Preliminary Full wwPDB EM Validation Report ⓘ

Dec 14, 2021 – 03:17 PM JST

Deposition ID : D_1300026309

This is a Preliminary Full wwPDB EM Validation Report.

This report is produced by the wwPDB Deposition System
during initial deposition but before 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 following versions of software and data (see references ⓘ) were used in the production of this report:

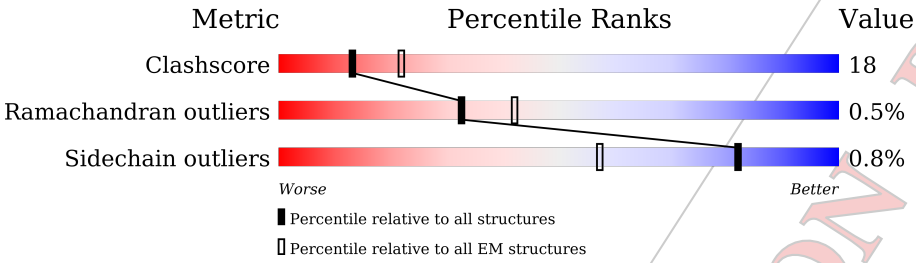
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

1 Overall quality at a glance

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 >=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	727	46% 70% 29% ·
1	B	727	10% 73% 26% ·
1	C	727	6% 73% 27% ·
1	D	727	7% 71% 28% ·
1	E	727	20% 67% 32% ·
1	F	727	61% 65% 34%
2	H	23	· 91% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33894 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.

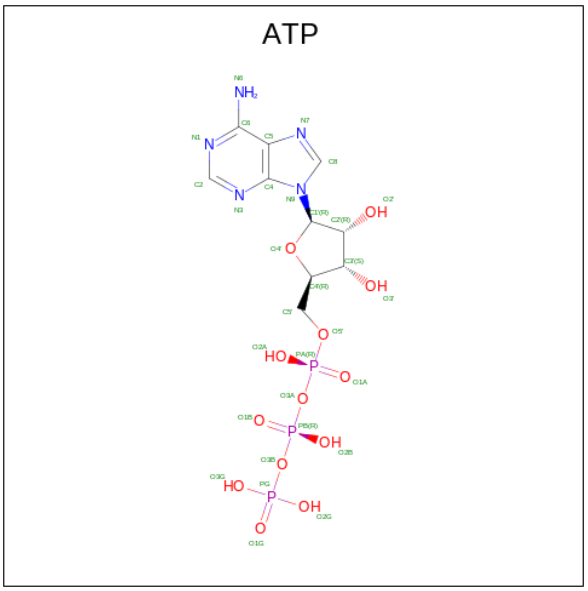
- Molecule 1 is a protein called Drg1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	727	Total	C	N	O	S	0	0
			5575	3522	956	1075	22		
1	B	727	Total	C	N	O	S	0	0
			5575	3522	956	1075	22		
1	D	727	Total	C	N	O	S	0	0
			5575	3522	956	1075	22		
1	E	727	Total	C	N	O	S	0	0
			5575	3522	956	1075	22		
1	F	725	Total	C	N	O	S	0	0
			5563	3516	954	1071	22		
1	C	727	Total	C	N	O	S	0	0
			5575	3522	956	1075	22		

- Molecule 2 is a protein called substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	H	23	Total	C	N	O	0	0
			115	69	23	23		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



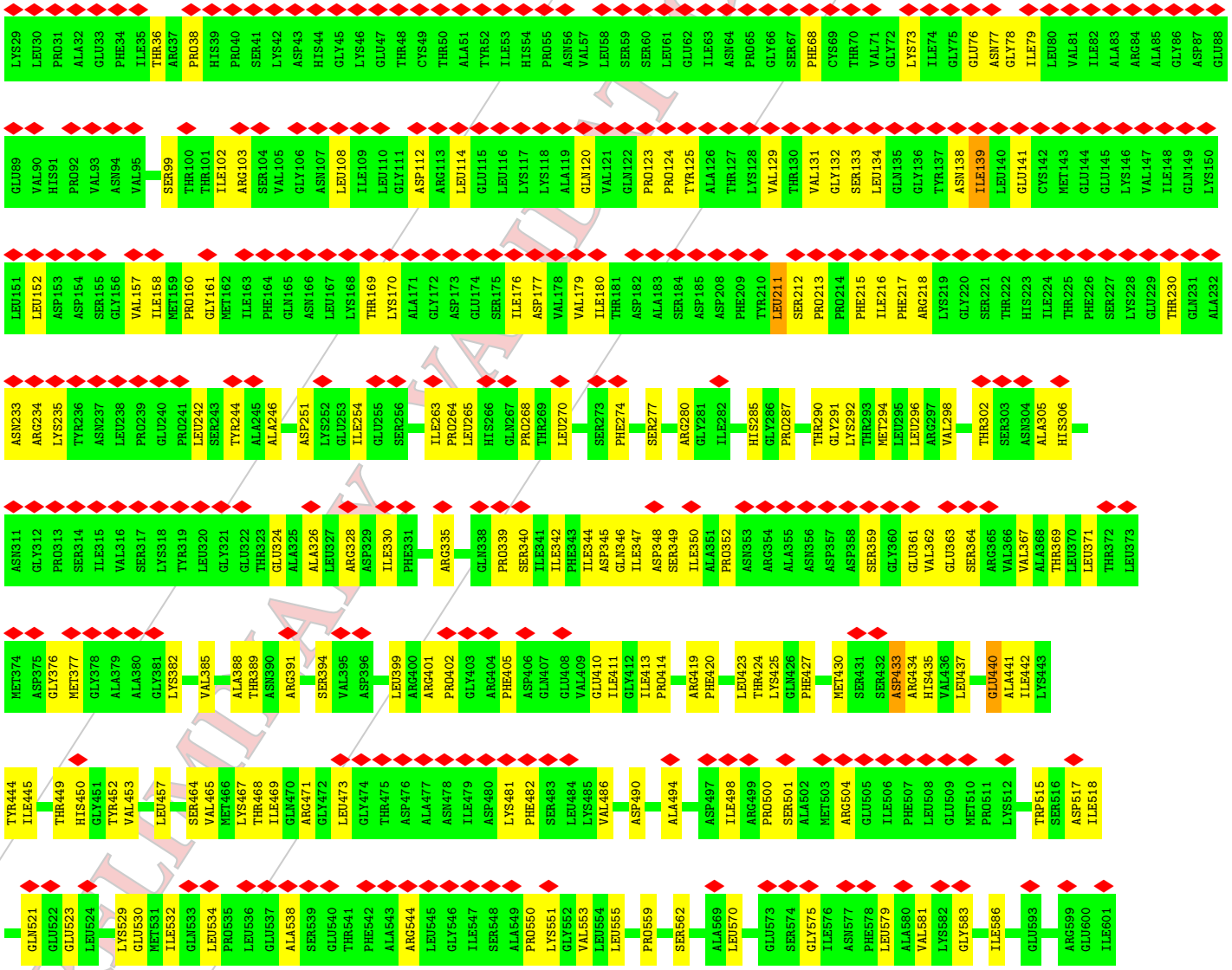
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	A	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	B	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	B	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	D	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	D	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	E	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	E	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	C	1	Total	C	N	O	P	0
			62	20	10	26	6	

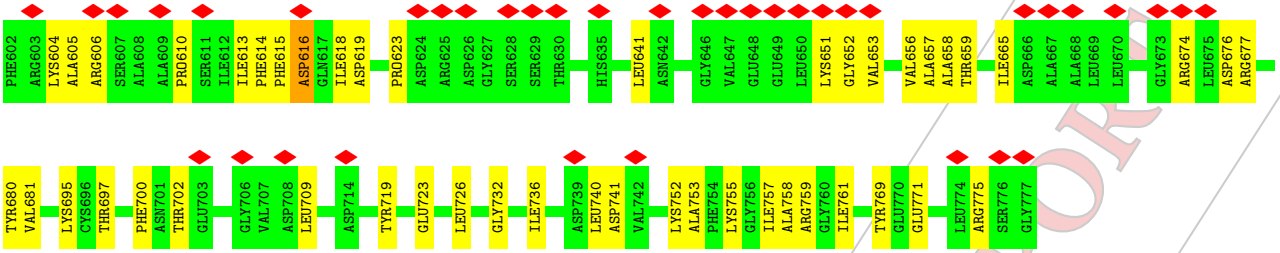
3 Residue-property plots (i)

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: Drg1

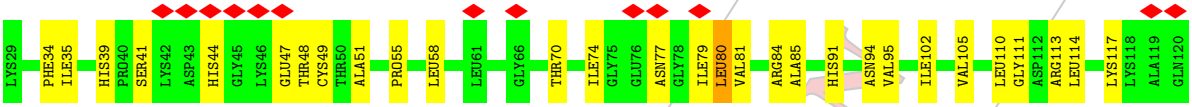
Chain A:

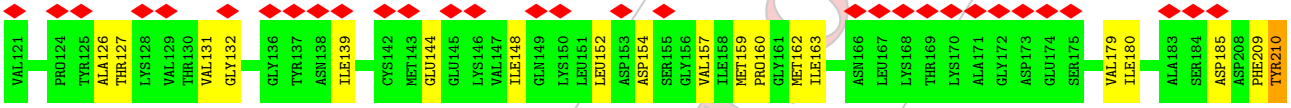


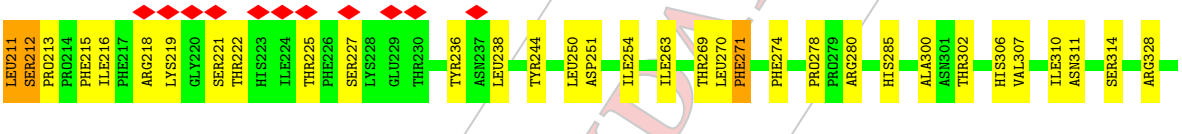


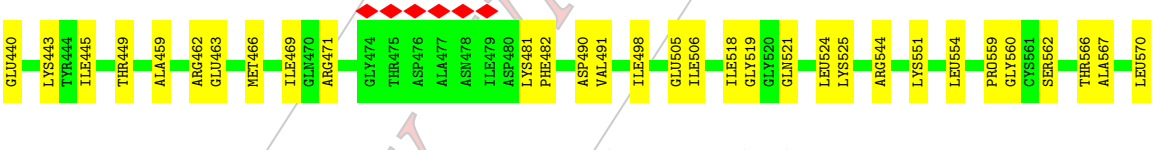
• Molecule 1: Drg1

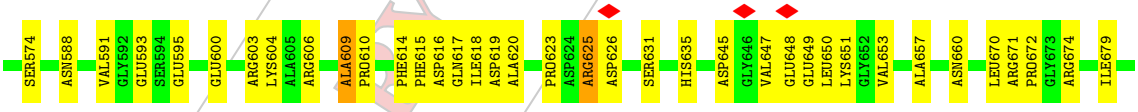
Chain B:





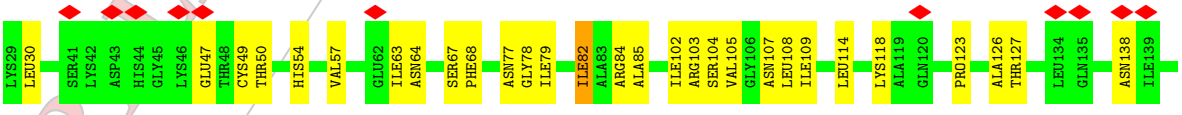






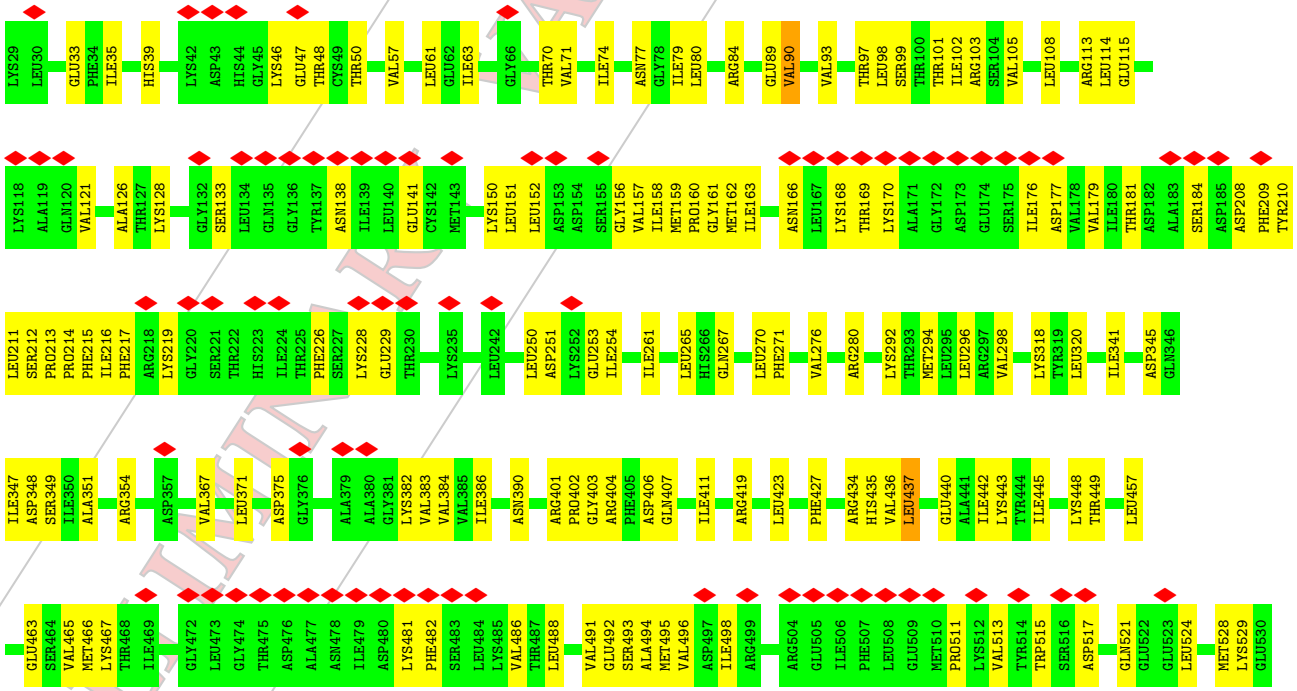
• Molecule 1: Drg1

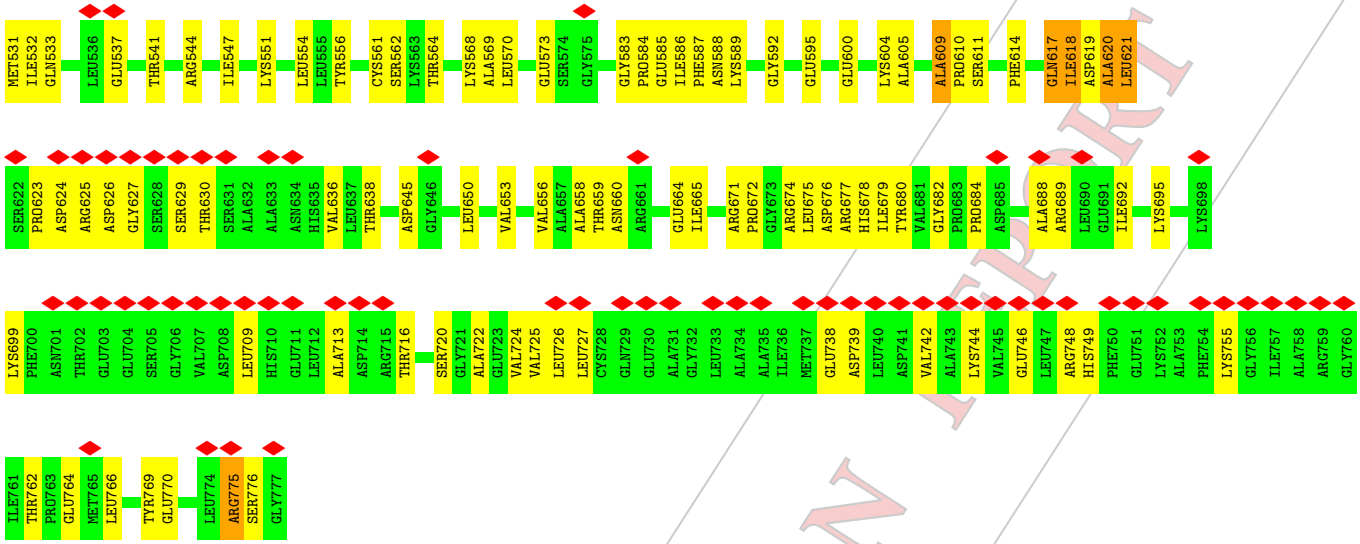
Chain D:



