	PT5	5	0
4	D	1204	YZY	1	0

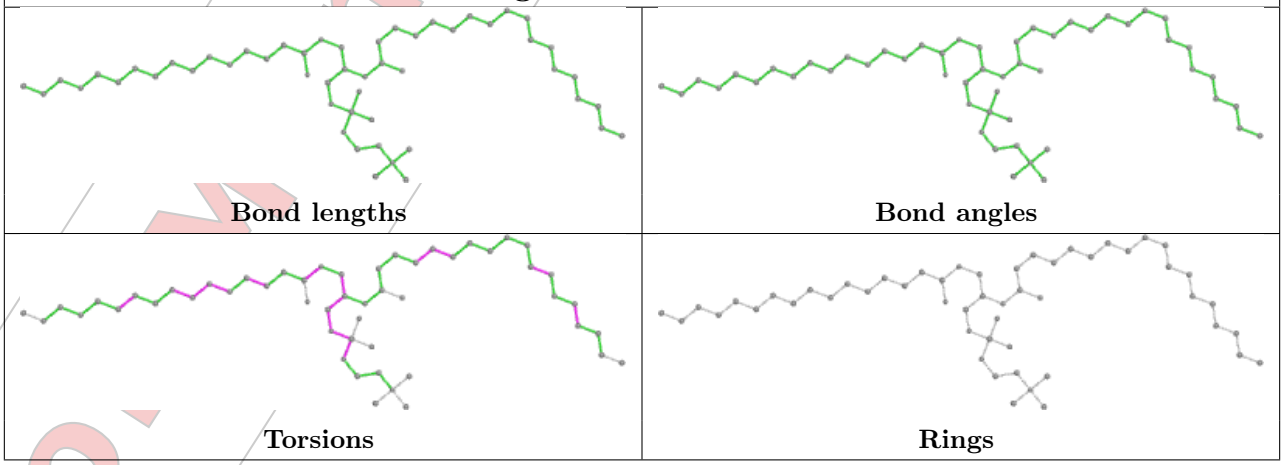
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

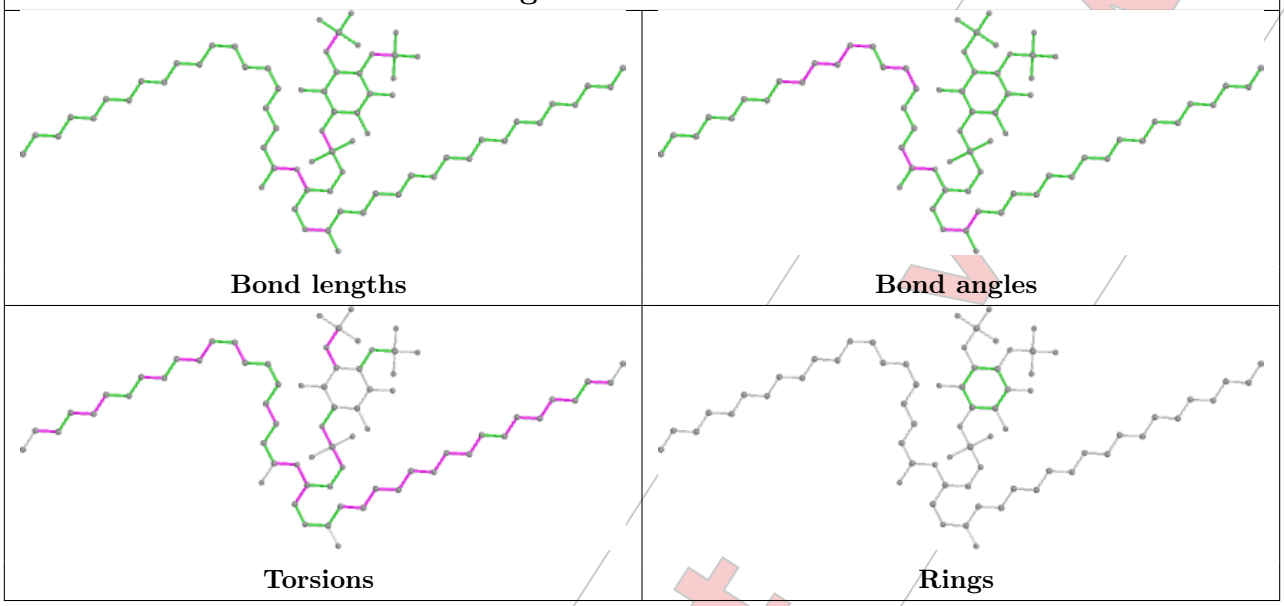
Ligand Y01 B 1206



Ligand POV D 1205



Ligand PT5 C 1207



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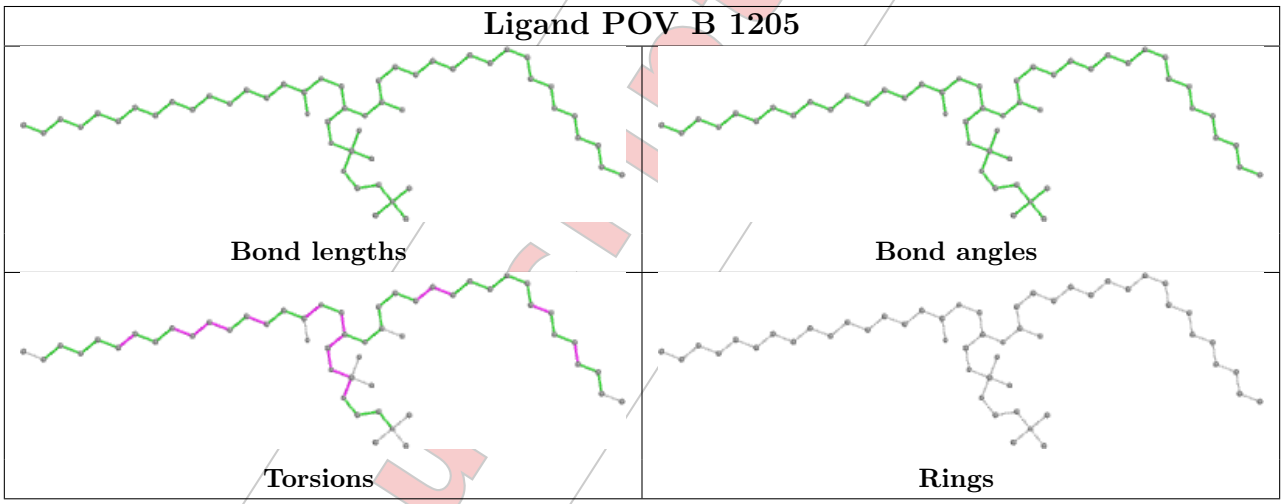
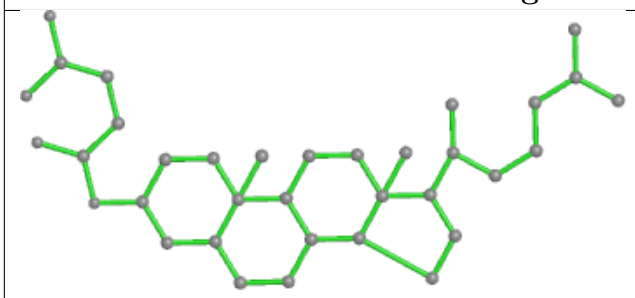
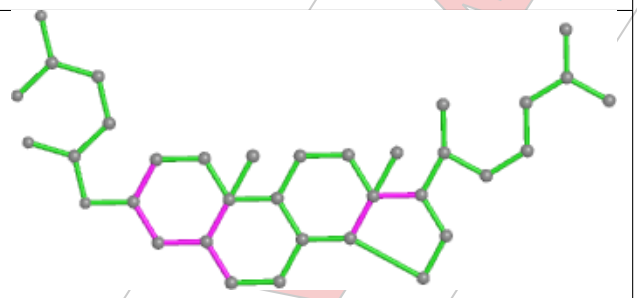


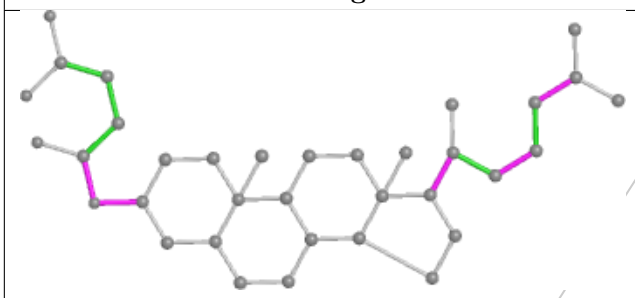
Ligand Y01 A 1206



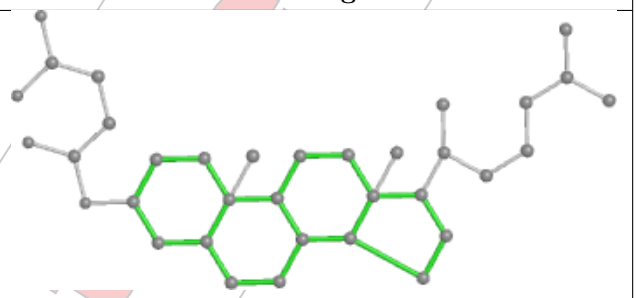
Bond lengths



Bond angles

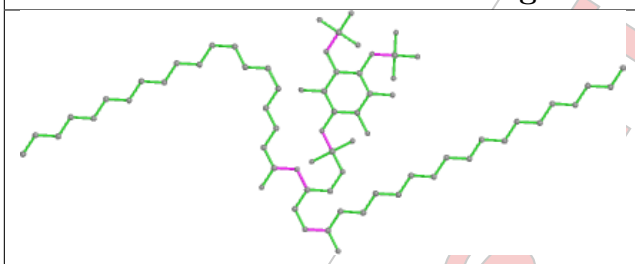


Torsions

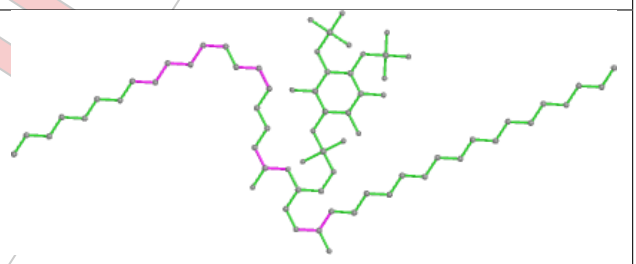


Rings

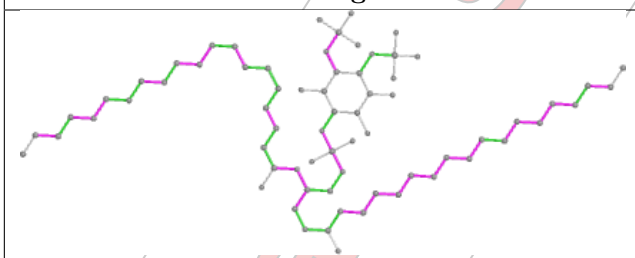
Ligand PT5 A 1207



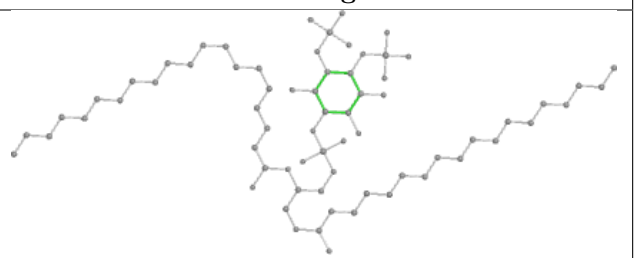
Bond lengths



Bond angles

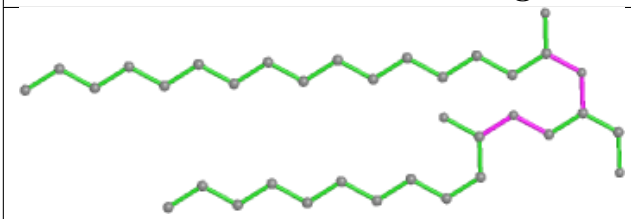


Torsions



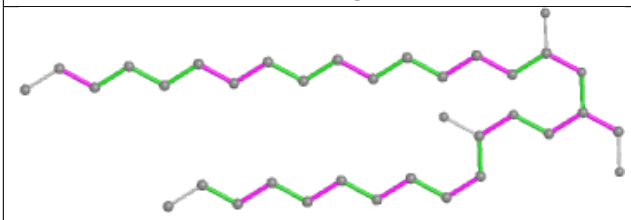
Rings

Ligand YZY A 1204

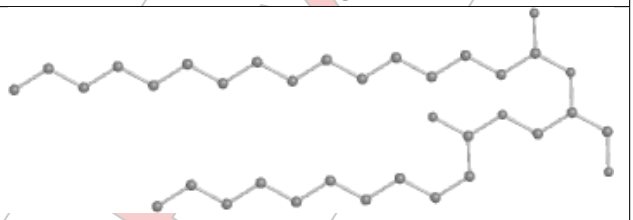


Bond lengths

Bond angles

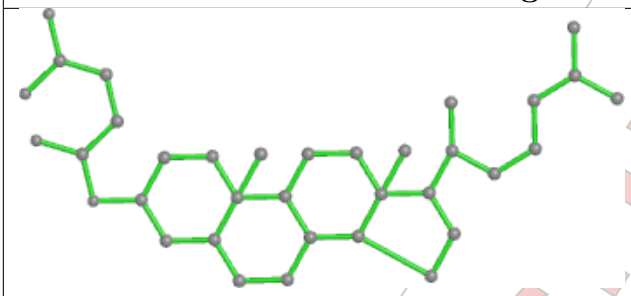


Torsions

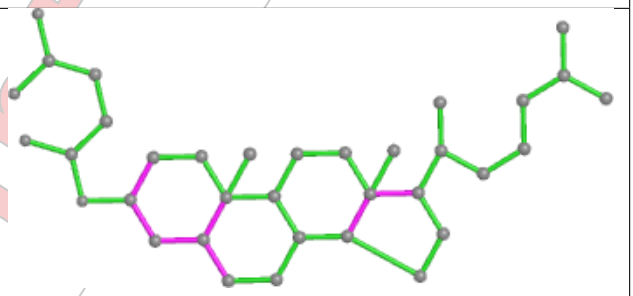


Rings

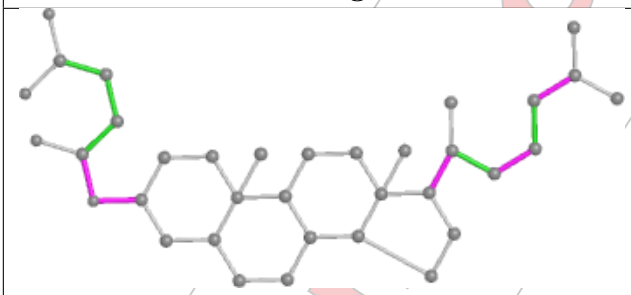
Ligand Y01 C 1206



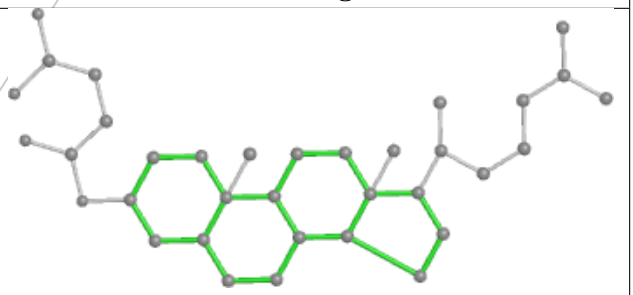
Bond lengths



Bond angles

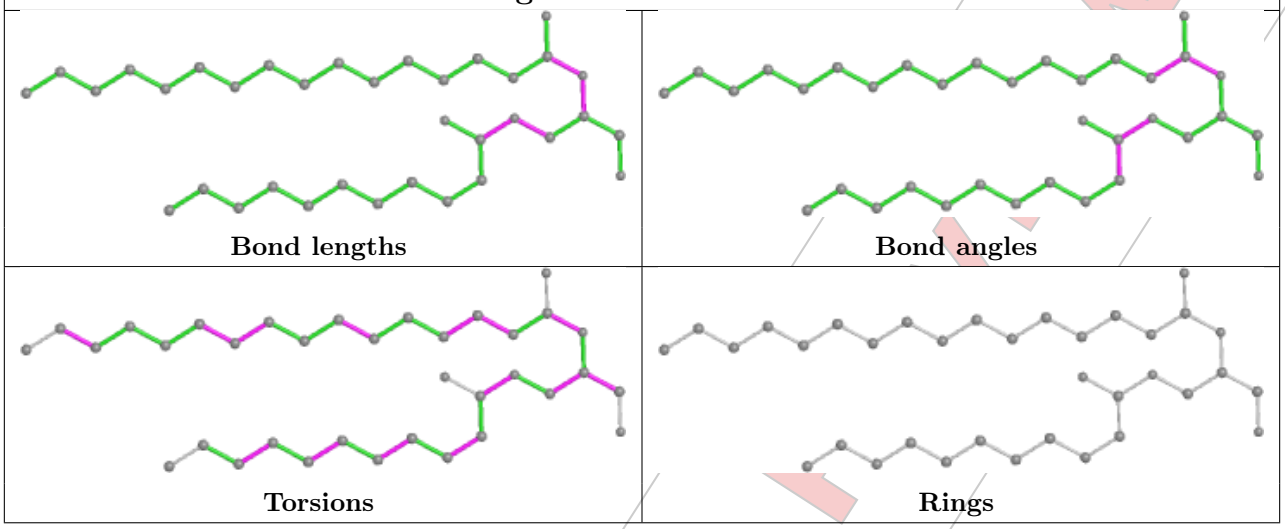


Torsions

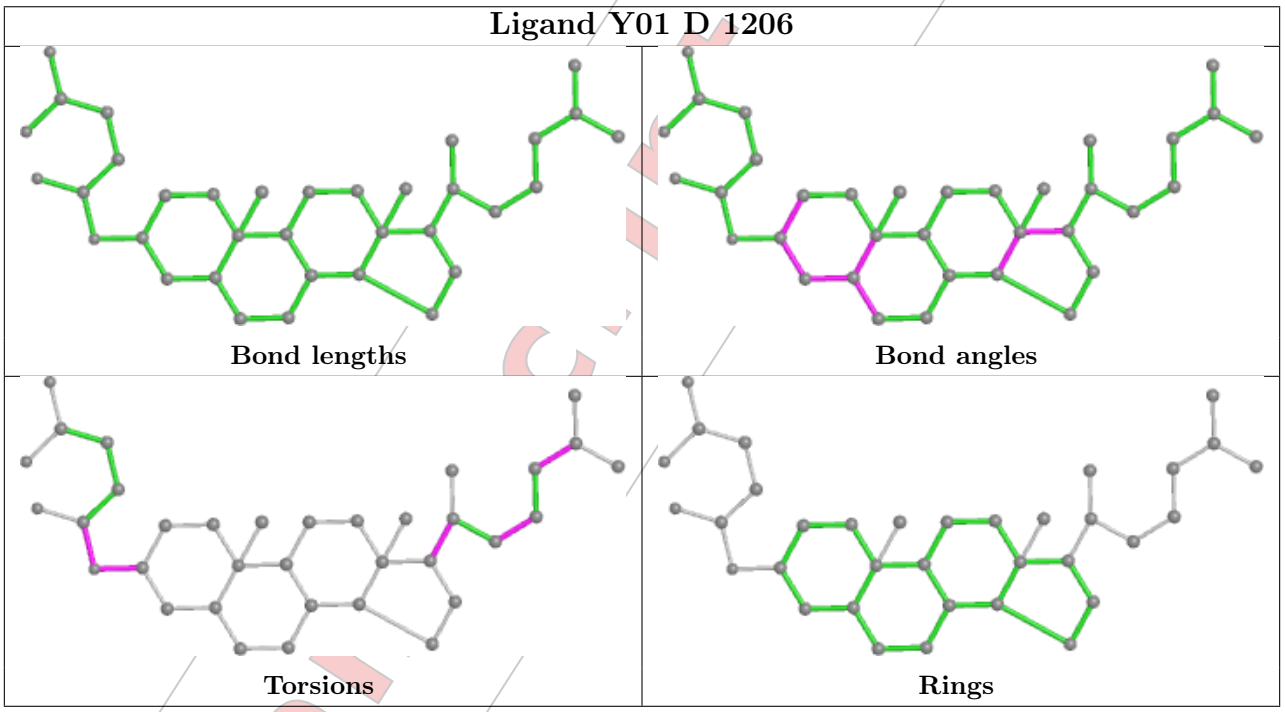


Rings

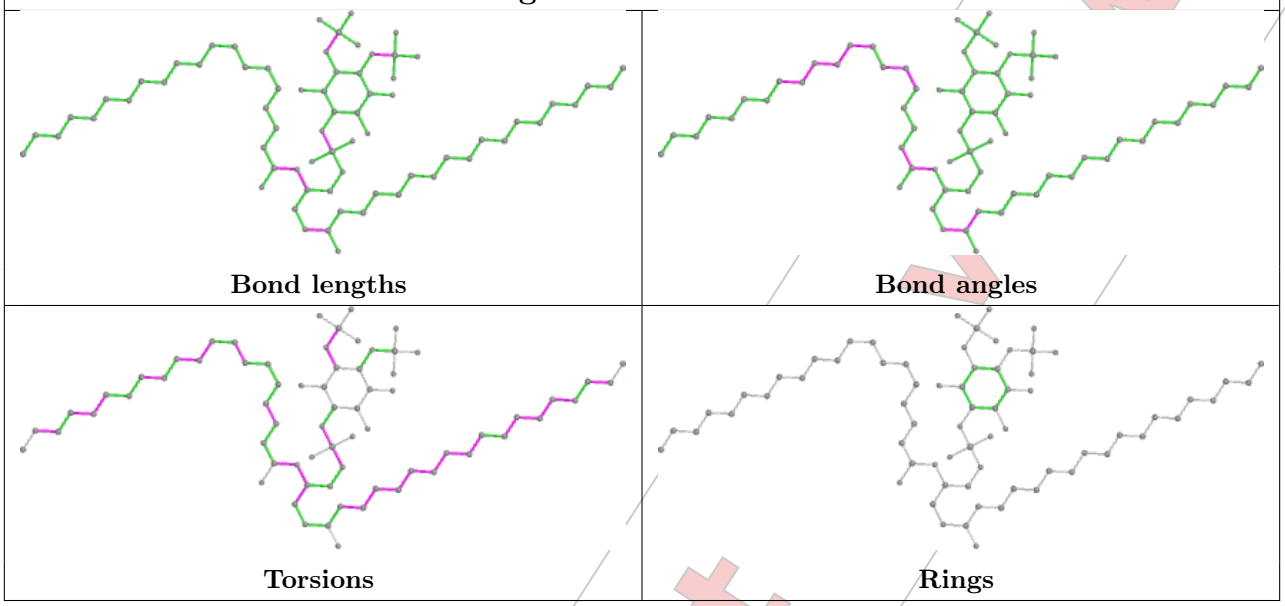
Ligand YZY B 1204



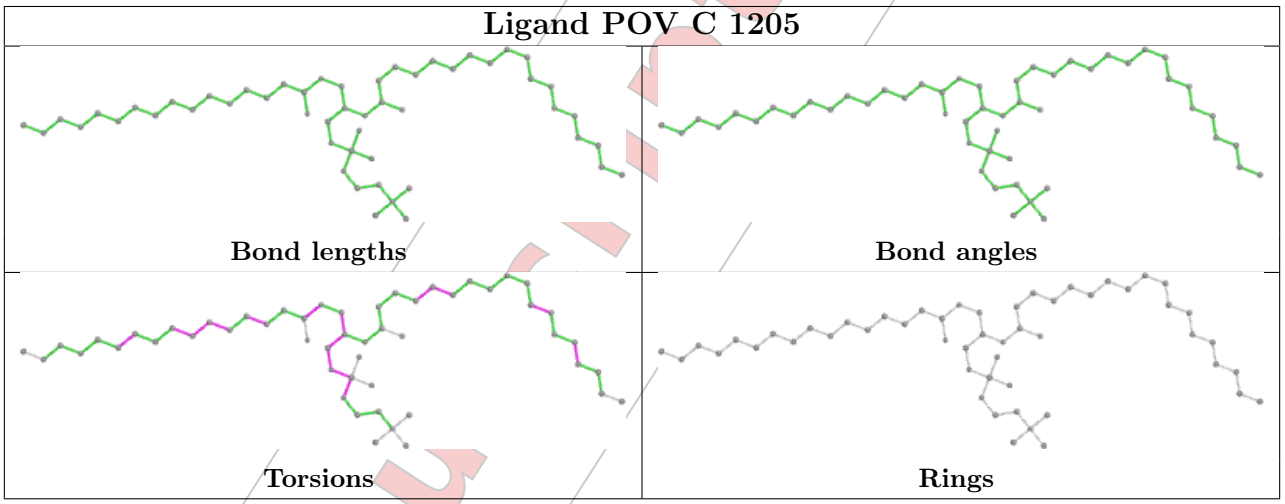
Ligand Y01 D 1206



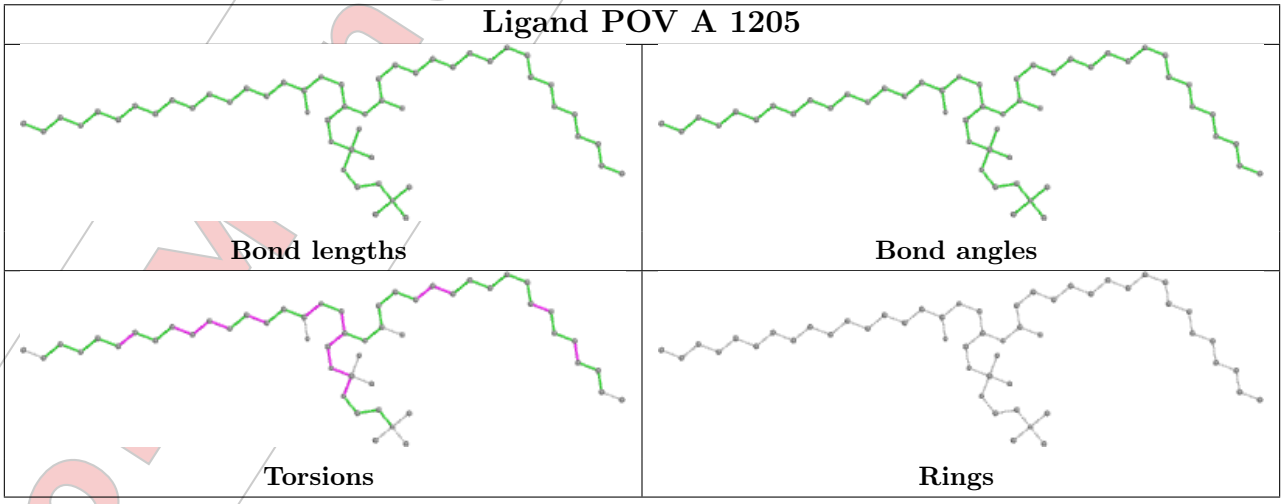
Ligand PT5 D 1207



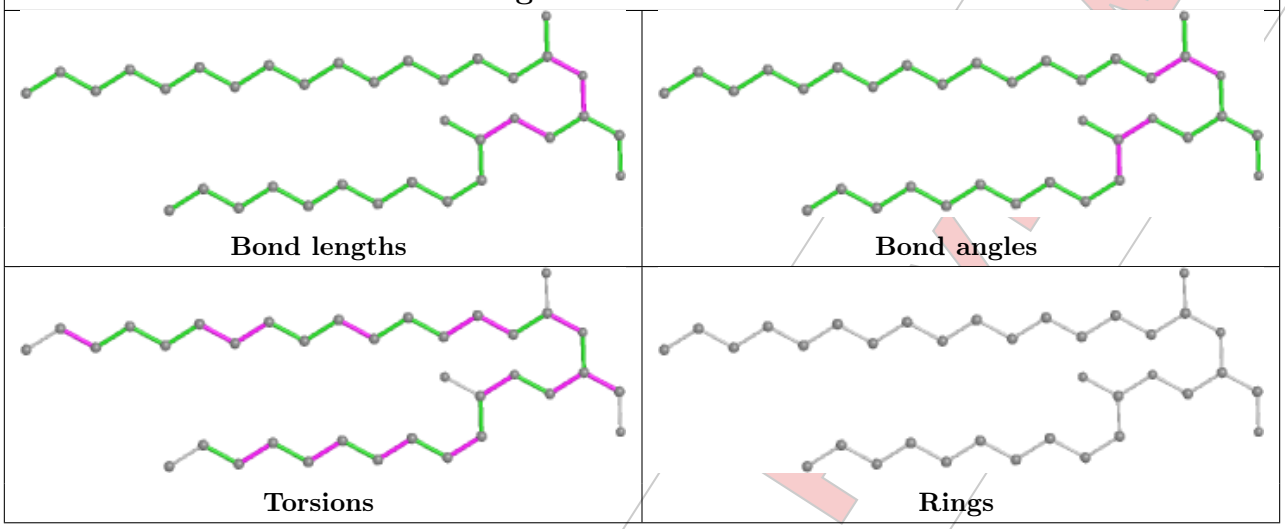
Ligand POV C 1205



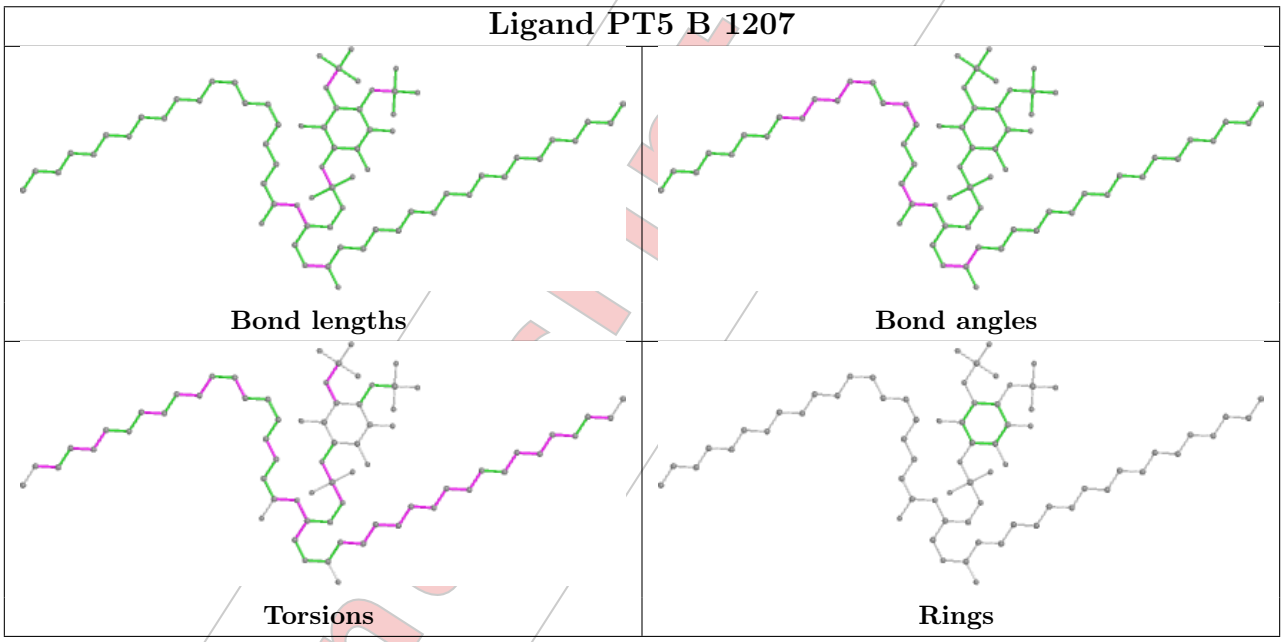
Ligand POV A 1205



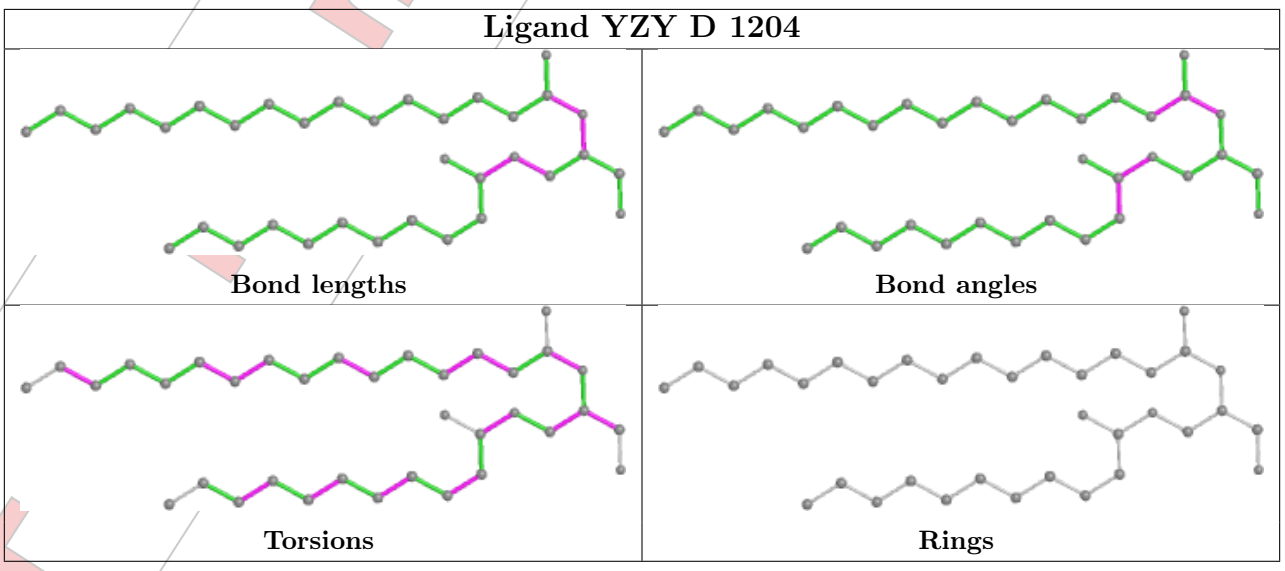
Ligand YZY C 1204



Ligand PT5 B 1207



Ligand YZY D 1204



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

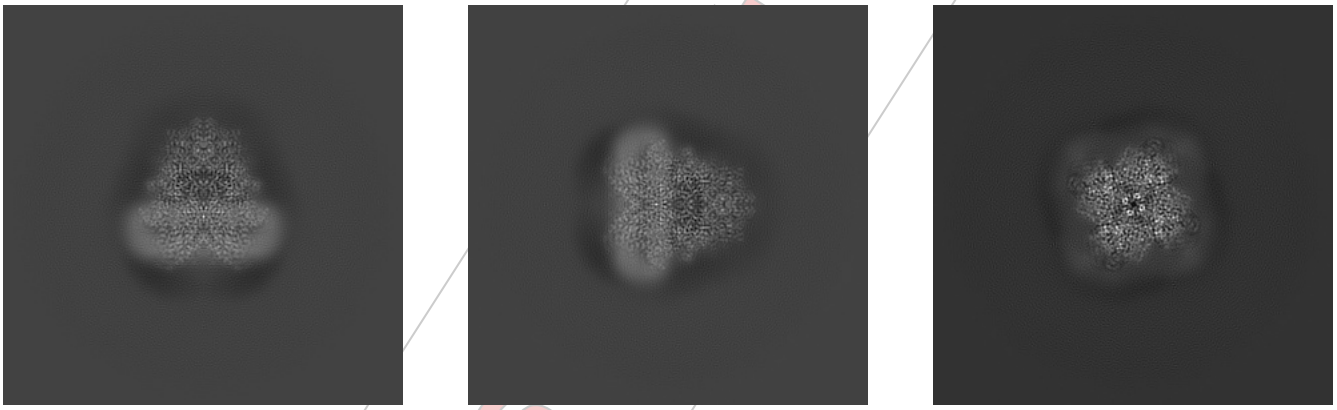
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-65273. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

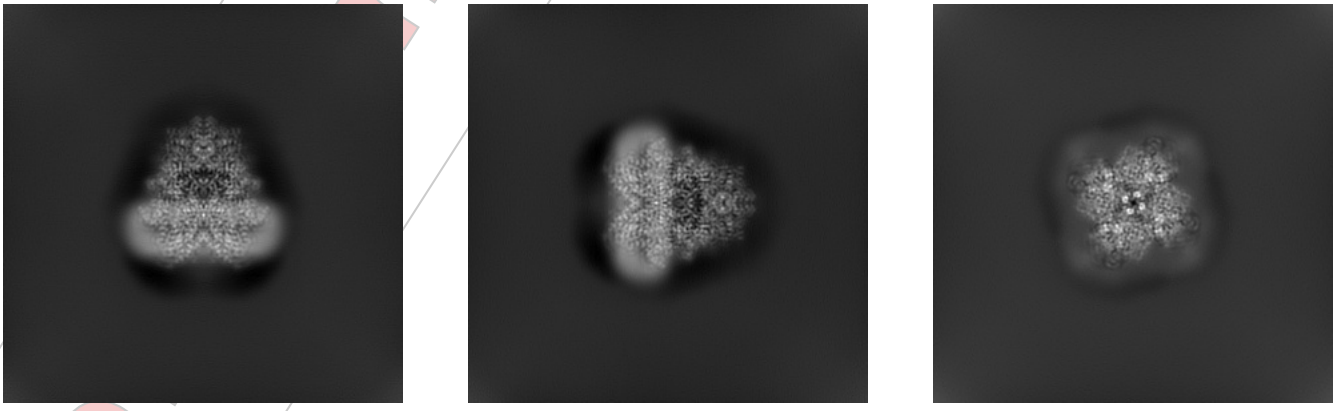
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

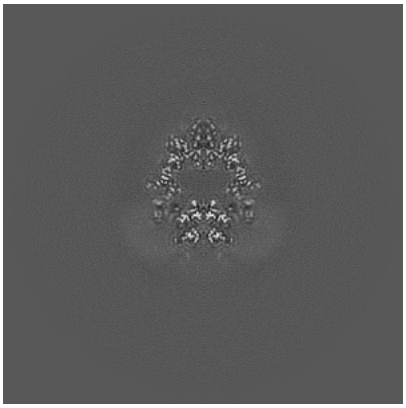


X Y Z

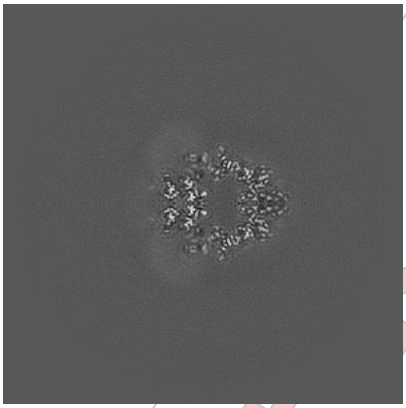
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

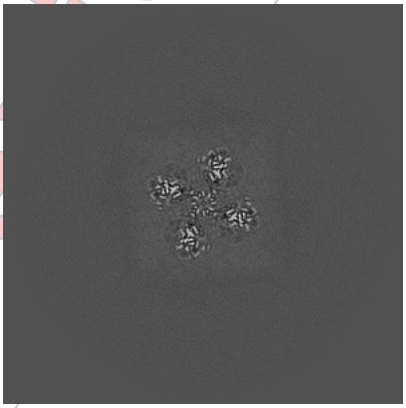
6.2.1 Primary map



X Index: 160

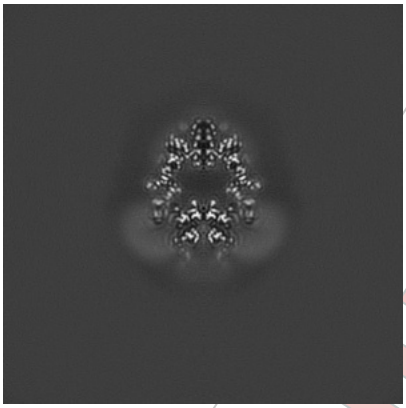


Y Index: 160

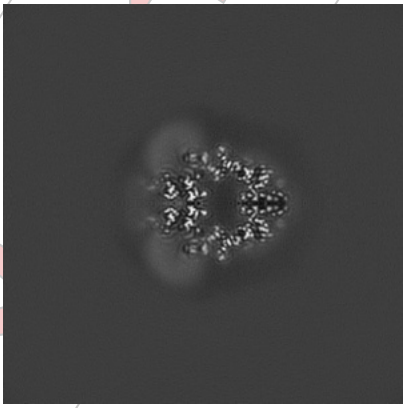


Z Index: 160

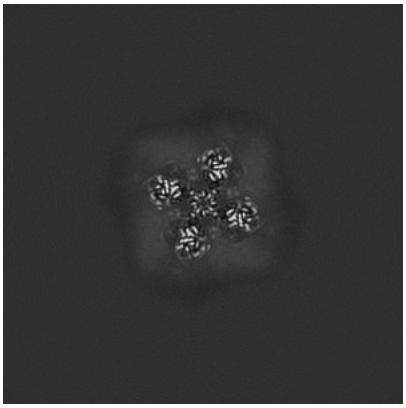
6.2.2 Raw map



X Index: 160



Y Index: 160

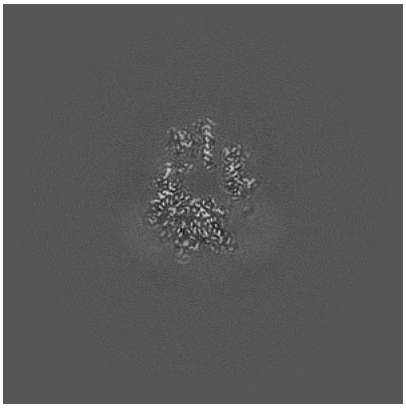


Z Index: 160

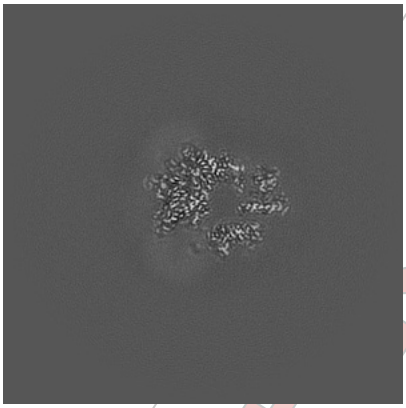
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

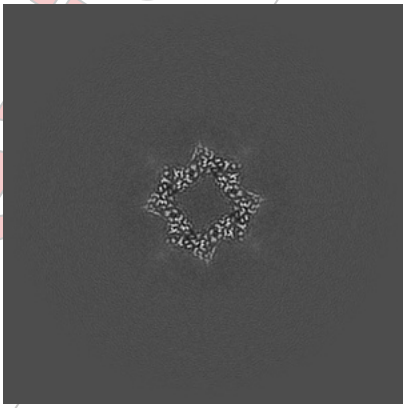
6.3.1 Primary map



X Index: 152

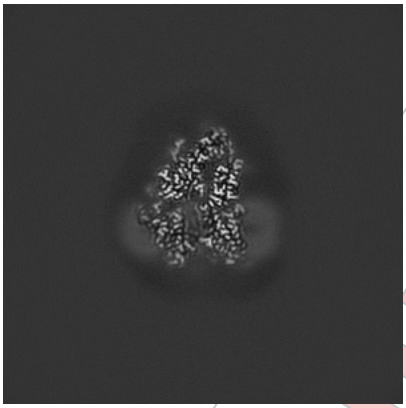


Y Index: 152

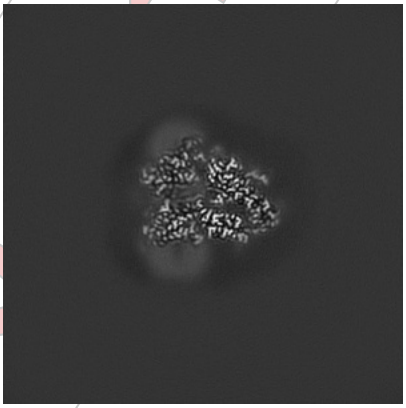


Z Index: 177

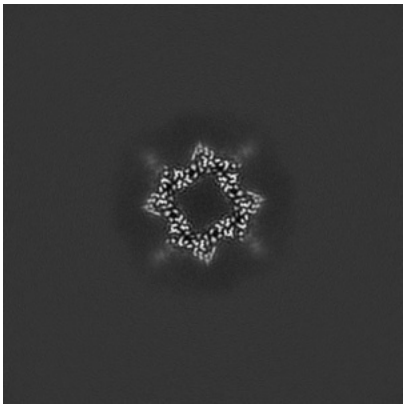
6.3.2 Raw map



X Index: 138



Y Index: 138

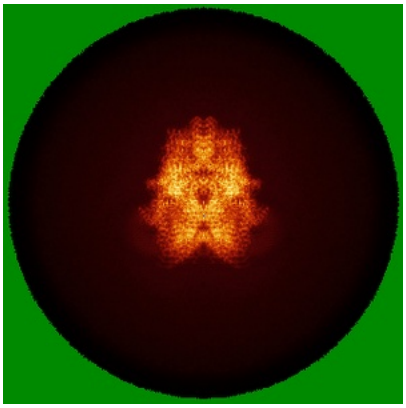


Z Index: 177

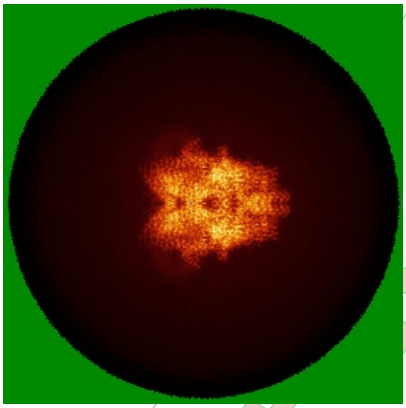
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

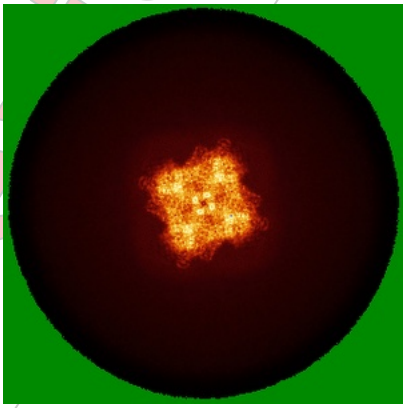
6.4.1 Primary map



X

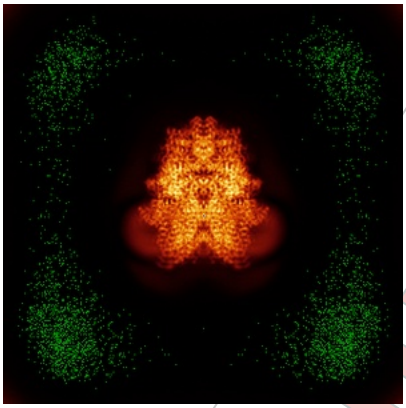


Y

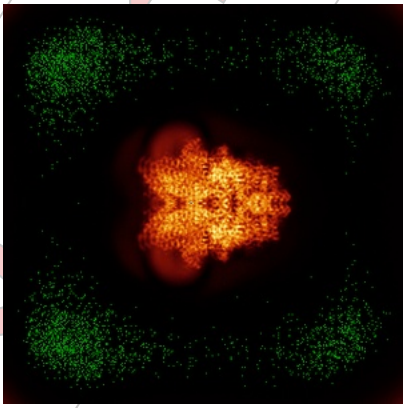


Z

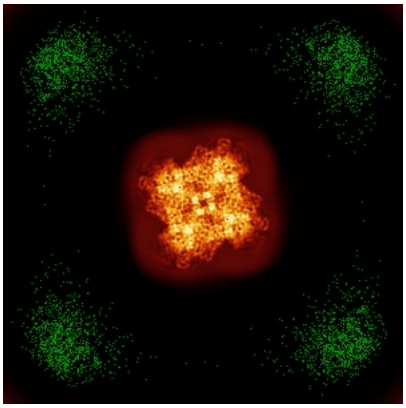
6.4.2 Raw map



X



Y

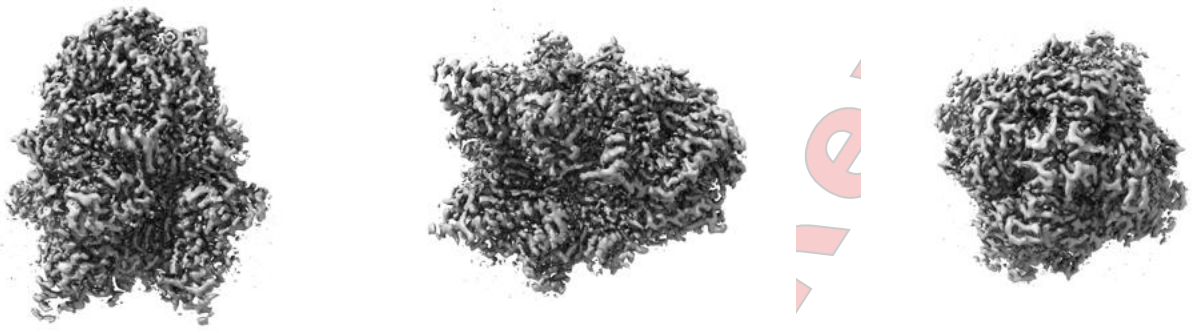


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

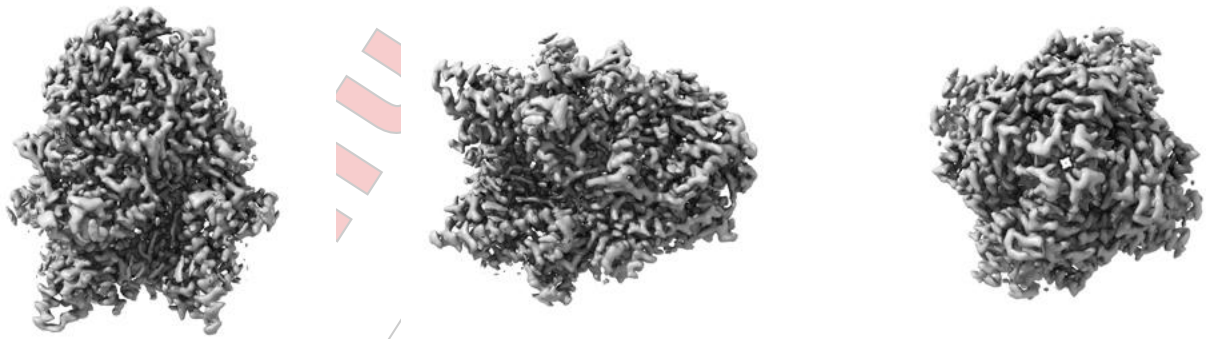
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

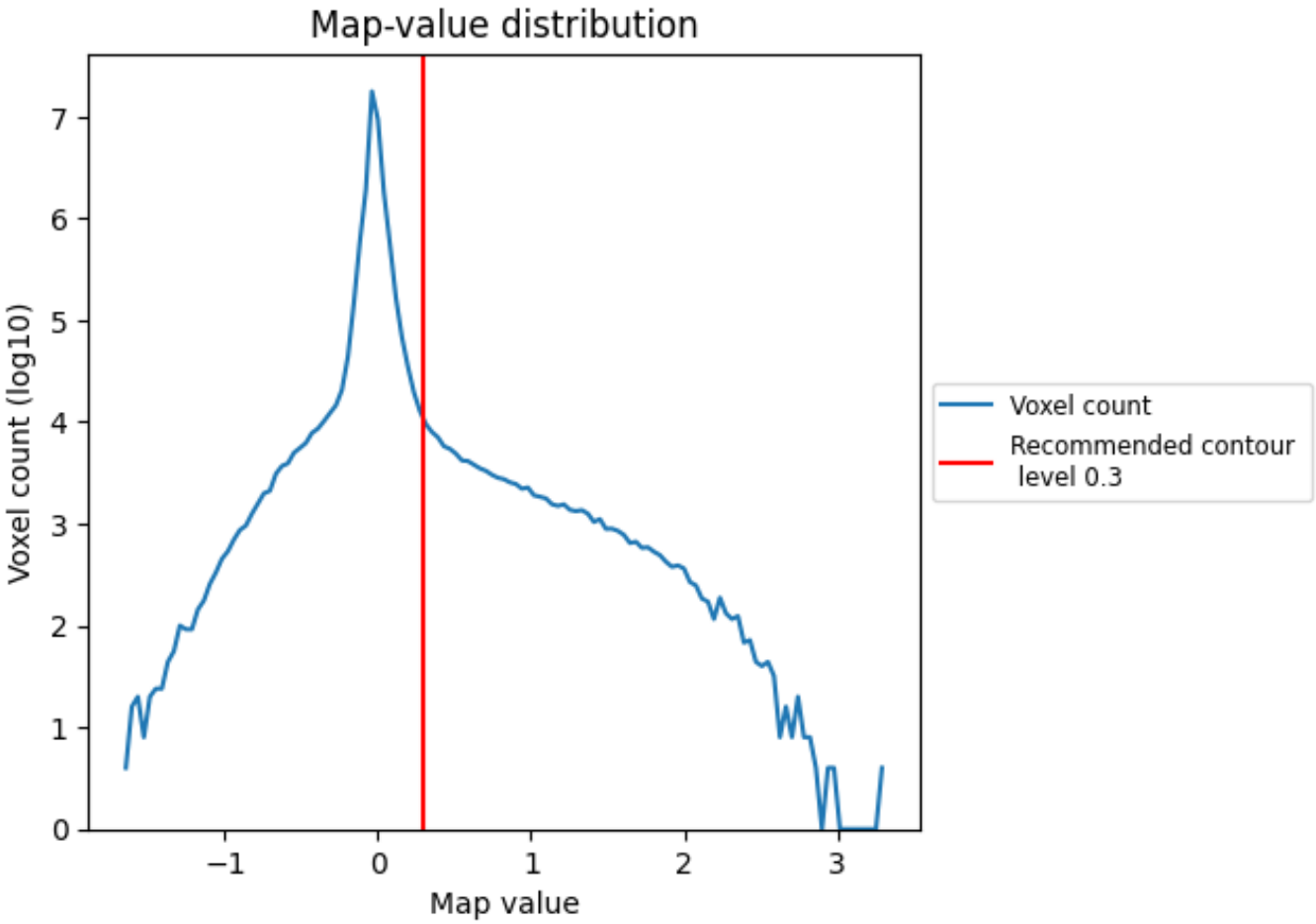
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

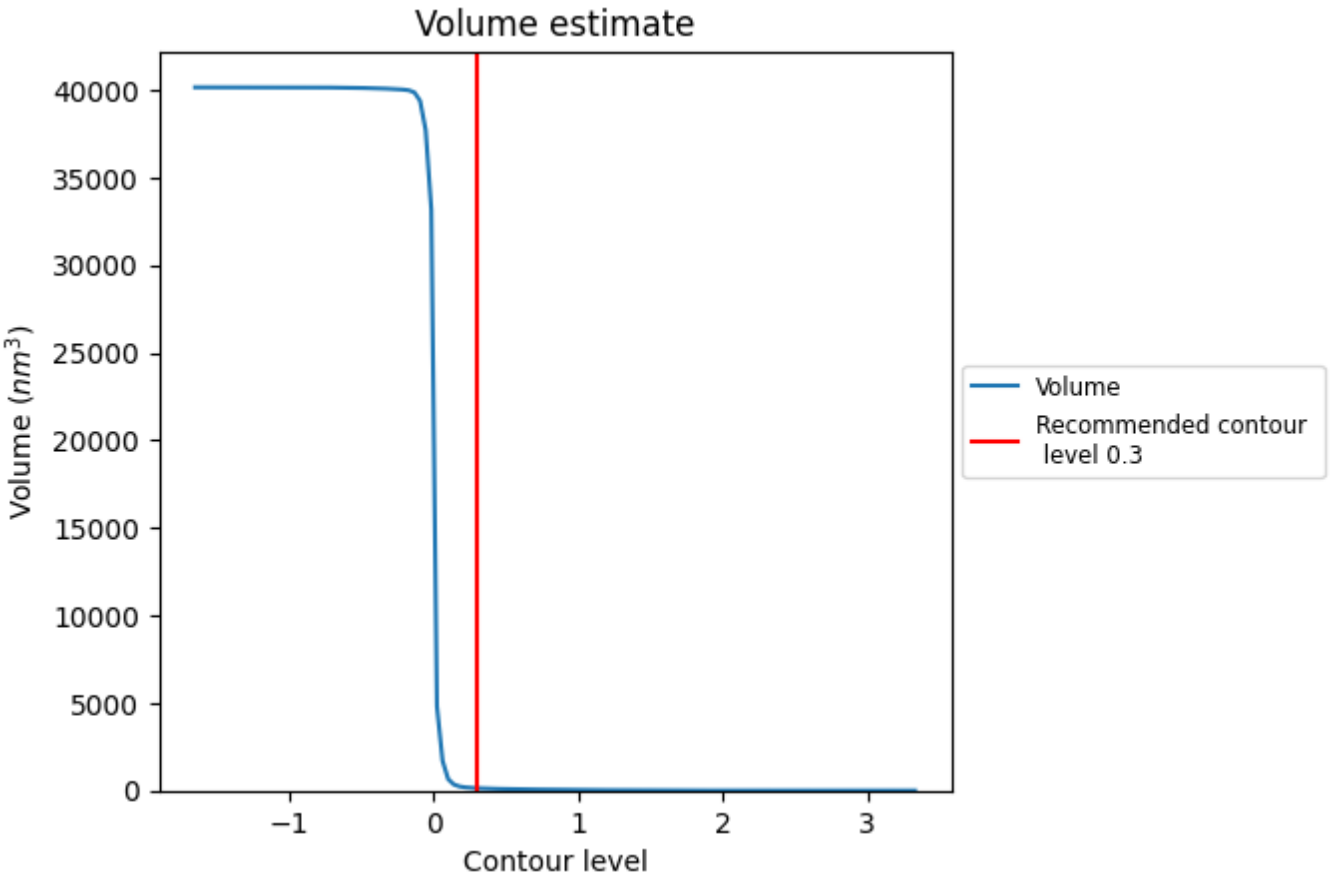
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

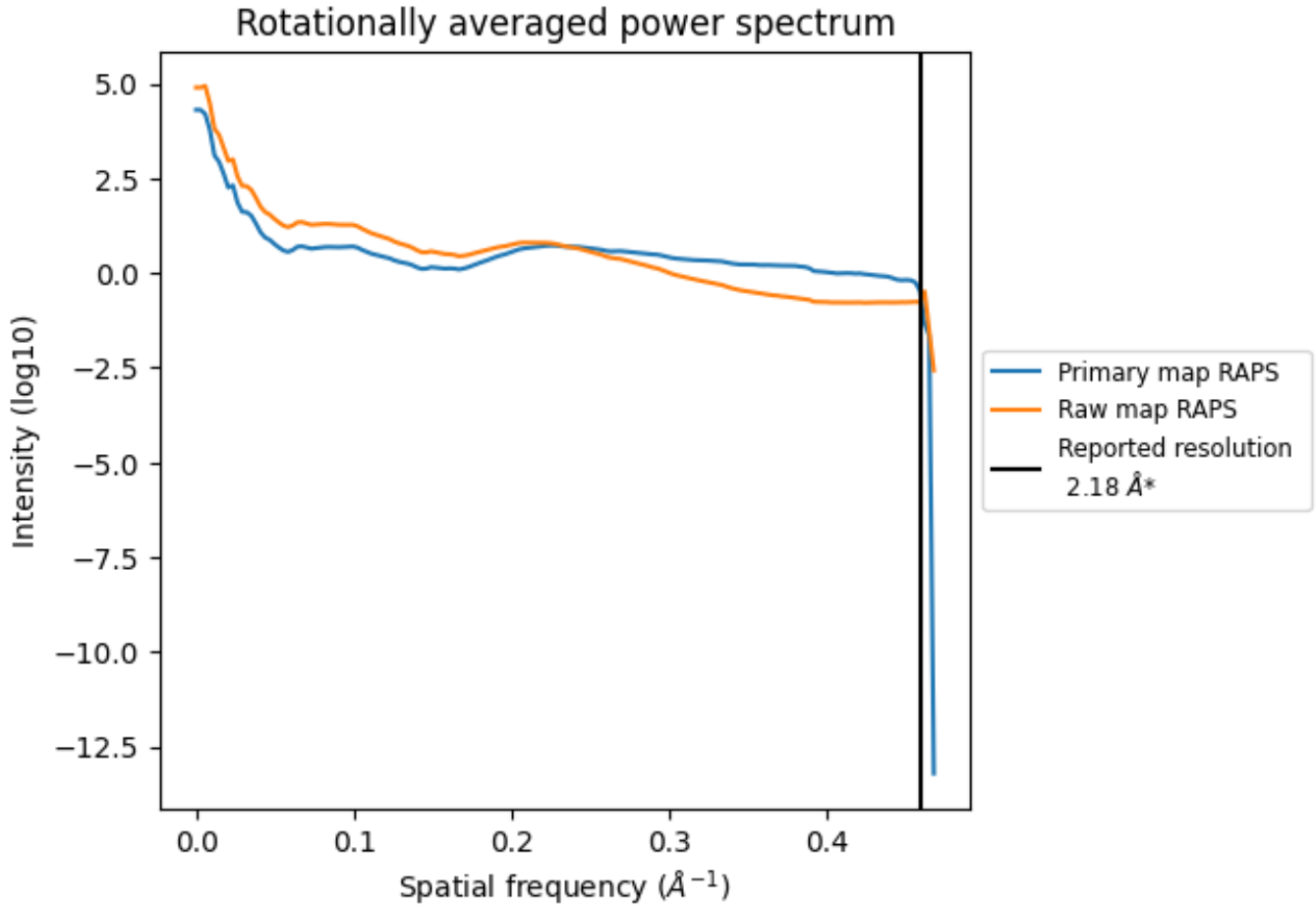
7.2 Volume estimate (i)



The volume at the recommended contour level is 135 nm^3; this corresponds to an approximate mass of 122 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

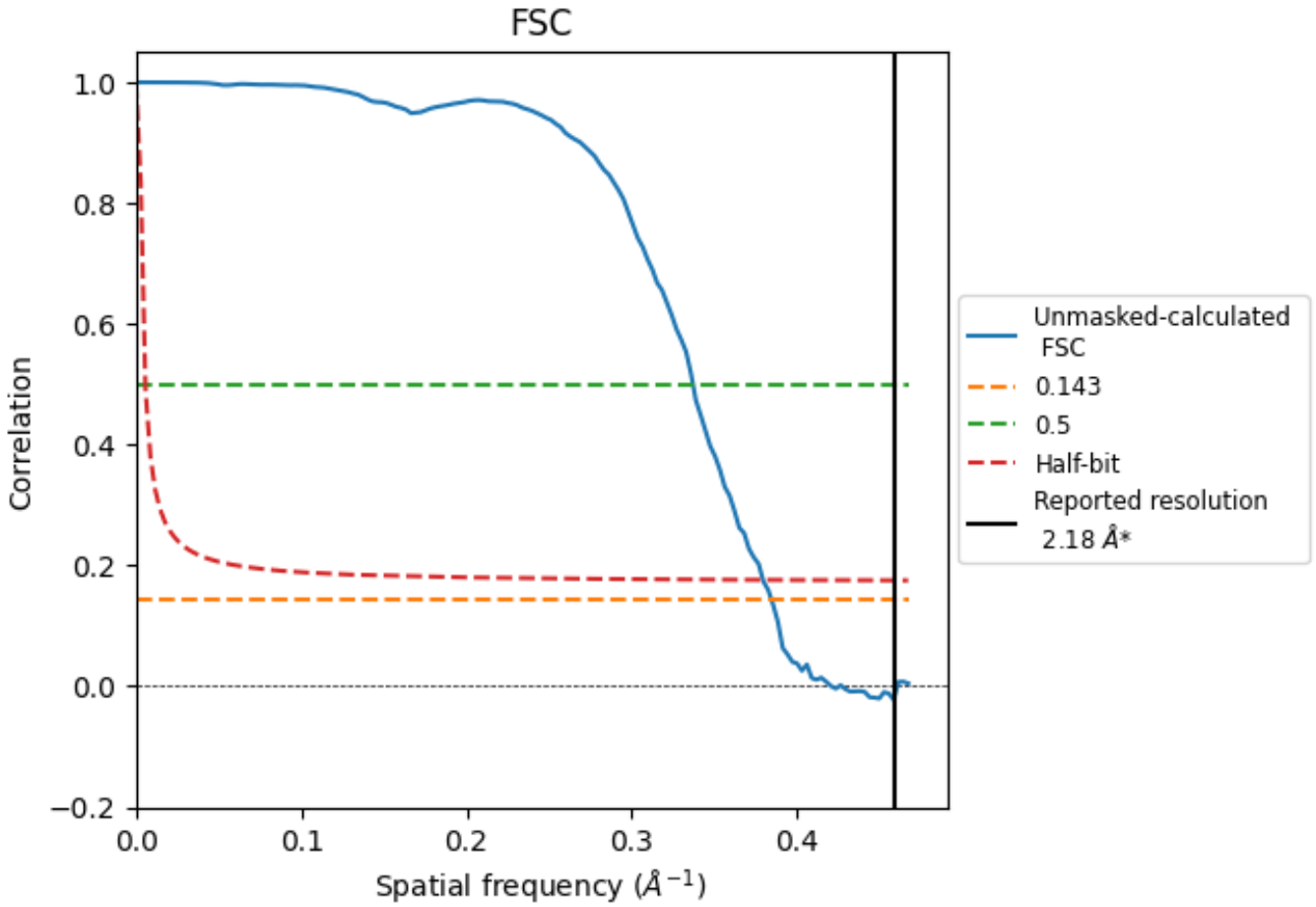


*Reported resolution corresponds to spatial frequency of 0.459 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.459 Å^{-1}

8.2 Resolution estimates (i)

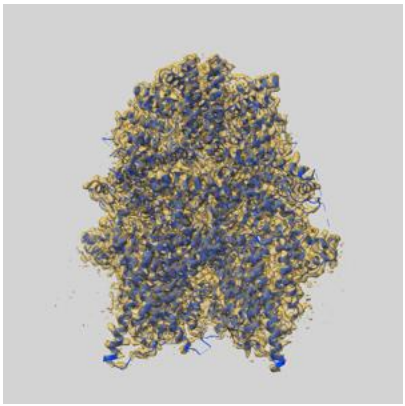
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.18	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.60	2.97	2.64

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.60 differs from the reported value 2.18 by more than 10 %

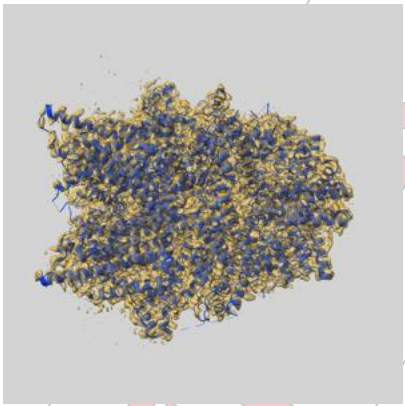
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-65273 and PDB model 9VQQ. Per-residue inclusion information can be found in section 3 on page 8.

