



# Preliminary Full wwPDB EM Validation Report ⓘ

Feb 4, 2024 – 10:23 PM EST

**This wwPDB validation report is NOT for manuscript review**

This is a Preliminary Full wwPDB EM Validation Report.

This report is produced by the standalone wwPDB validation server.  
**The structure in question has not been deposited to the wwPDB.**  
**This report should not be submitted to journals.**

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis	:	0.0.1.dev70
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

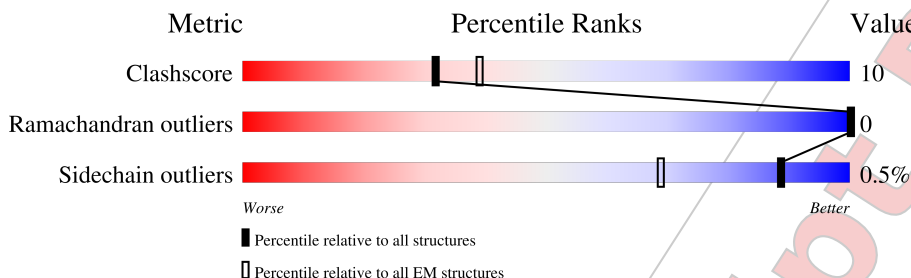
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is unknown.

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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  $\leq 5\%$ . 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	354	<div> <div>45%</div> <div>76%</div> <div>24%</div> </div>
2	F	107	<div> <div>51%</div> <div>83%</div> <div>17%</div> </div>
3	R	293	<div> <div>52%</div> <div>73%</div> <div>27%</div> </div>
4	L	15	<div> <div>53%</div> <div>67%</div> <div>27%</div> <div>7%</div> </div>

## 2 Entry composition [i](#)

There are 24 unique types of molecules in this entry. The entry contains 7463 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.

Mol	Chain	Residues	Atoms								AltConf	Trace
1	A	354	Total	C	Ca	Fe	N	O	S	Zn	5	6
			2881	1851	4	1	479	526	19	1		

- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	107	Total	C	N	O	S	0	0
			832	527	146	155	4		

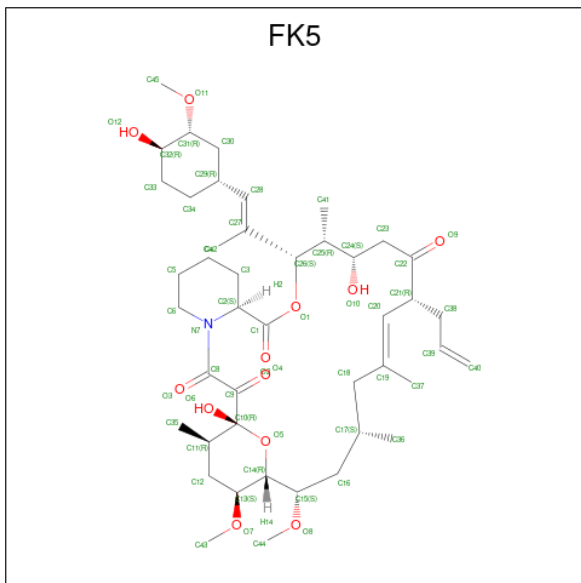
- Molecule 3 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	R	293	Total	C	N	O	S	0	0
			2323	1550	370	384	19		

- Molecule 4 is a protein called GLY-ASN-TRP-HIS-GLY-THR-SER-PRO-ASP-TRP-PHE-PHE-ASN-TYR-TYR.

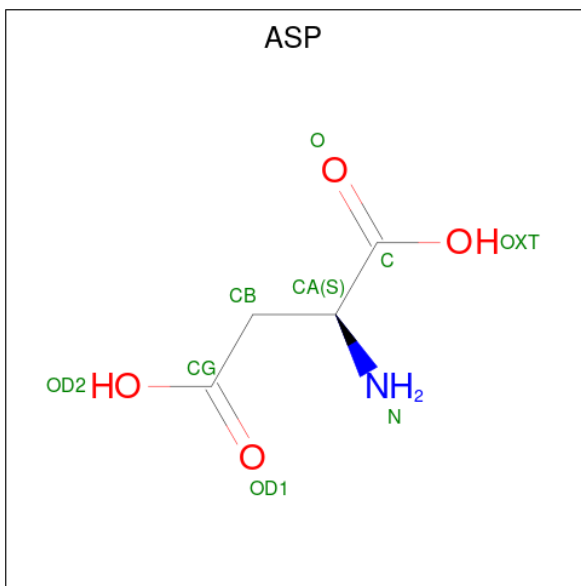
Mol	Chain	Residues	Atoms				AltConf	Trace
4	L	15	Total	C	N	O	0	0
			135	92	21	22		

- Molecule 5 is 8-DEETHYL-8-[BUT-3-ENYL]-ASCOMYCIN (three-letter code: FK5) (formula: C<sub>44</sub>H<sub>69</sub>NO<sub>12</sub>).



Mol	Chain	Residues	Atoms				AltConf
5	F	1	Total	C	N	O	0
			57	44	1	12	

- Molecule 6 is ASPARTIC ACID (three-letter code: ASP) (formula:  $C_4H_7NO_4$ ).



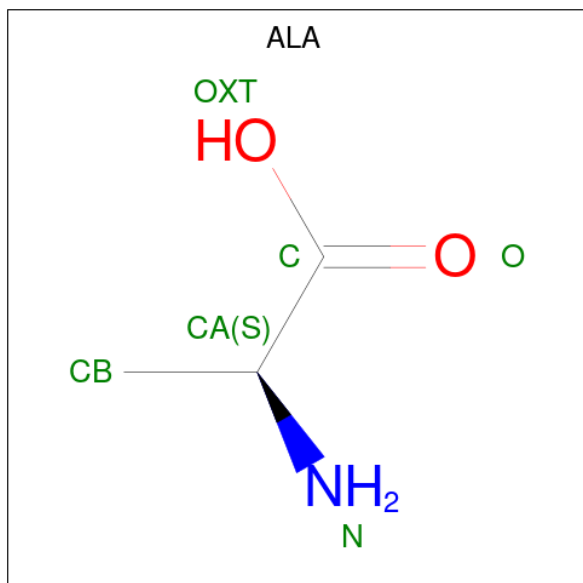
Mol	Chain	Residues	Atoms				AltConf
6	R	1	Total	C	N	O	0
			8	4	1	3	
6	R	1	Total	C	N	O	0
			8	4	1	3	
6	R	1	Total	C	N	O	0
			8	4	1	3	

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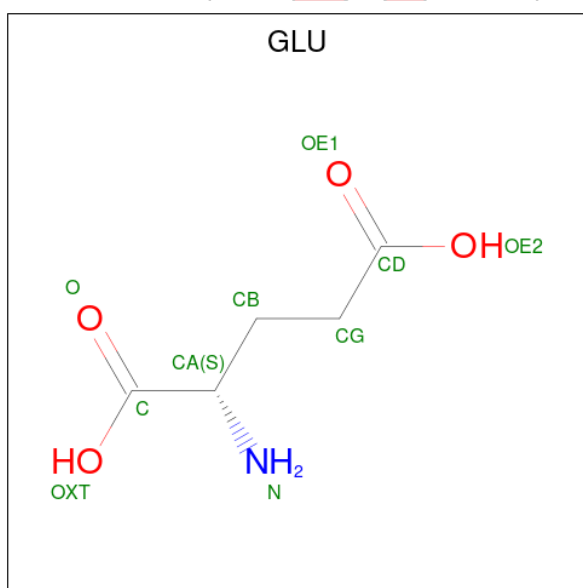
Mol	Chain	Residues	Atoms				AltConf
6	R	1	Total	C	N	O	0
			8	4	1	3	
6	R	1	Total	C	N	O	0
			8	4	1	3	
6	R	1	Total	C	N	O	0
			8	4	1	3	
6	R	1	Total	C	N	O	0
			8	4	1	3	
6	R	1	Total	C	N	O	0
			8	4	1	3	
6	R	1	Total	C	N	O	0
			8	4	1	3	
6	R	1	Total	C	N	O	0
			8	4	1	3	
6	R	1	Total	C	N	O	0
			8	4	1	3	
6	R	1	Total	C	N	O	0
			8	4	1	3	
6	R	1	Total	C	N	O	0
			8	4	1	3	
6	R	1	Total	C	N	O	0
			8	4	1	3	
6	R	1	Total	C	N	O	0
			8	4	1	3	
6	R	1	Total	C	N	O	0
			8	4	1	3	
6	R	1	Total	C	N	O	0
			8	4	1	3	
6	R	1	Total	C	N	O	0
			8	4	1	3	

- Molecule 7 is ALANINE (three-letter code: ALA) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>).



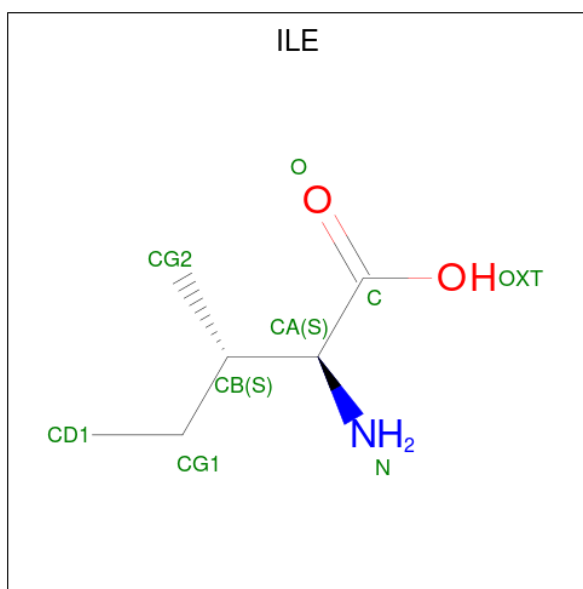
Mol	Chain	Residues	Atoms				AltConf
7	R	1	Total	C	N	O	0
			5	3	1	1	
7	R	1	Total	C	N	O	0
			5	3	1	1	
7	R	1	Total	C	N	O	0
			5	3	1	1	
7	R	1	Total	C	N	O	0
			5	3	1	1	

- Molecule 8 is GLUTAMIC ACID (three-letter code: GLU) (formula:  $C_5H_9NO_4$ ).



Mol	Chain	Residues	Atoms				AltConf
8	R	1	Total	C	N	O	0
			9	5	1	3	
8	R	1	Total	C	N	O	0
			9	5	1	3	
8	R	1	Total	C	N	O	0
			9	5	1	3	
8	R	1	Total	C	N	O	0
			9	5	1	3	
8	R	1	Total	C	N	O	0
			9	5	1	3	
8	R	1	Total	C	N	O	0
			9	5	1	3	
8	R	1	Total	C	N	O	0
			9	5	1	3	
8	R	1	Total	C	N	O	0
			9	5	1	3	

- Molecule 9 is ISOLEUCINE (three-letter code: ILE) (formula:  $C_6H_{13}NO_2$ ).



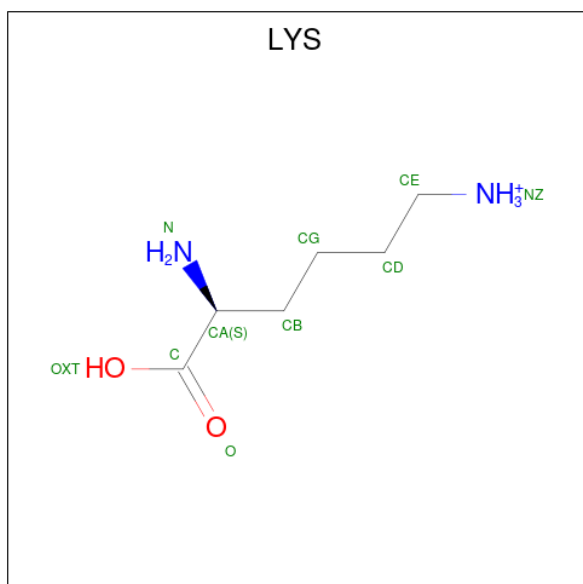
Mol	Chain	Residues	Atoms				AltConf
9	R	1	Total	C	N	O	0
			8	6	1	1	

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Mol	Chain	Residues	Atoms				AltConf
9	R	1	Total	C	N	O	0
			8	6	1	1	
9	R	1	Total	C	N	O	0
			8	6	1	1	
9	R	1	Total	C	N	O	0
			8	6	1	1	
9	R	1	Total	C	N	O	0
			8	6	1	1	
9	R	1	Total	C	N	O	0
			8	6	1	1	
9	R	1	Total	C	N	O	0
			8	6	1	1	
9	R	1	Total	C	N	O	0
			8	6	1	1	
9	R	1	Total	C	N	O	0
			8	6	1	1	

- Molecule 10 is LYSINE (three-letter code: LYS) (formula:  $C_6H_{15}N_2O_2$ ).



Mol	Chain	Residues	Atoms				AltConf
10	R	1	Total	C	N	O	0
			9	6	2	1	

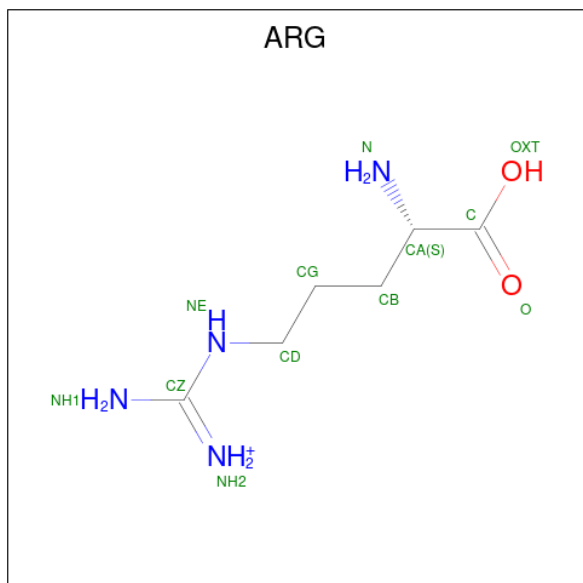
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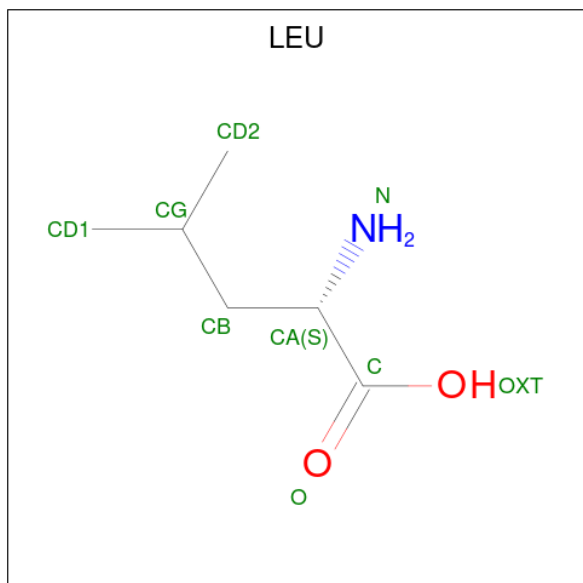
Mol	Chain	Residues	Atoms				AltConf
10	R	1	Total	C	N	O	0
			9	6	2	1	
10	R	1	Total	C	N	O	0
			9	6	2	1	
10	R	1	Total	C	N	O	0
			9	6	2	1	
10	R	1	Total	C	N	O	0
			9	6	2	1	
10	R	1	Total	C	N	O	0
			9	6	2	1	
10	R	1	Total	C	N	O	0
			9	6	2	1	
10	R	1	Total	C	N	O	0
			9	6	2	1	
10	R	1	Total	C	N	O	0
			9	6	2	1	
10	R	1	Total	C	N	O	0
			9	6	2	1	
10	R	1	Total	C	N	O	0
			9	6	2	1	
10	R	1	Total	C	N	O	0
			9	6	2	1	
10	R	1	Total	C	N	O	0
			9	6	2	1	

- Molecule 11 is ARGinine (three-letter code: ARG) (formula:  $C_6H_{15}N_4O_2$ ).