- Molecule 1: Drg1

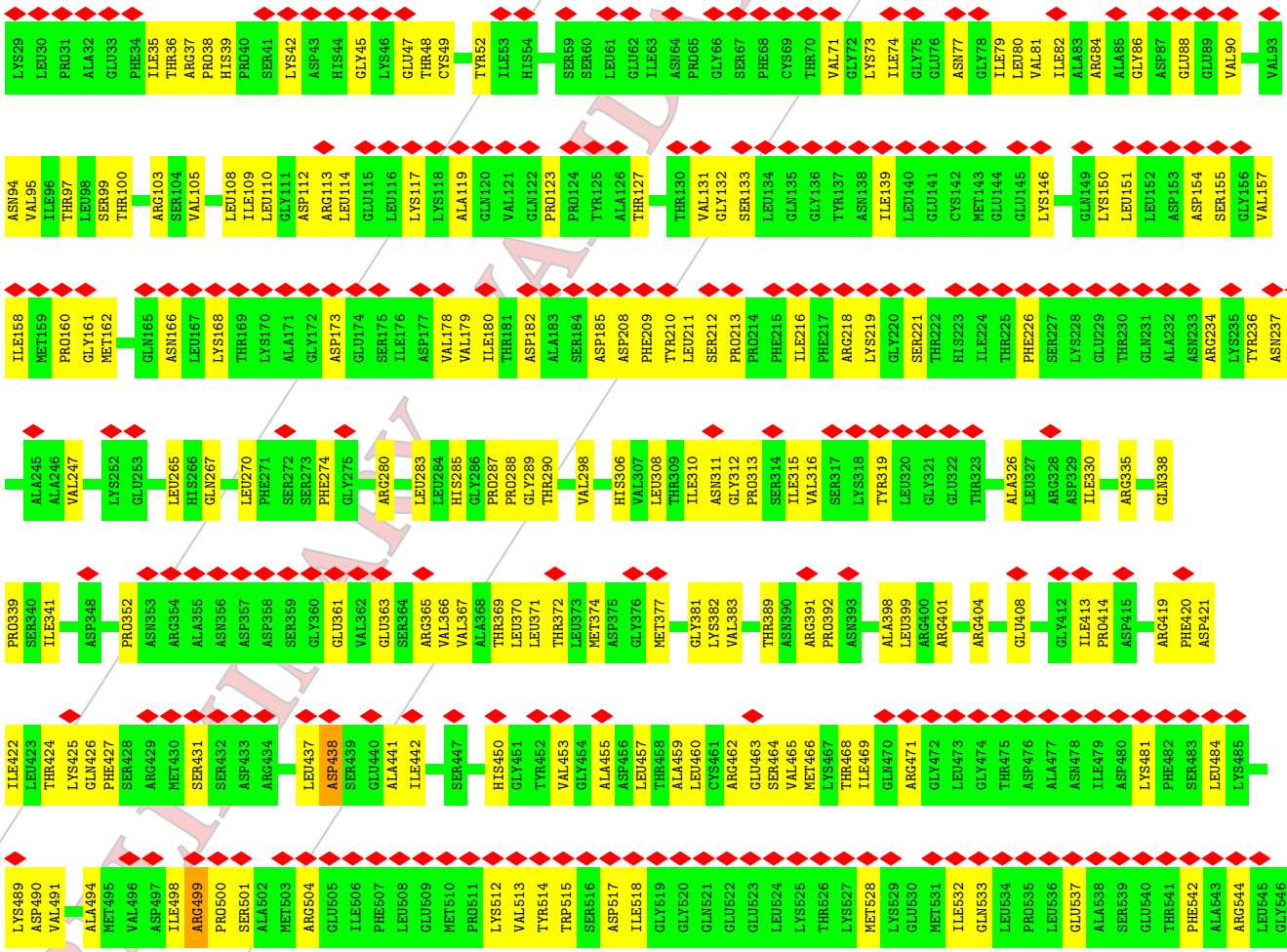
Chain E:

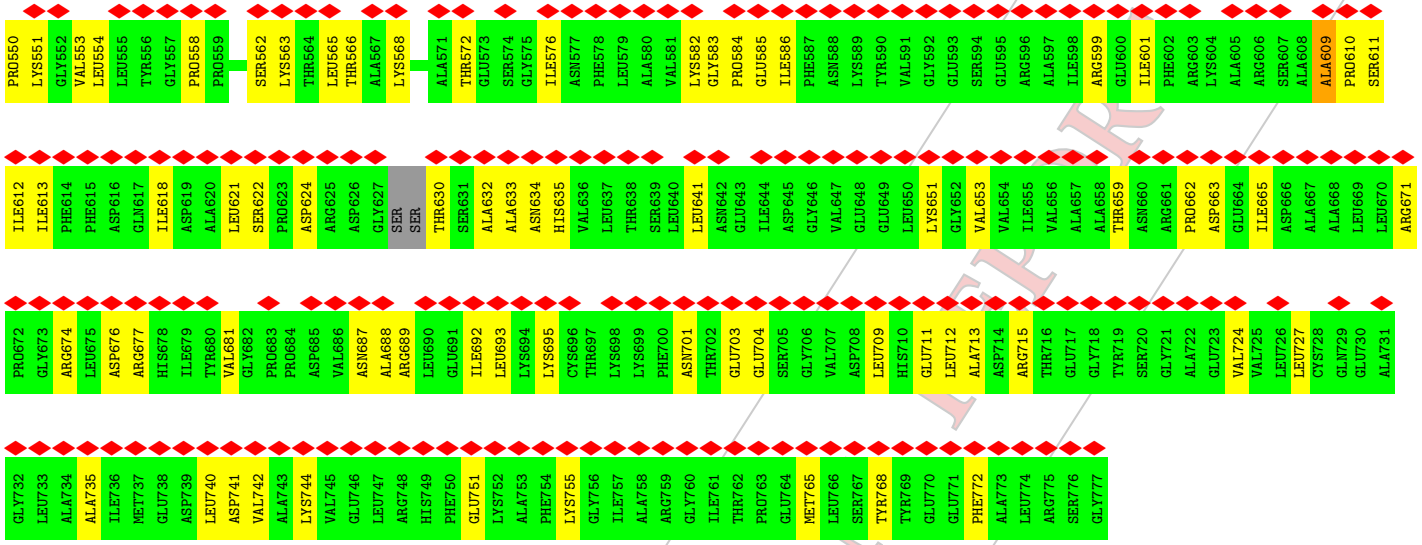




• Molecule 1: Drg1

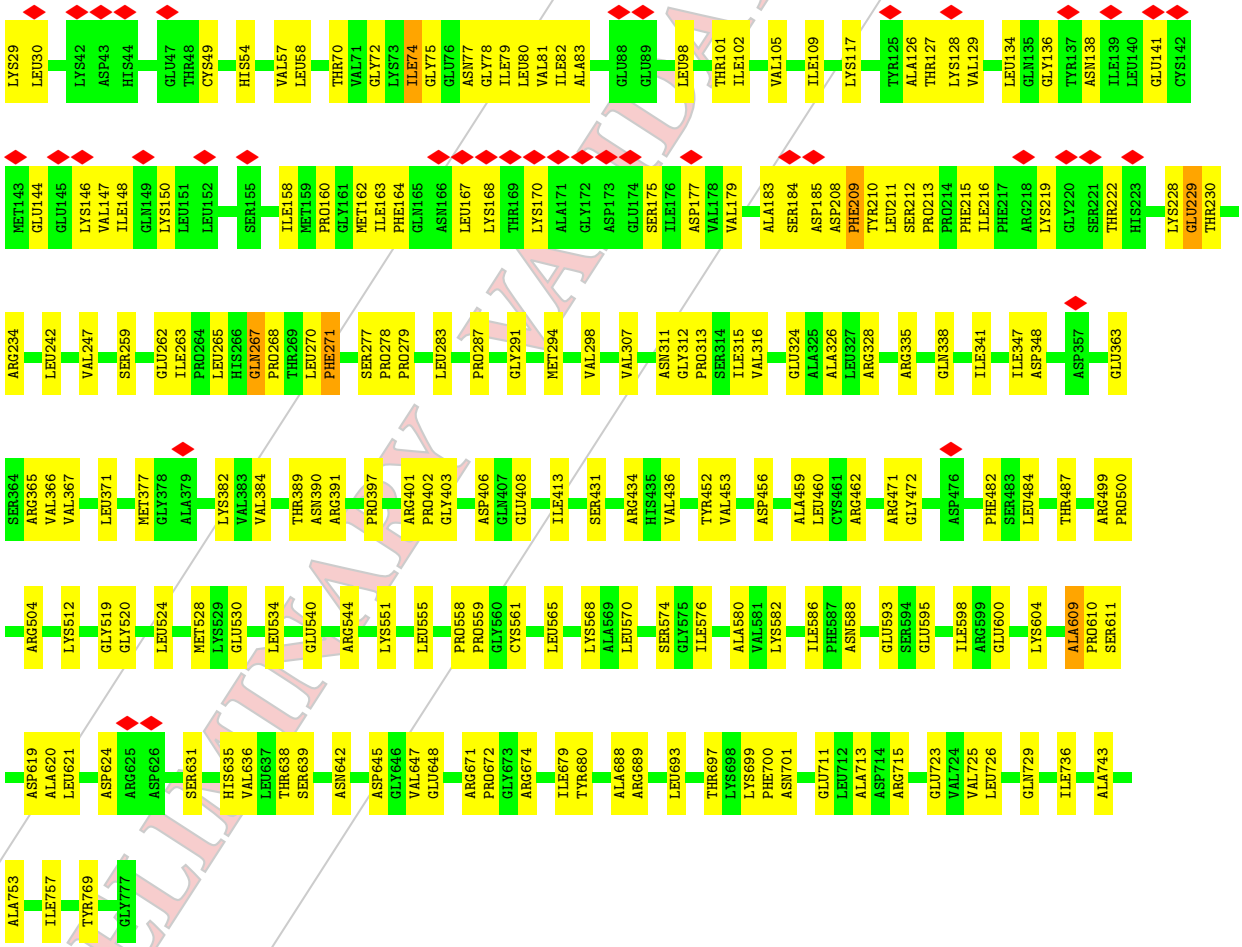
Chain F:





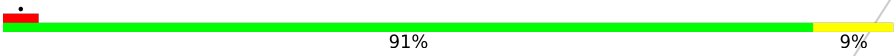
- Molecule 1: Drg1

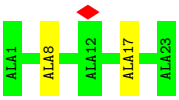
Chain C:



- Molecule 2: substrate

Chain H:





4 Experimental information (i)

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 ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	Not provided	
Maximum map value	0.130	Depositor
Minimum map value	-0.054	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	253.68001, 253.68001, 253.68001	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.057, 1.057, 1.057	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP

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	0.25	0/5672	0.51	0/7678
1	B	0.26	0/5672	0.52	1/7678 (0.0%)
1	C	0.27	0/5672	0.52	0/7678
1	D	0.26	0/5672	0.52	1/7678 (0.0%)
1	E	0.26	0/5672	0.54	0/7678
1	F	0.25	0/5659	0.51	1/7659 (0.0%)
2	H	0.24	0/114	0.68	0/158
All	All	0.26	0/34133	0.52	3/46207 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	30	LEU	CA-CB-CG	5.25	127.37	115.30
1	F	438	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	80	LEU	CA-CB-CG	5.09	127.00	115.30

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	5575	0	5654	246	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5575	0	5652	198	0
1	C	5575	0	5655	191	0
1	D	5575	0	5654	195	0
1	E	5575	0	5653	294	0
1	F	5563	0	5643	222	0
2	H	115	0	117	2	0
3	A	62	0	22	5	0
3	B	62	0	24	0	0
3	C	62	0	24	4	0
3	D	62	0	24	3	0
3	E	62	0	23	4	0
3	F	31	0	12	0	0
All	All	33894	0	34157	1245	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 18.