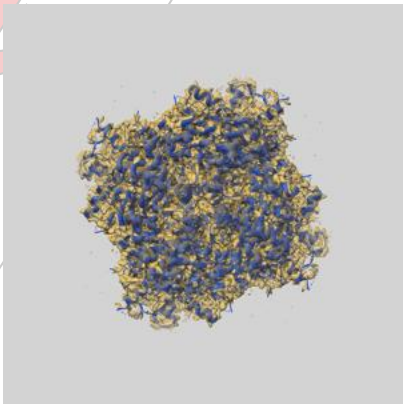
9.1 Map-model overlay



X



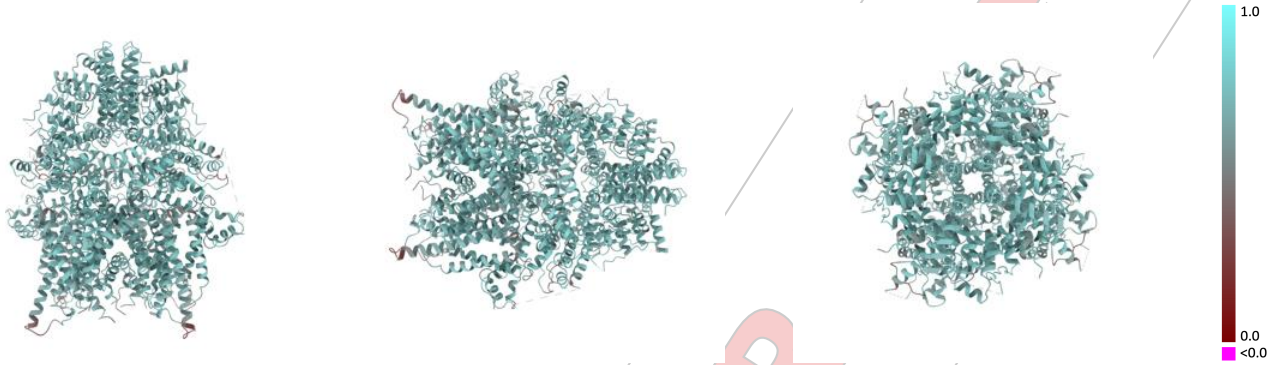
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

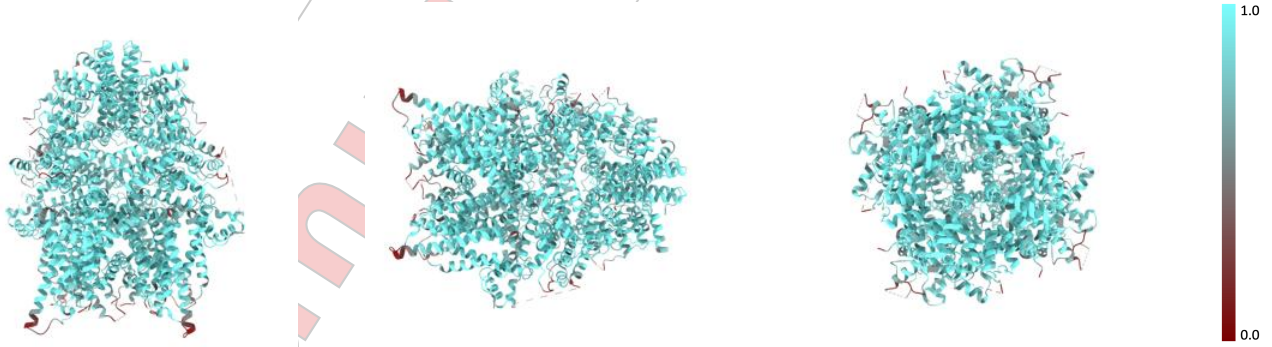
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

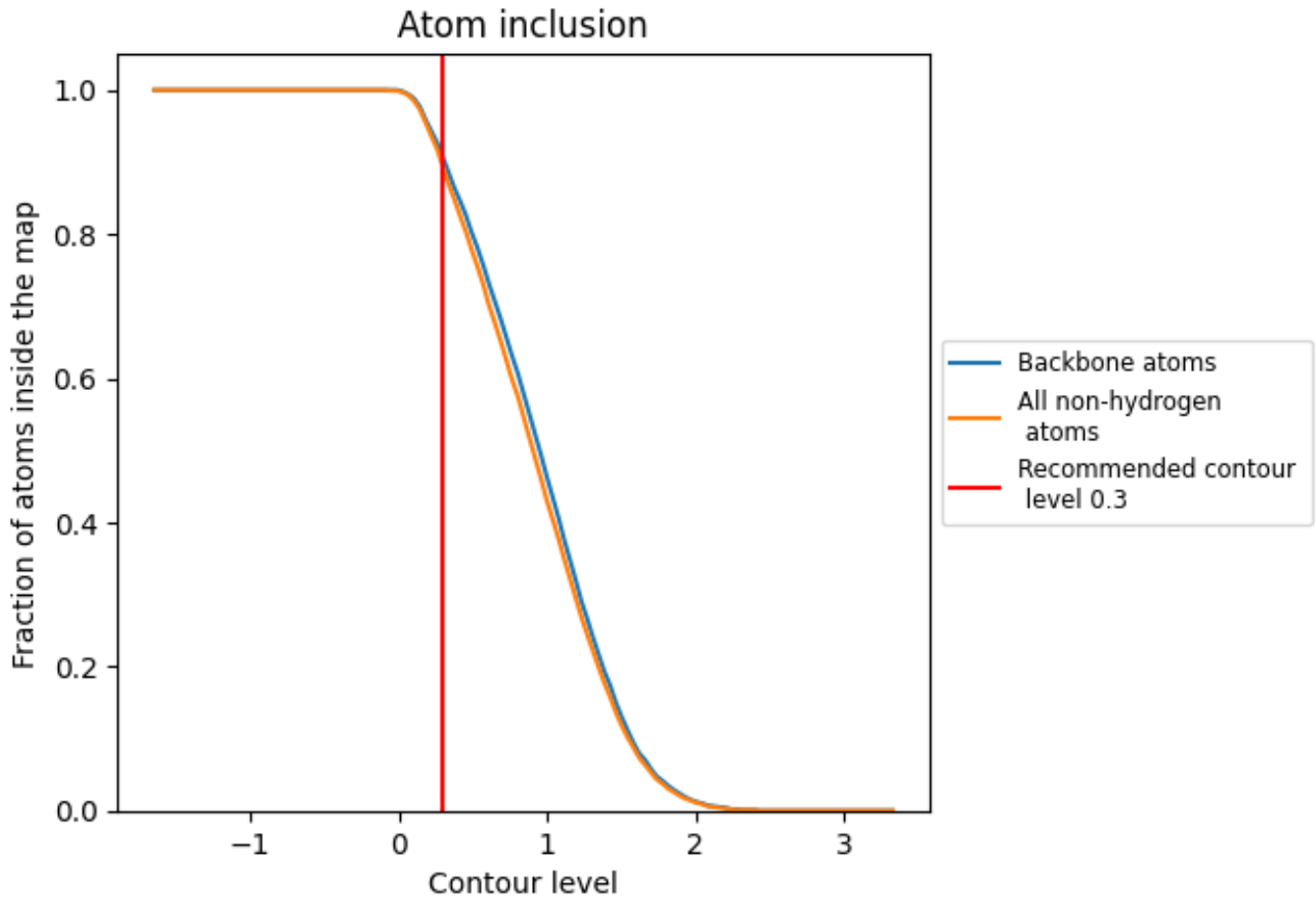
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8930	0.6750
A	0.8940	0.6740
B	0.8950	0.6750
C	0.8950	0.6740
D	0.8940	0.6750

Full wwPDB EM Validation Report ⓘ

Jul 20, 2025 – 02:16 PM JST

PDB ID	:	9VQW / pdb_00009vqw
EMDB ID	:	EMD-65279
Title	:	Cryo-EM structure of drosophila TRPgamma determined in GDN, state 2
Deposited on	:	2025-07-05
Resolution	:	2.29 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

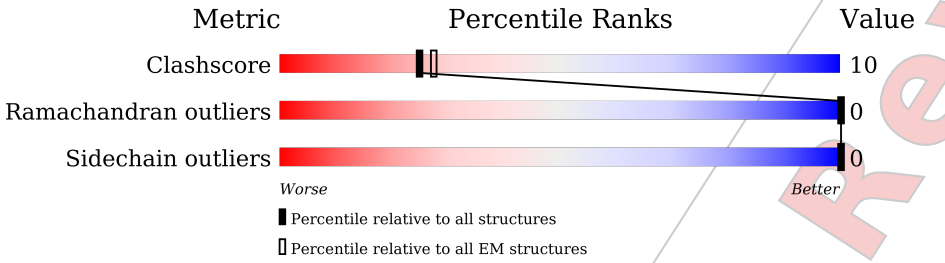
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.29 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1128	6% 52% 10% 38%
1	B	1128	6% 52% 10% 38%
1	C	1128	5% 52% 10% 38%
1	D	1128	5% 53% 9% 38%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PT5	A	1205	-	-	X	-
6	PT5	B	1205	-	-	X	-
6	PT5	C	1205	-	-	X	-
6	PT5	D	1206	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 23868 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transient receptor potential-gamma protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	705	Total 5769	C 3723	N 976	O 1036	S 34	0	0
1	B	705	Total 5769	C 3723	N 976	O 1036	S 34	0	0
1	C	705	Total 5769	C 3723	N 976	O 1036	S 34	0	0
1	D	705	Total 5769	C 3723	N 976	O 1036	S 34	0	0

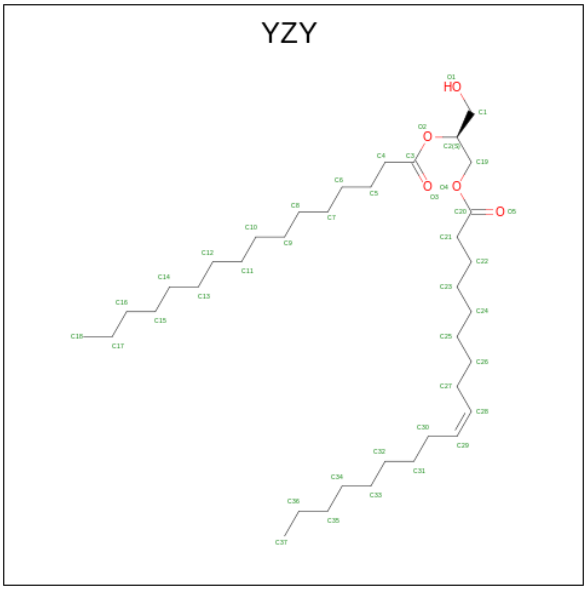
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total 1	Ca 1	0
2	B	1	Total 1	Ca 1	0
2	C	1	Total 1	Ca 1	0
2	D	1	Total 1	Ca 1	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

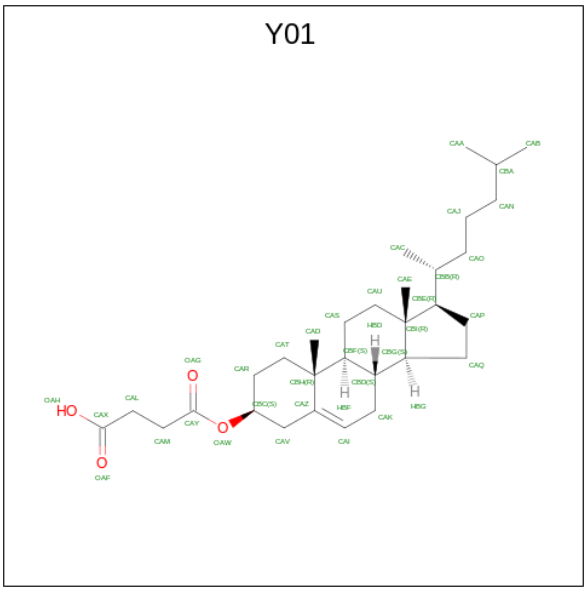
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total 1	Zn 1	0
3	B	1	Total 1	Zn 1	0
3	C	1	Total 1	Zn 1	0
3	D	1	Total 1	Zn 1	0

- Molecule 4 is (2S)-2-(hexadecanoyloxy)-3-hydroxypropyl (9Z)-octadec-9-enoate (CCD ID: YZY) (formula: $C_{37}H_{70}O_5$).



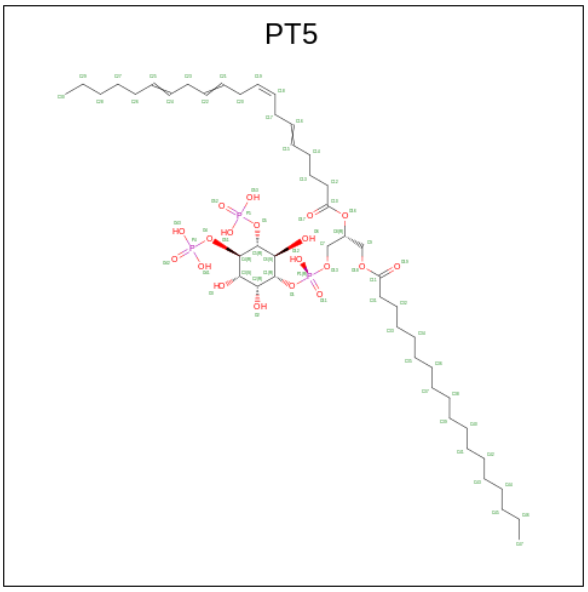
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
4	A	1	35	30	5	0
4	B	1	35	30	5	0
4	C	1	35	30	5	0
4	D	1	35	30	5	0

- Molecule 5 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $C_{31}H_{50}O_4$).



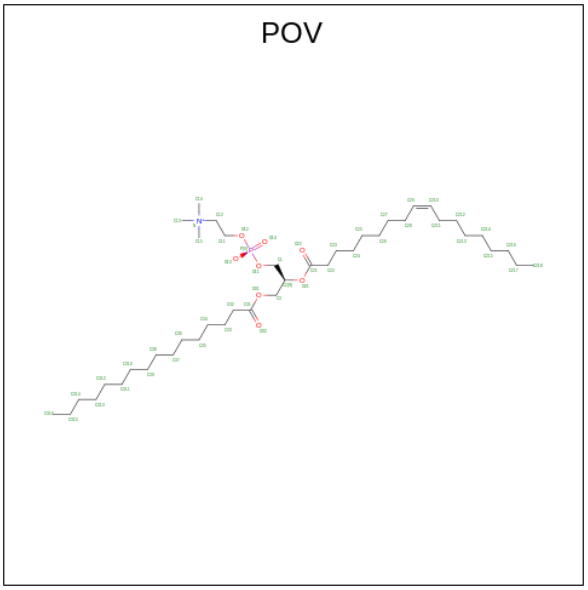
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C O 35 31 4	0
5	B	1	Total C O 35 31 4	0
5	C	1	Total C O 35 31 4	0
5	D	1	Total C O 35 31 4	0

- Molecule 6 is [(2R)-1-octadecanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phospho ryl]oxy-propan-2-yl] (8Z)-icosa-5,8,11,14-tetraenoate (CCD ID: PT5) (formula: $C_{47}H_{85}O_{19}P_3$).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	O	P	0
			69	47	19	3	
6	B	1	Total	C	O	P	0
			69	47	19	3	
6	C	1	Total	C	O	P	0
			69	47	19	3	
6	D	1	Total	C	O	P	0
			69	47	19	3	

- Molecule 7 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: $C_{42}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
7	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
7	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
7	D	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	A	5	Total	O	0
			5	5	

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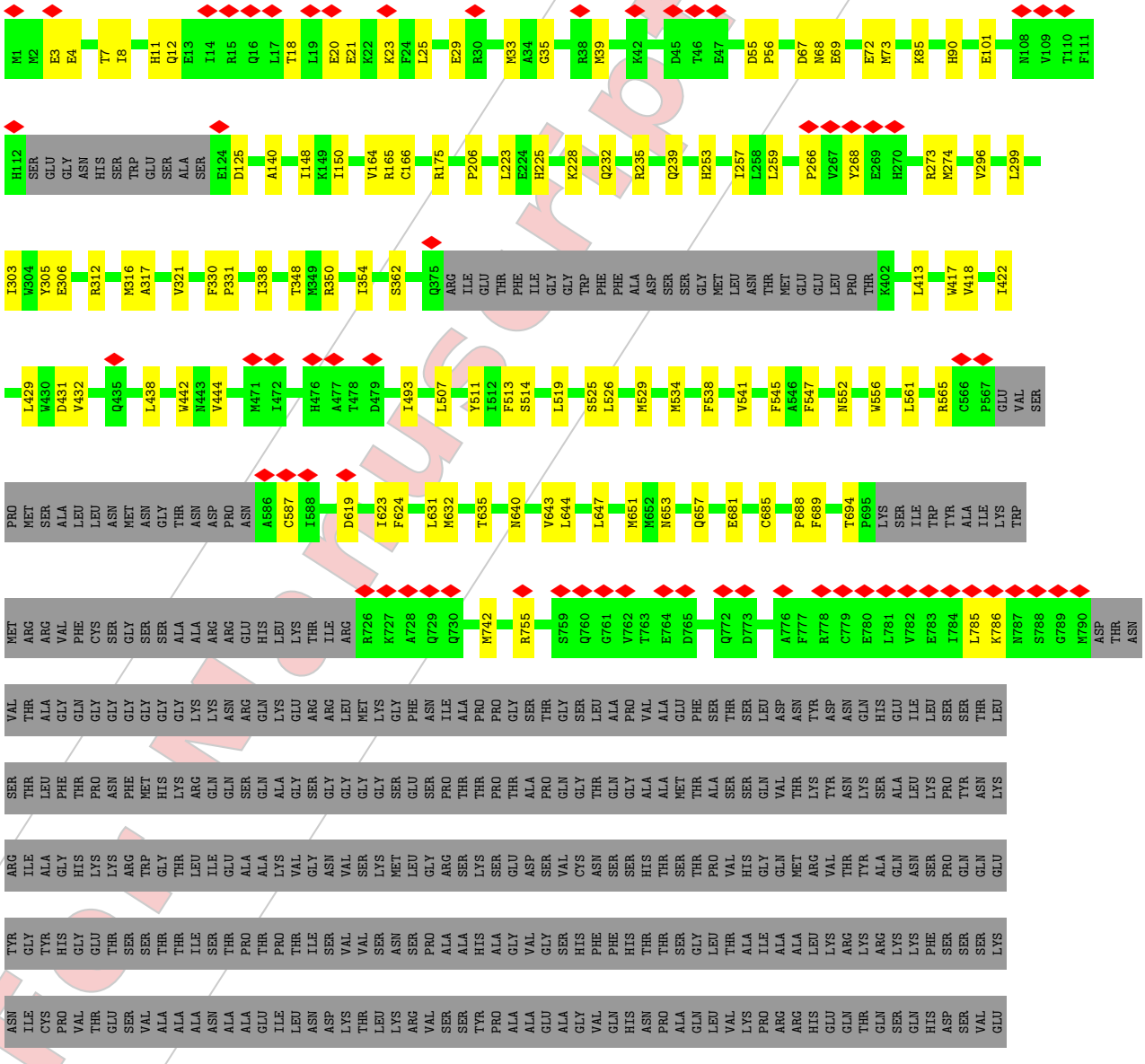
Mol	Chain	Residues	Atoms	AltConf
8	B	5	Total O 5 5	0
8	C	5	Total O 5 5	0
8	D	5	Total O 5 5	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

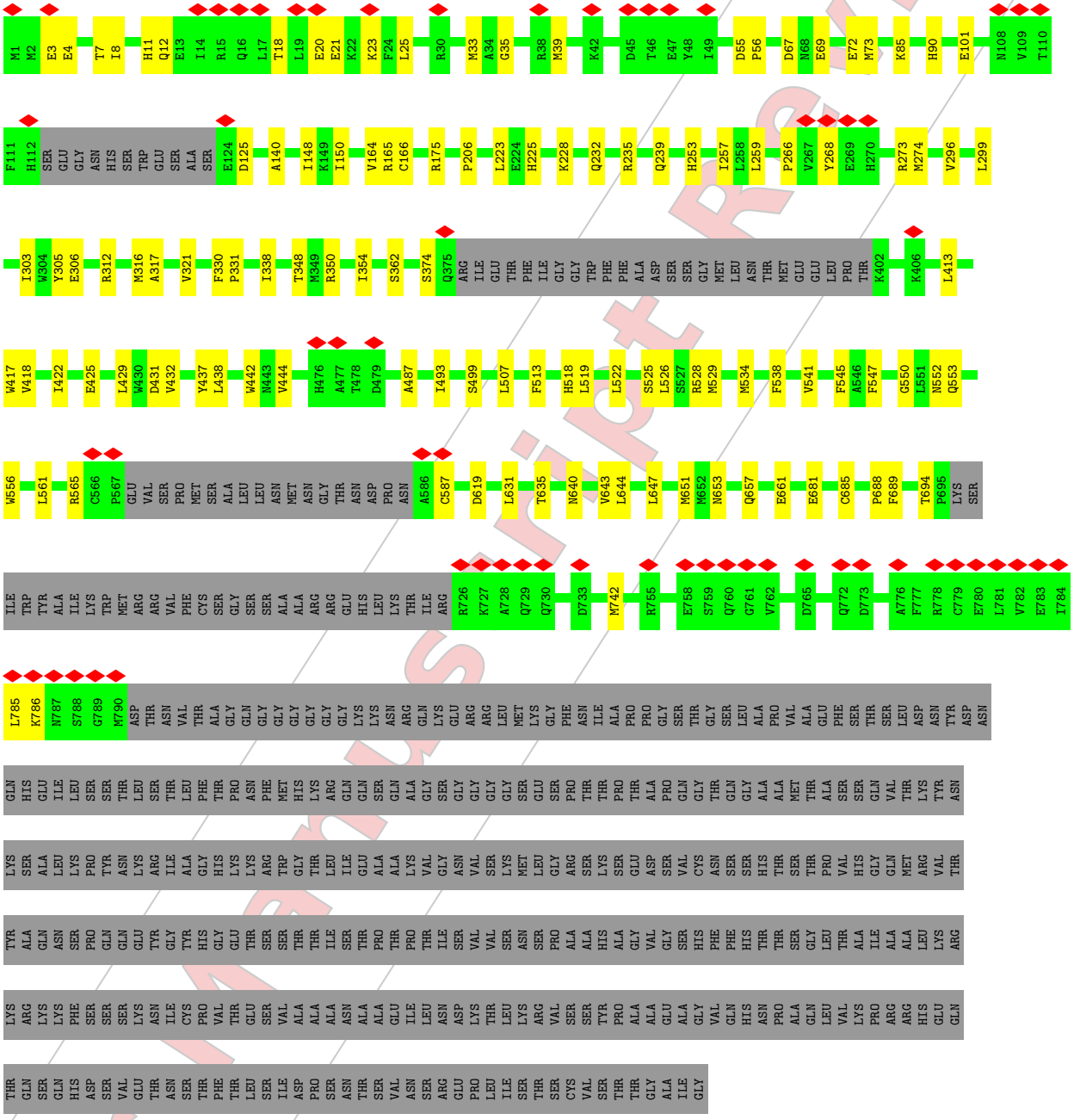
- Molecule 1: Transient receptor potential-gamma protein

Chain A:



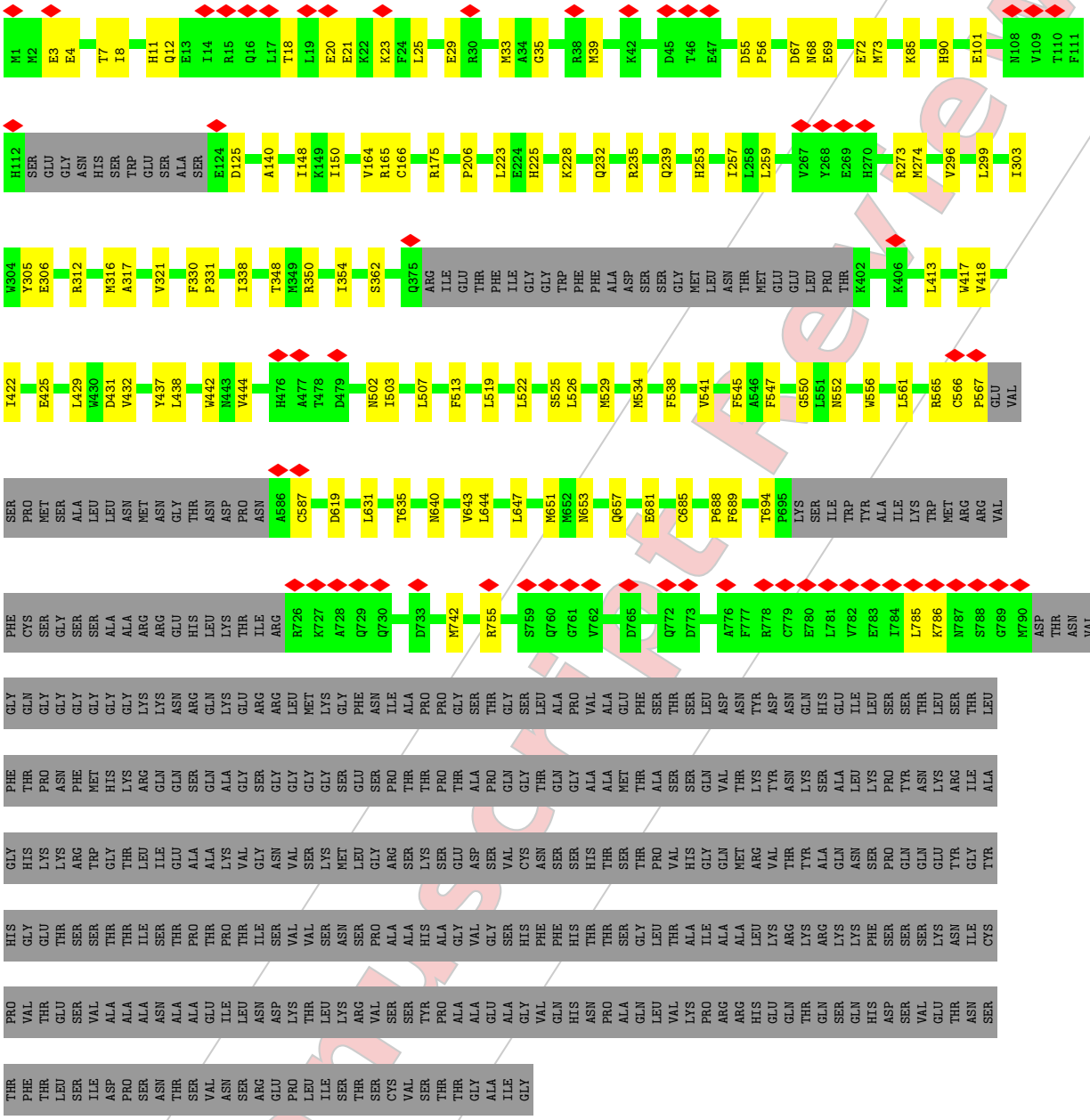
• Molecule 1: Transient receptor potential-gamma protein

Chain B:



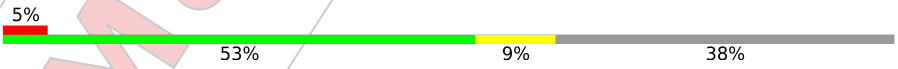
• Molecule 1: Transient receptor potential-gamma protein

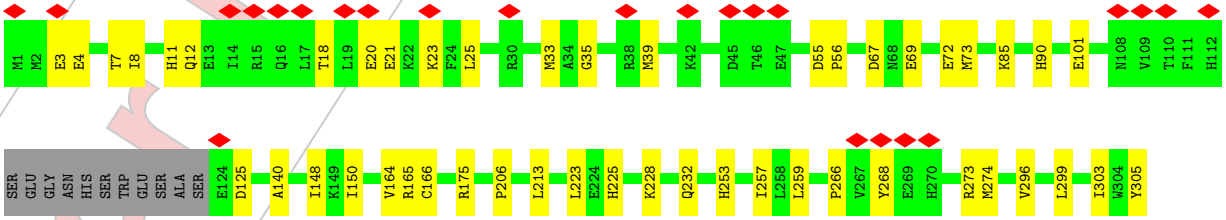
Chain C:

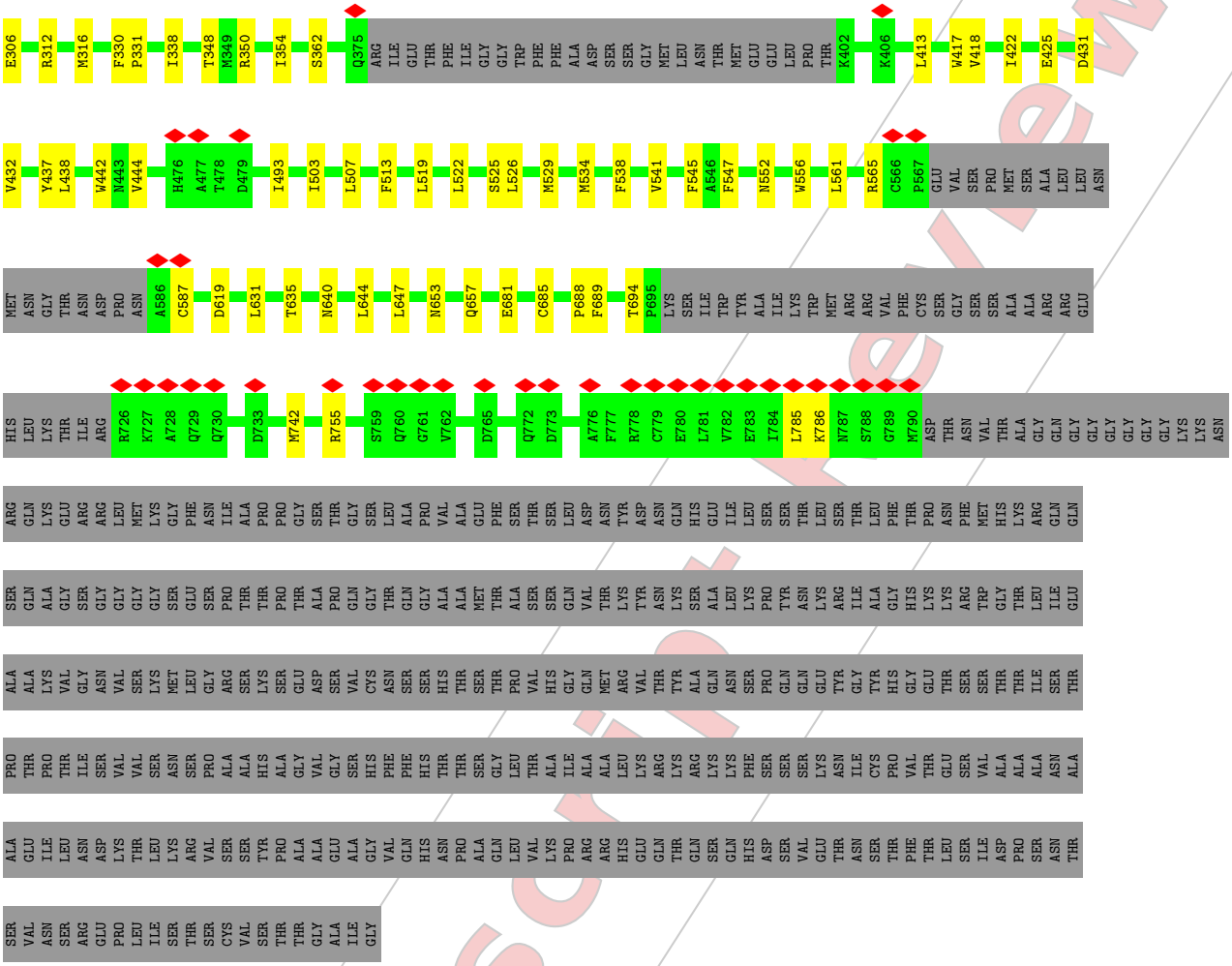


• Molecule 1: Transient receptor potential-gamma protein

Chain D:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	253312	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	-1400	Depositor
Maximum defocus (nm)	-2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.891	Depositor
Minimum map value	-1.377	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.28	Depositor
Map size (Å)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Y01, ZN, POV, YZY, CA, PT5

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.26	0/5901	0.38	0/7987
1	B	0.26	0/5901	0.38	0/7987
1	C	0.27	0/5901	0.38	0/7987
1	D	0.26	0/5901	0.38	0/7987
All	All	0.26	0/23604	0.38	0/31948

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5769	0	5765	129	0
1	B	5769	0	5765	131	0
1	C	5769	0	5765	123	0
1	D	5769	0	5765	113	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	35	0	53	4	0
4	B	35	0	53	4	0
4	C	35	0	53	5	0
4	D	35	0	53	5	0
5	A	35	0	49	13	0
5	B	35	0	49	16	0
5	C	35	0	49	13	0
5	D	35	0	49	14	0
6	A	69	0	80	23	0
6	B	69	0	80	22	0
6	C	69	0	80	22	0
6	D	69	0	80	23	0
7	A	52	0	82	10	0
7	B	52	0	82	11	0
7	C	52	0	82	11	0
7	D	52	0	82	10	0
8	A	5	0	0	0	0
8	B	5	0	0	0	0
8	C	5	0	0	0	0
8	D	5	0	0	0	0
All	All	23868	0	24116	496	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (496) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:HIS:CE1	7:B:1206:POV:H15A	1.54	1.43
1:C:225:HIS:CE1	7:C:1206:POV:H15A	1.55	1.42
1:C:225:HIS:CG	7:C:1206:POV:H15	1.63	1.34
1:B:225:HIS:CG	7:B:1206:POV:H15	1.63	1.31
1:D:225:HIS:CE1	7:D:1201:POV:H15A	1.69	1.27
1:A:225:HIS:CE1	7:A:1206:POV:H15A	1.68	1.26
1:A:225:HIS:CG	7:A:1206:POV:H15	1.70	1.25
1:B:225:HIS:CD2	7:B:1206:POV:H15	1.71	1.24
1:C:225:HIS:CD2	7:C:1206:POV:H15	1.72	1.23
1:D:225:HIS:CD2	7:D:1201:POV:H15	1.76	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:HIS:CD2	7:B:1206:POV:C15	2.25	1.19
1:C:225:HIS:CD2	7:C:1206:POV:C15	2.25	1.18
1:A:417:TRP:CZ3	1:A:688:PRO:HD3	1.79	1.17
1:B:417:TRP:CZ3	1:B:688:PRO:HD3	1.79	1.17
1:D:225:HIS:CG	7:D:1201:POV:H15	1.80	1.16
1:C:417:TRP:CZ3	1:C:688:PRO:HD3	1.79	1.16
1:D:417:TRP:CZ3	1:D:688:PRO:HD3	1.79	1.16
1:D:225:HIS:CD2	7:D:1201:POV:C15	2.32	1.11
1:A:225:HIS:CD2	7:A:1206:POV:C15	2.34	1.10
1:A:225:HIS:CD2	7:A:1206:POV:H15	1.86	1.10
1:C:225:HIS:CG	7:C:1206:POV:C15	2.34	1.09
1:A:225:HIS:CG	7:A:1206:POV:C15	2.38	1.07
6:A:1205:PT5:H21	1:B:316:MET:HE1	1.32	1.06
1:B:225:HIS:CG	7:B:1206:POV:C15	2.35	1.06
1:C:225:HIS:NE2	7:C:1206:POV:H15A	1.72	1.05
1:D:417:TRP:CH2	1:D:688:PRO:HG3	1.92	1.05
1:C:417:TRP:CH2	1:C:688:PRO:HG3	1.92	1.05
1:B:225:HIS:CE1	7:B:1206:POV:C15	2.40	1.04
1:B:225:HIS:NE2	7:B:1206:POV:H15A	1.71	1.04
1:B:417:TRP:CH2	1:B:688:PRO:HG3	1.92	1.04
1:A:417:TRP:CH2	1:A:688:PRO:HG3	1.92	1.04
1:D:225:HIS:NE2	7:D:1201:POV:H15A	1.74	1.03
1:C:362:SER:HG	1:C:417:TRP:HZ3	1.03	1.02
1:C:225:HIS:CE1	7:C:1206:POV:C15	2.41	1.02
1:C:534:MET:CE	6:C:1205:PT5:H63	1.90	1.01
1:B:534:MET:CE	6:B:1205:PT5:H63	1.90	1.01
1:D:534:MET:CE	6:D:1206:PT5:H63	1.90	1.01
1:A:534:MET:CE	6:A:1205:PT5:H63	1.90	1.00
1:D:362:SER:HG	1:D:417:TRP:HZ3	1.03	0.99
1:D:417:TRP:CZ3	1:D:688:PRO:CD	2.48	0.97
1:B:417:TRP:CZ3	1:B:688:PRO:CD	2.48	0.96
1:C:417:TRP:CZ3	1:C:688:PRO:CD	2.48	0.96
1:A:417:TRP:CZ3	1:A:688:PRO:CD	2.48	0.96
1:A:417:TRP:CE3	1:A:688:PRO:HD3	2.02	0.95
1:B:417:TRP:CE3	1:B:688:PRO:HD3	2.02	0.95
1:D:417:TRP:CE3	1:D:688:PRO:HD3	2.02	0.94
1:B:225:HIS:NE2	7:B:1206:POV:C15	2.27	0.94
6:C:1205:PT5:H21	1:D:316:MET:HE1	1.47	0.94
1:C:417:TRP:CE3	1:C:688:PRO:HD3	2.02	0.93
6:B:1205:PT5:H21	1:C:316:MET:HE1	1.49	0.92
1:C:225:HIS:NE2	7:C:1206:POV:C15	2.29	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:HIS:NE2	7:D:1201:POV:C15	2.33	0.92
1:D:225:HIS:CG	7:D:1201:POV:C15	2.51	0.91
1:A:225:HIS:NE2	7:A:1206:POV:H15A	1.85	0.90
1:D:225:HIS:CE1	7:D:1201:POV:C15	2.53	0.89
1:A:225:HIS:CE1	7:A:1206:POV:C15	2.56	0.89
1:A:316:MET:HE1	6:D:1206:PT5:H21	1.57	0.87
1:C:417:TRP:CZ3	1:C:688:PRO:HG3	2.11	0.85
1:A:417:TRP:CZ3	1:A:688:PRO:HG3	2.11	0.85
1:D:417:TRP:CZ3	1:D:688:PRO:HG3	2.11	0.85
1:B:417:TRP:CZ3	1:B:688:PRO:HG3	2.11	0.85
1:C:417:TRP:CZ3	1:C:688:PRO:CG	2.61	0.84
1:A:362:SER:HG	1:A:417:TRP:HZ3	1.25	0.83
1:B:362:SER:HG	1:B:417:TRP:HZ3	1.26	0.83
1:A:417:TRP:CZ3	1:A:688:PRO:CG	2.61	0.83
1:D:417:TRP:CZ3	1:D:688:PRO:CG	2.61	0.83
1:B:417:TRP:CZ3	1:B:688:PRO:CG	2.61	0.83
1:A:534:MET:HE3	6:A:1205:PT5:H63	1.61	0.82
1:B:534:MET:HE3	6:B:1205:PT5:H63	1.60	0.82
1:C:534:MET:HE3	6:C:1205:PT5:H63	1.61	0.81
1:D:534:MET:HE3	6:D:1206:PT5:H63	1.60	0.81
1:C:225:HIS:ND1	7:C:1206:POV:H15A	1.94	0.81
1:A:225:HIS:ND1	7:A:1206:POV:H15A	1.96	0.81
1:B:225:HIS:ND1	7:B:1206:POV:H15A	1.95	0.80
1:C:225:HIS:ND1	7:C:1206:POV:C15	2.44	0.80
6:A:1205:PT5:H21	1:B:316:MET:CE	2.12	0.80
1:B:225:HIS:ND1	7:B:1206:POV:C15	2.44	0.79
1:A:225:HIS:NE2	7:A:1206:POV:C15	2.45	0.79
1:A:635:THR:HG21	5:B:1204:Y01:HAO2	1.64	0.78
1:B:413:LEU:O	1:B:417:TRP:HD1	1.67	0.77
1:A:413:LEU:O	1:A:417:TRP:HD1	1.67	0.77
1:C:413:LEU:O	1:C:417:TRP:HD1	1.67	0.76
1:D:413:LEU:O	1:D:417:TRP:HD1	1.67	0.76
1:B:534:MET:CE	6:B:1205:PT5:C37	2.65	0.74
1:C:534:MET:CE	6:C:1205:PT5:C37	2.65	0.74
1:D:534:MET:CE	6:D:1206:PT5:C37	2.65	0.74
1:A:225:HIS:ND1	7:A:1206:POV:C15	2.51	0.73
1:A:534:MET:CE	6:A:1205:PT5:C37	2.65	0.73
1:A:547:PHE:CZ	5:B:1204:Y01:HAC2	2.25	0.72
1:C:647:LEU:HD22	1:D:526:LEU:HD13	1.73	0.71
1:A:417:TRP:CH2	1:A:688:PRO:CG	2.73	0.70
1:B:647:LEU:HD22	1:C:526:LEU:HD13	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:TRP:CH2	1:B:688:PRO:CG	2.73	0.70
1:D:685:CYS:SG	1:D:689:PHE:HB2	2.32	0.70
1:C:547:PHE:CZ	5:D:1205:Y01:HAC2	2.26	0.69
1:D:534:MET:HE2	6:D:1206:PT5:H60	1.75	0.69
1:A:534:MET:HE2	6:A:1205:PT5:H60	1.75	0.69
1:A:685:CYS:SG	1:A:689:PHE:HB2	2.32	0.69
1:C:685:CYS:SG	1:C:689:PHE:HB2	2.32	0.69
1:D:417:TRP:CH2	1:D:688:PRO:CG	2.73	0.68
1:A:413:LEU:O	1:A:417:TRP:CD1	2.46	0.68
1:B:547:PHE:CZ	5:C:1204:Y01:HAC2	2.27	0.68
1:B:413:LEU:O	1:B:417:TRP:CD1	2.46	0.68
1:B:685:CYS:SG	1:B:689:PHE:HB2	2.32	0.68
1:C:413:LEU:O	1:C:417:TRP:CD1	2.46	0.68
1:A:647:LEU:HD22	1:B:526:LEU:HD13	1.76	0.68
1:B:507:LEU:HD13	5:B:1204:Y01:HAS2	1.76	0.68
1:C:417:TRP:CH2	1:C:688:PRO:CG	2.73	0.68
1:C:507:LEU:HD13	5:C:1204:Y01:HAS2	1.76	0.68
1:A:507:LEU:HD13	5:A:1204:Y01:HAS2	1.76	0.68
1:C:534:MET:HE2	6:C:1205:PT5:H60	1.75	0.68
1:D:413:LEU:O	1:D:417:TRP:CD1	2.46	0.67
1:D:507:LEU:HD13	5:D:1205:Y01:HAS2	1.76	0.67
1:B:534:MET:HE2	6:B:1205:PT5:H60	1.75	0.67
1:A:785:LEU:HD12	1:A:786:LYS:N	2.10	0.66
1:D:785:LEU:HD12	1:D:786:LYS:N	2.10	0.66
1:C:635:THR:HG21	5:D:1205:Y01:HAO2	1.77	0.66
1:C:785:LEU:HD12	1:C:786:LYS:N	2.10	0.66
1:B:785:LEU:HD12	1:B:786:LYS:N	2.10	0.65
1:A:643:VAL:HG11	4:B:1203:YZY:H183	1.76	0.65
1:A:547:PHE:HZ	5:B:1204:Y01:HAC2	1.61	0.64
1:B:635:THR:HG21	5:C:1204:Y01:HAO2	1.79	0.64
1:B:538:PHE:HB2	6:B:1205:PT5:H64	1.80	0.64
1:B:541:VAL:HG21	6:B:1205:PT5:H67	1.79	0.64
1:D:541:VAL:HG21	6:D:1206:PT5:H67	1.79	0.64
1:A:541:VAL:HG21	6:A:1205:PT5:H67	1.79	0.63
1:D:538:PHE:HB2	6:D:1206:PT5:H64	1.80	0.63
4:A:1203:YZY:H42	1:D:631:LEU:HD12	1.78	0.63
1:C:541:VAL:HG21	6:C:1205:PT5:H67	1.79	0.62
1:B:507:LEU:CD1	5:B:1204:Y01:HAS2	2.29	0.62
1:C:538:PHE:HB2	6:C:1205:PT5:H64	1.80	0.62
1:A:538:PHE:HB2	6:A:1205:PT5:H64	1.80	0.62
1:C:507:LEU:CD1	5:C:1204:Y01:HAS2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:507:LEU:CD1	5:D:1205:Y01:HAS2	2.29	0.62
1:D:534:MET:HE2	6:D:1206:PT5:C35	2.30	0.62
1:A:507:LEU:CD1	5:A:1204:Y01:HAS2	2.29	0.61
1:D:225:HIS:ND1	7:D:1201:POV:C15	2.63	0.61
1:A:534:MET:HE2	6:A:1205:PT5:C35	2.30	0.61
1:D:140:ALA:HA	1:D:148:ILE:HD11	1.82	0.61
1:D:417:TRP:HZ3	1:D:688:PRO:HD3	1.60	0.61
1:B:534:MET:HE2	6:B:1205:PT5:C35	2.30	0.61
1:C:534:MET:HE2	6:C:1205:PT5:C35	2.30	0.60
1:A:556:TRP:NE1	1:B:374:SER:HB3	2.16	0.60
1:D:225:HIS:ND1	7:D:1201:POV:H15A	2.15	0.60
1:A:140:ALA:HA	1:A:148:ILE:HD11	1.82	0.60
1:B:417:TRP:HZ3	1:B:688:PRO:HD3	1.60	0.60
1:B:140:ALA:HA	1:B:148:ILE:HD11	1.82	0.60
1:B:362:SER:OG	1:B:417:TRP:HZ3	1.85	0.59
1:B:538:PHE:CD2	1:C:519:LEU:HD21	2.37	0.59
1:C:565:ARG:NH2	1:C:587:CYS:SG	2.75	0.59
1:A:565:ARG:NH2	1:A:587:CYS:SG	2.75	0.59
1:B:565:ARG:NH2	1:B:587:CYS:SG	2.75	0.59
6:B:1205:PT5:H26	6:B:1205:PT5:H56	1.84	0.59
1:C:140:ALA:HA	1:C:148:ILE:HD11	1.82	0.59
1:C:538:PHE:CD2	1:D:519:LEU:HD21	2.37	0.59
1:D:565:ARG:NH2	1:D:587:CYS:SG	2.75	0.59
6:A:1205:PT5:H26	6:A:1205:PT5:H56	1.84	0.59
6:C:1205:PT5:H26	6:C:1205:PT5:H56	1.84	0.59
1:D:20:GLU:O	1:D:23:LYS:NZ	2.36	0.59
6:D:1206:PT5:H26	6:D:1206:PT5:H56	1.84	0.59
1:A:362:SER:OG	1:A:417:TRP:HZ3	1.85	0.59
1:A:20:GLU:O	1:A:23:LYS:NZ	2.36	0.58
6:C:1205:PT5:H21	1:D:316:MET:CE	2.30	0.58
1:C:417:TRP:HZ3	1:C:688:PRO:HD3	1.60	0.58
1:C:20:GLU:O	1:C:23:LYS:NZ	2.36	0.58
1:A:538:PHE:CD2	1:B:519:LEU:HD21	2.39	0.58
1:A:631:LEU:HG	5:B:1204:Y01:HAB1	1.86	0.58
1:C:67:ASP:OD1	1:C:90:HIS:NE2	2.37	0.57
1:A:538:PHE:HD2	1:B:519:LEU:HD21	1.69	0.57
1:B:20:GLU:O	1:B:23:LYS:NZ	2.36	0.57
1:B:33:MET:HA	1:B:33:MET:HE2	1.86	0.57
1:C:33:MET:HE2	1:C:33:MET:HA	1.86	0.57
1:D:33:MET:HE2	1:D:33:MET:HA	1.86	0.57
1:A:632:MET:HE1	1:B:499:SER:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:GLU:O	1:B:8:ILE:HG13	2.05	0.57
1:C:4:GLU:O	1:C:8:ILE:HG13	2.05	0.57
1:A:316:MET:CE	6:D:1206:PT5:H21	2.33	0.57
1:D:4:GLU:O	1:D:8:ILE:HG13	2.05	0.57
1:D:67:ASP:OD1	1:D:90:HIS:NE2	2.37	0.57
1:A:4:GLU:O	1:A:8:ILE:HG13	2.05	0.56
1:D:18:THR:HG23	1:D:21:GLU:HB2	1.87	0.56
4:A:1203:YZY:H221	6:A:1205:PT5:H85	1.87	0.56
4:D:1204:YZY:H221	6:D:1206:PT5:H85	1.87	0.56
1:C:547:PHE:HZ	5:D:1205:Y01:HAC2	1.70	0.56
1:A:33:MET:HE2	1:A:33:MET:HA	1.86	0.55
1:A:67:ASP:OD1	1:A:90:HIS:NE2	2.37	0.55
4:C:1203:YZY:H221	6:C:1205:PT5:H85	1.87	0.55
1:A:18:THR:HG23	1:A:21:GLU:HB2	1.87	0.55
1:B:18:THR:HG23	1:B:21:GLU:HB2	1.87	0.55
1:C:18:THR:HG23	1:C:21:GLU:HB2	1.87	0.55
1:B:67:ASP:OD1	1:B:90:HIS:NE2	2.37	0.54
4:B:1203:YZY:H221	6:B:1205:PT5:H85	1.87	0.54
1:D:259:LEU:HD11	1:D:296:VAL:HG22	1.90	0.54
1:D:545:PHE:HB2	6:D:1206:PT5:H49	1.90	0.54
1:C:8:ILE:O	1:C:12:GLN:HG2	2.08	0.54
1:C:538:PHE:HD2	1:D:519:LEU:HD21	1.73	0.54
1:D:8:ILE:O	1:D:12:GLN:HG2	2.08	0.54
1:C:545:PHE:HB2	6:C:1205:PT5:H49	1.90	0.54
1:C:259:LEU:HD11	1:C:296:VAL:HG22	1.90	0.54
1:A:556:TRP:HE1	1:B:374:SER:HB3	1.71	0.54
1:D:164:VAL:HG11	1:D:223:LEU:HD23	1.90	0.53
1:A:545:PHE:HB2	6:A:1205:PT5:H49	1.90	0.53
1:A:8:ILE:O	1:A:12:GLN:HG2	2.08	0.53
1:B:8:ILE:O	1:B:12:GLN:HG2	2.08	0.53
1:A:534:MET:HE1	6:A:1205:PT5:C37	2.39	0.53
1:B:259:LEU:HD11	1:B:296:VAL:HG22	1.90	0.53
1:D:534:MET:HE1	6:D:1206:PT5:C37	2.39	0.53
1:A:623:ILE:HG22	1:B:487:ALA:HB1	1.91	0.53
1:A:164:VAL:HG11	1:A:223:LEU:HD23	1.90	0.53
1:C:534:MET:HE1	6:C:1205:PT5:C37	2.39	0.53
1:A:259:LEU:HD11	1:A:296:VAL:HG22	1.90	0.53
1:A:651:MET:SD	1:B:522:LEU:HD11	2.49	0.53
1:C:507:LEU:CD1	5:C:1204:Y01:CAE	2.87	0.53
1:D:3:GLU:O	1:D:7:THR:HG23	2.09	0.53
6:B:1205:PT5:H21	1:C:316:MET:CE	2.31	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:GLU:O	1:C:7:THR:HG23	2.09	0.53
1:B:507:LEU:CD1	5:B:1204:Y01:CAE	2.87	0.52
1:B:545:PHE:HB2	6:B:1205:PT5:H49	1.90	0.52
1:B:538:PHE:HD2	1:C:519:LEU:HD21	1.74	0.52
1:A:228:LYS:O	1:A:232:GLN:HG3	2.10	0.52
1:B:348:THR:HG22	1:B:354:ILE:HG21	1.92	0.52
1:B:534:MET:HE2	6:B:1205:PT5:C36	2.39	0.52
1:C:164:VAL:HG11	1:C:223:LEU:HD23	1.90	0.52
1:C:534:MET:HE2	6:C:1205:PT5:C36	2.39	0.52
1:B:164:VAL:HG11	1:B:223:LEU:HD23	1.90	0.52
1:D:228:LYS:O	1:D:232:GLN:HG3	2.10	0.52
1:B:3:GLU:O	1:B:7:THR:HG23	2.09	0.52
1:D:534:MET:HE2	6:D:1206:PT5:C36	2.39	0.52
1:C:72:GLU:H	1:C:72:GLU:CD	2.18	0.52
1:A:507:LEU:CD1	5:A:1204:Y01:CAE	2.87	0.52
1:A:348:THR:HG22	1:A:354:ILE:HG21	1.92	0.52
4:A:1203:YZY:H232	6:A:1205:PT5:C47	2.40	0.52
1:C:228:LYS:O	1:C:232:GLN:HG3	2.10	0.52
4:D:1204:YZY:H232	6:D:1206:PT5:C47	2.40	0.52
1:A:3:GLU:O	1:A:7:THR:HG23	2.09	0.52
1:A:35:GLY:O	1:A:39:MET:HG3	2.10	0.52
1:B:72:GLU:CD	1:B:72:GLU:H	2.18	0.52
1:A:253:HIS:O	1:A:257:ILE:HG12	2.11	0.51
1:D:507:LEU:CD1	5:D:1205:Y01:CAE	2.87	0.51
1:D:35:GLY:O	1:D:39:MET:HG3	2.10	0.51
6:B:1205:PT5:H46	6:B:1205:PT5:H77	1.92	0.51
1:C:643:VAL:HG11	4:D:1204:YZY:H183	1.91	0.51
5:A:1204:Y01:HAO2	1:D:635:THR:HG21	1.92	0.51
1:C:35:GLY:O	1:C:39:MET:HG3	2.10	0.51
6:C:1205:PT5:H46	6:C:1205:PT5:H77	1.92	0.51
1:D:72:GLU:CD	1:D:72:GLU:H	2.18	0.51
1:A:534:MET:HE2	6:A:1205:PT5:C36	2.39	0.51
1:B:228:LYS:O	1:B:232:GLN:HG3	2.10	0.51
4:C:1203:YZY:H232	6:C:1205:PT5:C47	2.40	0.51
1:D:253:HIS:O	1:D:257:ILE:HG12	2.11	0.51
1:D:348:THR:HG22	1:D:354:ILE:HG21	1.92	0.51
1:B:35:GLY:O	1:B:39:MET:HG3	2.10	0.51
1:C:348:THR:HG22	1:C:354:ILE:HG21	1.92	0.51
1:D:525:SER:O	1:D:529:MET:HG3	2.11	0.51
1:A:72:GLU:CD	1:A:72:GLU:H	2.18	0.51
6:A:1205:PT5:H77	6:A:1205:PT5:H46	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:MET:HE1	6:B:1205:PT5:C37	2.39	0.51
4:B:1203:YZY:H232	6:B:1205:PT5:C47	2.40	0.51
1:B:253:HIS:O	1:B:257:ILE:HG12	2.10	0.50
1:C:253:HIS:O	1:C:257:ILE:HG12	2.10	0.50
1:A:525:SER:O	1:A:529:MET:HG3	2.11	0.50
1:D:125:ASP:N	1:D:125:ASP:OD1	2.45	0.50
1:B:206:PRO:HD2	1:B:742:MET:HG2	1.94	0.50
1:C:55:ASP:HB2	1:C:56:PRO:HD2	1.94	0.50
1:C:525:SER:O	1:C:529:MET:HG3	2.11	0.50
1:D:55:ASP:HB2	1:D:56:PRO:HD2	1.94	0.50
1:A:624:PHE:CE2	1:B:493:ILE:HA	2.45	0.50
1:B:547:PHE:HZ	5:C:1204:Y01:HAC2	1.73	0.50
6:D:1206:PT5:H46	6:D:1206:PT5:H77	1.92	0.50
1:A:125:ASP:OD1	1:A:125:ASP:N	2.45	0.50
1:A:547:PHE:CZ	5:B:1204:Y01:CAC	2.95	0.50
1:C:507:LEU:CD1	5:C:1204:Y01:HAE1	2.42	0.50
1:A:55:ASP:HB2	1:A:56:PRO:HD2	1.94	0.49
1:B:507:LEU:CD1	5:B:1204:Y01:HAE1	2.42	0.49
1:C:206:PRO:HD2	1:C:742:MET:HG2	1.94	0.49
1:D:561:LEU:HB3	1:D:619:ASP:HB3	1.94	0.49
1:A:561:LEU:HB3	1:A:619:ASP:HB3	1.94	0.49
1:B:631:LEU:HD12	4:C:1203:YZY:H42	1.94	0.49
1:B:561:LEU:HB3	1:B:619:ASP:HB3	1.94	0.49
1:D:206:PRO:HD2	1:D:742:MET:HG2	1.94	0.49
1:D:507:LEU:HD11	5:D:1205:Y01:HAU2	1.95	0.49
1:A:507:LEU:HD11	5:A:1204:Y01:HAU2	1.95	0.49
1:B:507:LEU:HD11	5:B:1204:Y01:HAU2	1.94	0.49
1:C:125:ASP:OD1	1:C:125:ASP:N	2.45	0.49
1:C:507:LEU:HD11	5:C:1204:Y01:HAU2	1.94	0.49
1:A:507:LEU:CD1	5:A:1204:Y01:HAE1	2.42	0.49
1:B:125:ASP:OD1	1:B:125:ASP:N	2.45	0.49
1:B:525:SER:O	1:B:529:MET:HG3	2.11	0.49
1:A:206:PRO:HD2	1:A:742:MET:HG2	1.94	0.49
1:D:507:LEU:CD1	5:D:1205:Y01:HAE1	2.42	0.49
1:B:643:VAL:HG11	4:C:1203:YZY:H183	1.94	0.49
1:B:55:ASP:HB2	1:B:56:PRO:HD2	1.94	0.49
1:C:561:LEU:HB3	1:C:619:ASP:HB3	1.94	0.48
1:D:166:CYS:O	1:D:175:ARG:NH2	2.38	0.48
1:A:526:LEU:HD13	1:D:647:LEU:HD22	1.95	0.48
1:A:534:MET:CE	6:A:1205:PT5:C36	2.91	0.48
1:C:534:MET:CE	6:C:1205:PT5:C36	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:MET:CE	6:B:1205:PT5:C36	2.91	0.48
1:C:438:LEU:HD13	1:C:444:VAL:HG22	1.96	0.48
1:D:534:MET:CE	6:D:1206:PT5:C36	2.91	0.48
4:D:1204:YZY:H232	6:D:1206:PT5:H83	1.95	0.48
1:A:417:TRP:HZ3	1:A:688:PRO:CD	2.20	0.48
4:A:1203:YZY:H232	6:A:1205:PT5:H83	1.95	0.48
1:B:305:TYR:CE2	1:B:312:ARG:HD3	2.49	0.48
1:B:438:LEU:HD13	1:B:444:VAL:HG22	1.96	0.48
1:A:305:TYR:CE2	1:A:312:ARG:HD3	2.49	0.47
4:B:1203:YZY:H232	6:B:1205:PT5:H83	1.95	0.47
1:C:305:TYR:CE2	1:C:312:ARG:HD3	2.49	0.47
1:D:305:TYR:CE2	1:D:312:ARG:HD3	2.49	0.47
1:B:73:MET:HE3	1:B:73:MET:HA	1.96	0.47
4:C:1203:YZY:H232	6:C:1205:PT5:H83	1.95	0.47
1:A:438:LEU:HD13	1:A:444:VAL:HG22	1.96	0.47
5:A:1204:Y01:HAC2	1:D:547:PHE:CZ	2.49	0.47
1:D:438:LEU:HD13	1:D:444:VAL:HG22	1.96	0.47
1:C:273:ARG:NH1	1:C:306:GLU:OE1	2.48	0.47
1:A:85:LYS:HD2	1:A:85:LYS:HA	1.66	0.46
1:B:273:ARG:NH1	1:B:306:GLU:OE1	2.48	0.46
1:C:73:MET:HA	1:C:73:MET:HE3	1.96	0.46
1:A:417:TRP:HZ3	1:A:688:PRO:HD3	1.60	0.46
1:B:513:PHE:HB3	1:B:519:LEU:HD22	1.98	0.46
5:D:1205:Y01:HAJ1	5:D:1205:Y01:HAC3	1.80	0.46
1:C:631:LEU:HD12	4:D:1204:YZY:H42	1.97	0.46
1:D:273:ARG:NH1	1:D:306:GLU:OE1	2.48	0.46
1:A:73:MET:HA	1:A:73:MET:HE3	1.96	0.46
1:A:513:PHE:HB3	1:A:519:LEU:HD22	1.98	0.46
1:B:425:GLU:OE1	1:B:437:TYR:OH	2.29	0.46
1:C:538:PHE:HA	6:C:1205:PT5:H68	1.98	0.46
1:B:69:GLU:HG3	1:B:69:GLU:O	2.16	0.46
1:C:69:GLU:O	1:C:69:GLU:HG3	2.16	0.46
1:D:69:GLU:O	1:D:69:GLU:HG3	2.16	0.46
1:D:73:MET:HE3	1:D:73:MET:HA	1.96	0.46
1:A:69:GLU:O	1:A:69:GLU:HG3	2.16	0.46
1:A:350:ARG:NE	1:A:681:GLU:OE1	2.49	0.46
1:D:350:ARG:NE	1:D:681:GLU:OE1	2.49	0.46
1:D:538:PHE:HA	6:D:1206:PT5:H68	1.98	0.46
1:A:635:THR:HG21	5:B:1204:Y01:HAN2	1.96	0.46
1:C:350:ARG:NE	1:C:681:GLU:OE1	2.49	0.46
1:A:273:ARG:NH1	1:A:306:GLU:OE1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:PHE:CD2	1:B:331:PRO:HD3	2.52	0.45
1:D:513:PHE:HB3	1:D:519:LEU:HD22	1.98	0.45
1:A:519:LEU:HD21	1:D:538:PHE:CD2	2.51	0.45
1:A:785:LEU:CD1	1:A:786:LYS:N	2.80	0.45
1:C:513:PHE:HB3	1:C:519:LEU:HD22	1.98	0.45
1:B:166:CYS:O	1:B:175:ARG:NH2	2.38	0.45
1:B:538:PHE:CD1	6:B:1205:PT5:H71	2.52	0.45
1:B:785:LEU:CD1	1:B:786:LYS:N	2.80	0.45
1:C:538:PHE:CD1	6:C:1205:PT5:H71	2.52	0.45
1:C:651:MET:SD	1:D:522:LEU:HD11	2.57	0.45
1:B:225:HIS:ND1	7:B:1206:POV:C13	2.80	0.45
1:B:550:GLY:HA3	1:C:503:ILE:HG13	1.98	0.45
1:D:101:GLU:OE1	1:D:150:ILE:HD13	2.17	0.45
1:A:429:LEU:HD23	1:A:429:LEU:HA	1.86	0.45
1:A:538:PHE:CD1	6:A:1205:PT5:H71	2.52	0.45
1:B:350:ARG:NE	1:B:681:GLU:OE1	2.49	0.45
1:B:538:PHE:HA	6:B:1205:PT5:H68	1.98	0.45
1:C:101:GLU:OE1	1:C:150:ILE:HD13	2.17	0.45
1:C:429:LEU:HD23	1:C:429:LEU:HA	1.86	0.45
1:A:101:GLU:OE1	1:A:150:ILE:HD13	2.17	0.44
1:A:511:TYR:O	1:A:514:SER:OG	2.33	0.44
1:A:538:PHE:HA	6:A:1205:PT5:H68	1.98	0.44
1:D:534:MET:HE1	6:D:1206:PT5:H63	1.89	0.44
1:A:431:ASP:OD1	1:A:432:VAL:N	2.51	0.44
1:B:431:ASP:OD1	1:B:432:VAL:N	2.51	0.44
1:C:330:PHE:CD2	1:C:331:PRO:HD3	2.52	0.44
1:C:550:GLY:HA3	1:D:503:ILE:HG13	2.00	0.44
1:D:431:ASP:OD1	1:D:432:VAL:N	2.51	0.44
1:A:330:PHE:CD2	1:A:331:PRO:HD3	2.52	0.44
6:A:1205:PT5:H17	1:B:518:HIS:CE1	2.52	0.44
1:C:653:ASN:O	1:C:657:GLN:HG3	2.18	0.44
1:A:653:ASN:O	1:A:657:GLN:HG3	2.18	0.44
1:B:101:GLU:OE1	1:B:150:ILE:HD13	2.17	0.44
1:B:164:VAL:CG1	1:B:223:LEU:HD23	2.48	0.44
1:C:431:ASP:OD1	1:C:432:VAL:N	2.51	0.44
1:B:418:VAL:O	1:B:422:ILE:HG12	2.18	0.44
1:D:653:ASN:O	1:D:657:GLN:HG3	2.18	0.44
5:A:1204:Y01:HAJ1	5:A:1204:Y01:HAC3	1.80	0.44
1:D:330:PHE:CD2	1:D:331:PRO:HD3	2.52	0.44
1:A:507:LEU:HD12	5:A:1204:Y01:CAE	2.48	0.44
1:C:418:VAL:O	1:C:422:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:653:ASN:O	1:B:657:GLN:HG3	2.18	0.44
1:D:507:LEU:HD12	5:D:1205:Y01:CAE	2.48	0.43
1:D:538:PHE:CD1	6:D:1206:PT5:H71	2.52	0.43
1:A:164:VAL:CG1	1:A:223:LEU:HD23	2.48	0.43
1:C:785:LEU:CD1	1:C:786:LYS:H	2.32	0.43
1:B:785:LEU:CD1	1:B:786:LYS:H	2.32	0.43
1:C:225:HIS:ND1	7:C:1206:POV:C13	2.81	0.43
1:C:274:MET:HE2	1:C:303:ILE:HD11	2.01	0.43
1:A:785:LEU:CD1	1:A:786:LYS:H	2.32	0.43
1:C:164:VAL:CG1	1:C:223:LEU:HD23	2.48	0.43
1:C:223:LEU:HD12	1:C:223:LEU:HA	1.71	0.43
1:B:507:LEU:HD12	5:B:1204:Y01:CAE	2.48	0.43
1:A:418:VAL:O	1:A:422:ILE:HG12	2.18	0.43
1:B:223:LEU:HD12	1:B:223:LEU:HA	1.71	0.43
1:D:785:LEU:CD1	1:D:786:LYS:N	2.80	0.43
1:A:166:CYS:O	1:A:175:ARG:NH2	2.38	0.43
1:B:338:ILE:HG23	1:B:694:THR:HG22	2.01	0.43
1:B:552:ASN:O	1:B:556:TRP:HB3	2.19	0.43
1:C:7:THR:OG1	1:C:29:GLU:OE1	2.29	0.43
1:D:164:VAL:CG1	1:D:223:LEU:HD23	2.48	0.43
1:D:274:MET:HE2	1:D:303:ILE:HD11	2.00	0.43
1:B:661:GLU:H	1:B:661:GLU:HG3	1.70	0.42
1:C:338:ILE:HG23	1:C:694:THR:HG22	2.01	0.42
1:B:85:LYS:HD2	1:B:85:LYS:HA	1.66	0.42
1:B:274:MET:HE2	1:B:303:ILE:HD11	2.01	0.42
1:D:418:VAL:O	1:D:422:ILE:HG12	2.18	0.42
1:B:442:TRP:CZ2	5:B:1204:Y01:HAM2	2.55	0.42
1:C:507:LEU:HD12	5:C:1204:Y01:CAE	2.48	0.42
1:D:785:LEU:CD1	1:D:786:LYS:H	2.32	0.42
1:B:651:MET:SD	1:C:522:LEU:HD11	2.60	0.42
1:C:425:GLU:OE1	1:C:437:TYR:OH	2.29	0.42
1:D:85:LYS:HD2	1:D:85:LYS:HA	1.66	0.42
1:D:417:TRP:HZ3	1:D:688:PRO:CD	2.20	0.42
1:A:165:ARG:CZ	1:A:223:LEU:HD21	2.50	0.42
1:B:165:ARG:CZ	1:B:223:LEU:HD21	2.50	0.42
1:B:507:LEU:HD23	1:B:507:LEU:HA	1.90	0.42
1:A:338:ILE:HG23	1:A:694:THR:HG22	2.01	0.42
1:A:651:MET:SD	1:B:522:LEU:CD1	3.08	0.42
1:C:442:TRP:CZ2	5:C:1204:Y01:HAM2	2.55	0.42
1:D:338:ILE:HG23	1:D:694:THR:HG22	2.01	0.42
1:A:223:LEU:HD12	1:A:223:LEU:HA	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:ASN:O	1:A:556:TRP:HB3	2.19	0.42
1:B:442:TRP:HZ2	5:B:1204:Y01:HAM2	1.85	0.42
1:C:166:CYS:O	1:C:175:ARG:NH2	2.39	0.42
1:C:552:ASN:O	1:C:556:TRP:HB3	2.19	0.42
1:D:552:ASN:O	1:D:556:TRP:HB3	2.19	0.42
1:D:640:ASN:HA	1:D:644:LEU:HB2	2.01	0.42
1:A:274:MET:HE2	1:A:303:ILE:HD11	2.00	0.42
1:A:442:TRP:CZ2	5:A:1204:Y01:HAM2	2.54	0.42
1:B:274:MET:HE1	1:B:299:LEU:HD11	2.02	0.42
1:B:417:TRP:HZ3	1:B:688:PRO:CD	2.20	0.42
1:B:538:PHE:HD1	6:B:1205:PT5:H71	1.84	0.42
1:D:442:TRP:HZ2	5:D:1205:Y01:HAM2	1.85	0.42
1:D:538:PHE:HD1	6:D:1206:PT5:H71	1.85	0.42
5:B:1204:Y01:HAC3	5:B:1204:Y01:HAJ1	1.80	0.42
1:C:274:MET:HE1	1:C:299:LEU:HD11	2.02	0.42
1:C:305:TYR:CD2	1:C:312:ARG:HD3	2.55	0.42
1:D:442:TRP:CZ2	5:D:1205:Y01:HAM2	2.55	0.42
1:D:755:ARG:HA	1:D:755:ARG:HD3	1.88	0.42
1:B:429:LEU:HD23	1:B:429:LEU:HA	1.86	0.41
1:C:442:TRP:HZ2	5:C:1204:Y01:HAM2	1.85	0.41
1:D:274:MET:HE1	1:D:299:LEU:HD11	2.02	0.41
1:D:493:ILE:H	1:D:493:ILE:HG12	1.70	0.41
1:B:541:VAL:CG1	6:B:1205:PT5:H47	2.51	0.41
1:C:165:ARG:CZ	1:C:223:LEU:HD21	2.50	0.41
1:C:640:ASN:HA	1:C:644:LEU:HB2	2.02	0.41
1:A:305:TYR:CD2	1:A:312:ARG:HD3	2.55	0.41
1:B:305:TYR:CD2	1:B:312:ARG:HD3	2.55	0.41
1:B:640:ASN:HA	1:B:644:LEU:HB2	2.02	0.41
1:D:541:VAL:CG1	6:D:1206:PT5:H47	2.51	0.41
1:C:235:ARG:O	1:C:239:GLN:HG3	2.21	0.41
1:C:566:CYS:HA	1:C:567:PRO:HD3	1.94	0.41
1:A:235:ARG:O	1:A:239:GLN:HG3	2.21	0.41
1:B:507:LEU:HD11	5:B:1204:Y01:CAU	2.51	0.41
1:D:165:ARG:CZ	1:D:223:LEU:HD21	2.50	0.41
1:D:213:LEU:HD12	1:D:213:LEU:HA	1.90	0.41
1:A:266:PRO:HB2	1:A:268:TYR:CE1	2.55	0.41
1:A:442:TRP:HZ2	5:A:1204:Y01:HAM2	1.85	0.41
1:A:538:PHE:HD1	6:A:1205:PT5:H71	1.84	0.41
1:B:538:PHE:CE2	1:C:519:LEU:HD21	2.56	0.41
1:C:755:ARG:HD3	1:C:755:ARG:HA	1.88	0.41
5:C:1204:Y01:HAC3	5:C:1204:Y01:HAJ1	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:PRO:HB2	1:D:268:TYR:CE1	2.55	0.41
1:B:11:HIS:NE2	1:B:25:LEU:HB2	2.36	0.41
1:B:528:ARG:HD3	1:B:528:ARG:HA	1.86	0.41
1:D:305:TYR:CD2	1:D:312:ARG:HD3	2.55	0.41
1:A:493:ILE:H	1:A:493:ILE:HG12	1.70	0.41
1:B:553:GLN:HE21	1:C:502:ASN:ND2	2.19	0.41
1:C:85:LYS:HA	1:C:85:LYS:HD2	1.65	0.41
1:C:538:PHE:HD1	6:C:1205:PT5:H71	1.84	0.41
1:A:11:HIS:NE2	1:A:25:LEU:HB2	2.36	0.41
1:A:274:MET:HE1	1:A:299:LEU:HD11	2.02	0.41
1:B:235:ARG:O	1:B:239:GLN:HG3	2.21	0.41
1:C:317:ALA:O	1:C:321:VAL:HG23	2.21	0.41
1:C:541:VAL:CG1	6:C:1205:PT5:H47	2.51	0.41
1:A:507:LEU:HD11	5:A:1204:Y01:CAU	2.51	0.40
1:A:644:LEU:HD23	1:A:644:LEU:HA	1.91	0.40
1:B:266:PRO:HB2	1:B:268:TYR:CE1	2.55	0.40
1:B:317:ALA:O	1:B:321:VAL:HG23	2.21	0.40
1:C:4:GLU:OE2	1:C:4:GLU:HA	2.21	0.40
1:C:11:HIS:NE2	1:C:25:LEU:HB2	2.36	0.40
1:C:785:LEU:CD1	1:C:786:LYS:N	2.80	0.40
1:A:541:VAL:CG1	6:A:1205:PT5:H47	2.51	0.40
1:D:425:GLU:OE1	1:D:437:TYR:OH	2.29	0.40
1:D:507:LEU:HD11	5:D:1205:Y01:CAU	2.51	0.40
1:D:507:LEU:HD12	5:D:1205:Y01:HAE2	2.04	0.40
1:A:4:GLU:HA	1:A:4:GLU:OE2	2.21	0.40
1:A:317:ALA:O	1:A:321:VAL:HG23	2.21	0.40
1:A:507:LEU:HD12	5:A:1204:Y01:HAE2	2.04	0.40
1:A:507:LEU:HD23	1:A:507:LEU:HA	1.90	0.40
1:B:4:GLU:HA	1:B:4:GLU:OE2	2.21	0.40
1:C:29:GLU:O	1:C:68:ASN:ND2	2.55	0.40
1:D:11:HIS:NE2	1:D:25:LEU:HB2	2.36	0.40
1:A:29:GLU:O	1:A:68:ASN:ND2	2.55	0.40
1:A:640:ASN:HA	1:A:644:LEU:HB2	2.02	0.40
1:A:755:ARG:HA	1:A:755:ARG:HD3	1.88	0.40
1:C:507:LEU:HD11	5:C:1204:Y01:CAU	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	695/1128 (62%)	686 (99%)	9 (1%)	0	100	100
1	B	695/1128 (62%)	686 (99%)	9 (1%)	0	100	100
1	C	695/1128 (62%)	686 (99%)	9 (1%)	0	100	100
1	D	695/1128 (62%)	686 (99%)	9 (1%)	0	100	100
All	All	2780/4512 (62%)	2744 (99%)	36 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	634/985 (64%)	634 (100%)	0	100	100
1	B	634/985 (64%)	634 (100%)	0	100	100
1	C	634/985 (64%)	634 (100%)	0	100	100
1	D	634/985 (64%)	634 (100%)	0	100	100
All	All	2536/3940 (64%)	2536 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	68	ASN
1	A	239	GLN
1	A	428	GLN
1	A	523	GLN
1	A	553	GLN
1	A	654	HIS
1	A	657	GLN
1	B	44	GLN
1	B	68	ASN
1	B	239	GLN
1	B	428	GLN
1	B	523	GLN
1	B	552	ASN
1	B	553	GLN
1	B	653	ASN
1	B	657	GLN
1	C	44	GLN
1	C	68	ASN
1	C	239	GLN
1	C	428	GLN
1	C	523	GLN
1	C	553	GLN
1	C	654	HIS
1	C	657	GLN
1	D	44	GLN
1	D	68	ASN
1	D	239	GLN
1	D	428	GLN
1	D	523	GLN
1	D	553	GLN
1	D	654	HIS
1	D	657	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	YZY	A	1203	-	34,34,41	0.94	4 (11%)	36,36,43	1.23	2 (5%)
6	PT5	A	1205	-	69,69,69	1.21	6 (8%)	83,87,87	1.18	6 (7%)
5	Y01	A	1204	-	38,38,38	0.54	0	57,57,57	1.09	4 (7%)
4	YZY	B	1203	-	34,34,41	0.93	4 (11%)	36,36,43	1.23	2 (5%)
6	PT5	B	1205	-	69,69,69	1.21	6 (8%)	83,87,87	1.19	6 (7%)
4	YZY	C	1203	-	34,34,41	0.94	4 (11%)	36,36,43	1.23	2 (5%)
7	POV	B	1206	-	51,51,51	0.50	0	57,59,59	0.47	0
5	Y01	B	1204	-	38,38,38	0.54	0	57,57,57	1.09	4 (7%)
7	POV	A	1206	-	51,51,51	0.50	0	57,59,59	0.47	0
7	POV	C	1206	-	51,51,51	0.50	0	57,59,59	0.47	0
6	PT5	C	1205	-	69,69,69	1.21	6 (8%)	83,87,87	1.19	6 (7%)
5	Y01	C	1204	-	38,38,38	0.54	0	57,57,57	1.09	4 (7%)
6	PT5	D	1206	-	69,69,69	1.20	6 (8%)	83,87,87	1.18	6 (7%)
7	POV	D	1201	-	51,51,51	0.50	0	57,59,59	0.47	0
5	Y01	D	1205	-	38,38,38	0.54	0	57,57,57	1.09	4 (7%)
4	YZY	D	1204	-	34,34,41	0.94	4 (11%)	36,36,43	1.23	2 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	YZY	A	1203	-	-	18/36/36/43	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PT5	A	1205	-	-	37/66/90/90	0/1/1/1
5	Y01	A	1204	-	-	4/19/77/77	0/4/4/4
4	YZY	B	1203	-	-	18/36/36/43	-
6	PT5	B	1205	-	-	37/66/90/90	0/1/1/1
4	YZY	C	1203	-	-	18/36/36/43	-
7	POV	B	1206	-	-	26/55/55/55	-
5	Y01	B	1204	-	-	4/19/77/77	0/4/4/4
7	POV	A	1206	-	-	26/55/55/55	-
7	POV	C	1206	-	-	26/55/55/55	-
6	PT5	C	1205	-	-	37/66/90/90	0/1/1/1
5	Y01	C	1204	-	-	4/19/77/77	0/4/4/4
6	PT5	D	1206	-	-	37/66/90/90	0/1/1/1
7	POV	D	1201	-	-	26/55/55/55	-
5	Y01	D	1205	-	-	4/19/77/77	0/4/4/4
4	YZY	D	1204	-	-	18/36/36/43	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1205	PT5	P5-O5	4.16	1.67	1.59
6	D	1206	PT5	P5-O5	4.14	1.67	1.59
6	A	1205	PT5	P5-O5	4.13	1.67	1.59
6	B	1205	PT5	P5-O5	4.07	1.67	1.59
6	C	1205	PT5	P4-O4	3.84	1.66	1.59
6	B	1205	PT5	P4-O4	3.84	1.66	1.59
6	A	1205	PT5	P4-O4	3.83	1.66	1.59
6	D	1206	PT5	P4-O4	3.80	1.66	1.59
6	C	1205	PT5	O18-C11	2.88	1.41	1.33
6	A	1205	PT5	O18-C11	2.86	1.41	1.33
6	D	1206	PT5	O18-C11	2.85	1.41	1.33
6	B	1205	PT5	O18-C11	2.84	1.41	1.33
6	B	1205	PT5	O16-C10	2.65	1.41	1.34
6	C	1205	PT5	O16-C10	2.65	1.41	1.34
6	A	1205	PT5	O16-C10	2.64	1.41	1.34
6	D	1206	PT5	O16-C10	2.63	1.41	1.34
4	B	1203	YZY	O2-C2	-2.54	1.40	1.46
6	B	1205	PT5	O16-C8	-2.52	1.40	1.46
4	C	1203	YZY	O2-C2	-2.52	1.40	1.46
4	A	1203	YZY	O2-C2	-2.51	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1204	YZY	O2-C2	-2.49	1.40	1.46
6	C	1205	PT5	O16-C8	-2.49	1.40	1.46
6	A	1205	PT5	O16-C8	-2.48	1.40	1.46
6	B	1205	PT5	P1-O1	2.48	1.67	1.60
6	D	1206	PT5	O16-C8	-2.46	1.40	1.46
6	A	1205	PT5	P1-O1	2.46	1.66	1.60
6	C	1205	PT5	P1-O1	2.46	1.66	1.60
6	D	1206	PT5	P1-O1	2.46	1.66	1.60
4	D	1204	YZY	O4-C20	2.45	1.40	1.33
4	C	1203	YZY	O4-C20	2.43	1.40	1.33
4	A	1203	YZY	O4-C20	2.42	1.40	1.33
4	B	1203	YZY	O4-C20	2.40	1.40	1.33
4	C	1203	YZY	O2-C3	2.17	1.40	1.34
4	D	1204	YZY	O2-C3	2.17	1.40	1.34
4	A	1203	YZY	O2-C3	2.17	1.40	1.34
4	B	1203	YZY	O2-C3	2.16	1.40	1.34
4	A	1203	YZY	O4-C19	-2.06	1.40	1.45
4	C	1203	YZY	O4-C19	-2.05	1.40	1.45
4	D	1204	YZY	O4-C19	-2.05	1.40	1.45
4	B	1203	YZY	O4-C19	-2.03	1.40	1.45