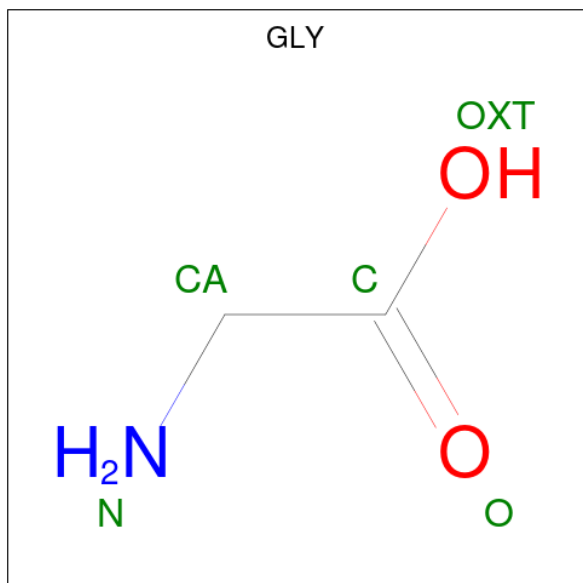
Mol	Chain	Residues	Atoms				AltConf
11	R	1	Total	C	N	O	0
			11	6	4	1	
11	R	1	Total	C	N	O	0
			11	6	4	1	
11	R	1	Total	C	N	O	0
			11	6	4	1	
11	R	1	Total	C	N	O	0
			11	6	4	1	
11	R	1	Total	C	N	O	0
			11	6	4	1	

- Molecule 12 is LEUCINE (three-letter code: LEU) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>2</sub>).



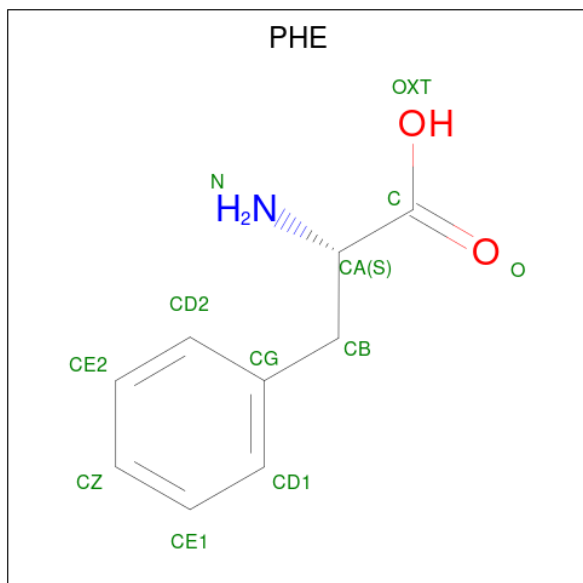
Mol	Chain	Residues	Atoms				AltConf
12	R	1	Total	C	N	O	0
			8	6	1	1	
12	R	1	Total	C	N	O	0
			8	6	1	1	
12	R	1	Total	C	N	O	0
			8	6	1	1	
12	R	1	Total	C	N	O	0
			8	6	1	1	
12	R	1	Total	C	N	O	0
			8	6	1	1	
12	R	1	Total	C	N	O	0
			8	6	1	1	
12	R	1	Total	C	N	O	0
			8	6	1	1	
12	R	1	Total	C	N	O	0
			8	6	1	1	
12	R	1	Total	C	N	O	0
			8	6	1	1	
12	R	1	Total	C	N	O	0
			8	6	1	1	

- Molecule 13 is GLYCINE (three-letter code: GLY) (formula: C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>).



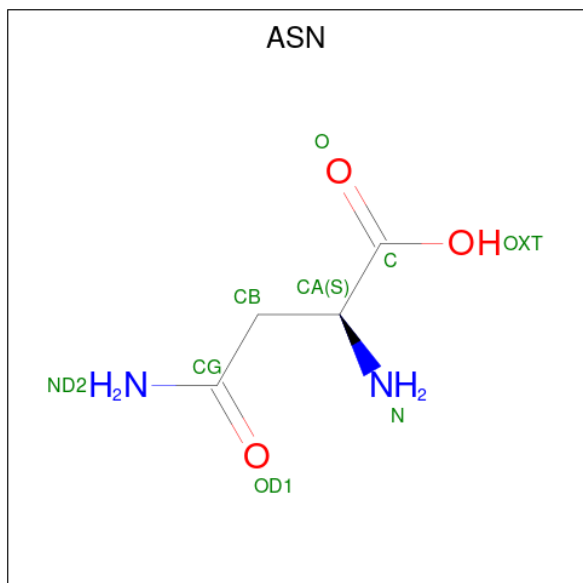
Mol	Chain	Residues	Atoms				AltConf
13	R	1	Total	C	N	O	0
			4	2	1	1	
13	R	1	Total	C	N	O	0
			4	2	1	1	
13	R	1	Total	C	N	O	0
			4	2	1	1	
13	R	1	Total	C	N	O	0
			4	2	1	1	
13	R	1	Total	C	N	O	0
			4	2	1	1	
13	R	1	Total	C	N	O	0
			4	2	1	1	
13	R	1	Total	C	N	O	0
			4	2	1	1	
13	R	1	Total	C	N	O	0
			4	2	1	1	
13	R	1	Total	C	N	O	0
			4	2	1	1	
13	R	1	Total	C	N	O	0
			4	2	1	1	

- Molecule 14 is PHENYLALANINE (three-letter code: PHE) (formula: C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub>).



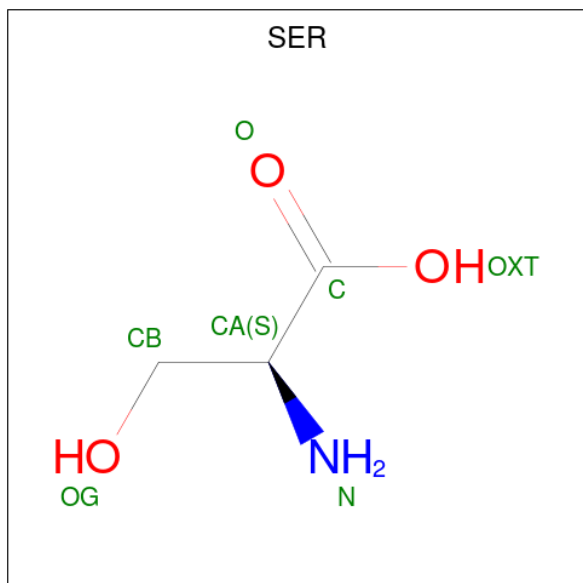
Mol	Chain	Residues	Atoms				AltConf
14	R	1	Total	C	N	O	0
			11	9	1	1	
14	R	1	Total	C	N	O	0
			11	9	1	1	
14	R	1	Total	C	N	O	0
			11	9	1	1	
14	R	1	Total	C	N	O	0
			11	9	1	1	
14	R	1	Total	C	N	O	0
			11	9	1	1	
14	R	1	Total	C	N	O	0
			11	9	1	1	
14	R	1	Total	C	N	O	0
			11	9	1	1	
14	R	1	Total	C	N	O	0
			11	9	1	1	

- Molecule 15 is ASPARAGINE (three-letter code: ASN) (formula:  $C_4H_8N_2O_3$ ).



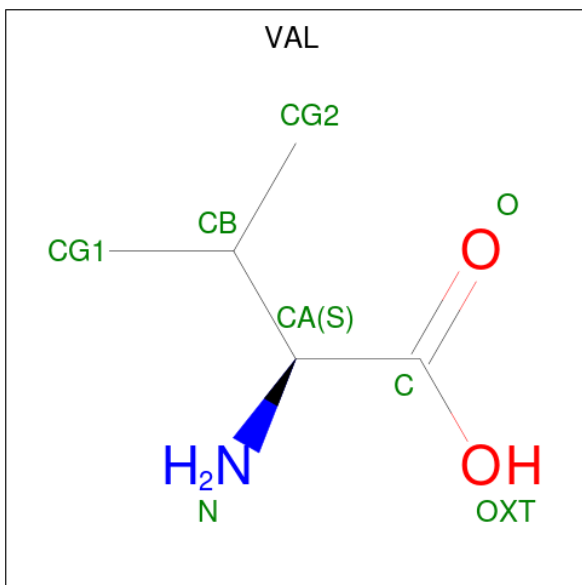
Mol	Chain	Residues	Atoms				AltConf
15	R	1	Total	C	N	O	0
			8	4	2	2	
15	R	1	Total	C	N	O	0
			8	4	2	2	
15	R	1	Total	C	N	O	0
			8	4	2	2	
15	R	1	Total	C	N	O	0
			8	4	2	2	
15	R	1	Total	C	N	O	0
			8	4	2	2	
15	R	1	Total	C	N	O	0
			8	4	2	2	

- Molecule 16 is SERINE (three-letter code: SER) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				AltConf
16	R	1	Total	C	N	O	0
			6	3	1	2	
16	R	1	Total	C	N	O	0
			6	3	1	2	
16	R	1	Total	C	N	O	0
			6	3	1	2	
16	R	1	Total	C	N	O	0
			6	3	1	2	
16	R	1	Total	C	N	O	0
			6	3	1	2	
16	R	1	Total	C	N	O	0
			6	3	1	2	
16	R	1	Total	C	N	O	0
			6	3	1	2	

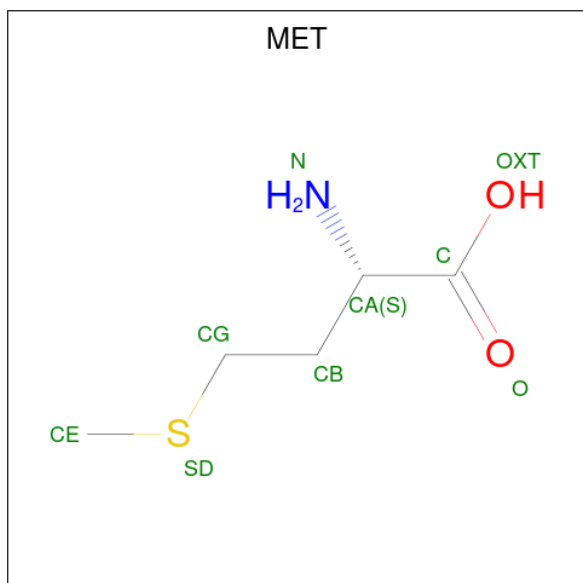
- Molecule 17 is VALINE (three-letter code: VAL) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				AltConf
17	R	1	Total	C	N	O	0
			7	5	1	1	
17	R	1	Total	C	N	O	0
			7	5	1	1	
17	R	1	Total	C	N	O	0
			7	5	1	1	
17	R	1	Total	C	N	O	0
			7	5	1	1	
17	R	1	Total	C	N	O	0
			7	5	1	1	
17	R	1	Total	C	N	O	0
			7	5	1	1	
17	R	1	Total	C	N	O	0
			7	5	1	1	
17	R	1	Total	C	N	O	0
			7	5	1	1	
17	R	1	Total	C	N	O	0
			7	5	1	1	
17	R	1	Total	C	N	O	0
			7	5	1	1	

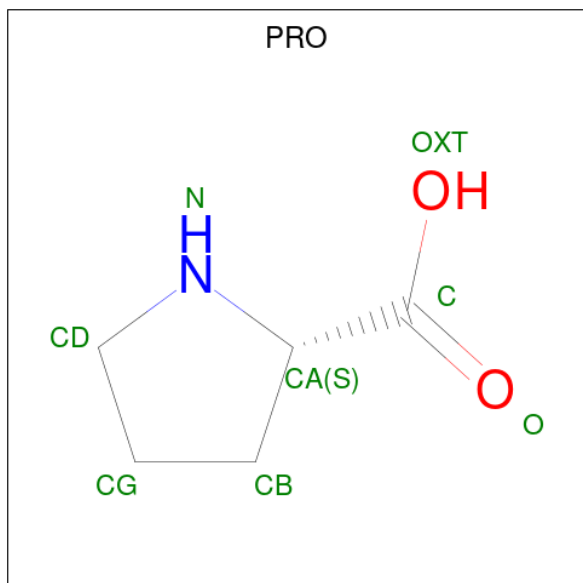


- Molecule 18 is METHIONINE (three-letter code: MET) (formula:  $C_5H_{11}NO_2S$ ).



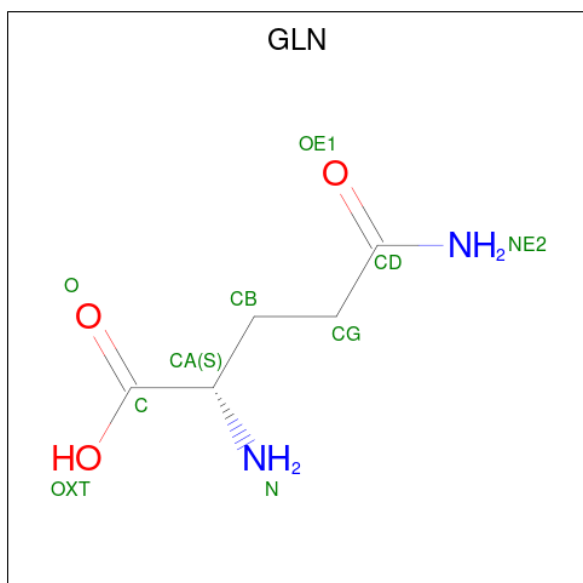
Mol	Chain	Residues	Atoms					AltConf
18	R	1	Total	C	N	O	S	0
			8	5	1	1	1	
18	R	1	Total	C	N	O	S	0
			8	5	1	1	1	
18	R	1	Total	C	N	O	S	0
			8	5	1	1	1	
18	R	1	Total	C	N	O	S	0
			8	5	1	1	1	
18	R	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 19 is PROLINE (three-letter code: PRO) (formula:  $C_5H_9NO_2$ ).