All (1245) 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:A:614:PHE:HD1	1:A:656:VAL:CG1	1.07	1.66
1:A:614:PHE:CD1	1:A:656:VAL:HG13	1.16	1.66
1:B:618:ILE:CD1	1:B:657:ALA:HB1	1.22	1.64
1:B:79:ILE:HG21	1:B:210:TYR:CD1	1.27	1.61
1:B:618:ILE:CD1	1:B:657:ALA:CB	1.86	1.52
1:C:79:ILE:HD11	1:C:211:LEU:CD2	1.36	1.51
1:F:77:ASN:HB2	1:F:211:LEU:CD2	1.39	1.51
1:A:270:LEU:CD1	1:F:469:ILE:HG21	1.41	1.51
1:E:481:LYS:CD	1:F:270:LEU:HD13	1.43	1.48
1:F:77:ASN:CB	1:F:211:LEU:CD2	1.88	1.48
1:B:482:PHE:CZ	1:C:270:LEU:CD2	1.97	1.48
1:B:482:PHE:CE2	1:C:270:LEU:CD2	1.96	1.46
1:C:77:ASN:HD22	1:C:210:TYR:N	1.04	1.44
1:E:481:LYS:HD2	1:F:270:LEU:CD1	1.48	1.43
1:C:77:ASN:ND2	1:C:210:TYR:H	1.12	1.43
1:E:435:HIS:CD2	1:E:437:LEU:HD21	1.52	1.42
1:B:79:ILE:CG2	1:B:210:TYR:HD1	1.32	1.42
1:A:344:ILE:HG22	1:A:347:ILE:CD1	1.54	1.36
1:D:185:ASP:OD1	1:D:215:PHE:CE1	1.78	1.34
1:A:270:LEU:CD1	1:F:469:ILE:CG2	2.01	1.34
1:E:624:ASP:CG	1:E:630:THR:HG23	1.49	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ILE:CG1	1:B:210:TYR:HA	1.59	1.30
1:B:482:PHE:CZ	1:C:270:LEU:HD23	1.60	1.29
1:D:78:GLY:N	1:D:211:LEU:HD21	1.43	1.29
1:F:77:ASN:CB	1:F:211:LEU:HD23	1.51	1.27
1:E:623:PRO:HB2	1:E:627:GLY:O	1.34	1.25
1:E:435:HIS:CD2	1:E:437:LEU:CD2	2.21	1.24
1:A:616:ASP:O	1:A:658:ALA:O	1.56	1.23
1:E:587:PHE:CE2	1:E:620:ALA:O	1.92	1.22
1:B:482:PHE:CE2	1:C:270:LEU:HD22	1.60	1.22
1:E:619:ASP:O	1:E:621:LEU:N	1.72	1.22
1:B:618:ILE:HD12	1:B:657:ALA:CB	1.53	1.21
1:E:435:HIS:CG	1:E:437:LEU:HD21	1.75	1.20
1:D:78:GLY:H	1:D:211:LEU:CD2	1.52	1.20
1:C:79:ILE:CD1	1:C:211:LEU:HD21	1.73	1.18
1:B:77:ASN:OD1	1:B:209:PHE:O	1.60	1.17
1:E:77:ASN:O	1:E:211:LEU:HD21	1.01	1.17
1:C:77:ASN:ND2	1:C:210:TYR:N	1.75	1.17
1:A:270:LEU:HD13	1:F:469:ILE:CG2	1.68	1.17
1:B:619:ASP:O	1:B:623:PRO:HD3	1.44	1.17
1:E:77:ASN:O	1:E:211:LEU:CD2	1.91	1.16
1:E:619:ASP:OD1	1:E:665:ILE:HD11	1.43	1.16
1:E:77:ASN:C	1:E:211:LEU:HD21	1.66	1.16
1:A:614:PHE:CE1	1:A:656:VAL:HG22	1.78	1.16
1:B:619:ASP:O	1:B:623:PRO:CD	1.92	1.15
1:A:614:PHE:CD1	1:A:656:VAL:CG1	1.93	1.15
1:D:78:GLY:N	1:D:211:LEU:CD2	2.08	1.15
1:D:185:ASP:CG	1:D:215:PHE:CE1	2.19	1.15
1:E:584:PRO:CD	1:E:617:GLN:OE1	1.94	1.15
1:A:270:LEU:HD22	1:F:469:ILE:HD12	1.19	1.14
1:A:614:PHE:HE1	1:A:656:VAL:CG2	1.57	1.14
1:E:587:PHE:HE2	1:E:620:ALA:C	1.49	1.14
1:B:618:ILE:HD11	1:B:657:ALA:CB	1.67	1.13
1:B:618:ILE:HD11	1:B:657:ALA:HB2	1.21	1.13
1:A:344:ILE:HG22	1:A:347:ILE:HD11	1.17	1.12
1:A:420:PHE:CD1	1:A:442:ILE:HG22	1.82	1.12
1:E:427:PHE:CD2	1:E:442:ILE:HD12	1.83	1.12
1:A:270:LEU:HD11	1:F:469:ILE:CG2	1.72	1.10
1:F:77:ASN:HB3	1:F:211:LEU:HD23	1.16	1.10
1:A:619:ASP:O	1:A:623:PRO:HD2	1.50	1.09
1:F:79:ILE:HD13	1:F:211:LEU:HD12	1.34	1.09
1:B:482:PHE:CE2	1:C:270:LEU:HD21	1.80	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:ILE:CD1	1:C:211:LEU:CD2	2.30	1.08
1:C:160:PRO:HD2	1:C:212:SER:OG	1.51	1.08
1:E:427:PHE:CD2	1:E:442:ILE:CD1	2.37	1.08
1:C:79:ILE:HD11	1:C:211:LEU:CG	1.83	1.08
1:A:344:ILE:CG2	1:A:347:ILE:HD11	1.82	1.08
1:F:77:ASN:CB	1:F:211:LEU:HD21	1.64	1.08
1:B:79:ILE:CB	1:B:210:TYR:HA	1.85	1.07
1:D:185:ASP:CG	1:D:215:PHE:HE1	1.56	1.07
1:F:79:ILE:CD1	1:F:211:LEU:HD12	1.84	1.06
1:A:270:LEU:HD13	1:F:469:ILE:HG21	1.28	1.05
1:E:624:ASP:OD2	1:E:629:SER:OG	1.75	1.04
1:A:270:LEU:HD22	1:F:469:ILE:CD1	1.88	1.04
1:A:614:PHE:HE1	1:A:656:VAL:HG22	0.90	1.04
1:B:567:ALA:HB2	1:B:614:PHE:CE1	1.92	1.04
1:F:77:ASN:HB3	1:F:211:LEU:CD2	1.73	1.03
1:A:435:HIS:HE1	1:A:437:LEU:HD12	1.22	1.03
1:D:185:ASP:OD2	1:D:215:PHE:CE1	2.12	1.03
1:E:445:ILE:HD12	1:E:491:VAL:HG11	1.37	1.03
1:A:270:LEU:HD11	1:F:469:ILE:HG23	1.41	1.02
1:A:211:LEU:HD13	1:A:211:LEU:H	1.22	1.01
1:D:619:ASP:O	1:D:623:PRO:CD	2.06	1.01
1:A:344:ILE:CG2	1:A:347:ILE:CD1	2.39	1.01
1:E:437:LEU:HD13	1:E:437:LEU:H	1.25	1.00
1:F:267:GLN:OE1	1:F:270:LEU:HD11	1.59	0.99
1:A:270:LEU:CD2	1:F:469:ILE:HD12	1.92	0.99
1:A:270:LEU:HD13	1:F:469:ILE:CG1	1.91	0.99
1:B:482:PHE:HE2	1:C:270:LEU:HD21	1.27	0.98
1:F:267:GLN:OE1	1:F:270:LEU:CD1	2.11	0.98
1:F:77:ASN:HB2	1:F:211:LEU:HD21	0.99	0.98
1:E:623:PRO:O	1:E:627:GLY:O	1.81	0.97
1:D:482:PHE:HE1	1:E:270:LEU:HG	1.29	0.97
1:E:584:PRO:HD3	1:E:617:GLN:OE1	1.61	0.97
1:E:586:ILE:HD11	1:E:621:LEU:HD22	1.47	0.97
1:E:624:ASP:CB	1:E:629:SER:OG	2.13	0.96
1:E:435:HIS:NE2	1:E:437:LEU:HD23	1.80	0.96
1:D:78:GLY:CA	1:D:211:LEU:HD21	1.96	0.95
1:B:79:ILE:HB	1:B:210:TYR:HB3	1.47	0.95
1:E:445:ILE:HD11	1:E:488:LEU:CD1	1.96	0.95
1:D:185:ASP:OD2	1:D:215:PHE:HE1	1.43	0.95
1:E:445:ILE:HD12	1:E:491:VAL:CG1	1.97	0.94
1:E:77:ASN:HB2	1:E:211:LEU:HD23	1.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:LEU:HD13	1:F:469:ILE:HG13	1.49	0.94
1:D:619:ASP:O	1:D:623:PRO:HD3	1.67	0.93
1:A:614:PHE:CE1	1:A:656:VAL:CG2	2.43	0.93
1:C:79:ILE:CD1	1:C:211:LEU:CG	2.47	0.93
1:B:482:PHE:HZ	1:C:270:LEU:HD23	1.16	0.93
1:E:583:GLY:C	1:E:620:ALA:CB	2.38	0.92
1:B:79:ILE:HG13	1:B:210:TYR:HA	1.49	0.92
1:D:78:GLY:H	1:D:211:LEU:HD21	1.00	0.92
1:E:619:ASP:O	1:E:620:ALA:C	2.07	0.92
1:B:79:ILE:CG1	1:B:210:TYR:CA	2.47	0.91
1:B:79:ILE:HB	1:B:210:TYR:HA	1.49	0.91
1:D:160:PRO:HD2	1:D:213:PRO:O	1.70	0.91
1:A:420:PHE:HD1	1:A:442:ILE:HG22	1.27	0.91
1:A:614:PHE:CD1	1:A:656:VAL:HG11	2.05	0.90
1:E:587:PHE:HE2	1:E:620:ALA:O	1.40	0.90
1:E:614:PHE:HD2	1:E:656:VAL:HG13	1.37	0.90
1:E:435:HIS:CG	1:E:437:LEU:CD2	2.50	0.90
1:A:344:ILE:HG22	1:A:347:ILE:CG1	2.01	0.89
1:A:270:LEU:CD1	1:F:469:ILE:HG23	1.94	0.89
1:B:79:ILE:HB	1:B:210:TYR:CB	2.03	0.89
1:E:77:ASN:C	1:E:211:LEU:CD2	2.37	0.89
1:A:344:ILE:CG2	1:A:347:ILE:HG13	2.02	0.89
1:B:79:ILE:HB	1:B:210:TYR:CA	2.03	0.88
1:A:344:ILE:HG21	1:A:347:ILE:HG13	1.56	0.88
1:A:344:ILE:CG2	1:A:347:ILE:CG1	2.50	0.88
1:D:160:PRO:HG2	1:D:213:PRO:HD2	1.55	0.87
1:D:619:ASP:O	1:D:623:PRO:HD2	1.72	0.87
1:C:79:ILE:CD1	1:C:211:LEU:HG	2.03	0.87
1:C:77:ASN:HD21	1:C:209:PHE:HA	1.38	0.87
1:E:267:GLN:HB3	1:E:270:LEU:HD13	1.53	0.86
1:B:79:ILE:HG12	1:B:210:TYR:HA	1.54	0.86
1:A:435:HIS:CE1	1:A:437:LEU:HD12	2.10	0.85
1:B:79:ILE:HG13	1:B:210:TYR:CA	2.07	0.85
1:A:348:ASP:O	1:A:352:PRO:HD3	1.77	0.85
1:E:624:ASP:OD1	1:E:630:THR:HG23	1.75	0.85
1:B:160:PRO:HG2	1:B:212:SER:HB2	1.59	0.85
1:D:77:ASN:HB2	1:D:211:LEU:HD23	1.56	0.85
1:E:587:PHE:CZ	1:E:620:ALA:O	2.29	0.84
1:A:614:PHE:CE1	1:A:656:VAL:HG13	2.09	0.84
1:E:587:PHE:CE2	1:E:620:ALA:C	2.38	0.84
1:E:624:ASP:CG	1:E:630:THR:CG2	2.40	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:584:PRO:HD2	1:E:617:GLN:OE1	1.78	0.84
1:C:79:ILE:HD11	1:C:211:LEU:HD21	0.84	0.84
1:D:271:PHE:O	1:D:274:PHE:O	1.96	0.83
1:D:185:ASP:OD1	1:D:215:PHE:CD1	2.31	0.83
1:C:271:PHE:HE2	1:C:279:PRO:HD3	1.43	0.83
1:A:270:LEU:HD12	1:F:469:ILE:HG21	1.55	0.82
1:E:445:ILE:CD1	1:E:491:VAL:HG11	2.08	0.82
1:C:160:PRO:HD2	1:C:212:SER:HG	1.39	0.82
1:A:344:ILE:CB	1:A:347:ILE:HD11	2.09	0.82
1:D:126:ALA:HB2	1:D:215:PHE:HB3	1.61	0.82
1:D:160:PRO:CD	1:D:213:PRO:O	2.27	0.82
1:A:435:HIS:HE1	1:A:437:LEU:CD1	1.91	0.82
1:C:77:ASN:HD22	1:C:210:TYR:CA	1.92	0.81
1:A:435:HIS:CE1	1:A:437:LEU:HB2	2.15	0.81
1:C:105:VAL:HG22	1:C:162:MET:H	1.46	0.81
1:E:619:ASP:OD1	1:E:665:ILE:CD1	2.28	0.81
1:A:424:THR:HG23	1:A:442:ILE:HG21	1.61	0.80
1:A:619:ASP:O	1:A:623:PRO:CD	2.29	0.80
1:B:347:ILE:HD12	1:B:387:ALA:HB1	1.63	0.80
1:E:270:LEU:HD12	1:E:270:LEU:H	1.44	0.80
1:B:79:ILE:CG2	1:B:210:TYR:CD1	2.23	0.80
1:A:420:PHE:CD1	1:A:442:ILE:CG2	2.65	0.80
1:E:427:PHE:CD2	1:E:442:ILE:HD11	2.15	0.80
1:F:160:PRO:HG2	1:F:212:SER:HB3	1.62	0.80
1:D:211:LEU:HD23	1:D:211:LEU:H	1.47	0.79
1:E:623:PRO:CB	1:E:627:GLY:O	2.25	0.79
1:A:581:VAL:CG1	1:A:615:PHE:HE1	1.95	0.79
1:E:624:ASP:CG	1:E:629:SER:OG	2.21	0.79
1:B:347:ILE:HD12	1:B:387:ALA:CB	2.13	0.79
1:E:296:LEU:CD2	1:E:345:ASP:OD1	2.30	0.79
1:A:211:LEU:H	1:A:211:LEU:CD1	1.95	0.79
1:E:524:LEU:HD13	1:E:679:ILE:HG21	1.64	0.79
1:D:127:THR:H	1:D:185:ASP:HB3	1.48	0.79
1:E:624:ASP:OD2	1:E:630:THR:HG23	1.81	0.78
1:E:435:HIS:NE2	1:E:437:LEU:CD2	2.41	0.78
1:E:619:ASP:O	1:E:621:LEU:C	2.21	0.78
1:F:77:ASN:CG	1:F:211:LEU:HD23	2.04	0.78
1:C:619:ASP:OD1	1:C:620:ALA:N	2.17	0.78
1:E:624:ASP:O	1:E:626:ASP:N	2.14	0.78
1:E:436:VAL:HG12	1:E:486:VAL:O	1.84	0.78
1:A:158:ILE:HG13	1:A:180:ILE:HD13	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:79:ILE:HD13	1:F:211:LEU:CD1	2.13	0.77
1:A:482:PHE:CE1	1:B:270:LEU:HD22	2.19	0.77
1:D:436:VAL:O	1:D:437:LEU:HD23	1.84	0.77
1:E:77:ASN:CB	1:E:211:LEU:HD23	2.14	0.77
1:B:79:ILE:CB	1:B:210:TYR:CA	2.62	0.77
1:A:614:PHE:CE1	1:A:656:VAL:CG1	2.66	0.77
1:B:311:ASN:CB	1:B:345:ASP:HB2	2.16	0.76
1:E:320:LEU:H	2:H:8:ALA:HB1	1.50	0.76
1:A:270:LEU:HD13	1:F:469:ILE:CB	2.15	0.76
1:E:619:ASP:C	1:E:621:LEU:N	2.37	0.76
1:A:581:VAL:HG11	1:A:615:PHE:HE1	1.51	0.76
1:B:440:GLU:OE1	1:B:443:LYS:HD2	1.84	0.76
1:B:616:ASP:OD2	1:C:642:ASN:ND2	2.19	0.75
1:C:595:GLU:OE1	1:C:639:SER:OG	2.04	0.75
1:E:481:LYS:HB2	1:F:270:LEU:HD22	1.68	0.75
1:B:328:ARG:HA	1:B:373:LEU:HD21	1.68	0.75
1:A:482:PHE:CE1	1:B:270:LEU:CD2	2.69	0.75
1:D:77:ASN:HB2	1:D:211:LEU:CD2	2.16	0.74
1:A:77:ASN:C	1:A:211:LEU:HD12	2.07	0.74
1:F:576:ILE:HG21	1:F:611:SER:HA	1.67	0.74
1:E:427:PHE:CE2	1:E:442:ILE:HD12	2.23	0.74
1:E:511:PRO:HB2	1:E:513:VAL:HG13	1.70	0.74
1:D:348:ASP:OD1	1:D:349:SER:N	2.21	0.73
1:E:160:PRO:HD2	1:E:212:SER:HB3	1.70	0.73
1:E:621:LEU:N	1:E:621:LEU:HD23	2.03	0.73
1:E:624:ASP:HB3	1:E:629:SER:OG	1.88	0.73
1:D:49:CYS:H	1:D:102:ILE:HD11	1.52	0.73
1:D:50:THR:HG22	1:D:82:ILE:HD11	1.69	0.73
1:B:70:THR:HG22	1:B:81:VAL:HG12	1.70	0.73
1:D:519:GLY:H	3:D:802:ATP:HN62	1.36	0.73
1:D:401:ARG:HH21	1:D:403:GLY:HA3	1.52	0.73
1:A:441:ALA:O	1:A:445:ILE:N	2.19	0.73
1:E:267:GLN:HB3	1:E:270:LEU:CD1	2.18	0.73
1:D:211:LEU:HD23	1:D:211:LEU:N	2.03	0.72
1:F:168:LYS:HE2	1:F:173:ASP:HA	1.71	0.72
1:B:311:ASN:HA	1:B:345:ASP:H	1.54	0.72
1:C:77:ASN:HB3	1:C:210:TYR:HA	1.71	0.72
1:D:160:PRO:CG	1:D:213:PRO:HG2	2.19	0.72
1:F:517:ASP:HA	1:F:695:LYS:HG3	1.71	0.72
1:B:723:GLU:HG2	1:C:672:PRO:HG2	1.72	0.72
1:C:271:PHE:HE2	1:C:279:PRO:CD	2.01	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLU:HB2	1:A:170:LYS:HD3	1.71	0.72
1:E:435:HIS:CE1	1:E:437:LEU:HD23	2.25	0.72
1:B:619:ASP:O	1:B:623:PRO:HD2	1.87	0.71
1:E:70:THR:HA	1:E:80:LEU:HA	1.72	0.71
1:E:775:ARG:NH1	1:E:776:SER:OG	2.23	0.71
1:A:344:ILE:C	1:A:347:ILE:HD11	2.10	0.71
1:F:735:ALA:HB1	1:F:742:VAL:HG11	1.72	0.71
1:B:617:GLN:HG3	1:C:638:THR:HG23	1.72	0.71
1:B:618:ILE:CD1	1:B:657:ALA:HB2	1.86	0.71
1:E:624:ASP:OD1	1:E:630:THR:CG2	2.38	0.71
1:A:361:GLU:HG2	1:A:362:VAL:HG23	1.72	0.70
1:C:77:ASN:HB3	1:C:210:TYR:CA	2.21	0.70
1:A:440:GLU:O	1:A:444:TYR:N	2.24	0.70
1:C:163:ILE:HG13	1:C:179:VAL:HG22	1.73	0.70
1:E:437:LEU:HD22	1:E:437:LEU:N	2.05	0.70
1:E:617:GLN:O	1:E:617:GLN:HG3	1.92	0.70
1:E:270:LEU:HD12	1:E:270:LEU:N	2.06	0.70
1:E:427:PHE:CE2	1:E:442:ILE:CD1	2.74	0.70
1:E:586:ILE:HD11	1:E:621:LEU:CD2	2.20	0.70
1:F:613:ILE:HG12	1:F:653:VAL:HG11	1.72	0.70
1:E:716:THR:HG23	1:E:724:VAL:HG11	1.73	0.70
1:F:105:VAL:HG22	1:F:162:MET:H	1.55	0.70
1:F:712:LEU:HD23	1:F:715:ARG:HH12	1.57	0.70
1:A:581:VAL:HG11	1:A:615:PHE:CE1	2.26	0.70
1:B:218:ARG:HE	1:B:219:LYS:H	1.39	0.70
1:E:437:LEU:H	1:E:437:LEU:CD1	1.96	0.70
1:A:346:GLN:N	1:A:388:ALA:O	2.24	0.70
1:C:598:ILE:HD11	1:C:636:VAL:HG13	1.74	0.70
1:C:609:ALA:HB1	1:C:610:PRO:HD2	1.74	0.70
1:D:482:PHE:CE1	1:E:270:LEU:HG	2.19	0.69
1:A:348:ASP:O	1:A:352:PRO:CD	2.40	0.69
1:A:606:ARG:HH22	1:A:652:GLY:H	1.38	0.69
1:E:609:ALA:HB1	1:E:610:PRO:HD2	1.74	0.69
1:E:583:GLY:C	1:E:620:ALA:HB2	2.13	0.69
1:F:160:PRO:CG	1:F:212:SER:HB3	2.23	0.69
1:F:701:ASN:ND2	1:F:704:GLU:OE1	2.26	0.69
1:C:401:ARG:HH21	1:C:403:GLY:HA3	1.58	0.69
1:D:185:ASP:CG	1:D:215:PHE:CD1	2.66	0.69
1:B:524:LEU:HD13	1:B:679:ILE:HG21	1.75	0.69
1:A:581:VAL:CG1	1:A:615:PHE:CE1	2.75	0.68
1:D:208:ASP:OD1	1:D:208:ASP:N	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:ASN:HB2	1:E:211:LEU:CD2	2.21	0.68
1:C:701:ASN:ND2	1:C:743:ALA:O	2.26	0.68
1:F:77:ASN:HB2	1:F:211:LEU:HD22	1.65	0.68
1:B:131:VAL:HG22	1:B:180:ILE:HG13	1.76	0.68
1:E:156:GLY:HA2	1:E:217:PHE:H	1.57	0.68
1:A:473:LEU:HD11	1:B:263:ILE:HD11	1.75	0.68
1:A:339:PRO:HA	1:A:382:LYS:HE3	1.76	0.68
1:E:481:LYS:CE	1:F:270:LEU:HD13	2.21	0.68
1:B:91:HIS:NE2	1:B:95:VAL:O	2.27	0.68
1:B:211:LEU:C	1:B:211:LEU:HD23	2.14	0.68
1:E:621:LEU:HD23	1:E:621:LEU:H	1.58	0.68
1:A:103:ARG:HA	1:A:108:LEU:HD12	1.75	0.67
1:B:434:ARG:NH1	1:B:482:PHE:O	2.27	0.67
1:B:438:ASP:OD1	1:B:438:ASP:N	2.27	0.67
1:E:726:LEU:HD11	1:F:671:ARG:HH21	1.58	0.67
1:C:74:ILE:HG23	1:C:75:GLY:H	1.59	0.67
1:A:364:SER:HA	1:A:367:VAL:HG12	1.76	0.67
1:C:434:ARG:NH1	1:C:482:PHE:O	2.27	0.67
1:F:160:PRO:HG2	1:F:212:SER:CB	2.24	0.67
1:F:160:PRO:HD2	1:F:212:SER:CB	2.24	0.67
1:A:618:ILE:HG21	1:A:657:ALA:HB1	1.76	0.67
1:B:402:PRO:HA	1:B:406:ASP:HB3	1.77	0.67
1:E:435:HIS:CE1	1:E:437:LEU:CD2	2.77	0.66
1:A:618:ILE:HD12	1:A:665:ILE:CD1	2.26	0.66
1:D:267:GLN:N	1:D:268:PRO:CD	2.58	0.66
1:E:126:ALA:HB2	1:E:215:PHE:HB3	1.76	0.66
1:E:270:LEU:H	1:E:270:LEU:CD1	2.07	0.66
1:F:468:THR:HG22	1:F:484:LEU:HD21	1.75	0.66
1:C:77:ASN:HD21	1:C:209:PHE:CA	2.07	0.66
1:A:344:ILE:HG21	1:A:347:ILE:CG1	2.21	0.66
1:D:185:ASP:OD2	1:D:215:PHE:CD1	2.48	0.66
1:A:517:ASP:HA	1:A:695:LYS:HE2	1.76	0.66
1:D:459:ALA:HB2	1:E:402:PRO:HB3	1.78	0.66
1:C:338:GLN:HB3	1:C:382:LYS:HD3	1.78	0.66
1:C:265:LEU:HD21	1:C:384:VAL:HG12	1.78	0.65
1:E:688:ALA:O	1:E:692:ILE:HD12	1.96	0.65
1:F:335:ARG:HH12	1:F:381:GLY:HA3	1.59	0.65
1:A:270:LEU:HG	1:F:481:LYS:HE2	1.78	0.65
1:A:501:SER:HA	1:A:504:ARG:HB2	1.79	0.65
1:B:482:PHE:HE2	1:C:270:LEU:CD2	1.78	0.65
1:E:445:ILE:HD11	1:E:488:LEU:HD12	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:ASN:ND2	1:C:209:PHE:C	2.50	0.65
1:D:406:ASP:O	1:C:504:ARG:NH2	2.30	0.65
1:E:170:LYS:HE3	1:E:176:ILE:HD13	1.78	0.65