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	1206	PT5	C21-C20-C19	4.98	136.56	112.02
6	B	1205	PT5	C21-C20-C19	4.98	136.54	112.02
6	A	1205	PT5	C21-C20-C19	4.98	136.54	112.02
6	C	1205	PT5	C21-C20-C19	4.98	136.53	112.02
6	C	1205	PT5	O16-C10-C12	3.98	120.07	111.50
6	A	1205	PT5	O16-C10-C12	3.96	120.03	111.50
6	B	1205	PT5	O16-C10-C12	3.96	120.03	111.50
6	D	1206	PT5	O16-C10-C12	3.94	120.00	111.50
4	B	1203	YZY	O2-C3-C4	3.91	119.94	111.50
4	A	1203	YZY	O2-C3-C4	3.91	119.92	111.50
4	C	1203	YZY	O2-C3-C4	3.90	119.91	111.50
4	D	1204	YZY	O2-C3-C4	3.89	119.88	111.50
5	B	1204	Y01	CBC-CAV-CAZ	3.81	117.44	111.52
5	D	1205	Y01	CBC-CAV-CAZ	3.79	117.40	111.52
5	A	1204	Y01	CBC-CAV-CAZ	3.78	117.40	111.52
5	C	1204	Y01	CBC-CAV-CAZ	3.77	117.38	111.52
6	B	1205	PT5	C17-C16-C15	3.43	152.53	123.57
6	A	1205	PT5	C17-C16-C15	3.43	152.51	123.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1205	PT5	C17-C16-C15	3.43	152.50	123.57
6	D	1206	PT5	C17-C16-C15	3.42	152.47	123.57
6	D	1206	PT5	C23-C22-C21	3.40	152.26	123.57
6	B	1205	PT5	C23-C22-C21	3.40	152.23	123.57
6	B	1205	PT5	C20-C19-C18	3.39	152.22	123.57
6	C	1205	PT5	C23-C22-C21	3.39	152.21	123.57
6	A	1205	PT5	C20-C19-C18	3.39	152.21	123.57
6	A	1205	PT5	C23-C22-C21	3.39	152.21	123.57
6	D	1206	PT5	C20-C19-C18	3.39	152.19	123.57
6	C	1205	PT5	C20-C19-C18	3.39	152.17	123.57
6	B	1205	PT5	O18-C11-C31	2.88	120.94	111.91
6	C	1205	PT5	O18-C11-C31	2.87	120.92	111.91
6	D	1206	PT5	O18-C11-C31	2.87	120.91	111.91
6	A	1205	PT5	O18-C11-C31	2.86	120.89	111.91
5	C	1204	Y01	CAR-CBC-CAV	2.79	115.15	110.99
5	A	1204	Y01	CAR-CBC-CAV	2.77	115.11	110.99
5	B	1204	Y01	CAR-CBC-CAV	2.76	115.10	110.99
5	D	1205	Y01	CAR-CBC-CAV	2.74	115.08	110.99
4	A	1203	YZY	O4-C20-C21	2.60	120.08	111.91
4	D	1204	YZY	O4-C20-C21	2.60	120.08	111.91
4	B	1203	YZY	O4-C20-C21	2.60	120.07	111.91
4	C	1203	YZY	O4-C20-C21	2.60	120.06	111.91
5	B	1204	Y01	CAV-CAZ-CAI	-2.51	116.99	120.61
5	A	1204	Y01	CAV-CAZ-CAI	-2.51	117.00	120.61
5	C	1204	Y01	CAV-CAZ-CAI	-2.51	117.00	120.61
5	D	1205	Y01	CAV-CAZ-CAI	-2.48	117.03	120.61
5	B	1204	Y01	CBG-CBI-CBE	2.07	102.53	100.07
5	C	1204	Y01	CBG-CBI-CBE	2.07	102.53	100.07
5	A	1204	Y01	CBG-CBI-CBE	2.05	102.50	100.07
5	D	1205	Y01	CBG-CBI-CBE	2.03	102.48	100.07

There are no chirality outliers.

All (340) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1204	Y01	CAR-CBC-OAW-CAY
5	B	1204	Y01	CAR-CBC-OAW-CAY
5	C	1204	Y01	CAR-CBC-OAW-CAY
5	D	1205	Y01	CAR-CBC-OAW-CAY
6	A	1205	PT5	C7-O13-P1-O12
6	A	1205	PT5	C7-O13-P1-O11
6	A	1205	PT5	C1-O1-P1-O12

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Mol	Chain	Res	Type	Atoms
6	A	1205	PT5	O17-C10-O16-C8
6	B	1205	PT5	C7-O13-P1-O12
6	B	1205	PT5	C7-O13-P1-O11
6	B	1205	PT5	C1-O1-P1-O12
6	B	1205	PT5	O17-C10-O16-C8
6	C	1205	PT5	C7-O13-P1-O12
6	C	1205	PT5	C7-O13-P1-O11
6	C	1205	PT5	C1-O1-P1-O12
6	C	1205	PT5	O17-C10-O16-C8
6	D	1206	PT5	C7-O13-P1-O12
6	D	1206	PT5	C7-O13-P1-O11
6	D	1206	PT5	C1-O1-P1-O12
6	D	1206	PT5	O17-C10-O16-C8
7	A	1206	POV	C1-O11-P-O13
7	A	1206	POV	C1-O11-P-O14
7	A	1206	POV	C11-O12-P-O11
7	A	1206	POV	C11-O12-P-O13
7	A	1206	POV	O21-C2-C3-O31
7	B	1206	POV	C1-O11-P-O13
7	B	1206	POV	C1-O11-P-O14
7	B	1206	POV	C11-O12-P-O11
7	B	1206	POV	C11-O12-P-O13
7	B	1206	POV	O21-C2-C3-O31
7	C	1206	POV	C1-O11-P-O13
7	C	1206	POV	C1-O11-P-O14
7	C	1206	POV	C11-O12-P-O11
7	C	1206	POV	C11-O12-P-O13
7	C	1206	POV	O21-C2-C3-O31
7	D	1201	POV	C1-O11-P-O13
7	D	1201	POV	C1-O11-P-O14
7	D	1201	POV	C11-O12-P-O11
7	D	1201	POV	C11-O12-P-O13
7	D	1201	POV	O21-C2-C3-O31
4	A	1203	YZY	O5-C20-O4-C19
4	B	1203	YZY	O5-C20-O4-C19
4	C	1203	YZY	O5-C20-O4-C19
4	D	1204	YZY	O5-C20-O4-C19
4	A	1203	YZY	C21-C20-O4-C19
4	B	1203	YZY	C21-C20-O4-C19
4	C	1203	YZY	C21-C20-O4-C19
4	D	1204	YZY	C21-C20-O4-C19
6	A	1205	PT5	C12-C10-O16-C8

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Mol	Chain	Res	Type	Atoms
6	B	1205	PT5	C12-C10-O16-C8
6	C	1205	PT5	C12-C10-O16-C8
6	D	1206	PT5	C12-C10-O16-C8
4	A	1203	YZY	C20-C21-C22-C23
4	B	1203	YZY	C20-C21-C22-C23
4	C	1203	YZY	C20-C21-C22-C23
4	D	1204	YZY	C20-C21-C22-C23
4	A	1203	YZY	C3-C4-C5-C6
4	B	1203	YZY	C3-C4-C5-C6
4	C	1203	YZY	C3-C4-C5-C6
4	D	1204	YZY	C3-C4-C5-C6
5	A	1204	Y01	CAM-CAY-OAW-CBC
5	B	1204	Y01	CAM-CAY-OAW-CBC
5	C	1204	Y01	CAM-CAY-OAW-CBC
5	D	1205	Y01	CAM-CAY-OAW-CBC
6	A	1205	PT5	C7-O13-P1-O1
6	B	1205	PT5	C7-O13-P1-O1
6	C	1205	PT5	C7-O13-P1-O1
6	D	1206	PT5	C7-O13-P1-O1
7	A	1206	POV	C1-O11-P-O12
7	B	1206	POV	C1-O11-P-O12
7	C	1206	POV	C1-O11-P-O12
7	D	1201	POV	C1-O11-P-O12
5	A	1204	Y01	OAG-CAY-OAW-CBC
5	B	1204	Y01	OAG-CAY-OAW-CBC
5	C	1204	Y01	OAG-CAY-OAW-CBC
5	D	1205	Y01	OAG-CAY-OAW-CBC
6	A	1205	PT5	C1-O1-P1-O13
6	B	1205	PT5	C1-O1-P1-O13
6	C	1205	PT5	C1-O1-P1-O13
6	D	1206	PT5	C1-O1-P1-O13
6	A	1205	PT5	C25-C26-C27-C28
6	B	1205	PT5	C25-C26-C27-C28
6	C	1205	PT5	C25-C26-C27-C28
6	D	1206	PT5	C25-C26-C27-C28
4	A	1203	YZY	C10-C11-C12-C13
4	B	1203	YZY	C10-C11-C12-C13
4	C	1203	YZY	C10-C11-C12-C13
4	D	1204	YZY	C10-C11-C12-C13
4	A	1203	YZY	C4-C3-O2-C2
4	B	1203	YZY	C4-C3-O2-C2
4	C	1203	YZY	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
4	D	1204	YZY	C4-C3-O2-C2
4	A	1203	YZY	O3-C3-O2-C2
4	B	1203	YZY	O3-C3-O2-C2
4	C	1203	YZY	O3-C3-O2-C2
4	D	1204	YZY	O3-C3-O2-C2
6	A	1205	PT5	C42-C43-C44-C45
6	B	1205	PT5	C42-C43-C44-C45
6	C	1205	PT5	C42-C43-C44-C45
6	D	1206	PT5	C42-C43-C44-C45
6	A	1205	PT5	C33-C34-C35-C36
6	B	1205	PT5	C33-C34-C35-C36
6	C	1205	PT5	C33-C34-C35-C36
6	D	1206	PT5	C33-C34-C35-C36
6	A	1205	PT5	C40-C41-C42-C43
6	B	1205	PT5	C40-C41-C42-C43
6	C	1205	PT5	C40-C41-C42-C43
6	D	1206	PT5	C40-C41-C42-C43
6	A	1205	PT5	C12-C13-C14-C15
6	B	1205	PT5	C12-C13-C14-C15
6	C	1205	PT5	C12-C13-C14-C15
6	D	1206	PT5	C12-C13-C14-C15
6	A	1205	PT5	C39-C40-C41-C42
6	B	1205	PT5	C39-C40-C41-C42
6	C	1205	PT5	C39-C40-C41-C42
6	D	1206	PT5	C39-C40-C41-C42
6	A	1205	PT5	C41-C42-C43-C44
6	B	1205	PT5	C41-C42-C43-C44
6	C	1205	PT5	C41-C42-C43-C44
6	D	1206	PT5	C41-C42-C43-C44
6	A	1205	PT5	C31-C32-C33-C34
6	B	1205	PT5	C31-C32-C33-C34
6	C	1205	PT5	C31-C32-C33-C34
6	D	1206	PT5	C31-C32-C33-C34
4	A	1203	YZY	C4-C5-C6-C7
4	B	1203	YZY	C4-C5-C6-C7
4	C	1203	YZY	C4-C5-C6-C7
4	D	1204	YZY	C4-C5-C6-C7
7	C	1206	POV	C311-C312-C313-C314
7	A	1206	POV	C311-C312-C313-C314
7	B	1206	POV	C311-C312-C313-C314
7	D	1201	POV	C311-C312-C313-C314
7	A	1206	POV	C210-C211-C212-C213

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Mol	Chain	Res	Type	Atoms
7	B	1206	POV	C210-C211-C212-C213
7	C	1206	POV	C210-C211-C212-C213
7	D	1201	POV	C210-C211-C212-C213
7	A	1206	POV	O11-C1-C2-C3
7	B	1206	POV	O11-C1-C2-C3
7	C	1206	POV	O11-C1-C2-C3
7	D	1201	POV	O11-C1-C2-C3
7	A	1206	POV	C213-C214-C215-C216
7	B	1206	POV	C213-C214-C215-C216
7	C	1206	POV	C213-C214-C215-C216
7	D	1201	POV	C213-C214-C215-C216
6	A	1205	PT5	C37-C38-C39-C40
6	B	1205	PT5	C37-C38-C39-C40
6	C	1205	PT5	C37-C38-C39-C40
6	D	1206	PT5	C37-C38-C39-C40
7	A	1206	POV	C26-C27-C28-C29
7	B	1206	POV	C26-C27-C28-C29
7	C	1206	POV	C26-C27-C28-C29
7	D	1201	POV	C26-C27-C28-C29
6	A	1205	PT5	C27-C28-C29-C30
6	B	1205	PT5	C36-C37-C38-C39
6	B	1205	PT5	C27-C28-C29-C30
6	C	1205	PT5	C36-C37-C38-C39
6	C	1205	PT5	C27-C28-C29-C30
6	D	1206	PT5	C27-C28-C29-C30
6	A	1205	PT5	C36-C37-C38-C39
6	D	1206	PT5	C36-C37-C38-C39
6	A	1205	PT5	C43-C44-C45-C46
6	B	1205	PT5	C43-C44-C45-C46
6	C	1205	PT5	C43-C44-C45-C46
6	D	1206	PT5	C43-C44-C45-C46
6	A	1205	PT5	C38-C39-C40-C41
6	B	1205	PT5	C38-C39-C40-C41
6	C	1205	PT5	C38-C39-C40-C41
6	D	1206	PT5	C38-C39-C40-C41
6	A	1205	PT5	C7-C8-C9-O18
6	B	1205	PT5	C7-C8-C9-O18
6	C	1205	PT5	C7-C8-C9-O18
6	D	1206	PT5	C7-C8-C9-O18
6	A	1205	PT5	C1-O1-P1-O11
6	B	1205	PT5	C1-O1-P1-O11
6	C	1205	PT5	C1-O1-P1-O11

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Mol	Chain	Res	Type	Atoms
6	D	1206	PT5	C1-O1-P1-O11
6	A	1205	PT5	C16-C17-C18-C19
6	A	1205	PT5	C18-C19-C20-C21
6	A	1205	PT5	C19-C20-C21-C22
6	B	1205	PT5	C16-C17-C18-C19
6	B	1205	PT5	C18-C19-C20-C21
6	B	1205	PT5	C19-C20-C21-C22
6	C	1205	PT5	C16-C17-C18-C19
6	C	1205	PT5	C18-C19-C20-C21
6	C	1205	PT5	C19-C20-C21-C22
6	D	1206	PT5	C16-C17-C18-C19
6	D	1206	PT5	C18-C19-C20-C21
6	D	1206	PT5	C19-C20-C21-C22
7	A	1206	POV	C25-C26-C27-C28
7	B	1206	POV	C25-C26-C27-C28
7	C	1206	POV	C25-C26-C27-C28
7	D	1201	POV	C25-C26-C27-C28
7	C	1206	POV	C36-C37-C38-C39
7	D	1201	POV	C36-C37-C38-C39
7	A	1206	POV	C36-C37-C38-C39
7	B	1206	POV	C36-C37-C38-C39
6	A	1205	PT5	O13-C7-C8-C9
6	B	1205	PT5	O13-C7-C8-C9
6	C	1205	PT5	O13-C7-C8-C9
6	D	1206	PT5	O13-C7-C8-C9
7	A	1206	POV	C32-C33-C34-C35
6	A	1205	PT5	C31-C11-O18-C9
6	B	1205	PT5	C31-C11-O18-C9
6	C	1205	PT5	C31-C11-O18-C9
6	D	1206	PT5	C31-C11-O18-C9
7	A	1206	POV	C32-C31-O31-C3
7	B	1206	POV	C32-C31-O31-C3
7	C	1206	POV	C32-C31-O31-C3
7	D	1201	POV	C32-C31-O31-C3
7	C	1206	POV	C32-C33-C34-C35
7	A	1206	POV	C1-C2-C3-O31
7	B	1206	POV	C1-C2-C3-O31
7	C	1206	POV	C1-C2-C3-O31
7	D	1201	POV	C1-C2-C3-O31
7	D	1201	POV	C32-C33-C34-C35
4	A	1203	YZY	C21-C22-C23-C24
4	B	1203	YZY	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
4	C	1203	YZY	C21-C22-C23-C24
4	D	1204	YZY	C21-C22-C23-C24
7	B	1206	POV	C32-C33-C34-C35
4	A	1203	YZY	O4-C19-C2-O2
4	B	1203	YZY	O4-C19-C2-O2
4	C	1203	YZY	O4-C19-C2-O2
4	D	1204	YZY	O4-C19-C2-O2
6	A	1205	PT5	O19-C11-O18-C9
6	B	1205	PT5	O19-C11-O18-C9
6	C	1205	PT5	O19-C11-O18-C9
6	D	1206	PT5	O19-C11-O18-C9
7	B	1206	POV	O32-C31-O31-C3
7	C	1206	POV	O32-C31-O31-C3
7	D	1201	POV	O32-C31-O31-C3
7	A	1206	POV	C11-O12-P-O14
7	B	1206	POV	C11-O12-P-O14
7	C	1206	POV	C11-O12-P-O14
7	D	1201	POV	C11-O12-P-O14
7	A	1206	POV	O32-C31-O31-C3
7	B	1206	POV	C310-C311-C312-C313
7	C	1206	POV	C310-C311-C312-C313
7	D	1201	POV	C310-C311-C312-C313
6	A	1205	PT5	O13-C7-C8-O16
6	B	1205	PT5	O13-C7-C8-O16
6	C	1205	PT5	O13-C7-C8-O16
6	D	1206	PT5	O13-C7-C8-O16
7	A	1206	POV	C310-C311-C312-C313
6	A	1205	PT5	O16-C8-C9-O18
6	B	1205	PT5	O16-C8-C9-O18
6	C	1205	PT5	O16-C8-C9-O18
6	D	1206	PT5	O16-C8-C9-O18
7	A	1206	POV	C35-C36-C37-C38
7	B	1206	POV	C35-C36-C37-C38
7	C	1206	POV	C35-C36-C37-C38
7	D	1201	POV	C35-C36-C37-C38
7	A	1206	POV	C211-C212-C213-C214
5	A	1204	Y01	CAJ-CAN-CBA-CAA
5	B	1204	Y01	CAJ-CAN-CBA-CAA
5	C	1204	Y01	CAJ-CAN-CBA-CAA
5	D	1205	Y01	CAJ-CAN-CBA-CAA
7	B	1206	POV	C211-C212-C213-C214
7	C	1206	POV	C211-C212-C213-C214

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Mol	Chain	Res	Type	Atoms
7	D	1201	POV	C211-C212-C213-C214
6	A	1205	PT5	C24-C25-C26-C27
6	B	1205	PT5	C24-C25-C26-C27
6	C	1205	PT5	C24-C25-C26-C27
6	D	1206	PT5	C24-C25-C26-C27
4	A	1203	YZY	C1-C2-O2-C3
4	B	1203	YZY	C1-C2-O2-C3
4	C	1203	YZY	C1-C2-O2-C3
4	D	1204	YZY	C1-C2-O2-C3
7	A	1206	POV	O11-C1-C2-O21
7	B	1206	POV	O11-C1-C2-O21
7	C	1206	POV	O11-C1-C2-O21
7	D	1201	POV	O11-C1-C2-O21
6	B	1205	PT5	C32-C33-C34-C35
6	D	1206	PT5	C32-C33-C34-C35
6	A	1205	PT5	C32-C33-C34-C35
6	C	1205	PT5	C32-C33-C34-C35
4	A	1203	YZY	O4-C19-C2-C1
4	B	1203	YZY	O4-C19-C2-C1
4	C	1203	YZY	O4-C19-C2-C1
4	D	1204	YZY	O4-C19-C2-C1
4	B	1203	YZY	C24-C25-C26-C27
4	D	1204	YZY	C24-C25-C26-C27
4	A	1203	YZY	C24-C25-C26-C27
4	C	1203	YZY	C24-C25-C26-C27
6	A	1205	PT5	C34-C35-C36-C37
6	C	1205	PT5	C34-C35-C36-C37
6	D	1206	PT5	C34-C35-C36-C37
6	B	1205	PT5	C34-C35-C36-C37
4	A	1203	YZY	C19-C2-O2-C3
4	B	1203	YZY	C19-C2-O2-C3
4	C	1203	YZY	C19-C2-O2-C3
4	D	1204	YZY	C19-C2-O2-C3
6	A	1205	PT5	C9-C8-O16-C10
6	B	1205	PT5	C9-C8-O16-C10
6	C	1205	PT5	C9-C8-O16-C10
6	D	1206	PT5	C9-C8-O16-C10
6	A	1205	PT5	C21-C22-C23-C24
6	B	1205	PT5	C21-C22-C23-C24
6	C	1205	PT5	C21-C22-C23-C24
6	D	1206	PT5	C21-C22-C23-C24
7	A	1206	POV	C11-C12-N-C13

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Mol	Chain	Res	Type	Atoms
7	B	1206	POV	C11-C12-N-C13
7	C	1206	POV	C11-C12-N-C13
7	D	1201	POV	C11-C12-N-C13
4	C	1203	YZY	C12-C13-C14-C15
4	A	1203	YZY	C12-C13-C14-C15
4	B	1203	YZY	C12-C13-C14-C15
4	D	1204	YZY	C12-C13-C14-C15
4	A	1203	YZY	C9-C10-C11-C12
4	B	1203	YZY	C9-C10-C11-C12
4	D	1204	YZY	C9-C10-C11-C12
4	C	1203	YZY	C9-C10-C11-C12
4	A	1203	YZY	C26-C27-C28-C29
4	B	1203	YZY	C26-C27-C28-C29
4	C	1203	YZY	C26-C27-C28-C29
4	D	1204	YZY	C26-C27-C28-C29
7	A	1206	POV	C11-C12-N-C15
7	B	1206	POV	C11-C12-N-C15
7	C	1206	POV	C11-C12-N-C15
7	D	1201	POV	C11-C12-N-C15
6	C	1205	PT5	C44-C45-C46-C47
6	D	1206	PT5	C44-C45-C46-C47
6	A	1205	PT5	C44-C45-C46-C47
6	B	1205	PT5	C44-C45-C46-C47
7	A	1206	POV	C11-C12-N-C14
7	B	1206	POV	C11-C12-N-C14
7	C	1206	POV	C11-C12-N-C14
7	D	1201	POV	C11-C12-N-C14
6	A	1205	PT5	C4-O4-P4-O41
6	B	1205	PT5	C4-O4-P4-O41
6	C	1205	PT5	C4-O4-P4-O41
6	D	1206	PT5	C4-O4-P4-O41
7	B	1206	POV	C37-C38-C39-C310
7	D	1201	POV	C37-C38-C39-C310
4	A	1203	YZY	C7-C8-C9-C10
7	A	1206	POV	C37-C38-C39-C310
4	B	1203	YZY	C7-C8-C9-C10
4	D	1204	YZY	C7-C8-C9-C10
7	C	1206	POV	C37-C38-C39-C310
4	C	1203	YZY	C7-C8-C9-C10

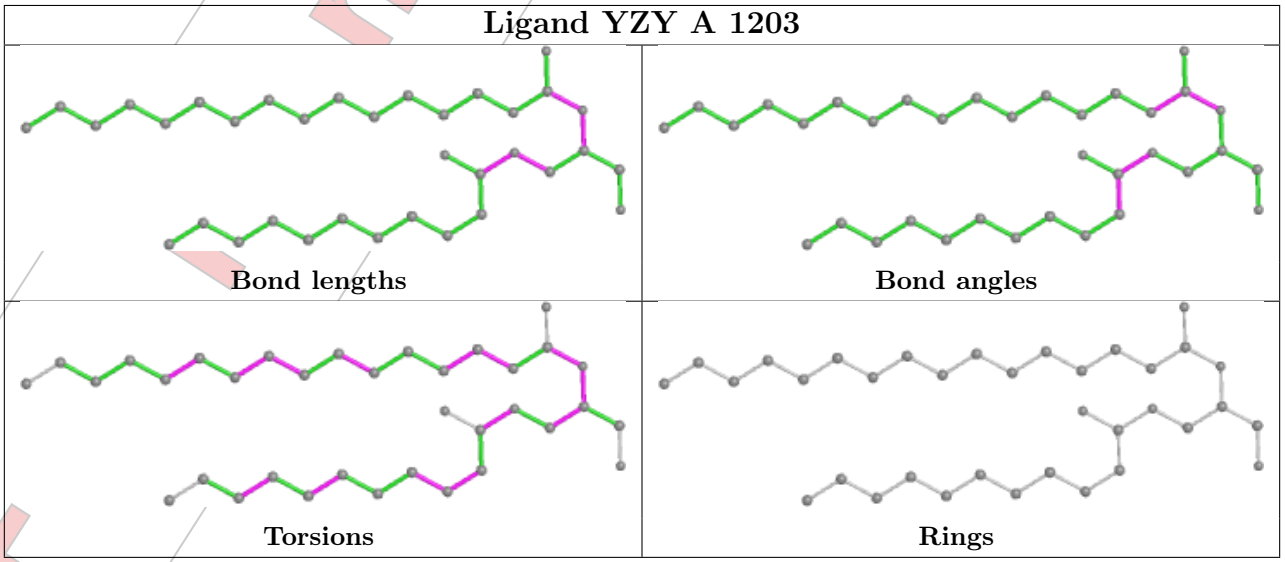
There are no ring outliers.

16 monomers are involved in 194 short contacts:

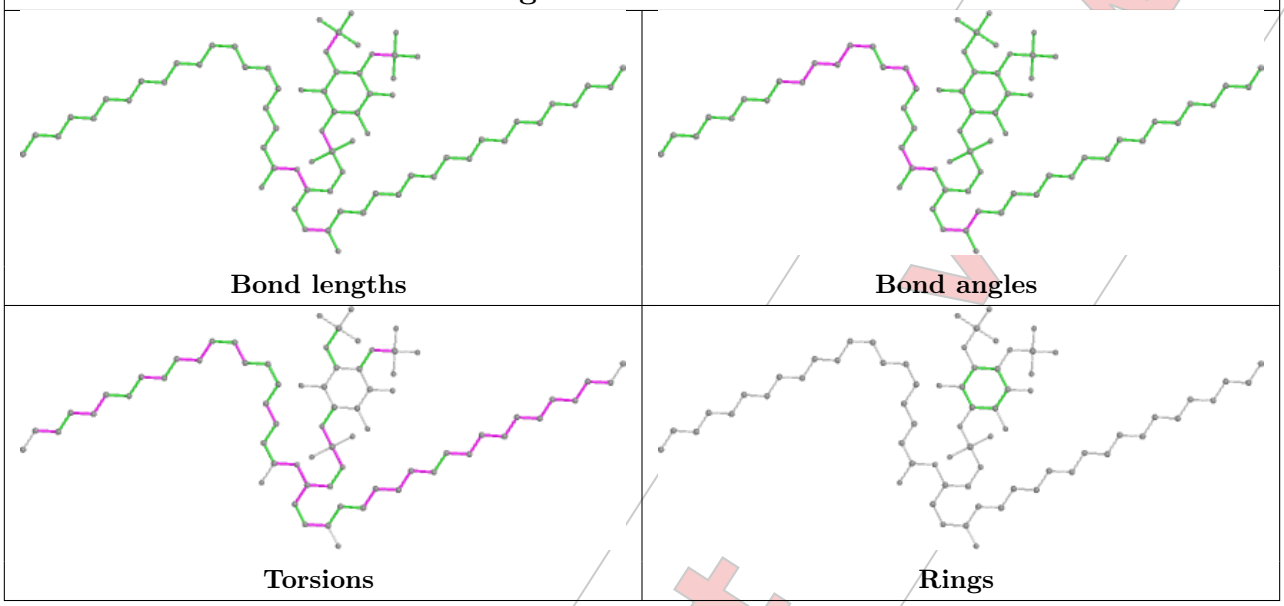
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1203	YZY	4	0
6	A	1205	PT5	23	0
5	A	1204	Y01	13	0
4	B	1203	YZY	4	0
6	B	1205	PT5	22	0
4	C	1203	YZY	5	0
7	B	1206	POV	11	0
5	B	1204	Y01	16	0
7	A	1206	POV	10	0
7	C	1206	POV	11	0
6	C	1205	PT5	22	0
5	C	1204	Y01	13	0
6	D	1206	PT5	23	0
7	D	1201	POV	10	0
5	D	1205	Y01	14	0
4	D	1204	YZY	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

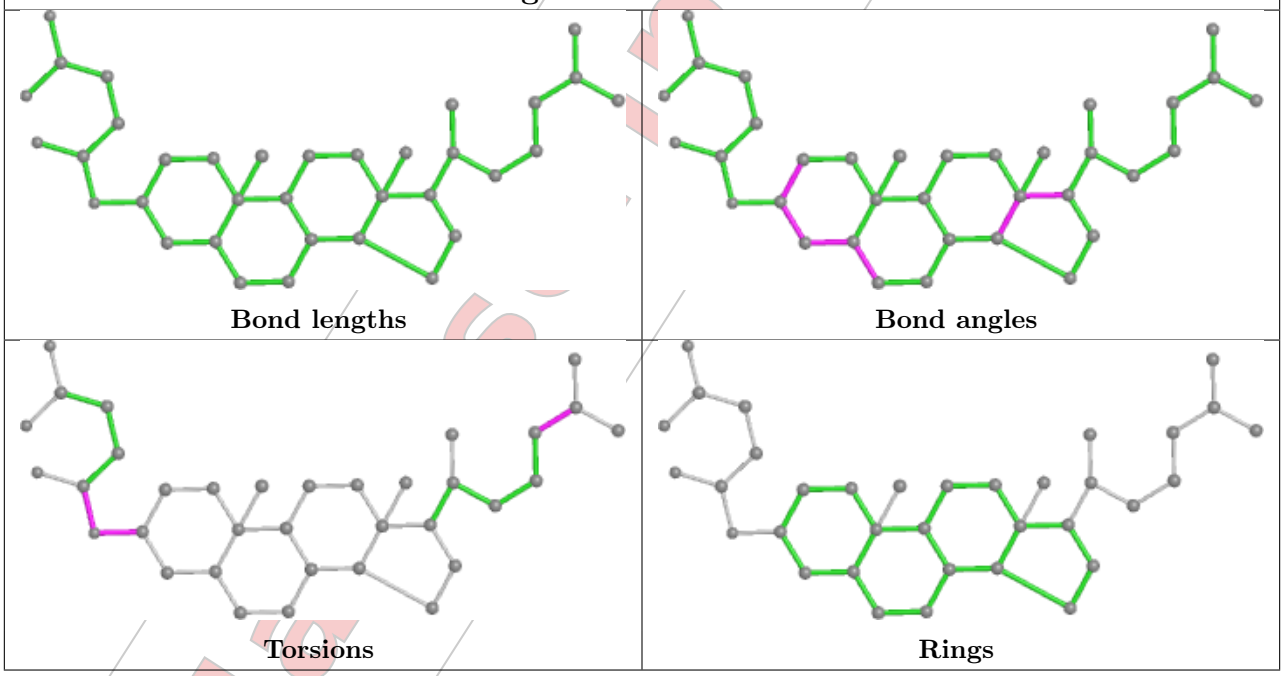
Ligand YZY A 1203



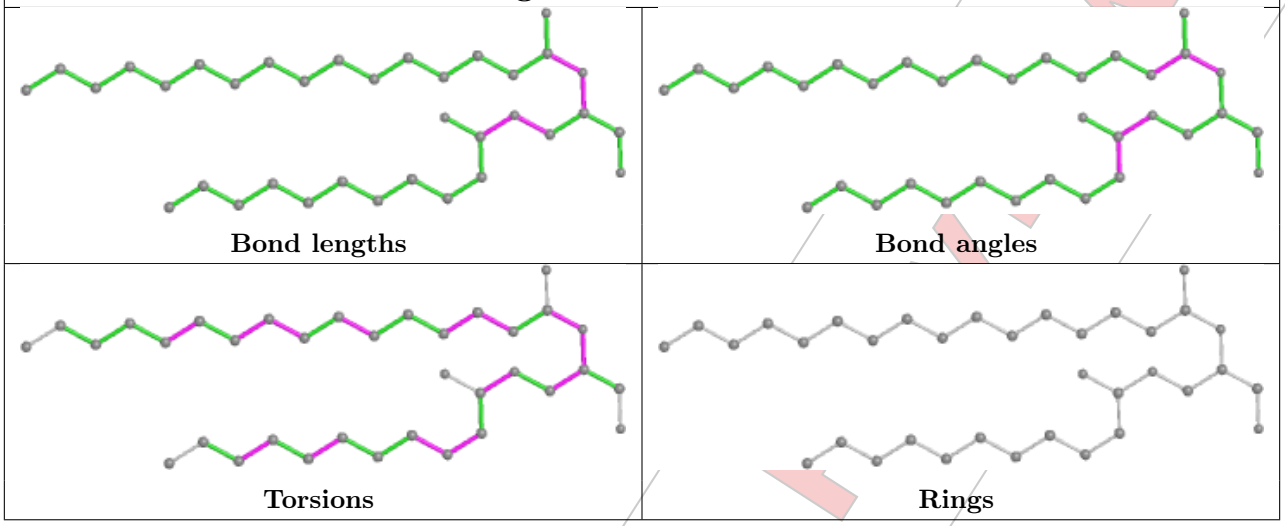
Ligand PT5 A 1205



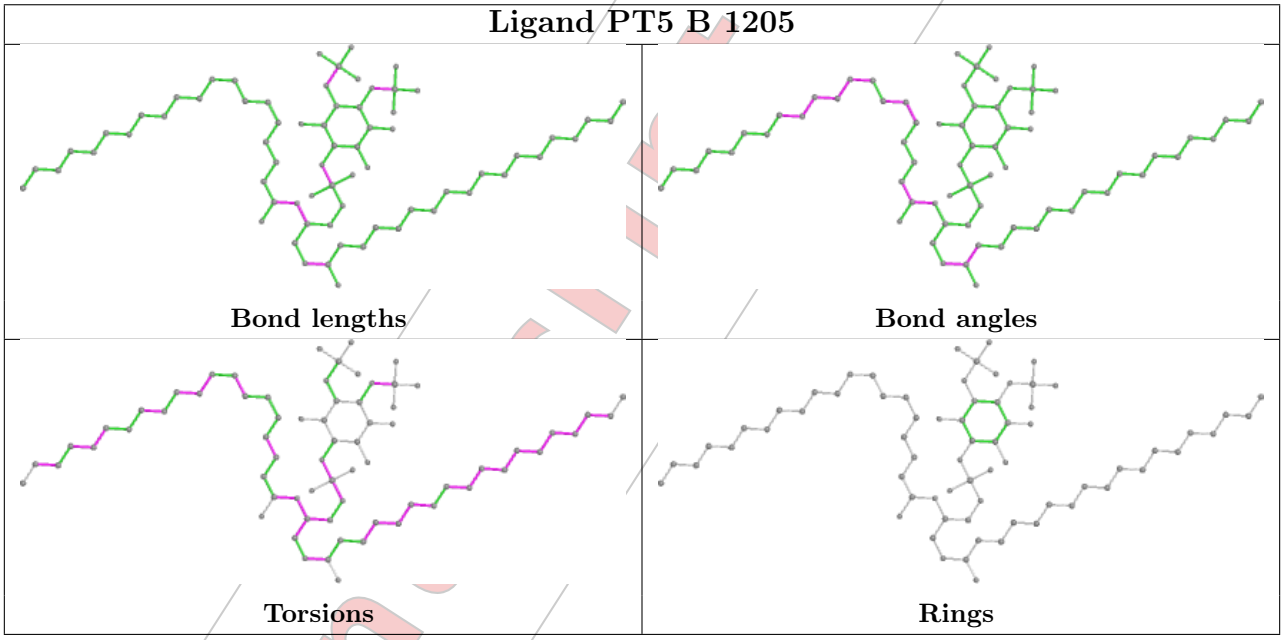
Ligand Y01 A 1204



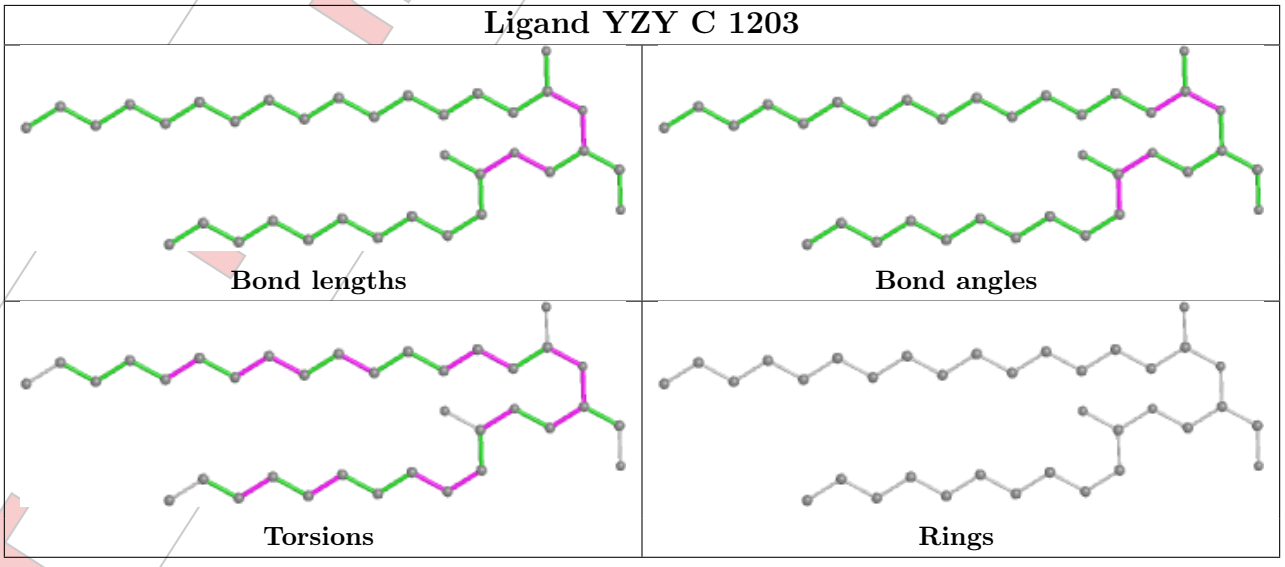
Ligand YZY B 1203



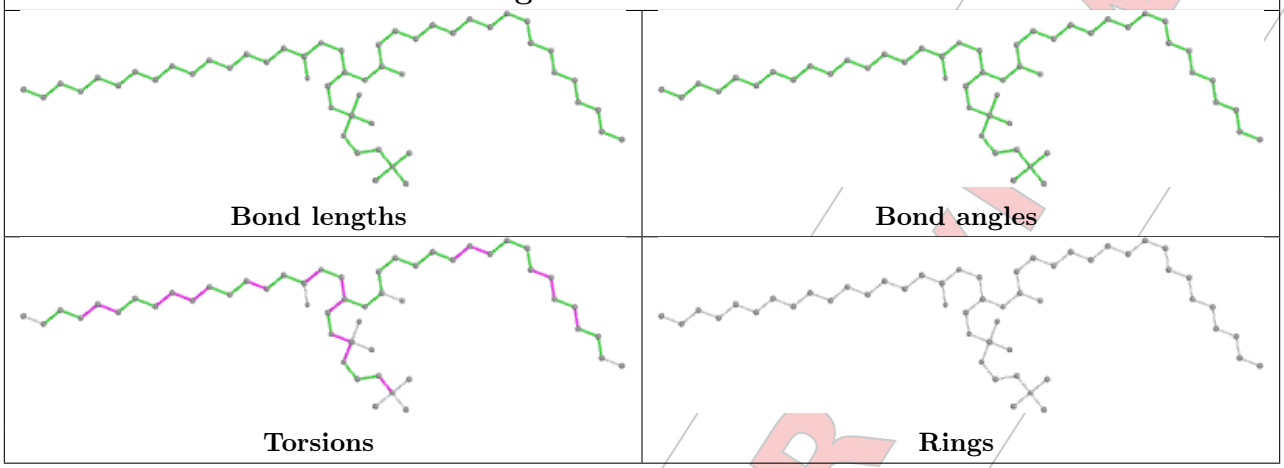
Ligand PT5 B 1205



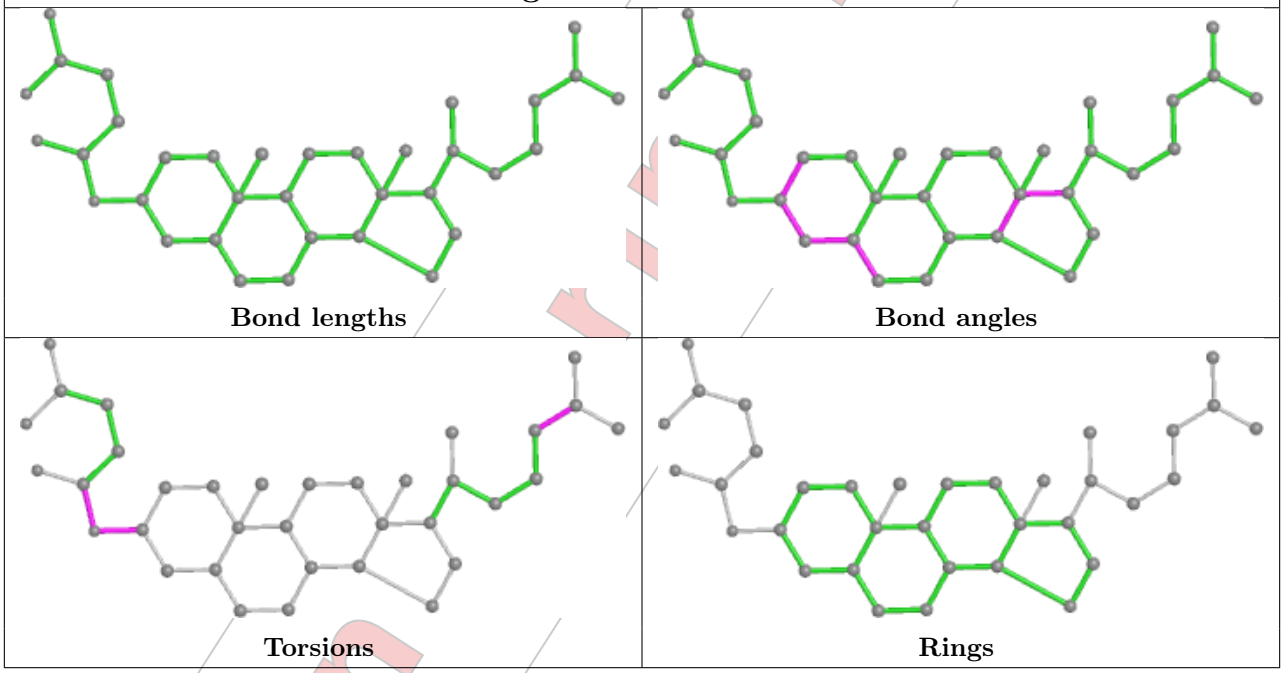
Ligand YZY C 1203



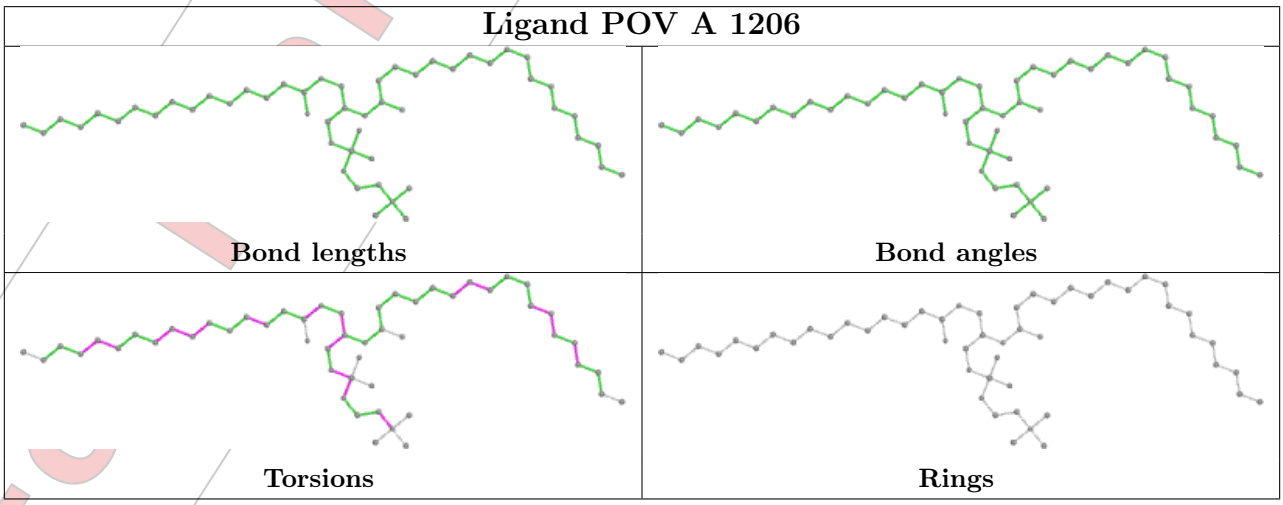
Ligand POV B 1206



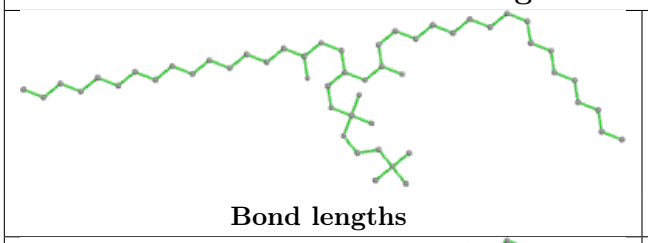
Ligand Y01 B 1204



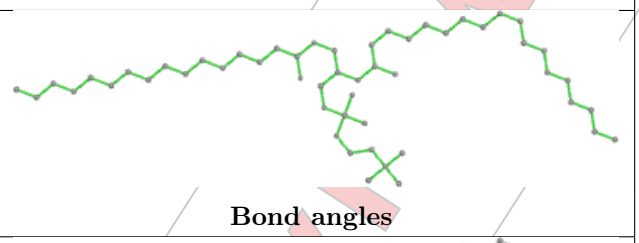
Ligand POV A 1206



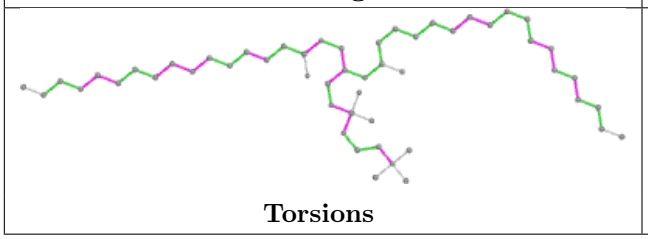
Ligand POV C 1206



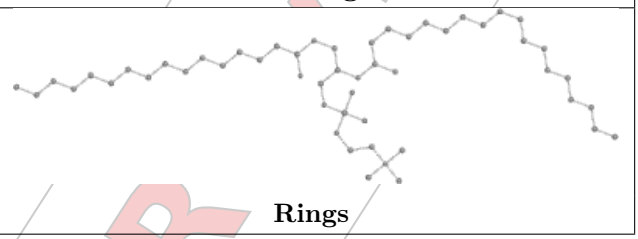
Bond lengths



Bond angles

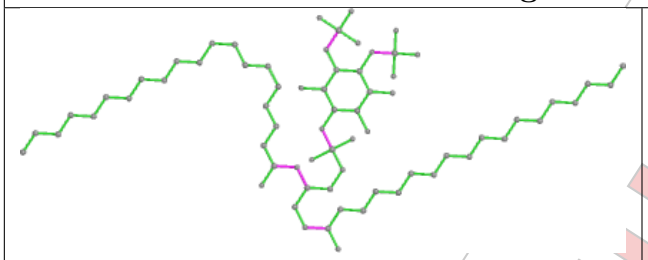


Torsions

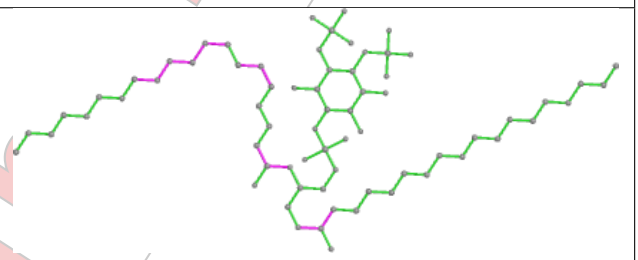


Rings

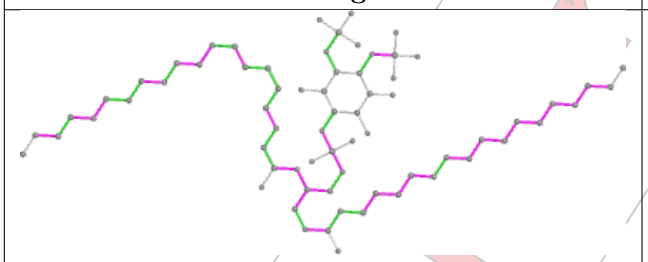
Ligand PT5 C 1205



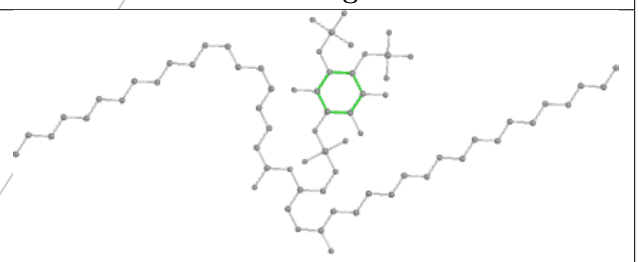
Bond lengths



Bond angles

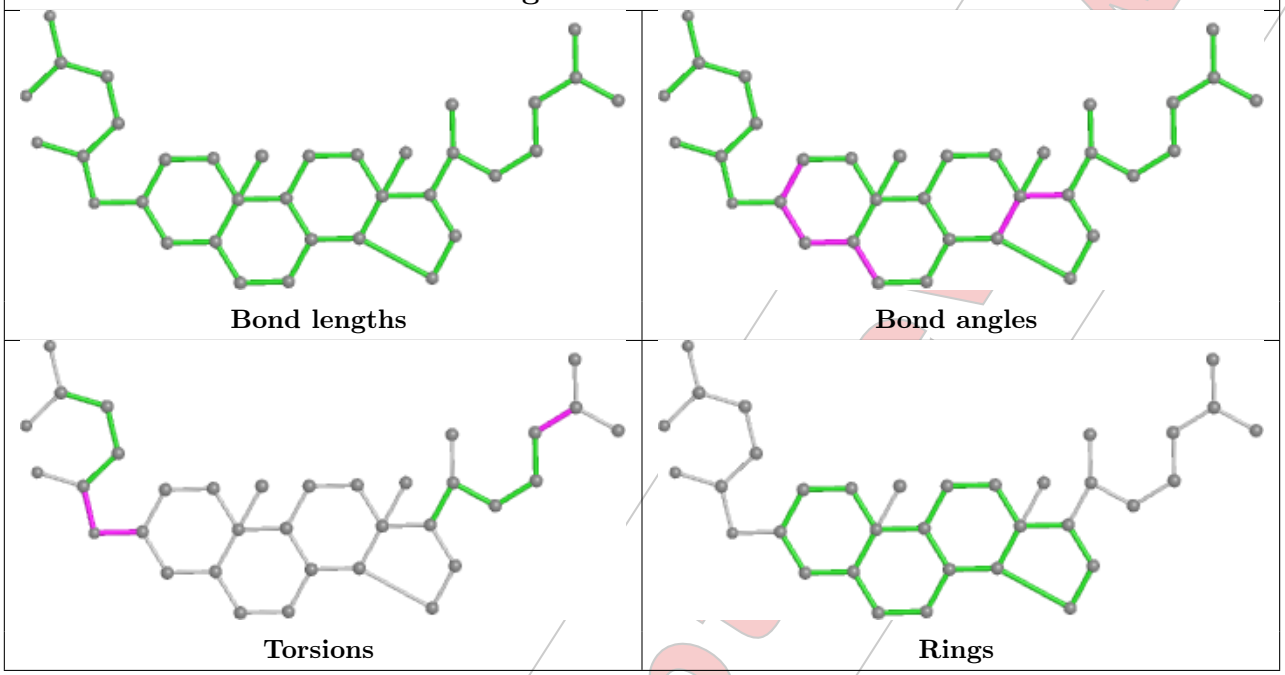


Torsions

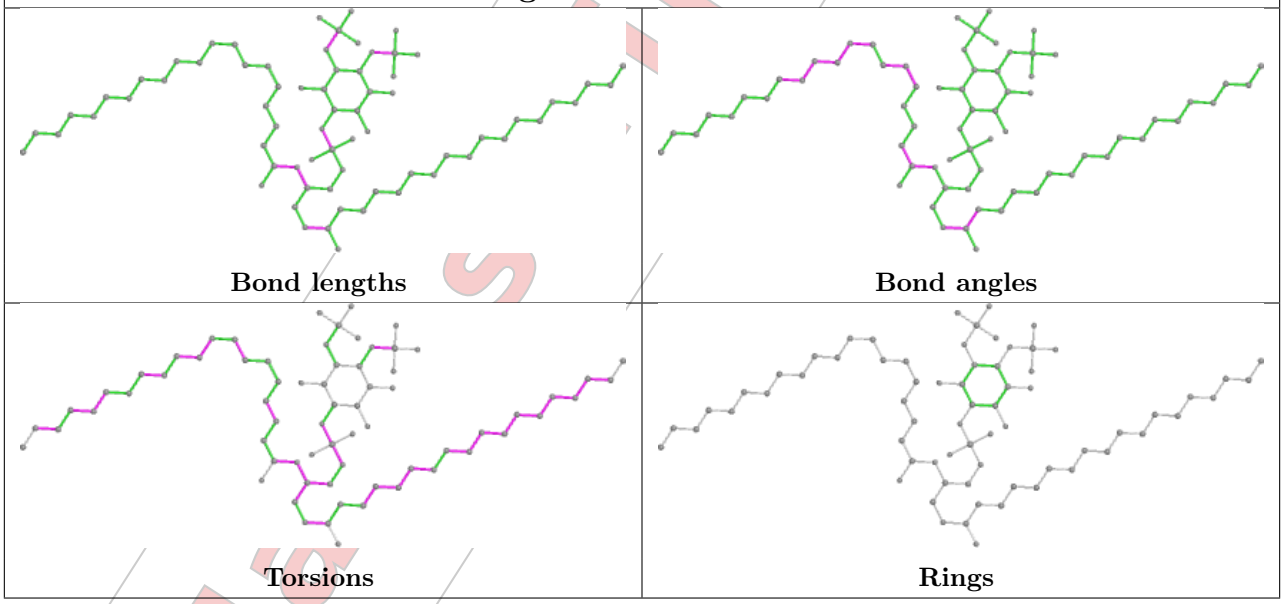


Rings

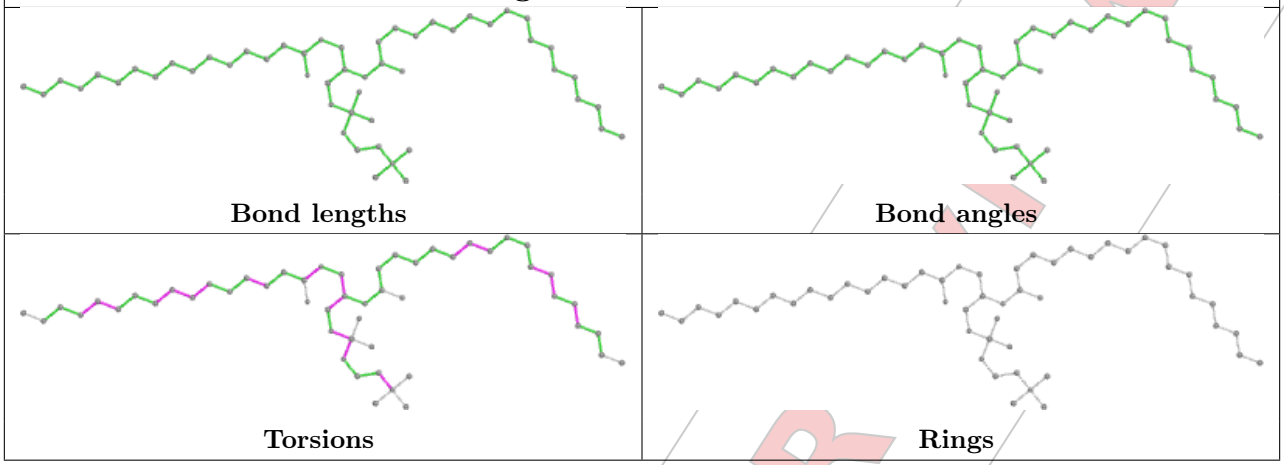
Ligand Y01 C 1204



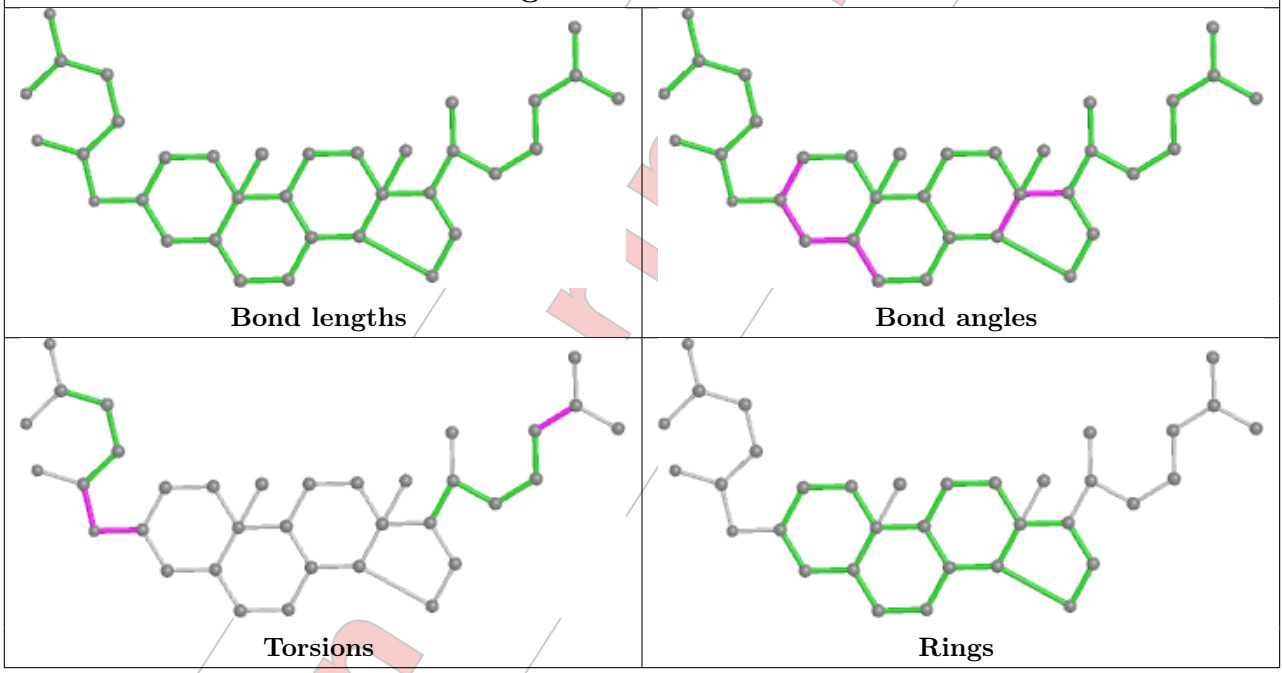
Ligand PT5 D 1206



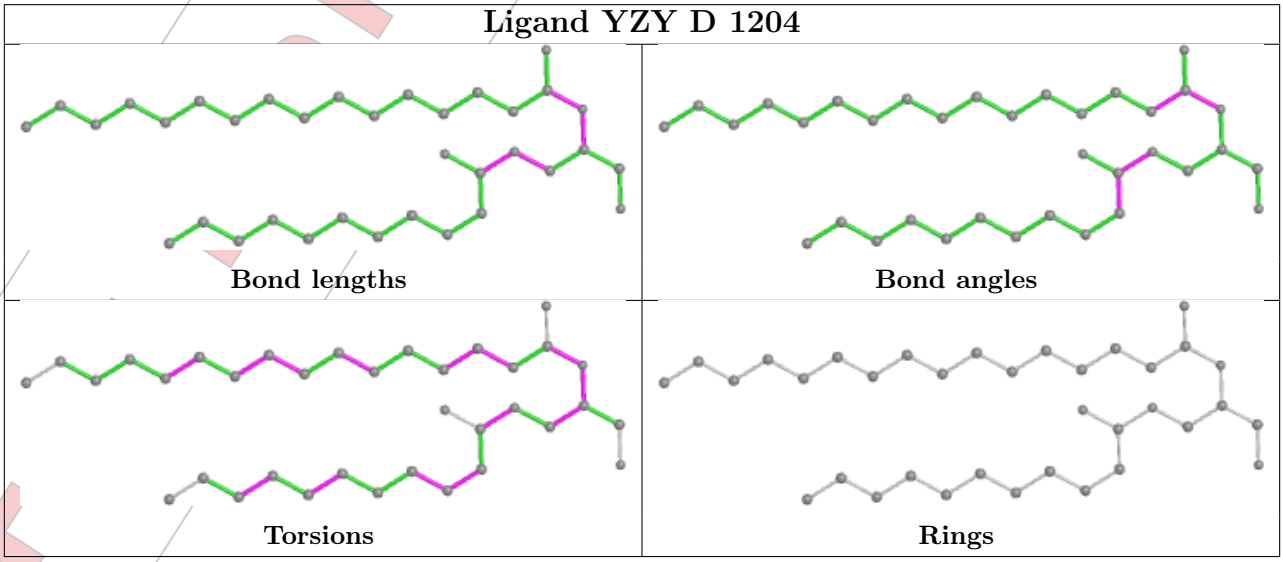
Ligand POV D 1201



Ligand Y01 D 1205



Ligand YZY D 1204



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

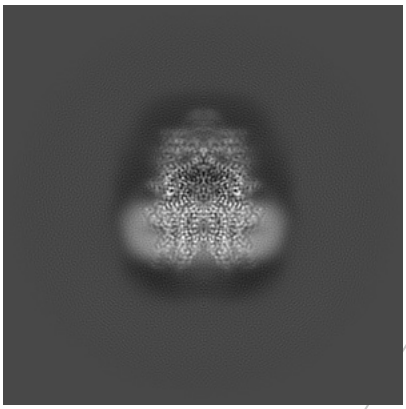
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-65279. These allow visual inspection of the internal detail of the map and identification of artifacts.