Mol	Chain	Residues	Atoms				AltConf
19	R	1	Total	C	N	O	0
			7	5	1	1	
19	R	1	Total	C	N	O	0
			7	5	1	1	

- Molecule 20 is GLUTAMINE (three-letter code: GLN) (formula:  $C_5H_{10}N_2O_3$ ).



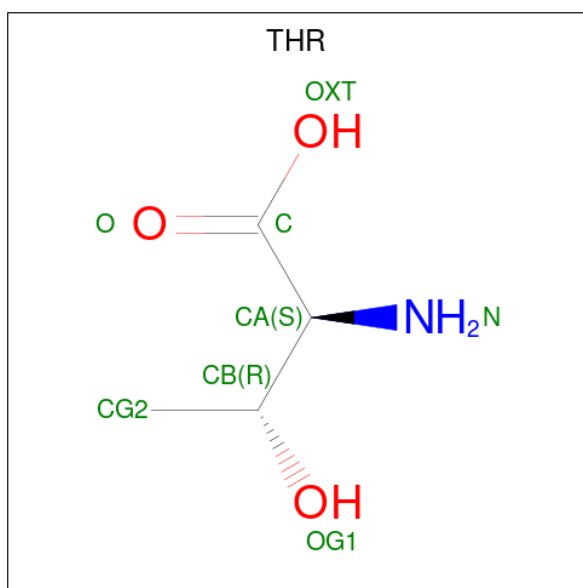
Mol	Chain	Residues	Atoms				AltConf
20	R	1	Total	C	N	O	0
			9	5	2	2	
20	R	1	Total	C	N	O	0
			9	5	2	2	

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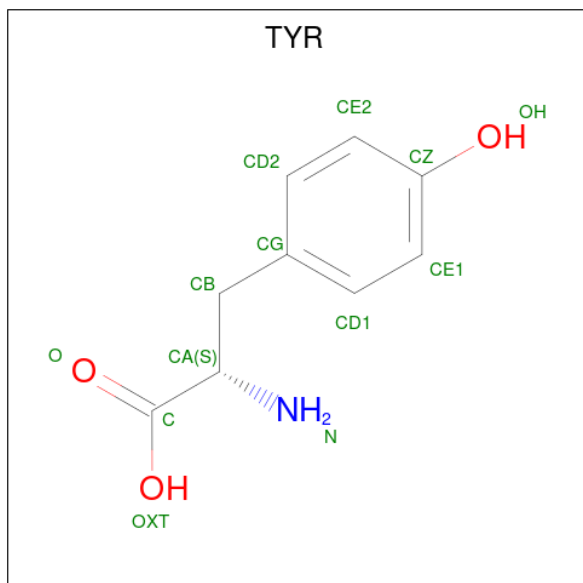
Mol	Chain	Residues	Atoms				AltConf
20	R	1	Total	C	N	O	0
			9	5	2	2	
20	R	1	Total	C	N	O	0
			9	5	2	2	
20	R	1	Total	C	N	O	0
			9	5	2	2	
20	R	1	Total	C	N	O	0
			9	5	2	2	
20	R	1	Total	C	N	O	0
			9	5	2	2	
20	R	1	Total	C	N	O	0
			9	5	2	2	

- Molecule 21 is THREONINE (three-letter code: THR) (formula: C<sub>4</sub>H<sub>9</sub>NO<sub>3</sub>).



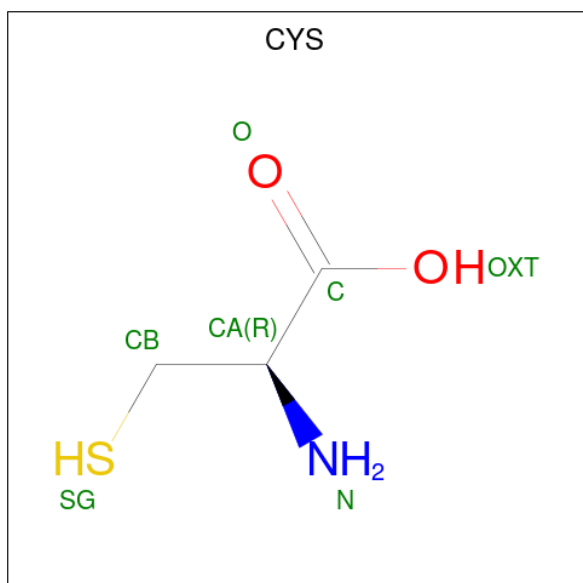
Mol	Chain	Residues	Atoms				AltConf
21	R	1	Total	C	N	O	0
			7	4	1	2	
21	R	1	Total	C	N	O	0
			7	4	1	2	
21	R	1	Total	C	N	O	0
			7	4	1	2	

- Molecule 22 is TYROSINE (three-letter code: TYR) (formula: C<sub>9</sub>H<sub>11</sub>NO<sub>3</sub>).



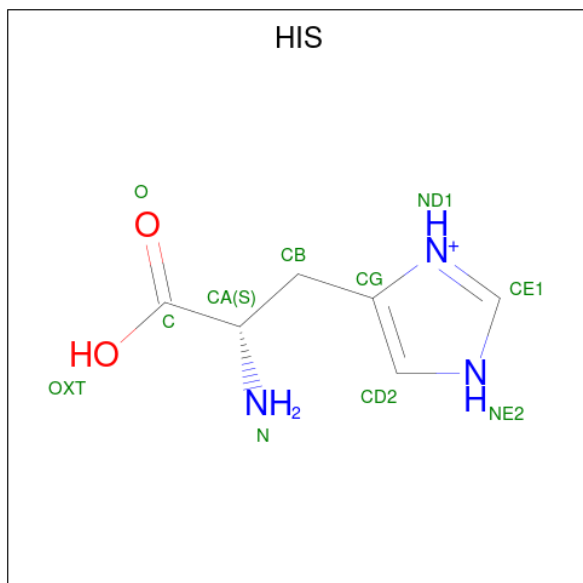
Mol	Chain	Residues	Atoms				AltConf
22	R	1	Total	C	N	O	0
			12	9	1	2	
22	R	1	Total	C	N	O	0
			12	9	1	2	

- Molecule 23 is CYSTEINE (three-letter code: CYS) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>S).



Mol	Chain	Residues	Atoms					AltConf
23	R	1	Total	C	N	O	S	0
			6	3	1	1	1	

- Molecule 24 is HISTIDINE (three-letter code: HIS) (formula: C<sub>6</sub>H<sub>10</sub>N<sub>3</sub>O<sub>2</sub>).

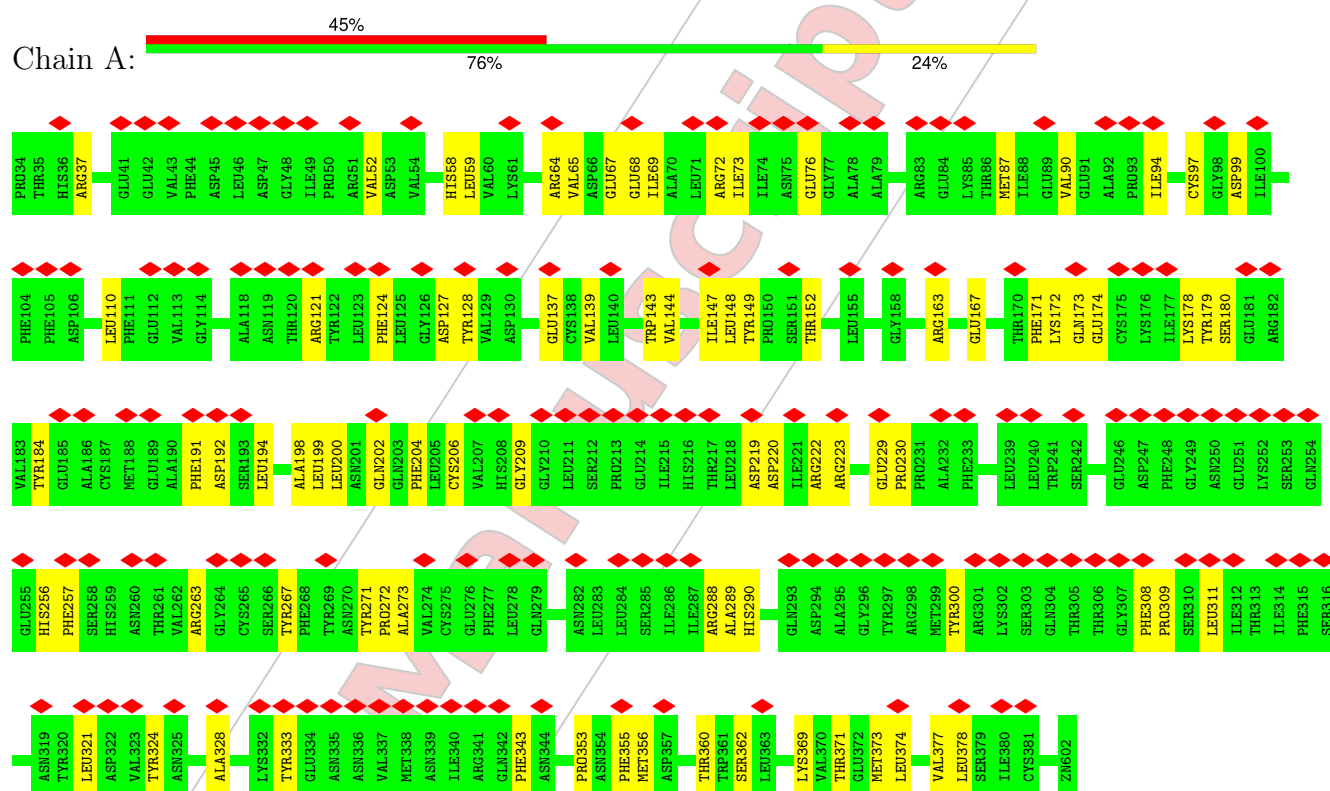


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
24	R	1	10	6	3	1	0

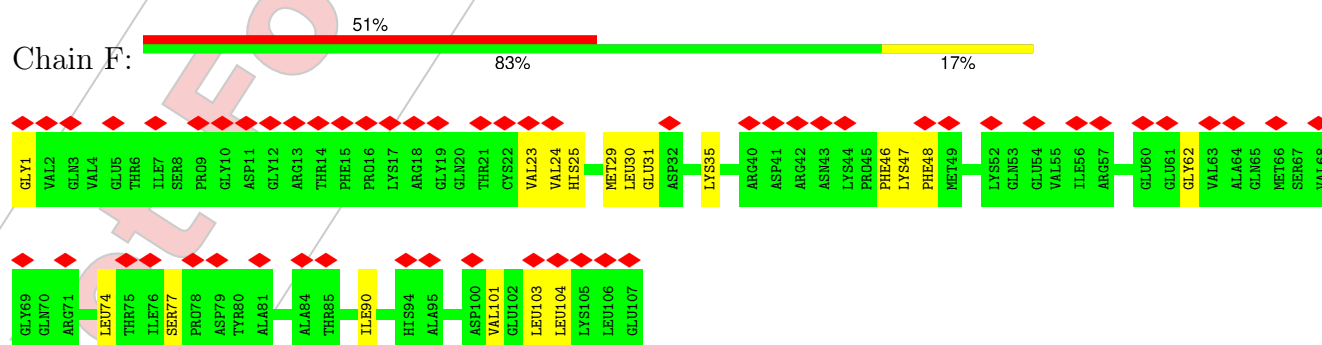
### 3 Residue-property plots

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.

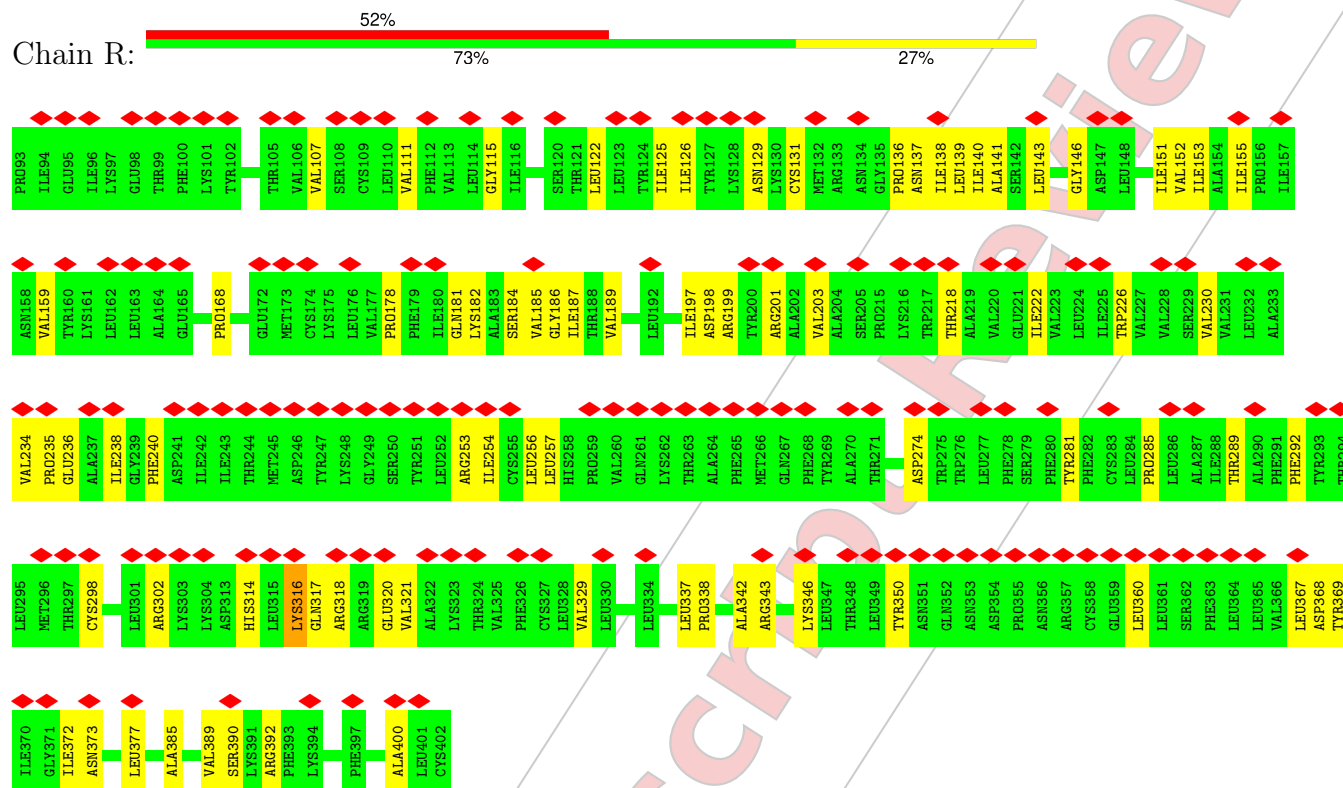
#### • Molecule 1:



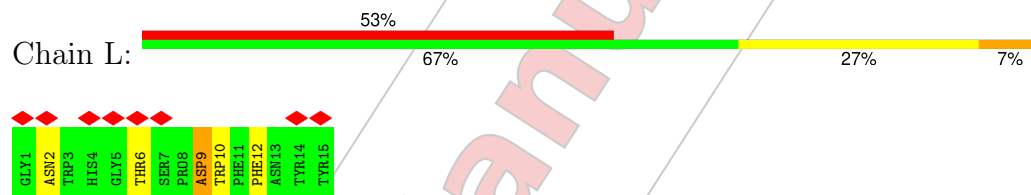
#### • Molecule 2:



#### • Molecule 3:



• Molecule 4: GLY-ASN-TRP-HIS-GLY-THR-SER-PRO-ASP-TRP-PHE-PHE-ASN-TYR-TYR



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	Not provided	
Voltage (kV)	Not provided	
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	Not provided	
Maximum map value	1.505	Depositor
Minimum map value	-0.941	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	232.0, 232.0, 232.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, ZN, FK5, CA

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	0/2962	0.51	0/4018
2	F	0.25	0/851	0.53	0/1146
3	R	0.26	0/2378	0.48	0/3233
4	L	0.25	0/144	0.52	0/197
All	All	0.26	0/6335	0.50	0/8594

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 [i](#)

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	2881	0	2792	55	0
2	F	832	0	831	10	0
3	R	2323	0	2430	58	0
4	L	135	0	104	7	0
5	F	57	0	69	2	0
6	R	152	0	75	2	0
7	R	20	0	20	0	0
8	R	99	0	66	3	0
9	R	88	0	121	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	R	135	0	195	3	0
11	R	66	0	78	0	0
12	R	104	0	143	6	0
13	R	52	0	39	1	0
14	R	121	0	99	4	0
15	R	56	0	42	1	0
16	R	48	0	39	2	0
17	R	98	0	126	7	0
18	R	40	0	45	3	0
19	R	14	0	14	0	0
20	R	81	0	72	2	0
21	R	21	0	21	0	0
22	R	24	0	18	1	0
23	R	6	0	5	1	0
24	R	10	0	7	1	0
All	All	7463	0	7451	142	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 (142) 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:R:182:LYS:HE3	3:R:236:GLU:HG3	1.63	0.80
2:F:24:VAL:HG12	2:F:103:LEU:HA	1.68	0.75
3:R:199:ARG:HH21	3:R:321:VAL:HG22	1.51	0.74
3:R:317:GLN:HG3	3:R:318:ARG:H	1.54	0.72
10:R:926:LYS:HE2	12:R:930:LEU:HD11	1.76	0.68
1:A:200:LEU:HB3	1:A:204:PHE:HB2	1.75	0.67
12:R:967:LEU:HD12	9:R:970:ILE:HD11	1.77	0.67
3:R:350:TYR:HA	3:R:360:LEU:HD21	1.77	0.66
1:A:219:ASP:OD1	1:A:222:ARG:NH2	2.29	0.65
3:R:254:ILE:HG22	3:R:256:LEU:HD22	1.78	0.65
3:R:274:ASP:OD2	3:R:343:ARG:NH2	2.29	0.65
3:R:199:ARG:HE	3:R:321:VAL:HG13	1.62	0.64
12:R:998:LEU:HB3	9:R:1000:ILE:HG12	1.79	0.64
2:F:29:MET:HG2	2:F:35:LYS:HA	1.79	0.64
3:R:289:THR:HG21	3:R:329:VAL:HG11	1.80	0.63
1:A:328:ALA:HB3	1:A:343:PHE:O	1.98	0.63
1:A:360:THR:HA	12:R:998:LEU:HD21	1.79	0.63
1:A:143:TRP:O	1:A:147:ILE:HG13	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:146:GLY:O	3:R:184:SER:OG	2.16	0.62
1:A:90:VAL:HG23	1:A:121:ARG:HH21	1.64	0.61
1:A:59:LEU:HD22	1:A:137:GLU:HG3	1.83	0.61
2:F:90:ILE:HG21	5:F:201:FK5:H353	1.84	0.60
3:R:369:TYR:O	3:R:373:ASN:ND2	2.35	0.59
3:R:320:GLU:OE2	3:R:390:SER:OG	2.18	0.58
1:A:139:VAL:O	1:A:143:TRP:HE3	1.86	0.58
1:A:257:PHE:HB3	1:A:267:TYR:HD2	1.69	0.58
3:R:178:PRO:HA	3:R:181:GLN:HG2	1.85	0.58
3:R:240:PHE:HE1	3:R:257:LEU:HD22	1.70	0.57
3:R:199:ARG:HH21	3:R:321:VAL:CG2	2.16	0.56
1:A:263:ARG:NH2	1:A:290:HIS:O	2.39	0.56
1:A:73:ILE:HG23	1:A:147:ILE:HD11	1.87	0.55
1:A:377:VAL:HG23	1:A:378:LEU:HG	1.89	0.54
2:F:25:HIS:ND1	2:F:104:LEU:HD11	2.22	0.54
3:R:199:ARG:NH2	3:R:321:VAL:HG22	2.22	0.54
3:R:346:LYS:NZ	4:L:2:ASN:O	2.30	0.53
1:A:143:TRP:HZ2	1:A:194:LEU:HD21	1.73	0.52
3:R:317:GLN:O	3:R:318:ARG:HB3	2.08	0.52
3:R:125:ILE:HD11	3:R:400:ALA:HB2	1.92	0.52
2:F:74:LEU:HD22	2:F:101:VAL:HG21	1.90	0.52
3:R:316:LYS:HG2	20:R:919:GLN:HE22	1.75	0.51
3:R:368:ASP:O	3:R:372:ILE:HG12	2.10	0.51
3:R:240:PHE:CE1	3:R:257:LEU:HD22	2.45	0.51
1:A:58:HIS:NE2	1:A:64:ARG:O	2.44	0.51
14:R:920:PHE:HA	10:R:929:LYS:HE3	1.94	0.50
1:A:97:CYS:SG	1:A:110:LEU:HD21	2.52	0.50
17:R:896:VAL:HA	9:R:899:ILE:HG22	1.94	0.49
3:R:139:LEU:HD23	3:R:222:ILE:HD11	1.94	0.49
3:R:182:LYS:HG2	4:L:10:TRP:CZ3	2.48	0.49
1:A:124:PHE:HB3	1:A:128:TYR:HE1	1.77	0.49
3:R:342:ALA:HB2	3:R:367:LEU:HG	1.95	0.49
17:R:893:VAL:O	9:R:897:ILE:HG12	2.13	0.49
3:R:189:VAL:HG23	3:R:285:PRO:HB3	1.96	0.48
3:R:317:GLN:HG3	3:R:318:ARG:N	2.26	0.48
1:A:369:LYS:HE3	15:R:890:ASN:ND2	2.28	0.48
10:R:926:LYS:HG3	24:R:1001:HIS:CG	2.48	0.48
2:F:30:LEU:HD23	2:F:31:GLU:N	2.29	0.48
1:A:256:HIS:HB3	1:A:273:ALA:HB2	1.96	0.48
3:R:137:ASN:O	3:R:140:ILE:HB	2.13	0.48
1:A:220:ASP:HA	1:A:223:ARG:NH2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:107:VAL:O	3:R:111:VAL:HG23	2.15	0.47
3:R:115:GLY:HA3	3:R:151:ILE:HD13	1.96	0.47
1:A:321:LEU:HD12	1:A:324:TYR:HE1	1.79	0.47
14:R:920:PHE:CD2	18:R:1004:MET:HB3	2.49	0.47
1:A:37:ARG:HH11	1:A:64:ARG:HB2	1.79	0.47
1:A:163:ARG:NH2	1:A:192:ASP:OD2	2.47	0.47
1:A:87:MET:HB3	1:A:222:ARG:HG2	1.96	0.47
1:A:172:LYS:HZ2	1:A:184:TYR:HE2	1.63	0.47
1:A:68[B]:GLU:HG3	1:A:69:ILE:N	2.31	0.46
3:R:131:CYS:HB2	8:R:989:GLU:OE1	2.16	0.46
3:R:168:PRO:HA	3:R:253:ARG:HH21	1.80	0.46
3:R:298:CYS:O	3:R:302:ARG:HG2	2.15	0.46
3:R:230:VAL:O	3:R:234:VAL:HG23	2.15	0.46
1:A:94:ILE:HG22	1:A:333:TYR:HB3	1.97	0.46
3:R:197:ILE:HG13	3:R:292:PHE:CE2	2.51	0.46
5:F:201:FK5:H371	5:F:201:FK5:H21	1.79	0.46
3:R:122:LEU:O	3:R:126:ILE:HG12	2.16	0.46
1:A:172:LYS:NZ	1:A:184:TYR:HE2	2.14	0.45
3:R:187:ILE:HD11	3:R:226:TRP:HA	1.97	0.45
16:R:875:SER:OG	8:R:907:GLU:OE1	2.23	0.45
1:A:171:PHE:CD2	1:A:184:TYR:HE1	2.33	0.45
3:R:185:VAL:HG12	3:R:281:TYR:HD2	1.80	0.45
3:R:131:CYS:SG	23:R:992:CYS:HB2	2.57	0.45
3:R:317:GLN:CG	3:R:318:ARG:H	2.28	0.45
1:A:288:ARG:HG2	1:A:289:ALA:H	1.82	0.45
4:L:9:ASP:OD1	4:L:10:TRP:N	2.50	0.45
3:R:126:ILE:HG21	3:R:141:ALA:HB2	1.98	0.45
12:R:967:LEU:HA	9:R:970:ILE:HG12	1.99	0.44
1:A:110:LEU:HD12	1:A:343:PHE:CZ	2.52	0.44
22:R:937:TYR:HA	17:R:953:VAL:HG21	1.99	0.44
1:A:199:LEU:HD21	1:A:202[A]:GLN:HA	1.99	0.44
1:A:374:LEU:HA	1:A:377:VAL:HG22	1.99	0.44
14:R:991:PHE:O	17:R:995:VAL:HG22	2.18	0.44
3:R:140:ILE:HA	3:R:143:LEU:HD12	1.99	0.44
3:R:337:LEU:HB3	3:R:338:PRO:HD3	1.99	0.44
1:A:209:GLY:O	1:A:288:ARG:HD2	2.18	0.44
3:R:385:ALA:O	3:R:389:VAL:HG12	2.18	0.43
1:A:191:PHE:HA	1:A:194:LEU:HD23	2.00	0.43
1:A:144:VAL:HA	1:A:147:ILE:HD12	1.99	0.43
3:R:138:ILE:HD11	3:R:218:THR:HG22	2.00	0.43
3:R:129:ASN:HD21	8:R:989:GLU:HG3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:1006:VAL:HG12	6:R:1007:ASP:N	2.33	0.43
1:A:198:ALA:HB3	1:A:206:CYS:HB2	2.01	0.43
1:A:149:TYR:HB3	1:A:152:THR:OG1	2.19	0.43
13:R:948:GLY:O	20:R:952:GLN:HG3	2.18	0.43
1:A:373:MET:HE1	17:R:893:VAL:HA	2.00	0.43
2:F:62:GLY:HA3	2:F:74:LEU:HD21	2.01	0.43
3:R:235:PRO:HA	3:R:238:ILE:HG22	2.01	0.43
1:A:271:TYR:HB3	1:A:272:PRO:HD3	2.00	0.42
2:F:23:VAL:HG22	2:F:47:LYS:HG2	2.01	0.42
1:A:199:LEU:HD21	1:A:202[B]:GLN:HA	2.01	0.42
1:A:288:ARG:NH1	1:A:289:ALA:O	2.53	0.42
3:R:198:ASP:O	3:R:201:ARG:HB3	2.18	0.42
3:R:254:ILE:HG23	4:L:6:THR:HA	2.02	0.42
1:A:308:PHE:CG	1:A:309:PRO:HD2	2.54	0.42
17:R:1006:VAL:HG12	6:R:1007:ASP:H	1.84	0.42
1:A:174:GLU:O	1:A:178:LYS:HB2	2.20	0.42
3:R:136:PRO:HB3	3:R:139:LEU:HD12	2.02	0.42
3:R:155:ILE:O	3:R:159:VAL:HG23	2.19	0.42
3:R:182:LYS:HG2	4:L:10:TRP:HZ3	1.84	0.42
3:R:314:HIS:HB2	16:R:918:SER:HB2	2.01	0.42
1:A:52:VAL:HB	1:A:148:LEU:HD11	2.01	0.42
3:R:152:VAL:HG23	3:R:153:ILE:HG12	2.01	0.42
3:R:131:CYS:HB3	3:R:392:ARG:HH22	1.85	0.41
3:R:343:ARG:HA	4:L:2:ASN:HD22	1.85	0.41
4:L:2:ASN:HA	4:L:12:PHE:HB2	2.02	0.41
1:A:173:GLN:HG3	1:A:355:PHE:HB2	2.01	0.41
1:A:99:ASP:OD1	1:A:127:ASP:HB2	2.21	0.41
1:A:229:GLU:CD	1:A:230:PRO:HD2	2.41	0.41
1:A:72:ARG:O	1:A:76:GLU:HG3	2.21	0.41
2:F:46:PHE:CZ	2:F:48:PHE:HB3	2.56	0.41
1:A:362:SER:HB3	12:R:954:LEU:HD11	2.01	0.41
1:A:67:GLU:OE1	1:A:180:SER:OG	2.38	0.41
1:A:139:VAL:HG13	1:A:143:TRP:CZ3	2.56	0.41
1:A:300:TYR:CE2	1:A:311:LEU:HD23	2.56	0.41
1:A:353:PRO:O	1:A:356:MET:HG2	2.21	0.41
3:R:199:ARG:O	3:R:203:VAL:HG23	2.20	0.41
1:A:371:THR:OG1	18:R:1004:MET:HA	2.20	0.40
14:R:920:PHE:HD2	18:R:1004:MET:HB3	1.86	0.40
2:F:1:GLY:N	2:F:77:SER:OG	2.48	0.40
1:A:65:VAL:HG22	1:A:179:TYR:OH	2.21	0.40
3:R:111:VAL:HG22	3:R:377:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:186:GLY:HA2	3:R:189:VAL:HG12	2.04	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	351/354 (99%)	335 (95%)	16 (5%)	0	100	100
2	F	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
3	R	287/293 (98%)	275 (96%)	12 (4%)	0	100	100
4	L	13/15 (87%)	11 (85%)	2 (15%)	0	100	100
All	All	756/769 (98%)	723 (96%)	33 (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	318/313 (102%)	316 (99%)	2 (1%)	86	86
2	F	89/89 (100%)	89 (100%)	0	100	100
3	R	254/259 (98%)	253 (100%)	1 (0%)	91	91
4	L	13/13 (100%)	12 (92%)	1 (8%)	13	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	674/674 (100%)	670 (99%)	4 (1%)	89	86

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167[A]	GLU
1	A	167[B]	GLU
3	R	316	LYS
4	L	9	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

156 ligands are modelled in this entry.