1:B:482:PHE:CZ	1:C:270:LEU:HD21	2.09	0.65
1:E:427:PHE:CG	1:E:442:ILE:HD11	2.32	0.65
1:A:270:LEU:CG	1:F:481:LYS:HE2	2.26	0.65
1:A:344:ILE:HG22	1:A:347:ILE:HD12	1.69	0.65
1:B:218:ARG:HB3	1:B:221:SER:HB3	1.78	0.65
1:F:450:HIS:HD2	1:F:512:LYS:HB2	1.61	0.65
1:F:79:ILE:HD12	1:F:211:LEU:HD12	1.79	0.65
1:B:462:ARG:NH1	1:C:277:SER:O	2.29	0.64
1:F:100:THR:HG23	1:F:103:ARG:HH21	1.60	0.64
1:B:79:ILE:CB	1:B:210:TYR:HB3	2.26	0.64
1:E:437:LEU:HD13	1:E:437:LEU:N	2.05	0.64
1:E:517:ASP:HA	1:E:695:LYS:HE3	1.78	0.64
1:D:280:ARG:NH2	1:D:380:ALA:O	2.31	0.64
1:E:445:ILE:CD1	1:E:488:LEU:CD1	2.73	0.64
1:F:553:VAL:HG11	1:F:677:ARG:HB2	1.80	0.64
1:B:645:ASP:OD1	1:B:674:ARG:NH1	2.31	0.64
1:D:583:GLY:HA2	1:D:621:LEU:HD23	1.77	0.64
1:E:621:LEU:HB3	1:E:636:VAL:HG11	1.79	0.64
1:F:82:ILE:HD11	1:F:157:VAL:HG21	1.80	0.64
1:D:619:ASP:OD1	1:D:620:ALA:N	2.31	0.64
1:D:671:ARG:HD3	1:C:559:PRO:HB2	1.78	0.64
1:F:518:ILE:HG23	1:F:565:LEU:HG	1.80	0.64
1:A:616:ASP:OD1	1:A:616:ASP:N	2.18	0.64
1:B:437:LEU:HD11	1:B:491:VAL:HG21	1.78	0.64
1:A:550:PRO:HB3	1:A:676:ASP:HB2	1.79	0.63
1:D:617:GLN:HG2	1:E:638:THR:HG23	1.80	0.63
1:E:141:GLU:HG3	1:E:170:LYS:HG2	1.79	0.63
1:E:583:GLY:C	1:E:620:ALA:HB3	2.19	0.63
1:F:218:ARG:HE	1:F:219:LYS:H	1.43	0.63
1:F:306:HIS:O	1:F:341:ILE:N	2.29	0.63
1:B:126:ALA:HB2	1:B:215:PHE:HB3	1.81	0.63
1:F:352:PRO:HD2	1:F:363:GLU:HG3	1.80	0.63
1:C:160:PRO:CD	1:C:212:SER:OG	2.38	0.63
1:A:723:GLU:HG2	1:B:672:PRO:HG2	1.79	0.63
1:A:73:LYS:NZ	1:A:112:ASP:OD2	2.32	0.63
1:D:213:PRO:HB2	1:D:215:PHE:HE2	1.63	0.63
1:D:365:ARG:NH2	1:C:363:GLU:OE2	2.31	0.63
1:D:672:PRO:HG2	1:C:723:GLU:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:181:THR:HG21	1:E:229:GLU:HB3	1.80	0.63
1:F:288:PRO:HD3	1:F:391:ARG:HH12	1.62	0.63
1:B:746:GLU:OE1	1:B:748:ARG:NH1	2.32	0.63
1:F:267:GLN:OE1	1:F:270:LEU:HD12	1.96	0.63
1:A:99:SER:HB3	1:A:102:ILE:HB	1.81	0.63
1:A:424:THR:HG22	1:A:442:ILE:HD13	1.79	0.62
1:E:624:ASP:OD1	1:E:630:THR:OG1	2.13	0.62
1:F:361:GLU:O	1:F:365:ARG:HG3	1.98	0.62
1:F:562:SER:O	1:F:566:THR:N	2.26	0.62
1:B:645:ASP:OD2	1:B:671:ARG:NH2	2.32	0.62
1:D:213:PRO:HG3	1:D:236:TYR:CE1	2.34	0.62
1:E:619:ASP:O	1:E:621:LEU:CA	2.48	0.62
1:F:437:LEU:HD13	1:F:442:ILE:HD11	1.80	0.62
1:F:689:ARG:HH11	1:F:713:ALA:HB1	1.64	0.62
1:C:271:PHE:CD2	1:C:278:PRO:HA	2.34	0.62
1:F:79:ILE:HG23	1:F:81:VAL:HG23	1.80	0.62
1:A:420:PHE:CE1	1:A:442:ILE:HG22	2.33	0.62
1:A:435:HIS:CE1	1:A:437:LEU:CG	2.83	0.62
1:A:719:TYR:HE1	1:A:759:ARG:HG2	1.64	0.62
1:B:79:ILE:HG13	1:B:210:TYR:N	2.14	0.62
1:E:532:ILE:HD11	1:E:570:LEU:HG	1.80	0.62
1:C:228:LYS:O	1:C:229:GLU:HG2	1.98	0.62
1:B:567:ALA:HB2	1:B:614:PHE:CD1	2.34	0.62
1:F:724:VAL:HA	1:F:727:LEU:HD12	1.81	0.62
1:C:146:LYS:O	1:C:150:LYS:N	2.32	0.62
1:B:310:ILE:HD11	1:B:344:ILE:HG12	1.81	0.61
1:A:328:ARG:HH22	1:A:369:THR:HG21	1.65	0.61
1:E:435:HIS:O	1:E:435:HIS:ND1	2.33	0.61
1:C:77:ASN:ND2	1:C:209:PHE:HA	2.13	0.61
1:D:109:ILE:HD12	1:D:307:VAL:HG21	1.82	0.61
1:E:296:LEU:HD22	1:E:345:ASP:OD1	2.00	0.61
1:B:79:ILE:CB	1:B:210:TYR:CB	2.76	0.61
1:B:285:HIS:HB2	1:B:392:PRO:HG3	1.81	0.61
1:D:138:ASN:HA	1:D:228:LYS:HE2	1.83	0.61
1:A:758:ALA:HB1	1:B:776:SER:HB3	1.82	0.61
1:D:426:GLN:OE1	1:D:429:ARG:NH2	2.34	0.61
1:E:79:ILE:HG23	1:E:159:MET:HE3	1.82	0.61
1:D:701:ASN:ND2	1:D:743:ALA:O	2.33	0.61
1:A:292:LYS:HG2	1:A:411:ILE:HD11	1.83	0.61
1:B:148:ILE:HG23	1:B:152:LEU:HD12	1.82	0.61
1:E:401:ARG:HG2	1:E:402:PRO:HD2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:PRO:HG2	1:D:213:PRO:CD	2.27	0.61
1:F:751:GLU:OE2	1:F:755:LYS:NZ	2.34	0.61
1:B:311:ASN:HB2	1:B:345:ASP:CB	2.31	0.60
1:D:438:ASP:OD1	1:D:438:ASP:N	2.34	0.60
1:E:152:LEU:HD21	1:E:219:LYS:HD2	1.81	0.60
1:A:726:LEU:HD22	1:B:672:PRO:HB3	1.83	0.60
1:D:674:ARG:NH2	3:C:802:ATP:O1G	2.34	0.60
1:D:726:LEU:HD22	1:E:672:PRO:HB3	1.83	0.60
1:E:618:ILE:C	1:E:618:ILE:HD13	2.21	0.60
1:A:274:PHE:HE2	1:F:469:ILE:HD11	1.65	0.60
1:A:277:SER:O	1:F:462:ARG:NH2	2.27	0.60
1:B:311:ASN:HB3	1:B:345:ASP:HB2	1.83	0.60
1:C:311:ASN:OD1	1:C:312:GLY:N	2.33	0.60
1:E:671:ARG:NH1	1:E:672:PRO:O	2.34	0.60
1:F:401:ARG:HH11	1:F:404:ARG:HH22	1.48	0.60
1:B:211:LEU:HD23	1:B:211:LEU:O	2.01	0.60
1:D:605:ALA:HB1	1:D:653:VAL:HG11	1.84	0.60
1:C:315:ILE:HG23	1:C:326:ALA:HB3	1.82	0.60
1:B:560:GLY:HA3	1:C:671:ARG:HD2	1.83	0.60
1:E:133:SER:HA	1:E:179:VAL:HB	1.84	0.60
1:E:624:ASP:C	1:E:625:ARG:HG3	2.22	0.60
1:A:469:ILE:HD12	1:A:481:LYS:HD3	1.84	0.60
1:E:375:ASP:OD1	1:E:404:ARG:NH1	2.35	0.60
1:D:630:THR:HA	1:D:634:ASN:HB3	1.84	0.60
1:E:427:PHE:HD2	1:E:442:ILE:HD12	1.59	0.60
1:C:283:LEU:HB3	1:C:408:GLU:HG2	1.84	0.59
1:A:280:ARG:NH2	1:A:376:GLY:O	2.35	0.59
1:D:271:PHE:O	1:D:274:PHE:N	2.35	0.59
1:F:265:LEU:O	1:F:382:LYS:NZ	2.34	0.59
1:A:160:PRO:HG3	1:A:213:PRO:HD2	1.85	0.59
1:A:732:GLY:O	1:A:736:ILE:HG12	2.03	0.59
1:E:592:GLY:HA2	1:E:595:GLU:HG2	1.84	0.59
1:A:346:GLN:HA	1:A:389:THR:HA	1.84	0.59
1:E:423:LEU:HD21	1:E:457:LEU:HD22	1.83	0.59
1:E:742:VAL:O	1:F:544:ARG:NH1	2.35	0.59
1:B:79:ILE:HG21	1:B:210:TYR:CG	2.20	0.59
1:B:250:LEU:HD11	1:B:411:ILE:HG23	1.84	0.59
1:D:269:THR:O	1:D:269:THR:HG22	2.03	0.59
1:D:619:ASP:O	1:D:620:ALA:C	2.41	0.59
1:E:605:ALA:HB1	1:E:653:VAL:HG11	1.84	0.59
1:E:746:GLU:HG2	1:E:748:ARG:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:775:ARG:NH2	1:B:776:SER:OG	2.35	0.59
1:B:649:GLU:O	1:B:651:LYS:NZ	2.32	0.59
1:B:251:ASP:O	1:B:254:ILE:N	2.35	0.59
1:F:160:PRO:CD	1:F:212:SER:CB	2.80	0.59
1:B:436:VAL:O	1:B:436:VAL:HG22	2.01	0.59
1:B:55:PRO:HA	1:B:58:LEU:HD12	1.84	0.58
1:C:77:ASN:ND2	1:C:209:PHE:CA	2.65	0.58
1:A:414:PRO:O	1:A:419:ARG:NH1	2.36	0.58
1:A:434:ARG:HH21	1:A:482:PHE:HB3	1.66	0.58
1:E:208:ASP:HA	1:E:210:TYR:CE2	2.38	0.58
1:A:435:HIS:HE1	1:A:437:LEU:CG	2.15	0.58
1:A:741:ASP:OD2	1:B:544:ARG:NE	2.31	0.58
1:D:163:ILE:HG13	1:D:179:VAL:HG22	1.85	0.58
1:E:74:ILE:HG22	1:E:115:GLU:HG2	1.85	0.58
1:D:614:PHE:HD1	1:D:656:VAL:HG13	1.68	0.58
1:E:587:PHE:CZ	1:E:621:LEU:HA	2.39	0.58
1:F:427:PHE:O	1:F:431:SER:N	2.36	0.58
1:C:160:PRO:CD	1:C:212:SER:HG	2.15	0.58
1:E:152:LEU:HD12	1:E:217:PHE:HE2	1.68	0.58
1:E:48:THR:HA	1:E:102:ILE:HD11	1.84	0.58
1:B:127:THR:HA	1:B:222:THR:HG21	1.86	0.58
1:B:506:ILE:HD11	1:B:604:LYS:HD3	1.85	0.58
1:D:78:GLY:H	1:D:211:LEU:HD22	1.57	0.58
1:D:77:ASN:CB	1:D:211:LEU:HD23	2.31	0.58
1:C:452:TYR:HE2	1:C:460:LEU:HD12	1.68	0.58
3:A:802:ATP:O1G	1:B:674:ARG:NH2	2.37	0.57
1:E:296:LEU:HD23	1:E:345:ASP:OD1	2.01	0.57
1:B:163:ILE:HG13	1:B:179:VAL:HG22	1.86	0.57
1:F:94:ASN:OD1	1:F:95:VAL:N	2.38	0.57
1:B:347:ILE:HG22	1:B:389:THR:HB	1.86	0.57
1:C:247:VAL:HG22	1:C:294:MET:HE3	1.86	0.57
1:A:367:VAL:O	1:A:371:LEU:HG	2.04	0.57
1:E:138:ASN:HB3	1:E:228:LYS:HB2	1.86	0.57
1:E:292:LYS:NZ	1:E:390:ASN:OD1	2.37	0.57
1:B:625:ARG:NH1	1:B:626:ASP:HB2	2.19	0.57
1:D:77:ASN:HB3	1:D:209:PHE:O	2.03	0.57
1:D:160:PRO:HD3	1:D:213:PRO:O	2.04	0.57
1:E:98:LEU:HD12	1:E:102:ILE:HD13	1.85	0.57
1:D:68:PHE:HD1	1:D:82:ILE:HG22	1.70	0.57
1:D:547:ILE:HD12	1:C:729:GLN:HA	1.86	0.57
1:A:413:ILE:HD11	1:A:610:PRO:HD2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:LEU:HD22	1:D:219:LYS:HD2	1.87	0.57
1:E:645:ASP:OD2	1:E:671:ARG:NH2	2.33	0.57
1:A:36:THR:HB	1:A:114:LEU:HD11	1.85	0.57
1:A:211:LEU:HD13	1:A:211:LEU:N	2.06	0.57
1:A:420:PHE:CE1	1:A:442:ILE:CG2	2.87	0.57
1:D:468:THR:HG21	1:D:486:VAL:HG22	1.86	0.57
1:E:401:ARG:HH21	1:E:403:GLY:HA3	1.70	0.57
1:E:435:HIS:CD2	1:E:437:LEU:HD23	2.17	0.57
1:F:421:ASP:O	1:F:425:LYS:HG2	2.05	0.57
1:F:688:ALA:O	1:F:692:ILE:HG12	2.05	0.57
1:A:433:ASP:OD1	1:A:434:ARG:N	2.37	0.56
1:D:463:GLU:HB3	1:D:494:ALA:HB1	1.87	0.56
1:C:77:ASN:HB3	1:C:210:TYR:C	2.25	0.56
1:A:618:ILE:HG12	1:A:659:THR:HB	1.87	0.56
1:B:469:ILE:HG23	1:B:481:LYS:HD2	1.87	0.56
1:D:68:PHE:CD1	1:D:82:ILE:HG22	2.40	0.56
1:D:453:VAL:HG22	1:D:454:GLY:H	1.71	0.56
1:D:672:PRO:HB3	1:C:726:LEU:HD22	1.87	0.56
1:F:160:PRO:CD	1:F:212:SER:HB3	2.35	0.56
1:A:435:HIS:CE1	1:A:437:LEU:CB	2.86	0.56
1:D:78:GLY:C	1:D:211:LEU:HD21	2.26	0.56
1:C:49:CYS:H	1:C:102:ILE:HD11	1.71	0.56
1:D:647:VAL:HG21	1:C:580:ALA:HB1	1.88	0.56
1:A:242:LEU:HB3	1:A:298:VAL:HG22	1.86	0.56
1:A:287:PRO:HG2	1:A:413:ILE:HG23	1.87	0.56
1:A:78:GLY:N	1:A:211:LEU:HD12	2.21	0.56
1:E:533:GLN:NE2	1:E:537:GLU:OE2	2.39	0.56
1:E:584:PRO:CG	1:E:617:GLN:OE1	2.54	0.56
1:F:247:VAL:HG11	1:F:298:VAL:HG21	1.87	0.56
1:D:694:LYS:HG2	1:D:709:LEU:HD21	1.86	0.56
1:C:265:LEU:HD11	1:C:341:ILE:HG12	1.88	0.56
1:A:494:ALA:O	1:A:498:ILE:HG23	2.06	0.55
1:B:618:ILE:HD12	1:B:657:ALA:HB1	0.56	0.55
1:E:445:ILE:CD1	1:E:488:LEU:HD11	2.35	0.55
1:F:212:SER:O	1:F:213:PRO:C	2.43	0.55
1:C:291:GLY:N	3:C:801:ATP:O2B	2.34	0.55
1:B:341:ILE:HG23	1:B:384:VAL:HG13	1.87	0.55
1:E:528:MET:SD	1:E:570:LEU:HD23	2.46	0.55
1:E:570:LEU:HD12	1:E:573:GLU:HB3	1.88	0.55
1:E:163:ILE:HG12	1:E:179:VAL:HG22	1.88	0.55
1:E:436:VAL:CG1	1:E:486:VAL:O	2.52	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:GLY:HA3	1:C:78:GLY:HA2	1.89	0.55
1:A:618:ILE:CG2	1:A:657:ALA:HB1	2.36	0.55
1:A:619:ASP:OD1	1:A:619:ASP:N	2.35	0.55
1:E:33:GLU:OE2	1:E:114:LEU:N	2.39	0.55
1:E:611:SER:HB3	1:E:653:VAL:HG12	1.87	0.55
1:A:618:ILE:HD12	1:A:665:ILE:HD12	1.88	0.55
1:B:160:PRO:CG	1:B:212:SER:HB2	2.34	0.55
1:E:465:VAL:HG13	1:F:274:PHE:HD2	1.72	0.55
1:F:377:MET:HG2	1:F:383:VAL:HG11	1.88	0.55
1:F:42:LYS:HD2	1:F:42:LYS:O	2.06	0.55
1:C:74:ILE:HG23	1:C:75:GLY:N	2.22	0.55
1:D:103:ARG:O	1:D:108:LEU:N	2.35	0.55
1:E:624:ASP:OD2	1:E:630:THR:CG2	2.50	0.55
1:F:398:ALA:O	1:F:404:ARG:NH2	2.27	0.55
1:A:251:ASP:O	1:A:254:ILE:N	2.40	0.55
1:C:401:ARG:HG2	1:C:402:PRO:HD2	1.88	0.55
1:D:625:ARG:HG3	1:D:626:ASP:H	1.72	0.55
1:E:160:PRO:HG3	1:E:213:PRO:HD2	1.88	0.55
1:F:110:LEU:HB3	1:F:306:HIS:HA	1.88	0.55
1:B:331:PHE:HB2	1:B:373:LEU:HD23	1.89	0.54
1:E:121:VAL:HG21	1:F:90:VAL:HG23	1.89	0.54
1:F:630:THR:OG1	1:F:633:ALA:HB2	2.06	0.54
1:A:348:ASP:O	1:A:352:PRO:N	2.40	0.54
1:A:482:PHE:CZ	1:B:270:LEU:CD2	2.89	0.54
1:A:581:VAL:HG12	1:A:615:PHE:HE1	1.71	0.54
1:E:80:LEU:HD23	1:E:210:TYR:CE1	2.42	0.54
1:E:614:PHE:CD2	1:E:656:VAL:HG13	2.29	0.54
1:E:676:ASP:OD1	1:E:677:ARG:N	2.40	0.54
1:C:262:GLU:HA	1:C:262:GLU:OE1	2.07	0.54
1:A:270:LEU:CG	1:F:481:LYS:CE	2.81	0.54
1:E:160:PRO:CD	1:E:212:SER:HB3	2.37	0.54
1:E:434:ARG:NH2	1:E:482:PHE:HA	2.21	0.54
1:C:452:TYR:HE1	1:C:500:PRO:HG3	1.72	0.54
1:A:132:GLY:O	1:A:179:VAL:N	2.28	0.54
1:D:629:SER:HB3	1:D:633:ALA:HB3	1.90	0.54
1:F:632:ALA:O	1:F:635:HIS:N	2.39	0.54
1:A:618:ILE:CG1	1:A:659:THR:HB	2.37	0.54
1:F:499:ARG:HB2	1:F:500:PRO:HD2	1.89	0.54
1:E:77:ASN:O	1:E:211:LEU:CG	2.55	0.54
1:F:414:PRO:HD2	1:F:453:VAL:HA	1.89	0.54
1:C:271:PHE:CE2	1:C:279:PRO:HD3	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:THR:CG2	1:A:442:ILE:HG21	2.33	0.54
1:A:553:VAL:HG12	1:A:677:ARG:HB2	1.90	0.54
1:E:584:PRO:N	1:E:620:ALA:HB2	2.22	0.54
1:F:550:PRO:HB3	1:F:676:ASP:HB2	1.90	0.54
1:D:619:ASP:O	1:D:621:LEU:N	2.41	0.54
1:E:619:ASP:C	1:E:621:LEU:H	2.10	0.54
1:D:107:ASN:ND2	1:D:301:ASN:OD1	2.33	0.54
1:D:257:LEU:O	1:D:261:ILE:HG12	2.08	0.54
1:F:542:PHE:HA	1:F:547:ILE:HD12	1.90	0.54
1:A:79:ILE:HA	1:A:211:LEU:HD21	1.90	0.53
1:A:532:ILE:HG12	1:A:570:LEU:HD11	1.90	0.53
1:B:244:TYR:HD1	1:B:254:ILE:HD11	1.73	0.53
1:C:101:THR:O	1:C:105:VAL:HG23	2.07	0.53
1:E:600:GLU:OE2	1:E:604:LYS:NZ	2.42	0.53
1:F:77:ASN:CG	1:F:211:LEU:CD2	2.69	0.53
1:F:310:ILE:HG23	1:F:315:ILE:HG13	1.91	0.53
1:F:582:LYS:HE2	1:F:585:GLU:HB2	1.90	0.53
1:A:68:PHE:HB2	1:A:120:GLN:HG2	1.88	0.53
1:A:161:GLY:N	1:A:180:ILE:O	2.39	0.53
1:B:482:PHE:CZ	1:C:270:LEU:HD22	1.96	0.53
1:D:308:LEU:HD22	1:D:330:ILE:HG23	1.89	0.53
1:B:311:ASN:CB	1:B:345:ASP:CB	2.84	0.53
1:E:99:SER:O	1:E:101:THR:N	2.42	0.53
1:E:583:GLY:CA	1:E:620:ALA:CB	2.87	0.53
1:A:468:THR:HG21	1:A:486:VAL:HG22	1.89	0.53
1:E:554:LEU:HD12	1:E:675:LEU:HD23	1.91	0.53
1:E:521:GLN:NE2	1:E:682:GLY:O	2.38	0.52
1:A:335:ARG:NH1	1:F:208:ASP:OD2	2.42	0.52
1:A:244:TYR:CE2	1:A:302:THR:HG21	2.44	0.52
3:A:801:ATP:O1G	1:B:401:ARG:NH2	2.41	0.52
1:D:160:PRO:HG3	1:D:213:PRO:HG2	1.91	0.52
1:E:157:VAL:H	1:E:216:ILE:HA	1.74	0.52
1:F:618:ILE:HG13	1:F:621:LEU:HD11	1.91	0.52
1:C:520:GLY:HA2	1:C:688:ALA:HB1	1.91	0.52
1:A:424:THR:HG22	1:A:442:ILE:CD1	2.39	0.52
1:A:618:ILE:HD12	1:A:665:ILE:HD11	1.90	0.52
1:D:47:GLU:OE1	1:D:47:GLU:N	2.42	0.52
1:E:672:PRO:HA	1:E:676:ASP:HB3	1.90	0.52
1:C:348:ASP:OD2	1:C:389:THR:OG1	2.25	0.52
1:A:217:PHE:O	1:A:218:ARG:NE	2.41	0.52
1:B:609:ALA:HB1	1:B:610:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:103:ARG:HA	1:E:108:LEU:HB2	1.92	0.52
1:F:287:PRO:HG2	1:F:290:THR:HG21	1.92	0.52
1:F:462:ARG:O	1:F:466:MET:HG2	2.10	0.52
1:F:701:ASN:HD21	1:F:744:LYS:HB3	1.73	0.52
1:A:606:ARG:NH2	1:A:652:GLY:H	2.06	0.52
1:B:34:PHE:O	1:B:114:LEU:N	2.42	0.52
1:B:144:GLU:HB3	1:B:148:ILE:HG13	1.91	0.52
1:B:697:THR:HG23	1:B:700:PHE:HD2	1.73	0.52
1:D:64:ASN:OD1	1:D:67:SER:N	2.42	0.52
1:A:482:PHE:CE1	1:B:270:LEU:HD23	2.44	0.52
1:C:168:LYS:NZ	1:C:170:LYS:O	2.37	0.52
1:D:319:TYR:HB2	1:D:322:GLU:HG2	1.92	0.52
1:D:741:ASP:OD2	1:E:544:ARG:NH1	2.43	0.52
1:F:48:THR:OG1	1:F:154:ASP:HB2	2.10	0.52
1:B:160:PRO:O	1:B:180:ILE:HB	2.10	0.52
1:D:707:VAL:HG21	1:D:750:PHE:HE2	1.75	0.52
1:E:39:HIS:ND1	1:E:97:THR:HG22	2.25	0.52
1:D:159:MET:HG3	1:D:212:SER:OG	2.10	0.52
1:E:261:ILE:HD11	1:E:386:ILE:HD11	1.91	0.52
1:C:79:ILE:CG1	1:C:211:LEU:HD21	2.38	0.52
1:C:402:PRO:HA	1:C:406:ASP:HB3	1.90	0.52
1:B:127:THR:HG22	1:B:185:ASP:HB3	1.92	0.51
1:D:547:ILE:HD11	1:C:700:PHE:HZ	1.75	0.51
1:E:618:ILE:CG2	1:E:659:THR:HG22	2.41	0.51
1:F:109:ILE:N	1:F:112:ASP:OD2	2.43	0.51
1:B:84:ARG:HE	1:B:85:ALA:H	1.59	0.51
1:B:360:GLY:H	1:B:363:GLU:CD	2.13	0.51
1:B:459:ALA:HB2	1:C:402:PRO:HB3	1.91	0.51
1:E:347:ILE:HG12	1:E:347:ILE:O	2.09	0.51