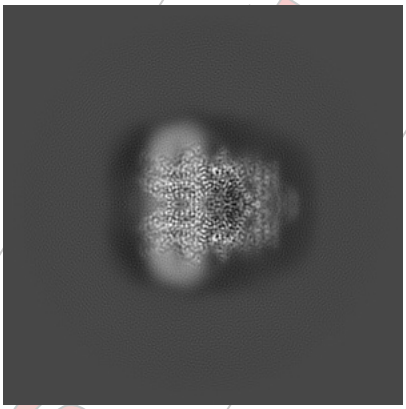
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

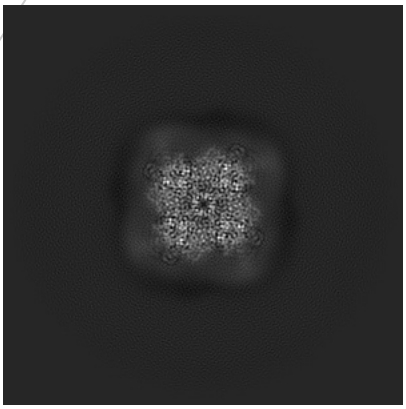
6.1.1 Primary map



X

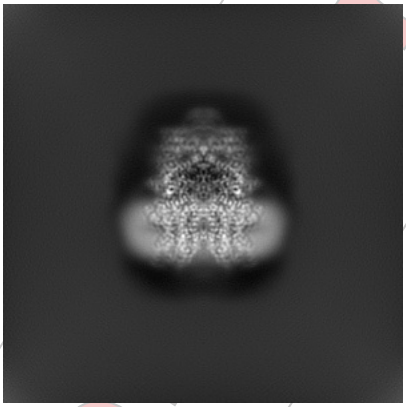


Y

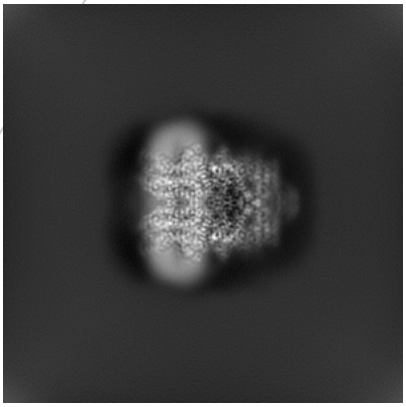


Z

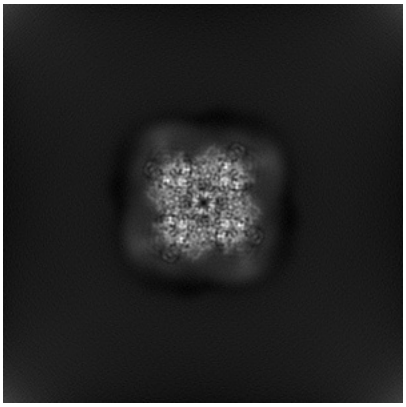
6.1.2 Raw map



X



Y

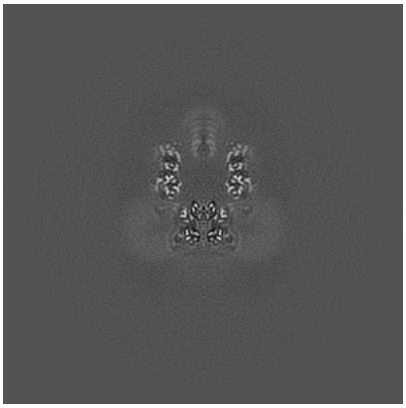


Z

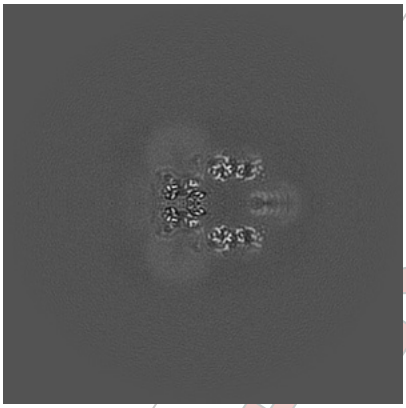
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

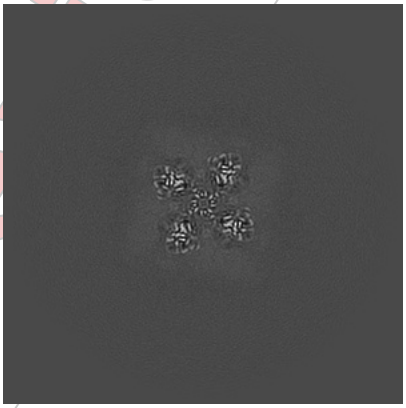
6.2.1 Primary map



X Index: 160

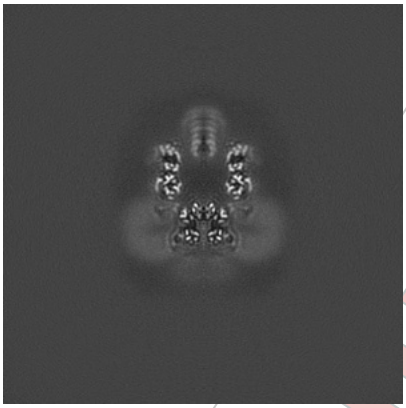


Y Index: 160

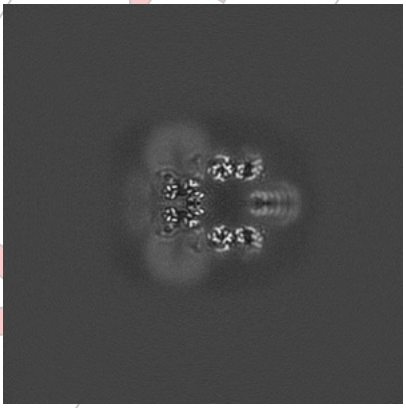


Z Index: 160

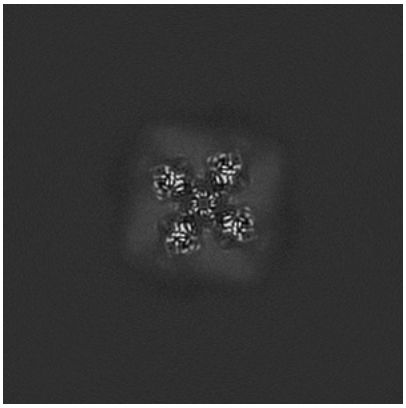
6.2.2 Raw map



X Index: 160



Y Index: 160

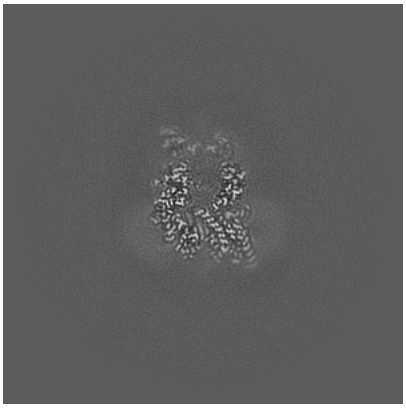


Z Index: 160

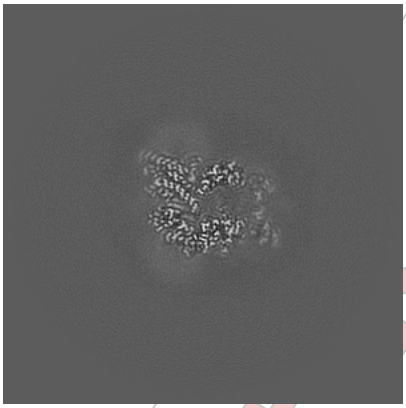
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

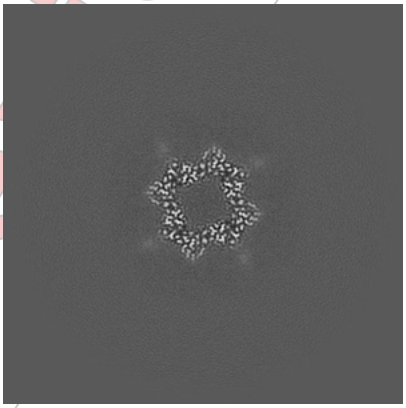
6.3.1 Primary map



X Index: 143

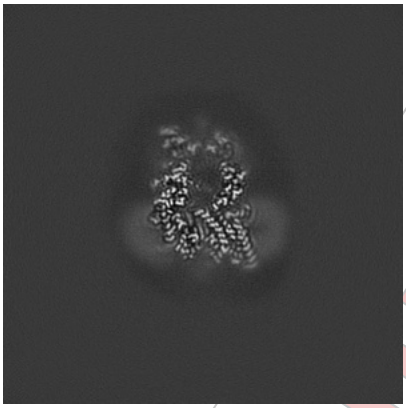


Y Index: 177

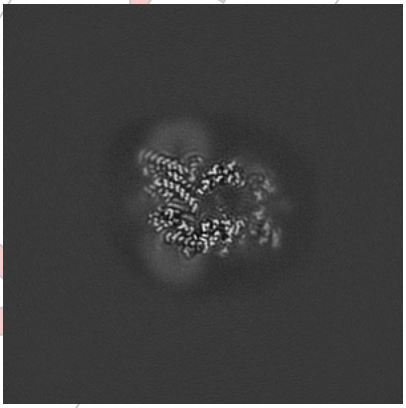


Z Index: 177

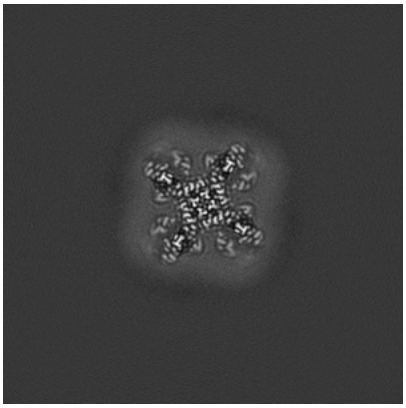
6.3.2 Raw map



X Index: 143



Y Index: 177

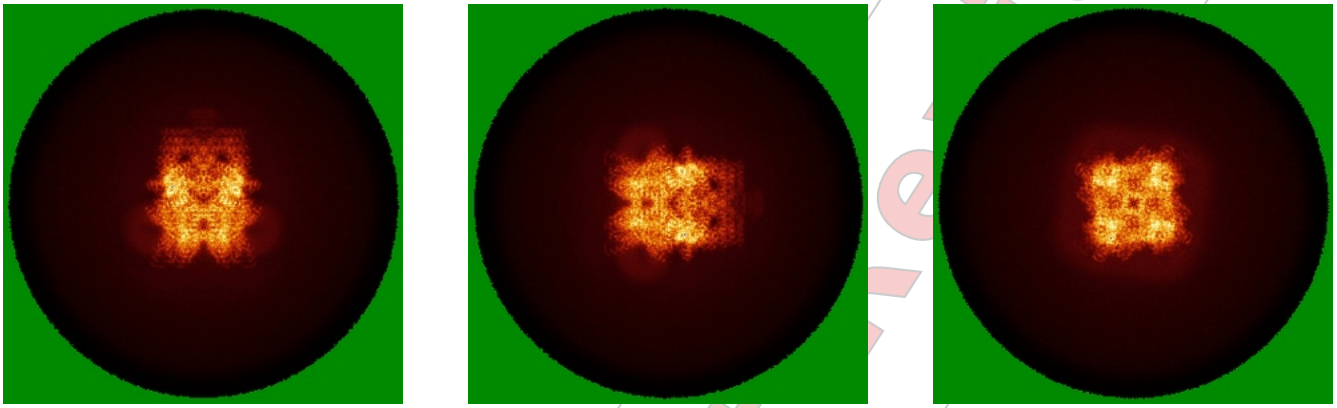


Z Index: 154

The images above show the largest variance slices of the map in three orthogonal directions.

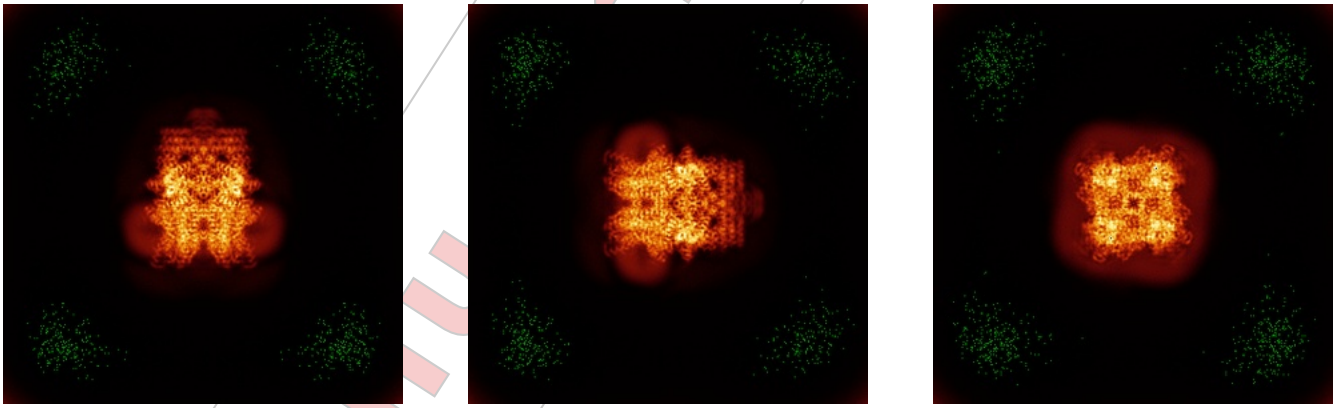
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

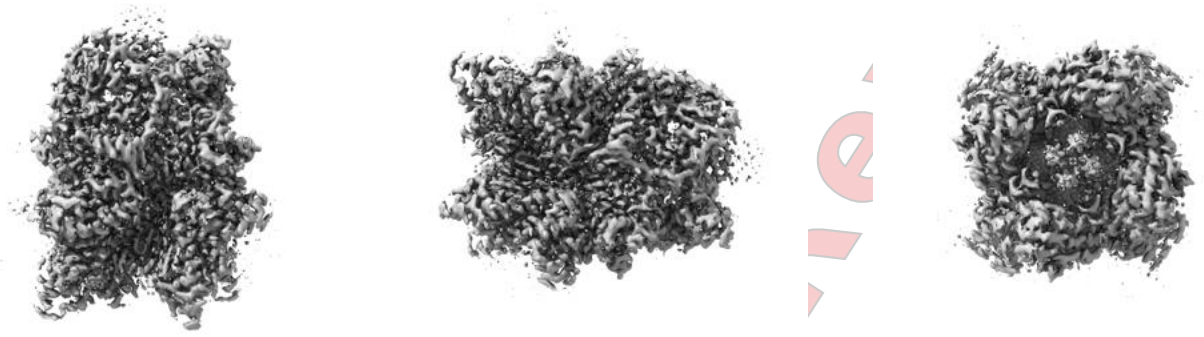


X Y Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

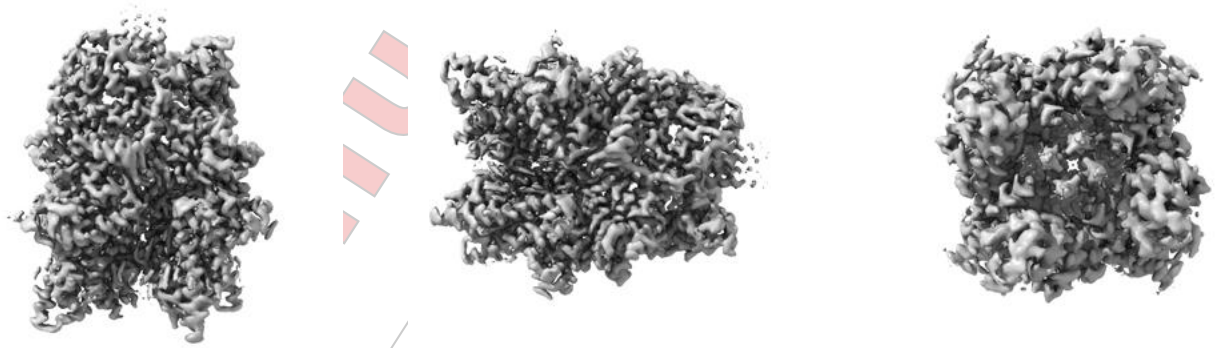
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.28. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

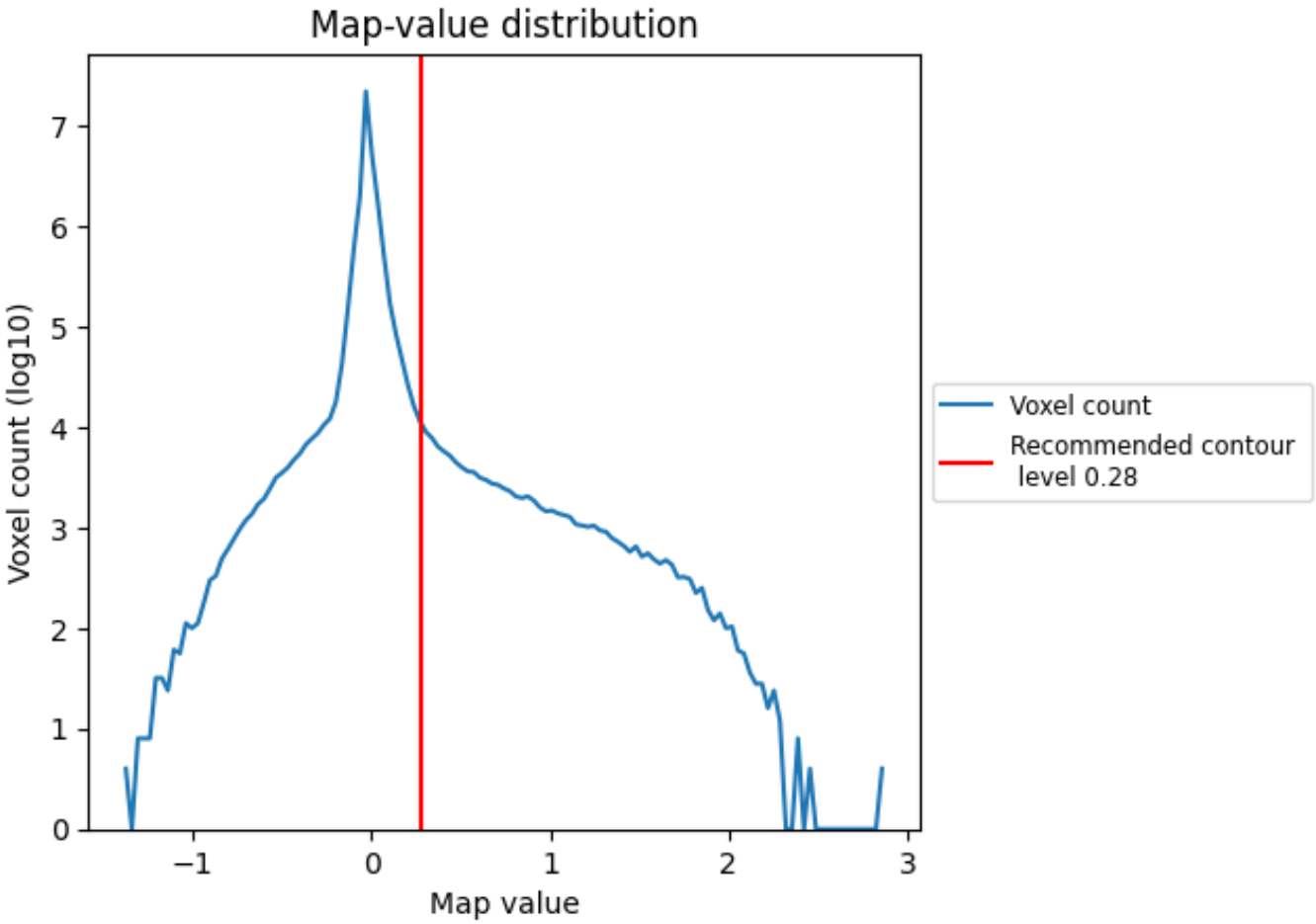
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

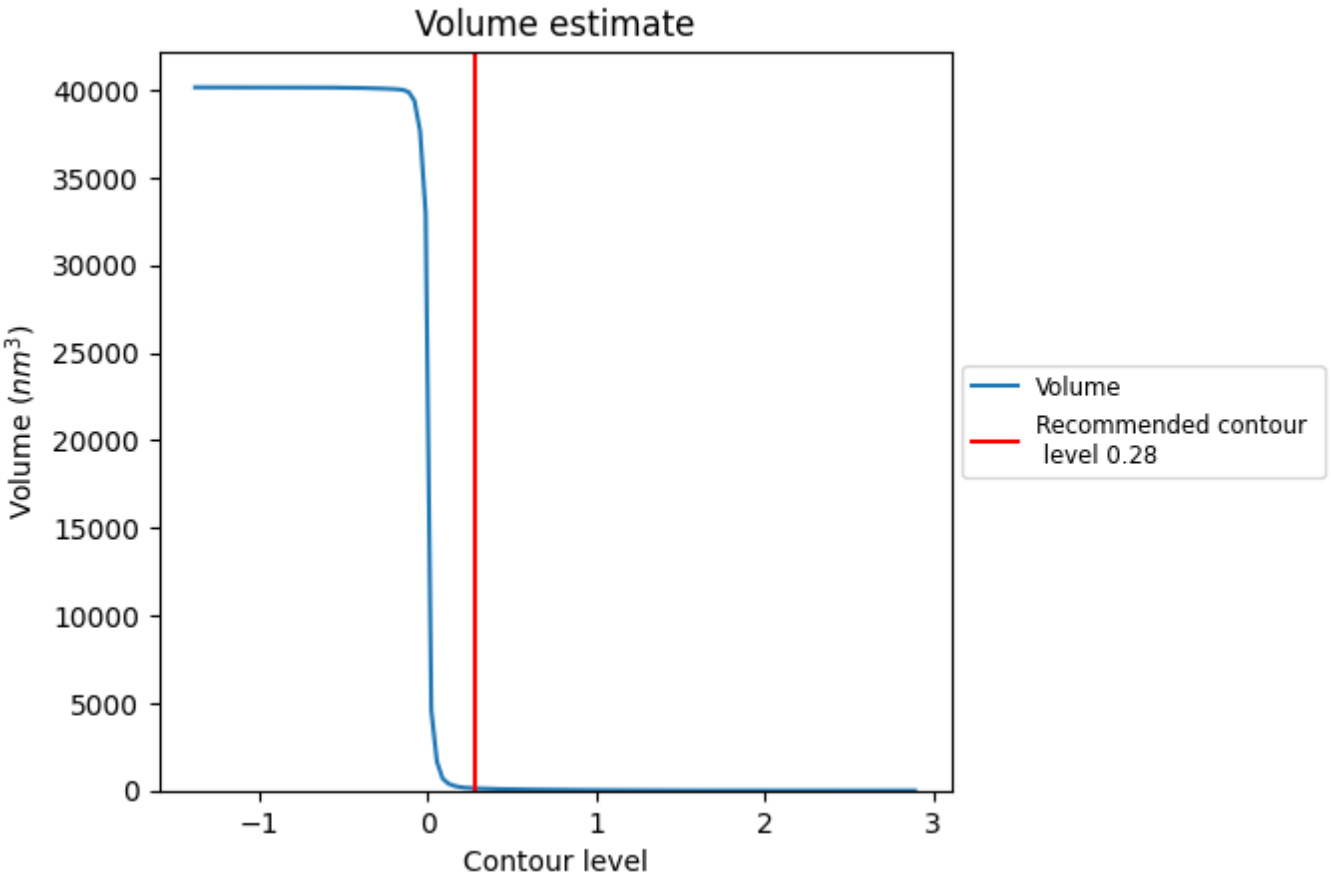
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

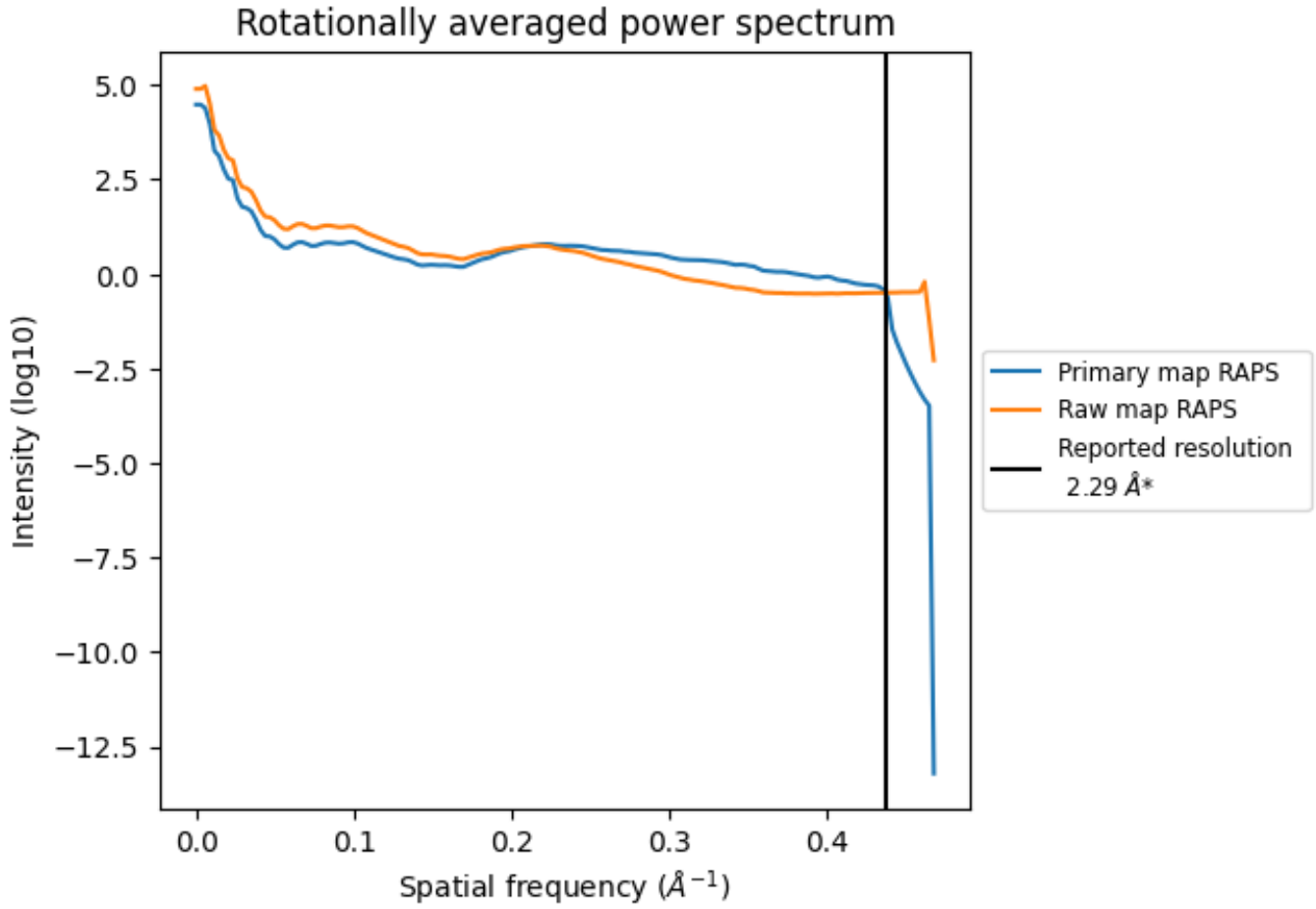
7.2 Volume estimate (i)



The volume at the recommended contour level is 129 nm^3; this corresponds to an approximate mass of 117 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

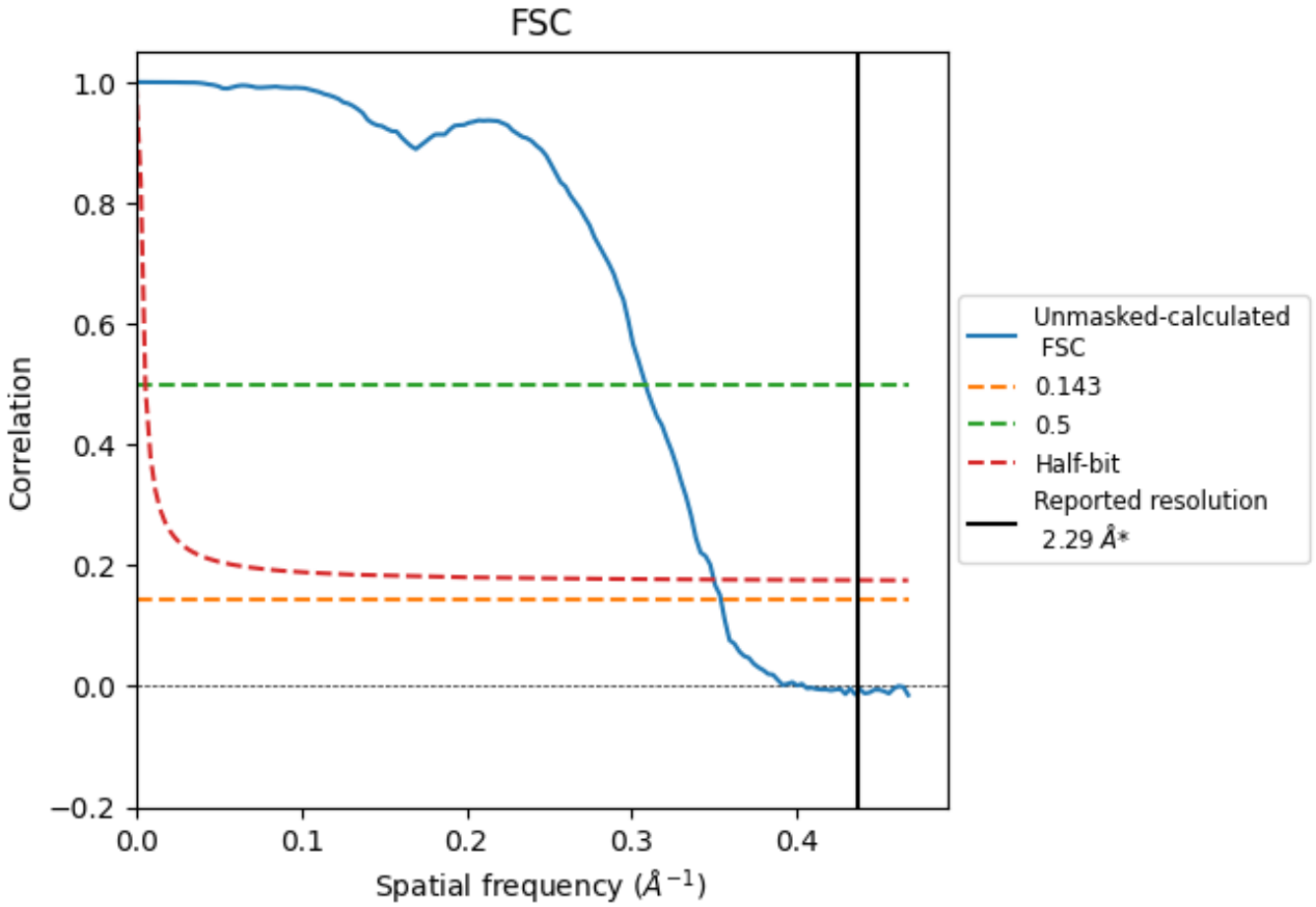


*Reported resolution corresponds to spatial frequency of 0.437 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.437 Å^{-1}

8.2 Resolution estimates (i)

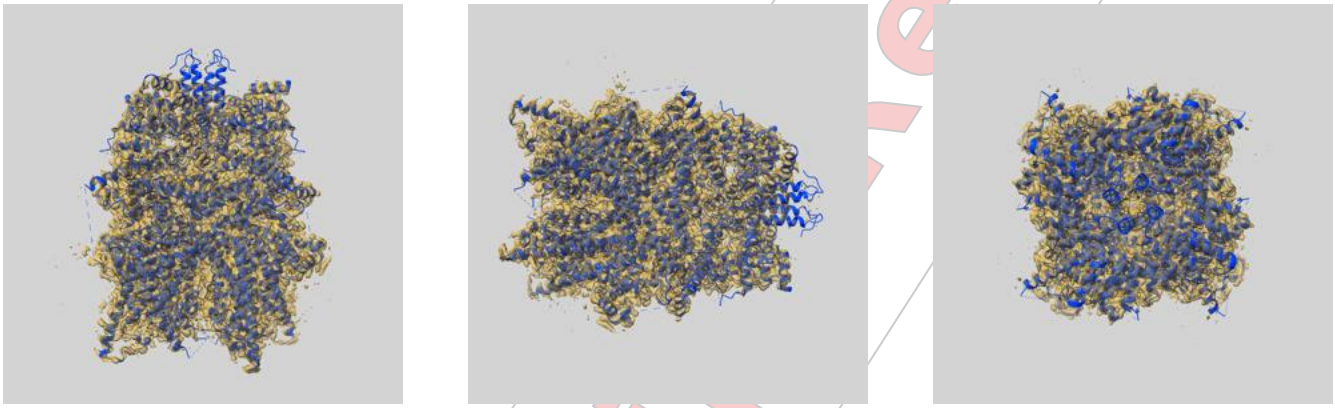
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.29	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.82	3.24	2.86

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.82 differs from the reported value 2.29 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-65279 and PDB model 9VQW. Per-residue inclusion information can be found in section 3 on page 9.

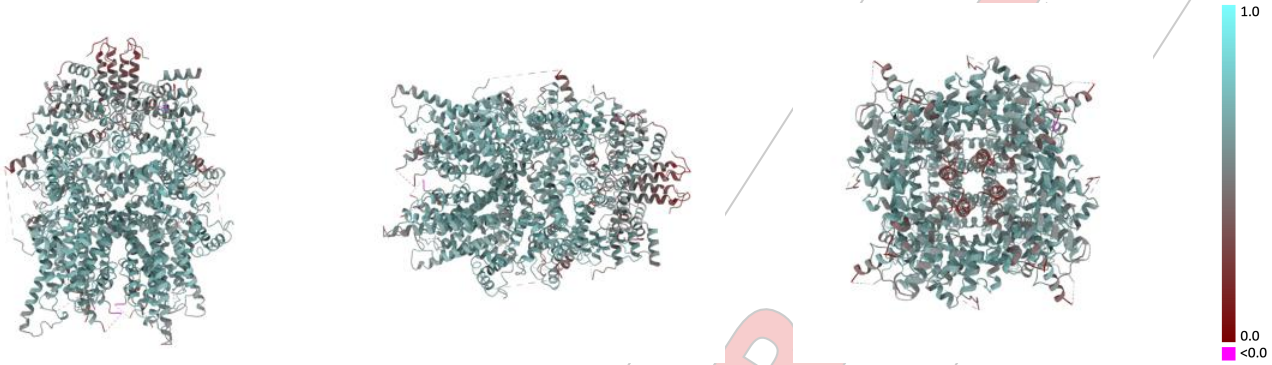
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.28 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

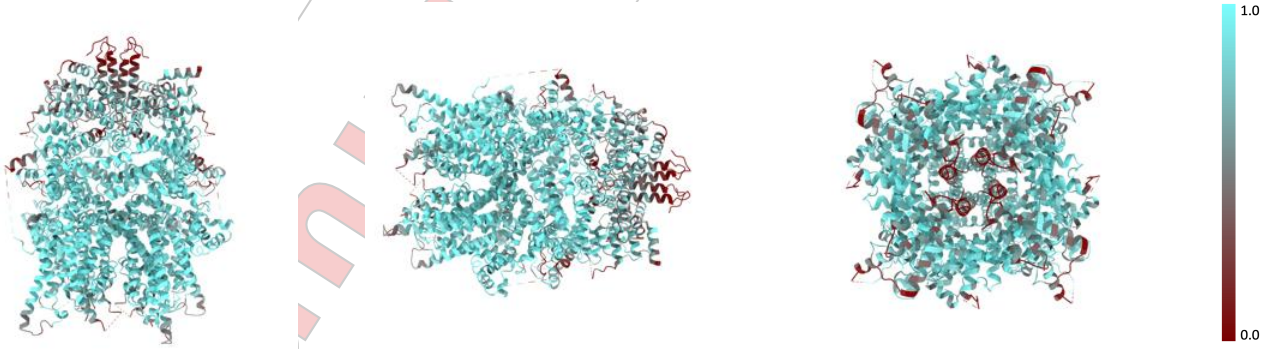
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

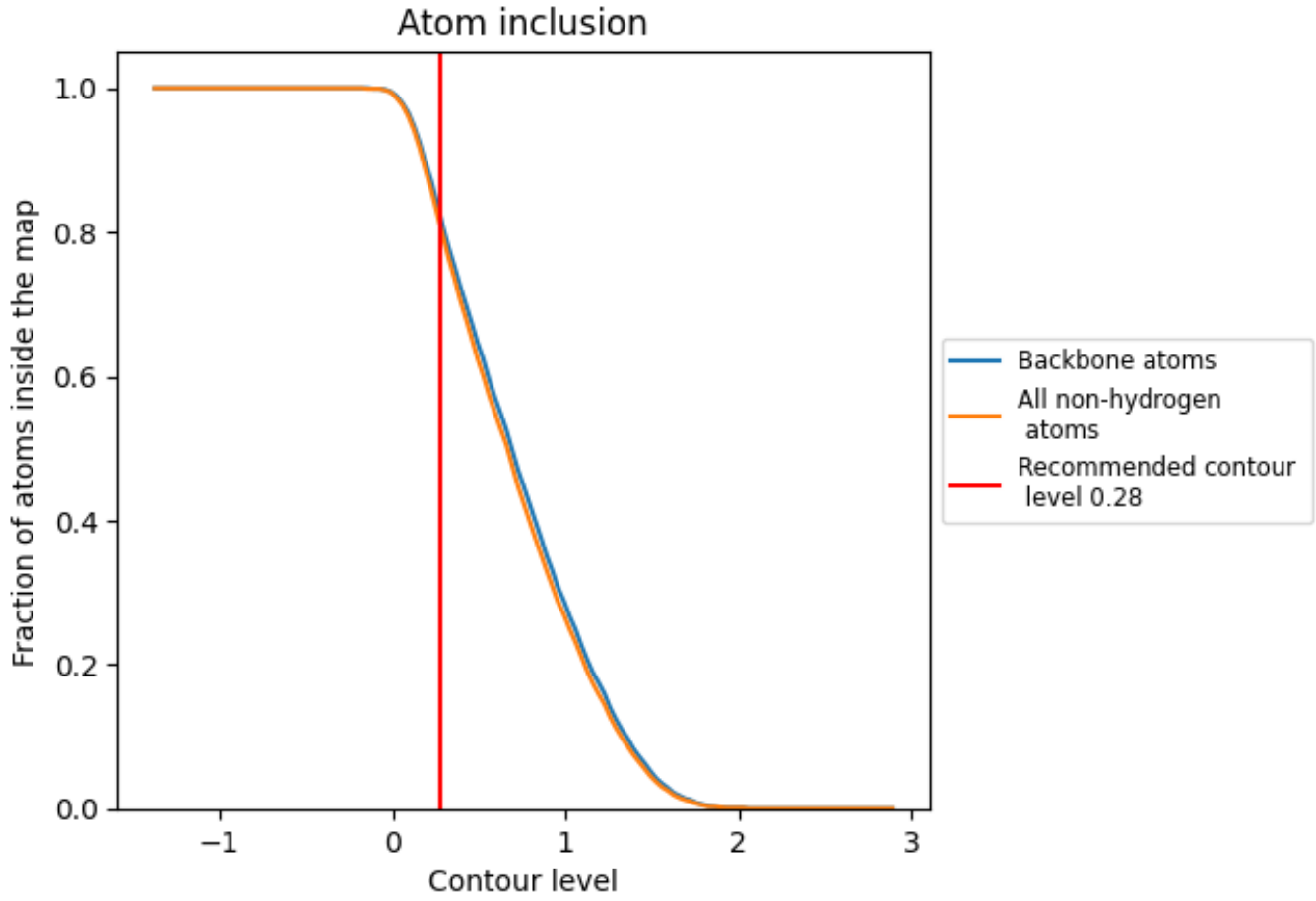
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.28).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8050	0.5900
A	0.8030	0.5840
B	0.8100	0.5910
C	0.8110	0.5920
D	0.8110	0.5930

Full wwPDB EM Validation Report ⓘ

Jul 20, 2025 – 02:21 PM JST

PDB ID	:	9VQX / pdb_00009vqx
EMDB ID	:	EMD-65280
Title	:	Cryo-EM structure of drosophila TRPgamma in low calcium state
Deposited on	:	2025-07-05
Resolution	:	2.46 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

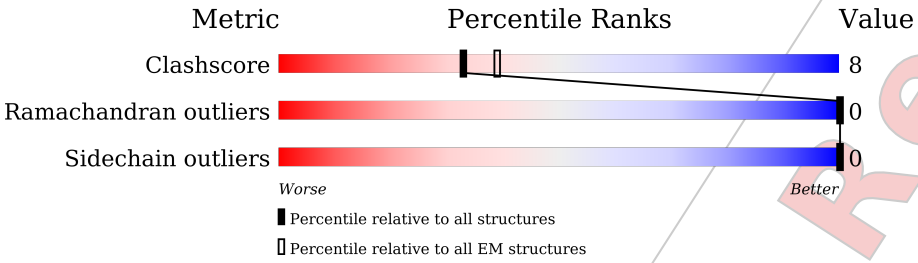
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.46 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1128	9% 54% 9% 38%
1	B	1128	9% 53% 9% 38%
1	C	1128	9% 53% 9% 38%
1	D	1128	9% 53% 9% 38%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 23868 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

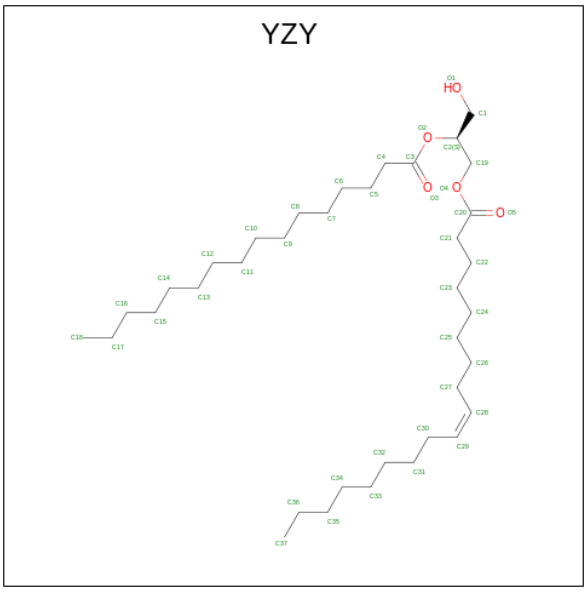
- Molecule 1 is a protein called Transient receptor potential-gamma protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	705	Total 5769	C 3723	N 976	O 1036	S 34	0	0
1	B	705	Total 5769	C 3723	N 976	O 1036	S 34	0	0
1	C	705	Total 5769	C 3723	N 976	O 1036	S 34	0	0
1	D	705	Total 5769	C 3723	N 976	O 1036	S 34	0	0

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

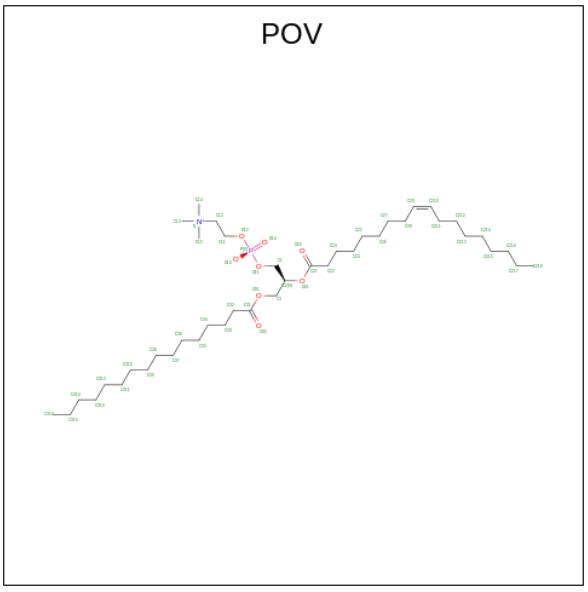
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total 1	Zn 1	0
2	B	1	Total 1	Zn 1	0
2	C	1	Total 1	Zn 1	0
2	D	1	Total 1	Zn 1	0

- Molecule 3 is (2S)-2-(hexadecanoyloxy)-3-hydroxypropyl (9Z)-octadec-9-enoate (CCD ID: YZY) (formula: $C_{37}H_{70}O_5$).



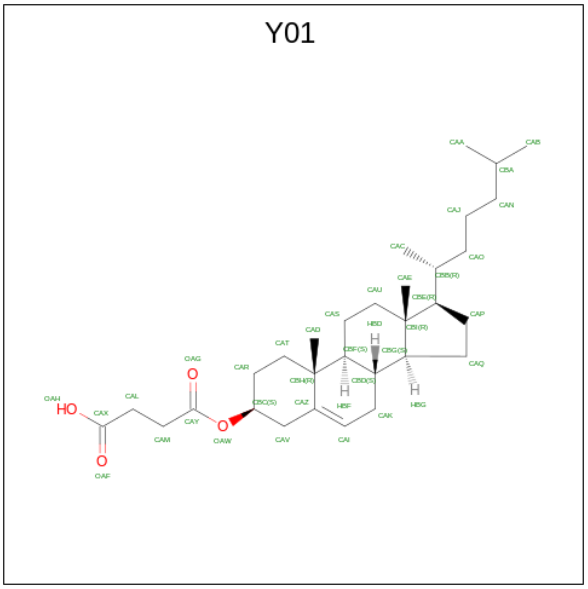
Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C O 35 30 5	0
3	B	1	Total C O 35 30 5	0
3	C	1	Total C O 35 30 5	0
3	D	1	Total C O 35 30 5	0

- Molecule 4 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: $C_{42}H_{82}NO_8P$).



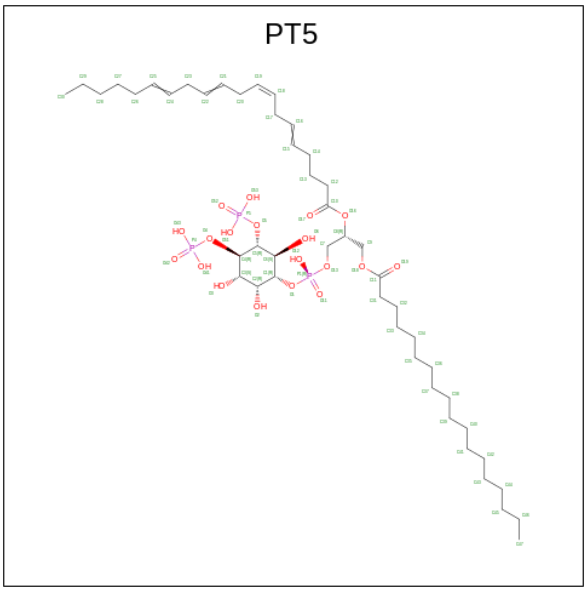
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	D	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 5 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			35	31	4	
5	B	1	Total	C	O	0
			35	31	4	
5	C	1	Total	C	O	0
			35	31	4	
5	D	1	Total	C	O	0
			35	31	4	

- Molecule 6 is [(2R)-1-octadecanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phospho ryl]oxy-propan-2-yl] (8Z)-icosa-5,8,11,14-tetraenoate (CCD ID: PT5) (formula: $C_{47}H_{85}O_{19}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	O	P	0
			69	47	19	3	
6	B	1	Total	C	O	P	0
			69	47	19	3	
6	C	1	Total	C	O	P	0
			69	47	19	3	
6	D	1	Total	C	O	P	0
			69	47	19	3	

- Molecule 7 is water.

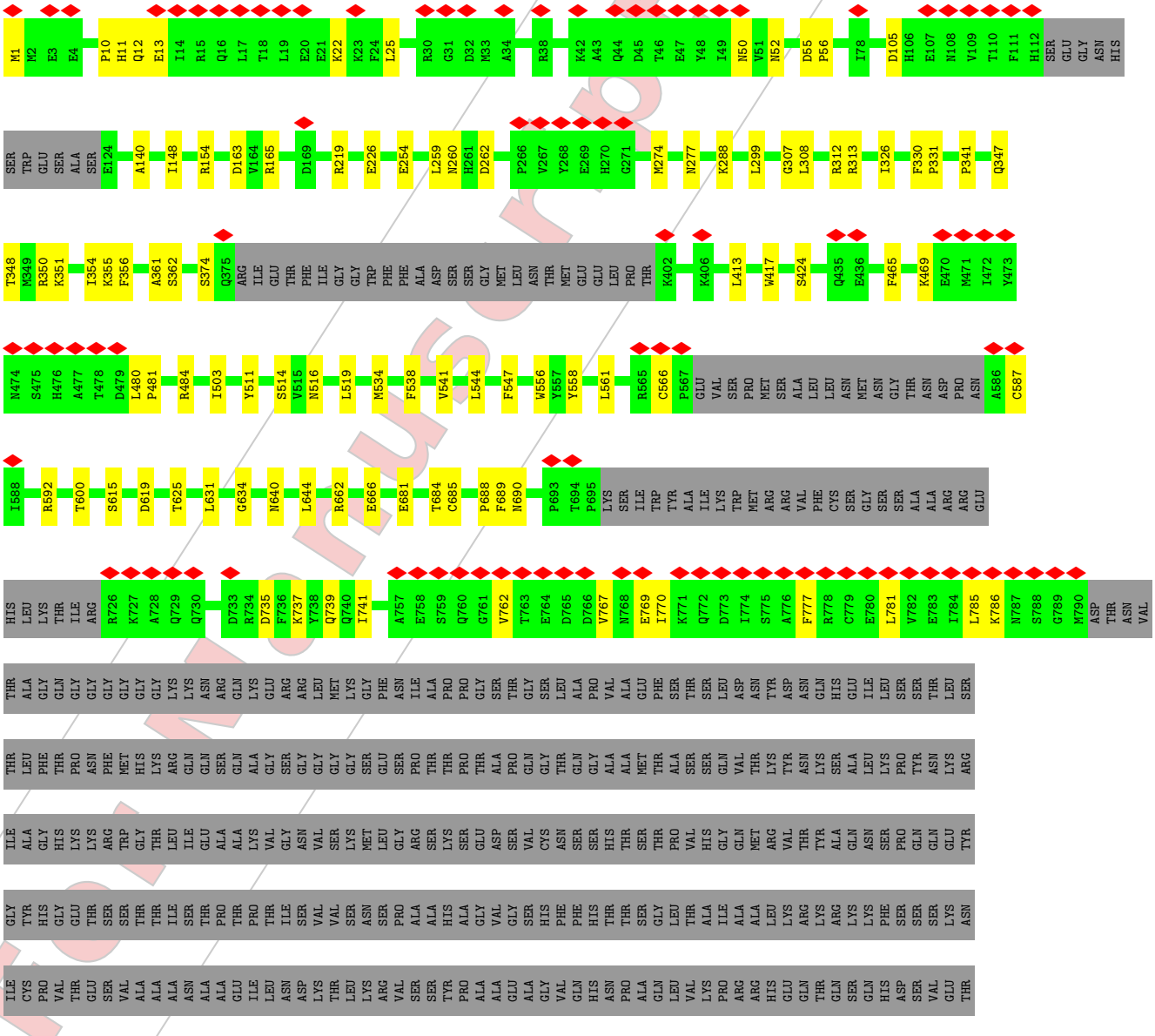
Mol	Chain	Residues	Atoms		AltConf
7	A	6	Total	O	0
			6	6	
7	B	6	Total	O	0
			6	6	
7	C	6	Total	O	0
			6	6	
7	D	6	Total	O	0
			6	6	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

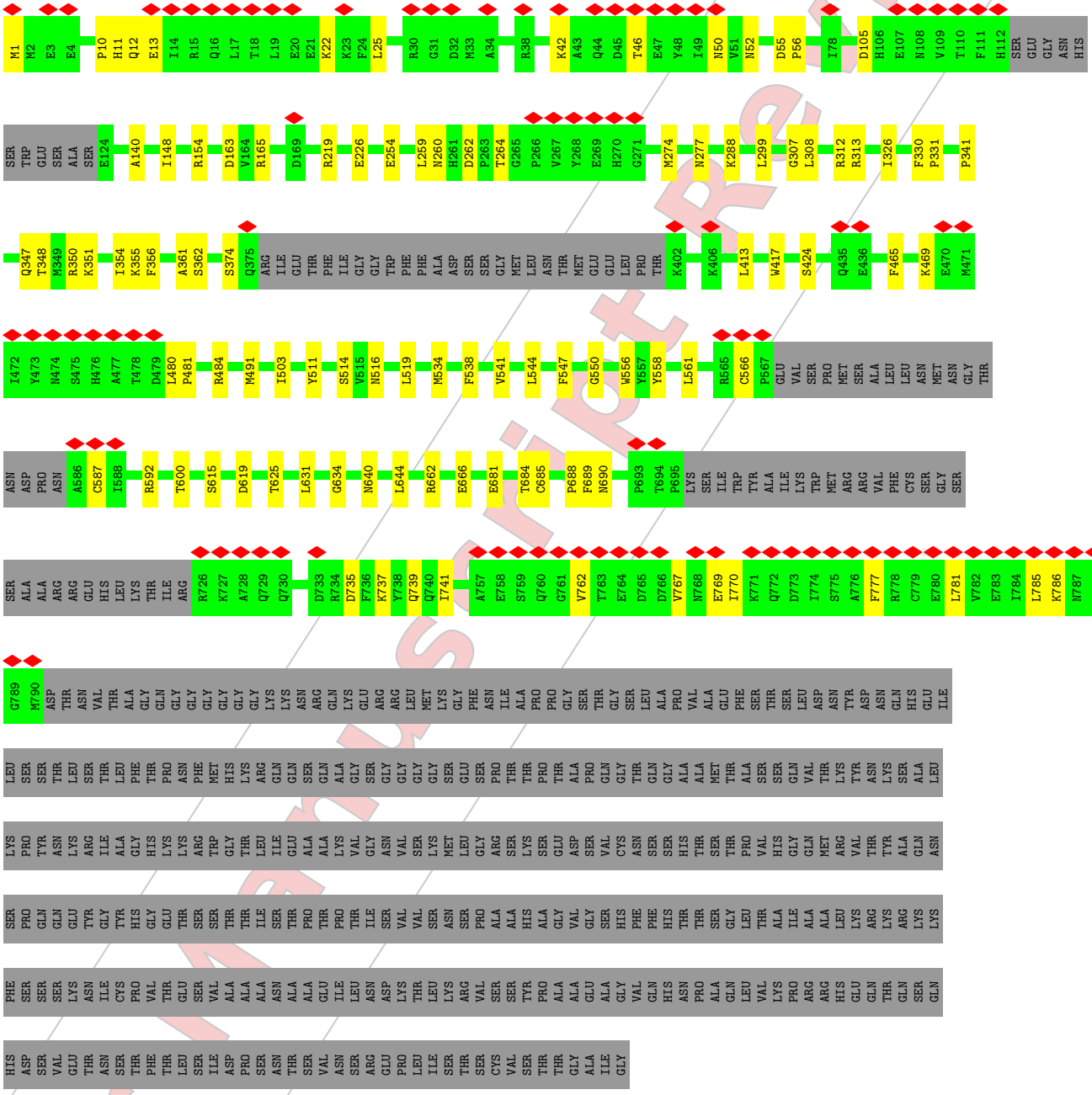
- Molecule 1: Transient receptor potential-gamma protein

Chain A:



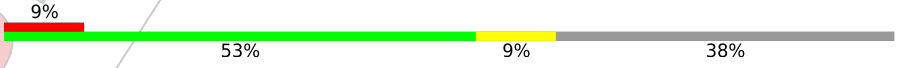
• Molecule 1: Transient receptor potential-gamma protein

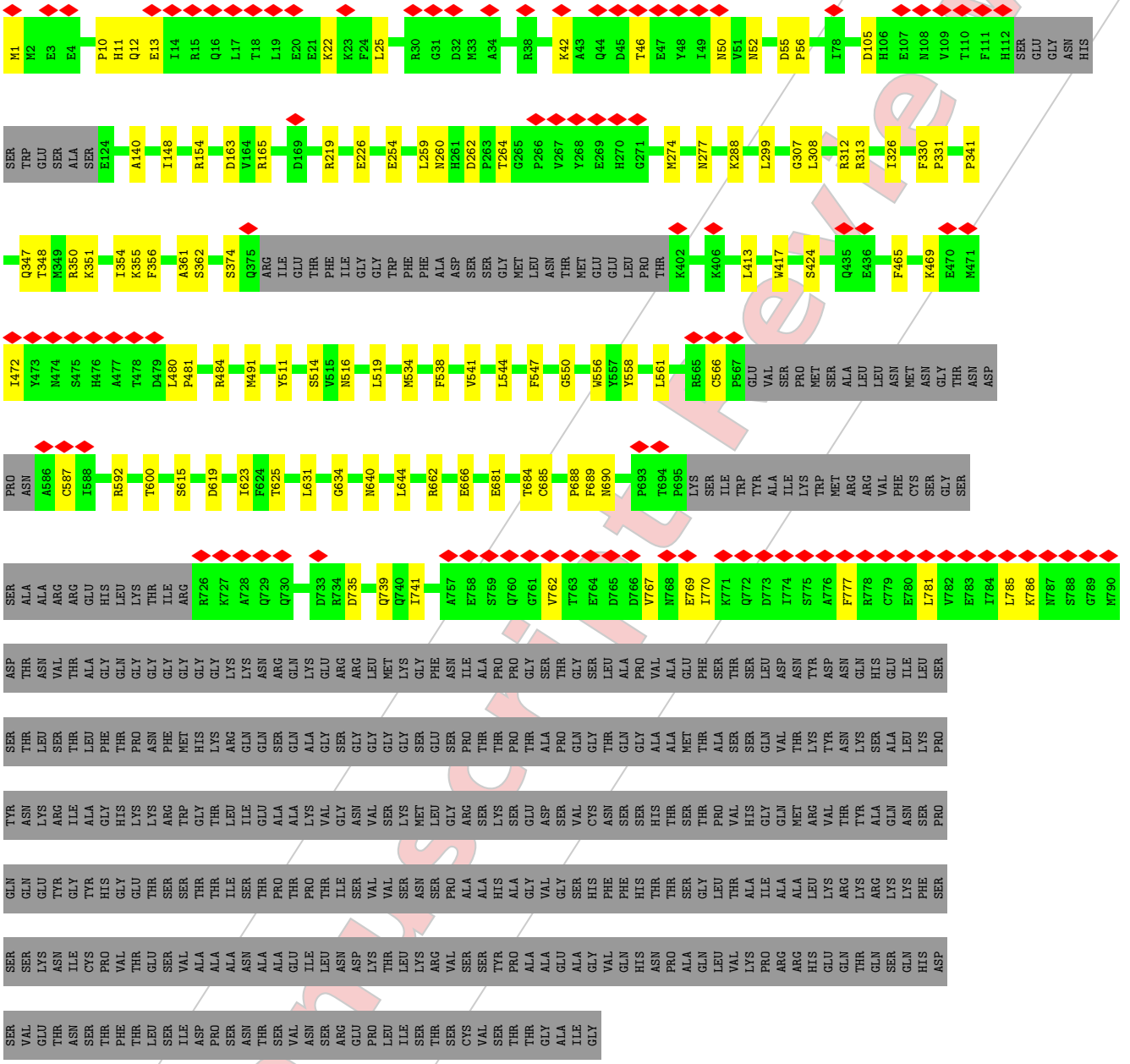
Chain B:



• Molecule 1: Transient receptor potential-gamma protein

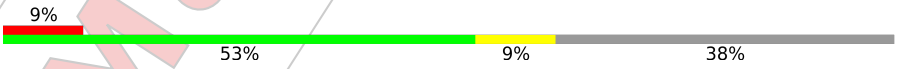
Chain C:

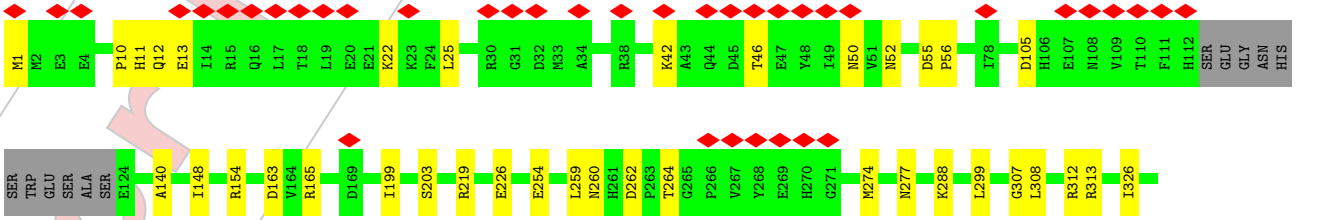


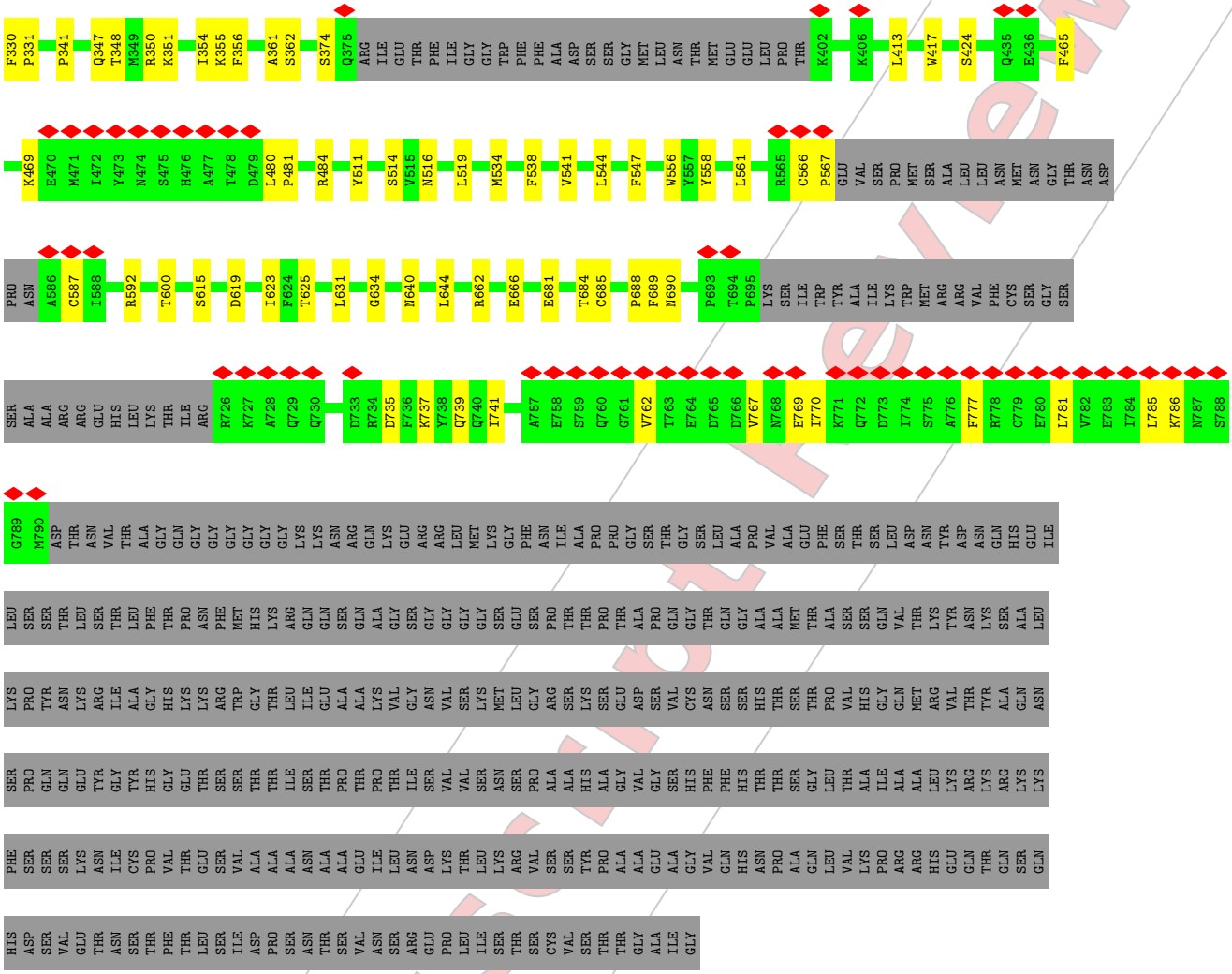


• Molecule 1: Transient receptor potential-gamma protein

Chain D:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91279	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	-1300	Depositor
Maximum defocus (nm)	-1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.098	Depositor
Minimum map value	-1.178	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	316.41602, 316.41602, 316.41602	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82400006, 0.82400006, 0.82400006	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, Y01, PT5, POV, YZY

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.11	0/5901	0.28	0/7987
1	B	0.11	0/5901	0.28	0/7987
1	C	0.11	0/5901	0.28	0/7987
1	D	0.11	0/5901	0.28	0/7987
All	All	0.11	0/23604	0.28	0/31948