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	$\# Z  > 2$
8	GLU	R	880	1	7,8,9	0.90	0	4,9,11	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	ILE	R	976	-	6,7,8	0.48	0	4,8,10	0.74	0
17	VAL	R	917	-	4,6,7	0.62	0	6,7,9	0.88	0
10	LYS	R	923	-	7,8,9	0.52	0	3,8,10	0.40	0
13	GLY	R	984	-	3,3,4	0.60	0	1,2,4	0.03	0
6	ASP	R	942	1	6,7,8	0.97	0	4,8,10	0.85	0
12	LEU	R	876	-	5,7,8	0.56	0	6,8,10	0.24	0
8	GLU	R	915	-	7,8,9	0.90	0	4,9,11	1.01	0
13	GLY	R	996	-	3,3,4	0.61	0	1,2,4	0.09	0
8	GLU	R	989	-	7,8,9	0.88	0	4,9,11	1.06	0
14	PHE	R	991	-	10,11,12	0.43	0	8,13,15	0.19	0
12	LEU	R	962	-	5,7,8	0.56	0	6,8,10	0.32	0
15	ASN	R	905	1	6,7,8	0.52	0	4,8,10	0.17	0
14	PHE	R	934	-	10,11,12	0.40	0	8,13,15	0.21	0
7	ALA	R	855	-	3,4,5	0.75	0	2,4,6	1.12	0
22	TYR	R	944	1	11,12,13	0.44	0	10,15,17	0.16	0
6	ASP	R	983	1	6,7,8	0.92	0	4,8,10	1.04	0
20	GLN	R	894	-	7,8,9	0.50	0	4,9,11	0.04	0
12	LEU	R	868	-	5,7,8	0.58	0	6,8,10	0.33	0
8	GLU	R	949	1	7,8,9	0.92	0	4,9,11	0.99	0
12	LEU	R	967	-	5,7,8	0.58	0	6,8,10	0.11	0
16	SER	R	987	-	4,5,6	0.67	0	1,5,7	0.60	0
10	LYS	R	1003	-	7,8,9	0.52	0	3,8,10	0.43	0
10	LYS	R	980	-	7,8,9	0.51	0	3,8,10	0.23	0
18	MET	R	957	-	6,7,8	0.52	0	2,7,9	0.65	0
8	GLU	R	927	-	7,8,9	0.90	0	4,9,11	1.01	0
17	VAL	R	1005	-	4,6,7	0.61	0	6,7,9	0.64	0
9	ILE	R	914	-	6,7,8	0.49	0	4,8,10	0.86	0
9	ILE	R	970	-	6,7,8	0.51	0	4,8,10	1.10	1 (25%)
6	ASP	R	869	-	6,7,8	0.93	0	4,8,10	1.02	0
18	MET	R	882	-	6,7,8	0.52	0	2,7,9	0.12	0
6	ASP	R	854	-	6,7,8	0.96	0	4,8,10	1.01	0
8	GLU	R	907	1	7,8,9	0.91	0	4,9,11	1.01	0
15	ASN	R	977	-	6,7,8	0.50	0	4,8,10	0.17	0
8	GLU	R	912	1	7,8,9	0.90	0	4,9,11	0.99	0
10	LYS	R	955	-	7,8,9	0.51	0	3,8,10	0.45	0
12	LEU	R	887	-	5,7,8	0.60	0	6,8,10	0.48	0
20	GLN	R	969	-	7,8,9	0.50	0	4,9,11	0.04	0
17	VAL	R	893	-	4,6,7	0.61	0	6,7,9	0.76	0
20	GLN	R	919	-	7,8,9	0.49	0	4,9,11	0.04	0
6	ASP	R	925	-	6,7,8	0.96	0	4,8,10	0.95	0
6	ASP	R	909	-	6,7,8	0.97	0	4,8,10	0.93	0
11	ARG	R	860	-	9,10,11	0.47	0	5,11,13	0.60	0
14	PHE	R	881	-	10,11,12	0.45	0	8,13,15	0.18	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	ASP	R	999	-	6,7,8	0.91	0	4,8,10	1.01	0
16	SER	R	873	1	4,5,6	0.65	0	1,5,7	0.84	0
18	MET	R	956	-	6,7,8	0.53	0	2,7,9	0.15	0
8	GLU	R	879	-	7,8,9	0.92	0	4,9,11	1.00	0
9	ILE	R	936	-	6,7,8	0.49	0	4,8,10	0.81	0
7	ALA	R	993	-	3,4,5	0.75	0	2,4,6	0.84	0
16	SER	R	877	-	4,5,6	0.64	0	1,5,7	0.39	0
11	ARG	R	931	-	9,10,11	0.47	0	5,11,13	0.61	0
14	PHE	R	932	-	10,11,12	0.46	0	8,13,15	0.21	0
9	ILE	R	858	-	6,7,8	0.48	0	4,8,10	0.86	0
13	GLY	R	874	-	3,3,4	0.55	0	1,2,4	0.04	0
13	GLY	R	904	-	3,3,4	0.56	0	1,2,4	0.04	0
13	GLY	R	982	-	3,3,4	0.57	0	1,2,4	0.32	0
8	GLU	R	990	1	7,8,9	0.92	0	4,9,11	1.00	0
17	VAL	R	1006	-	4,6,7	0.60	0	6,7,9	0.74	0
20	GLN	R	889	-	7,8,9	0.50	0	4,9,11	0.03	0
11	ARG	R	985	1	9,10,11	0.46	0	5,11,13	0.61	0
6	ASP	R	903	1	6,7,8	0.94	0	4,8,10	0.93	0
12	LEU	R	870	-	5,7,8	0.57	0	6,8,10	0.14	0
6	ASP	R	972	-	6,7,8	0.95	0	4,8,10	1.02	0
10	LYS	R	941	-	7,8,9	0.44	0	3,8,10	0.42	0
17	VAL	R	958	-	4,6,7	0.60	0	6,7,9	1.15	0
8	GLU	R	886	-	7,8,9	0.93	0	4,9,11	0.99	0
10	LYS	R	911	-	7,8,9	0.50	0	3,8,10	0.37	0
10	LYS	R	1002	-	7,8,9	0.52	0	3,8,10	0.42	0
13	GLY	R	924	-	3,3,4	0.59	0	1,2,4	0.48	0
17	VAL	R	971	-	4,6,7	0.61	0	6,7,9	0.72	0
10	LYS	R	963	-	7,8,9	0.53	0	3,8,10	0.41	0
17	VAL	R	995	-	4,6,7	0.60	0	6,7,9	1.01	0
20	GLN	R	888	-	7,8,9	0.49	0	4,9,11	0.04	0
14	PHE	R	910	-	10,11,12	0.40	0	8,13,15	0.21	0
21	THR	R	902	-	5,6,7	0.53	0	5,7,9	1.07	1 (20%)
9	ILE	R	975	-	6,7,8	0.47	0	4,8,10	0.79	0
15	ASN	R	872	-	6,7,8	0.45	0	4,8,10	0.11	0
21	THR	R	974	-	5,6,7	0.57	0	5,7,9	0.88	0
17	VAL	R	896	-	4,6,7	0.66	0	6,7,9	0.75	0
20	GLN	R	952	-	7,8,9	0.49	0	4,9,11	0.08	0
14	PHE	R	900	-	10,11,12	0.40	0	8,13,15	0.19	0
14	PHE	R	913	-	10,11,12	0.43	0	8,13,15	0.18	0
6	ASP	R	901	-	6,7,8	0.95	0	4,8,10	0.88	0
16	SER	R	918	-	4,5,6	0.62	0	1,5,7	0.99	0
20	GLN	R	968	-	7,8,9	0.50	0	4,9,11	0.03	0
12	LEU	R	998	-	5,7,8	0.57	0	6,8,10	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	ASP	R	856	-	6,7,8	0.93	0	4,8,10	1.01	0
23	CYS	R	992	-	4,5,6	0.84	0	1,5,7	0.56	0
14	PHE	R	951	-	10,11,12	0.42	0	8,13,15	0.19	0
10	LYS	R	859	-	7,8,9	0.49	0	3,8,10	0.41	0
10	LYS	R	867	-	7,8,9	0.51	0	3,8,10	0.38	0
6	ASP	R	981	1	6,7,8	0.93	0	4,8,10	1.03	0
20	GLN	R	966	-	7,8,9	0.50	0	4,9,11	0.04	0
15	ASN	R	960	-	6,7,8	0.52	0	4,8,10	0.11	0
16	SER	R	921	-	4,5,6	0.66	0	1,5,7	0.66	0
13	GLY	R	943	-	3,3,4	0.59	0	1,2,4	0.01	0
10	LYS	R	866	-	7,8,9	0.52	0	3,8,10	0.38	0
11	ARG	R	895	-	9,10,11	0.47	0	5,11,13	0.59	0
15	ASN	R	947	-	6,7,8	0.53	0	4,8,10	0.13	0
5	FK5	F	201	-	54,60,60	3.63	10 (18%)	64,86,86	1.61	9 (14%)
17	VAL	R	878	-	4,6,7	0.60	0	6,7,9	0.71	0
11	ARG	R	864	-	9,10,11	0.45	0	5,11,13	0.59	0
14	PHE	R	865	-	10,11,12	0.42	0	8,13,15	0.19	0
17	VAL	R	922	-	4,6,7	0.60	0	6,7,9	1.03	0
10	LYS	R	863	-	7,8,9	0.52	0	3,8,10	0.42	0
6	ASP	R	938	1	6,7,8	0.95	0	4,8,10	0.96	0
12	LEU	R	930	-	5,7,8	0.57	0	6,8,10	0.24	0
17	VAL	R	953	-	4,6,7	0.64	0	6,7,9	0.71	0
14	PHE	R	920	-	10,11,12	0.50	0	8,13,15	0.22	0
16	SER	R	883	-	4,5,6	0.65	0	1,5,7	0.92	0
18	MET	R	1004	-	6,7,8	0.52	0	2,7,9	0.09	0
18	MET	R	939	-	6,7,8	0.52	0	2,7,9	0.12	0
12	LEU	R	892	-	5,7,8	0.59	0	6,8,10	0.28	0
6	ASP	R	979	-	6,7,8	0.93	0	4,8,10	0.92	0
13	GLY	R	997	-	3,3,4	0.55	0	1,2,4	0.24	0
9	ILE	R	897	-	6,7,8	0.50	0	4,8,10	0.79	0
17	VAL	R	1008	-	6,6,7	1.85	1 (16%)	4,7,9	2.12	1 (25%)
6	ASP	R	1007	-	6,7,8	0.96	0	4,8,10	1.00	0
6	ASP	R	871	1	6,7,8	0.96	0	4,8,10	0.91	0
16	SER	R	875	1	4,5,6	0.66	0	1,5,7	0.38	0
6	ASP	R	940	1	6,7,8	0.95	0	4,8,10	0.93	0
24	HIS	R	1001	-	5,10,11	0.66	0	3,12,14	1.71	1 (33%)
6	ASP	R	898	-	6,7,8	0.96	0	4,8,10	1.04	0
16	SER	R	946	-	4,5,6	0.67	0	1,5,7	0.04	0
9	ILE	R	986	-	6,7,8	0.49	0	4,8,10	0.83	0
12	LEU	R	950	-	5,7,8	0.61	0	6,8,10	0.37	0
8	GLU	R	857	-	7,8,9	0.90	0	4,9,11	1.00	0
9	ILE	R	1000	-	6,7,8	0.50	0	4,8,10	1.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	TYR	R	937	-	11,12,13	0.46	0	10,15,17	0.22	0
13	GLY	R	959	-	3,3,4	0.59	0	1,2,4	0.81	0
7	ALA	R	978	-	3,4,5	0.77	0	2,4,6	1.14	0
10	LYS	R	973	-	7,8,9	0.53	0	3,8,10	0.47	0
13	GLY	R	916	-	3,3,4	0.58	0	1,2,4	0.36	0
12	LEU	R	861	-	5,7,8	0.56	0	6,8,10	0.20	0
12	LEU	R	954	-	5,7,8	0.53	0	6,8,10	0.27	0
19	PRO	R	885	-	6,7,8	0.60	0	7,8,10	1.26	2 (28%)
15	ASN	R	961	-	6,7,8	0.51	0	4,8,10	0.12	0
15	ASN	R	890	-	6,7,8	0.61	0	4,8,10	0.24	0
19	PRO	R	891	-	6,7,8	0.98	0	7,8,10	1.20	1 (14%)
9	ILE	R	899	-	6,7,8	0.63	0	4,8,10	1.13	0
13	GLY	R	948	-	3,3,4	0.57	0	1,2,4	0.23	0
10	LYS	R	929	-	7,8,9	0.52	0	3,8,10	0.37	0
7	ALA	R	933	-	3,4,5	0.75	0	2,4,6	0.86	0
9	ILE	R	945	-	6,7,8	0.49	0	4,8,10	0.82	0
14	PHE	R	988	-	10,11,12	0.46	0	8,13,15	0.21	0
17	VAL	R	908	-	4,6,7	0.61	0	6,7,9	0.91	0
13	GLY	R	862	-	3,3,4	0.60	0	1,2,4	0.44	0
13	GLY	R	906	-	3,3,4	0.62	0	1,2,4	0.10	0
6	ASP	R	964	-	6,7,8	0.94	0	4,8,10	1.01	0
17	VAL	R	994	-	4,6,7	0.58	0	6,7,9	0.77	0
21	THR	R	965	-	5,6,7	0.55	0	5,7,9	0.84	0
20	GLN	R	928	-	7,8,9	0.50	0	4,9,11	0.07	0
12	LEU	R	884	-	5,7,8	0.62	0	6,8,10	0.29	0
10	LYS	R	926	-	7,8,9	0.52	0	3,8,10	0.49	0
11	ARG	R	935	-	9,10,11	0.48	0	5,11,13	0.72	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
8	GLU	R	880	1	-	2/6/7/9	-
9	ILE	R	976	-	-	1/7/8/10	-
17	VAL	R	917	-	-	0/5/6/8	-
10	LYS	R	923	-	-	0/6/7/9	-
13	GLY	R	984	-	-	0/0/1/2	-
6	ASP	R	942	1	-	0/5/6/8	-
12	LEU	R	876	-	-	0/5/6/8	-
8	GLU	R	915	-	-	0/6/7/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	GLY	R	996	-	-	0/0/1/2	-
8	GLU	R	989	-	-	0/6/7/9	-
14	PHE	R	991	-	-	1/5/6/8	0/1/1/1
12	LEU	R	962	-	-	0/5/6/8	-
15	ASN	R	905	1	-	0/5/6/8	-
14	PHE	R	934	-	-	0/5/6/8	0/1/1/1
7	ALA	R	855	-	-	0/1/2/4	-
22	TYR	R	944	1	-	1/5/6/8	0/1/1/1
6	ASP	R	983	1	-	0/5/6/8	-
20	GLN	R	894	-	-	0/6/7/9	-
12	LEU	R	868	-	-	2/5/6/8	-
8	GLU	R	949	1	-	0/6/7/9	-
12	LEU	R	967	-	-	0/5/6/8	-
16	SER	R	987	-	-	0/2/4/6	-
10	LYS	R	1003	-	-	0/6/7/9	-
10	LYS	R	980	-	-	1/6/7/9	-
18	MET	R	957	-	-	0/5/6/8	-
8	GLU	R	927	-	-	1/6/7/9	-
17	VAL	R	1005	-	-	1/5/6/8	-
9	ILE	R	914	-	-	0/7/8/10	-
9	ILE	R	970	-	-	0/7/8/10	-
6	ASP	R	869	-	-	1/5/6/8	-
18	MET	R	882	-	-	0/5/6/8	-
6	ASP	R	854	-	-	0/5/6/8	-
8	GLU	R	907	1	-	0/6/7/9	-
15	ASN	R	977	-	-	2/5/6/8	-
8	GLU	R	912	1	-	0/6/7/9	-
10	LYS	R	955	-	-	0/6/7/9	-
12	LEU	R	887	-	-	0/5/6/8	-
20	GLN	R	969	-	-	0/6/7/9	-
17	VAL	R	893	-	-	0/5/6/8	-
20	GLN	R	919	-	-	0/6/7/9	-
6	ASP	R	925	-	-	1/5/6/8	-
6	ASP	R	909	-	-	0/5/6/8	-
11	ARG	R	860	-	-	0/8/9/11	-
14	PHE	R	881	-	-	2/5/6/8	0/1/1/1
6	ASP	R	999	-	-	0/5/6/8	-
16	SER	R	873	1	-	2/2/4/6	-
18	MET	R	956	-	-	1/5/6/8	-
8	GLU	R	879	-	-	0/6/7/9	-
9	ILE	R	936	-	-	3/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ALA	R	993	-	-	1/1/2/4	-
16	SER	R	877	-	-	0/2/4/6	-
11	ARG	R	931	-	-	1/8/9/11	-
14	PHE	R	932	-	-	0/5/6/8	0/1/1/1
9	ILE	R	858	-	-	2/7/8/10	-
13	GLY	R	874	-	-	0/0/1/2	-
13	GLY	R	904	-	-	0/0/1/2	-
13	GLY	R	982	-	-	0/0/1/2	-
8	GLU	R	990	1	-	0/6/7/9	-
17	VAL	R	1006	-	-	0/5/6/8	-
20	GLN	R	889	-	-	1/6/7/9	-
11	ARG	R	985	1	-	0/8/9/11	-
6	ASP	R	903	1	-	0/5/6/8	-
12	LEU	R	870	-	-	0/5/6/8	-
6	ASP	R	972	-	-	2/5/6/8	-
10	LYS	R	941	-	-	0/6/7/9	-
17	VAL	R	958	-	-	0/5/6/8	-
8	GLU	R	886	-	-	0/6/7/9	-
10	LYS	R	911	-	-	1/6/7/9	-
10	LYS	R	1002	-	-	0/6/7/9	-
13	GLY	R	924	-	-	0/0/1/2	-
17	VAL	R	971	-	-	1/5/6/8	-
10	LYS	R	963	-	-	0/6/7/9	-
17	VAL	R	995	-	-	0/5/6/8	-
20	GLN	R	888	-	-	0/6/7/9	-
14	PHE	R	910	-	-	2/5/6/8	0/1/1/1
21	THR	R	902	-	-	1/5/6/8	-
9	ILE	R	975	-	-	0/7/8/10	-
15	ASN	R	872	-	-	2/5/6/8	-
21	THR	R	974	-	-	1/5/6/8	-
17	VAL	R	896	-	-	0/5/6/8	-
20	GLN	R	952	-	-	2/6/7/9	-
14	PHE	R	900	-	-	2/5/6/8	0/1/1/1
14	PHE	R	913	-	-	0/5/6/8	0/1/1/1
6	ASP	R	901	-	-	2/5/6/8	-
16	SER	R	918	-	-	2/2/4/6	-
20	GLN	R	968	-	-	0/6/7/9	-
12	LEU	R	998	-	-	2/5/6/8	-
6	ASP	R	856	-	-	0/5/6/8	-
23	CYS	R	992	-	-	0/1/4/6	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	PHE	R	951	-	-	0/5/6/8	0/1/1/1
10	LYS	R	859	-	-	1/6/7/9	-
10	LYS	R	867	-	-	1/6/7/9	-
6	ASP	R	981	1	-	0/5/6/8	-
20	GLN	R	966	-	-	0/6/7/9	-
15	ASN	R	960	-	-	0/5/6/8	-
16	SER	R	921	-	-	0/2/4/6	-
13	GLY	R	943	-	-	0/0/1/2	-
10	LYS	R	866	-	-	0/6/7/9	-
11	ARG	R	895	-	-	1/8/9/11	-
15	ASN	R	947	-	-	0/5/6/8	-
5	FK5	F	201	-	-	3/68/114/114	0/3/4/4
17	VAL	R	878	-	-	1/5/6/8	-
11	ARG	R	864	-	-	1/8/9/11	-
14	PHE	R	865	-	-	0/5/6/8	0/1/1/1
17	VAL	R	922	-	-	1/5/6/8	-
10	LYS	R	863	-	-	0/6/7/9	-
6	ASP	R	938	1	-	1/5/6/8	-
12	LEU	R	930	-	-	0/5/6/8	-
17	VAL	R	953	-	-	0/5/6/8	-
14	PHE	R	920	-	-	0/5/6/8	0/1/1/1
16	SER	R	883	-	-	2/2/4/6	-
18	MET	R	1004	-	-	0/5/6/8	-
18	MET	R	939	-	-	0/5/6/8	-
12	LEU	R	892	-	-	2/5/6/8	-
6	ASP	R	979	-	-	1/5/6/8	-
13	GLY	R	997	-	-	0/0/1/2	-
9	ILE	R	897	-	-	0/7/8/10	-
17	VAL	R	1008	-	-	3/6/6/8	-
6	ASP	R	1007	-	-	1/5/6/8	-
6	ASP	R	871	1	-	0/5/6/8	-
16	SER	R	875	1	-	1/2/4/6	-
6	ASP	R	940	1	-	0/5/6/8	-
24	HIS	R	1001	-	-	0/5/6/8	0/1/1/1
6	ASP	R	898	-	-	0/5/6/8	-
16	SER	R	946	-	-	0/2/4/6	-
9	ILE	R	986	-	-	0/7/8/10	-
12	LEU	R	950	-	-	0/5/6/8	-
8	GLU	R	857	-	-	0/6/7/9	-
9	ILE	R	1000	-	-	1/7/8/10	-
22	TYR	R	937	-	-	0/5/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	GLY	R	959	-	-	0/0/1/2	-
7	ALA	R	978	-	-	1/1/2/4	-
10	LYS	R	973	-	-	1/6/7/9	-
13	GLY	R	916	-	-	0/0/1/2	-
12	LEU	R	861	-	-	0/5/6/8	-
12	LEU	R	954	-	-	1/5/6/8	-
19	PRO	R	885	-	-	0/0/9/11	0/1/1/1
15	ASN	R	961	-	-	1/5/6/8	-
15	ASN	R	890	-	-	0/5/6/8	-
19	PRO	R	891	-	-	0/0/9/11	0/1/1/1
9	ILE	R	899	-	-	0/7/8/10	-
13	GLY	R	948	-	-	0/0/1/2	-
10	LYS	R	929	-	-	0/6/7/9	-
7	ALA	R	933	-	-	0/1/2/4	-
9	ILE	R	945	-	-	0/7/8/10	-
14	PHE	R	988	-	-	0/5/6/8	0/1/1/1
17	VAL	R	908	-	-	0/5/6/8	-
13	GLY	R	862	-	-	0/0/1/2	-
13	GLY	R	906	-	-	0/0/1/2	-
6	ASP	R	964	-	-	0/5/6/8	-
17	VAL	R	994	-	-	0/5/6/8	-
21	THR	R	965	-	-	1/5/6/8	-
20	GLN	R	928	-	-	2/6/7/9	-
12	LEU	R	884	-	-	0/5/6/8	-
10	LYS	R	926	-	-	0/6/7/9	-
11	ARG	R	935	-	-	0/8/9/11	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	201	FK5	O9-C22	12.03	1.41	1.21
5	F	201	FK5	O4-C9	10.97	1.41	1.22
5	F	201	FK5	C8-C9	-10.61	1.40	1.53
5	F	201	FK5	C20-C19	9.95	1.47	1.33
5	F	201	FK5	O3-C8	8.97	1.41	1.23
5	F	201	FK5	O2-C1	7.99	1.41	1.21
5	F	201	FK5	C28-C27	6.32	1.47	1.33
17	R	1008	VAL	OXT-C	-4.50	1.23	1.42
5	F	201	FK5	O1-C1	-3.78	1.25	1.34
5	F	201	FK5	O6-C10	3.68	1.45	1.39
5	F	201	FK5	C40-C39	2.84	1.47	1.29