1:C:141:GLU:HB2	1:C:170:LYS:HD2	1.92	0.51
1:D:401:ARG:HG2	1:D:402:PRO:HD2	1.92	0.51
1:C:136:GLY:O	1:C:228:LYS:NZ	2.43	0.51
1:E:318:LYS:HD3	1:F:319:TYR:HD2	1.75	0.51
1:F:513:VAL:HG21	1:F:568:LYS:HD2	1.91	0.51
1:B:471:ARG:NH1	1:B:490:ASP:OD2	2.44	0.51
1:E:513:VAL:HG21	1:E:568:LYS:HG3	1.93	0.51
1:D:79:ILE:HD11	1:D:159:MET:HG3	1.92	0.51
1:D:524:LEU:HD13	1:D:679:ILE:HG21	1.91	0.51
1:D:532:ILE:HG13	1:D:533:GLN:N	2.26	0.51
1:E:77:ASN:CA	1:E:211:LEU:HD21	2.38	0.51
1:F:528:MET:O	1:F:532:ILE:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:LEU:HD13	1:F:469:ILE:CD1	2.40	0.51
1:B:41:SER:HB2	1:B:44:HIS:ND1	2.26	0.51
1:B:94:ASN:OD1	1:B:95:VAL:N	2.44	0.51
1:D:159:MET:HB2	1:D:212:SER:OG	2.11	0.51
1:F:52:TYR:HA	1:F:84:ARG:HB2	1.92	0.51
1:C:551:LYS:HD2	1:C:551:LYS:O	2.10	0.51
1:A:152:LEU:HD11	1:A:218:ARG:HA	1.93	0.51
1:A:328:ARG:HE	1:F:74:ILE:HG13	1.74	0.51
1:D:707:VAL:HG12	1:D:747:LEU:HD12	1.92	0.51
1:E:584:PRO:N	1:E:620:ALA:CB	2.73	0.51
1:C:70:THR:HG21	1:C:210:TYR:HE1	1.76	0.51
1:A:285:HIS:NE2	1:A:410:GLU:HB3	2.26	0.51
1:C:134:LEU:HB2	1:C:179:VAL:HG23	1.93	0.51
1:C:689:ARG:NH1	1:C:713:ALA:O	2.44	0.51
1:A:697:THR:HG23	1:A:700:PHE:HD2	1.75	0.50
1:D:618:ILE:CG2	1:D:659:THR:HB	2.41	0.50
1:C:80:LEU:HD11	1:C:210:TYR:CZ	2.46	0.50
1:C:144:GLU:HA	1:C:147:VAL:HB	1.93	0.50
1:D:528:MET:O	1:D:532:ILE:HG12	2.12	0.50
1:F:127:THR:HB	1:F:185:ASP:HB3	1.93	0.50
1:F:514:TYR:HA	1:F:572:THR:HG21	1.92	0.50
1:D:609:ALA:HB1	1:D:610:PRO:HD2	1.93	0.50
1:E:739:ASP:OD1	1:E:739:ASP:N	2.43	0.50
1:D:642:ASN:HD22	1:C:582:LYS:HB3	1.76	0.50
1:C:126:ALA:N	1:C:216:ILE:O	2.36	0.50
1:A:414:PRO:HB2	1:A:419:ARG:HG3	1.93	0.50
1:E:724:VAL:HA	1:E:727:LEU:HD12	1.94	0.50
1:B:431:SER:HB2	1:B:434:ARG:HG2	1.92	0.50
1:D:209:PHE:HB2	1:D:210:TYR:CE2	2.46	0.50
1:D:283:LEU:HB3	1:D:408:GLU:HG2	1.93	0.50
1:E:292:LYS:HG2	1:E:411:ILE:HD13	1.93	0.50
1:F:463:GLU:HG2	1:F:494:ALA:HB1	1.94	0.50
1:C:530:GLU:HA	1:C:534:LEU:HD23	1.94	0.50
1:B:251:ASP:HA	1:B:254:ILE:HG22	1.94	0.50
1:E:624:ASP:OD1	1:E:630:THR:CB	2.60	0.50
1:E:684:PRO:HG2	1:E:689:ARG:HD2	1.94	0.50
1:F:88:GLU:HG3	1:F:90:VAL:HG12	1.94	0.50
1:F:283:LEU:HB3	1:F:408:GLU:HG3	1.92	0.50
1:E:738:GLU:OE1	1:E:749:HIS:NE2	2.42	0.50
1:F:413:ILE:HG13	1:F:453:VAL:HG12	1.94	0.50
1:A:123:PRO:HB2	1:A:215:PHE:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:PHE:CD2	1:B:271:PHE:C	2.86	0.49
1:A:138:ASN:OD1	1:A:139:ILE:HG13	2.13	0.49
1:B:271:PHE:CE2	1:B:278:PRO:HA	2.48	0.49
1:F:117:LYS:HD3	1:F:119:ALA:HB3	1.94	0.49
1:A:344:ILE:HB	1:A:347:ILE:HD11	1.92	0.49
1:B:762:THR:HG23	1:B:765:MET:H	1.77	0.49
1:F:414:PRO:O	1:F:419:ARG:NH1	2.44	0.49
1:E:151:LEU:HD22	1:E:158:ILE:HD13	1.94	0.49
1:E:445:ILE:HD12	1:E:491:VAL:HG12	1.87	0.49
1:A:435:HIS:CE1	1:A:437:LEU:CD1	2.82	0.49
1:C:363:GLU:HA	1:C:366:VAL:HG12	1.94	0.49
1:C:540:GLU:O	1:C:544:ARG:HG3	2.13	0.49
1:C:624:ASP:OD1	1:C:624:ASP:N	2.43	0.49
1:A:326:ALA:O	1:A:330:ILE:HG12	2.12	0.49
1:A:435:HIS:NE2	1:A:437:LEU:HB2	2.28	0.49
1:F:160:PRO:HD2	1:F:212:SER:HB2	1.92	0.49
1:C:753:ALA:O	1:C:757:ILE:HG12	2.13	0.49
1:B:154:ASP:N	1:B:154:ASP:OD1	2.43	0.49
1:B:619:ASP:O	1:B:623:PRO:CG	2.59	0.49
1:D:213:PRO:HB2	1:D:215:PHE:CE2	2.46	0.49
1:D:310:ILE:HG22	1:D:330:ILE:HD13	1.94	0.49
1:D:762:THR:HG23	1:D:764:GLU:HG3	1.95	0.49
1:E:70:THR:HG22	1:E:80:LEU:HB3	1.95	0.49
1:E:77:ASN:CB	1:E:211:LEU:CD2	2.85	0.49
1:E:208:ASP:HA	1:E:210:TYR:HE2	1.77	0.49
1:F:499:ARG:HB2	1:F:500:PRO:CD	2.43	0.49
1:A:265:LEU:HG	1:A:382:LYS:HD3	1.95	0.49
1:A:467:LYS:HB3	1:A:490:ASP:HB2	1.93	0.49
1:A:680:TYR:HE1	1:A:769:TYR:HB3	1.77	0.49
1:C:313:PRO:O	1:C:316:VAL:HG22	2.13	0.49
1:C:341:ILE:HG23	1:C:384:VAL:HG13	1.94	0.49
1:A:581:VAL:HG12	1:A:615:PHE:CE1	2.47	0.49
1:F:103:ARG:O	1:F:108:LEU:N	2.41	0.49
1:F:369:THR:HA	1:F:372:THR:HG22	1.95	0.49
1:C:453:VAL:H	1:C:456:ASP:HB2	1.77	0.49
1:A:361:GLU:O	1:A:363:GLU:N	2.40	0.48
1:D:617:GLN:OE1	1:D:617:GLN:N	2.46	0.48
1:F:663:ASP:OD2	1:F:768:TYR:OH	2.27	0.48
1:C:287:PRO:HG2	1:C:413:ILE:HG13	1.95	0.48
1:A:38:PRO:HB3	1:A:103:ARG:HH22	1.77	0.48
1:A:434:ARG:HG2	1:B:274:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:ALA:O	1:A:757:ILE:HG12	2.13	0.48
1:B:619:ASP:C	1:B:623:PRO:HD3	2.27	0.48
1:C:54:HIS:HB3	1:C:57:VAL:HG12	1.95	0.48
1:C:472:GLY:HA3	1:C:484:LEU:HD11	1.95	0.48
1:A:234:ARG:NH2	1:B:269:THR:O	2.46	0.48
1:A:246:ALA:HA	1:A:425:LYS:HE2	1.93	0.48
1:A:551:LYS:HE3	1:A:651:LYS:HB3	1.94	0.48
1:D:402:PRO:HB3	1:C:459:ALA:HB2	1.94	0.48
1:D:554:LEU:HD12	1:D:675:LEU:HD23	1.95	0.48
3:D:801:ATP:O1G	1:E:401:ARG:NH1	2.46	0.48
1:E:492:GLU:HA	1:E:495:MET:HG3	1.95	0.48
1:A:424:THR:CG2	1:A:442:ILE:HD13	2.43	0.48
1:C:128:LYS:N	1:C:222:THR:OG1	2.47	0.48
1:A:129:VAL:HB	1:A:158:ILE:HD12	1.96	0.48
1:B:762:THR:OG1	1:B:764:GLU:OE1	2.27	0.48
1:D:84:ARG:HG3	1:D:85:ALA:H	1.79	0.48
1:D:282:ILE:HD13	1:D:407:GLN:HB3	1.94	0.48
1:E:583:GLY:CA	1:E:620:ALA:HB2	2.43	0.48
1:C:109:ILE:HD12	1:C:307:VAL:HG21	1.94	0.48
1:C:471:ARG:HH22	1:C:487:THR:HG22	1.77	0.48
1:E:465:VAL:HG13	1:F:274:PHE:CD2	2.48	0.48
1:F:38:PRO:HD3	1:F:110:LEU:HD11	1.96	0.48
1:A:618:ILE:CD1	1:A:665:ILE:HD11	2.44	0.48
1:D:609:ALA:HB1	1:D:610:PRO:CD	2.44	0.48
1:C:134:LEU:HA	1:C:230:THR:HG23	1.96	0.48
1:C:335:ARG:O	1:C:338:GLN:NE2	2.43	0.48
1:C:697:THR:HG23	1:C:700:PHE:HD2	1.78	0.48
1:A:305:ALA:HB1	1:A:339:PRO:O	2.14	0.48
1:B:469:ILE:HD12	1:B:481:LYS:HB3	1.96	0.48
1:D:267:GLN:N	1:D:268:PRO:HD3	2.28	0.48
1:F:49:CYS:HA	1:F:81:VAL:HG13	1.94	0.48
1:F:182:ASP:OD1	1:F:236:TYR:OH	2.27	0.48
1:F:457:LEU:HA	1:F:460:LEU:HD13	1.95	0.48
1:C:558:PRO:HG2	1:C:561:CYS:SG	2.54	0.48
1:B:311:ASN:HB2	1:B:345:ASP:HB3	1.96	0.48
1:D:165:GLN:OE1	1:D:175:SER:OG	2.30	0.48
1:D:671:ARG:HH21	1:D:674:ARG:CZ	2.27	0.48
1:E:427:PHE:HB3	1:E:435:HIS:NE2	2.29	0.48
1:C:267:GLN:HG3	1:C:267:GLN:O	2.13	0.48
1:A:348:ASP:CG	1:A:389:THR:OG1	2.52	0.47
1:A:614:PHE:CE1	1:A:656:VAL:HG21	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:GLU:HG3	1:B:498:ILE:HD11	1.95	0.47
1:D:619:ASP:HA	1:D:622:SER:OG	2.14	0.47
1:D:729:GLN:HA	1:E:547:ILE:HD12	1.94	0.47
1:C:58:LEU:HD11	1:C:83:ALA:HB1	1.95	0.47
1:A:606:ARG:HH21	1:A:653:VAL:HG22	1.77	0.47
1:A:579:LEU:HB3	1:A:613:ILE:HG22	1.95	0.47
1:E:102:ILE:H	1:E:102:ILE:HD12	1.79	0.47
1:E:280:ARG:HH12	1:E:383:VAL:H	1.62	0.47
1:E:619:ASP:O	1:E:621:LEU:O	2.32	0.47
1:C:588:ASN:HB3	1:C:593:GLU:HB3	1.97	0.47
1:A:296:LEU:HD22	1:A:345:ASP:OD1	2.15	0.47
1:B:159:MET:HE3	1:B:212:SER:O	2.14	0.47
1:C:105:VAL:HG22	1:C:162:MET:N	2.22	0.47
1:C:699:LYS:HA	1:C:699:LYS:HD3	1.66	0.47
1:B:35:ILE:HG13	1:B:95:VAL:HG23	1.97	0.47
1:B:618:ILE:HD13	1:B:657:ALA:CB	2.22	0.47
1:F:371:LEU:O	1:F:374:MET:HG2	2.14	0.47
1:F:450:HIS:CD2	1:F:512:LYS:HE2	2.48	0.47
1:F:558:PRO:HA	1:F:765:MET:HE2	1.96	0.47
1:C:631:SER:O	1:C:635:HIS:ND1	2.47	0.47
1:A:544:ARG:NH2	1:F:741:ASP:OD1	2.47	0.47
1:B:615:PHE:HB3	1:B:618:ILE:HG13	1.96	0.47
1:D:584:PRO:HA	1:D:587:PHE:HD2	1.79	0.47
1:E:77:ASN:CA	1:E:211:LEU:CD2	2.92	0.47
1:E:725:VAL:HG21	3:E:802:ATP:H1'	1.96	0.47
1:A:324:GLU:HB2	1:A:328:ARG:NH1	2.30	0.47
1:A:771:GLU:OE2	1:A:775:ARG:NE	2.36	0.47
1:E:166:ASN:OD1	1:E:176:ILE:HG13	2.15	0.47
1:E:495:MET:HA	1:E:498:ILE:HG22	1.96	0.47
1:C:29:LYS:HG3	1:C:30:LEU:H	1.79	0.47
1:A:702:THR:HG21	1:A:709:LEU:HD11	1.97	0.47
1:B:466:MET:SD	1:C:271:PHE:CZ	3.08	0.47
1:F:133:SER:HA	1:F:178:VAL:HA	1.95	0.47
1:C:126:ALA:HB2	1:C:215:PHE:HB3	1.96	0.47
1:A:521:GLN:HG3	1:A:523:GLU:H	1.79	0.47
1:A:562:SER:HB3	3:A:802:ATP:C8	2.50	0.47
1:E:676:ASP:OD1	1:E:677:ARG:HG2	2.14	0.47
1:C:600:GLU:OE1	1:C:604:LYS:NZ	2.47	0.47
1:D:252:LYS:HD2	1:D:252:LYS:HA	1.71	0.47
1:D:712:LEU:O	1:D:716:THR:HG22	2.14	0.47
1:F:515:TRP:H	1:F:572:THR:HG21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:618:ILE:O	1:F:622:SER:OG	2.18	0.47
1:C:271:PHE:CE2	1:C:279:PRO:CD	2.90	0.47
1:A:605:ALA:HB1	1:A:653:VAL:HG11	1.96	0.46
1:E:583:GLY:HA3	1:E:620:ALA:HB2	1.97	0.46
1:B:244:TYR:CE2	1:B:302:THR:HG21	2.50	0.46
1:B:348:ASP:OD2	1:B:389:THR:OG1	2.33	0.46
1:E:481:LYS:HD2	1:F:270:LEU:CG	2.35	0.46
1:F:160:PRO:CG	1:F:212:SER:CB	2.90	0.46
1:A:132:GLY:N	1:A:179:VAL:O	2.48	0.46
1:A:270:LEU:HD22	1:F:469:ILE:HD11	1.89	0.46
1:A:538:ALA:HB2	1:F:740:LEU:HD12	1.98	0.46
1:B:660:ASN:O	1:B:769:TYR:OH	2.18	0.46
1:D:63:ILE:HD11	1:D:118:LYS:HE2	1.97	0.46
1:D:209:PHE:HB2	1:D:210:TYR:CD2	2.50	0.46
1:D:272:SER:O	1:C:234:ARG:NH1	2.48	0.46
1:F:563:LYS:HB3	1:F:681:VAL:HG21	1.96	0.46
1:C:138:ASN:ND2	1:C:228:LYS:HD3	2.30	0.46
1:A:157:VAL:HG11	1:A:215:PHE:C	2.36	0.46
1:E:419:ARG:NE	1:E:449:THR:O	2.49	0.46
1:E:588:ASN:OD1	1:E:589:LYS:N	2.49	0.46
1:D:290:THR:HB	1:D:411:ILE:HG22	1.97	0.46
1:D:480:ASP:OD1	1:D:481:LYS:N	2.48	0.46
1:E:271:PHE:HB3	1:E:276:VAL:O	2.16	0.46
1:F:35:ILE:HG13	1:F:95:VAL:HG23	1.97	0.46
1:F:551:LYS:HE3	1:F:651:LYS:HA	1.98	0.46
1:F:624:ASP:OD2	1:F:634:ASN:HA	2.15	0.46
1:C:162:MET:HB3	1:C:164:PHE:CE1	2.50	0.46
1:A:529:LYS:HA	1:A:532:ILE:HG22	1.98	0.46
1:D:102:ILE:HD12	1:D:102:ILE:H	1.80	0.46
1:D:210:TYR:CD2	1:D:210:TYR:N	2.84	0.46
1:E:406:ASP:OD1	1:E:407:GLN:N	2.48	0.46
1:C:148:ILE:HG21	1:C:219:LYS:HG3	1.96	0.46
1:A:515:TRP:HA	1:A:518:ILE:HG22	1.97	0.46
1:F:160:PRO:HA	1:F:180:ILE:O	2.15	0.46
1:C:127:THR:OG1	1:C:185:ASP:HB3	2.15	0.46
1:C:129:VAL:HG11	1:C:158:ILE:HD11	1.97	0.46
1:A:377:MET:HG3	1:F:237:ASN:HB2	1.97	0.46
1:B:236:TYR:CE2	1:B:238:LEU:HD23	2.51	0.46
1:D:160:PRO:CG	1:D:213:PRO:CG	2.93	0.46
1:E:434:ARG:CZ	1:F:274:PHE:HE1	2.29	0.46
1:F:366:VAL:HA	1:F:369:THR:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:662:PRO:HB2	1:F:772:PHE:CZ	2.51	0.46
1:A:124:PRO:O	1:A:216:ILE:N	2.49	0.46
1:B:567:ALA:CB	1:B:614:PHE:CD1	2.99	0.46
1:D:666:ASP:OD1	1:D:667:ALA:N	2.48	0.46
1:E:35:ILE:HG12	1:E:113:ARG:HH22	1.81	0.46
1:A:131:VAL:HG12	1:A:180:ILE:HG12	1.96	0.46
1:B:111:GLY:O	1:B:113:ARG:NH1	2.48	0.46
1:B:244:TYR:CD1	1:B:254:ILE:HD11	2.50	0.46
1:B:631:SER:O	1:B:635:HIS:ND1	2.39	0.46
1:D:464:SER:O	1:D:468:THR:HG23	2.16	0.46
1:A:291:GLY:H	3:A:801:ATP:PB	2.39	0.45
1:A:342:ILE:HD13	1:A:385:VAL:HG22	1.98	0.45
1:A:347:ILE:HD12	1:A:347:ILE:N	2.30	0.45
1:B:49:CYS:SG	1:B:157:VAL:N	2.88	0.45
1:D:527:LYS:O	1:D:530:GLU:HG2	2.16	0.45
1:E:265:LEU:HD11	1:E:341:ILE:HD11	1.98	0.45
1:E:624:ASP:HB2	1:E:629:SER:OG	2.09	0.45
1:D:300:ALA:HB2	1:D:343:PHE:CE2	2.51	0.45
1:E:618:ILE:HG22	1:E:658:ALA:O	2.17	0.45
1:C:524:LEU:HD13	1:C:679:ILE:HG21	1.98	0.45
1:A:423:LEU:HD21	1:A:457:LEU:HD22	1.97	0.45
1:D:105:VAL:HG22	1:D:161:GLY:O	2.15	0.45
1:F:460:LEU:O	1:F:464:SER:OG	2.29	0.45
1:F:687:ASN:OD1	1:F:688:ALA:N	2.49	0.45
1:B:337:TYR:O	1:B:339:PRO:HD2	2.15	0.45
1:D:244:TYR:CD1	1:D:254:ILE:HD11	2.52	0.45
1:D:467:LYS:HB3	1:D:490:ASP:HB2	1.98	0.45
1:F:468:THR:OG1	1:F:490:ASP:OD2	2.20	0.45
1:F:471:ARG:HH12	1:F:489:LYS:HB2	1.80	0.45
1:C:117:LYS:HB3	1:C:117:LYS:HE2	1.70	0.45
1:D:108:LEU:HD22	1:D:114:LEU:HD21	1.99	0.45
1:E:709:LEU:O	1:E:713:ALA:N	2.46	0.45
1:F:52:TYR:HB3	1:F:86:GLY:HA2	1.99	0.45
1:F:123:PRO:HG2	1:F:216:ILE:HG13	1.97	0.45
1:F:132:GLY:O	1:F:179:VAL:N	2.31	0.45
1:A:419:ARG:NE	1:A:449:THR:O	2.50	0.45
1:A:555:LEU:HB2	1:A:658:ALA:HA	1.97	0.45
1:B:620:ALA:HB2	1:C:638:THR:HG21	1.99	0.45
1:D:160:PRO:CD	1:D:213:PRO:HG2	2.46	0.45
1:D:266:HIS:C	1:D:268:PRO:CD	2.85	0.45
1:D:313:PRO:O	1:D:316:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:735:ALA:HB1	1:D:742:VAL:HG21	1.99	0.45
1:E:541:THR:HA	1:E:544:ARG:HD2	1.97	0.45
1:F:99:SER:O	1:F:103:ARG:HG3	2.16	0.45
1:F:370:LEU:HD22	1:F:399:LEU:HD21	1.98	0.45
1:D:285:HIS:HB2	1:D:392:PRO:HG3	1.99	0.45
1:F:151:LEU:HB3	1:F:158:ILE:HD11	1.97	0.45
1:A:481:LYS:HZ1	1:B:263:ILE:HD12	1.82	0.45
1:B:367:VAL:O	1:B:371:LEU:HG	2.16	0.45
1:D:77:ASN:HB3	1:D:210:TYR:HA	1.99	0.45
1:E:621:LEU:N	1:E:621:LEU:CD2	2.73	0.45
1:E:621:LEU:CD2	1:E:621:LEU:H	2.24	0.45
1:E:624:ASP:C	1:E:626:ASP:N	2.69	0.45
1:C:70:THR:HG21	1:C:210:TYR:CE1	2.52	0.45
1:C:406:ASP:OD1	1:C:406:ASP:N	2.48	0.45
1:B:159:MET:HE3	1:B:212:SER:OG	2.17	0.45
1:B:773:ALA:O	1:B:777:GLY:N	2.42	0.45
1:D:182:ASP:HA	1:D:236:TYR:HE2	1.82	0.45
1:E:209:PHE:CD2	1:E:209:PHE:O	2.70	0.45
1:E:583:GLY:O	1:E:620:ALA:CB	2.62	0.45
1:F:533:GLN:O	1:F:537:GLU:N	2.34	0.45
1:C:271:PHE:HD2	1:C:278:PRO:HA	1.77	0.45
1:E:159:MET:HE2	1:E:214:PRO:HB3	1.99	0.45
1:E:614:PHE:HD2	1:E:656:VAL:CG1	2.20	0.45
1:D:619:ASP:HB3	1:D:665:ILE:CD1	2.47	0.44
1:E:209:PHE:O	1:E:209:PHE:CG	2.71	0.44
1:E:492:GLU:O	1:E:496:VAL:HG13	2.17	0.44
1:E:621:LEU:HD13	1:E:636:VAL:CG1	2.47	0.44
1:C:528:MET:SD	1:C:570:LEU:HD21	2.57	0.44
1:B:39:HIS:HE1	1:B:47:GLU:HB2	1.82	0.44
1:D:271:PHE:O	1:D:274:PHE:C	2.55	0.44
1:D:739:ASP:OD1	1:D:739:ASP:N	2.49	0.44
1:E:128:LYS:HG3	1:E:184:SER:HB3	1.99	0.44
1:F:39:HIS:NE2	1:F:47:GLU:HB2	2.33	0.44
1:F:338:GLN:HB3	1:F:339:PRO:HD3	1.99	0.44
1:C:242:LEU:HB3	1:C:298:VAL:HG22	1.99	0.44
1:D:251:ASP:HA	1:D:254:ILE:HG22	1.99	0.44
1:D:600:GLU:OE1	1:D:603:ARG:NE	2.46	0.44
1:E:624:ASP:OD2	1:E:629:SER:CB	2.49	0.44
1:E:624:ASP:C	1:E:625:ARG:CG	2.85	0.44
1:E:689:ARG:HG2	1:E:716:THR:HG22	1.98	0.44
1:F:308:LEU:HD22	1:F:330:ILE:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:528:MET:SD	1:C:570:LEU:HD11	2.57	0.44
1:B:505:GLU:OE2	1:C:397:PRO:HB3	2.17	0.44
1:D:576:ILE:HG22	1:D:611:SER:HA	2.00	0.44
1:E:71:VAL:O	1:E:79:ILE:N	2.51	0.44
1:E:150:LYS:NZ	1:E:166:ASN:HA	2.32	0.44
1:E:513:VAL:HG23	1:E:569:ALA:HA	1.99	0.44
1:E:689:ARG:HH22	1:E:720:SER:C	2.15	0.44
1:F:420:PHE:O	1:F:424:THR:HG23	2.17	0.44
1:F:460:LEU:HD12	1:F:498:ILE:HD13	2.00	0.44
1:F:609:ALA:HB1	1:F:610:PRO:HD2	1.98	0.44
1:A:435:HIS:CE1	1:A:437:LEU:HG	2.52	0.44
1:D:270:LEU:C	1:D:270:LEU:CD2	2.85	0.44
1:F:80:LEU:HD11	1:F:210:TYR:OH	2.17	0.44
1:F:335:ARG:NH1	1:F:377:MET:O	2.50	0.44
1:C:208:ASP:OD2	1:C:208:ASP:N	2.48	0.44
1:C:565:LEU:HA	1:C:568:LYS:HE3	1.99	0.44