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5769	0	5767	93	0
1	B	5769	0	5767	99	0
1	C	5769	0	5767	100	0
1	D	5769	0	5767	98	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	35	0	53	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	35	0	53	11	0
3	C	35	0	53	11	0
3	D	35	0	53	11	0
4	A	52	0	82	2	0
4	B	52	0	82	2	0
4	C	52	0	82	3	0
4	D	52	0	82	3	0
5	A	35	0	49	10	0
5	B	35	0	49	11	0
5	C	35	0	49	10	0
5	D	35	0	49	11	0
6	A	69	0	80	12	0
6	B	69	0	80	13	0
6	C	69	0	80	13	0
6	D	69	0	80	13	0
7	A	6	0	0	0	0
7	B	6	0	0	0	0
7	C	6	0	0	0	0
7	D	6	0	0	0	0
All	All	23868	0	24124	392	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (392) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1202:YZY:C15	5:D:1204:Y01:HAK2	1.79	1.12
3:C:1202:YZY:C15	5:C:1204:Y01:HAK2	1.79	1.12
3:A:1202:YZY:C15	5:A:1204:Y01:HAK2	1.79	1.11
3:B:1202:YZY:C15	5:B:1204:Y01:HAK2	1.79	1.11
3:C:1202:YZY:H151	5:C:1204:Y01:HAK2	1.30	1.09
3:D:1202:YZY:H151	5:D:1204:Y01:HAK2	1.30	1.09
3:A:1202:YZY:H151	5:A:1204:Y01:HAK2	1.30	1.09
1:A:417:TRP:CZ3	1:A:688:PRO:HD3	1.89	1.08
1:B:417:TRP:CZ3	1:B:688:PRO:HD3	1.89	1.08
1:D:417:TRP:CZ3	1:D:688:PRO:HD3	1.89	1.06
1:C:417:TRP:CZ3	1:C:688:PRO:HD3	1.89	1.06
1:A:417:TRP:CH2	1:A:688:PRO:HG3	1.91	1.05
1:B:417:TRP:CH2	1:B:688:PRO:HG3	1.91	1.05
3:B:1202:YZY:H151	5:B:1204:Y01:HAK2	1.30	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:TRP:CH2	1:D:688:PRO:HG3	1.91	1.04
1:C:417:TRP:CH2	1:C:688:PRO:HG3	1.91	1.04
1:D:417:TRP:CZ3	1:D:688:PRO:HG3	1.95	1.01
1:B:417:TRP:CZ3	1:B:688:PRO:HG3	1.95	1.01
1:C:417:TRP:CZ3	1:C:688:PRO:HG3	1.95	1.00
1:A:417:TRP:CZ3	1:A:688:PRO:HG3	1.95	1.00
1:A:417:TRP:CZ3	1:A:688:PRO:CG	2.50	0.94
1:D:417:TRP:CZ3	1:D:688:PRO:CG	2.50	0.94
1:A:417:TRP:CE3	1:A:688:PRO:HD3	2.02	0.94
1:D:417:TRP:CZ3	1:D:688:PRO:CD	2.51	0.94
1:D:417:TRP:CE3	1:D:688:PRO:HD3	2.02	0.94
1:B:417:TRP:CZ3	1:B:688:PRO:CD	2.51	0.94
1:C:417:TRP:CZ3	1:C:688:PRO:CG	2.50	0.93
1:C:417:TRP:CZ3	1:C:688:PRO:CD	2.51	0.93
1:C:417:TRP:CE3	1:C:688:PRO:HD3	2.02	0.93
1:B:417:TRP:CZ3	1:B:688:PRO:CG	2.50	0.93
1:A:417:TRP:CZ3	1:A:688:PRO:CD	2.51	0.93
1:B:417:TRP:CE3	1:B:688:PRO:HD3	2.02	0.93
1:A:55:ASP:OD1	1:A:56:PRO:HD2	1.70	0.92
1:D:55:ASP:OD1	1:D:56:PRO:HD2	1.70	0.92
1:B:55:ASP:OD1	1:B:56:PRO:HD2	1.70	0.92
1:C:55:ASP:OD1	1:C:56:PRO:HD2	1.70	0.90
1:A:55:ASP:CG	1:A:56:PRO:HD2	1.97	0.89
1:B:55:ASP:CG	1:B:56:PRO:HD2	1.97	0.89
1:D:566:CYS:SG	1:D:587:CYS:HB3	2.12	0.89
1:C:566:CYS:SG	1:C:587:CYS:HB3	2.12	0.89
1:A:566:CYS:SG	1:A:587:CYS:HB3	2.12	0.89
1:D:55:ASP:CG	1:D:56:PRO:HD2	1.97	0.88
1:C:55:ASP:CG	1:C:56:PRO:HD2	1.97	0.88
1:B:566:CYS:SG	1:B:587:CYS:HB3	2.12	0.87
6:A:1205:PT5:H26	1:D:519:LEU:HD11	1.62	0.81
1:C:519:LEU:HD11	6:D:1205:PT5:H26	1.62	0.81
1:B:362:SER:HG	1:B:417:TRP:HZ3	1.28	0.81
1:A:519:LEU:HD11	6:B:1205:PT5:H26	1.62	0.80
1:C:362:SER:HG	1:C:417:TRP:HZ3	1.30	0.80
1:B:519:LEU:HD11	6:C:1205:PT5:H26	1.62	0.80
1:C:785:LEU:HD12	1:C:786:LYS:HG3	1.64	0.80
1:D:785:LEU:HD12	1:D:786:LYS:HG3	1.64	0.79
1:B:785:LEU:HD12	1:B:786:LYS:HG3	1.64	0.78
1:A:785:LEU:HD12	1:A:786:LYS:HG3	1.64	0.77
3:D:1202:YZY:H161	5:D:1204:Y01:CAI	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1202:YZY:H161	5:A:1204:Y01:CAI	2.15	0.77
3:C:1202:YZY:H161	5:C:1204:Y01:CAI	2.15	0.76
3:B:1202:YZY:H161	5:B:1204:Y01:CAI	2.15	0.76
5:B:1204:Y01:HAC2	1:C:547:PHE:CZ	2.21	0.75
5:C:1204:Y01:HAC2	1:D:547:PHE:CZ	2.22	0.75
5:A:1204:Y01:HAC2	1:B:547:PHE:CZ	2.21	0.74
1:A:547:PHE:CZ	5:D:1204:Y01:HAC2	2.22	0.74
1:A:413:LEU:O	1:A:417:TRP:HD1	1.72	0.72
1:D:413:LEU:O	1:D:417:TRP:HD1	1.72	0.72
1:B:413:LEU:O	1:B:417:TRP:HD1	1.72	0.71
1:C:413:LEU:O	1:C:417:TRP:HD1	1.73	0.70
1:D:538:PHE:HD1	6:D:1205:PT5:C41	2.05	0.70
1:A:417:TRP:CH2	1:A:688:PRO:CG	2.73	0.69
1:A:538:PHE:HD1	6:A:1205:PT5:C41	2.05	0.69
1:C:538:PHE:HD1	6:C:1205:PT5:C41	2.05	0.69
1:D:362:SER:HG	1:D:417:TRP:HZ3	1.40	0.69
1:B:538:PHE:HD1	6:B:1205:PT5:C41	2.05	0.69
1:D:260:ASN:HD21	1:D:274:MET:HE3	1.58	0.69
1:A:260:ASN:HD21	1:A:274:MET:HE3	1.58	0.68
1:D:417:TRP:CH2	1:D:688:PRO:CG	2.73	0.68
1:D:534:MET:HB3	6:D:1205:PT5:H56	1.76	0.68
1:A:769:GLU:HG2	1:B:1:MET:N	2.08	0.68
1:C:534:MET:HB3	6:C:1205:PT5:H56	1.76	0.68
1:B:260:ASN:HD21	1:B:274:MET:HE3	1.58	0.68
1:C:260:ASN:HD21	1:C:274:MET:HE3	1.58	0.68
1:B:769:GLU:HG2	1:C:1:MET:N	2.09	0.67
1:C:769:GLU:HG2	1:D:1:MET:N	2.08	0.67
1:B:417:TRP:CH2	1:B:688:PRO:CG	2.73	0.67
1:B:534:MET:HB3	6:B:1205:PT5:H56	1.76	0.66
1:C:55:ASP:CG	1:C:56:PRO:CD	2.68	0.66
1:A:1:MET:N	1:D:769:GLU:HG2	2.10	0.66
1:A:55:ASP:CG	1:A:56:PRO:CD	2.68	0.66
1:B:55:ASP:CG	1:B:56:PRO:CD	2.68	0.66
1:A:534:MET:HB3	6:A:1205:PT5:H56	1.76	0.66
1:D:55:ASP:CG	1:D:56:PRO:CD	2.68	0.66
1:D:516:ASN:HB3	1:D:519:LEU:HB2	1.78	0.65
1:B:516:ASN:HB3	1:B:519:LEU:HB2	1.78	0.65
1:A:516:ASN:HB3	1:A:519:LEU:HB2	1.78	0.65
1:C:516:ASN:HB3	1:C:519:LEU:HB2	1.78	0.64
1:C:417:TRP:CH2	1:C:688:PRO:CG	2.73	0.63
1:A:413:LEU:O	1:A:417:TRP:CD1	2.52	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:LEU:O	1:B:417:TRP:CD1	2.52	0.62
1:A:785:LEU:HD12	1:A:786:LYS:N	2.14	0.62
1:B:361:ALA:HB2	4:B:1203:POV:H38	1.82	0.62
1:B:538:PHE:HD1	6:B:1205:PT5:H71	1.64	0.62
1:C:413:LEU:O	1:C:417:TRP:CD1	2.52	0.62
1:D:785:LEU:HD12	1:D:786:LYS:N	2.14	0.62
1:C:361:ALA:HB2	4:C:1203:POV:H38	1.82	0.62
1:B:785:LEU:HD12	1:B:786:LYS:N	2.14	0.62
1:D:361:ALA:HB2	4:D:1203:POV:H38	1.82	0.62
1:A:361:ALA:HB2	4:A:1203:POV:H38	1.82	0.62
1:A:538:PHE:HD1	6:A:1205:PT5:H71	1.65	0.62
1:D:413:LEU:O	1:D:417:TRP:CD1	2.52	0.62
1:D:538:PHE:HD1	6:D:1205:PT5:H71	1.65	0.62
3:D:1202:YZY:H152	5:D:1204:Y01:HAK2	1.81	0.61
1:A:341:PRO:O	1:A:347:GLN:NE2	2.33	0.61
1:A:541:VAL:HG21	6:A:1205:PT5:H67	1.82	0.61
1:C:785:LEU:HD12	1:C:786:LYS:N	2.14	0.61
1:D:541:VAL:HG21	6:D:1205:PT5:H67	1.82	0.61
1:D:55:ASP:OD1	1:D:56:PRO:CD	2.48	0.61
1:C:538:PHE:HD1	6:C:1205:PT5:H71	1.65	0.61
1:D:341:PRO:O	1:D:347:GLN:NE2	2.33	0.61
1:D:785:LEU:CD1	1:D:786:LYS:H	2.14	0.61
1:B:519:LEU:CD1	6:C:1205:PT5:H26	2.31	0.60
1:A:55:ASP:OD1	1:A:56:PRO:CD	2.48	0.60
1:A:785:LEU:CD1	1:A:786:LYS:H	2.14	0.60
1:A:312:ARG:NH2	1:B:226:GLU:OE2	2.35	0.60
1:B:541:VAL:HG21	6:B:1205:PT5:H67	1.82	0.60
1:A:519:LEU:CD1	6:B:1205:PT5:H26	2.31	0.60
1:B:341:PRO:O	1:B:347:GLN:NE2	2.33	0.60
1:C:785:LEU:CD1	1:C:786:LYS:H	2.14	0.60
1:C:341:PRO:O	1:C:347:GLN:NE2	2.33	0.60
1:B:55:ASP:OD1	1:B:56:PRO:CD	2.48	0.60
1:C:312:ARG:NH2	1:D:226:GLU:OE2	2.35	0.60
1:A:226:GLU:OE2	1:D:312:ARG:NH2	2.34	0.60
1:C:541:VAL:HG21	6:C:1205:PT5:H67	1.82	0.60
1:B:785:LEU:CD1	1:B:786:LYS:H	2.14	0.59
1:C:480:LEU:HD12	1:C:481:PRO:HD2	1.85	0.59
1:B:274:MET:HE1	1:B:299:LEU:HD21	1.85	0.59
1:C:313:ARG:O	1:D:165:ARG:NH2	2.36	0.59
3:C:1202:YZY:H152	5:C:1204:Y01:HAK2	1.81	0.58
1:C:274:MET:HE1	1:C:299:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1205:PT5:H26	1:D:519:LEU:CD1	2.31	0.58
1:B:312:ARG:NH2	1:C:226:GLU:OE2	2.35	0.58
1:C:55:ASP:OD1	1:C:56:PRO:CD	2.48	0.58
1:D:480:LEU:HD12	1:D:481:PRO:HD2	1.85	0.58
1:A:313:ARG:O	1:B:165:ARG:NH2	2.35	0.58
1:A:480:LEU:HD12	1:A:481:PRO:HD2	1.85	0.58
1:A:165:ARG:NH2	1:D:313:ARG:O	2.36	0.58
5:C:1204:Y01:HAC2	1:D:547:PHE:HZ	1.69	0.58
1:D:362:SER:OG	1:D:417:TRP:HZ3	1.87	0.58
5:B:1204:Y01:HAC2	1:C:547:PHE:HZ	1.68	0.57
1:B:480:LEU:HD12	1:B:481:PRO:HD2	1.85	0.57
1:A:362:SER:OG	1:A:417:TRP:HZ3	1.87	0.57
1:A:547:PHE:HZ	5:D:1204:Y01:HAC2	1.69	0.57
5:A:1204:Y01:HAC2	1:B:547:PHE:HZ	1.68	0.57
1:D:685:CYS:SG	1:D:689:PHE:HB2	2.45	0.57
1:A:163:ASP:OD1	1:A:219:ARG:NH2	2.38	0.57
1:D:274:MET:HE1	1:D:299:LEU:HD21	1.85	0.57
1:A:762:VAL:HG22	1:B:762:VAL:HG11	1.86	0.57
1:B:313:ARG:O	1:C:165:ARG:NH2	2.37	0.57
1:B:538:PHE:HD1	6:B:1205:PT5:H72	1.70	0.57
1:C:362:SER:OG	1:C:417:TRP:HZ3	1.87	0.57
1:C:538:PHE:HD1	6:C:1205:PT5:H72	1.70	0.57
1:C:685:CYS:SG	1:C:689:PHE:HB2	2.45	0.57
1:A:274:MET:HE1	1:A:299:LEU:HD21	1.85	0.56
1:C:519:LEU:CD1	6:D:1205:PT5:H26	2.31	0.56
1:C:762:VAL:HG22	1:D:762:VAL:HG11	1.86	0.56
1:B:362:SER:OG	1:B:417:TRP:HZ3	1.87	0.56
1:B:163:ASP:OD1	1:B:219:ARG:NH2	2.38	0.56
1:A:685:CYS:SG	1:A:689:PHE:HB2	2.45	0.56
1:A:762:VAL:HG11	1:D:762:VAL:HG22	1.86	0.56
1:D:538:PHE:HD1	6:D:1205:PT5:H72	1.70	0.56
3:A:1202:YZY:H41	1:B:634:GLY:HA3	1.88	0.56
1:B:685:CYS:SG	1:B:689:PHE:HB2	2.45	0.56
1:B:762:VAL:HG22	1:C:762:VAL:HG11	1.86	0.56
1:B:10:PRO:HA	1:B:13:GLU:HG2	1.89	0.55
1:A:538:PHE:HD1	6:A:1205:PT5:H72	1.70	0.55
1:D:11:HIS:ND1	1:D:55:ASP:OD1	2.37	0.55
1:D:163:ASP:OD1	1:D:219:ARG:NH2	2.38	0.55
1:C:10:PRO:HA	1:C:13:GLU:HG2	1.88	0.55
1:C:163:ASP:OD1	1:C:219:ARG:NH2	2.38	0.55
3:B:1202:YZY:H152	5:B:1204:Y01:HAK2	1.80	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:GLY:HA3	3:D:1202:YZY:H41	1.89	0.54
3:C:1202:YZY:H41	1:D:634:GLY:HA3	1.89	0.54
1:A:10:PRO:HA	1:A:13:GLU:HG2	1.88	0.54
3:B:1202:YZY:H41	1:C:634:GLY:HA3	1.89	0.54
1:A:11:HIS:ND1	1:A:55:ASP:OD1	2.37	0.54
1:D:10:PRO:HA	1:D:13:GLU:HG2	1.89	0.54
1:D:424:SER:OG	1:D:690:ASN:ND2	2.41	0.54
1:A:140:ALA:HA	1:A:148:ILE:HD11	1.90	0.53
5:B:1204:Y01:HAB1	1:C:631:LEU:HG	1.90	0.53
1:B:592:ARG:NH1	1:B:615:SER:OG	2.41	0.53
1:C:254:GLU:HA	1:C:741:ILE:HD13	1.90	0.53
1:C:770:ILE:HD11	1:D:767:VAL:HB	1.91	0.53
1:B:424:SER:OG	1:B:690:ASN:ND2	2.41	0.53
1:A:424:SER:OG	1:A:690:ASN:ND2	2.41	0.53
1:B:254:GLU:HA	1:B:741:ILE:HD13	1.90	0.53
1:C:140:ALA:HA	1:C:148:ILE:HD11	1.90	0.53
1:C:424:SER:OG	1:C:690:ASN:ND2	2.41	0.53
1:A:592:ARG:NH1	1:A:615:SER:OG	2.41	0.53
1:C:12:GLN:HA	1:C:22:LYS:HD3	1.91	0.53
1:C:592:ARG:NH1	1:C:615:SER:OG	2.41	0.53
1:D:254:GLU:HA	1:D:741:ILE:HD13	1.90	0.53
1:B:140:ALA:HA	1:B:148:ILE:HD11	1.90	0.52
3:C:1202:YZY:H221	6:C:1205:PT5:H83	1.91	0.52
1:A:770:ILE:HD11	1:B:767:VAL:HB	1.91	0.52
1:C:11:HIS:ND1	1:C:55:ASP:OD1	2.37	0.52
1:C:538:PHE:CD1	6:C:1205:PT5:H71	2.44	0.52
3:A:1202:YZY:H221	6:A:1205:PT5:H83	1.91	0.52
3:D:1202:YZY:H221	6:D:1205:PT5:H83	1.91	0.52
1:A:254:GLU:HA	1:A:741:ILE:HD13	1.90	0.52
1:A:767:VAL:HB	1:D:770:ILE:HD11	1.92	0.52
3:A:1202:YZY:H152	5:A:1204:Y01:HAK2	1.81	0.52
1:B:12:GLN:HA	1:B:22:LYS:HD3	1.91	0.52
1:B:770:ILE:HD11	1:C:767:VAL:HB	1.91	0.52
3:B:1202:YZY:H221	6:B:1205:PT5:H83	1.91	0.52
1:A:631:LEU:HG	5:D:1204:Y01:HAB1	1.91	0.52
1:A:777:PHE:CZ	1:B:781:LEU:HD21	2.44	0.52
1:C:777:PHE:CZ	1:D:781:LEU:HD21	2.44	0.52
1:B:538:PHE:CD1	6:B:1205:PT5:H71	2.44	0.51
1:D:12:GLN:HA	1:D:22:LYS:HD3	1.91	0.51
1:A:781:LEU:HD21	1:D:777:PHE:CZ	2.45	0.51
1:D:538:PHE:CD1	6:D:1205:PT5:H71	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1202:YZY:H151	5:A:1204:Y01:CAK	2.22	0.51
5:C:1204:Y01:HAB1	1:D:631:LEU:HG	1.91	0.51
1:C:417:TRP:HZ3	1:C:688:PRO:CD	2.20	0.51
1:C:511:TYR:O	1:C:514:SER:OG	2.29	0.51
3:D:1202:YZY:H151	5:D:1204:Y01:CAK	2.22	0.51
1:A:12:GLN:HA	1:A:22:LYS:HD3	1.91	0.51
1:D:140:ALA:HA	1:D:148:ILE:HD11	1.90	0.51
1:D:592:ARG:NH1	1:D:615:SER:OG	2.41	0.51
1:B:11:HIS:ND1	1:B:55:ASP:OD1	2.37	0.51
1:C:11:HIS:CE1	1:C:25:LEU:HB2	2.46	0.51
1:A:538:PHE:CD1	6:A:1205:PT5:H71	2.44	0.50
1:B:11:HIS:CE1	1:B:25:LEU:HB2	2.46	0.50
1:B:777:PHE:CZ	1:C:781:LEU:HD21	2.46	0.50
1:C:544:LEU:HD21	1:C:600:THR:HG23	1.94	0.50
1:A:544:LEU:HD21	1:A:600:THR:HG23	1.93	0.50
1:B:511:TYR:O	1:B:514:SER:OG	2.28	0.50
1:B:785:LEU:HD12	1:B:786:LYS:H	1.76	0.50
1:D:544:LEU:HD21	1:D:600:THR:HG23	1.93	0.50
5:A:1204:Y01:HAB1	1:B:631:LEU:HG	1.92	0.50
1:D:11:HIS:CE1	1:D:25:LEU:HB2	2.46	0.50
1:B:544:LEU:HD21	1:B:600:THR:HG23	1.94	0.49
1:B:538:PHE:CD1	6:B:1205:PT5:C41	2.93	0.49
1:A:465:PHE:O	1:A:469:LYS:HG2	2.13	0.49
1:B:105:ASP:OD1	1:B:154:ARG:NH2	2.46	0.49
1:A:11:HIS:CE1	1:A:25:LEU:HB2	2.46	0.49
1:C:465:PHE:O	1:C:469:LYS:HG2	2.13	0.49
1:A:785:LEU:HD12	1:A:786:LYS:H	1.76	0.49
1:D:465:PHE:O	1:D:469:LYS:HG2	2.13	0.49
3:A:1202:YZY:C16	5:A:1204:Y01:HAK2	2.42	0.49
1:B:465:PHE:O	1:B:469:LYS:HG2	2.13	0.48
1:A:105:ASP:OD1	1:A:154:ARG:NH2	2.46	0.48
3:A:1202:YZY:H151	5:A:1204:Y01:HBG	1.96	0.48
1:C:105:ASP:OD1	1:C:154:ARG:NH2	2.46	0.48
1:D:105:ASP:OD1	1:D:154:ARG:NH2	2.46	0.48
1:C:481:PRO:HG2	1:C:484:ARG:HB2	1.96	0.48
3:C:1202:YZY:H151	5:C:1204:Y01:HBG	1.96	0.47
1:C:417:TRP:HZ3	1:C:688:PRO:HD3	1.68	0.47
3:C:1202:YZY:H151	5:C:1204:Y01:CAK	2.22	0.47
1:D:481:PRO:HG2	1:D:484:ARG:HB2	1.96	0.47
1:D:538:PHE:HA	6:D:1205:PT5:H68	1.95	0.47
1:A:481:PRO:HG2	1:A:484:ARG:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:PRO:HG2	1:B:484:ARG:HB2	1.96	0.47
1:A:538:PHE:HA	6:A:1205:PT5:H68	1.95	0.47
3:B:1202:YZY:H151	5:B:1204:Y01:CAK	2.22	0.47
3:B:1202:YZY:H151	5:B:1204:Y01:HBG	1.96	0.47
3:D:1202:YZY:H151	5:D:1204:Y01:HBG	1.96	0.47
1:A:511:TYR:O	1:A:514:SER:OG	2.28	0.47
3:B:1202:YZY:H51	1:C:631:LEU:HD12	1.96	0.47
1:D:511:TYR:O	1:D:514:SER:OG	2.28	0.47
1:D:538:PHE:CD1	6:D:1205:PT5:C41	2.93	0.47
1:A:538:PHE:CD1	6:A:1205:PT5:C41	2.93	0.47
1:B:538:PHE:HA	6:B:1205:PT5:H68	1.95	0.47
1:D:785:LEU:CD1	1:D:786:LYS:N	2.77	0.47
1:B:785:LEU:CD1	1:B:786:LYS:N	2.77	0.47
1:C:538:PHE:CD1	6:C:1205:PT5:C41	2.93	0.46
3:B:1202:YZY:C16	5:B:1204:Y01:HAK2	2.42	0.46
1:A:417:TRP:HZ3	1:A:688:PRO:CD	2.20	0.46
1:C:538:PHE:HA	6:C:1205:PT5:H68	1.95	0.46
3:C:1202:YZY:H51	1:D:631:LEU:HD12	1.97	0.46
1:A:259:LEU:HD12	1:A:299:LEU:HD23	1.97	0.46
1:B:735:ASP:O	1:B:739:GLN:HG2	2.16	0.46
1:D:735:ASP:O	1:D:739:GLN:HG2	2.16	0.46
1:C:735:ASP:O	1:C:739:GLN:HG2	2.16	0.46
3:D:1202:YZY:C16	5:D:1204:Y01:HAK2	2.42	0.46
1:B:259:LEU:HD12	1:B:299:LEU:HD23	1.98	0.46
1:D:259:LEU:HD12	1:D:299:LEU:HD23	1.97	0.46
3:A:1202:YZY:H51	1:B:631:LEU:HD12	1.98	0.46
1:A:769:GLU:HG2	1:B:1:MET:H3	1.80	0.45
1:C:259:LEU:HD12	1:C:299:LEU:HD23	1.97	0.45
1:A:631:LEU:HD12	3:D:1202:YZY:H51	1.96	0.45
3:C:1202:YZY:C16	5:C:1204:Y01:HAK2	2.42	0.45
1:B:640:ASN:HA	1:B:644:LEU:HB2	1.99	0.45
1:A:735:ASP:O	1:A:739:GLN:HG2	2.16	0.45
1:D:199:ILE:O	1:D:203:SER:OG	2.27	0.45
1:A:785:LEU:CD1	1:A:786:LYS:N	2.77	0.45
1:A:308:LEU:HD21	1:A:326:ILE:HD11	1.98	0.45
1:D:737:LYS:HB2	1:D:737:LYS:HE2	1.75	0.45
5:D:1204:Y01:HAJ1	5:D:1204:Y01:HAC3	1.82	0.45
1:B:264:THR:O	1:B:264:THR:OG1	2.33	0.45
1:C:308:LEU:HD21	1:C:326:ILE:HD11	1.98	0.45
1:C:538:PHE:CD1	6:C:1205:PT5:H72	2.52	0.44
1:B:308:LEU:HD21	1:B:326:ILE:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:640:ASN:HA	1:C:644:LEU:HB2	1.99	0.44
1:A:288:LYS:NZ	1:A:666:GLU:OE1	2.40	0.44
1:D:640:ASN:HA	1:D:644:LEU:HB2	1.99	0.44
1:B:307:GLY:HA3	1:B:351:LYS:HD3	2.00	0.44
1:A:262:ASP:OD2	1:A:277:ASN:ND2	2.51	0.44
1:A:640:ASN:HA	1:A:644:LEU:HB2	1.99	0.44
1:B:769:GLU:HG2	1:C:1:MET:H3	1.81	0.44
1:C:785:LEU:CD1	1:C:786:LYS:N	2.77	0.44
1:D:308:LEU:HD21	1:D:326:ILE:HD11	1.98	0.44
1:C:307:GLY:HA3	1:C:351:LYS:HD3	2.00	0.44
1:A:307:GLY:HA3	1:A:351:LYS:HD3	2.00	0.43
1:B:662:ARG:NH1	1:B:666:GLU:OE2	2.51	0.43
1:C:264:THR:O	1:C:264:THR:OG1	2.33	0.43
1:D:348:THR:HG22	1:D:354:ILE:HG21	2.00	0.43
1:A:561:LEU:HB3	1:A:619:ASP:HB3	2.00	0.43
1:B:561:LEU:HB3	1:B:619:ASP:HB3	2.00	0.43
1:D:561:LEU:HB3	1:D:619:ASP:HB3	2.00	0.43
1:A:348:THR:HG22	1:A:354:ILE:HG21	2.00	0.43
1:B:262:ASP:OD2	1:B:277:ASN:ND2	2.51	0.43
1:B:288:LYS:NZ	1:B:666:GLU:OE1	2.40	0.43
3:B:1202:YZY:H221	6:B:1205:PT5:C47	2.49	0.43
1:A:356:PHE:CE2	4:A:1203:POV:H33A	2.54	0.43
1:C:262:ASP:OD2	1:C:277:ASN:ND2	2.51	0.43
1:C:769:GLU:HG2	1:D:1:MET:H3	1.80	0.43
1:D:262:ASP:OD2	1:D:277:ASN:ND2	2.51	0.43
1:B:519:LEU:HD21	1:C:538:PHE:CE2	2.53	0.43
1:C:356:PHE:CE2	4:C:1203:POV:H33A	2.54	0.43
3:C:1202:YZY:H221	6:C:1205:PT5:C47	2.49	0.43
1:D:307:GLY:HA3	1:D:351:LYS:HD3	2.00	0.43
1:B:356:PHE:CE2	4:B:1203:POV:H33A	2.54	0.43
1:B:538:PHE:CD1	6:B:1205:PT5:H72	2.52	0.43
3:A:1202:YZY:H221	6:A:1205:PT5:C47	2.49	0.42
1:C:348:THR:HG22	1:C:354:ILE:HG21	2.00	0.42
1:C:561:LEU:HB3	1:C:619:ASP:HB3	2.00	0.42
1:D:417:TRP:HZ3	1:D:688:PRO:CD	2.20	0.42
1:A:355:LYS:HE2	1:A:684:THR:HG23	2.02	0.42
1:C:519:LEU:HD21	1:D:538:PHE:CE2	2.54	0.42
1:D:355:LYS:HE2	1:D:684:THR:HG23	2.02	0.42
1:A:737:LYS:HB2	1:A:737:LYS:HE2	1.75	0.42
1:D:264:THR:O	1:D:264:THR:OG1	2.33	0.42
1:D:356:PHE:CE2	4:D:1203:POV:H33A	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1202:YZY:H221	6:D:1205:PT5:C47	2.49	0.42
1:B:374:SER:HB3	1:C:556:TRP:NE1	2.34	0.42
1:B:491:MET:HE2	1:B:491:MET:HB2	1.86	0.42
1:C:472:ILE:H	1:C:472:ILE:HG13	1.68	0.42
1:D:330:PHE:CD2	1:D:331:PRO:HD3	2.55	0.42
1:A:374:SER:HB3	1:B:556:TRP:NE1	2.34	0.42
1:D:538:PHE:CD1	6:D:1205:PT5:H72	2.52	0.42
1:A:662:ARG:NH1	1:A:666:GLU:OE2	2.51	0.42
1:B:348:THR:HG22	1:B:354:ILE:HG21	2.00	0.42
1:A:519:LEU:HD21	1:B:538:PHE:CE2	2.55	0.42
1:B:50:ASN:ND2	1:B:52:ASN:O	2.53	0.42
1:B:355:LYS:HE2	1:B:684:THR:HG23	2.01	0.42
1:C:355:LYS:HE2	1:C:684:THR:HG23	2.02	0.42
1:C:42:LYS:O	1:C:46:THR:N	2.51	0.42
1:C:374:SER:HB3	1:D:556:TRP:NE1	2.35	0.42
1:C:662:ARG:NH1	1:C:666:GLU:OE2	2.51	0.42
1:D:288:LYS:NZ	1:D:666:GLU:OE1	2.40	0.42
1:A:330:PHE:CD2	1:A:331:PRO:HD3	2.55	0.42
1:D:50:ASN:ND2	1:D:52:ASN:O	2.53	0.42
1:A:538:PHE:CE2	1:D:519:LEU:HD21	2.54	0.41
1:D:42:LYS:O	1:D:46:THR:N	2.51	0.41
1:D:662:ARG:NH1	1:D:666:GLU:OE2	2.51	0.41
1:A:556:TRP:NE1	1:D:374:SER:HB3	2.35	0.41
1:B:330:PHE:CD2	1:B:331:PRO:HD3	2.55	0.41
5:B:1204:Y01:HAC3	5:B:1204:Y01:HAJ1	1.82	0.41
1:C:623:ILE:HD12	1:C:623:ILE:HA	1.87	0.41
1:C:50:ASN:ND2	1:C:52:ASN:O	2.53	0.41
1:C:330:PHE:CD2	1:C:331:PRO:HD3	2.55	0.41
1:B:737:LYS:HB2	1:B:737:LYS:HE2	1.75	0.41
1:A:1:MET:H3	1:D:769:GLU:HG2	1.82	0.41
1:D:623:ILE:HD12	1:D:623:ILE:HA	1.87	0.41
1:A:558:TYR:CE2	1:A:625:THR:HG21	2.56	0.41
1:B:350:ARG:NE	1:B:681:GLU:OE2	2.54	0.41
1:B:503:ILE:HG13	1:C:550:GLY:HA3	2.03	0.41
1:C:491:MET:HE2	1:C:491:MET:HB2	1.86	0.41
1:A:50:ASN:ND2	1:A:52:ASN:O	2.53	0.41
1:A:350:ARG:NE	1:A:681:GLU:OE2	2.54	0.41
1:B:558:TYR:CE2	1:B:625:THR:HG21	2.56	0.41
1:C:312:ARG:H	1:C:312:ARG:HG3	1.73	0.41
4:C:1203:POV:H21B	4:C:1203:POV:H215	1.91	0.41
1:B:42:LYS:O	1:B:46:THR:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:558:TYR:CE2	1:C:625:THR:HG21	2.56	0.40
1:C:350:ARG:NE	1:C:681:GLU:OE2	2.54	0.40
1:D:566:CYS:HA	1:D:567:PRO:HD3	1.97	0.40
1:A:503:ILE:HG13	1:B:550:GLY:HA3	2.04	0.40
4:D:1203:POV:H21B	4:D:1203:POV:H215	1.91	0.40
1:B:417:TRP:HZ3	1:B:688:PRO:CD	2.20	0.40
1:C:288:LYS:NZ	1:C:666:GLU:OE1	2.40	0.40
1:D:350:ARG:NE	1:D:681:GLU:OE2	2.54	0.40
1:D:558:TYR:CE2	1:D:625:THR:HG21	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	695/1128 (62%)	683 (98%)	12 (2%)	0	100	100
1	B	695/1128 (62%)	683 (98%)	12 (2%)	0	100	100
1	C	695/1128 (62%)	683 (98%)	12 (2%)	0	100	100
1	D	695/1128 (62%)	683 (98%)	12 (2%)	0	100	100
All	All	2780/4512 (62%)	2732 (98%)	48 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	634/985 (64%)	634 (100%)	0	100	100
1	B	634/985 (64%)	634 (100%)	0	100	100
1	C	634/985 (64%)	634 (100%)	0	100	100
1	D	634/985 (64%)	634 (100%)	0	100	100
All	All	2536/3940 (64%)	2536 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	502	ASN
1	A	516	ASN
1	A	523	GLN
1	A	552	ASN
1	A	653	ASN
1	B	50	ASN
1	B	502	ASN
1	B	516	ASN
1	B	552	ASN
1	B	653	ASN
1	B	690	ASN
1	C	50	ASN
1	C	502	ASN
1	C	516	ASN
1	C	552	ASN
1	C	653	ASN
1	D	502	ASN
1	D	516	ASN
1	D	523	GLN
1	D	552	ASN
1	D	653	ASN
1	D	690	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	PT5	C	1205	-	69,69,69	1.21	6 (8%)	83,87,87	1.21	6 (7%)
5	Y01	B	1204	-	38,38,38	0.54	0	57,57,57	1.16	4 (7%)
3	YZY	A	1202	-	34,34,41	0.93	4 (11%)	36,36,43	1.26	2 (5%)
6	PT5	D	1205	-	69,69,69	1.21	6 (8%)	83,87,87	1.21	6 (7%)
4	POV	A	1203	-	51,51,51	0.50	0	57,59,59	0.46	0
5	Y01	C	1204	-	38,38,38	0.54	0	57,57,57	1.16	4 (7%)
5	Y01	D	1204	-	38,38,38	0.54	0	57,57,57	1.16	4 (7%)
4	POV	C	1203	-	51,51,51	0.49	0	57,59,59	0.46	0
4	POV	B	1203	-	51,51,51	0.50	0	57,59,59	0.46	0
5	Y01	A	1204	-	38,38,38	0.54	0	57,57,57	1.16	4 (7%)
6	PT5	B	1205	-	69,69,69	1.21	6 (8%)	83,87,87	1.21	6 (7%)
6	PT5	A	1205	-	69,69,69	1.21	6 (8%)	83,87,87	1.21	6 (7%)
3	YZY	D	1202	-	34,34,41	0.94	4 (11%)	36,36,43	1.27	2 (5%)
3	YZY	B	1202	-	34,34,41	0.93	4 (11%)	36,36,43	1.26	2 (5%)
3	YZY	C	1202	-	34,34,41	0.93	4 (11%)	36,36,43	1.26	2 (5%)
4	POV	D	1203	-	51,51,51	0.50	0	57,59,59	0.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PT5	C	1205	-	-	36/66/90/90	0/1/1/1
5	Y01	B	1204	-	-	5/19/77/77	0/4/4/4
3	YZY	A	1202	-	-	19/36/36/43	-
6	PT5	D	1205	-	-	36/66/90/90	0/1/1/1
4	POV	A	1203	-	-	22/55/55/55	-
5	Y01	C	1204	-	-	5/19/77/77	0/4/4/4
5	Y01	D	1204	-	-	5/19/77/77	0/4/4/4
4	POV	C	1203	-	-	22/55/55/55	-
4	POV	B	1203	-	-	22/55/55/55	-
5	Y01	A	1204	-	-	5/19/77/77	0/4/4/4
6	PT5	B	1205	-	-	36/66/90/90	0/1/1/1
6	PT5	A	1205	-	-	36/66/90/90	0/1/1/1
3	YZY	D	1202	-	-	19/36/36/43	-
3	YZY	B	1202	-	-	19/36/36/43	-
3	YZY	C	1202	-	-	19/36/36/43	-
4	POV	D	1203	-	-	22/55/55/55	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1205	PT5	P5-O5	4.34	1.67	1.59
6	D	1205	PT5	P5-O5	4.34	1.67	1.59
6	B	1205	PT5	P5-O5	4.32	1.67	1.59
6	C	1205	PT5	P5-O5	4.32	1.67	1.59
6	A	1205	PT5	P4-O4	3.80	1.66	1.59
6	B	1205	PT5	P4-O4	3.80	1.66	1.59
6	C	1205	PT5	P4-O4	3.80	1.66	1.59
6	D	1205	PT5	P4-O4	3.80	1.66	1.59
6	D	1205	PT5	O18-C11	2.84	1.41	1.33
6	A	1205	PT5	O18-C11	2.84	1.41	1.33
6	C	1205	PT5	O18-C11	2.84	1.41	1.33
6	B	1205	PT5	O18-C11	2.83	1.41	1.33
6	A	1205	PT5	O16-C10	2.65	1.41	1.34
6	B	1205	PT5	O16-C10	2.65	1.41	1.34
6	C	1205	PT5	O16-C10	2.65	1.41	1.34
6	D	1205	PT5	O16-C10	2.65	1.41	1.34
6	A	1205	PT5	O16-C8	-2.48	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1205	PT5	O16-C8	-2.48	1.40	1.46
6	C	1205	PT5	O16-C8	-2.48	1.40	1.46
6	D	1205	PT5	O16-C8	-2.48	1.40	1.46
6	A	1205	PT5	P1-O1	2.44	1.66	1.60
6	B	1205	PT5	P1-O1	2.44	1.66	1.60
6	C	1205	PT5	P1-O1	2.44	1.66	1.60
6	D	1205	PT5	P1-O1	2.44	1.66	1.60
3	A	1202	YZY	O4-C20	2.41	1.40	1.33
3	B	1202	YZY	O4-C20	2.41	1.40	1.33
3	C	1202	YZY	O4-C20	2.41	1.40	1.33
3	D	1202	YZY	O4-C20	2.41	1.40	1.33
3	D	1202	YZY	O2-C3	2.37	1.41	1.34
3	A	1202	YZY	O2-C3	2.34	1.40	1.34
3	B	1202	YZY	O2-C3	2.34	1.40	1.34
3	C	1202	YZY	O2-C3	2.34	1.40	1.34
3	D	1202	YZY	O2-C2	-2.13	1.41	1.46
3	A	1202	YZY	O2-C2	-2.11	1.41	1.46
3	C	1202	YZY	O2-C2	-2.11	1.41	1.46
3	C	1202	YZY	O4-C19	-2.09	1.40	1.45
3	B	1202	YZY	O2-C2	-2.08	1.41	1.46
3	A	1202	YZY	O4-C19	-2.07	1.40	1.45
3	B	1202	YZY	O4-C19	-2.07	1.40	1.45
3	D	1202	YZY	O4-C19	-2.07	1.40	1.45

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1204	Y01	CBC-CAV-CAZ	5.14	119.51	111.52
5	A	1204	Y01	CBC-CAV-CAZ	5.13	119.49	111.52
5	D	1204	Y01	CBC-CAV-CAZ	5.13	119.49	111.52
5	B	1204	Y01	CBC-CAV-CAZ	5.12	119.48	111.52
6	D	1205	PT5	C21-C20-C19	5.00	136.63	112.02
6	A	1205	PT5	C21-C20-C19	4.99	136.60	112.02
6	C	1205	PT5	C21-C20-C19	4.99	136.60	112.02
6	B	1205	PT5	C21-C20-C19	4.99	136.58	112.02
3	A	1202	YZY	O2-C3-C4	4.41	121.01	111.50
3	B	1202	YZY	O2-C3-C4	4.41	121.01	111.50
3	C	1202	YZY	O2-C3-C4	4.41	121.01	111.50
3	D	1202	YZY	O2-C3-C4	4.41	121.00	111.50
6	A	1205	PT5	O16-C10-C12	3.98	120.08	111.50
6	B	1205	PT5	O16-C10-C12	3.98	120.08	111.50
6	C	1205	PT5	O16-C10-C12	3.98	120.08	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	1205	PT5	O16-C10-C12	3.98	120.08	111.50
6	A	1205	PT5	C20-C19-C18	3.51	153.23	123.57
6	B	1205	PT5	C20-C19-C18	3.51	153.23	123.57
6	C	1205	PT5	C20-C19-C18	3.51	153.23	123.57
6	D	1205	PT5	C20-C19-C18	3.51	153.17	123.57
6	C	1205	PT5	C17-C16-C15	3.45	152.71	123.57
6	D	1205	PT5	C17-C16-C15	3.45	152.66	123.57
6	A	1205	PT5	C17-C16-C15	3.45	152.66	123.57
6	B	1205	PT5	C17-C16-C15	3.44	152.64	123.57
6	D	1205	PT5	C23-C22-C21	3.44	152.57	123.57
6	A	1205	PT5	C23-C22-C21	3.43	152.53	123.57
6	B	1205	PT5	C23-C22-C21	3.43	152.53	123.57
6	C	1205	PT5	C23-C22-C21	3.43	152.53	123.57
5	B	1204	Y01	CAR-CBC-CAV	3.35	115.98	110.99
5	A	1204	Y01	CAR-CBC-CAV	3.34	115.96	110.99
5	D	1204	Y01	CAR-CBC-CAV	3.34	115.96	110.99
5	C	1204	Y01	CAR-CBC-CAV	3.32	115.94	110.99
5	A	1204	Y01	CAV-CAZ-CBH	2.94	120.33	116.42
5	D	1204	Y01	CAV-CAZ-CBH	2.94	120.33	116.42
5	B	1204	Y01	CAV-CAZ-CBH	2.93	120.32	116.42
5	C	1204	Y01	CAV-CAZ-CBH	2.93	120.31	116.42
6	B	1205	PT5	O18-C11-C31	2.66	120.24	111.91
6	A	1205	PT5	O18-C11-C31	2.65	120.24	111.91
6	C	1205	PT5	O18-C11-C31	2.65	120.24	111.91
6	D	1205	PT5	O18-C11-C31	2.64	120.20	111.91
3	A	1202	YZY	O4-C20-C21	2.58	119.99	111.91
3	B	1202	YZY	O4-C20-C21	2.58	119.99	111.91
3	C	1202	YZY	O4-C20-C21	2.58	119.99	111.91
3	D	1202	YZY	O4-C20-C21	2.58	119.99	111.91
5	C	1204	Y01	CAV-CAZ-CAI	-2.05	117.66	120.61
5	A	1204	Y01	CAV-CAZ-CAI	-2.04	117.66	120.61
5	B	1204	Y01	CAV-CAZ-CAI	-2.04	117.66	120.61
5	D	1204	Y01	CAV-CAZ-CAI	-2.04	117.66	120.61

There are no chirality outliers.

All (328) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1202	YZY	O1-C1-C2-O2
3	A	1202	YZY	O1-C1-C2-C19
3	A	1202	YZY	C19-C2-O2-C3
3	A	1202	YZY	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
3	B	1202	YZY	O1-C1-C2-O2
3	B	1202	YZY	O1-C1-C2-C19
3	B	1202	YZY	C19-C2-O2-C3
3	B	1202	YZY	C4-C3-O2-C2
3	C	1202	YZY	O1-C1-C2-O2
3	C	1202	YZY	O1-C1-C2-C19
3	C	1202	YZY	C19-C2-O2-C3
3	C	1202	YZY	C4-C3-O2-C2
3	D	1202	YZY	O1-C1-C2-O2
3	D	1202	YZY	O1-C1-C2-C19
3	D	1202	YZY	C19-C2-O2-C3
3	D	1202	YZY	C4-C3-O2-C2
4	A	1203	POV	C1-O11-P-O12
4	A	1203	POV	C1-O11-P-O14
4	A	1203	POV	C11-O12-P-O13
4	A	1203	POV	C2-C1-O11-P
4	A	1203	POV	O12-C11-C12-N
4	A	1203	POV	C12-C11-O12-P
4	B	1203	POV	C1-O11-P-O12
4	B	1203	POV	C1-O11-P-O14
4	B	1203	POV	C11-O12-P-O13
4	B	1203	POV	C2-C1-O11-P
4	B	1203	POV	O12-C11-C12-N
4	B	1203	POV	C12-C11-O12-P
4	C	1203	POV	C1-O11-P-O12
4	C	1203	POV	C1-O11-P-O14
4	C	1203	POV	C11-O12-P-O13
4	C	1203	POV	C2-C1-O11-P
4	C	1203	POV	O12-C11-C12-N
4	C	1203	POV	C12-C11-O12-P
4	D	1203	POV	C1-O11-P-O12
4	D	1203	POV	C1-O11-P-O14
4	D	1203	POV	C11-O12-P-O13
4	D	1203	POV	C2-C1-O11-P
4	D	1203	POV	O12-C11-C12-N
4	D	1203	POV	C12-C11-O12-P
5	A	1204	Y01	CAR-CBC-OAW-CAY
5	B	1204	Y01	CAR-CBC-OAW-CAY
5	C	1204	Y01	CAR-CBC-OAW-CAY
5	D	1204	Y01	CAR-CBC-OAW-CAY
6	A	1205	PT5	C7-O13-P1-O12
6	A	1205	PT5	C7-O13-P1-O11

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Mol	Chain	Res	Type	Atoms
6	A	1205	PT5	C1-O1-P1-O12
6	A	1205	PT5	C6-C5-O5-P5
6	A	1205	PT5	C5-O5-P5-O53
6	A	1205	PT5	O17-C10-O16-C8
6	A	1205	PT5	C19-C20-C21-C22
6	B	1205	PT5	C7-O13-P1-O12
6	B	1205	PT5	C7-O13-P1-O11
6	B	1205	PT5	C1-O1-P1-O12
6	B	1205	PT5	C6-C5-O5-P5
6	B	1205	PT5	C5-O5-P5-O53
6	B	1205	PT5	O17-C10-O16-C8
6	B	1205	PT5	C19-C20-C21-C22
6	C	1205	PT5	C7-O13-P1-O12
6	C	1205	PT5	C7-O13-P1-O11
6	C	1205	PT5	C1-O1-P1-O12
6	C	1205	PT5	C6-C5-O5-P5
6	C	1205	PT5	C5-O5-P5-O53
6	C	1205	PT5	O17-C10-O16-C8
6	C	1205	PT5	C19-C20-C21-C22
6	D	1205	PT5	C7-O13-P1-O12
6	D	1205	PT5	C7-O13-P1-O11
6	D	1205	PT5	C1-O1-P1-O12
6	D	1205	PT5	C6-C5-O5-P5
6	D	1205	PT5	C5-O5-P5-O53
6	D	1205	PT5	O17-C10-O16-C8
6	D	1205	PT5	C19-C20-C21-C22
3	A	1202	YZY	O5-C20-O4-C19
3	B	1202	YZY	O5-C20-O4-C19
3	C	1202	YZY	O5-C20-O4-C19
3	D	1202	YZY	O5-C20-O4-C19
3	A	1202	YZY	C21-C20-O4-C19
3	B	1202	YZY	C21-C20-O4-C19
3	C	1202	YZY	C21-C20-O4-C19
3	D	1202	YZY	C21-C20-O4-C19
3	A	1202	YZY	O3-C3-O2-C2
3	B	1202	YZY	O3-C3-O2-C2
3	C	1202	YZY	O3-C3-O2-C2
3	D	1202	YZY	O3-C3-O2-C2
6	A	1205	PT5	C12-C10-O16-C8
6	B	1205	PT5	C12-C10-O16-C8
6	C	1205	PT5	C12-C10-O16-C8
6	D	1205	PT5	C12-C10-O16-C8

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Mol	Chain	Res	Type	Atoms
5	A	1204	Y01	CAM-CAY-OAW-CBC
5	B	1204	Y01	CAM-CAY-OAW-CBC
5	C	1204	Y01	CAM-CAY-OAW-CBC
5	D	1204	Y01	CAM-CAY-OAW-CBC
4	A	1203	POV	C11-O12-P-O11
4	B	1203	POV	C11-O12-P-O11
4	C	1203	POV	C11-O12-P-O11
4	D	1203	POV	C11-O12-P-O11
6	A	1205	PT5	C7-O13-P1-O1
6	B	1205	PT5	C7-O13-P1-O1
6	C	1205	PT5	C7-O13-P1-O1
6	D	1205	PT5	C7-O13-P1-O1
5	A	1204	Y01	OAG-CAY-OAW-CBC
5	B	1204	Y01	OAG-CAY-OAW-CBC
5	C	1204	Y01	OAG-CAY-OAW-CBC
5	D	1204	Y01	OAG-CAY-OAW-CBC
6	A	1205	PT5	C40-C41-C42-C43
6	B	1205	PT5	C40-C41-C42-C43
6	C	1205	PT5	C40-C41-C42-C43
6	D	1205	PT5	C40-C41-C42-C43
4	A	1203	POV	C36-C37-C38-C39
4	B	1203	POV	C36-C37-C38-C39
4	C	1203	POV	C36-C37-C38-C39
4	D	1203	POV	C36-C37-C38-C39
6	A	1205	PT5	C1-O1-P1-O13
6	B	1205	PT5	C1-O1-P1-O13
6	C	1205	PT5	C1-O1-P1-O13
6	D	1205	PT5	C1-O1-P1-O13
3	A	1202	YZY	C7-C8-C9-C10
3	B	1202	YZY	C7-C8-C9-C10
3	C	1202	YZY	C7-C8-C9-C10
3	D	1202	YZY	C7-C8-C9-C10
6	A	1205	PT5	C42-C43-C44-C45
6	B	1205	PT5	C42-C43-C44-C45
6	C	1205	PT5	C42-C43-C44-C45
6	D	1205	PT5	C42-C43-C44-C45
6	A	1205	PT5	C35-C36-C37-C38
6	B	1205	PT5	C35-C36-C37-C38
6	C	1205	PT5	C35-C36-C37-C38
6	D	1205	PT5	C35-C36-C37-C38
6	A	1205	PT5	C32-C33-C34-C35
6	B	1205	PT5	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
6	C	1205	PT5	C32-C33-C34-C35
6	D	1205	PT5	C32-C33-C34-C35
6	A	1205	PT5	C41-C42-C43-C44
6	B	1205	PT5	C41-C42-C43-C44
6	C	1205	PT5	C41-C42-C43-C44
6	D	1205	PT5	C41-C42-C43-C44
4	A	1203	POV	C39-C310-C311-C312
4	B	1203	POV	C39-C310-C311-C312
4	C	1203	POV	C39-C310-C311-C312
4	D	1203	POV	C39-C310-C311-C312
6	A	1205	PT5	C37-C38-C39-C40
6	B	1205	PT5	C37-C38-C39-C40
6	C	1205	PT5	C37-C38-C39-C40
6	D	1205	PT5	C37-C38-C39-C40
3	A	1202	YZY	C9-C10-C11-C12
3	B	1202	YZY	C9-C10-C11-C12
3	C	1202	YZY	C9-C10-C11-C12
6	A	1205	PT5	C31-C32-C33-C34
6	B	1205	PT5	C31-C32-C33-C34
6	C	1205	PT5	C31-C32-C33-C34
6	D	1205	PT5	C31-C32-C33-C34
3	D	1202	YZY	C9-C10-C11-C12
6	A	1205	PT5	C43-C44-C45-C46
6	B	1205	PT5	C43-C44-C45-C46
6	C	1205	PT5	C43-C44-C45-C46
6	D	1205	PT5	C43-C44-C45-C46
4	A	1203	POV	C210-C211-C212-C213
4	B	1203	POV	C210-C211-C212-C213
4	C	1203	POV	C210-C211-C212-C213
4	D	1203	POV	C210-C211-C212-C213
3	A	1202	YZY	C3-C4-C5-C6
3	B	1202	YZY	C3-C4-C5-C6
3	C	1202	YZY	C3-C4-C5-C6
3	D	1202	YZY	C3-C4-C5-C6
4	A	1203	POV	C212-C213-C214-C215
4	D	1203	POV	C212-C213-C214-C215
4	C	1203	POV	C212-C213-C214-C215
4	B	1203	POV	C212-C213-C214-C215
3	A	1202	YZY	C20-C21-C22-C23
3	B	1202	YZY	C20-C21-C22-C23
3	C	1202	YZY	C20-C21-C22-C23
3	D	1202	YZY	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
3	A	1202	YZY	C21-C22-C23-C24
3	B	1202	YZY	C21-C22-C23-C24
3	C	1202	YZY	C21-C22-C23-C24
3	D	1202	YZY	C21-C22-C23-C24
4	A	1203	POV	C31-C32-C33-C34
4	B	1203	POV	C31-C32-C33-C34
4	C	1203	POV	C31-C32-C33-C34
4	D	1203	POV	C31-C32-C33-C34
6	A	1205	PT5	C13-C14-C15-C16
6	B	1205	PT5	C13-C14-C15-C16
6	C	1205	PT5	C13-C14-C15-C16
6	D	1205	PT5	C13-C14-C15-C16
3	A	1202	YZY	O4-C19-C2-C1
3	B	1202	YZY	O4-C19-C2-C1
3	C	1202	YZY	O4-C19-C2-C1
3	D	1202	YZY	O4-C19-C2-C1
6	A	1205	PT5	C7-C8-C9-O18
6	B	1205	PT5	C7-C8-C9-O18
6	C	1205	PT5	C7-C8-C9-O18
6	D	1205	PT5	C7-C8-C9-O18
3	A	1202	YZY	C25-C26-C27-C28
3	B	1202	YZY	C25-C26-C27-C28
3	C	1202	YZY	C25-C26-C27-C28
3	D	1202	YZY	C25-C26-C27-C28
6	A	1205	PT5	C31-C11-O18-C9
6	B	1205	PT5	C31-C11-O18-C9
6	C	1205	PT5	C31-C11-O18-C9
6	D	1205	PT5	C31-C11-O18-C9
3	A	1202	YZY	C22-C23-C24-C25
3	B	1202	YZY	C22-C23-C24-C25
3	C	1202	YZY	C22-C23-C24-C25
3	D	1202	YZY	C22-C23-C24-C25
4	A	1203	POV	C32-C33-C34-C35
4	B	1203	POV	C32-C33-C34-C35
4	C	1203	POV	C32-C33-C34-C35
4	D	1203	POV	C32-C33-C34-C35
6	A	1205	PT5	C27-C28-C29-C30
6	B	1205	PT5	C27-C28-C29-C30
6	C	1205	PT5	C27-C28-C29-C30
6	D	1205	PT5	C27-C28-C29-C30
6	A	1205	PT5	C1-O1-P1-O11
6	B	1205	PT5	C1-O1-P1-O11

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Mol	Chain	Res	Type	Atoms
6	C	1205	PT5	C1-O1-P1-O11
6	D	1205	PT5	C1-O1-P1-O11
6	A	1205	PT5	C21-C22-C23-C24
6	B	1205	PT5	C21-C22-C23-C24
6	C	1205	PT5	C21-C22-C23-C24
6	D	1205	PT5	C21-C22-C23-C24
6	A	1205	PT5	C39-C40-C41-C42
6	B	1205	PT5	C39-C40-C41-C42
6	C	1205	PT5	C39-C40-C41-C42
6	D	1205	PT5	C39-C40-C41-C42
3	A	1202	YZY	C10-C11-C12-C13
3	B	1202	YZY	C10-C11-C12-C13
3	C	1202	YZY	C10-C11-C12-C13
3	D	1202	YZY	C10-C11-C12-C13
6	A	1205	PT5	O19-C11-O18-C9
6	B	1205	PT5	O19-C11-O18-C9
6	C	1205	PT5	O19-C11-O18-C9
6	D	1205	PT5	O19-C11-O18-C9
6	A	1205	PT5	C12-C13-C14-C15
6	B	1205	PT5	C12-C13-C14-C15
6	C	1205	PT5	C12-C13-C14-C15
6	D	1205	PT5	C12-C13-C14-C15
4	A	1203	POV	O11-C1-C2-C3
4	B	1203	POV	O11-C1-C2-C3
4	C	1203	POV	O11-C1-C2-C3
4	D	1203	POV	O11-C1-C2-C3
3	A	1202	YZY	O4-C19-C2-O2
3	B	1202	YZY	O4-C19-C2-O2
3	C	1202	YZY	O4-C19-C2-O2
3	D	1202	YZY	O4-C19-C2-O2
6	A	1205	PT5	O16-C8-C9-O18
6	B	1205	PT5	O16-C8-C9-O18
6	C	1205	PT5	O16-C8-C9-O18
6	D	1205	PT5	O16-C8-C9-O18
3	C	1202	YZY	C14-C15-C16-C17
3	A	1202	YZY	C14-C15-C16-C17
3	B	1202	YZY	C14-C15-C16-C17
3	D	1202	YZY	C14-C15-C16-C17
4	C	1203	POV	C25-C26-C27-C28
4	D	1203	POV	C25-C26-C27-C28
4	A	1203	POV	C25-C26-C27-C28
4	B	1203	POV	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
6	A	1205	PT5	C11-C31-C32-C33
6	B	1205	PT5	C11-C31-C32-C33
6	C	1205	PT5	C11-C31-C32-C33
6	D	1205	PT5	C11-C31-C32-C33
4	A	1203	POV	C37-C38-C39-C310
4	B	1203	POV	C37-C38-C39-C310
4	C	1203	POV	C37-C38-C39-C310
4	D	1203	POV	C37-C38-C39-C310
4	D	1203	POV	C311-C310-C39-C38
4	A	1203	POV	C311-C310-C39-C38
4	B	1203	POV	C311-C310-C39-C38
4	C	1203	POV	C311-C310-C39-C38
3	B	1202	YZY	C23-C24-C25-C26
3	A	1202	YZY	C23-C24-C25-C26
3	C	1202	YZY	C23-C24-C25-C26
3	D	1202	YZY	C23-C24-C25-C26
4	A	1203	POV	O11-C1-C2-O21
4	B	1203	POV	O11-C1-C2-O21
4	C	1203	POV	O11-C1-C2-O21
4	D	1203	POV	O11-C1-C2-O21
6	D	1205	PT5	C26-C27-C28-C29
6	A	1205	PT5	C26-C27-C28-C29
6	B	1205	PT5	C26-C27-C28-C29
6	C	1205	PT5	C26-C27-C28-C29
6	A	1205	PT5	C7-C8-O16-C10
6	B	1205	PT5	C7-C8-O16-C10
6	C	1205	PT5	C7-C8-O16-C10
6	D	1205	PT5	C7-C8-O16-C10
4	D	1203	POV	C34-C35-C36-C37
4	B	1203	POV	C34-C35-C36-C37
4	C	1203	POV	C34-C35-C36-C37
4	A	1203	POV	C34-C35-C36-C37
6	A	1205	PT5	C10-C12-C13-C14
6	B	1205	PT5	C10-C12-C13-C14
6	C	1205	PT5	C10-C12-C13-C14
6	D	1205	PT5	C10-C12-C13-C14
4	C	1203	POV	C310-C311-C312-C313
4	A	1203	POV	C310-C311-C312-C313
4	B	1203	POV	C310-C311-C312-C313
4	D	1203	POV	C310-C311-C312-C313
6	C	1205	PT5	C36-C37-C38-C39
6	A	1205	PT5	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
6	B	1205	PT5	C36-C37-C38-C39
6	D	1205	PT5	C36-C37-C38-C39
6	B	1205	PT5	C33-C34-C35-C36
6	A	1205	PT5	C33-C34-C35-C36
6	C	1205	PT5	C33-C34-C35-C36
6	D	1205	PT5	C33-C34-C35-C36
6	A	1205	PT5	C9-C8-O16-C10
6	B	1205	PT5	C9-C8-O16-C10
6	C	1205	PT5	C9-C8-O16-C10
6	D	1205	PT5	C9-C8-O16-C10
4	A	1203	POV	C214-C215-C216-C217
4	B	1203	POV	C214-C215-C216-C217
4	C	1203	POV	C214-C215-C216-C217
4	D	1203	POV	C214-C215-C216-C217
6	A	1205	PT5	C24-C25-C26-C27
6	B	1205	PT5	C24-C25-C26-C27
6	C	1205	PT5	C24-C25-C26-C27
6	D	1205	PT5	C24-C25-C26-C27
4	D	1203	POV	C21-C22-C23-C24
4	A	1203	POV	C21-C22-C23-C24
4	B	1203	POV	C21-C22-C23-C24
4	C	1203	POV	C21-C22-C23-C24
5	A	1204	Y01	CAL-CAM-CAY-OAW
5	C	1204	Y01	CAL-CAM-CAY-OAW
5	D	1204	Y01	CAL-CAM-CAY-OAW
5	B	1204	Y01	CAL-CAM-CAY-OAW
5	A	1204	Y01	CAL-CAM-CAY-OAG
5	C	1204	Y01	CAL-CAM-CAY-OAG
5	B	1204	Y01	CAL-CAM-CAY-OAG
5	D	1204	Y01	CAL-CAM-CAY-OAG

There are no ring outliers.

16 monomers are involved in 111 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1205	PT5	13	0
5	B	1204	Y01	11	0
3	A	1202	YZY	11	0
6	D	1205	PT5	13	0
4	A	1203	POV	2	0
5	C	1204	Y01	10	0
5	D	1204	Y01	11	0

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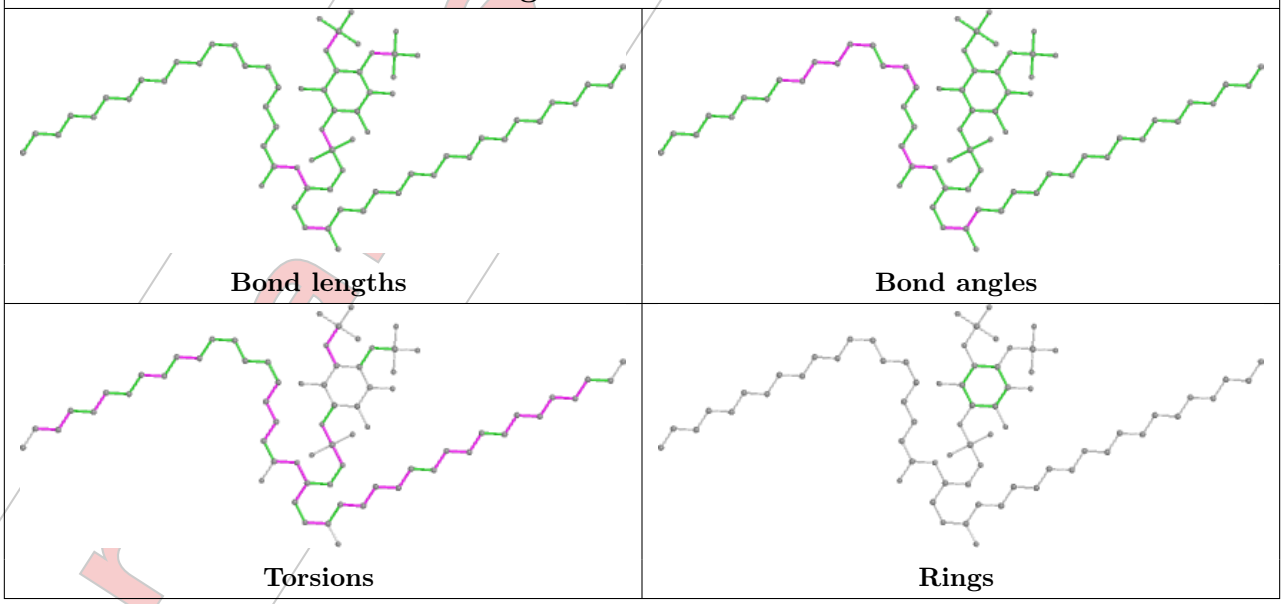
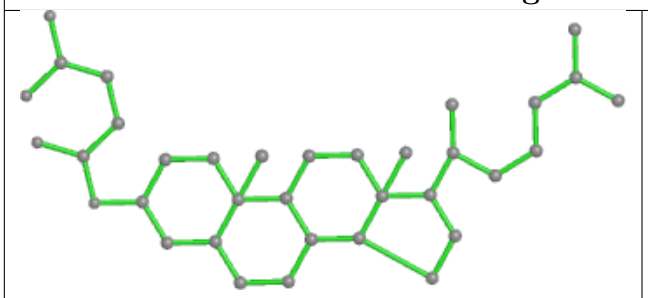
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1203	POV	3	0
4	B	1203	POV	2	0
5	A	1204	Y01	10	0
6	B	1205	PT5	13	0
6	A	1205	PT5	12	0
3	D	1202	YZY	11	0
3	B	1202	YZY	11	0
3	C	1202	YZY	11	0
4	D	1203	POV	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