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	201	FK5	C21-C20-C19	-7.58	120.40	127.63
5	F	201	FK5	O1-C1-C2	4.65	120.46	110.80
17	R	1008	VAL	OXT-C-CA	4.18	120.61	111.55
5	F	201	FK5	O1-C26-C25	2.59	108.88	105.91
5	F	201	FK5	O1-C1-O2	-2.52	119.39	123.95
5	F	201	FK5	C6-N7-C2	2.46	120.90	115.81
5	F	201	FK5	O3-C8-C9	2.34	120.12	116.28
19	R	891	PRO	O-C-CA	-2.26	118.95	124.77
21	R	902	THR	O-C-CA	-2.18	119.16	124.77
5	F	201	FK5	C37-C19-C18	2.09	119.93	115.28
19	R	885	PRO	CD-N-CA	2.09	112.51	107.21
9	R	970	ILE	O-C-CA	-2.08	119.42	124.77
24	R	1001	HIS	CD2-NE2-CE1	2.07	108.99	105.72
19	R	885	PRO	O-C-CA	-2.02	119.58	124.77
5	F	201	FK5	C9-C8-N7	2.01	121.54	119.25
5	F	201	FK5	C42-C27-C26	2.00	119.91	115.96

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	201	FK5	C15-C16-C17-C36
6	R	869	ASP	O-C-CA-CB
6	R	901	ASP	O-C-CA-CB
6	R	938	ASP	O-C-CA-CB
6	R	979	ASP	O-C-CA-CB
6	R	1007	ASP	O-C-CA-CB
7	R	978	ALA	O-C-CA-CB
7	R	993	ALA	O-C-CA-CB
8	R	880	GLU	O-C-CA-CB
8	R	927	GLU	C-CA-CB-CG
9	R	936	ILE	C-CA-CB-CG2
9	R	976	ILE	C-CA-CB-CG2
9	R	1000	ILE	O-C-CA-CB
11	R	864	ARG	C-CA-CB-CG
12	R	892	LEU	O-C-CA-CB
12	R	954	LEU	O-C-CA-CB
14	R	881	PHE	C-CA-CB-CG
14	R	991	PHE	C-CA-CB-CG
15	R	961	ASN	O-C-CA-CB
15	R	977	ASN	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
16	R	873	SER	C-CA-CB-OG
16	R	875	SER	C-CA-CB-OG
16	R	883	SER	C-CA-CB-OG
17	R	922	VAL	O-C-CA-CB
17	R	971	VAL	C-CA-CB-CG1
17	R	1008	VAL	OXT-C-CA-N
17	R	1008	VAL	OXT-C-CA-CB
20	R	889	GLN	O-C-CA-CB
21	R	902	THR	O-C-CA-CB
22	R	944	TYR	O-C-CA-CB
18	R	956	MET	CB-CG-SD-CE
15	R	977	ASN	CA-CB-CG-ND2
14	R	900	PHE	CA-CB-CG-CD1
14	R	900	PHE	CA-CB-CG-CD2
14	R	881	PHE	N-CA-CB-CG
9	R	858	ILE	CG2-CB-CG1-CD1
14	R	910	PHE	CA-CB-CG-CD1
14	R	910	PHE	CA-CB-CG-CD2
9	R	858	ILE	CA-CB-CG1-CD1
6	R	972	ASP	CA-CB-CG-OD2
12	R	998	LEU	N-CA-CB-CG
6	R	972	ASP	CA-CB-CG-OD1
10	R	973	LYS	CE-CD-CG-CB
20	R	928	GLN	OE1-CD-CG-CB
10	R	911	LYS	C-CA-CB-CG
15	R	872	ASN	CA-CB-CG-ND2
20	R	952	GLN	CA-CB-CG-CD
5	F	201	FK5	C19-C20-C21-C22
12	R	998	LEU	C-CA-CB-CG
11	R	931	ARG	NE-CD-CG-CB
15	R	872	ASN	CA-CB-CG-OD1
9	R	936	ILE	CG2-CB-CG1-CD1
17	R	1005	VAL	O-C-CA-CB
17	R	878	VAL	C-CA-CB-CG1
20	R	928	GLN	NE2-CD-CG-CB
16	R	873	SER	N-CA-CB-OG
16	R	883	SER	N-CA-CB-OG
16	R	918	SER	N-CA-CB-OG
6	R	901	ASP	CA-CB-CG-OD1
17	R	1008	VAL	N-CA-CB-CG1
10	R	867	LYS	CE-CD-CG-CB
9	R	936	ILE	CA-CB-CG1-CD1

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Mol	Chain	Res	Type	Atoms
12	R	868	LEU	CA-CB-CG-CD1
11	R	895	ARG	CG-CD-NE-CZ
6	R	925	ASP	CA-CB-CG-OD1
12	R	868	LEU	CA-CB-CG-CD2
5	F	201	FK5	C15-C16-C17-C18
8	R	880	GLU	C-CA-CB-CG
10	R	980	LYS	C-CA-CB-CG
10	R	859	LYS	CA-CB-CG-CD
21	R	965	THR	O-C-CA-CB
21	R	974	THR	O-C-CA-CB
12	R	892	LEU	CA-CB-CG-CD2
16	R	918	SER	C-CA-CB-OG
20	R	952	GLN	N-CA-CB-CG

There are no ring outliers.