1:C:680:TYR:HE1	1:C:769:TYR:HB3	1.83	0.44
1:A:349:SER:O	1:A:352:PRO:HD3	2.17	0.44
1:B:554:LEU:HD13	1:B:670:LEU:HD21	1.99	0.44
1:D:54:HIS:HB3	1:D:57:VAL:HG12	2.00	0.44
1:F:160:PRO:HB2	1:F:238:LEU:HD11	1.98	0.44
1:C:645:ASP:HB2	1:C:674:ARG:HG2	2.00	0.44
1:A:465:VAL:O	1:A:469:ILE:HG12	2.17	0.44
1:B:280:ARG:NH1	1:B:383:VAL:H	2.15	0.44
1:B:519:GLY:HA3	1:B:691:GLU:OE1	2.18	0.44
1:D:123:PRO:HG2	1:D:216:ILE:HD11	1.98	0.44
1:D:366:VAL:HA	1:D:369:THR:HG22	1.99	0.44
1:D:662:PRO:HB2	1:D:772:PHE:CZ	2.53	0.44
1:E:280:ARG:NH1	1:E:383:VAL:H	2.16	0.44
1:E:367:VAL:O	1:E:371:LEU:HG	2.17	0.44
1:E:463:GLU:HA	1:E:466:MET:HG3	2.00	0.44
1:E:564:THR:HG23	1:E:614:PHE:HE1	1.82	0.44
1:F:218:ARG:HB3	1:F:221:SER:OG	2.17	0.44
1:C:70:THR:HG22	1:C:80:LEU:HG	2.00	0.44
1:A:157:VAL:HG12	1:A:158:ILE:N	2.33	0.44
1:E:551:LYS:HE2	1:E:551:LYS:HB3	1.86	0.44
1:C:367:VAL:O	1:C:371:LEU:HG	2.18	0.44
1:C:436:VAL:O	1:C:436:VAL:HG13	2.18	0.44
1:B:606:ARG:NH2	1:B:648:GLU:OE1	2.50	0.44
1:D:532:ILE:HG13	1:D:533:GLN:HG3	2.00	0.44
1:E:84:ARG:HA	1:E:84:ARG:HD3	1.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:168:LYS:HG3	1:E:169:THR:H	1.82	0.44
1:E:250:LEU:HD21	1:E:411:ILE:HG23	1.99	0.44
1:E:435:HIS:C	1:E:437:LEU:HD22	2.38	0.44
1:F:73:LYS:HA	1:F:113:ARG:O	2.18	0.44
1:F:518:ILE:HD13	1:F:692:ILE:HD12	1.99	0.44
1:A:73:LYS:HE2	1:A:108:LEU:HA	2.00	0.43
1:A:263:ILE:CG2	1:A:264:PRO:HD3	2.48	0.43
1:A:481:LYS:HD2	1:B:270:LEU:HB3	2.00	0.43
1:B:126:ALA:N	1:B:216:ILE:O	2.46	0.43
1:E:265:LEU:HD23	1:E:382:LYS:HB3	2.00	0.43
1:F:711:GLU:OE1	1:F:715:ARG:NH1	2.41	0.43
1:B:79:ILE:C	1:B:80:LEU:HD23	2.38	0.43
1:B:567:ALA:HB2	1:B:614:PHE:CZ	2.49	0.43
1:D:693:LEU:HB3	1:D:709:LEU:HD11	2.00	0.43
1:E:423:LEU:HD12	1:E:427:PHE:CE2	2.53	0.43
1:E:435:HIS:ND1	1:E:437:LEU:CD2	2.80	0.43
1:E:624:ASP:C	1:E:626:ASP:H	2.13	0.43
1:C:431:SER:O	1:C:434:ARG:HB2	2.18	0.43
1:A:413:ILE:HG22	1:A:453:VAL:HG23	1.99	0.43
1:B:559:PRO:HB3	1:B:660:ASN:HD21	1.83	0.43
1:B:591:VAL:HG22	2:H:17:ALA:HB2	1.99	0.43
1:E:351:ALA:HB1	1:E:367:VAL:HG22	2.01	0.43
1:C:259:SER:O	1:C:263:ILE:HG12	2.19	0.43
1:A:263:ILE:HD11	1:F:469:ILE:HG21	2.00	0.43
1:B:51:ALA:H	1:B:84:ARG:HB3	1.84	0.43
1:B:406:ASP:OD1	1:B:406:ASP:N	2.50	0.43
1:D:102:ILE:HA	1:D:105:VAL:HG23	2.00	0.43
1:D:436:VAL:O	1:D:436:VAL:HG13	2.19	0.43
1:F:583:GLY:O	1:F:586:ILE:HG12	2.17	0.43
1:C:671:ARG:HE	1:C:674:ARG:NH1	2.15	0.43
1:A:157:VAL:HG11	1:A:215:PHE:O	2.19	0.43
1:E:660:ASN:O	1:E:769:TYR:OH	2.19	0.43
1:F:150:LYS:NZ	1:F:166:ASN:HD22	2.15	0.43
1:F:326:ALA:O	1:F:330:ILE:HG12	2.19	0.43
1:C:49:CYS:H	1:C:102:ILE:CD1	2.31	0.43
1:C:81:VAL:HG11	1:C:98:LEU:HD22	1.99	0.43
1:A:344:ILE:O	1:A:347:ILE:HD11	2.19	0.43
1:A:530:GLU:HG3	1:A:534:LEU:HD22	1.99	0.43
1:B:570:LEU:O	1:B:574:SER:OG	2.31	0.43
1:E:515:TRP:CZ2	1:E:570:LEU:HB2	2.54	0.43
1:F:45:GLY:O	1:F:154:ASP:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:265:LEU:HD12	1:F:382:LYS:HD3	2.00	0.43
1:F:422:ILE:O	1:F:426:GLN:HG3	2.18	0.43
1:F:438:ASP:O	1:F:442:ILE:HG13	2.19	0.43
1:F:450:HIS:HA	1:F:512:LYS:HE3	2.00	0.43
1:D:300:ALA:HB2	1:D:343:PHE:HE2	1.82	0.43
1:D:354:ARG:CZ	1:C:391:ARG:HH12	2.31	0.43
1:E:253:GLU:OE2	1:E:411:ILE:HG13	2.18	0.43
1:E:762:THR:HG23	1:E:764:GLU:HG2	2.01	0.43
1:F:611:SER:OG	1:F:612:ILE:N	2.52	0.43
1:F:651:LYS:HD2	1:F:651:LYS:O	2.19	0.43
1:C:267:GLN:N	1:C:268:PRO:CD	2.82	0.43
1:A:464:SER:O	1:A:468:THR:HG23	2.19	0.43
1:A:641:LEU:HA	1:A:674:ARG:NH2	2.34	0.43
1:B:132:GLY:HA2	1:B:227:SER:O	2.18	0.43
1:B:671:ARG:HE	1:B:674:ARG:NH2	2.17	0.43
1:E:445:ILE:CD1	1:E:491:VAL:CG1	2.79	0.43
1:E:448:LYS:HE2	1:E:492:GLU:OE2	2.19	0.43
1:E:583:GLY:CA	1:E:620:ALA:HB3	2.48	0.43
1:F:582:LYS:HG2	1:F:584:PRO:HD2	1.99	0.43
1:C:29:LYS:HG3	1:C:30:LEU:N	2.33	0.43
1:D:506:ILE:HD11	1:D:604:LYS:HD3	2.00	0.43
1:E:105:VAL:HG22	1:E:161:GLY:O	2.18	0.43
1:E:177:ASP:OD1	1:E:177:ASP:N	2.49	0.43
1:E:251:ASP:O	1:E:254:ILE:N	2.51	0.43
1:E:294:MET:O	1:E:298:VAL:HG23	2.19	0.43
1:F:161:GLY:O	1:F:179:VAL:HG13	2.18	0.43
1:A:161:GLY:HA2	1:A:179:VAL:HG13	2.01	0.43
1:A:427:PHE:HA	1:A:430:MET:HB3	2.01	0.43
1:A:450:HIS:ND1	1:A:575:GLY:HA2	2.34	0.43
1:B:300:ALA:HB2	1:B:343:PHE:CE2	2.54	0.43
1:B:562:SER:O	1:B:566:THR:HG23	2.19	0.43
1:B:746:GLU:HB2	1:B:749:HIS:CE1	2.54	0.43
1:D:406:ASP:OD1	1:D:406:ASP:N	2.51	0.43
1:F:247:VAL:O	1:F:425:LYS:NZ	2.49	0.43
1:F:285:HIS:CG	1:F:392:PRO:HG3	2.54	0.43
1:C:267:GLN:HG3	1:C:270:LEU:HD12	2.01	0.43
1:A:605:ALA:HB1	1:A:653:VAL:HG21	2.01	0.42
1:B:280:ARG:HH21	1:B:379:ALA:HA	1.83	0.42
1:B:588:ASN:HB3	1:B:593:GLU:HB3	2.01	0.42
1:E:371:LEU:HD22	1:E:404:ARG:HE	1.84	0.42
1:F:490:ASP:OD1	1:F:491:VAL:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:PHE:HD2	1:C:278:PRO:HB3	1.84	0.42
1:A:169:THR:HG21	1:A:176:ILE:HG12	2.01	0.42
1:A:287:PRO:O	1:A:290:THR:OG1	2.33	0.42
1:D:160:PRO:HG2	1:D:213:PRO:CG	2.48	0.42
1:D:445:ILE:HD13	1:D:491:VAL:HG11	2.00	0.42
1:D:453:VAL:H	1:D:456:ASP:HB2	1.83	0.42
1:E:265:LEU:HD21	1:E:384:VAL:HG22	2.01	0.42
1:C:324:GLU:HB2	1:C:328:ARG:HH21	1.84	0.42
1:C:499:ARG:HG3	1:C:500:PRO:HD2	2.01	0.42
1:C:519:GLY:O	3:C:802:ATP:N6	2.49	0.42
1:A:583:GLY:O	1:A:586:ILE:HG12	2.20	0.42
1:D:159:MET:CG	1:D:212:SER:OG	2.66	0.42
1:D:343:PHE:HD1	1:D:386:ILE:HB	1.83	0.42
1:E:435:HIS:CG	1:E:435:HIS:O	2.72	0.42
1:F:71:VAL:O	1:F:79:ILE:HG22	2.18	0.42
1:A:280:ARG:O	1:A:385:VAL:N	2.47	0.42
1:B:600:GLU:OE2	1:B:603:ARG:NH1	2.53	0.42
1:E:61:LEU:HB3	1:E:63:ILE:HG12	2.01	0.42
1:E:133:SER:OG	1:E:177:ASP:O	2.23	0.42
1:E:443:LYS:HE3	1:E:443:LYS:HB2	1.89	0.42
1:E:611:SER:O	1:E:653:VAL:HA	2.20	0.42
1:F:36:THR:HB	1:F:114:LEU:HD11	2.02	0.42
1:C:167:LEU:O	1:C:175:SER:HB2	2.20	0.42
1:A:604:LYS:HA	1:A:604:LYS:HD3	1.74	0.42
1:B:110:LEU:O	1:B:307:VAL:HG22	2.19	0.42
1:B:712:LEU:O	1:B:716:THR:HG22	2.19	0.42
1:E:515:TRP:CZ2	1:E:529:LYS:HE2	2.55	0.42
1:E:561:CYS:N	3:E:802:ATP:O2B	2.52	0.42
1:E:585:GLU:HA	1:F:635:HIS:CD2	2.54	0.42
1:C:80:LEU:HD11	1:C:210:TYR:CE1	2.54	0.42
1:C:452:TYR:CE1	1:C:500:PRO:HG3	2.54	0.42
1:C:647:VAL:HG13	1:C:648:GLU:HG3	2.01	0.42
1:A:399:LEU:O	1:A:405:PHE:HB2	2.19	0.42
1:A:441:ALA:O	1:A:445:ILE:HG12	2.19	0.42
1:B:79:ILE:HG13	1:B:209:PHE:C	2.39	0.42
1:D:244:TYR:CE2	1:D:302:THR:HG21	2.55	0.42
1:D:347:ILE:HG22	1:D:389:THR:HB	2.02	0.42
1:E:89:GLU:O	1:E:90:VAL:HG22	2.20	0.42
1:E:250:LEU:O	1:E:254:ILE:N	2.52	0.42
1:E:766:LEU:O	1:E:770:GLU:HG2	2.20	0.42
1:F:131:VAL:HA	1:F:180:ILE:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:VAL:O	1:C:150:LYS:HB3	2.20	0.42
1:A:134:LEU:HA	1:A:230:THR:OG1	2.20	0.42
1:A:264:PRO:O	1:A:268:PRO:HG3	2.19	0.42
1:A:349:SER:C	1:A:352:PRO:HD3	2.40	0.42
1:A:559:PRO:HB2	1:B:671:ARG:HG2	2.01	0.42
1:D:104:SER:OG	1:D:163:ILE:HD13	2.18	0.42
1:D:279:PRO:HD3	1:C:462:ARG:HD3	2.01	0.42
1:E:434:ARG:NH2	1:E:482:PHE:HD1	2.18	0.42
1:E:744:LYS:NZ	1:E:746:GLU:HA	2.35	0.42
1:A:306:HIS:HB3	1:A:340:SER:HA	2.01	0.42
1:A:618:ILE:HG21	1:A:657:ALA:CB	2.45	0.42
1:B:91:HIS:CD2	1:B:95:VAL:HG13	2.55	0.42
1:D:49:CYS:O	1:D:82:ILE:HG12	2.20	0.42
1:D:218:ARG:HB3	1:D:221:SER:OG	2.19	0.42
1:F:312:GLY:O	1:F:316:VAL:HG12	2.20	0.42
1:A:614:PHE:CE1	1:A:656:VAL:CB	3.02	0.42
1:A:736:ILE:HA	1:A:740:LEU:O	2.20	0.42
1:B:338:GLN:HB3	1:B:339:PRO:CD	2.50	0.42
1:B:650:LEU:HB3	1:B:653:VAL:HG22	2.02	0.42
1:E:348:ASP:N	1:E:348:ASP:OD1	2.48	0.42
1:E:463:GLU:HB3	1:E:494:ALA:HB1	2.02	0.42
1:F:139:ILE:HG23	1:F:226:PHE:HE2	1.85	0.42
1:F:438:ASP:H	1:F:441:ALA:HB3	1.84	0.42
1:F:554:LEU:HD22	1:F:665:ILE:HD12	2.02	0.42
1:C:81:VAL:HG12	1:C:81:VAL:O	2.19	0.42
1:C:711:GLU:OE2	1:C:715:ARG:HD2	2.20	0.42
1:A:291:GLY:N	3:A:801:ATP:O2B	2.53	0.42
1:A:402:PRO:HG2	1:F:459:ALA:HB2	2.02	0.42
1:B:212:SER:HA	1:B:213:PRO:HD2	1.94	0.42
1:D:551:LYS:HE2	1:D:551:LYS:HB3	1.80	0.42
1:E:47:GLU:HG2	1:E:48:THR:N	2.35	0.42
1:C:347:ILE:HG23	1:C:348:ASP:N	2.35	0.42
1:A:359:SER:O	1:A:363:GLU:HB2	2.20	0.41
1:A:467:LYS:O	1:A:471:ARG:HG3	2.19	0.41
1:D:280:ARG:NH1	1:D:374:MET:O	2.53	0.41
1:D:699:LYS:HD3	1:D:699:LYS:HA	1.72	0.41
1:E:168:LYS:HD2	1:E:168:LYS:HA	1.88	0.41
1:F:100:THR:HA	1:F:103:ARG:HE	1.85	0.41
1:F:280:ARG:NH2	1:F:381:GLY:O	2.40	0.41
1:C:79:ILE:HD13	1:C:211:LEU:HG	1.96	0.41
1:A:348:ASP:OD2	1:A:391:ARG:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:TYR:CE1	1:A:500:PRO:HG2	2.55	0.41
1:B:77:ASN:CG	1:B:209:PHE:O	2.50	0.41
1:D:672:PRO:HA	1:D:676:ASP:HB3	2.01	0.41
1:E:39:HIS:CE1	1:E:99:SER:HG	2.38	0.41
1:E:671:ARG:HE	1:E:674:ARG:CZ	2.33	0.41
1:E:755:LYS:HA	1:E:755:LYS:HD3	1.88	0.41
1:F:82:ILE:HD12	1:F:82:ILE:H	1.85	0.41
1:C:183:ALA:HB3	1:C:215:PHE:CD2	2.55	0.41
1:C:693:LEU:O	1:C:697:THR:OG1	2.24	0.41
1:A:344:ILE:C	1:A:347:ILE:CD1	2.83	0.41
1:A:757:ILE:HG22	1:A:759:ARG:H	1.85	0.41
1:D:542:PHE:CZ	1:C:736:ILE:HD11	2.55	0.41
1:E:251:ASP:HA	1:E:254:ILE:HG22	2.02	0.41
1:E:354:ARG:HD2	1:E:367:VAL:HG11	2.01	0.41
1:F:47:GLU:HG3	1:F:48:THR:HG23	2.02	0.41
1:A:73:LYS:HB2	1:A:76:GLU:HB2	2.01	0.41
1:B:616:ASP:CG	1:C:642:ASN:HD21	2.24	0.41
1:D:315:ILE:HG23	1:D:326:ALA:HB3	2.03	0.41
1:D:406:ASP:OD2	1:C:462:ARG:NH1	2.53	0.41
1:D:567:ALA:HB2	1:D:614:PHE:CE1	2.56	0.41
1:D:615:PHE:HE2	1:D:655:ILE:CD1	2.34	0.41
1:E:680:TYR:HE1	1:E:769:TYR:HB3	1.84	0.41
1:F:52:TYR:HB2	1:F:97:THR:OG1	2.20	0.41
1:F:367:VAL:O	1:F:371:LEU:HG	2.20	0.41
1:F:701:ASN:HD21	1:F:744:LYS:CB	2.32	0.41
1:C:134:LEU:HB3	1:C:177:ASP:HB2	2.03	0.41
1:A:125:TYR:HA	1:A:216:ILE:HB	2.03	0.41
1:B:595:GLU:OE2	1:B:635:HIS:HB3	2.21	0.41
1:F:146:LYS:O	1:F:150:LYS:N	2.51	0.41
1:C:570:LEU:O	1:C:574:SER:OG	2.26	0.41
1:B:139:ILE:O	1:B:139:ILE:HG22	2.21	0.41
1:D:369:THR:O	1:D:373:LEU:HD23	2.20	0.41
1:D:527:LYS:O	1:D:531:MET:HG2	2.21	0.41
1:E:208:ASP:HA	1:E:210:TYR:CD2	2.55	0.41
1:F:287:PRO:CB	1:F:453:VAL:HG11	2.50	0.41
1:F:311:ASN:C	1:F:313:PRO:HD2	2.41	0.41
1:C:555:LEU:HD23	1:C:679:ILE:HB	2.03	0.41
1:C:586:ILE:HD11	1:C:621:LEU:HD11	2.01	0.41
1:A:305:ALA:HB1	1:A:339:PRO:HB2	2.02	0.41
1:B:70:THR:OG1	1:B:117:LYS:HB3	2.19	0.41
1:D:168:LYS:O	1:D:169:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:ILE:HG22	1:D:217:PHE:N	2.36	0.41
1:E:467:LYS:HE3	1:E:493:SER:O	2.20	0.41
1:E:531:MET:HE1	1:E:677:ARG:HG3	2.03	0.41
1:E:738:GLU:OE2	1:E:748:ARG:NH1	2.46	0.41
1:F:49:CYS:HB2	1:F:155:SER:HB2	2.02	0.41
1:F:703:GLU:HG2	1:F:704:GLU:N	2.34	0.41
1:C:725:VAL:HG21	3:C:802:ATP:H1'	2.03	0.41
1:A:233:ASN:ND2	1:A:235:LYS:HG2	2.35	0.41
1:B:466:MET:SD	1:C:271:PHE:CE1	3.14	0.41
1:E:39:HIS:CG	1:E:99:SER:HG	2.39	0.41
1:E:583:GLY:O	1:E:620:ALA:HB3	2.20	0.41
1:F:132:GLY:N	1:F:179:VAL:O	2.29	0.41
1:F:693:LEU:HB3	1:F:709:LEU:HD12	2.02	0.41
1:B:48:THR:HG21	1:B:154:ASP:OD2	2.21	0.41
1:B:225:THR:O	1:B:225:THR:OG1	2.36	0.41
1:B:518:ILE:O	1:B:525:LYS:NZ	2.32	0.41
1:D:271:PHE:HB3	1:D:276:VAL:O	2.21	0.41
1:D:564:THR:HB	3:D:802:ATP:O2A	2.20	0.41
1:D:618:ILE:HG22	1:D:659:THR:HB	2.03	0.41
1:E:138:ASN:HA	1:E:226:PHE:HE2	1.86	0.41
1:E:159:MET:HB2	1:E:162:MET:HE3	2.03	0.41
1:E:348:ASP:OD1	1:E:349:SER:N	2.53	0.41
1:E:562:SER:N	3:E:802:ATP:O2B	2.53	0.41
1:E:699:LYS:HA	1:E:699:LYS:HD3	1.71	0.41
1:F:37:ARG:HH11	1:F:38:PRO:HD2	1.86	0.41
1:F:285:HIS:HB3	1:F:389:THR:HG23	2.03	0.41
1:F:632:ALA:O	1:F:633:ALA:C	2.59	0.41
1:C:134:LEU:O	1:C:230:THR:OG1	2.30	0.41
1:C:160:PRO:HG2	1:C:213:PRO:HD2	2.02	0.41
1:C:576:ILE:HG22	1:C:611:SER:HA	2.03	0.41
1:A:350:ILE:O	1:A:363:GLU:CD	2.59	0.41
1:B:39:HIS:CE1	1:B:47:GLU:HB2	2.56	0.41
1:B:102:ILE:O	1:B:105:VAL:HG12	2.21	0.41
1:B:521:GLN:H	1:B:521:GLN:CD	2.23	0.41
1:D:354:ARG:HH22	1:C:390:ASN:HD21	1.69	0.41
1:D:430:MET:O	1:D:431:SER:OG	2.32	0.41
1:E:551:LYS:HD2	1:E:650:LEU:HD23	2.03	0.41
1:E:689:ARG:HE	1:E:716:THR:C	2.24	0.41
1:F:47:GLU:O	1:F:99:SER:HB2	2.20	0.41
1:F:287:PRO:HA	1:F:288:PRO:HD3	1.93	0.41
1:C:570:LEU:O	1:C:574:SER:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ILE:HG13	1:A:180:ILE:HG21	2.02	0.40
1:A:211:LEU:HD22	1:A:212:SER:H	1.87	0.40
1:B:445:ILE:O	1:B:449:THR:HG23	2.21	0.40
1:D:770:GLU:HG3	1:D:774:LEU:HD23	2.03	0.40
1:E:57:VAL:HG21	1:E:93:VAL:HG13	2.02	0.40
1:F:47:GLU:HG3	1:F:48:THR:N	2.36	0.40
1:F:601:ILE:HD12	1:F:601:ILE:HA	1.92	0.40
1:C:77:ASN:HB3	1:C:211:LEU:N	2.36	0.40
1:B:251:ASP:O	1:B:254:ILE:HG22	2.21	0.40
1:B:306:HIS:O	1:B:341:ILE:N	2.48	0.40
1:B:314:SER:OG	1:C:328:ARG:NH1	2.54	0.40
1:B:370:LEU:HD23	1:B:399:LEU:HD11	2.03	0.40
1:E:437:LEU:H	1:E:437:LEU:HD22	1.84	0.40
1:E:619:ASP:OD2	1:E:664:GLU:OE2	2.37	0.40
1:A:133:SER:HA	1:A:177:ASP:O	2.22	0.40
1:A:291:GLY:O	1:A:294:MET:HG2	2.21	0.40
1:A:296:LEU:CD2	1:A:345:ASP:OD1	2.69	0.40
1:E:556:TYR:HE1	1:E:678:HIS:HB3	1.85	0.40
1:E:722:ALA:HB2	3:E:802:ATP:H5'1	2.03	0.40
1:F:618:ILE:HG22	1:F:659:THR:HB	2.04	0.40
1:A:134:LEU:HD13	1:A:177:ASP:HB3	2.03	0.40
1:A:348:ASP:HB2	1:A:394:SER:HB2	2.02	0.40
1:A:401:ARG:HD3	1:A:401:ARG:HA	1.85	0.40
1:A:452:TYR:CE2	1:A:498:ILE:HD11	2.56	0.40
1:F:289:GLY:O	1:F:455:ALA:HA	2.21	0.40
1:F:465:VAL:O	1:F:469:ILE:HG12	2.21	0.40
1:C:128:LYS:HG3	1:C:184:SER:HB3	2.04	0.40
1:C:512:LYS:HE2	1:C:512:LYS:HB2	1.88	0.40
1:A:752:LYS:O	1:A:755:LYS:HG2	2.21	0.40
1:B:162:MET:O	1:B:179:VAL:HA	2.21	0.40
1:B:311:ASN:HD22	1:C:377:MET:HG2	1.85	0.40
1:D:154:ASP:OD1	1:D:155:SER:N	2.55	0.40
1:E:46:LYS:HB3	1:E:50:THR:HG21	2.02	0.40
1:F:501:SER:HA	1:F:504:ARG:HG3	2.04	0.40
1:F:641:LEU:HD11	1:F:674:ARG:NH1	2.36	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	723/727 (99%)	673 (93%)	46 (6%)	4 (1%)	25	25
1	B	723/727 (99%)	676 (94%)	41 (6%)	6 (1%)	19	19
1	C	723/727 (99%)	668 (92%)	51 (7%)	4 (1%)	25	25
1	D	723/727 (99%)	678 (94%)	43 (6%)	2 (0%)	41	41
1	E	723/727 (99%)	668 (92%)	52 (7%)	3 (0%)	34	34
1	F	719/727 (99%)	670 (93%)	47 (6%)	2 (0%)	41	41
2	H	21/23 (91%)	19 (90%)	2 (10%)	0	100	100
All	All	4355/4385 (99%)	4052 (93%)	282 (6%)	21 (0%)	32	29