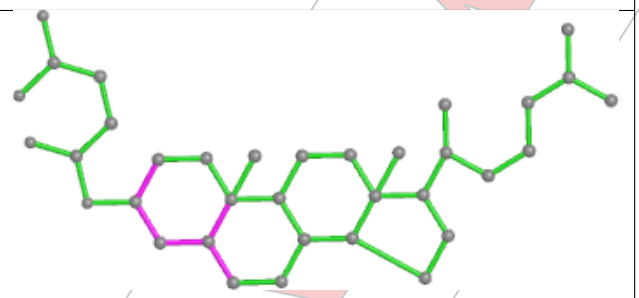
Ligand PT5 C 1205



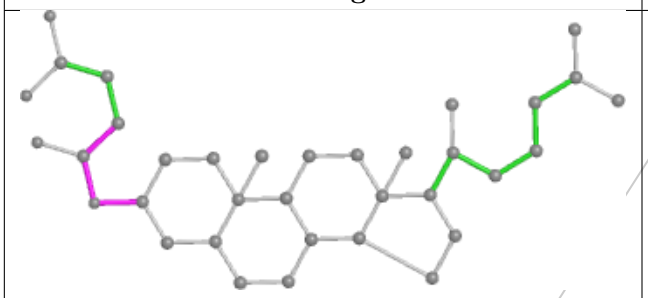
Ligand Y01 B 1204



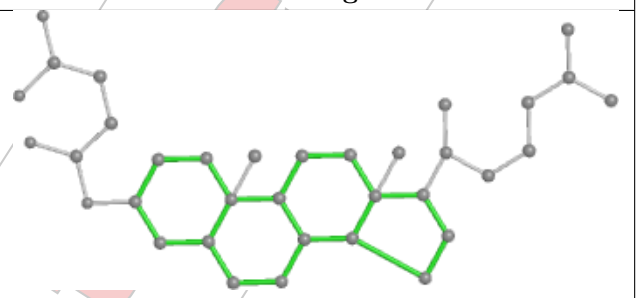
Bond lengths



Bond angles

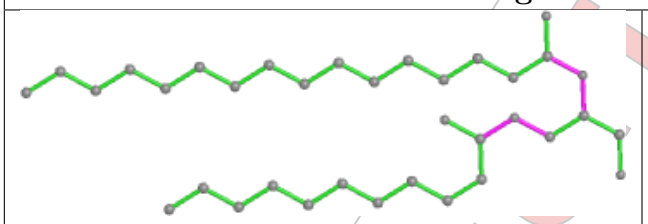


Torsions

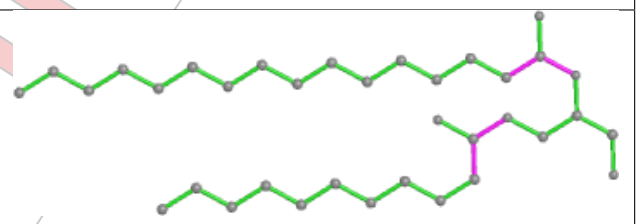


Rings

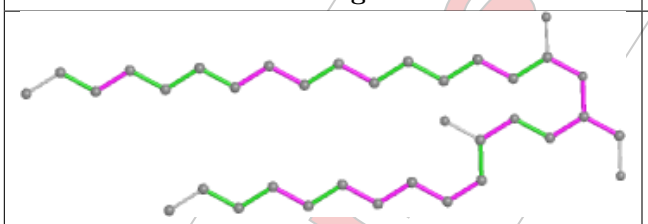
Ligand YZY A 1202



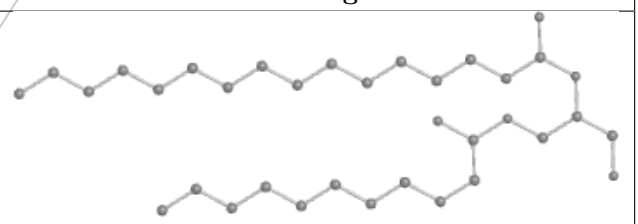
Bond lengths



Bond angles

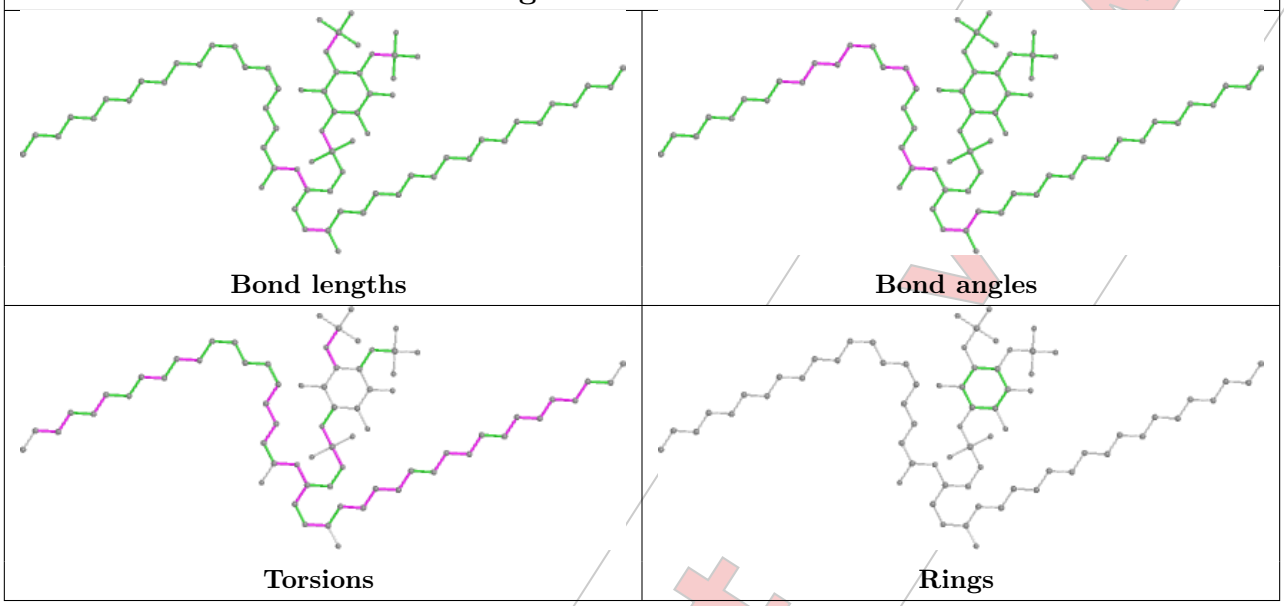


Torsions

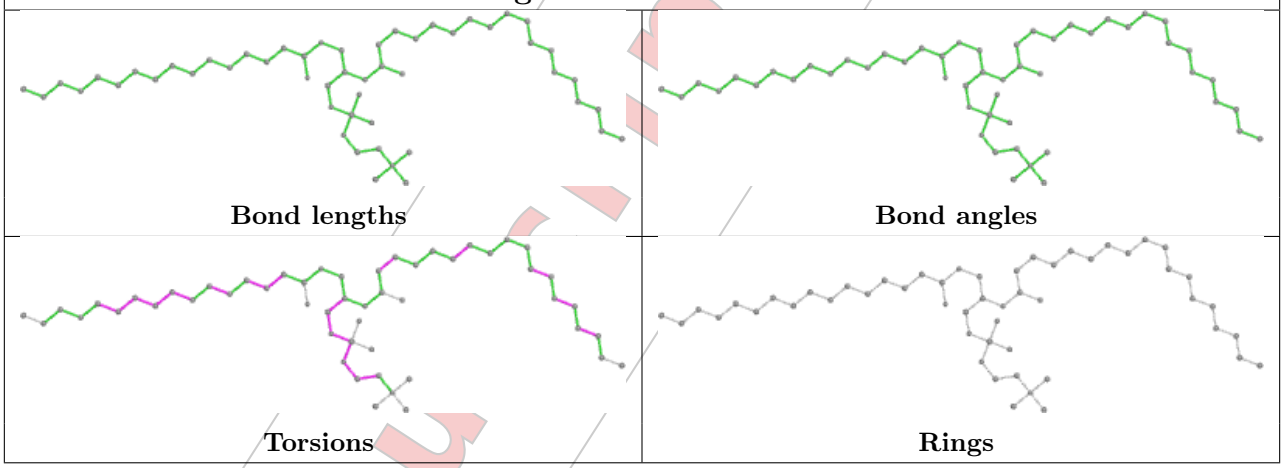


Rings

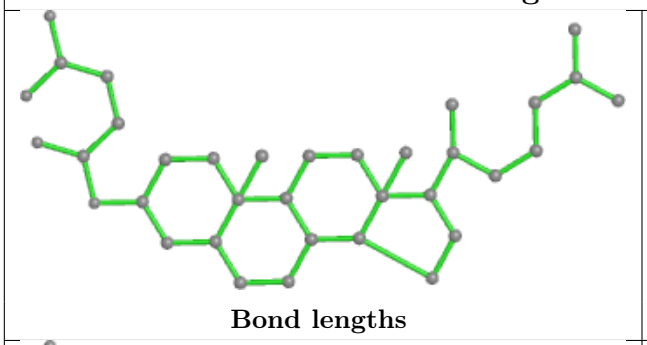
Ligand PT5 D 1205



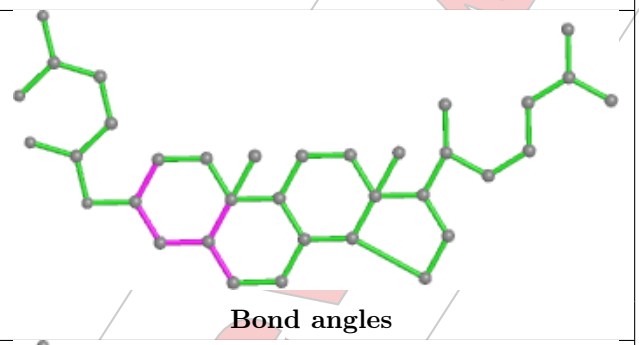
Ligand POV A 1203



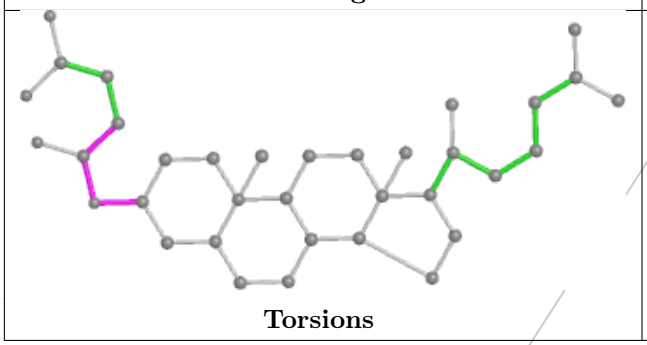
Ligand Y01 C 1204



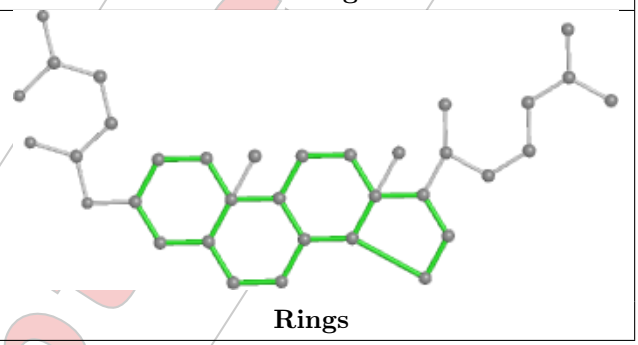
Bond lengths



Bond angles

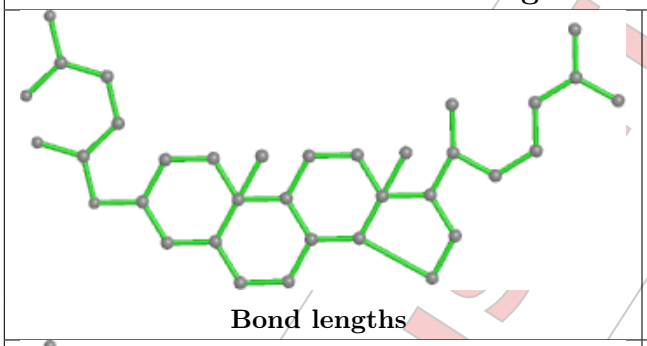


Torsions

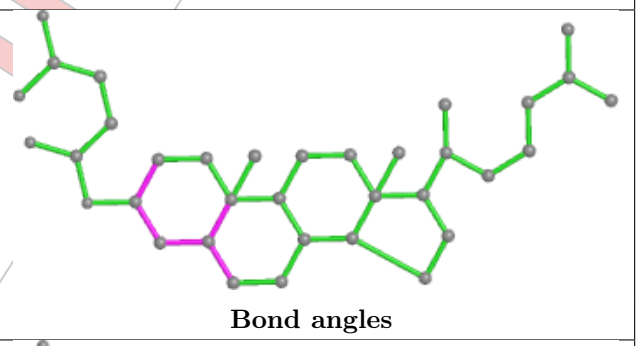


Rings

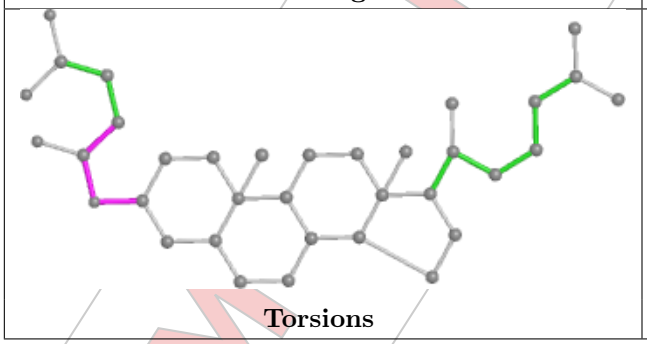
Ligand Y01 D 1204



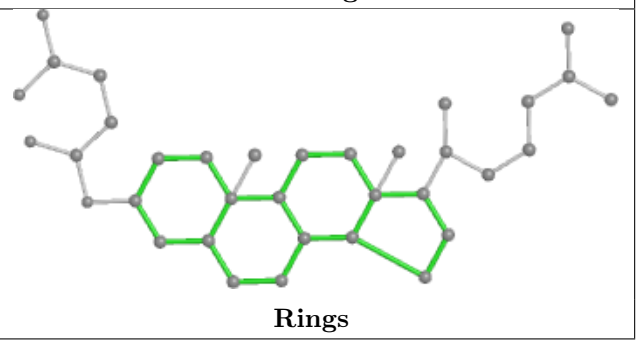
Bond lengths



Bond angles

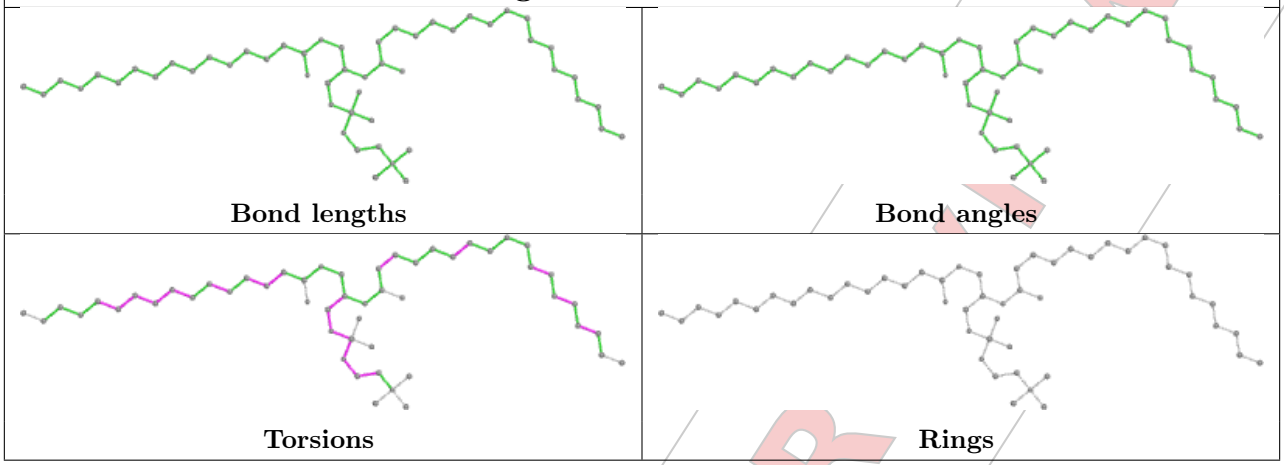


Torsions

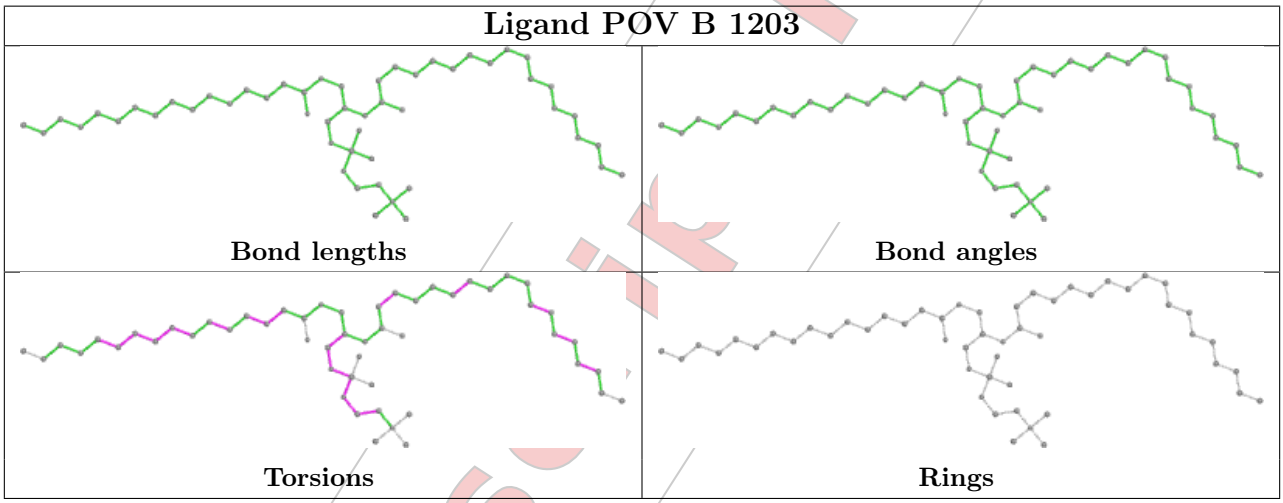


Rings

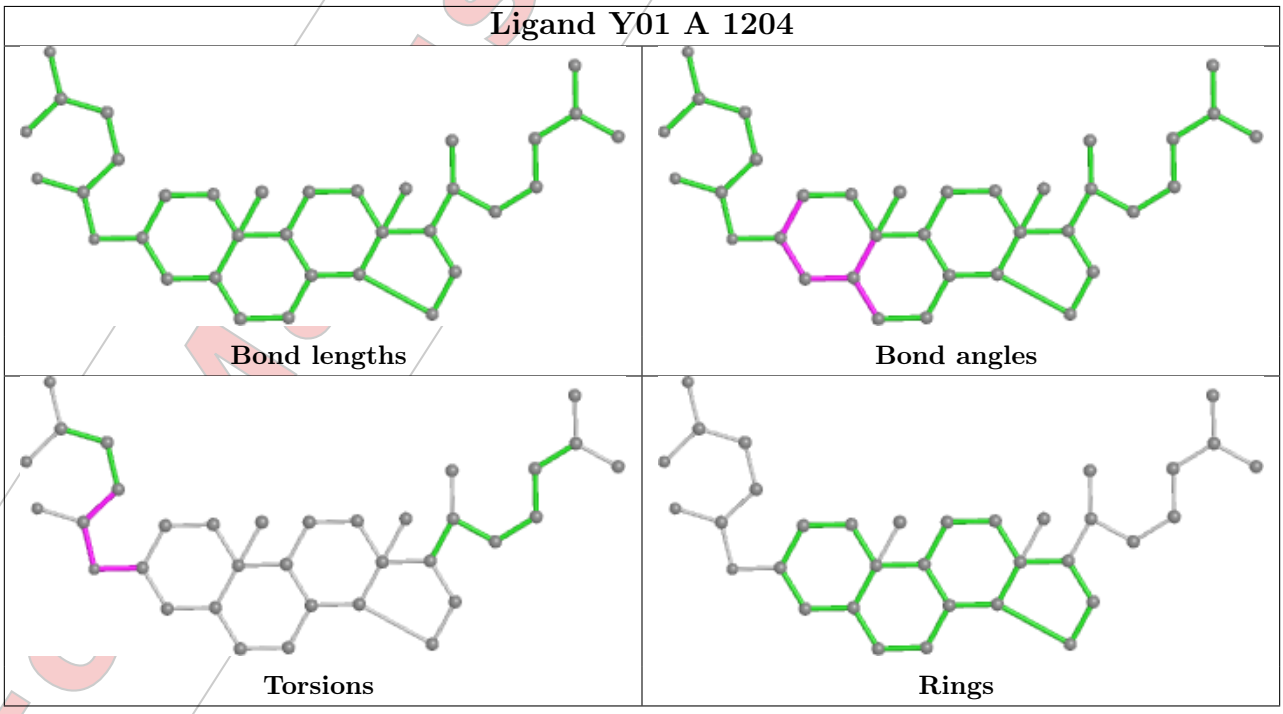
Ligand POV C 1203



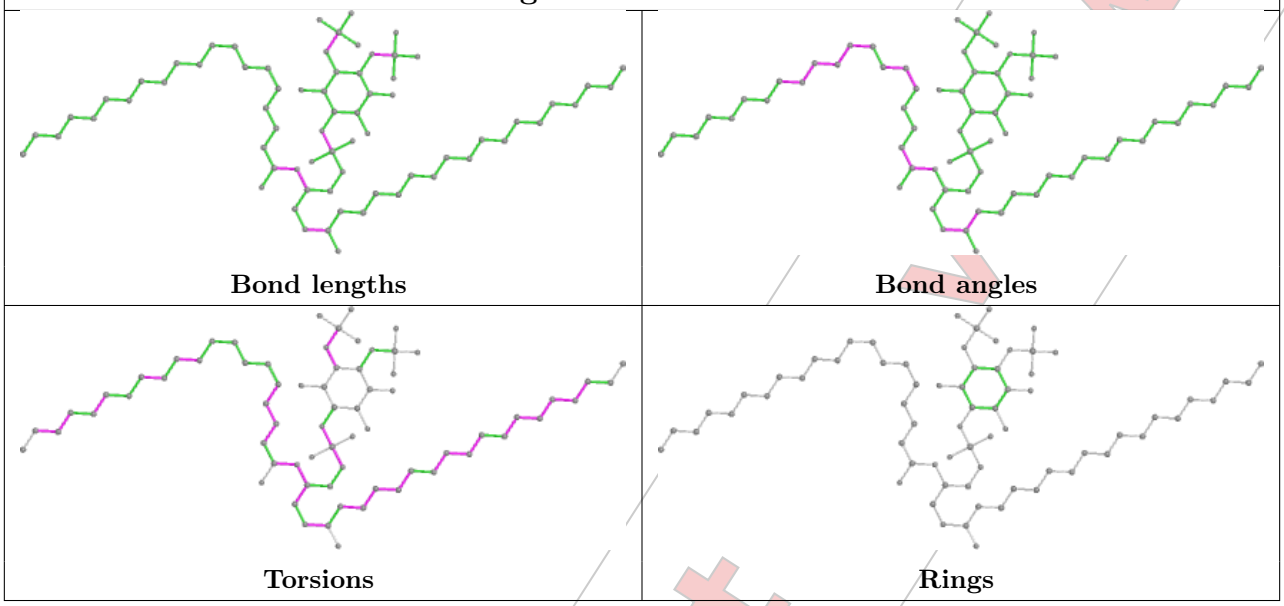
Ligand POV B 1203



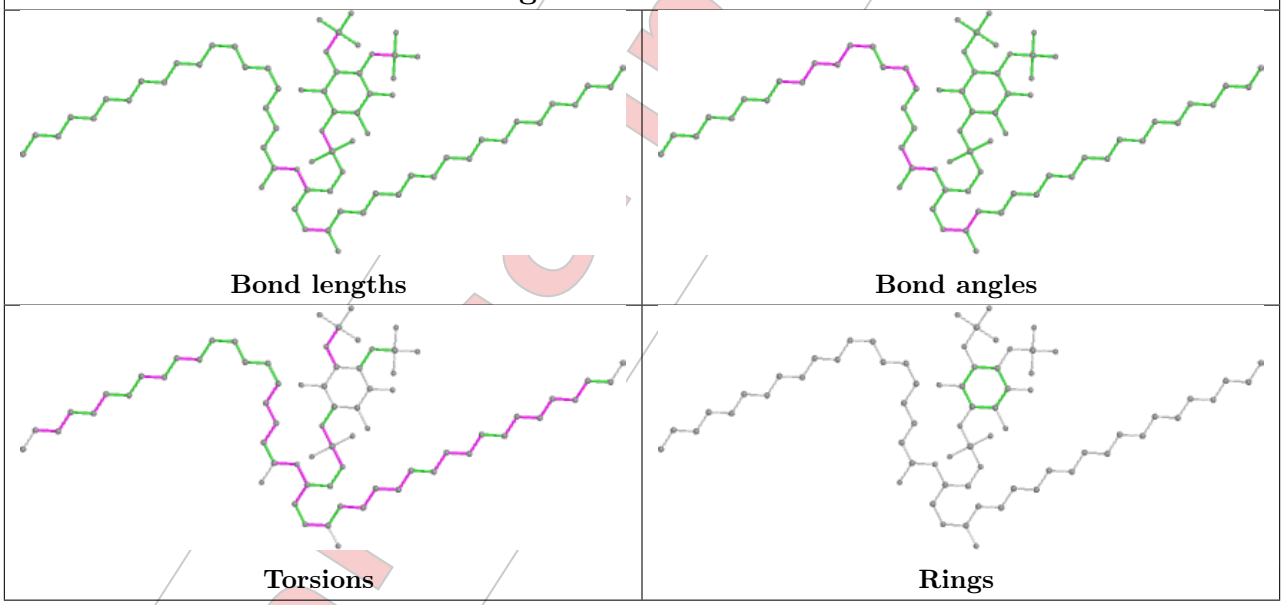
Ligand Y01 A 1204



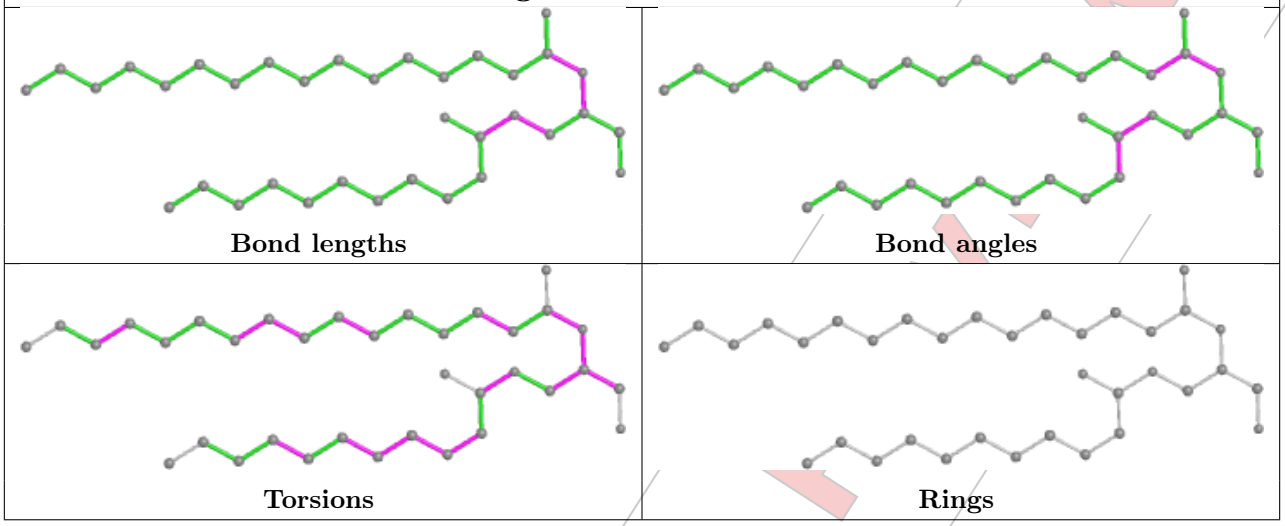
Ligand PT5 B 1205



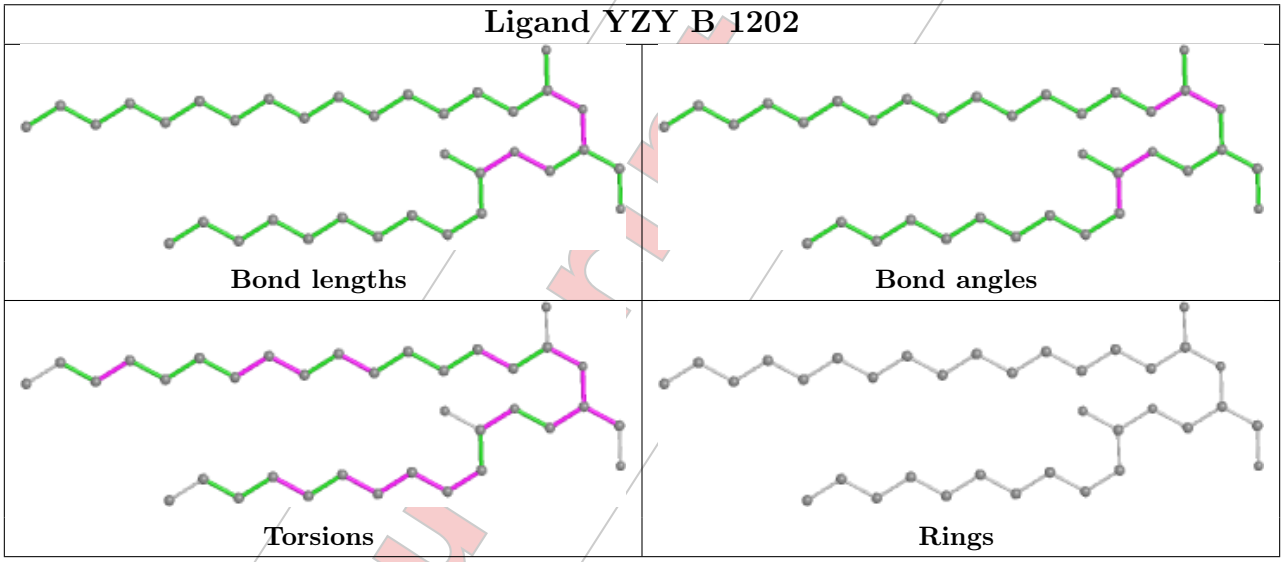
Ligand PT5 A 1205



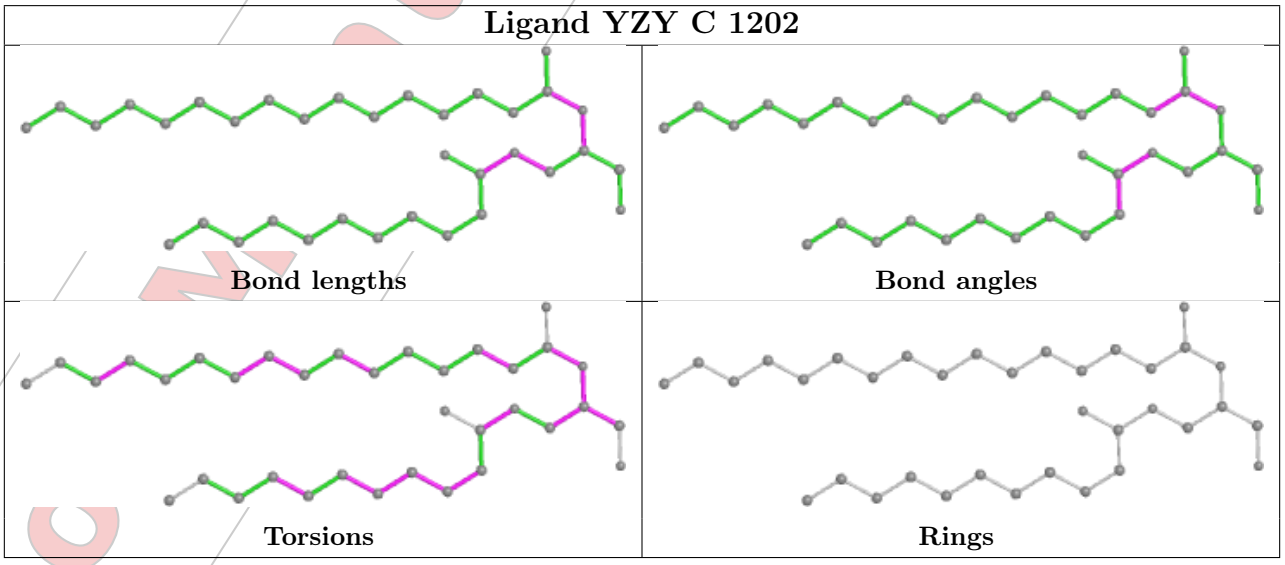
Ligand YZY D 1202

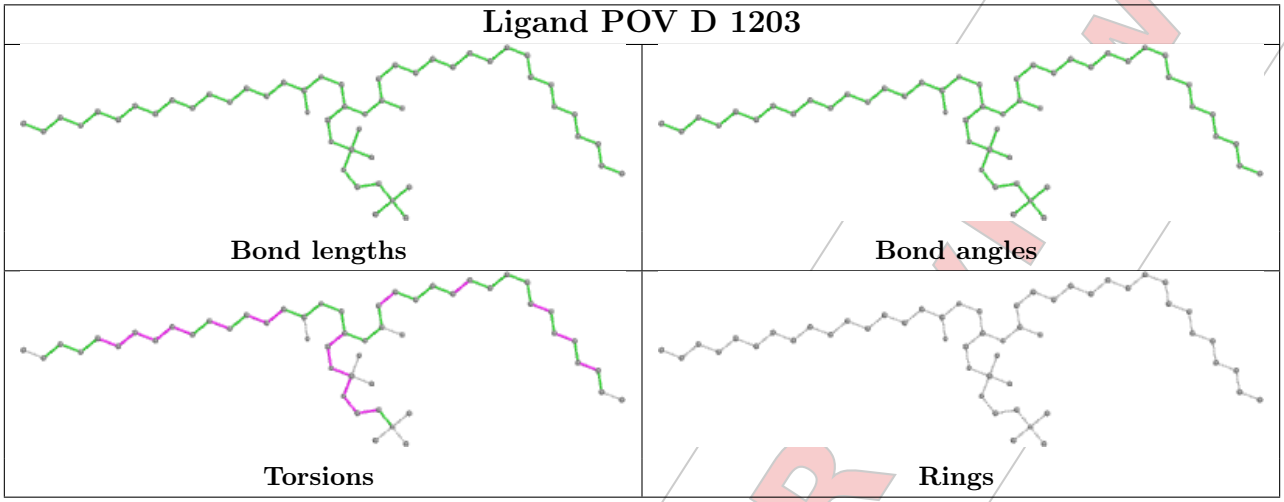


Ligand YZY B 1202



Ligand YZY C 1202





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

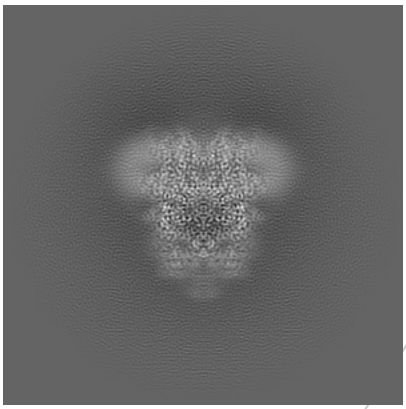
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-65280. These allow visual inspection of the internal detail of the map and identification of artifacts.

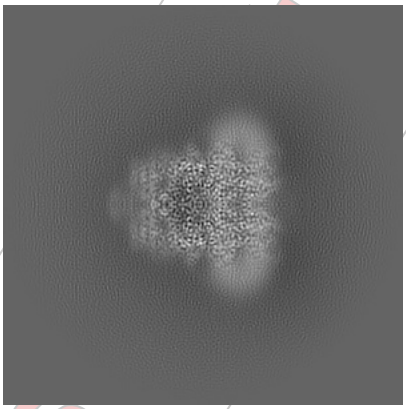
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

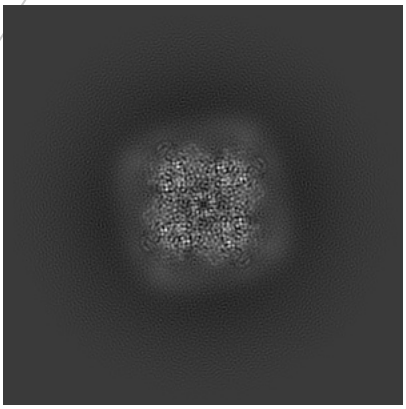
6.1.1 Primary map



X

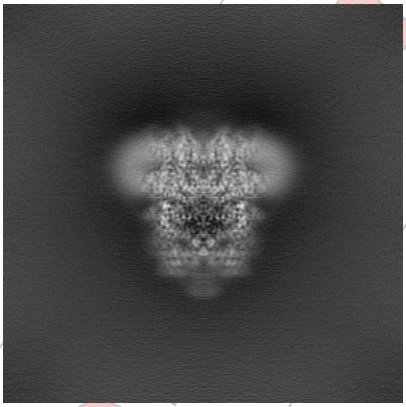


Y

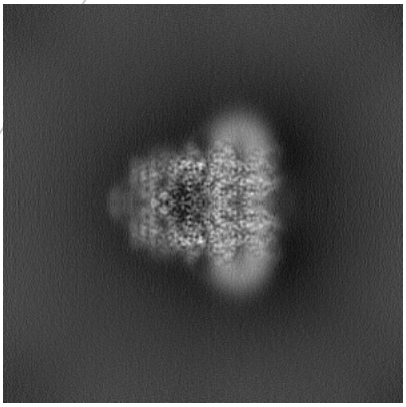


Z

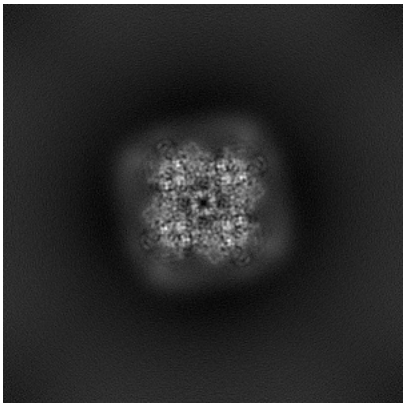
6.1.2 Raw map



X



Y

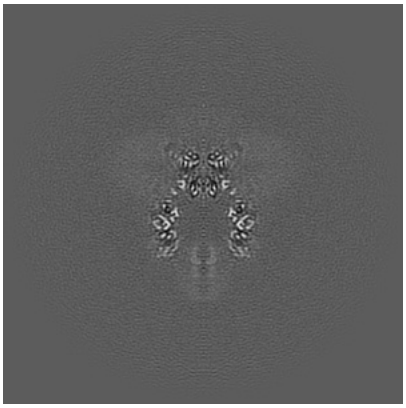


Z

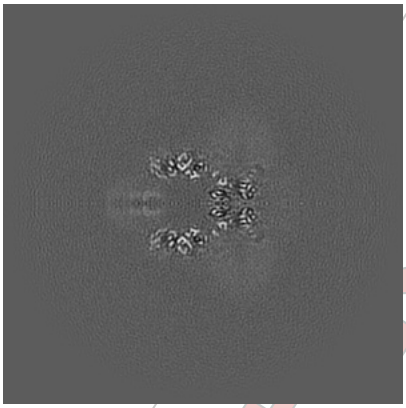
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

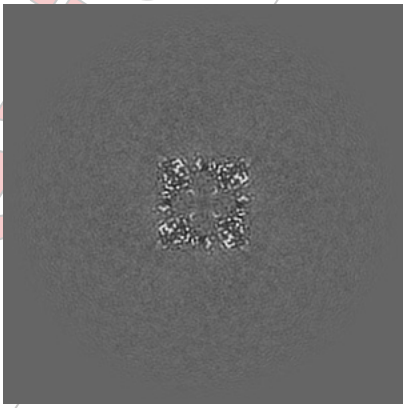
6.2.1 Primary map



X Index: 192

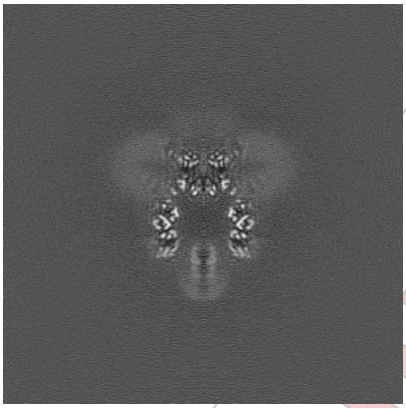


Y Index: 192

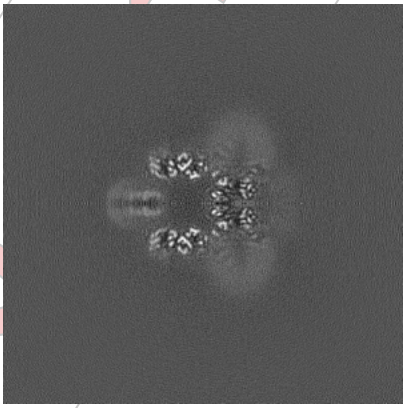


Z Index: 192

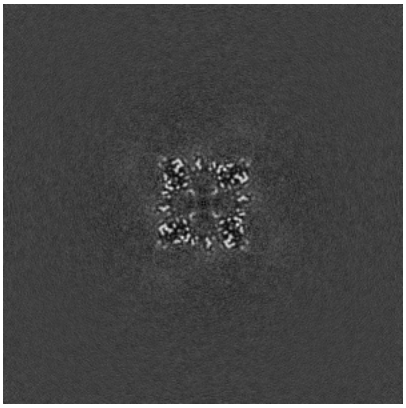
6.2.2 Raw map



X Index: 192



Y Index: 192

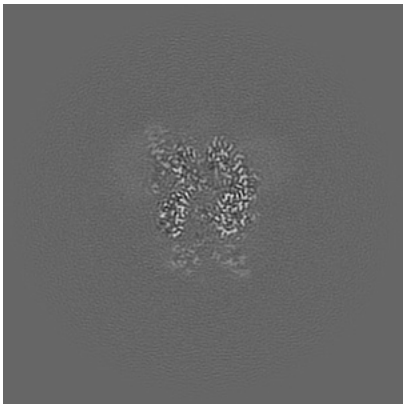


Z Index: 192

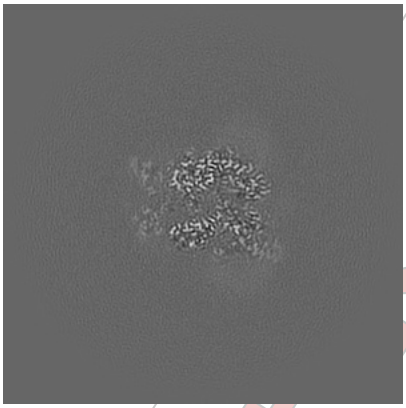
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

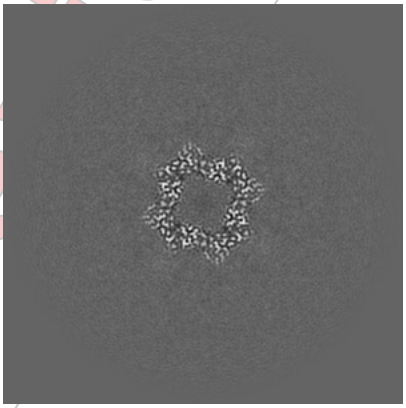
6.3.1 Primary map



X Index: 168

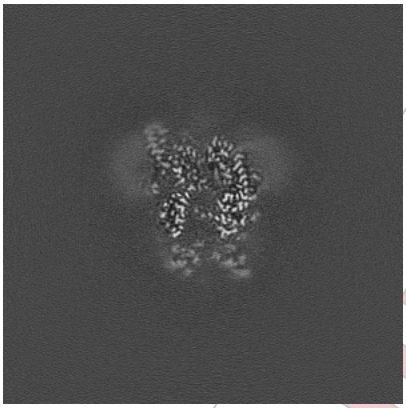


Y Index: 216

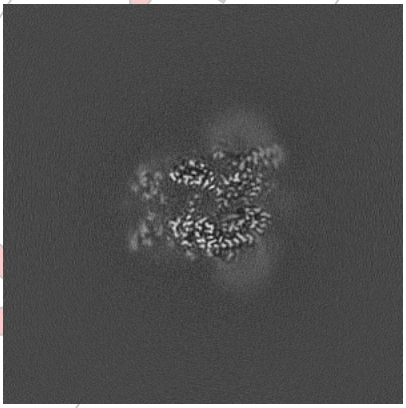


Z Index: 178

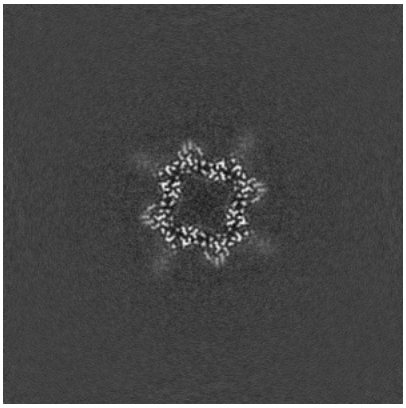
6.3.2 Raw map



X Index: 168



Y Index: 168

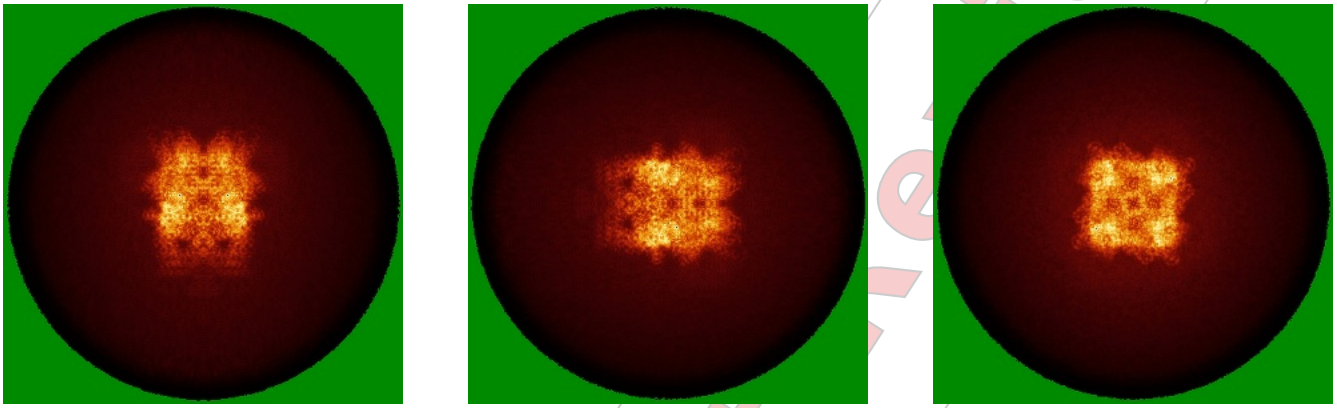


Z Index: 178

The images above show the largest variance slices of the map in three orthogonal directions.

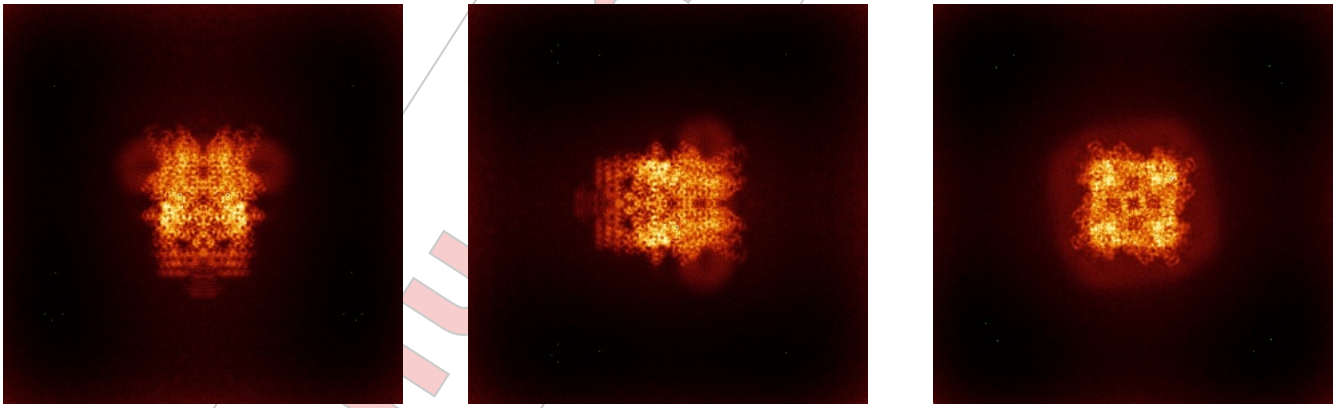
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



X Y Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

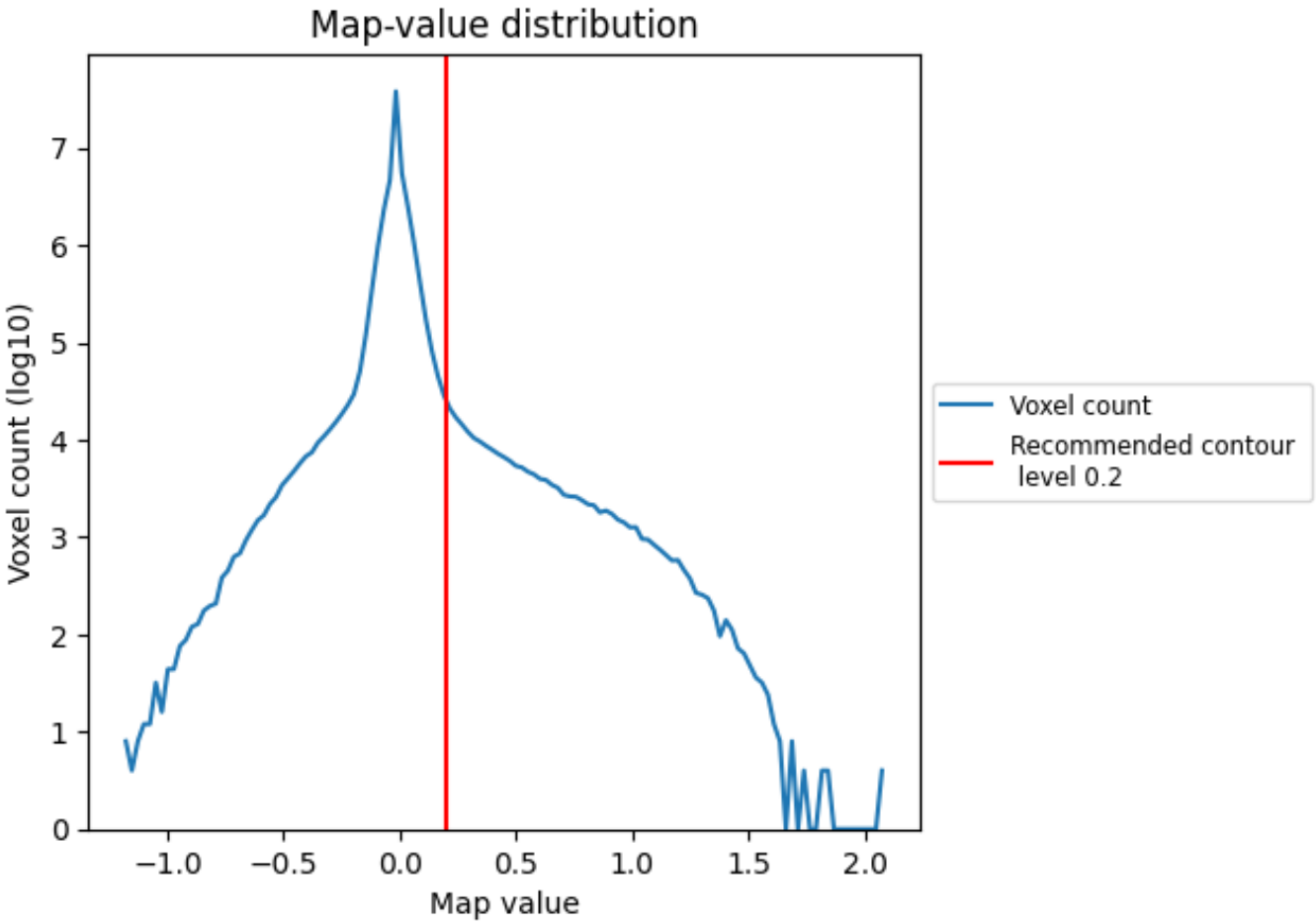
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

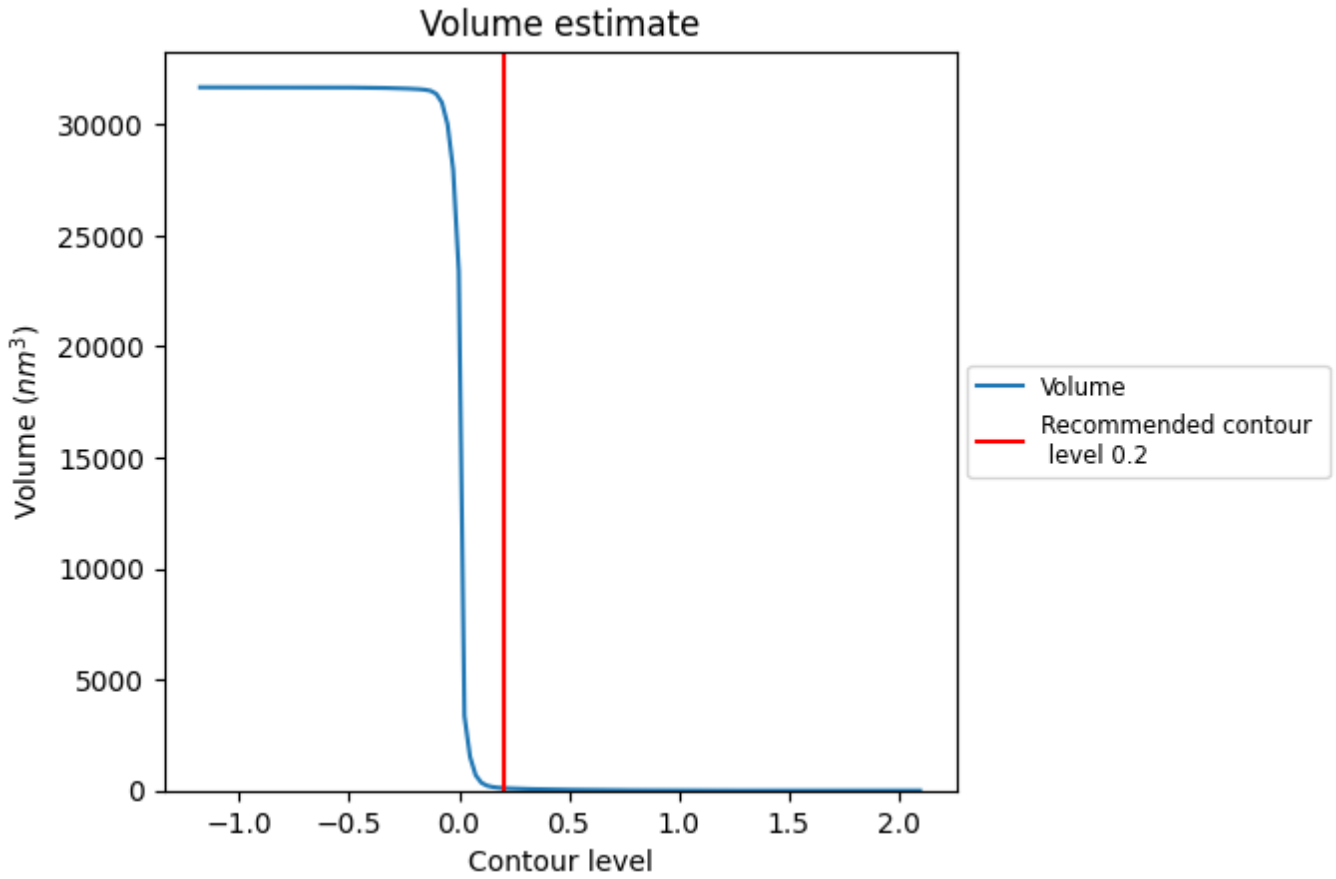
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

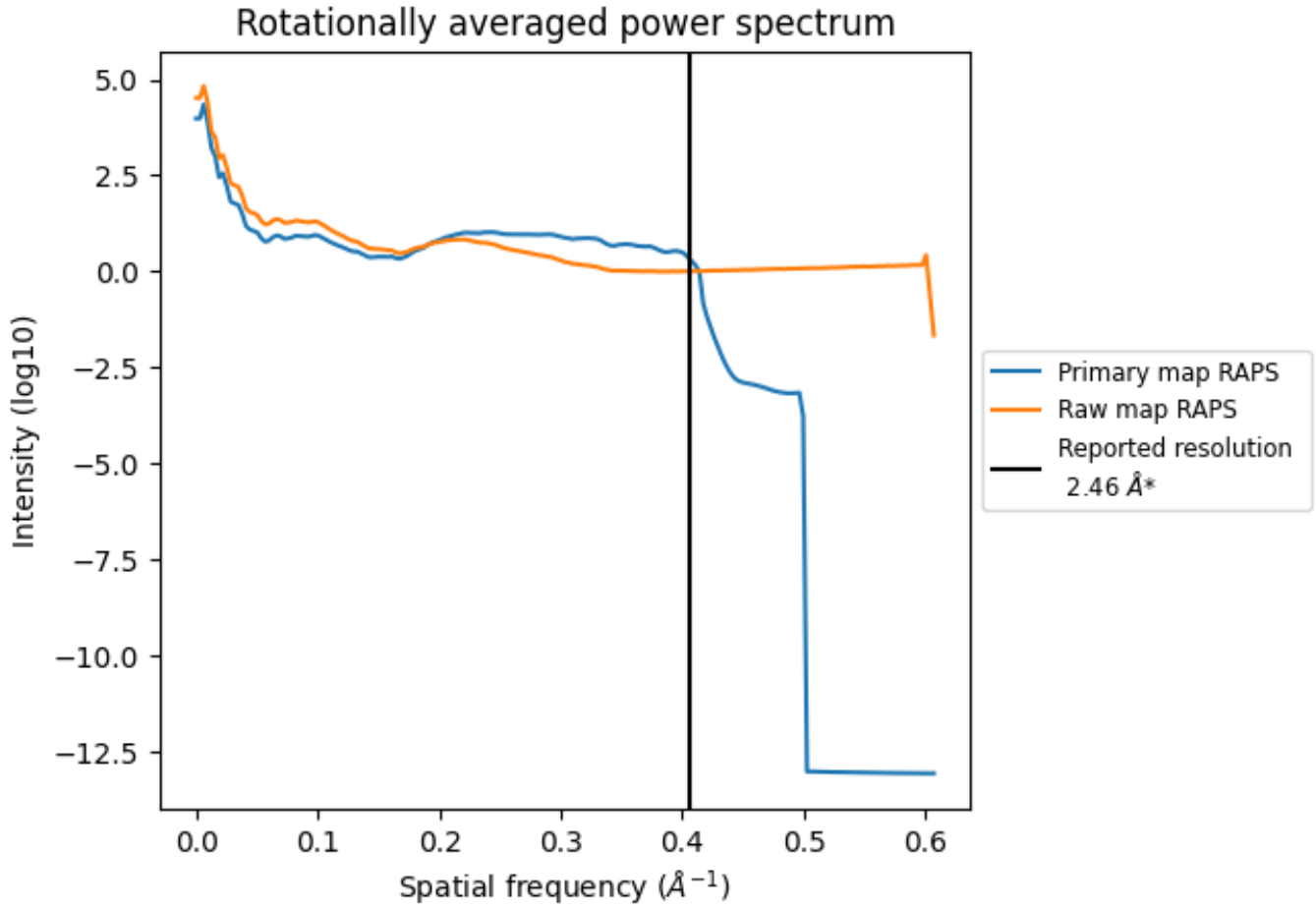
7.2 Volume estimate



The volume at the recommended contour level is 114 nm^3; this corresponds to an approximate mass of 103 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

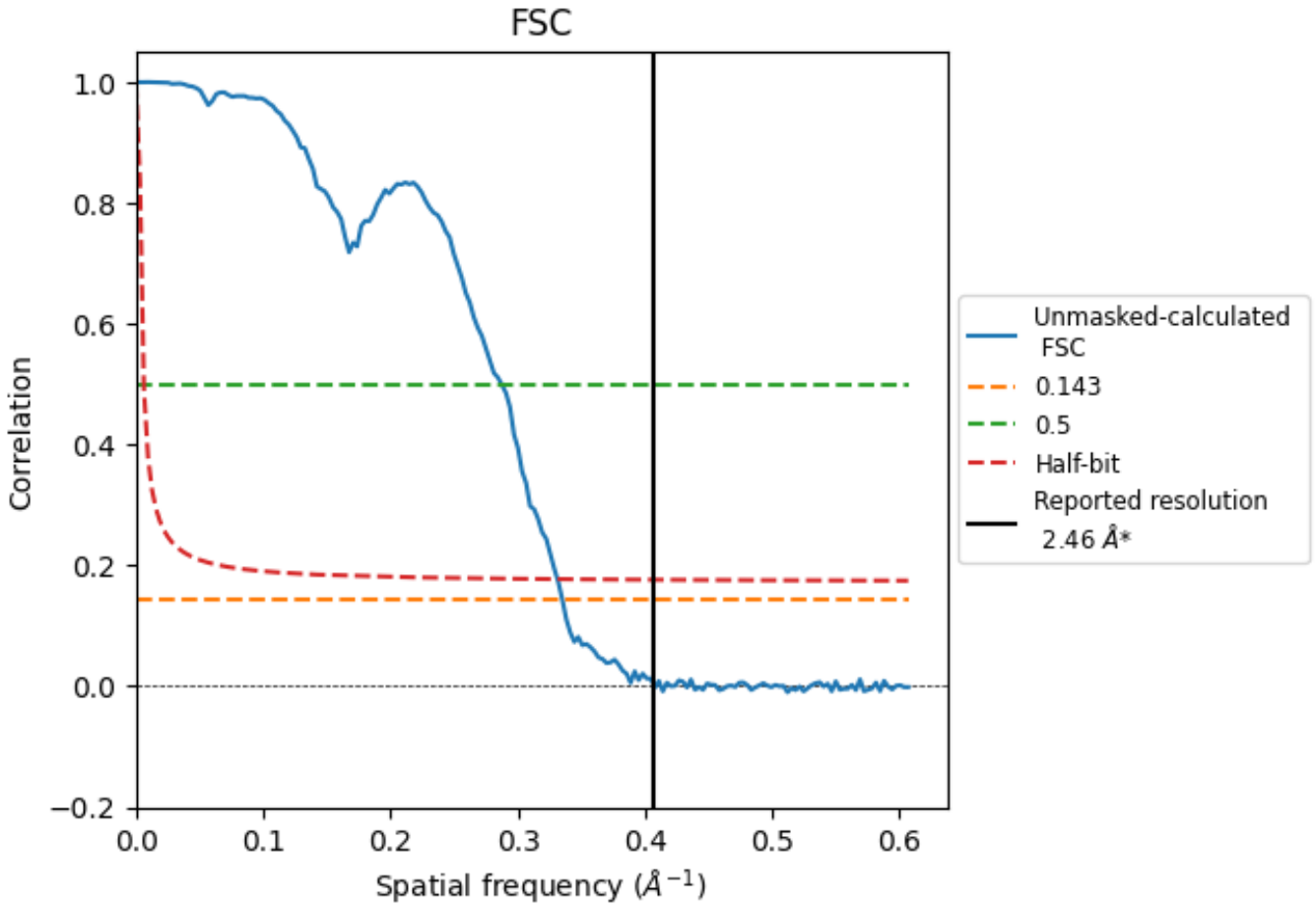


*Reported resolution corresponds to spatial frequency of 0.407 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.407 Å^{-1}

8.2 Resolution estimates (i)

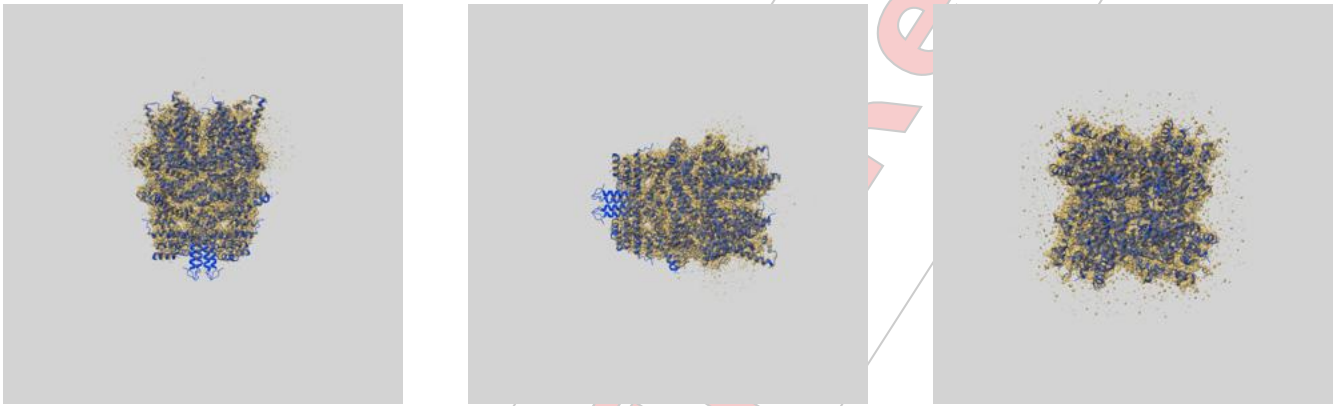
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.46	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.98	3.48	3.02

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.98 differs from the reported value 2.46 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-65280 and PDB model 9VQX. Per-residue inclusion information can be found in section 3 on page 7.

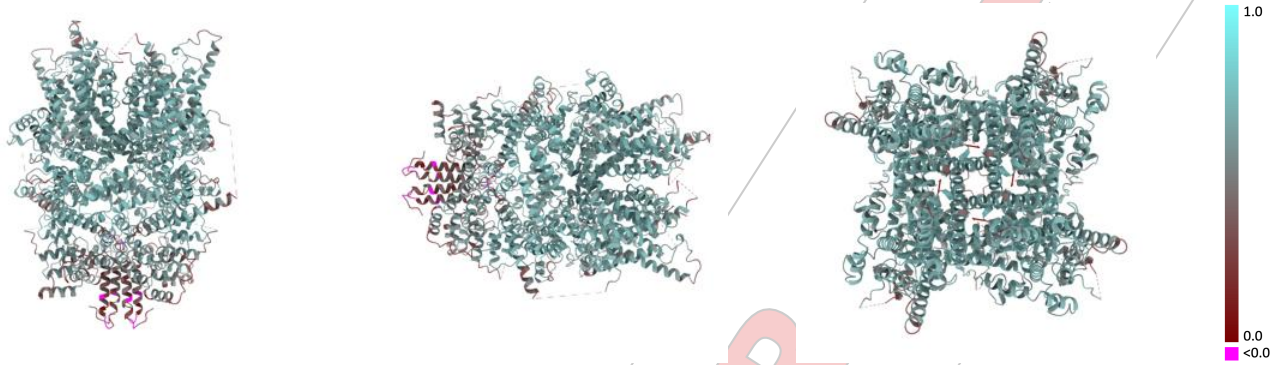
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

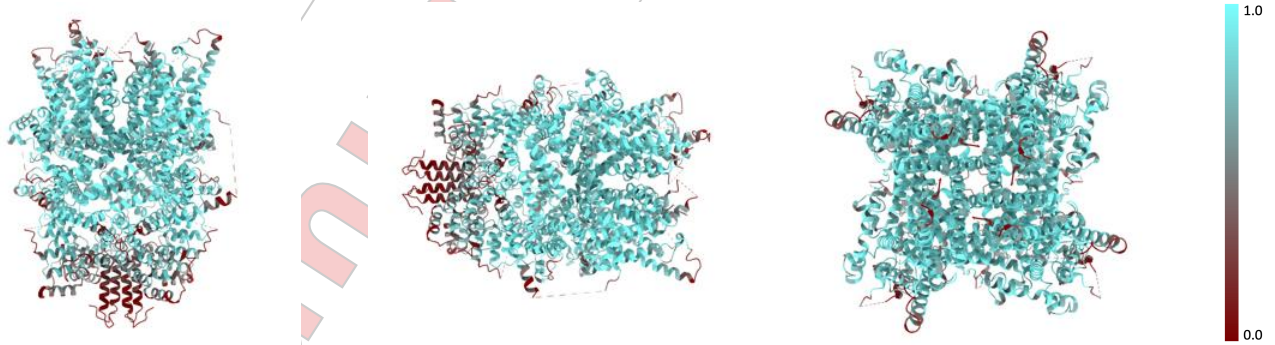
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

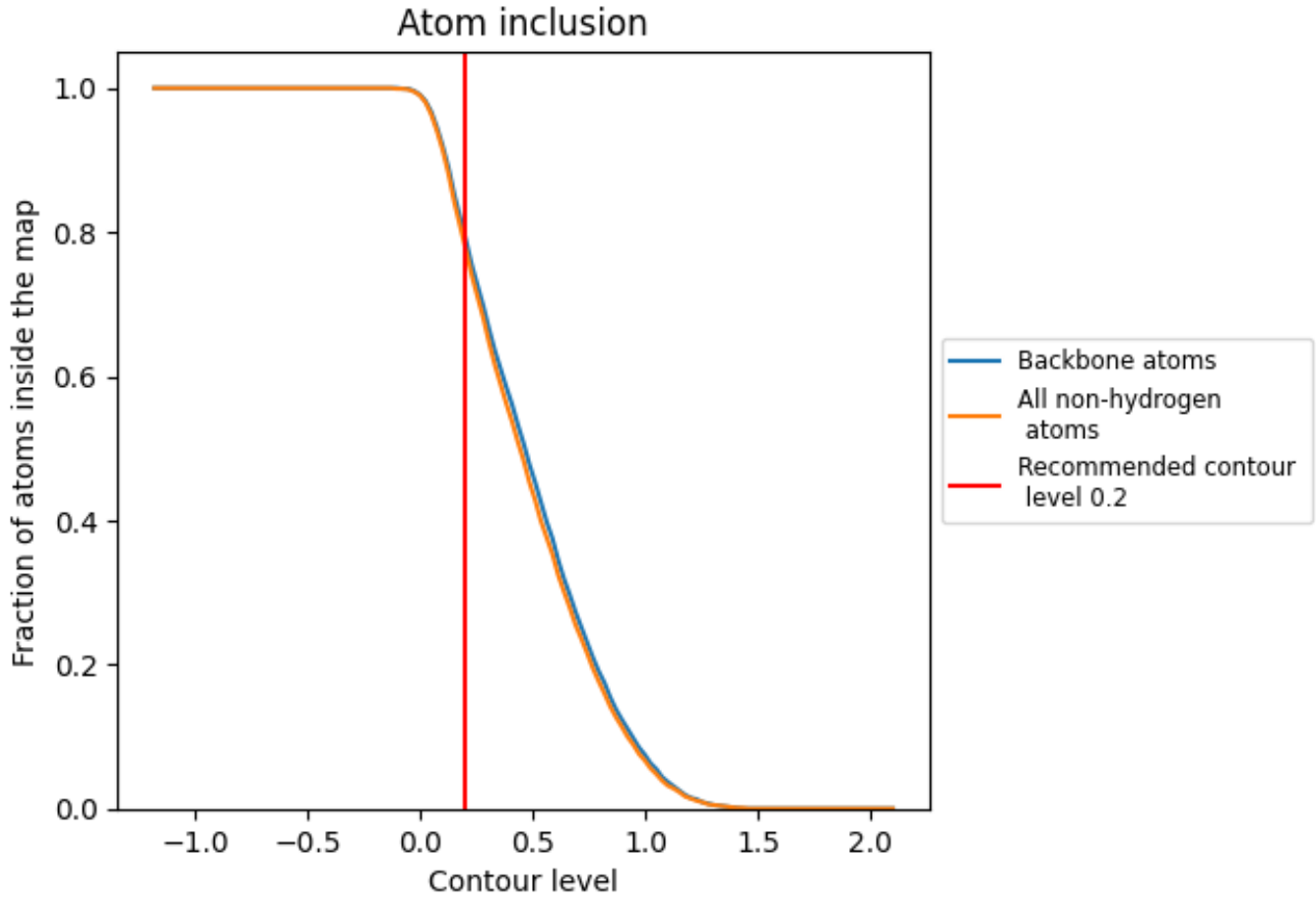
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7800	0.5950
A	0.7810	0.5950
B	0.7820	0.5950
C	0.7820	0.5940
D	0.7820	0.5950

Full wwPDB EM Validation Report ⓘ

Jul 20, 2025 – 02:21 PM JST

PDB ID	:	9VQY / pdb_00009vqy
EMDB ID	:	EMD-65281
Title	:	Cryo-EM structure of drosophila TRPgamma in complex with camphor
Deposited on	:	2025-07-05
Resolution	:	3.44 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

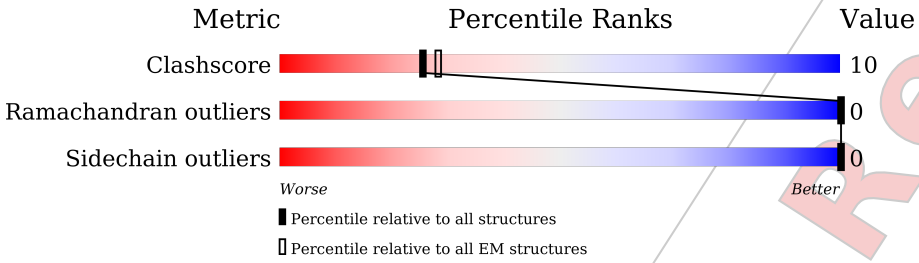
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.44 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1128	9% 53% 9% 38%
1	B	1128	9% 52% 9% 38%
1	C	1128	9% 53% 9% 38%
1	D	1128	9% 52% 9% 38%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CAM	A	1206	-	-	X	-
6	CAM	B	1206	-	-	X	-
6	CAM	C	1206	-	-	X	-
6	CAM	D	1206	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 23141 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transient receptor potential-gamma protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	694	Total 5681	C 3671	N 958	O 1022	S 30	0	0
1	B	694	Total 5681	C 3671	N 958	O 1022	S 30	0	0
1	C	694	Total 5681	C 3671	N 958	O 1022	S 30	0	0
1	D	694	Total 5681	C 3671	N 958	O 1022	S 30	0	0

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

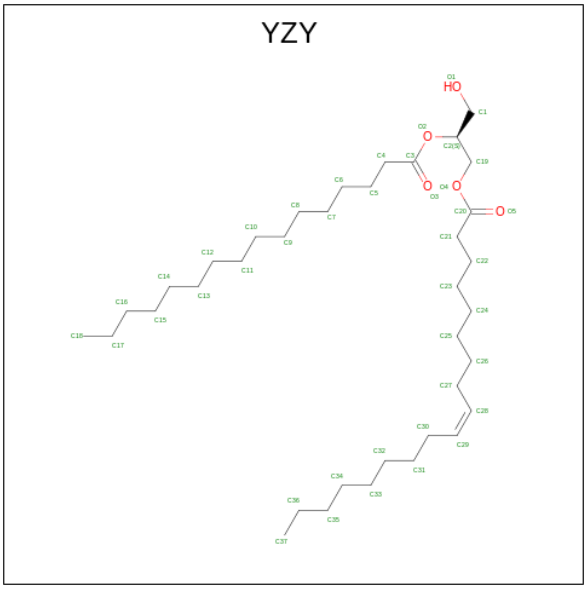
Mol	Chain	Residues	Atoms		AltConf
2	A	2	Total 2	Ca 2	0
2	B	2	Total 2	Ca 2	0
2	C	2	Total 2	Ca 2	0
2	D	2	Total 2	Ca 2	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total 1	Zn 1	0
3	B	1	Total 1	Zn 1	0
3	C	1	Total 1	Zn 1	0
3	D	1	Total 1	Zn 1	0

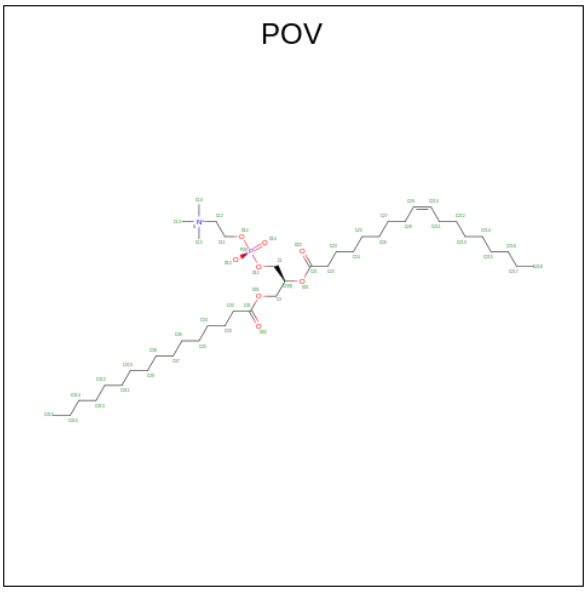
- Molecule 4 is (2S)-2-(hexadecanoyloxy)-3-hydroxypropyl (9Z)-octadec-9-enoate (CCD ID:

YZY) (formula: $C_{37}H_{70}O_5$).



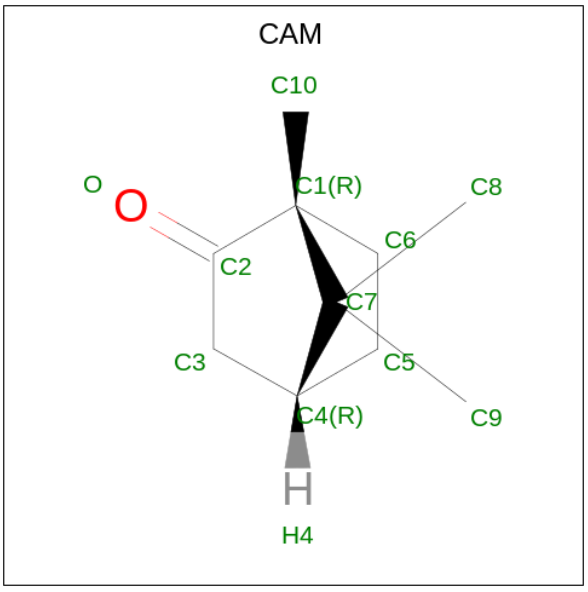
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C O 35 30 5	0
4	B	1	Total C O 35 30 5	0
4	C	1	Total C O 35 30 5	0
4	D	1	Total C O 35 30 5	0

- Molecule 5 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: $C_{42}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	D	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 6 is CAMPHOR (CCD ID: CAM) (formula: $C_{10}H_{16}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total 11	C 10	O 1	0
6	B	1	Total 11	C 10	O 1	0
6	C	1	Total 11	C 10	O 1	0
6	D	1	Total 11	C 10	O 1	0

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
7	A	5	Total 5	Na 5	0

- Molecule 8 is water.