31 monomers are involved in 28 short contacts:

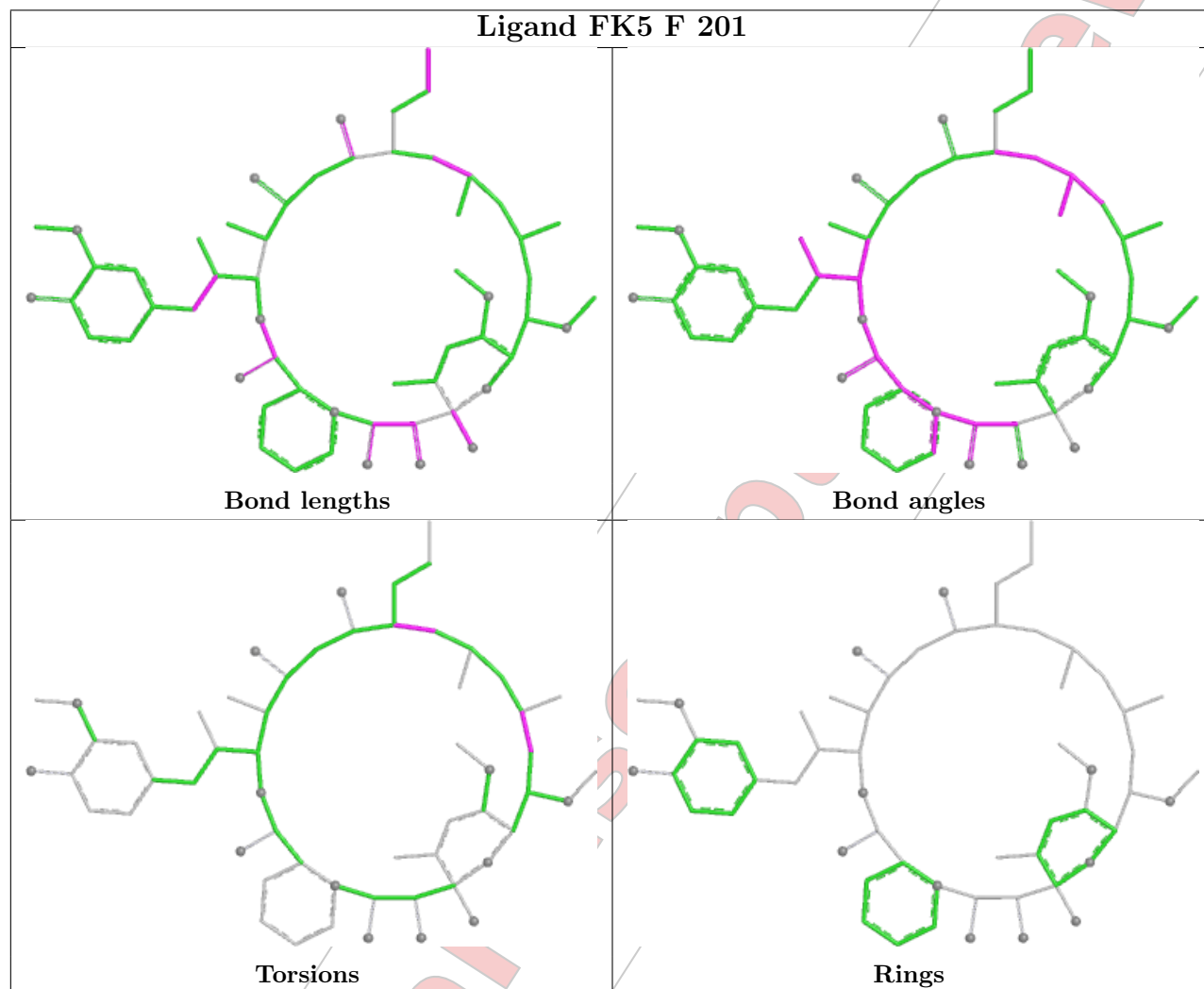
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	R	989	GLU	2	0
14	R	991	PHE	1	0
12	R	967	LEU	2	0
9	R	970	ILE	2	0
8	R	907	GLU	1	0
17	R	893	VAL	2	0
20	R	919	GLN	1	0
17	R	1006	VAL	2	0
17	R	995	VAL	1	0
17	R	896	VAL	1	0
20	R	952	GLN	1	0
16	R	918	SER	1	0
12	R	998	LEU	2	0
23	R	992	CYS	1	0
5	F	201	FK5	2	0
12	R	930	LEU	1	0
17	R	953	VAL	1	0
14	R	920	PHE	3	0
18	R	1004	MET	3	0
9	R	897	ILE	1	0
6	R	1007	ASP	2	0
16	R	875	SER	1	0
24	R	1001	HIS	1	0
9	R	1000	ILE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	R	937	TYR	1	0
12	R	954	LEU	1	0
15	R	890	ASN	1	0
9	R	899	ILE	1	0
13	R	948	GLY	1	0
10	R	929	LYS	1	0
10	R	926	LYS	2	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 than 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.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	6
3	R	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	494:CA	CA	601:FE	FE	41.61

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	381:CYS	C	491:CA	CA	22.40
1	A	492:CA	CA	493:CA	CA	20.58
1	R	205:SER	C	215:PRO	N	16.45
1	R	304:LYS	C	313:ASP	N	11.31
1	A	493:CA	CA	494:CA	CA	11.26
1	A	491:CA	CA	492:CA	CA	10.87
1	A	601:FE	FE	602:ZN	ZN	3.20

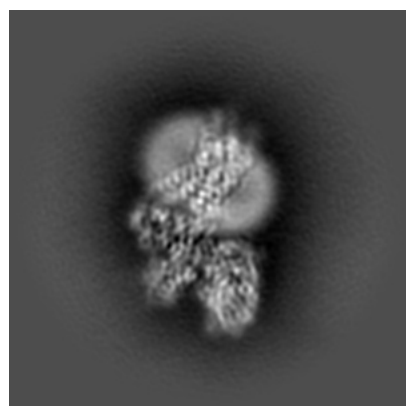
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry D\_9100090016. These allow visual inspection of the internal detail of the map and identification of artifacts.

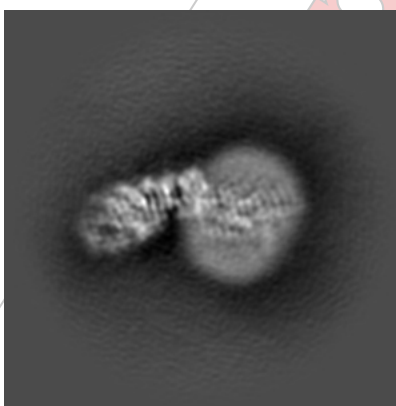
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

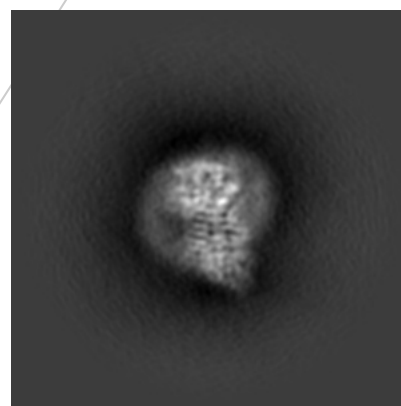
#### 6.1.1 Primary map



X



Y

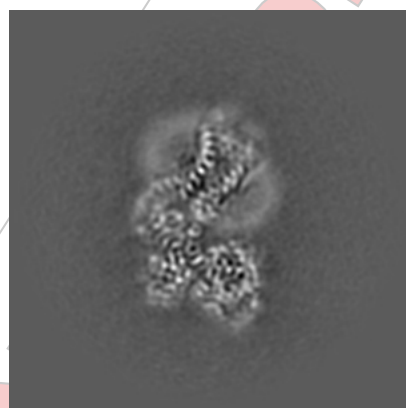


Z

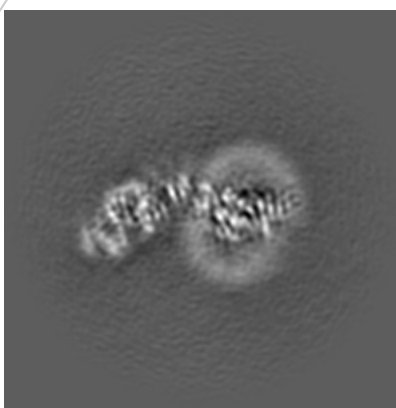
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

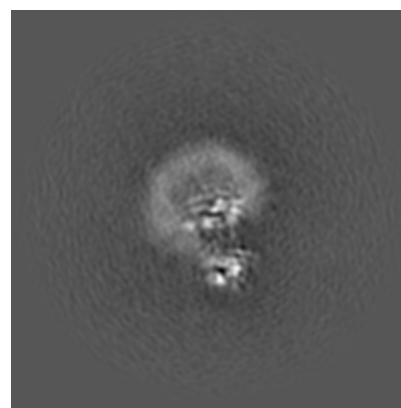
#### 6.2.1 Primary map



X Index: 100



Y Index: 100

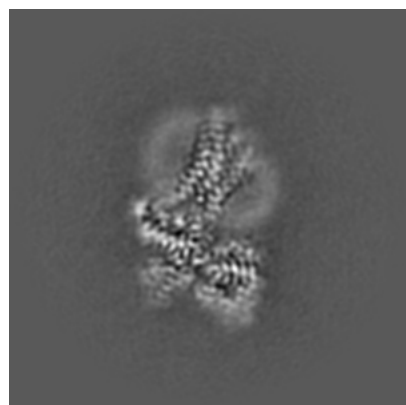


Z Index: 100

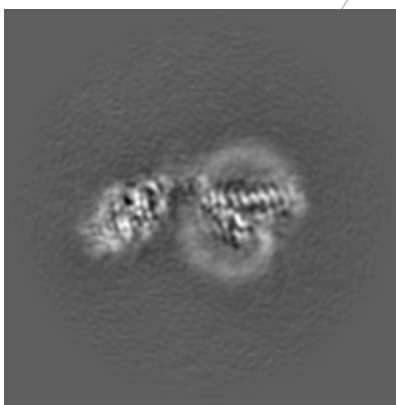
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

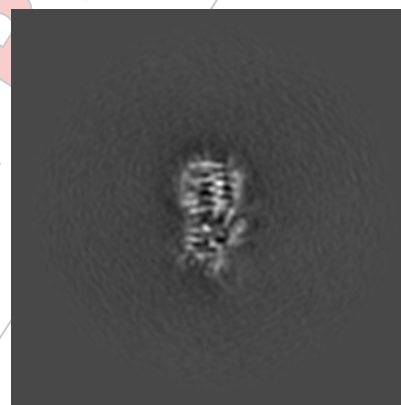
### 6.3.1 Primary map



X Index: 104



Y Index: 104

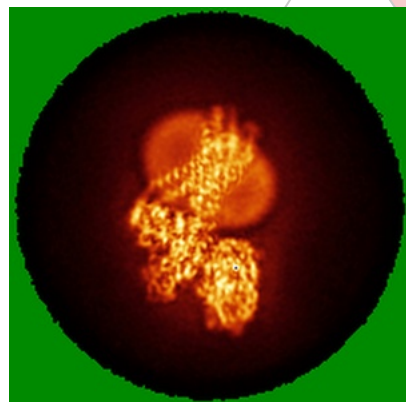


Z Index: 70

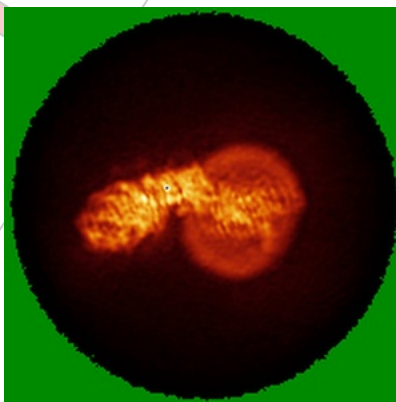
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

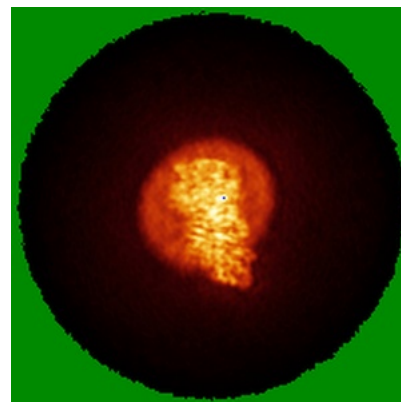
### 6.4.1 Primary map



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



The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation [i](#)

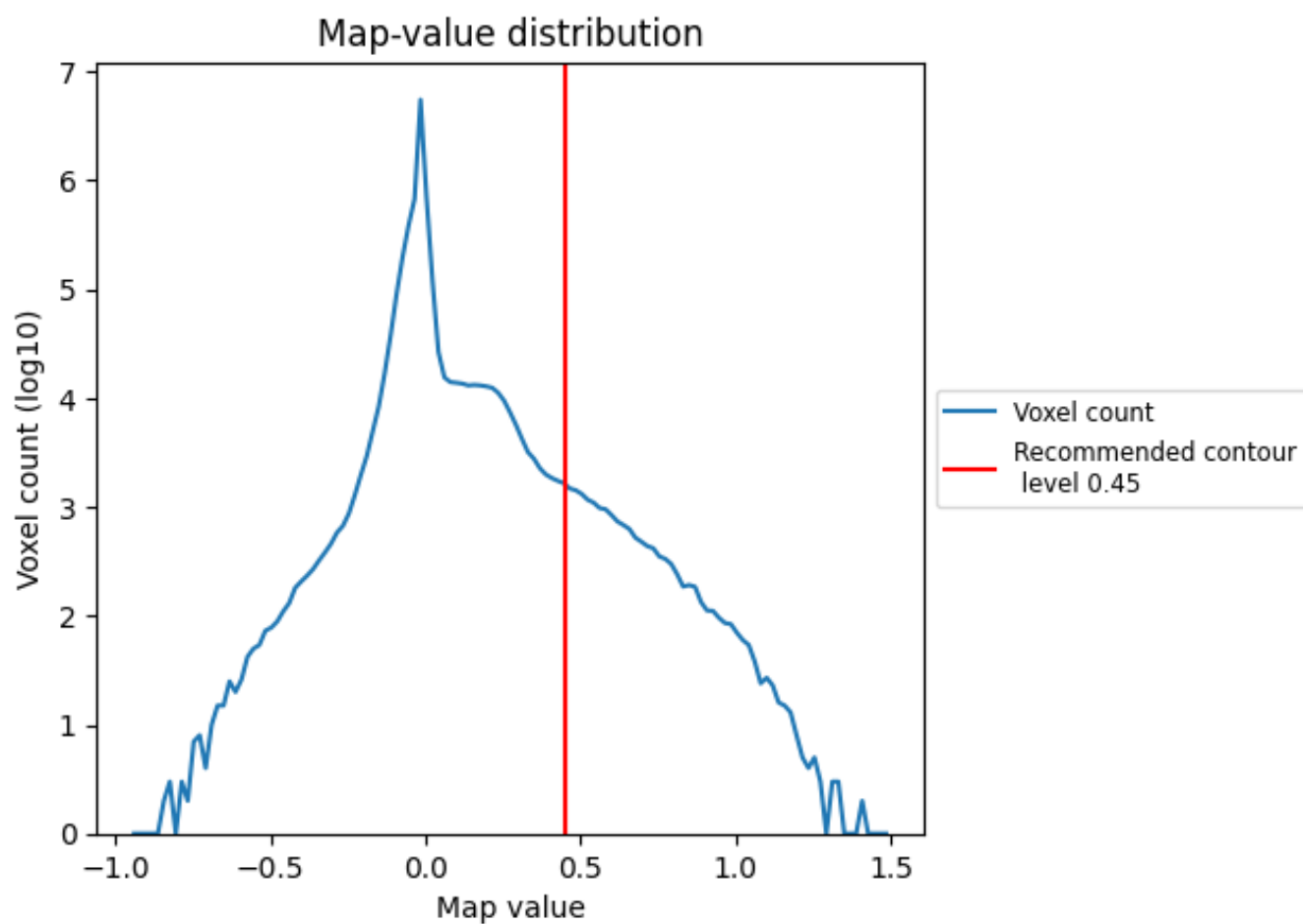
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis ⓘ