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	338	GLN
1	B	439	SER
1	B	647	VAL
1	D	609	ALA
1	E	609	ALA
1	E	620	ALA
1	F	609	ALA
1	B	609	ALA
1	D	82	ILE
1	F	499	ARG
1	C	82	ILE
1	C	609	ALA
1	B	212	SER
1	C	74	ILE
1	A	139	ILE
1	C	229	GLU
1	A	433	ASP
1	B	74	ILE

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Mol	Chain	Res	Type
1	A	681	VAL
1	E	90	VAL
1	A	761	ILE

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	612/612 (100%)	609 (100%)	3 (0%)	88	88
1	B	612/612 (100%)	605 (99%)	7 (1%)	73	73
1	C	612/612 (100%)	608 (99%)	4 (1%)	84	84
1	D	612/612 (100%)	605 (99%)	7 (1%)	73	73
1	E	612/612 (100%)	606 (99%)	6 (1%)	76	76
1	F	610/612 (100%)	607 (100%)	3 (0%)	88	88
All	All	3670/3672 (100%)	3640 (99%)	30 (1%)	82	81

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	LEU
1	A	440	GLU
1	A	616	ASP
1	B	210	TYR
1	B	211	LEU
1	B	271	PHE
1	B	347	ILE
1	B	438	ASP
1	B	551	LYS
1	B	625	ARG
1	D	208	ASP
1	D	209	PHE
1	D	210	TYR
1	D	211	LEU
1	D	270	LEU