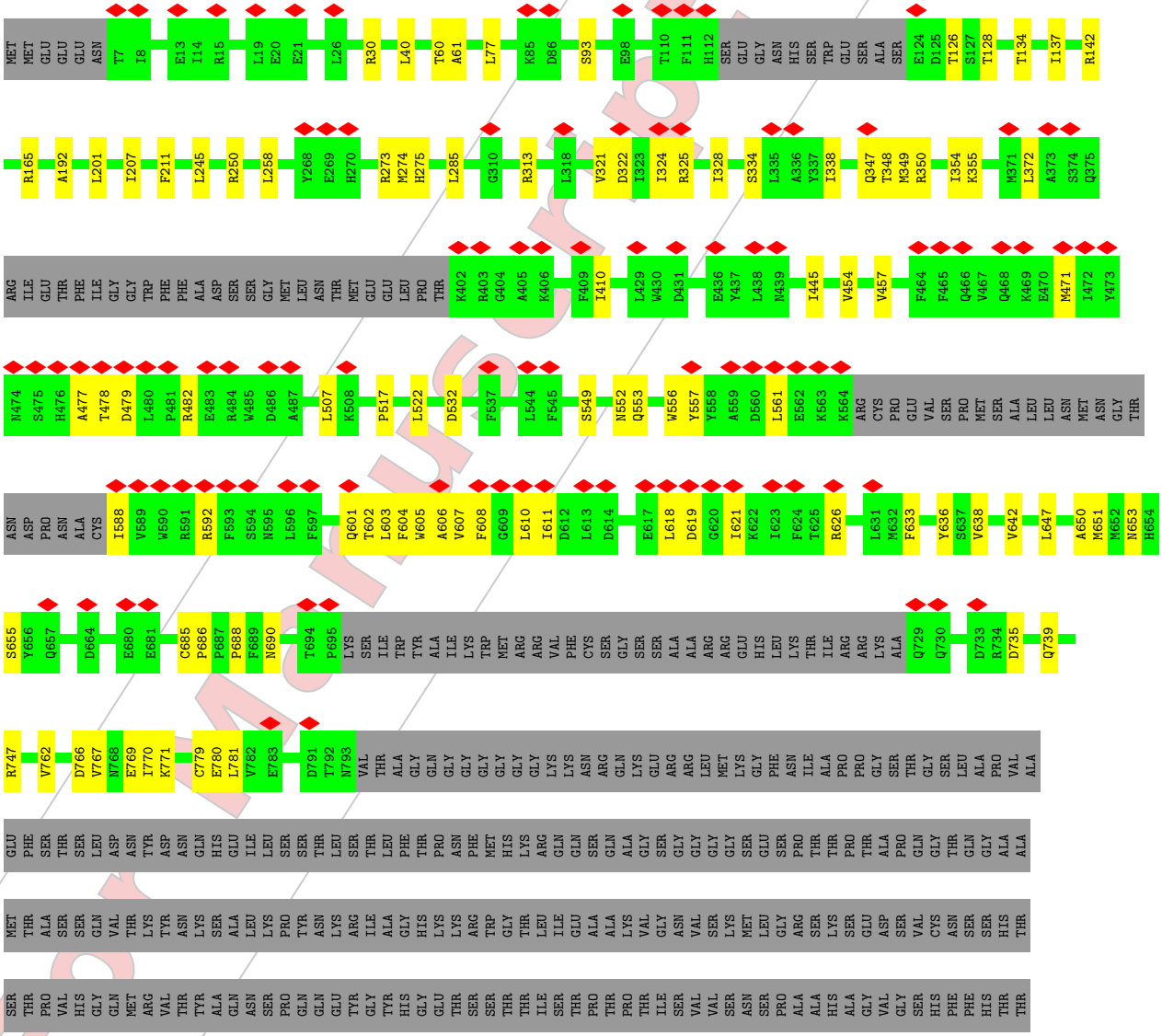
Mol	Chain	Residues	Atoms		AltConf
8	A	2	Total 2	O 2	0
8	B	2	Total 2	O 2	0
8	C	2	Total 2	O 2	0
8	D	2	Total 2	O 2	0

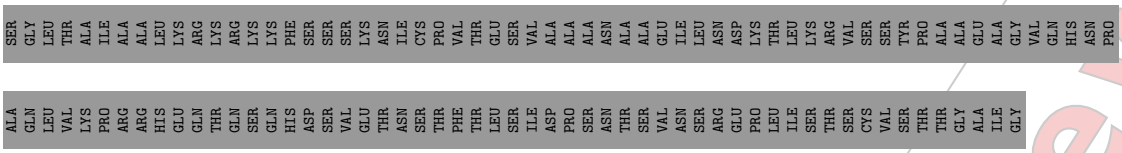
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Transient receptor potential-gamma protein

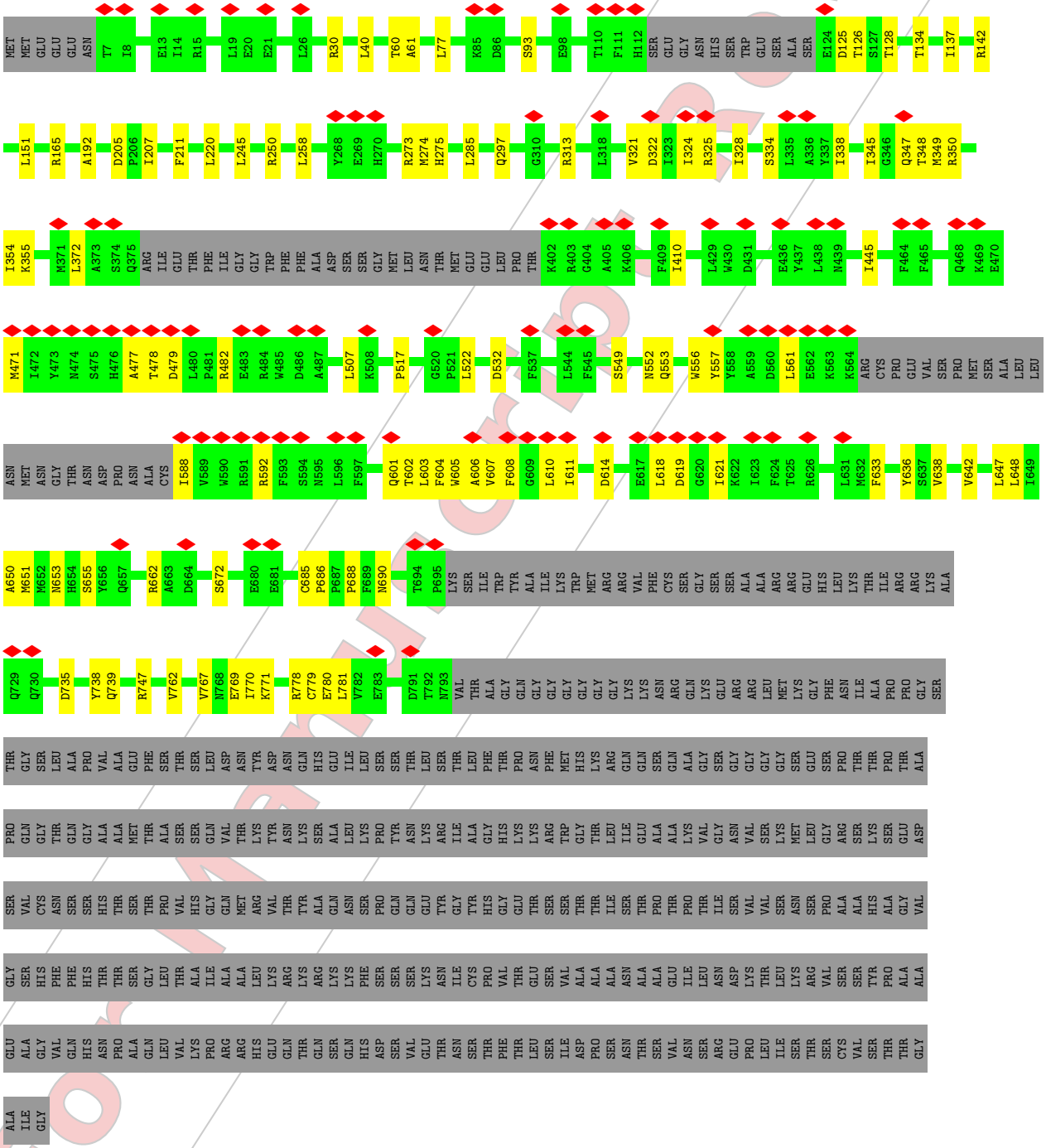
Chain A:





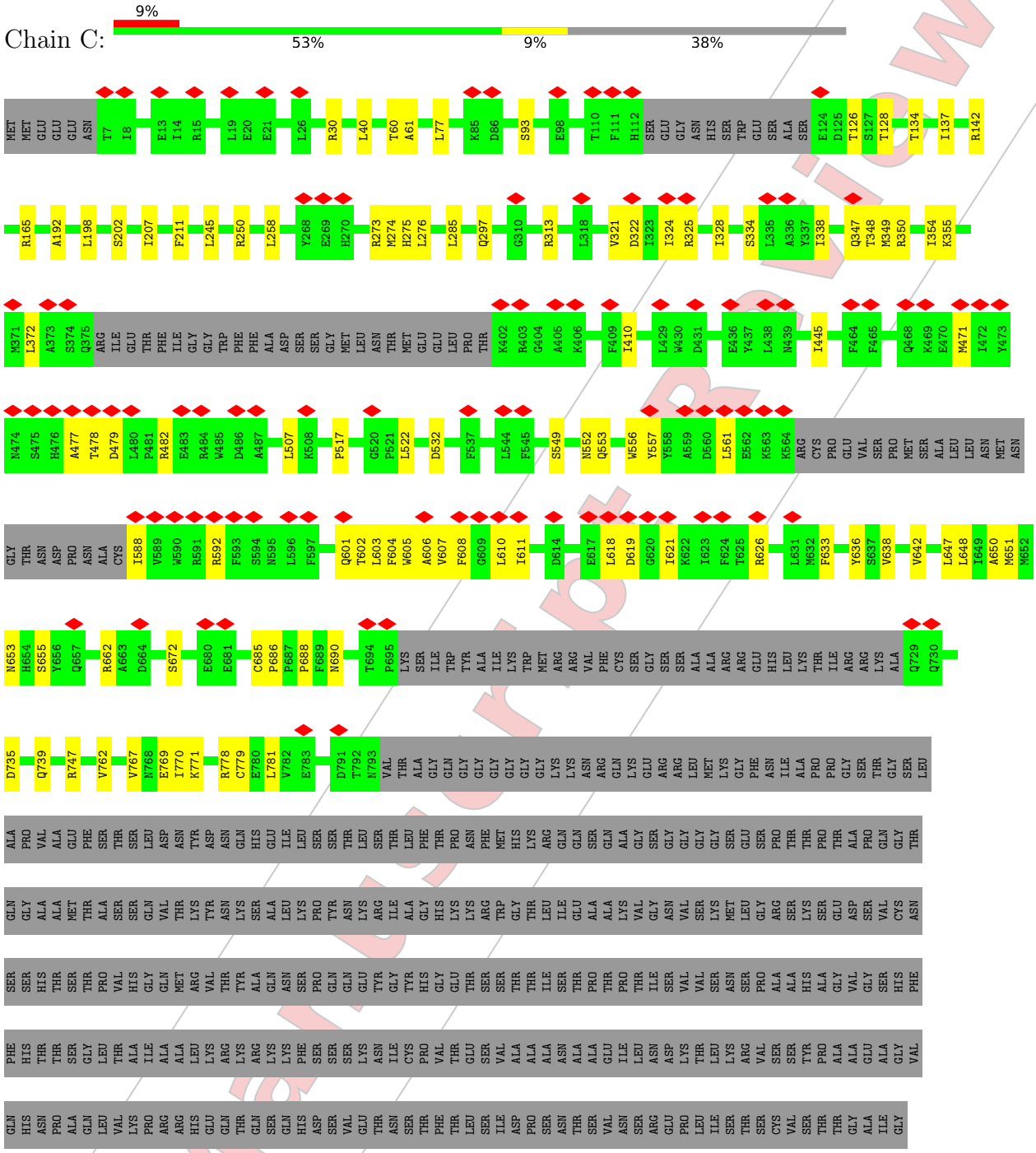
• Molecule 1: Transient receptor potential-gamma protein

Chain B:



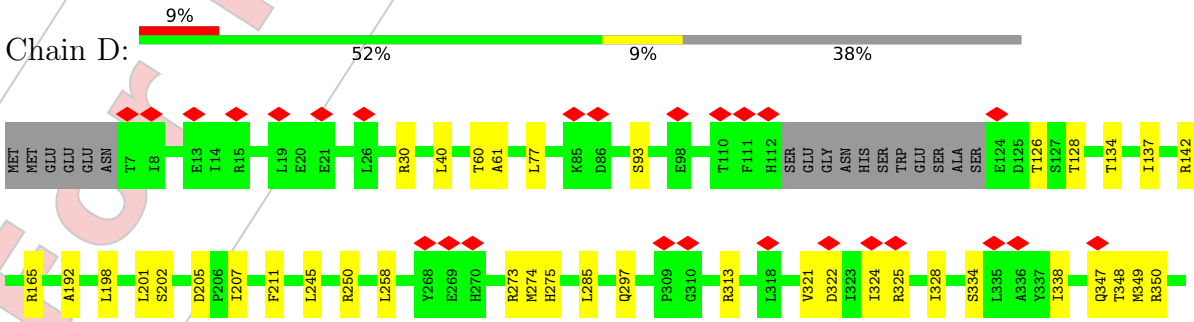
• Molecule 1: Transient receptor potential-gamma protein

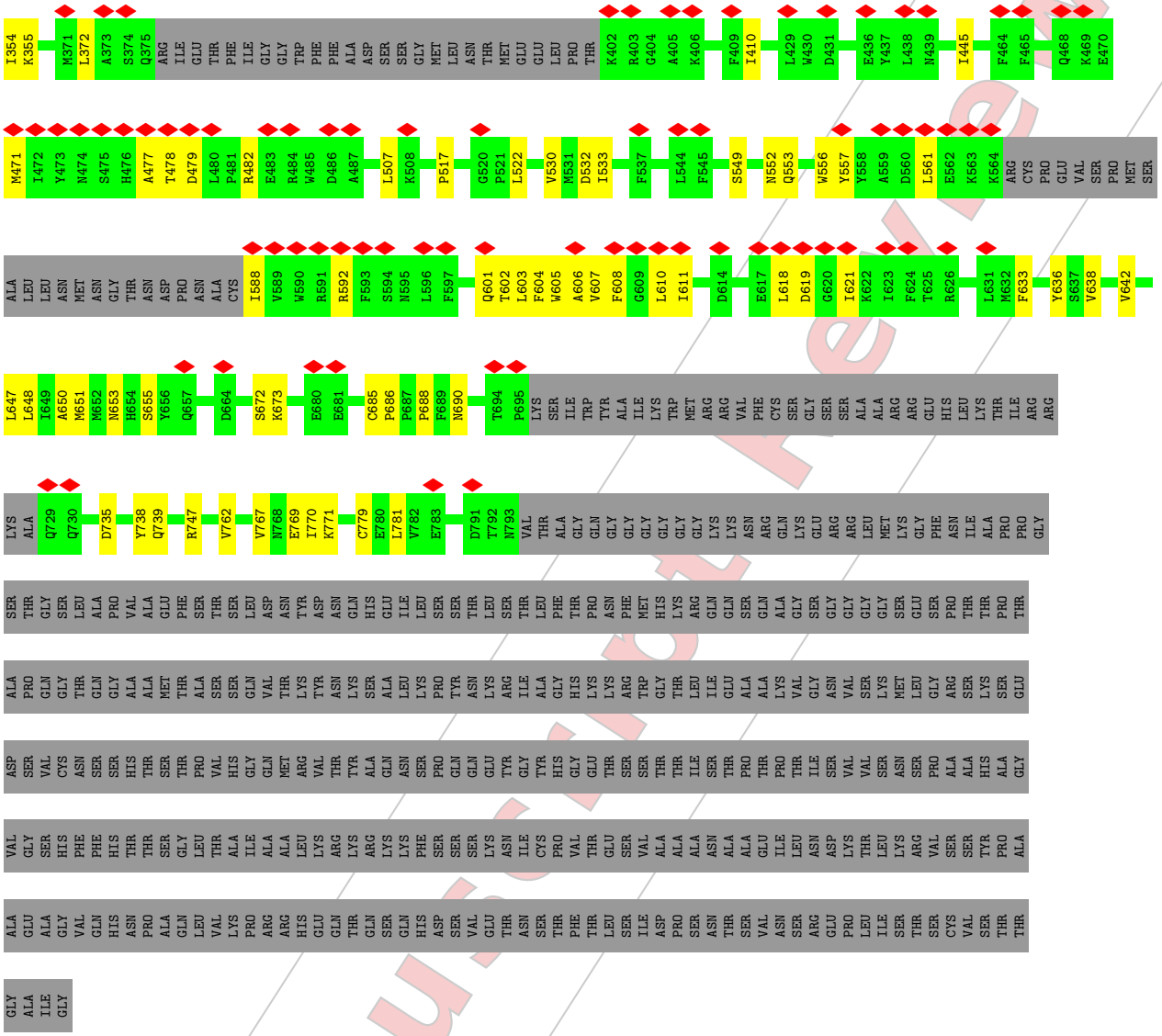
Chain C:



• Molecule 1: Transient receptor potential-gamma protein

Chain D:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3587	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	-1300	Depositor
Maximum defocus (nm)	-1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.534	Depositor
Minimum map value	-0.319	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	316.41602, 316.41602, 316.41602	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82400006, 0.82400006, 0.82400006	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CAM, CA, POV, YZY, NA, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.19	0/5812	0.40	0/7871
1	B	0.19	0/5812	0.40	0/7871
1	C	0.19	0/5812	0.40	0/7871
1	D	0.19	0/5812	0.40	0/7871
All	All	0.19	0/23248	0.40	0/31484

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5681	0	5674	123	0
1	B	5681	0	5674	132	0
1	C	5681	0	5674	126	0
1	D	5681	0	5674	128	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	35	0	53	9	0
4	B	35	0	53	9	0
4	C	35	0	53	10	0
4	D	35	0	53	9	0
5	A	52	0	82	8	0
5	B	52	0	82	9	0
5	C	52	0	82	8	0
5	D	52	0	82	8	0
6	A	11	0	16	9	0
6	B	11	0	16	8	0
6	C	11	0	16	9	0
6	D	11	0	16	9	0
7	A	5	0	0	0	0
8	A	2	0	0	0	0
8	B	2	0	0	0	0
8	C	2	0	0	0	0
8	D	2	0	0	0	0
All	All	23141	0	23300	471	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (471) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:610:LEU:O	1:C:610:LEU:HD12	1.29	1.29
1:B:610:LEU:HD12	1:B:610:LEU:O	1.29	1.28
1:D:610:LEU:HD12	1:D:610:LEU:O	1.29	1.26
1:A:610:LEU:O	1:A:610:LEU:HD12	1.29	1.25
1:D:606:ALA:HA	1:D:611:ILE:HD12	1.28	1.15
1:A:606:ALA:HA	1:A:611:ILE:HD12	1.28	1.11
1:C:328:ILE:HD12	5:C:1205:POV:H31F	1.31	1.11
1:D:328:ILE:HD12	5:D:1205:POV:H31F	1.31	1.10
1:C:273:ARG:O	1:C:274:MET:HG2	1.51	1.09
1:C:606:ALA:HA	1:C:611:ILE:HD12	1.28	1.09
1:A:273:ARG:O	1:A:274:MET:HG2	1.51	1.08
1:C:372:LEU:HD12	1:C:410:ILE:HD13	1.36	1.08
1:D:273:ARG:O	1:D:274:MET:HG2	1.51	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ILE:HD12	5:A:1205:POV:H31F	1.31	1.07
1:B:273:ARG:O	1:B:274:MET:HG2	1.51	1.07
1:A:207:ILE:HD13	1:A:258:LEU:HD11	1.35	1.07
1:B:606:ALA:HA	1:B:611:ILE:HD12	1.28	1.06
1:B:328:ILE:HD12	5:B:1205:POV:H31F	1.31	1.06
1:D:372:LEU:HD12	1:D:410:ILE:HD13	1.36	1.06
1:C:207:ILE:HD13	1:C:258:LEU:HD11	1.35	1.06
1:A:372:LEU:HD12	1:A:410:ILE:HD13	1.36	1.05
1:B:207:ILE:HD13	1:B:258:LEU:HD11	1.35	1.05
1:D:207:ILE:HD13	1:D:258:LEU:HD11	1.35	1.05
1:C:605:TRP:HH2	4:C:1204:YZY:H11	1.19	1.04
1:D:605:TRP:HH2	4:D:1204:YZY:H11	1.19	1.03
1:A:605:TRP:HH2	4:A:1204:YZY:H11	1.19	1.03
1:B:372:LEU:HD12	1:B:410:ILE:HD13	1.36	1.02
1:B:605:TRP:HH2	4:B:1204:YZY:H11	1.19	1.02
1:A:606:ALA:HA	1:A:611:ILE:CD1	1.91	1.01
1:B:606:ALA:HA	1:B:611:ILE:CD1	1.91	1.01
1:C:606:ALA:HA	1:C:611:ILE:CD1	1.91	1.01
1:B:561:LEU:HD23	1:B:619:ASP:CG	1.87	1.00
1:C:561:LEU:HD23	1:C:619:ASP:CG	1.87	1.00
1:D:561:LEU:HD23	1:D:619:ASP:CG	1.87	1.00
1:D:606:ALA:HA	1:D:611:ILE:CD1	1.91	1.00
1:A:561:LEU:HD23	1:A:619:ASP:CG	1.87	0.99
1:C:517:PRO:HG3	5:C:1205:POV:H15A	1.46	0.97
1:D:517:PRO:HG3	5:D:1205:POV:H15A	1.46	0.97
1:B:517:PRO:HG3	5:B:1205:POV:H15A	1.47	0.95
1:A:517:PRO:HG3	5:A:1205:POV:H15A	1.46	0.95
4:B:1204:YZY:H121	6:B:1206:CAM:C10	1.97	0.95
4:D:1204:YZY:H121	6:D:1206:CAM:C10	1.97	0.94
4:A:1204:YZY:H121	6:A:1206:CAM:C10	1.97	0.94
4:C:1204:YZY:H121	6:C:1206:CAM:C10	1.97	0.94
1:A:522:LEU:HD21	1:B:651:MET:CE	1.98	0.93
1:D:372:LEU:HD12	1:D:410:ILE:CD1	1.99	0.93
1:A:372:LEU:HD12	1:A:410:ILE:CD1	1.99	0.93
1:C:372:LEU:CD1	1:C:410:ILE:HD13	1.99	0.92
1:D:372:LEU:CD1	1:D:410:ILE:HD13	1.99	0.92
1:C:605:TRP:CH2	4:C:1204:YZY:H11	2.04	0.92
1:B:372:LEU:CD1	1:B:410:ILE:HD13	1.99	0.92
1:B:522:LEU:HD21	1:C:651:MET:CE	2.00	0.92
1:D:605:TRP:CH2	4:D:1204:YZY:H11	2.05	0.91
1:A:762:VAL:HG11	1:B:767:VAL:HG21	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:LEU:HD12	1:B:410:ILE:CD1	1.99	0.91
1:A:372:LEU:CD1	1:A:410:ILE:HD13	1.99	0.91
1:B:605:TRP:CH2	4:B:1204:YZY:H11	2.04	0.91
1:C:522:LEU:HD21	1:D:651:MET:CE	2.00	0.91
1:C:372:LEU:HD12	1:C:410:ILE:CD1	1.99	0.91
1:D:610:LEU:O	1:D:610:LEU:CD1	2.18	0.90
1:A:605:TRP:CH2	4:A:1204:YZY:H11	2.05	0.90
1:A:610:LEU:O	1:A:610:LEU:CD1	2.18	0.90
1:A:651:MET:CE	1:D:522:LEU:HD21	2.02	0.90
1:B:610:LEU:O	1:B:610:LEU:CD1	2.18	0.90
1:A:762:VAL:HG11	1:B:767:VAL:CG2	2.01	0.90
1:A:767:VAL:HG21	1:D:762:VAL:HG11	1.54	0.90
1:C:762:VAL:HG11	1:D:767:VAL:HG21	1.53	0.90
1:C:762:VAL:HG11	1:D:767:VAL:CG2	2.03	0.89
1:B:762:VAL:HG11	1:C:767:VAL:HG21	1.54	0.89
1:B:762:VAL:HG11	1:C:767:VAL:CG2	2.03	0.88
1:D:611:ILE:HG21	1:D:633:PHE:CZ	2.09	0.88
1:C:611:ILE:HG21	1:C:633:PHE:CZ	2.09	0.87
1:C:610:LEU:O	1:C:610:LEU:CD1	2.18	0.87
1:A:611:ILE:HG21	1:A:633:PHE:CZ	2.09	0.87
1:B:607:VAL:HG23	1:B:608:PHE:CD2	2.10	0.87
1:D:607:VAL:HG23	1:D:608:PHE:CD2	2.10	0.87
1:A:522:LEU:HD21	1:B:651:MET:HE1	1.56	0.87
1:A:372:LEU:CD1	1:A:410:ILE:CD1	2.53	0.86
1:A:767:VAL:CG2	1:D:762:VAL:HG11	2.05	0.86
1:C:372:LEU:CD1	1:C:410:ILE:CD1	2.53	0.86
1:B:372:LEU:CD1	1:B:410:ILE:CD1	2.53	0.86
1:B:611:ILE:HG21	1:B:633:PHE:CZ	2.09	0.86
1:A:607:VAL:HG23	1:A:608:PHE:CD2	2.10	0.86
1:C:607:VAL:HG23	1:C:608:PHE:CD2	2.10	0.86
1:D:372:LEU:CD1	1:D:410:ILE:CD1	2.53	0.85
1:D:607:VAL:HG23	1:D:608:PHE:HD2	1.42	0.85
1:C:522:LEU:HD21	1:D:651:MET:HE1	1.59	0.85
1:A:651:MET:HE1	1:D:522:LEU:HD21	1.59	0.84
1:A:611:ILE:O	1:A:611:ILE:HG22	1.77	0.84
1:B:522:LEU:HD21	1:C:651:MET:HE1	1.58	0.84
1:A:134:THR:OG1	1:A:137:ILE:HG12	1.78	0.83
1:C:611:ILE:O	1:C:611:ILE:HG22	1.77	0.83
1:D:134:THR:OG1	1:D:137:ILE:HG12	1.78	0.83
1:B:611:ILE:HG22	1:B:611:ILE:O	1.77	0.83
1:C:134:THR:OG1	1:C:137:ILE:HG12	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:THR:OG1	1:B:137:ILE:HG12	1.78	0.82
1:C:328:ILE:CD1	5:C:1205:POV:H31F	2.09	0.82
1:C:607:VAL:HG23	1:C:608:PHE:HD2	1.42	0.82
1:A:607:VAL:HG23	1:A:608:PHE:HD2	1.42	0.82
4:D:1204:YZY:H121	6:D:1206:CAM:H102	1.61	0.82
1:B:328:ILE:CD1	5:B:1205:POV:H31F	2.10	0.82
4:B:1204:YZY:H121	6:B:1206:CAM:H102	1.61	0.81
1:D:611:ILE:HG22	1:D:611:ILE:O	1.77	0.81
1:B:607:VAL:HG23	1:B:608:PHE:HD2	1.42	0.81
4:C:1204:YZY:H121	6:C:1206:CAM:H102	1.61	0.81
1:A:328:ILE:CD1	5:A:1205:POV:H31F	2.10	0.80
4:A:1204:YZY:H121	6:A:1206:CAM:H102	1.61	0.79
1:D:328:ILE:CD1	5:D:1205:POV:H31F	2.10	0.79
1:D:349:MET:HE1	1:D:686:PRO:HD3	1.66	0.78
1:B:349:MET:HE1	1:B:686:PRO:HD3	1.66	0.77
1:C:349:MET:HE1	1:C:686:PRO:HD3	1.66	0.77
4:A:1204:YZY:H121	6:A:1206:CAM:H101	1.65	0.77
4:B:1204:YZY:H121	6:B:1206:CAM:H101	1.65	0.77
1:A:349:MET:HE1	1:A:686:PRO:HD3	1.67	0.77
4:D:1204:YZY:H121	6:D:1206:CAM:H101	1.65	0.77
1:B:618:LEU:HD12	1:B:621:ILE:HD11	1.68	0.76
4:C:1204:YZY:H121	6:C:1206:CAM:H101	1.65	0.75
1:A:618:LEU:HD12	1:A:621:ILE:HD11	1.68	0.75
1:A:328:ILE:HD12	5:A:1205:POV:C315	2.14	0.75
1:C:618:LEU:HD12	1:C:621:ILE:HD11	1.68	0.75
1:B:328:ILE:HD12	5:B:1205:POV:C315	2.14	0.74
1:D:618:LEU:HD12	1:D:621:ILE:HD11	1.68	0.74
1:A:762:VAL:CG1	1:B:767:VAL:HG21	2.18	0.73
1:C:328:ILE:HD12	5:C:1205:POV:C315	2.14	0.73
1:D:328:ILE:HD12	5:D:1205:POV:C315	2.14	0.73
1:B:762:VAL:CG1	1:C:767:VAL:HG21	2.20	0.72
1:A:482:ARG:HD3	1:B:557:TYR:CE2	2.25	0.72
1:C:762:VAL:CG1	1:D:767:VAL:HG21	2.20	0.71
1:C:552:ASN:O	1:C:556:TRP:HB3	1.91	0.71
1:A:273:ARG:O	1:A:274:MET:CG	2.37	0.70
1:B:552:ASN:O	1:B:556:TRP:HB3	1.91	0.70
1:B:478:THR:HG22	1:B:479:ASP:N	2.07	0.70
1:C:207:ILE:HD13	1:C:258:LEU:CD1	2.19	0.70
1:A:767:VAL:HG21	1:D:762:VAL:CG1	2.22	0.69
1:D:207:ILE:HD13	1:D:258:LEU:CD1	2.19	0.69
1:A:478:THR:HG22	1:A:479:ASP:N	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:ASN:O	1:A:556:TRP:HB3	1.91	0.69
1:D:552:ASN:O	1:D:556:TRP:HB3	1.91	0.69
1:D:207:ILE:CD1	1:D:258:LEU:HD11	2.19	0.69
1:D:478:THR:HG22	1:D:479:ASP:N	2.07	0.68
1:C:478:THR:HG22	1:C:479:ASP:N	2.07	0.68
1:C:561:LEU:HD23	1:C:619:ASP:OD1	1.93	0.68
1:A:207:ILE:HD13	1:A:258:LEU:CD1	2.19	0.68
1:A:557:TYR:CE2	1:D:482:ARG:HD3	2.29	0.68
1:B:561:LEU:HD23	1:B:619:ASP:OD1	1.93	0.68
1:B:207:ILE:HD13	1:B:258:LEU:CD1	2.19	0.68
1:D:561:LEU:HD23	1:D:619:ASP:OD1	1.93	0.68
1:A:561:LEU:HD23	1:A:619:ASP:OD1	1.93	0.68
1:A:781:LEU:HD11	1:B:781:LEU:HD13	1.75	0.68
1:C:207:ILE:CD1	1:C:258:LEU:HD11	2.20	0.68
1:A:207:ILE:CD1	1:A:258:LEU:HD11	2.20	0.67
1:B:207:ILE:CD1	1:B:258:LEU:HD11	2.19	0.67
1:B:482:ARG:HD3	1:C:557:TYR:CE2	2.29	0.67
1:C:781:LEU:HD11	1:D:781:LEU:HD13	1.77	0.67
1:C:482:ARG:HD3	1:D:557:TYR:CE2	2.30	0.66
1:D:273:ARG:O	1:D:274:MET:CG	2.37	0.66
1:D:372:LEU:HD13	1:D:410:ILE:CD1	2.27	0.65
1:A:372:LEU:HD13	1:A:410:ILE:CD1	2.27	0.64
1:B:781:LEU:HD11	1:C:781:LEU:HD13	1.78	0.64
1:A:372:LEU:CD1	1:A:410:ILE:HD11	2.27	0.64
1:B:372:LEU:HD13	1:B:410:ILE:CD1	2.27	0.64
1:C:273:ARG:O	1:C:274:MET:CG	2.37	0.64
1:C:372:LEU:HD13	1:C:410:ILE:CD1	2.27	0.64
1:A:781:LEU:HD13	1:D:781:LEU:HD11	1.80	0.64
1:C:372:LEU:CD1	1:C:410:ILE:HD11	2.27	0.64
1:B:273:ARG:O	1:B:274:MET:CG	2.37	0.64
1:D:372:LEU:CD1	1:D:410:ILE:HD11	2.27	0.63
1:B:372:LEU:CD1	1:B:410:ILE:HD11	2.27	0.62
1:D:273:ARG:C	1:D:274:MET:HG2	2.26	0.61
1:A:165:ARG:HH21	1:D:313:ARG:HB3	1.65	0.61
1:A:606:ALA:CA	1:A:611:ILE:CD1	2.75	0.61
1:A:313:ARG:HB3	1:B:165:ARG:HH21	1.65	0.61
1:A:273:ARG:C	1:A:274:MET:HG2	2.26	0.61
1:C:273:ARG:C	1:C:274:MET:HG2	2.26	0.60
1:B:313:ARG:HB3	1:C:165:ARG:HH21	1.65	0.60
1:B:604:PHE:HD2	1:B:605:TRP:CE3	2.20	0.60
1:B:608:PHE:O	1:B:608:PHE:CD1	2.55	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:606:ALA:CA	1:D:611:ILE:CD1	2.75	0.60
1:D:608:PHE:CD1	1:D:608:PHE:O	2.55	0.60
1:D:604:PHE:HD2	1:D:605:TRP:CE3	2.20	0.59
1:C:313:ARG:HB3	1:D:165:ARG:HH21	1.66	0.59
1:C:604:PHE:HD2	1:C:605:TRP:CE3	2.20	0.59
1:C:608:PHE:O	1:C:608:PHE:CD1	2.55	0.59
1:B:638:VAL:O	1:B:642:VAL:HB	2.03	0.59
1:B:273:ARG:C	1:B:274:MET:HG2	2.26	0.59
1:A:608:PHE:O	1:A:608:PHE:CD1	2.55	0.59
1:D:638:VAL:O	1:D:642:VAL:HB	2.03	0.59
1:A:372:LEU:HD13	1:A:410:ILE:HD11	1.85	0.59
1:A:638:VAL:O	1:A:642:VAL:HB	2.03	0.59
1:A:482:ARG:HD3	1:B:557:TYR:CD2	2.37	0.58
1:C:638:VAL:O	1:C:642:VAL:HB	2.03	0.58
1:A:604:PHE:HD2	1:A:605:TRP:CE3	2.20	0.58
1:B:349:MET:O	1:B:355:LYS:NZ	2.37	0.58
1:A:349:MET:O	1:A:355:LYS:NZ	2.37	0.58
1:C:606:ALA:CA	1:C:611:ILE:CD1	2.75	0.58
1:D:372:LEU:HD13	1:D:410:ILE:HD11	1.85	0.58
1:B:372:LEU:HD13	1:B:410:ILE:HD11	1.85	0.58
1:B:606:ALA:CA	1:B:611:ILE:CD1	2.75	0.58
1:A:618:LEU:HD12	1:A:621:ILE:CD1	2.34	0.57
1:D:618:LEU:HD12	1:D:621:ILE:CD1	2.34	0.57
1:A:605:TRP:HH2	4:A:1204:YZY:C1	2.07	0.57
1:B:478:THR:CG2	1:B:479:ASP:N	2.67	0.57
1:C:478:THR:CG2	1:C:479:ASP:N	2.67	0.57
1:C:349:MET:O	1:C:355:LYS:NZ	2.37	0.57
1:D:478:THR:CG2	1:D:479:ASP:N	2.67	0.57
1:D:349:MET:O	1:D:355:LYS:NZ	2.37	0.57
5:B:1205:POV:H311	5:B:1205:POV:H21F	1.87	0.57
1:C:685:CYS:HB2	1:C:690:ASN:HB3	1.88	0.56
5:C:1205:POV:H21F	5:C:1205:POV:H311	1.87	0.56
1:A:478:THR:CG2	1:A:479:ASP:N	2.67	0.56
5:A:1205:POV:H21F	5:A:1205:POV:H311	1.87	0.56
5:D:1205:POV:H311	5:D:1205:POV:H21F	1.87	0.56
1:C:372:LEU:HD13	1:C:410:ILE:HD11	1.85	0.56
1:D:611:ILE:O	1:D:611:ILE:CG2	2.50	0.56
1:A:507:LEU:CD2	6:A:1206:CAM:H51	2.36	0.56
1:B:507:LEU:CD2	6:B:1206:CAM:H51	2.36	0.56
1:A:767:VAL:HG23	1:D:762:VAL:HG11	1.88	0.56
4:D:1204:YZY:C12	6:D:1206:CAM:C10	2.80	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1204:YZY:C12	6:A:1206:CAM:C10	2.80	0.55
1:C:507:LEU:CD2	6:C:1206:CAM:C5	2.85	0.55
1:D:507:LEU:CD2	6:D:1206:CAM:H51	2.36	0.55
1:D:507:LEU:CD2	6:D:1206:CAM:C5	2.85	0.55
1:B:482:ARG:HD3	1:C:557:TYR:CD2	2.42	0.55
1:C:507:LEU:CD2	6:C:1206:CAM:H51	2.36	0.55
1:A:522:LEU:HD21	1:B:651:MET:HE3	1.86	0.55
1:D:685:CYS:HB2	1:D:690:ASN:HB3	1.88	0.55
1:A:685:CYS:HB2	1:A:690:ASN:HB3	1.88	0.55
1:B:605:TRP:HH2	4:B:1204:YZY:C1	2.07	0.55
1:C:482:ARG:HD3	1:D:557:TYR:CD2	2.42	0.55
1:C:618:LEU:HD12	1:C:621:ILE:CD1	2.34	0.55
1:A:507:LEU:CD2	6:A:1206:CAM:C5	2.85	0.55
1:C:445:ILE:CD1	1:C:507:LEU:HD11	2.37	0.55
1:B:507:LEU:HD22	6:B:1206:CAM:H52	1.89	0.55
1:B:685:CYS:HB2	1:B:690:ASN:HB3	1.88	0.55
4:B:1204:YZY:C12	6:B:1206:CAM:C10	2.80	0.54
1:C:522:LEU:HD21	1:D:651:MET:HE3	1.88	0.54
1:D:445:ILE:CD1	1:D:507:LEU:HD11	2.37	0.54
1:B:445:ILE:CD1	1:B:507:LEU:HD11	2.37	0.54
1:D:605:TRP:HH2	4:D:1204:YZY:C1	2.07	0.54
1:B:507:LEU:CD2	6:B:1206:CAM:C5	2.85	0.54
1:B:618:LEU:HD12	1:B:621:ILE:CD1	2.34	0.54
1:A:507:LEU:HD22	6:A:1206:CAM:H52	1.90	0.54
1:C:605:TRP:HH2	4:C:1204:YZY:C1	2.07	0.54
1:C:762:VAL:HG11	1:D:767:VAL:HG23	1.87	0.54
1:A:611:ILE:O	1:A:611:ILE:CG2	2.50	0.54
1:A:762:VAL:HG11	1:B:767:VAL:HG23	1.84	0.54
1:B:445:ILE:HD12	1:B:507:LEU:HD11	1.90	0.54
1:C:517:PRO:HG3	5:C:1205:POV:C15	2.30	0.54
1:C:507:LEU:HD22	6:C:1206:CAM:H52	1.89	0.54
1:A:557:TYR:CD2	1:D:482:ARG:HD3	2.42	0.53
1:C:445:ILE:HD12	1:C:507:LEU:HD11	1.90	0.53
1:D:507:LEU:HD22	6:D:1206:CAM:H52	1.90	0.53
1:D:532:ASP:OD2	1:D:655:SER:OG	2.25	0.53
4:B:1204:YZY:H261	4:B:1204:YZY:H51	1.90	0.53
1:D:561:LEU:CD2	1:D:619:ASP:CG	2.74	0.53
1:A:445:ILE:CD1	1:A:507:LEU:HD11	2.37	0.53
4:A:1204:YZY:H51	4:A:1204:YZY:H261	1.90	0.53
1:A:606:ALA:CA	1:A:611:ILE:HD12	2.20	0.53
1:D:445:ILE:HD12	1:D:507:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:PRO:HG3	5:B:1205:POV:C15	2.30	0.53
4:C:1204:YZY:H51	4:C:1204:YZY:H261	1.90	0.53
1:D:592:ARG:HH21	1:D:602:THR:HG23	1.74	0.53
1:B:522:LEU:HD21	1:C:651:MET:HE3	1.88	0.53
4:D:1204:YZY:H261	4:D:1204:YZY:H51	1.90	0.53
1:C:93:SER:OG	1:C:142:ARG:NH1	2.42	0.53
1:B:592:ARG:HH21	1:B:602:THR:HG23	1.74	0.52
1:B:762:VAL:HG11	1:C:767:VAL:HG23	1.87	0.52
1:A:445:ILE:HD12	1:A:507:LEU:HD11	1.90	0.52
1:C:592:ARG:HH21	1:C:602:THR:HG23	1.74	0.52
1:A:93:SER:OG	1:A:142:ARG:NH1	2.42	0.52
1:D:93:SER:OG	1:D:142:ARG:NH1	2.42	0.52
1:A:592:ARG:HH21	1:A:602:THR:HG23	1.74	0.52
1:D:601:GLN:O	1:D:605:TRP:HE3	1.93	0.52
1:A:601:GLN:O	1:A:605:TRP:HE3	1.92	0.52
1:B:618:LEU:HB2	1:B:621:ILE:CD1	2.40	0.52
1:C:601:GLN:O	1:C:605:TRP:HE3	1.93	0.52
1:A:328:ILE:CD1	5:A:1205:POV:C315	2.84	0.52
1:A:650:ALA:HA	1:D:653:ASN:ND2	2.25	0.52
1:C:606:ALA:CA	1:C:611:ILE:HD12	2.20	0.52
1:B:93:SER:OG	1:B:142:ARG:NH1	2.42	0.51
1:B:561:LEU:CD2	1:B:619:ASP:CG	2.74	0.51
1:B:601:GLN:O	1:B:605:TRP:HE3	1.92	0.51
1:C:30:ARG:NH1	1:C:779:CYS:SG	2.83	0.51
1:A:561:LEU:CD2	1:A:619:ASP:CG	2.74	0.51
1:B:735:ASP:O	1:B:739:GLN:HG2	2.10	0.51
1:D:735:ASP:O	1:D:739:GLN:HG2	2.10	0.51
1:A:30:ARG:NH1	1:A:779:CYS:SG	2.83	0.51
1:A:618:LEU:HB2	1:A:621:ILE:CD1	2.40	0.51
1:B:30:ARG:NH1	1:B:779:CYS:SG	2.83	0.51
1:D:603:LEU:O	1:D:636:TYR:OH	2.26	0.51
1:C:618:LEU:HB2	1:C:621:ILE:CD1	2.40	0.51
1:A:735:ASP:O	1:A:739:GLN:HG2	2.10	0.51
1:C:769:GLU:OE1	1:D:771:LYS:NZ	2.41	0.51
1:A:517:PRO:HG3	5:A:1205:POV:C15	2.30	0.51
1:C:735:ASP:O	1:C:739:GLN:HG2	2.10	0.51
4:C:1204:YZY:C12	6:C:1206:CAM:C10	2.80	0.51
1:D:30:ARG:NH1	1:D:779:CYS:SG	2.83	0.51
1:D:618:LEU:HB2	1:D:621:ILE:CD1	2.40	0.50
1:C:40:LEU:HD11	1:C:77:LEU:HD23	1.94	0.50
1:A:767:VAL:HG13	1:D:770:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:ASP:OD2	1:B:655:SER:OG	2.25	0.50
1:D:40:LEU:HD11	1:D:77:LEU:HD23	1.94	0.50
1:B:770:ILE:HD11	1:C:767:VAL:HG13	1.94	0.50
1:A:769:GLU:OE1	1:B:771:LYS:NZ	2.40	0.49
1:B:40:LEU:HD11	1:B:77:LEU:HD23	1.94	0.49
1:A:274:MET:O	1:A:275:HIS:HB2	2.13	0.49
1:D:517:PRO:HG3	5:D:1205:POV:C15	2.30	0.49
1:A:603:LEU:O	1:A:636:TYR:OH	2.26	0.49
1:A:40:LEU:HD11	1:A:77:LEU:HD23	1.94	0.49
1:C:274:MET:O	1:C:275:HIS:HB2	2.13	0.49
1:C:770:ILE:HD11	1:D:767:VAL:HG13	1.94	0.49
1:A:770:ILE:HD11	1:B:767:VAL:HG13	1.94	0.49
1:C:60:THR:HG22	1:C:61:ALA:N	2.28	0.49
1:C:532:ASP:OD2	1:C:655:SER:OG	2.25	0.49
1:B:274:MET:O	1:B:275:HIS:HB2	2.13	0.48
1:D:274:MET:O	1:D:275:HIS:HB2	2.13	0.48
1:B:207:ILE:CD1	1:B:258:LEU:CD1	2.88	0.48
1:A:651:MET:HE3	1:D:522:LEU:HD21	1.91	0.48
1:D:60:THR:HG22	1:D:61:ALA:N	2.28	0.48
1:B:60:THR:HG22	1:B:61:ALA:N	2.28	0.48
1:A:60:THR:HG22	1:A:61:ALA:N	2.28	0.48
1:A:207:ILE:CD1	1:A:258:LEU:CD1	2.88	0.48
1:C:611:ILE:O	1:C:611:ILE:CG2	2.50	0.48
1:A:321:VAL:HA	1:A:324:ILE:HG22	1.96	0.47
1:C:328:ILE:CD1	5:C:1205:POV:C315	2.84	0.47
1:C:250:ARG:NH2	1:D:128:THR:O	2.47	0.47
1:A:126:THR:HA	1:D:747:ARG:HH22	1.79	0.47
1:B:603:LEU:O	1:B:636:TYR:OH	2.26	0.47
1:D:606:ALA:CA	1:D:611:ILE:HD12	2.20	0.47
1:A:128:THR:O	1:D:250:ARG:NH2	2.48	0.47
1:C:747:ARG:HH22	1:D:126:THR:HA	1.80	0.47
1:D:321:VAL:HA	1:D:324:ILE:HG22	1.96	0.47
4:C:1204:YZY:C12	6:C:1206:CAM:H101	2.42	0.47
1:A:653:ASN:ND2	1:B:650:ALA:HA	2.30	0.47
1:B:478:THR:CG2	1:B:479:ASP:H	2.28	0.47
1:B:653:ASN:ND2	1:C:650:ALA:HA	2.29	0.47
1:B:769:GLU:OE1	1:C:771:LYS:NZ	2.42	0.47
1:D:588:ILE:N	1:D:610:LEU:HD21	2.30	0.47
1:C:478:THR:CG2	1:C:479:ASP:H	2.28	0.47
1:C:653:ASN:ND2	1:D:650:ALA:HA	2.29	0.47
1:D:478:THR:CG2	1:D:479:ASP:H	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:747:ARG:HH22	1:B:126:THR:HA	1.80	0.47
1:C:588:ILE:N	1:C:610:LEU:HD21	2.30	0.47
1:C:603:LEU:O	1:C:636:TYR:OH	2.26	0.47
1:A:211:PHE:HB3	1:A:285:LEU:HD12	1.97	0.46
1:B:747:ARG:HH22	1:C:126:THR:HA	1.80	0.46
1:C:207:ILE:CD1	1:C:258:LEU:CD1	2.88	0.46
1:B:321:VAL:HA	1:B:324:ILE:HG22	1.96	0.46
1:C:211:PHE:HB3	1:C:285:LEU:HD12	1.97	0.46
1:D:207:ILE:CD1	1:D:258:LEU:CD1	2.88	0.46
1:A:647:LEU:O	1:A:651:MET:HG3	2.16	0.46
1:A:686:PRO:HB2	1:A:688:PRO:HD2	1.98	0.46
1:A:250:ARG:NH2	1:B:128:THR:O	2.48	0.46
1:C:647:LEU:O	1:C:651:MET:HG3	2.16	0.46
1:D:211:PHE:HB3	1:D:285:LEU:HD12	1.97	0.46
1:D:347:GLN:OE1	1:D:350:ARG:NH1	2.49	0.46
1:D:647:LEU:O	1:D:651:MET:HG3	2.16	0.46
1:A:588:ILE:N	1:A:610:LEU:HD21	2.30	0.46
1:B:588:ILE:N	1:B:610:LEU:HD21	2.30	0.46
1:C:321:VAL:HA	1:C:324:ILE:HG22	1.96	0.46
1:D:328:ILE:CD1	5:D:1205:POV:C315	2.84	0.46
1:D:606:ALA:HA	1:D:611:ILE:HD11	1.91	0.46
1:B:686:PRO:HB2	1:B:688:PRO:HD2	1.98	0.46
1:D:686:PRO:HB2	1:D:688:PRO:HD2	1.98	0.46
4:D:1204:YZY:C12	6:D:1206:CAM:H101	2.42	0.46
5:D:1205:POV:H2	5:D:1205:POV:O14	2.15	0.46
1:B:250:ARG:NH2	1:C:128:THR:O	2.47	0.45
5:B:1205:POV:H2	5:B:1205:POV:O14	2.15	0.45
1:A:478:THR:CG2	1:A:479:ASP:H	2.28	0.45
1:C:561:LEU:CD2	1:C:619:ASP:CG	2.74	0.45
1:B:647:LEU:O	1:B:651:MET:HG3	2.16	0.45
1:C:347:GLN:OE1	1:C:350:ARG:NH1	2.49	0.45
5:C:1205:POV:O14	5:C:1205:POV:H2	2.15	0.45
5:A:1205:POV:H2	5:A:1205:POV:O14	2.15	0.45
1:B:347:GLN:OE1	1:B:350:ARG:NH1	2.49	0.45
1:C:561:LEU:HD23	1:C:619:ASP:OD2	2.16	0.45
1:A:322:ASP:HA	1:A:325:ARG:HG2	1.99	0.45
1:B:211:PHE:HB3	1:B:285:LEU:HD12	1.97	0.45
1:D:322:ASP:HA	1:D:325:ARG:HG2	1.99	0.45
1:D:348:THR:HG22	1:D:354:ILE:HG21	1.99	0.45
1:A:642:VAL:HG13	1:D:648:LEU:HD21	1.98	0.45
1:D:198:LEU:O	1:D:202:SER:OG	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:GLN:OE1	1:A:350:ARG:NH1	2.49	0.44
1:C:686:PRO:HB2	1:C:688:PRO:HD2	1.98	0.44
1:C:348:THR:HG22	1:C:354:ILE:HG21	1.99	0.44
1:C:618:LEU:HB2	1:C:621:ILE:HD11	1.98	0.44
1:A:348:THR:HG22	1:A:354:ILE:HG21	1.99	0.44
1:B:245:LEU:HD23	1:B:245:LEU:HA	1.84	0.44
1:B:328:ILE:CD1	5:B:1205:POV:C315	2.84	0.44
1:B:205:ASP:OD1	1:B:738:TYR:OH	2.28	0.44
1:B:618:LEU:HB2	1:B:621:ILE:HD11	1.99	0.44
1:C:137:ILE:HG23	1:C:192:ALA:HB2	1.99	0.44
1:C:549:SER:O	1:C:553:GLN:HG2	2.18	0.44
1:D:245:LEU:HD23	1:D:245:LEU:HA	1.84	0.44
1:A:618:LEU:HB2	1:A:621:ILE:HD11	1.98	0.44
1:A:771:LYS:NZ	1:D:769:GLU:OE1	2.43	0.44
1:B:348:THR:HG22	1:B:354:ILE:HG21	1.99	0.44
1:C:322:ASP:HA	1:C:325:ARG:HG2	1.99	0.44
1:D:137:ILE:HG23	1:D:192:ALA:HB2	1.99	0.44
1:B:549:SER:O	1:B:553:GLN:HG2	2.18	0.44
1:D:618:LEU:HB2	1:D:621:ILE:HD11	1.98	0.44
1:B:137:ILE:HG23	1:B:192:ALA:HB2	1.99	0.43
1:B:592:ARG:NH1	1:B:610:LEU:CD1	2.81	0.43
1:C:507:LEU:HD22	6:C:1206:CAM:C5	2.49	0.43
1:A:592:ARG:NH1	1:A:610:LEU:CD1	2.81	0.43
1:A:780:GLU:OE1	1:B:778:ARG:NE	2.48	0.43
1:B:322:ASP:HA	1:B:325:ARG:HG2	1.99	0.43
1:B:606:ALA:HA	1:B:611:ILE:HD11	1.91	0.43
1:D:507:LEU:HD22	6:D:1206:CAM:C5	2.49	0.43
1:A:137:ILE:HG23	1:A:192:ALA:HB2	1.99	0.43
1:A:245:LEU:HD23	1:A:245:LEU:HA	1.84	0.43
1:A:618:LEU:CD1	1:A:621:ILE:HD11	2.45	0.43
1:C:592:ARG:NH1	1:C:610:LEU:CD1	2.81	0.43
1:D:592:ARG:NH1	1:D:610:LEU:CD1	2.81	0.43
1:B:605:TRP:CH2	4:B:1204:YZY:C1	2.91	0.43
1:D:471:MET:CE	1:D:477:ALA:HB3	2.49	0.43
1:B:648:LEU:HD21	1:C:642:VAL:HG13	2.01	0.43
1:C:471:MET:CE	1:C:477:ALA:HB3	2.49	0.43
1:D:549:SER:O	1:D:553:GLN:HG2	2.18	0.43
1:C:618:LEU:CD1	1:C:621:ILE:HD11	2.45	0.43
1:B:611:ILE:O	1:B:611:ILE:CG2	2.50	0.43
1:C:605:TRP:CH2	4:C:1204:YZY:C1	2.91	0.43
1:C:648:LEU:HD21	1:D:642:VAL:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:SER:O	1:A:553:GLN:HG2	2.18	0.43
1:B:471:MET:CE	1:B:477:ALA:HB3	2.49	0.43
1:B:507:LEU:HD22	6:B:1206:CAM:C5	2.49	0.43
1:A:471:MET:CE	1:A:477:ALA:HB3	2.49	0.43
1:A:532:ASP:OD2	1:A:655:SER:OG	2.25	0.43
1:C:245:LEU:HD23	1:C:245:LEU:HA	1.84	0.42
1:A:507:LEU:HD22	6:A:1206:CAM:C5	2.49	0.42
1:D:561:LEU:HD23	1:D:619:ASP:OD2	2.16	0.42
1:A:766:ASP:HB3	1:B:767:VAL:HG11	2.02	0.42
1:B:297:GLN:NE2	1:B:672:SER:OG	2.43	0.42
4:A:1204:YZY:C12	6:A:1206:CAM:H101	2.42	0.42
1:C:603:LEU:HA	1:C:606:ALA:HB2	2.02	0.42
1:D:297:GLN:NE2	1:D:672:SER:OG	2.43	0.42
1:B:603:LEU:HA	1:B:606:ALA:HB2	2.02	0.42
1:B:780:GLU:OE1	1:C:778:ARG:NE	2.51	0.41
1:A:201:LEU:HD23	1:A:201:LEU:HA	1.93	0.41
1:A:334:SER:O	1:A:338:ILE:HG12	2.21	0.41
1:B:608:PHE:O	1:B:608:PHE:HD1	2.03	0.41
1:B:662:ARG:HE	1:B:662:ARG:HB2	1.75	0.41
1:C:662:ARG:HE	1:C:662:ARG:HB2	1.75	0.41
1:D:603:LEU:HA	1:D:606:ALA:HB2	2.02	0.41
1:D:673:LYS:HE2	1:D:673:LYS:HB3	1.91	0.41
1:C:198:LEU:O	1:C:202:SER:OG	2.33	0.41
1:D:205:ASP:OD1	1:D:738:TYR:OH	2.28	0.41
5:B:1205:POV:H13B	5:B:1205:POV:H11	1.91	0.41
1:B:220:LEU:HD23	1:B:220:LEU:HA	1.91	0.41
1:B:345:ILE:HD12	1:B:345:ILE:HA	1.97	0.41
1:B:471:MET:HE2	1:B:477:ALA:HB3	2.03	0.41
1:B:614:ASP:OD1	1:B:614:ASP:N	2.54	0.41
1:D:201:LEU:HD23	1:D:201:LEU:HA	1.93	0.41
1:D:334:SER:O	1:D:338:ILE:HG12	2.21	0.41
1:A:606:ALA:HA	1:A:611:ILE:HD11	1.91	0.41
1:B:478:THR:HG22	1:B:479:ASP:H	1.82	0.41
1:C:297:GLN:NE2	1:C:672:SER:OG	2.43	0.41
1:C:621:ILE:HG22	1:C:626:ARG:HG2	2.02	0.41
1:B:334:SER:O	1:B:338:ILE:HG12	2.21	0.41
1:B:618:LEU:CD1	1:B:621:ILE:HD11	2.45	0.41
1:D:530:VAL:HA	1:D:533:ILE:HD12	2.03	0.41
1:A:603:LEU:HA	1:A:606:ALA:HB2	2.02	0.40
1:D:608:PHE:O	1:D:608:PHE:HD1	2.03	0.40
1:D:618:LEU:CD1	1:D:621:ILE:HD11	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ASP:OD1	1:B:125:ASP:N	2.55	0.40
1:A:454:VAL:HA	1:A:457:VAL:HG22	2.03	0.40
1:D:478:THR:HG22	1:D:479:ASP:H	1.82	0.40
1:A:621:ILE:HG22	1:A:626:ARG:HG2	2.02	0.40
1:B:151:LEU:HD23	1:B:151:LEU:HA	1.92	0.40
1:C:275:HIS:O	1:C:276:LEU:C	2.65	0.40
1:C:334:SER:O	1:C:338:ILE:HG12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	684/1128 (61%)	659 (96%)	25 (4%)	0	100	100
1	B	684/1128 (61%)	660 (96%)	24 (4%)	0	100	100
1	C	684/1128 (61%)	659 (96%)	25 (4%)	0	100	100
1	D	684/1128 (61%)	659 (96%)	25 (4%)	0	100	100
All	All	2736/4512 (61%)	2637 (96%)	99 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	625/985 (64%)	625 (100%)	0	100	100
1	B	625/985 (64%)	625 (100%)	0	100	100
1	C	625/985 (64%)	625 (100%)	0	100	100
1	D	625/985 (64%)	625 (100%)	0	100	100
All	All	2500/3940 (64%)	2500 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	GLN
1	A	237	GLN
1	A	553	GLN
1	A	595	ASN
1	A	654	HIS
1	A	768	ASN
1	B	237	GLN
1	B	595	ASN
1	B	653	ASN
1	B	654	HIS
1	B	768	ASN
1	C	237	GLN
1	C	553	GLN
1	C	595	ASN
1	C	654	HIS
1	C	768	ASN
1	D	237	GLN
1	D	553	GLN
1	D	595	ASN
1	D	653	ASN
1	D	654	HIS
1	D	768	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 29 ligands modelled in this entry, 17 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	POV	D	1205	-	51,51,51	0.50	0	57,59,59	0.46	0
5	POV	A	1205	-	51,51,51	0.50	0	57,59,59	0.46	0
4	YZY	D	1204	-	34,34,41	0.93	4 (11%)	36,36,43	1.22	2 (5%)
6	CAM	C	1206	-	12,12,12	0.21	0	20,21,21	0.46	0
5	POV	C	1205	-	51,51,51	0.50	0	57,59,59	0.46	0
5	POV	B	1205	-	51,51,51	0.50	0	57,59,59	0.46	0
4	YZY	B	1204	-	34,34,41	0.93	4 (11%)	36,36,43	1.21	2 (5%)
6	CAM	A	1206	-	12,12,12	0.21	0	20,21,21	0.46	0
4	YZY	C	1204	-	34,34,41	0.94	4 (11%)	36,36,43	1.22	2 (5%)
6	CAM	D	1206	-	12,12,12	0.21	0	20,21,21	0.46	0
4	YZY	A	1204	-	34,34,41	0.93	4 (11%)	36,36,43	1.22	2 (5%)
6	CAM	B	1206	-	12,12,12	0.19	0	20,21,21	0.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	POV	D	1205	-	-	20/55/55/55	-
5	POV	A	1205	-	-	20/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	YZY	D	1204	-	-	15/36/36/43	-
6	CAM	C	1206	-	-	-	0/3/2/2
5	POV	C	1205	-	-	20/55/55/55	-
5	POV	B	1205	-	-	20/55/55/55	-
4	YZY	B	1204	-	-	15/36/36/43	-
6	CAM	A	1206	-	-	-	0/3/2/2
4	YZY	C	1204	-	-	15/36/36/43	-
6	CAM	D	1206	-	-	-	0/3/2/2
4	YZY	A	1204	-	-	15/36/36/43	-
6	CAM	B	1206	-	-	-	0/3/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1204	YZY	O2-C2	-2.47	1.40	1.46
4	D	1204	YZY	O2-C2	-2.45	1.40	1.46
4	A	1204	YZY	O2-C2	-2.44	1.40	1.46
4	B	1204	YZY	O2-C2	-2.44	1.40	1.46
4	A	1204	YZY	O4-C20	2.39	1.40	1.33
4	B	1204	YZY	O4-C20	2.39	1.40	1.33
4	C	1204	YZY	O4-C20	2.39	1.40	1.33
4	D	1204	YZY	O4-C20	2.37	1.40	1.33
4	C	1204	YZY	O2-C3	2.21	1.40	1.34
4	D	1204	YZY	O2-C3	2.21	1.40	1.34
4	A	1204	YZY	O2-C3	2.20	1.40	1.34
4	B	1204	YZY	O2-C3	2.20	1.40	1.34
4	B	1204	YZY	O4-C19	-2.09	1.40	1.45
4	A	1204	YZY	O4-C19	-2.08	1.40	1.45
4	C	1204	YZY	O4-C19	-2.08	1.40	1.45
4	D	1204	YZY	O4-C19	-2.08	1.40	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1204	YZY	O2-C3-C4	4.08	120.30	111.50
4	C	1204	YZY	O2-C3-C4	4.08	120.29	111.50
4	D	1204	YZY	O2-C3-C4	4.08	120.29	111.50
4	B	1204	YZY	O2-C3-C4	4.06	120.24	111.50
4	C	1204	YZY	O4-C20-C21	2.54	119.89	111.91
4	A	1204	YZY	O4-C20-C21	2.54	119.86	111.91
4	D	1204	YZY	O4-C20-C21	2.53	119.84	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1204	YZY	O4-C20-C21	2.52	119.82	111.91

There are no chirality outliers.

All (140) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1204	YZY	O1-C1-C2-O2
4	A	1204	YZY	O1-C1-C2-C19
4	B	1204	YZY	O1-C1-C2-O2
4	B	1204	YZY	O1-C1-C2-C19
4	C	1204	YZY	O1-C1-C2-O2
4	C	1204	YZY	O1-C1-C2-C19
4	D	1204	YZY	O1-C1-C2-O2
4	D	1204	YZY	O1-C1-C2-C19
5	A	1205	POV	C2-C1-O11-P
5	A	1205	POV	C12-C11-O12-P
5	B	1205	POV	C2-C1-O11-P
5	B	1205	POV	C12-C11-O12-P
5	C	1205	POV	C2-C1-O11-P
5	C	1205	POV	C12-C11-O12-P
5	D	1205	POV	C2-C1-O11-P
5	D	1205	POV	C12-C11-O12-P
4	A	1204	YZY	C21-C20-O4-C19
4	B	1204	YZY	C21-C20-O4-C19
4	C	1204	YZY	C21-C20-O4-C19
4	D	1204	YZY	C21-C20-O4-C19
4	A	1204	YZY	O5-C20-O4-C19
4	B	1204	YZY	O5-C20-O4-C19
4	C	1204	YZY	O5-C20-O4-C19
4	D	1204	YZY	O5-C20-O4-C19
5	A	1205	POV	C310-C311-C312-C313
5	B	1205	POV	C310-C311-C312-C313
5	C	1205	POV	C310-C311-C312-C313
5	D	1205	POV	C310-C311-C312-C313
4	A	1204	YZY	C20-C21-C22-C23
4	B	1204	YZY	C20-C21-C22-C23
4	C	1204	YZY	C20-C21-C22-C23
4	D	1204	YZY	C20-C21-C22-C23
5	B	1205	POV	C36-C37-C38-C39
5	C	1205	POV	C36-C37-C38-C39
5	A	1205	POV	C36-C37-C38-C39
5	D	1205	POV	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
5	A	1205	POV	C11-O12-P-O11
5	B	1205	POV	C11-O12-P-O11
5	C	1205	POV	C11-O12-P-O11
5	D	1205	POV	C11-O12-P-O11
4	A	1204	YZY	C3-C4-C5-C6
4	B	1204	YZY	C3-C4-C5-C6
4	C	1204	YZY	C3-C4-C5-C6
4	D	1204	YZY	C3-C4-C5-C6
4	A	1204	YZY	C4-C3-O2-C2
4	B	1204	YZY	C4-C3-O2-C2
4	C	1204	YZY	C4-C3-O2-C2
4	D	1204	YZY	C4-C3-O2-C2
4	B	1204	YZY	C22-C23-C24-C25
4	D	1204	YZY	C22-C23-C24-C25
4	A	1204	YZY	C22-C23-C24-C25
4	C	1204	YZY	C22-C23-C24-C25
5	A	1205	POV	C213-C214-C215-C216
5	B	1205	POV	C213-C214-C215-C216
5	C	1205	POV	C213-C214-C215-C216
5	D	1205	POV	C213-C214-C215-C216
4	A	1204	YZY	O3-C3-O2-C2
4	B	1204	YZY	O3-C3-O2-C2
4	C	1204	YZY	O3-C3-O2-C2
4	D	1204	YZY	O3-C3-O2-C2
4	C	1204	YZY	C4-C5-C6-C7
5	A	1205	POV	O11-C1-C2-C3
5	B	1205	POV	O11-C1-C2-C3
5	C	1205	POV	O11-C1-C2-C3
5	D	1205	POV	O11-C1-C2-C3
4	A	1204	YZY	C4-C5-C6-C7
4	B	1204	YZY	C4-C5-C6-C7
4	D	1204	YZY	C4-C5-C6-C7
4	A	1204	YZY	O4-C19-C2-C1
4	B	1204	YZY	O4-C19-C2-C1
4	C	1204	YZY	O4-C19-C2-C1
4	D	1204	YZY	O4-C19-C2-C1
5	B	1205	POV	C22-C23-C24-C25
5	A	1205	POV	C22-C23-C24-C25
5	C	1205	POV	C22-C23-C24-C25
5	D	1205	POV	C22-C23-C24-C25
4	A	1204	YZY	C7-C8-C9-C10
4	B	1204	YZY	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
4	C	1204	YZY	C7-C8-C9-C10
4	D	1204	YZY	C7-C8-C9-C10
5	A	1205	POV	C33-C34-C35-C36
5	C	1205	POV	C33-C34-C35-C36
5	B	1205	POV	C33-C34-C35-C36
5	D	1205	POV	C33-C34-C35-C36
5	A	1205	POV	C37-C38-C39-C310
5	B	1205	POV	C37-C38-C39-C310
5	D	1205	POV	C37-C38-C39-C310
5	C	1205	POV	C37-C38-C39-C310
5	A	1205	POV	C11-O12-P-O14
5	B	1205	POV	C11-O12-P-O14
5	C	1205	POV	C11-O12-P-O14
5	D	1205	POV	C11-O12-P-O14
5	A	1205	POV	C39-C310-C311-C312
5	B	1205	POV	C39-C310-C311-C312
5	C	1205	POV	C39-C310-C311-C312
5	D	1205	POV	C39-C310-C311-C312
5	A	1205	POV	O11-C1-C2-O21
5	B	1205	POV	O11-C1-C2-O21
5	C	1205	POV	O11-C1-C2-O21
5	D	1205	POV	O11-C1-C2-O21
4	D	1204	YZY	C6-C7-C8-C9
4	A	1204	YZY	C6-C7-C8-C9
4	B	1204	YZY	C6-C7-C8-C9
4	C	1204	YZY	C6-C7-C8-C9
5	B	1205	POV	C24-C25-C26-C27
5	C	1205	POV	C24-C25-C26-C27
5	D	1205	POV	C24-C25-C26-C27
5	A	1205	POV	C24-C25-C26-C27
4	A	1204	YZY	O4-C19-C2-O2
4	B	1204	YZY	O4-C19-C2-O2
4	C	1204	YZY	O4-C19-C2-O2
4	D	1204	YZY	O4-C19-C2-O2
5	A	1205	POV	C22-C21-O21-C2
5	B	1205	POV	C22-C21-O21-C2
5	C	1205	POV	C22-C21-O21-C2
5	D	1205	POV	C22-C21-O21-C2
5	A	1205	POV	O22-C21-O21-C2
5	B	1205	POV	O22-C21-O21-C2
5	C	1205	POV	O22-C21-O21-C2
5	D	1205	POV	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
5	A	1205	POV	C1-O11-P-O12
5	B	1205	POV	C1-O11-P-O12
5	C	1205	POV	C1-O11-P-O12
5	D	1205	POV	C1-O11-P-O12
5	D	1205	POV	C31-C32-C33-C34
5	A	1205	POV	C31-C32-C33-C34
5	B	1205	POV	C31-C32-C33-C34
5	C	1205	POV	C31-C32-C33-C34
4	D	1204	YZY	C10-C11-C12-C13
4	A	1204	YZY	C10-C11-C12-C13
4	B	1204	YZY	C10-C11-C12-C13
4	C	1204	YZY	C10-C11-C12-C13
5	A	1205	POV	C210-C211-C212-C213
5	B	1205	POV	C210-C211-C212-C213
5	C	1205	POV	C210-C211-C212-C213
5	D	1205	POV	C210-C211-C212-C213
5	A	1205	POV	C1-O11-P-O14
5	B	1205	POV	C1-O11-P-O14
5	C	1205	POV	C1-O11-P-O14
5	D	1205	POV	C1-O11-P-O14

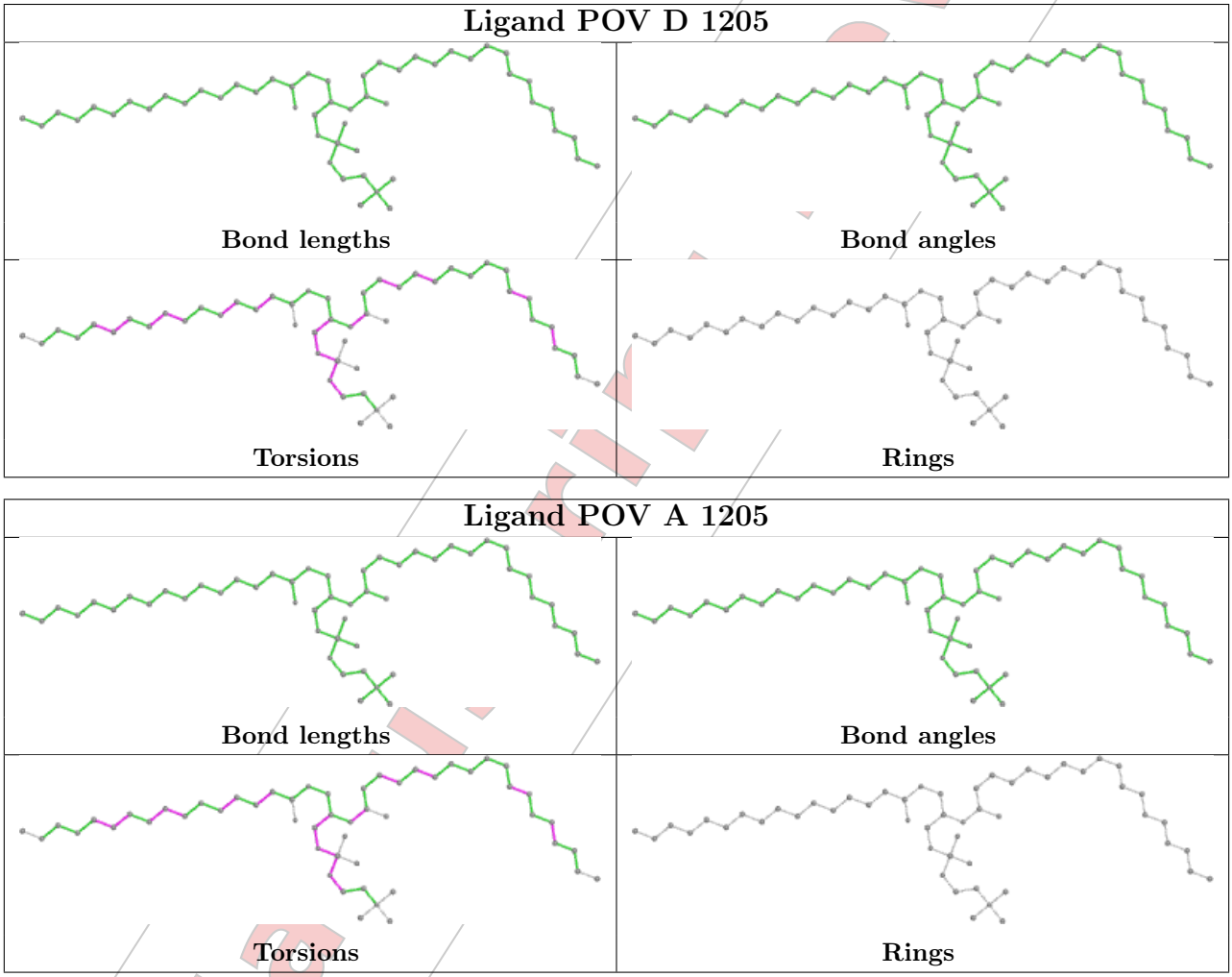
There are no ring outliers.