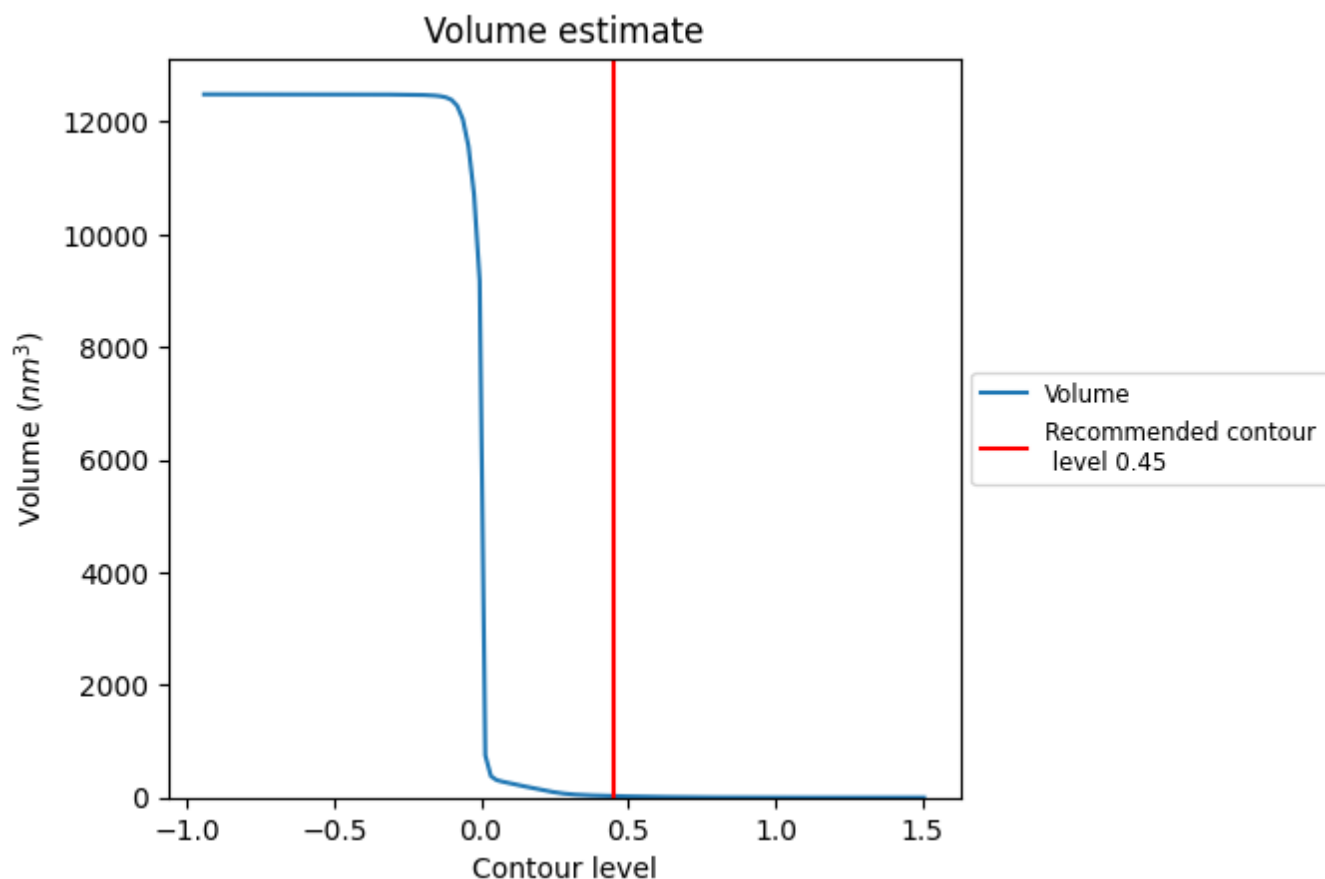
This section contains the results of statistical analysis of the map.

### 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.

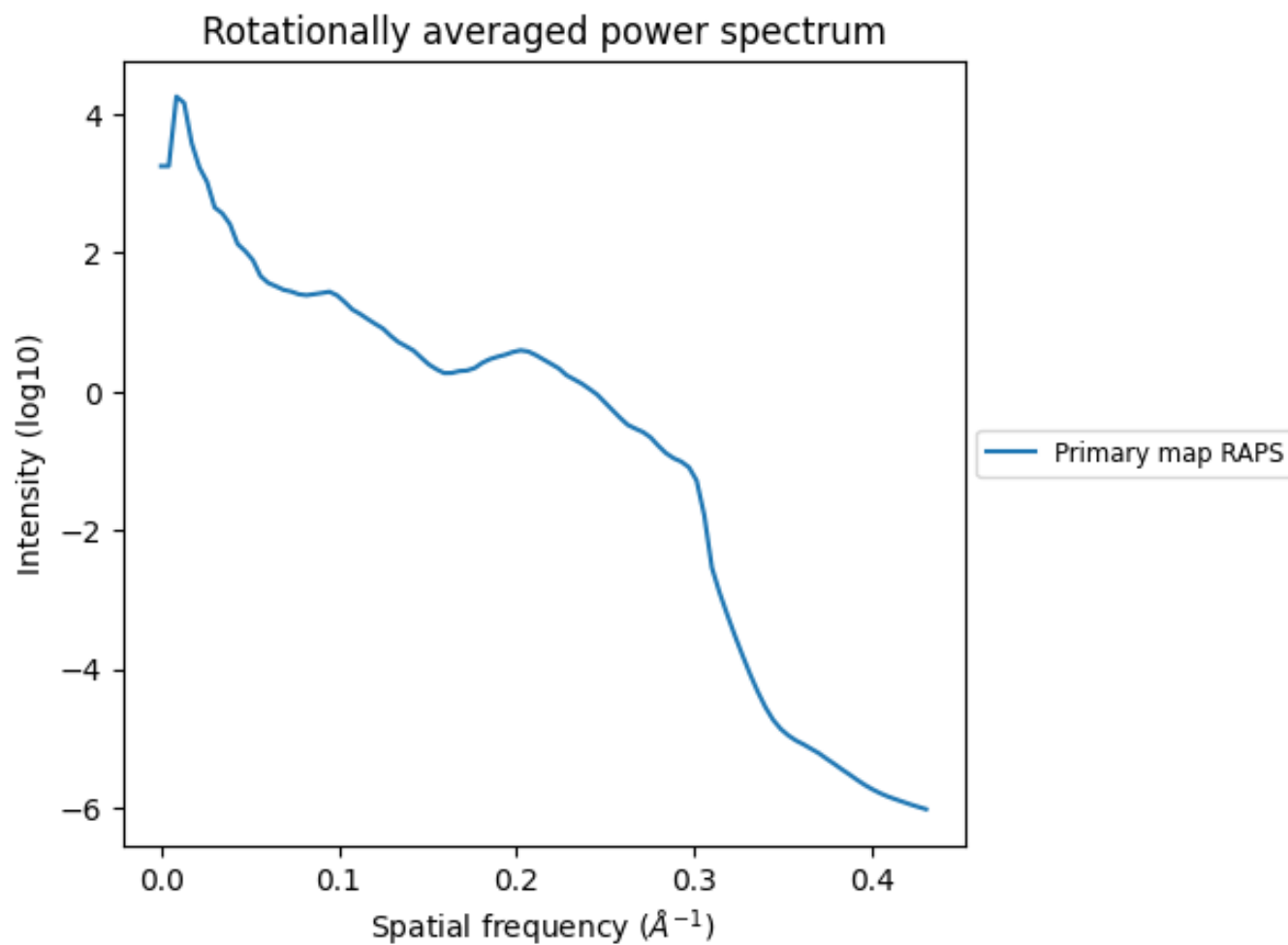
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 27 nm<sup>3</sup>; this corresponds to an approximate mass of 24 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 ⓘ



## 8 Fourier-Shell correlation ⓘ

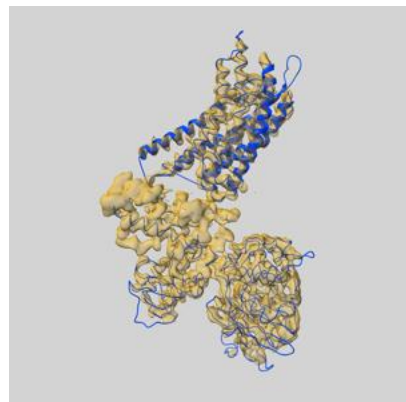
This section was not generated. No FSC curve or half-maps provided.

Not For Manuscript Review

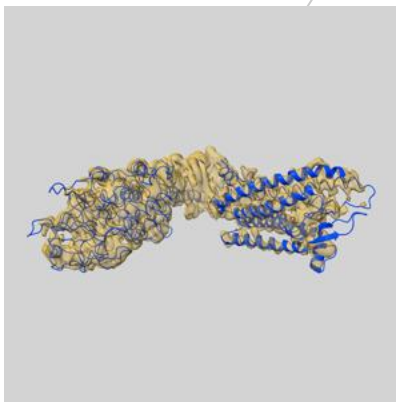
## 9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map D\_9100090016 and PDB model D\_9100090016. Per-residue inclusion information can be found in section 3 on page 22.

### 9.1 Map-model overlay ⓘ



X



Y



Z

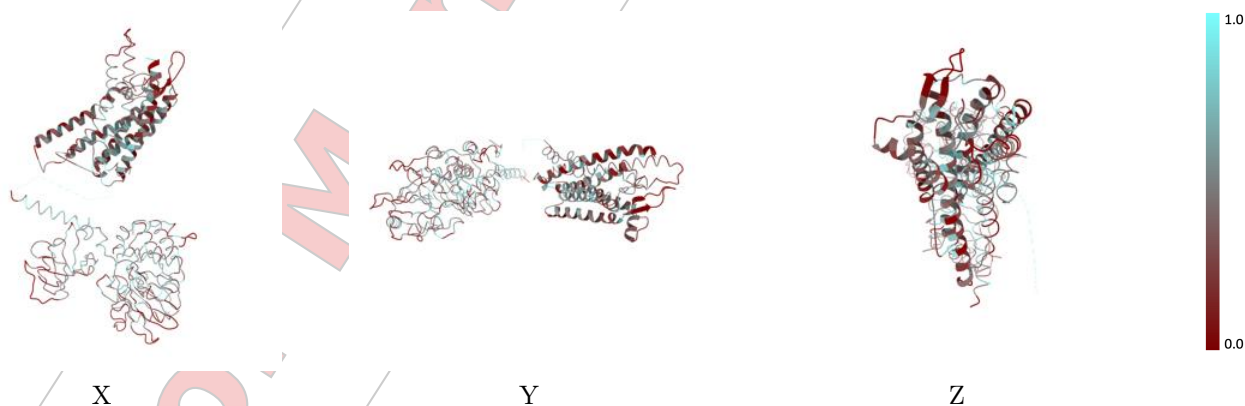
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



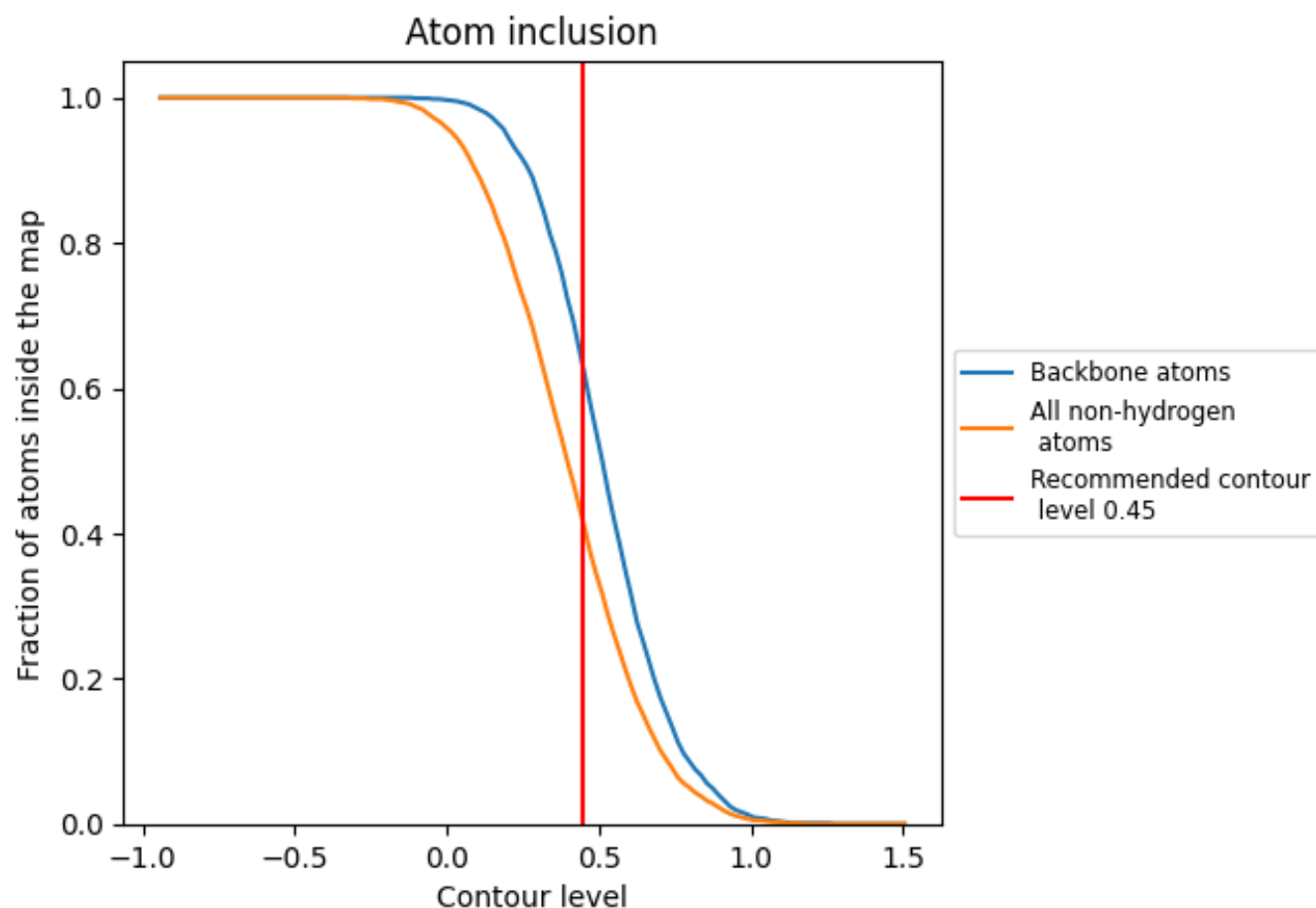
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 [i](#)



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 (0.45).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 63% of all backbone atoms, 41% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4130	0.3250
A	0.4350	0.3350
F	0.3570	0.3480
L	0.3590	0.2650
R	0.4110	0.3140