12 monomers are involved in 86 short contacts:

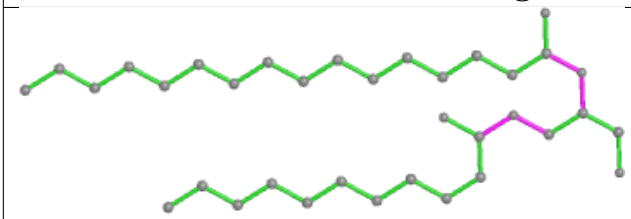
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1205	POV	8	0
5	A	1205	POV	8	0
4	D	1204	YZY	9	0
6	C	1206	CAM	9	0
5	C	1205	POV	8	0
5	B	1205	POV	9	0
4	B	1204	YZY	9	0
6	A	1206	CAM	9	0
4	C	1204	YZY	10	0
6	D	1206	CAM	9	0
4	A	1204	YZY	9	0
6	B	1206	CAM	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

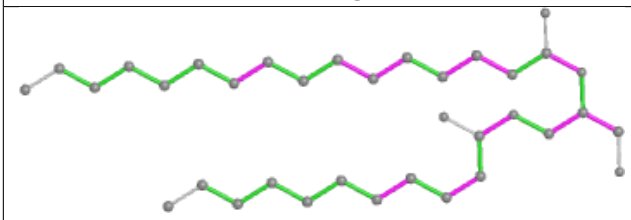


Ligand YZY D 1204

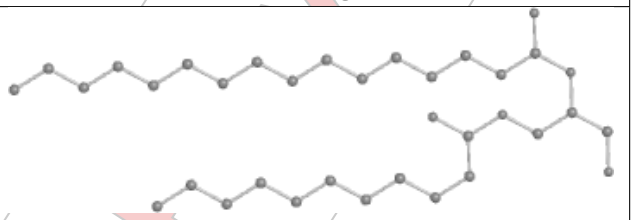


Bond lengths

Bond angles

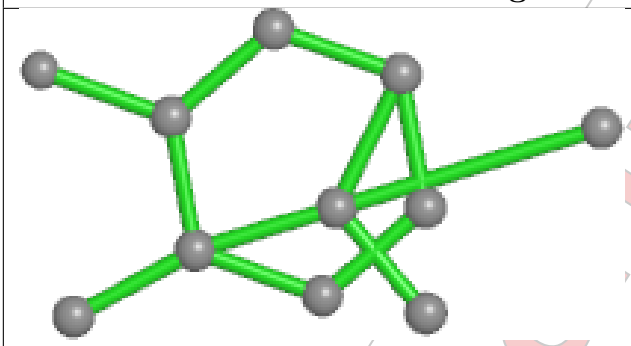


Torsions

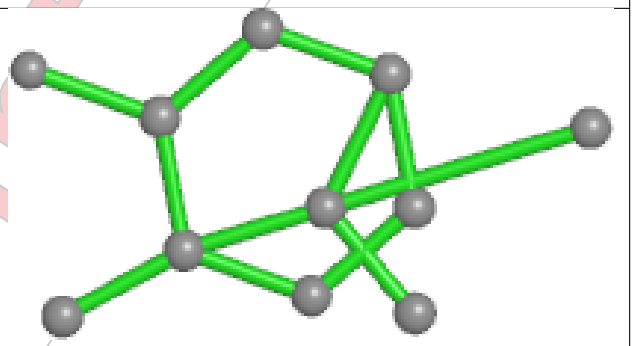


Rings

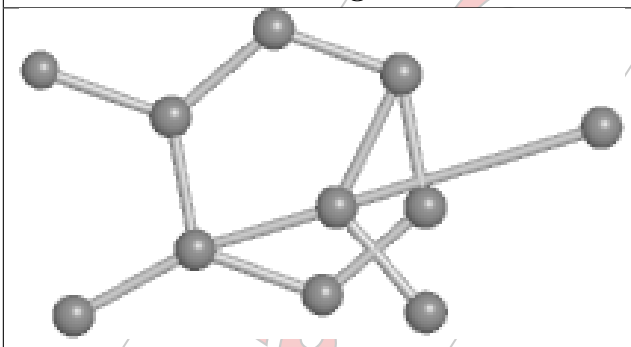
Ligand CAM C 1206



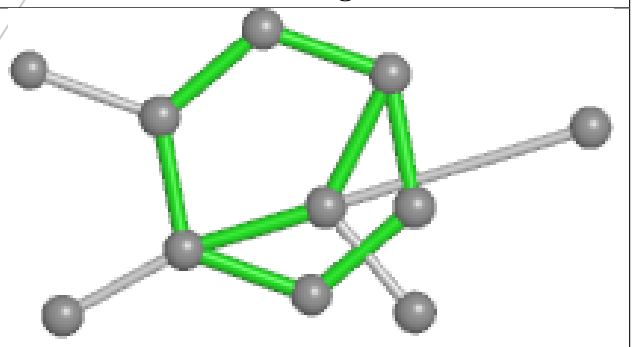
Bond lengths



Bond angles

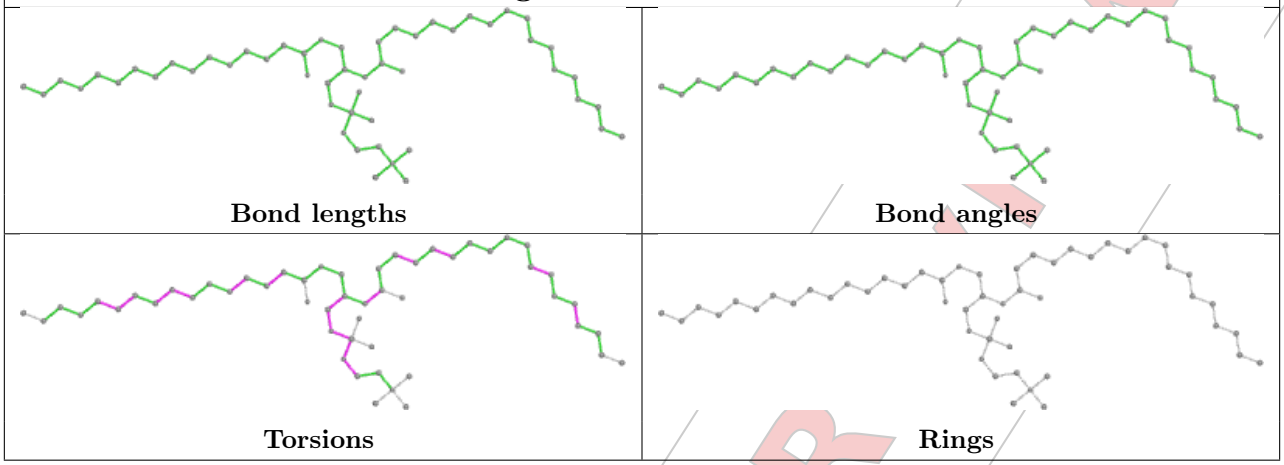


Torsions

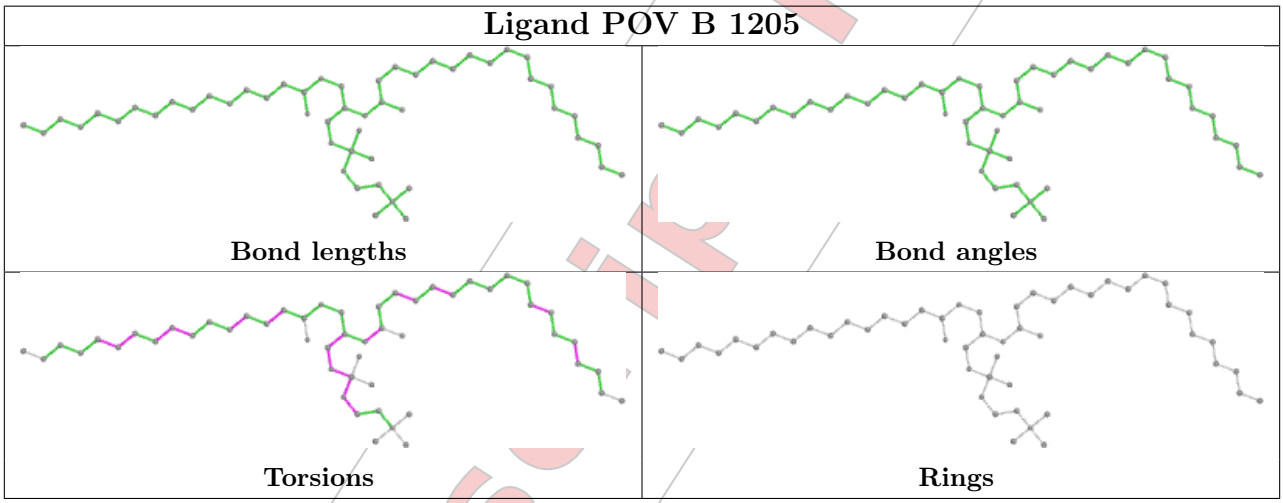


Rings

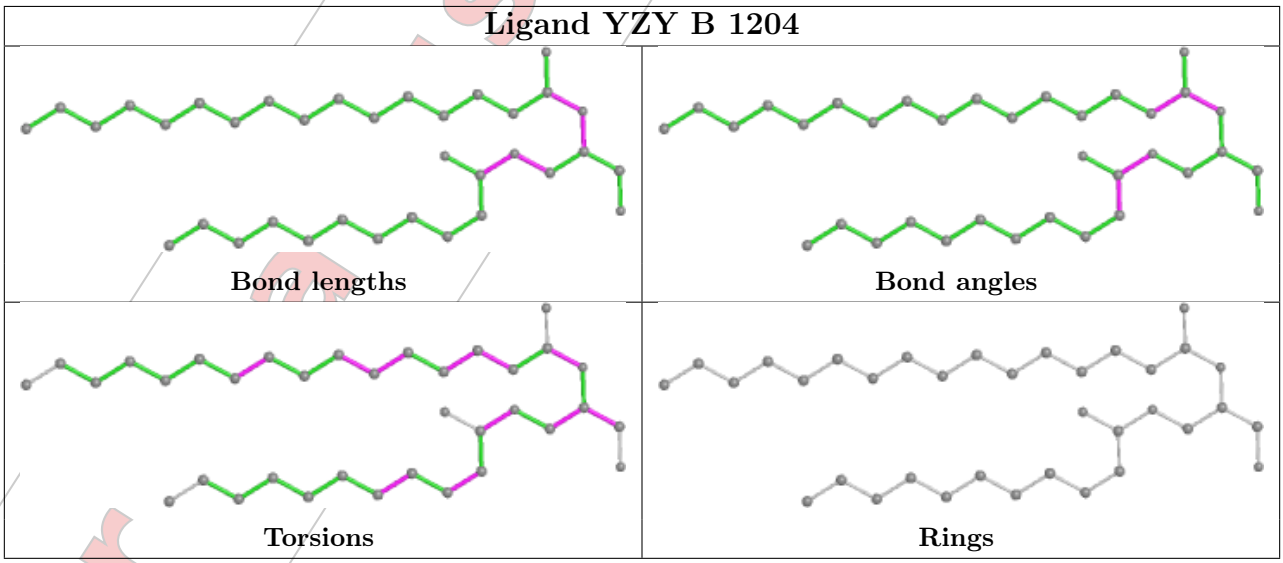
Ligand POV C 1205



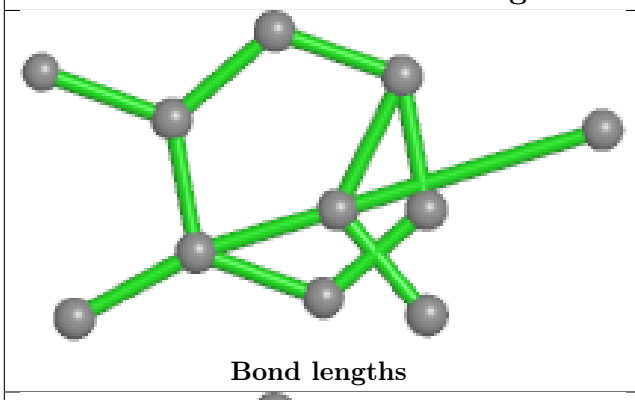
Ligand POV B 1205



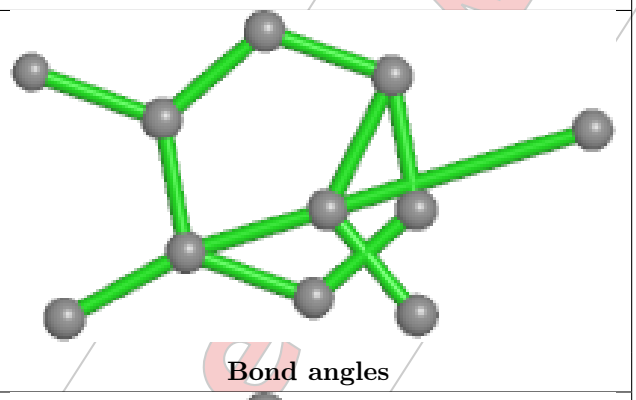
Ligand YZY B 1204



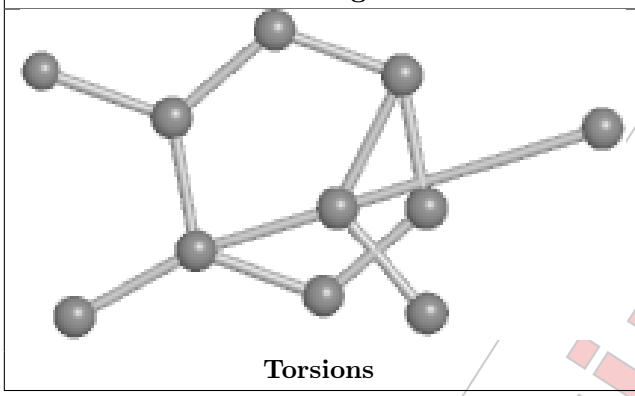
Ligand CAM A 1206



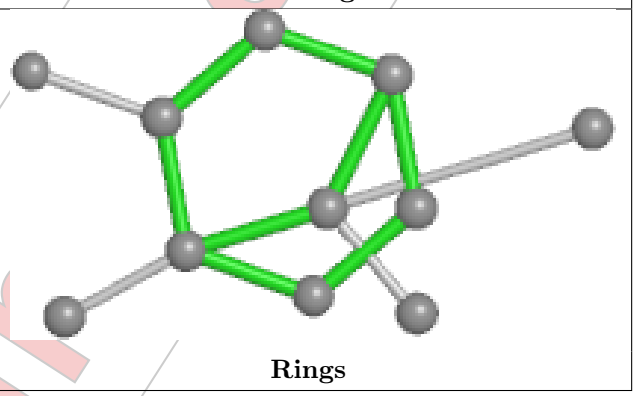
Bond lengths



Bond angles

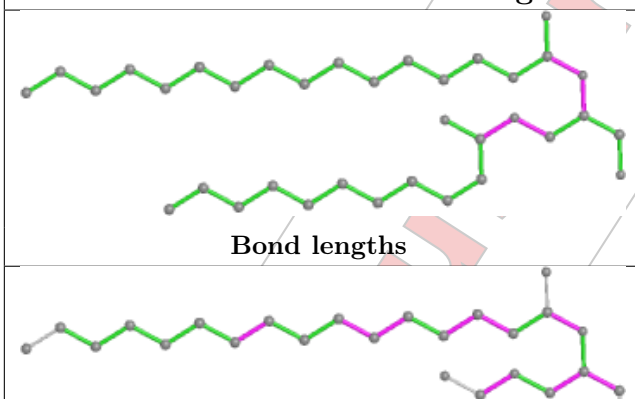


Torsions

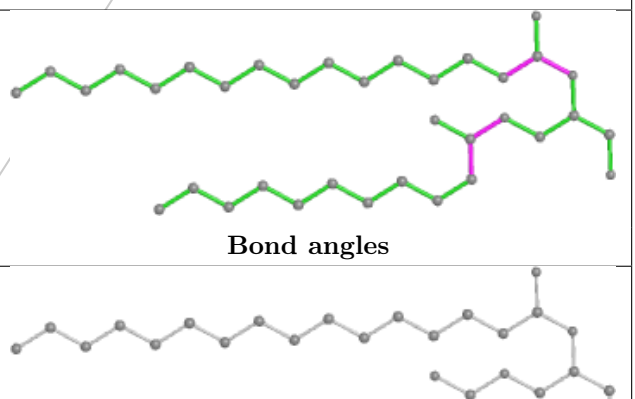


Rings

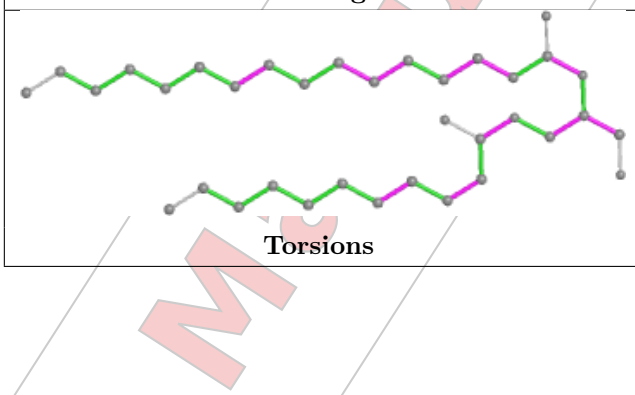
Ligand YZY C 1204



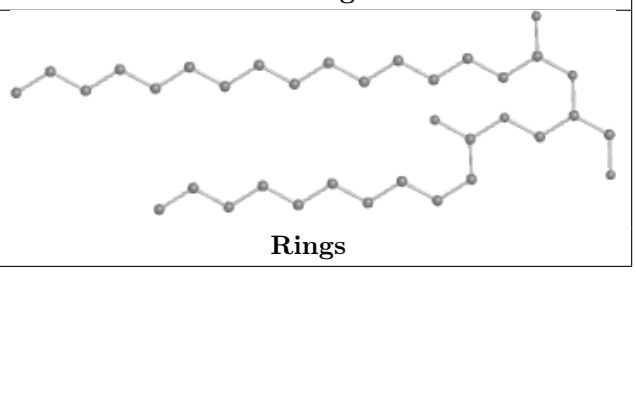
Bond lengths



Bond angles

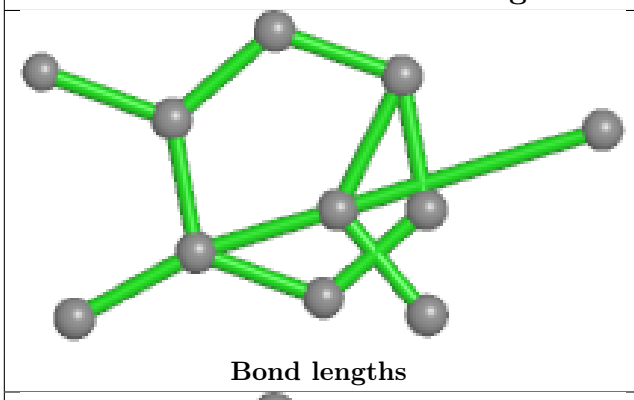


Torsions

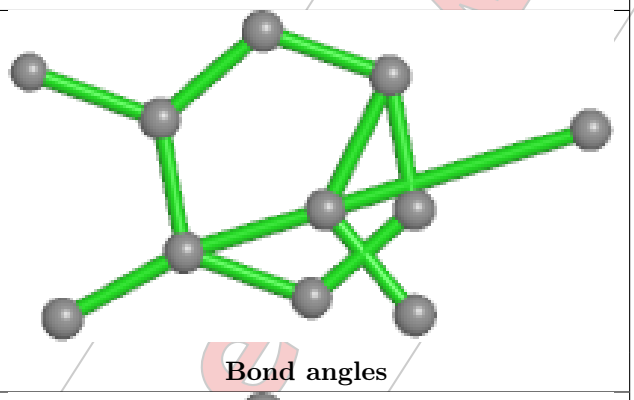


Rings

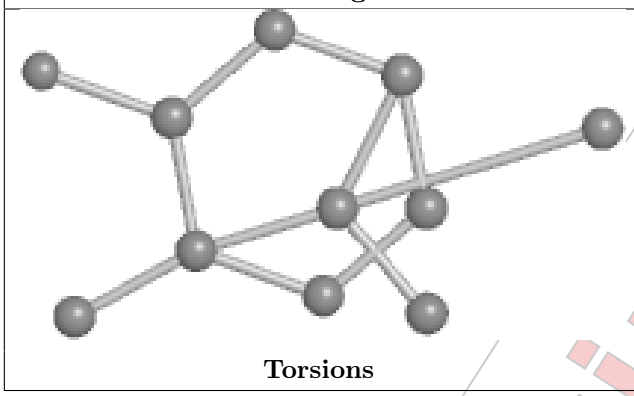
Ligand CAM D 1206



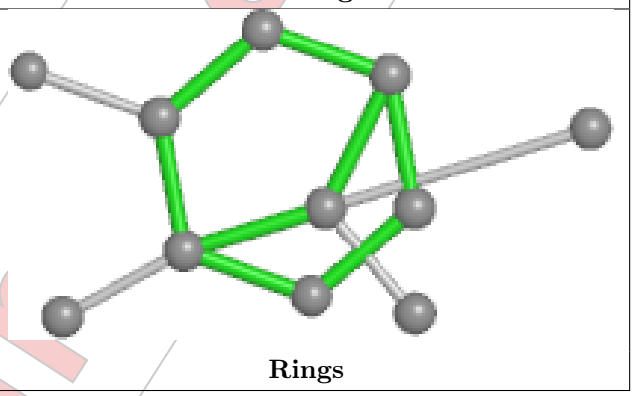
Bond lengths



Bond angles

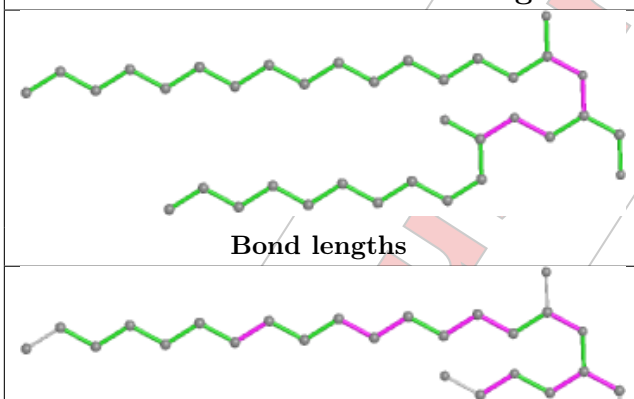


Torsions

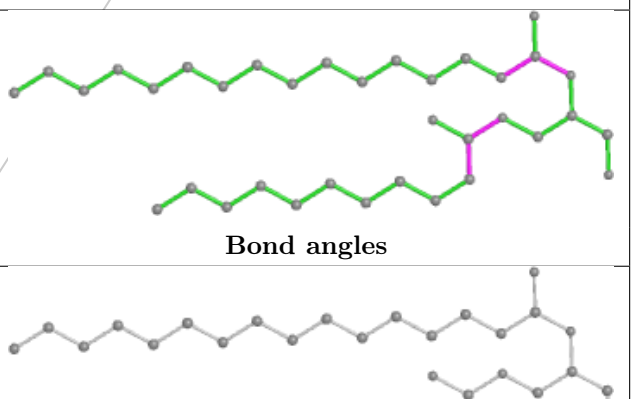


Rings

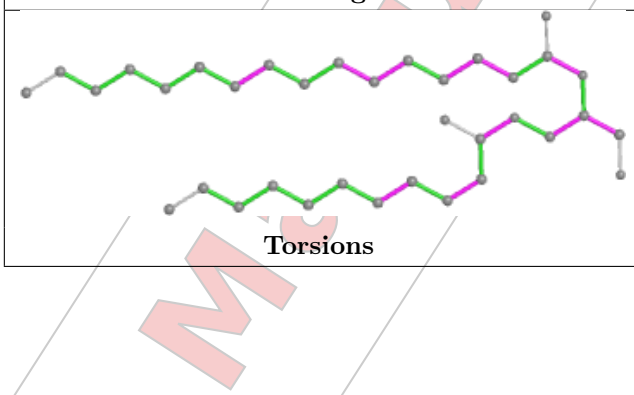
Ligand YZY A 1204



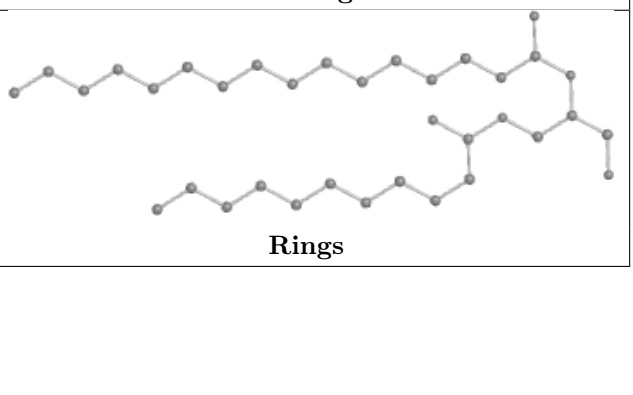
Bond lengths



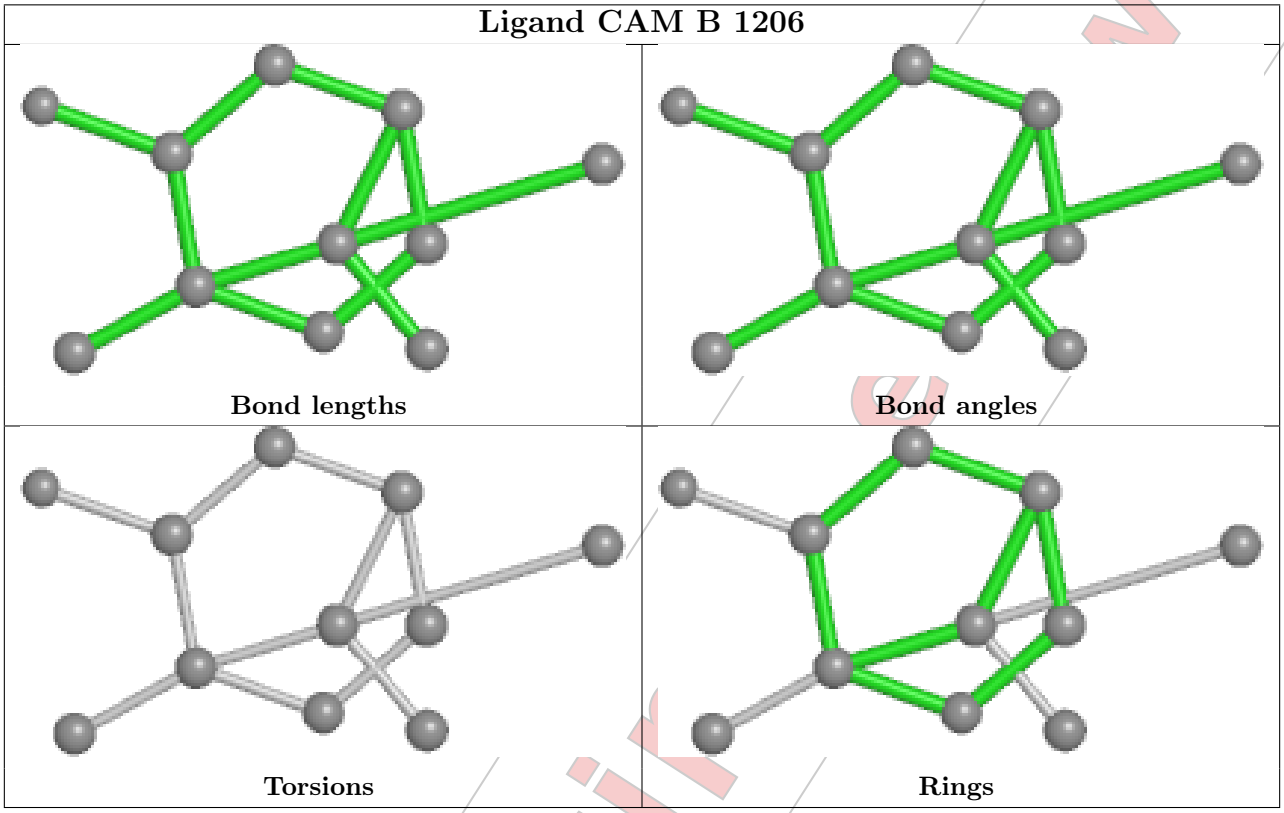
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

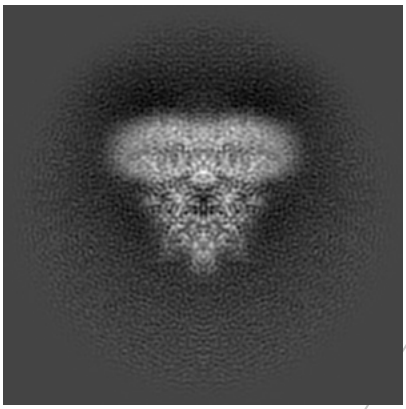
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-65281. These allow visual inspection of the internal detail of the map and identification of artifacts.

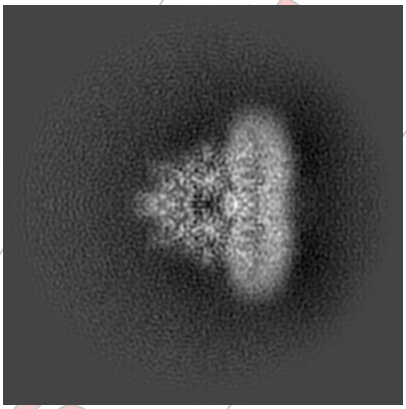
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

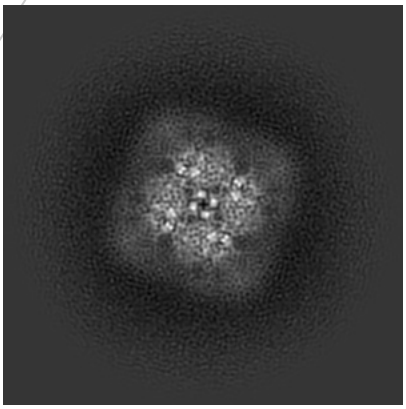
6.1.1 Primary map



X

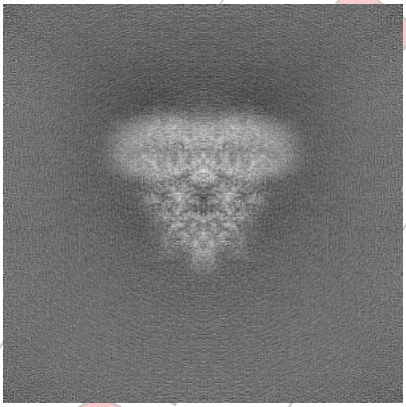


Y

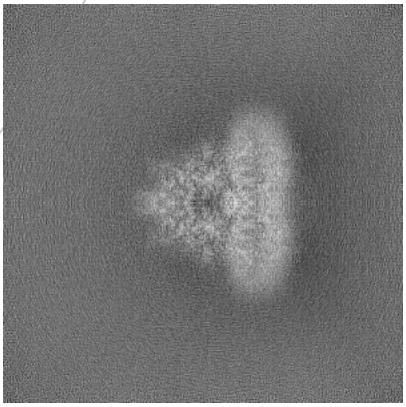


Z

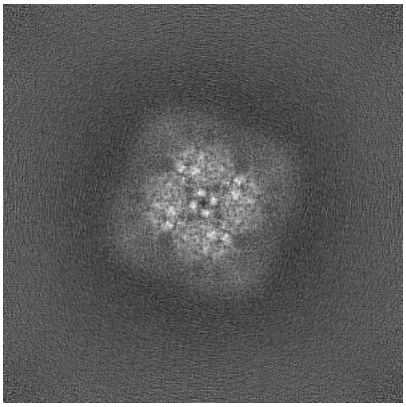
6.1.2 Raw map



X



Y

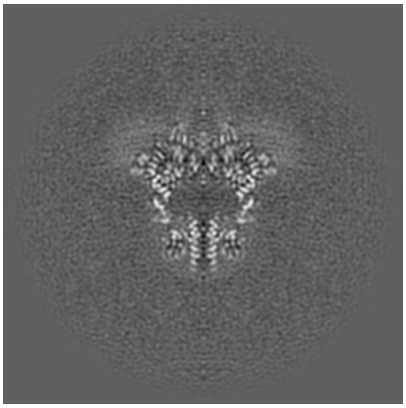


Z

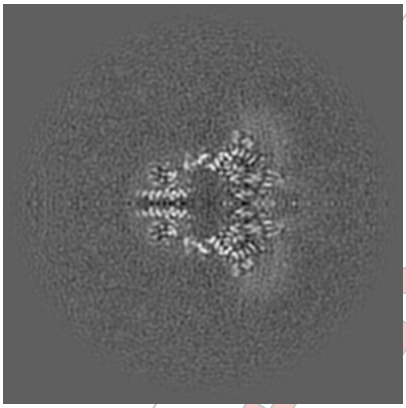
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

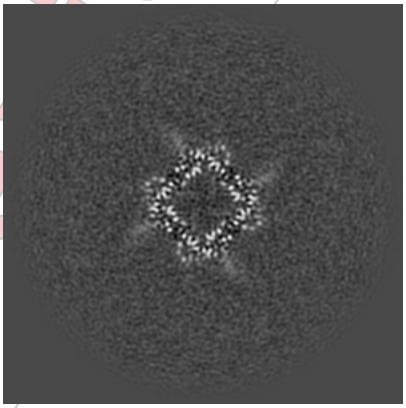
6.2.1 Primary map



X Index: 192

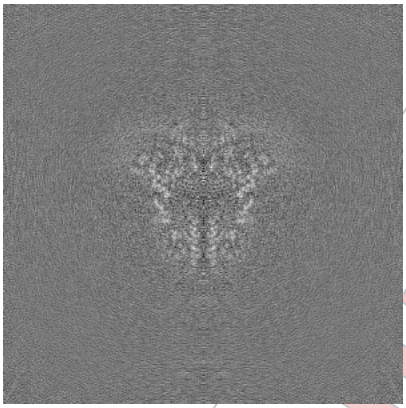


Y Index: 192

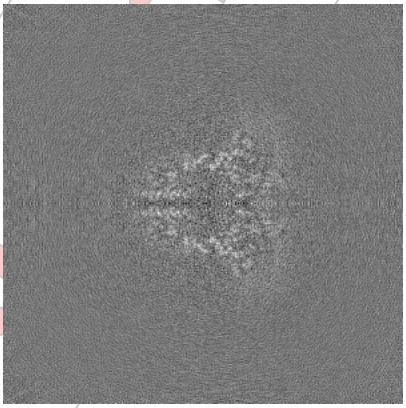


Z Index: 192

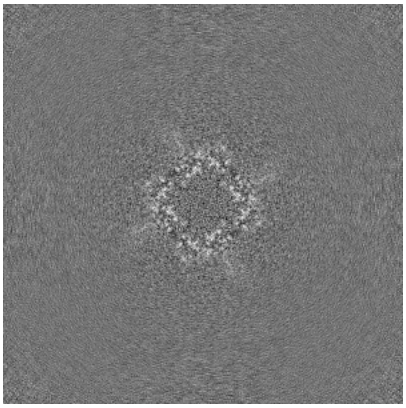
6.2.2 Raw map



X Index: 192



Y Index: 192

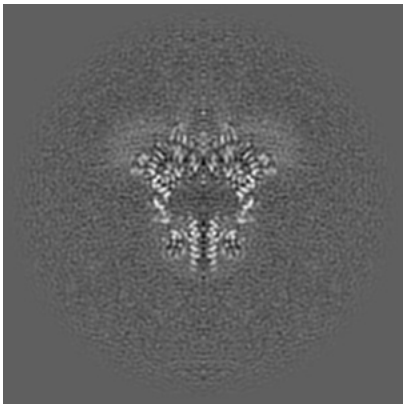


Z Index: 192

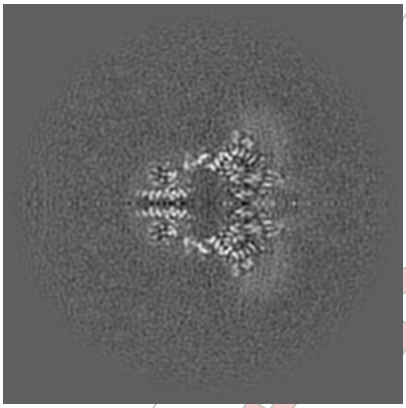
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

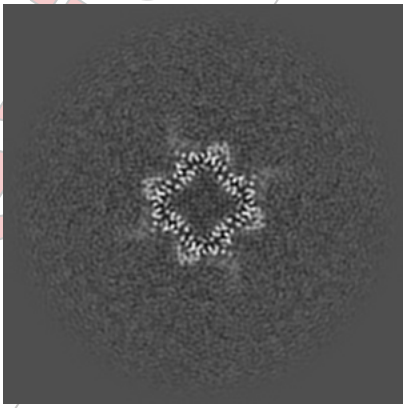
6.3.1 Primary map



X Index: 192

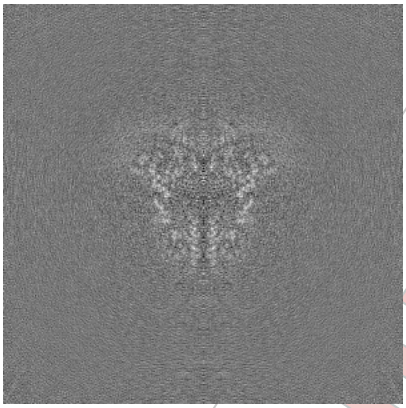


Y Index: 192

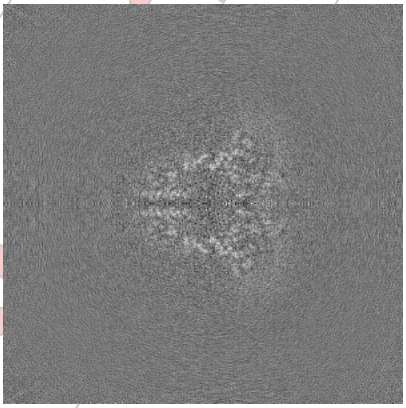


Z Index: 195

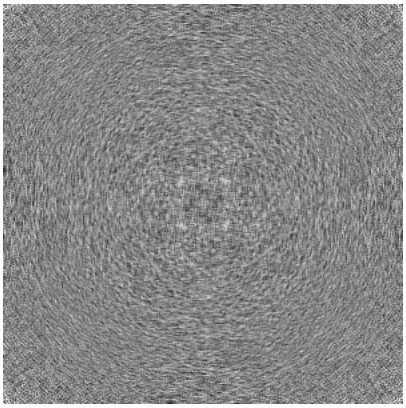
6.3.2 Raw map



X Index: 192



Y Index: 192

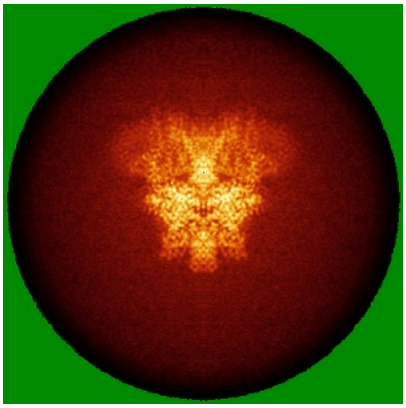


Z Index: 0

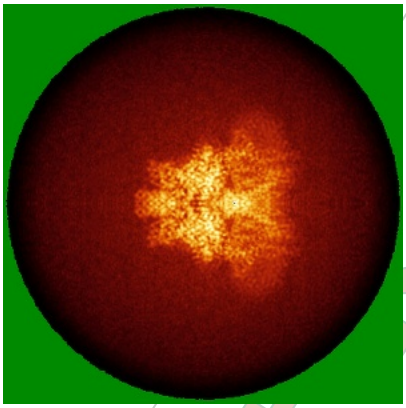
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

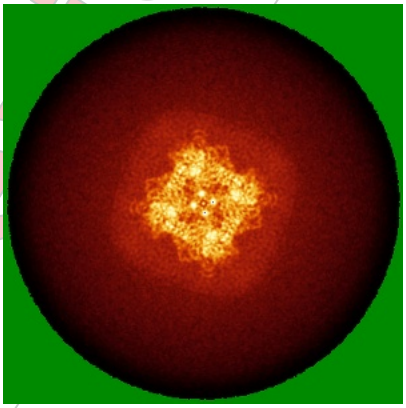
6.4.1 Primary map



X

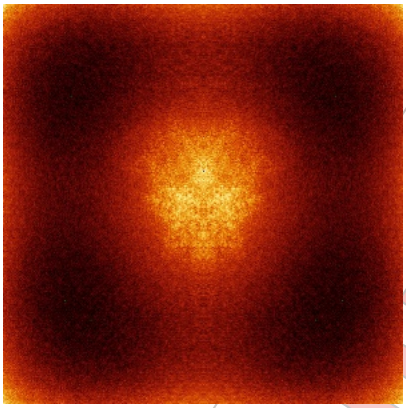


Y

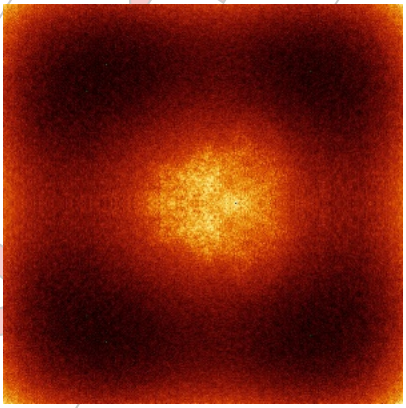


Z

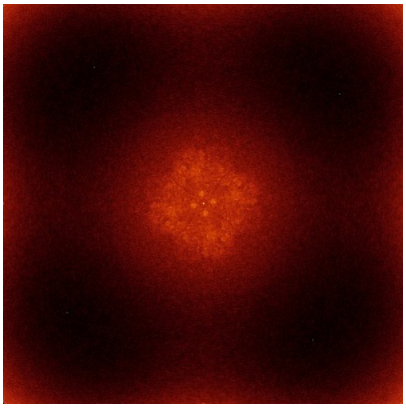
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

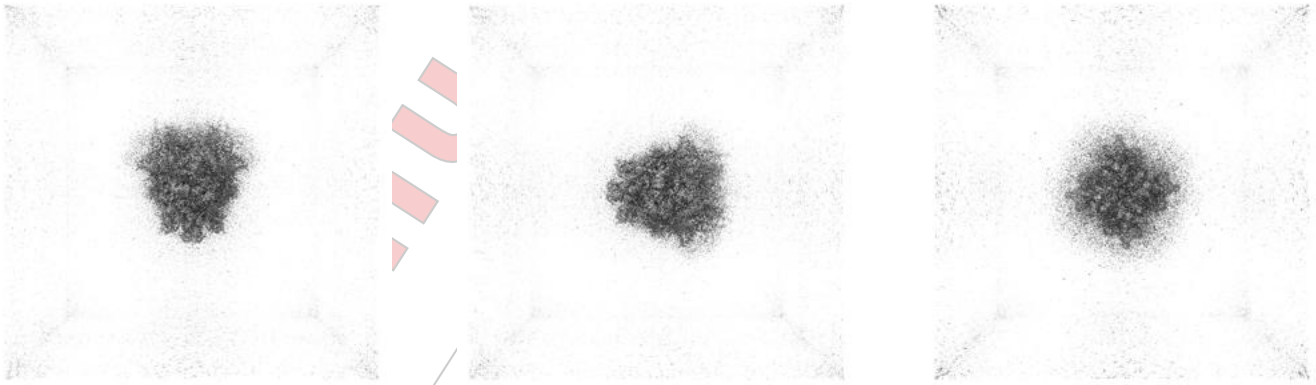
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

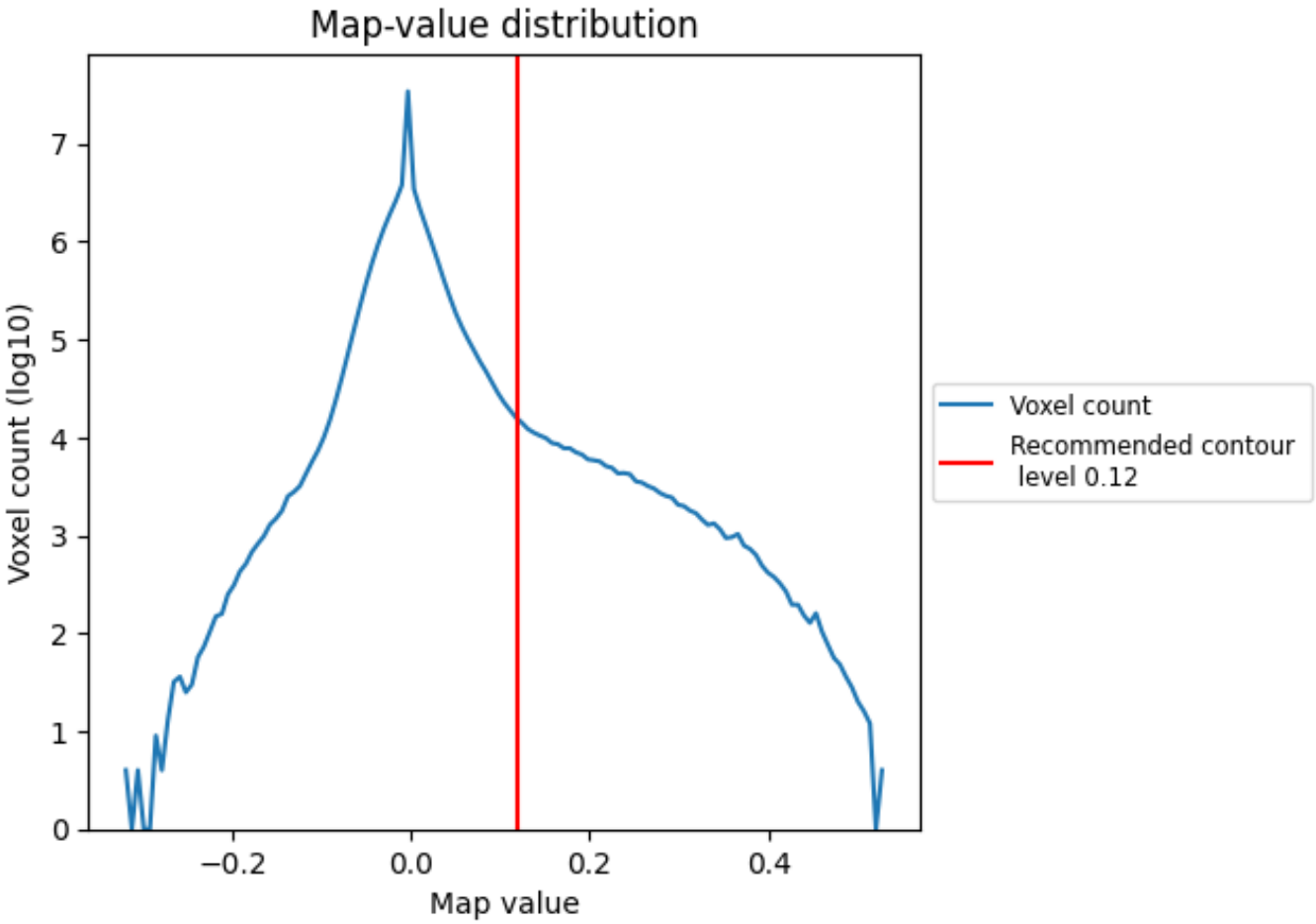
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

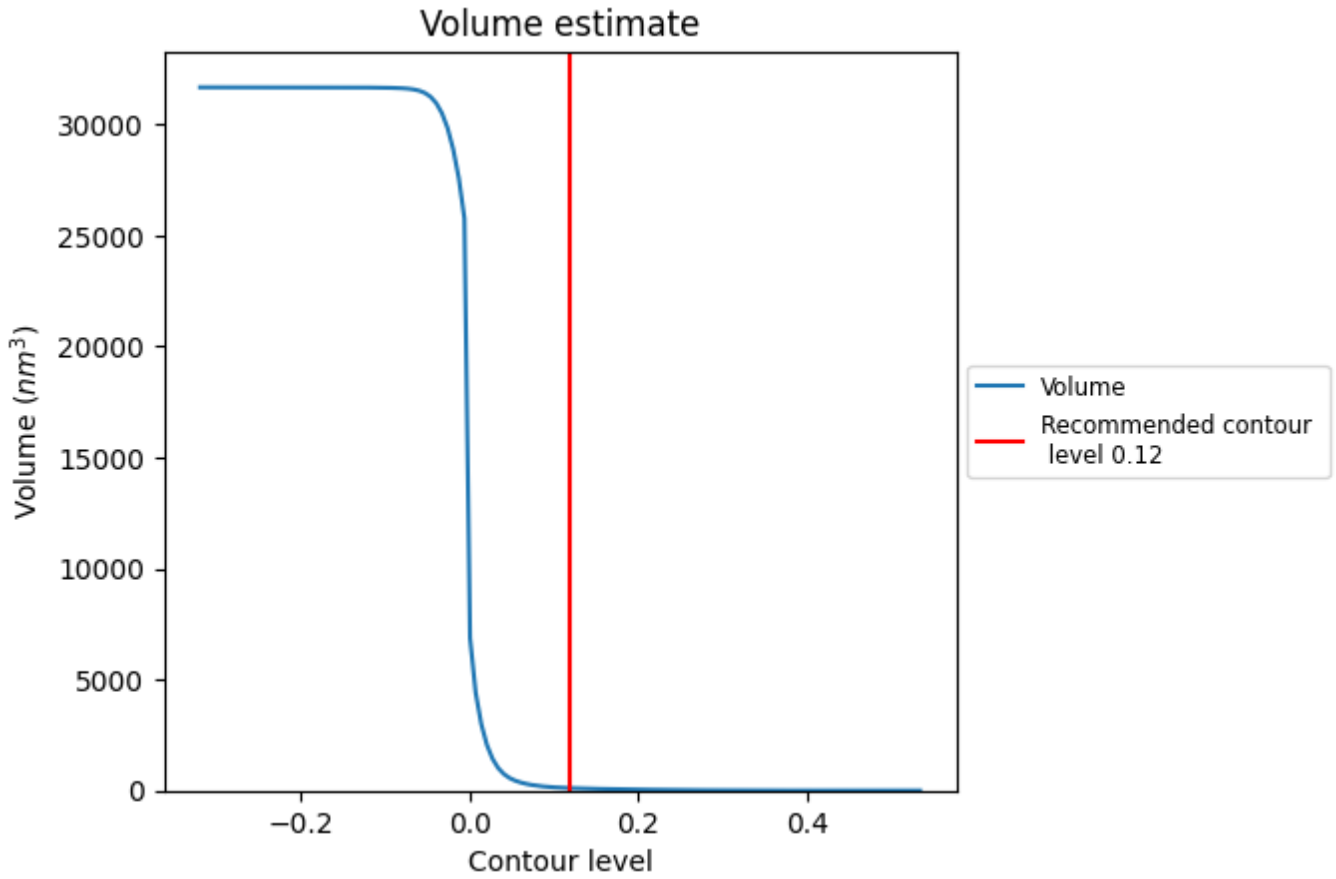
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

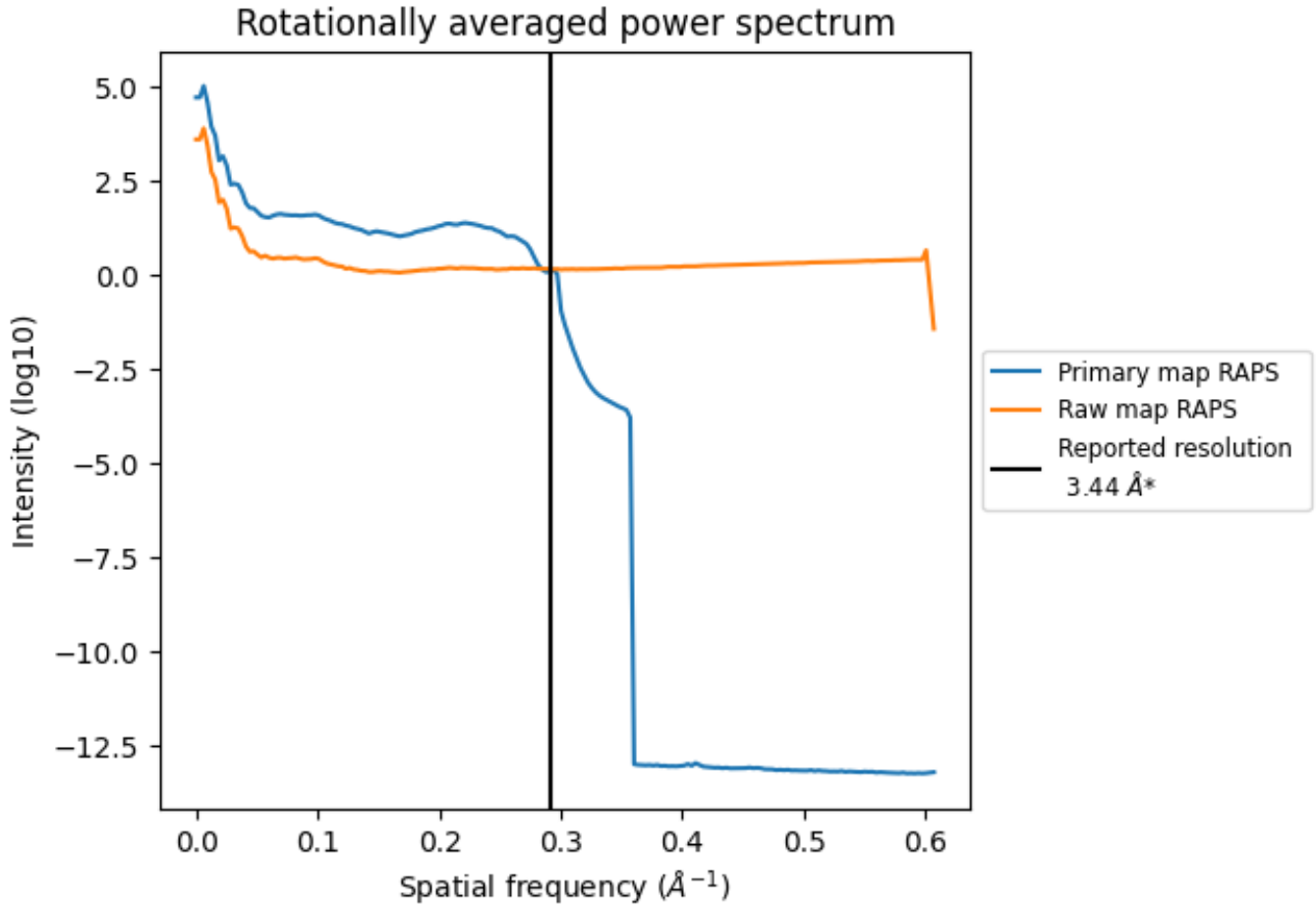
7.2 Volume estimate (i)



The volume at the recommended contour level is 110 nm^3; this corresponds to an approximate mass of 99 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

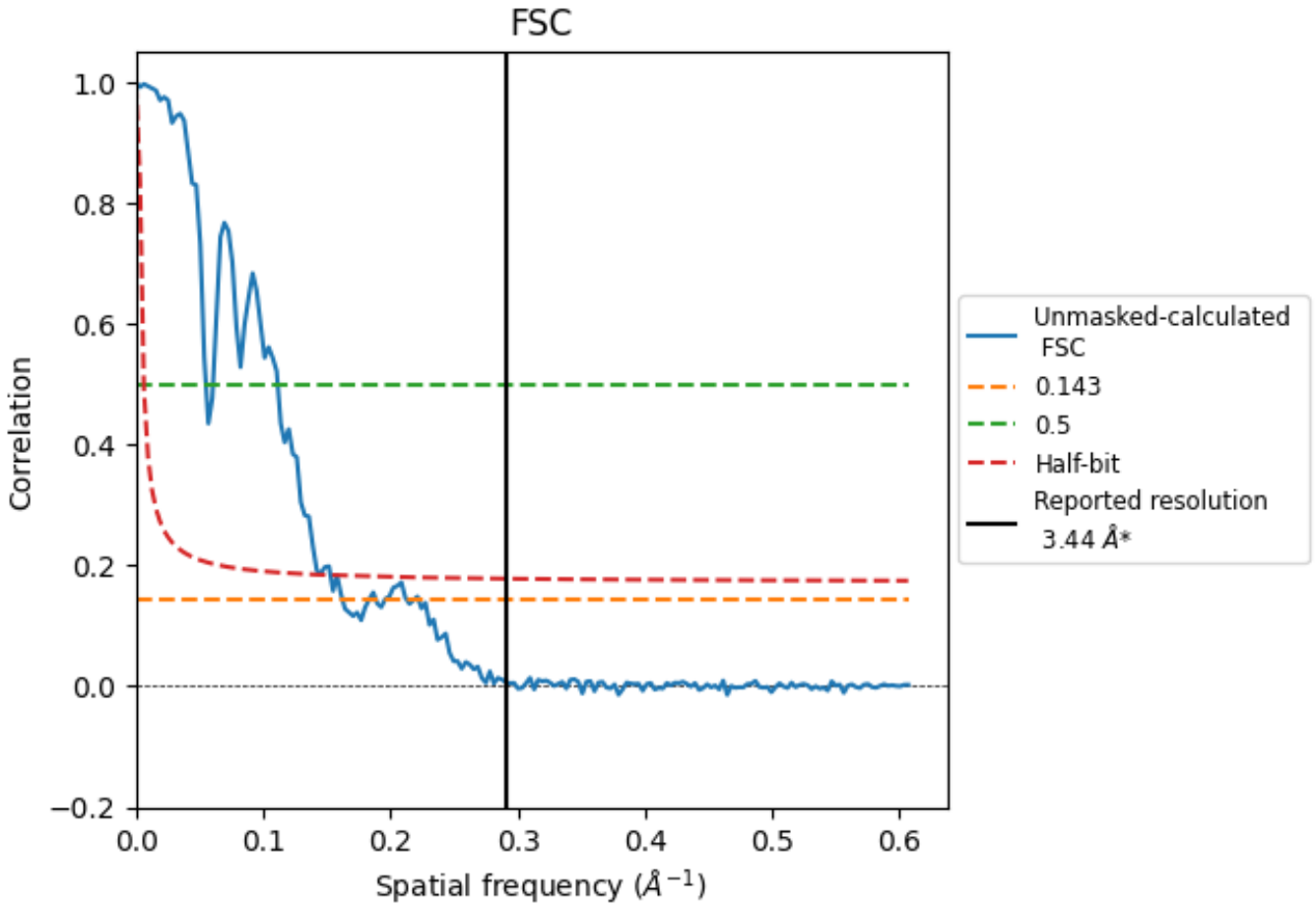


*Reported resolution corresponds to spatial frequency of 0.291 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.291 Å^{-1}

8.2 Resolution estimates (i)

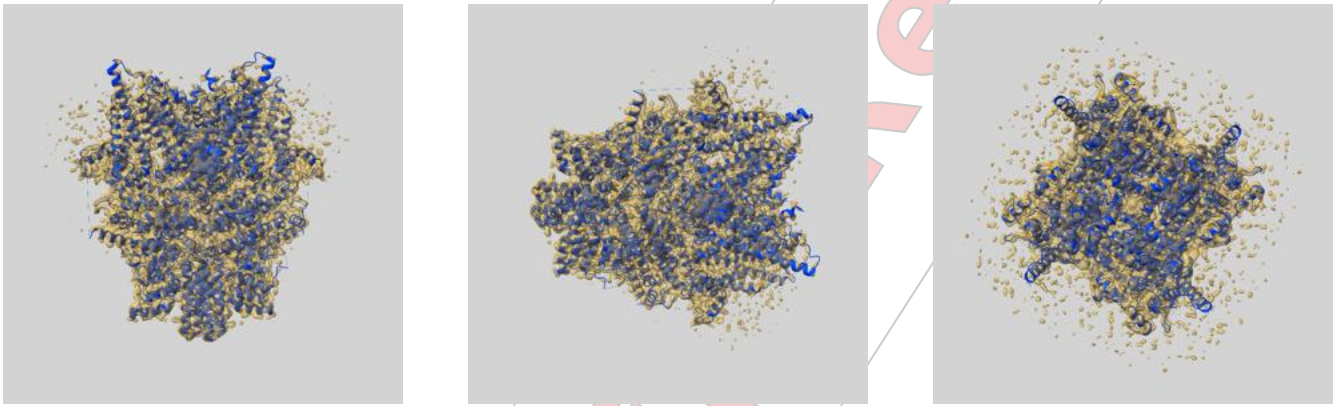
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.44	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.16	18.18	6.54

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.16 differs from the reported value 3.44 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-65281 and PDB model 9VQY. Per-residue inclusion information can be found in section 3 on page 8.

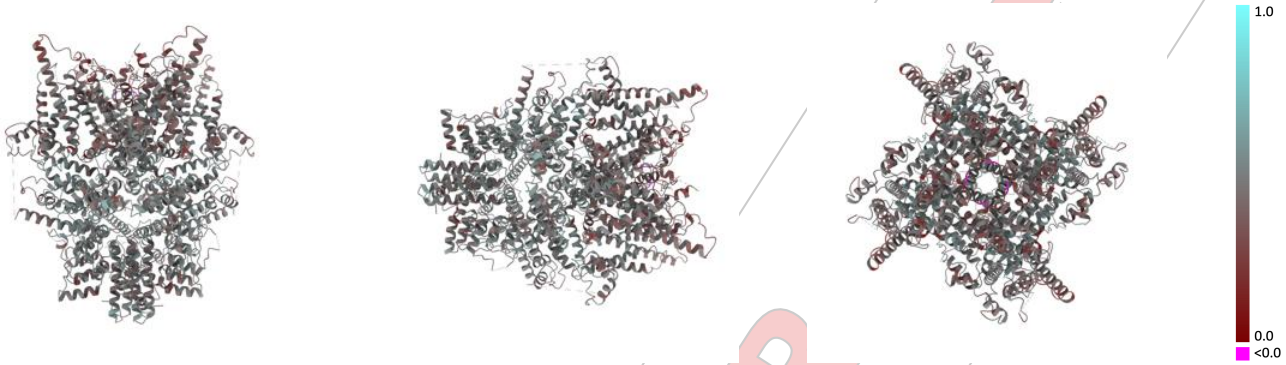
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

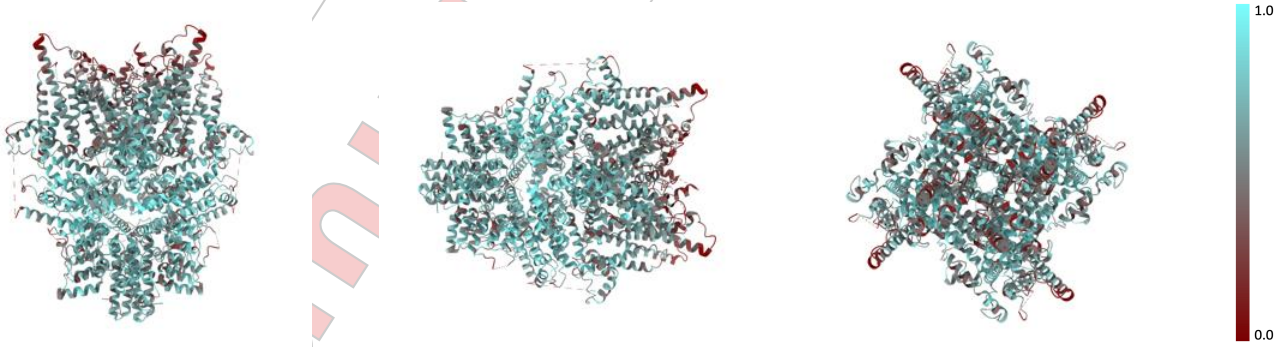
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

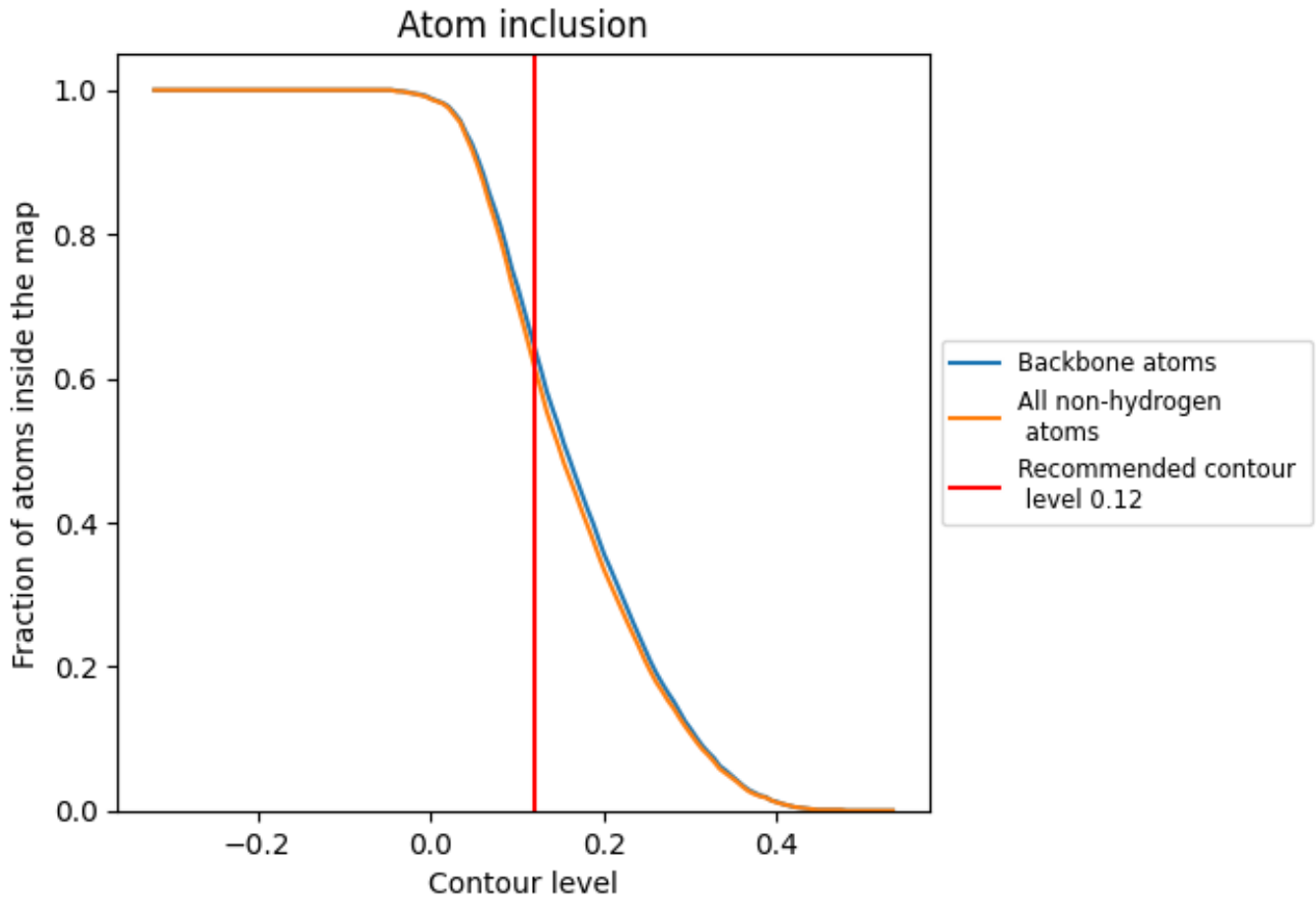
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 64% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6160	0.4540
A	0.6250	0.4550
B	0.6250	0.4540
C	0.6250	0.4540
D	0.6250	0.4540