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Mol	Chain	Res	Type
1	D	438	ASP
1	D	617	GLN
1	E	437	LEU
1	E	440	GLU
1	E	617	GLN
1	E	618	ILE
1	E	621	LEU
1	E	775	ARG
1	F	209	PHE
1	F	234	ARG
1	F	599	ARG
1	C	209	PHE
1	C	267	GLN
1	C	271	PHE
1	C	365	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	435	HIS
1	F	166	ASN
1	F	450	HIS
1	F	701	ASN
1	C	77	ASN

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

11 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	$\#\|Z\| > 2$
3	ATP	E	802	1	26,33,33	0.60	0	31,52,52	0.77	2 (6%)
3	ATP	D	801	-	26,33,33	0.62	0	31,52,52	0.78	2 (6%)
3	ATP	A	802	1	26,33,33	0.61	0	31,52,52	0.74	2 (6%)
3	ATP	C	801	-	26,33,33	0.61	0	31,52,52	0.75	2 (6%)
3	ATP	A	801	1	26,33,33	0.61	0	31,52,52	0.76	2 (6%)
3	ATP	F	802	1	26,33,33	0.62	0	31,52,52	0.73	2 (6%)
3	ATP	B	801	-	26,33,33	0.62	0	31,52,52	0.77	2 (6%)
3	ATP	D	802	1	26,33,33	0.62	0	31,52,52	0.77	2 (6%)
3	ATP	C	802	-	26,33,33	0.63	0	31,52,52	0.75	2 (6%)
3	ATP	B	802	1	26,33,33	0.60	0	31,52,52	0.76	2 (6%)
3	ATP	E	801	-	26,33,33	0.61	0	31,52,52	0.76	2 (6%)

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
3	ATP	E	802	1	-	4/18/38/38	0/3/3/3
3	ATP	D	801	-	-	6/18/38/38	0/3/3/3
3	ATP	A	802	1	-	3/18/38/38	0/3/3/3
3	ATP	C	801	-	-	3/18/38/38	0/3/3/3
3	ATP	A	801	1	-	6/18/38/38	0/3/3/3
3	ATP	F	802	1	-	5/18/38/38	0/3/3/3
3	ATP	B	801	-	-	3/18/38/38	0/3/3/3
3	ATP	D	802	1	-	8/18/38/38	0/3/3/3
3	ATP	C	802	-	-	5/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	802	1	-	6/18/38/38	0/3/3/3
3	ATP	E	801	-	-	4/18/38/38	0/3/3/3

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	802	ATP	C5-C6-N6	2.34	123.91	120.35
3	C	801	ATP	C5-C6-N6	2.32	123.88	120.35
3	E	801	ATP	C5-C6-N6	2.32	123.88	120.35
3	A	802	ATP	C5-C6-N6	2.32	123.87	120.35
3	D	801	ATP	C5-C6-N6	2.31	123.86	120.35
3	D	802	ATP	C5-C6-N6	2.30	123.85	120.35
3	C	802	ATP	C5-C6-N6	2.30	123.84	120.35
3	B	801	ATP	C5-C6-N6	2.29	123.84	120.35
3	B	802	ATP	C5-C6-N6	2.28	123.82	120.35
3	A	801	ATP	C5-C6-N6	2.28	123.82	120.35
3	F	802	ATP	C5-C6-N6	2.20	123.70	120.35
3	B	802	ATP	PB-O3B-PG	2.08	139.96	132.83
3	E	801	ATP	PB-O3B-PG	2.05	139.86	132.83
3	C	801	ATP	PB-O3B-PG	2.04	139.84	132.83
3	A	802	ATP	PB-O3B-PG	2.04	139.81	132.83
3	A	801	ATP	PB-O3B-PG	2.03	139.79	132.83
3	C	802	ATP	PB-O3B-PG	2.03	139.78	132.83
3	E	802	ATP	PB-O3B-PG	2.02	139.77	132.83
3	F	802	ATP	PB-O3B-PG	2.02	139.75	132.83
3	B	801	ATP	PB-O3B-PG	2.01	139.74	132.83
3	D	801	ATP	PB-O3B-PG	2.01	139.73	132.83
3	D	802	ATP	PB-O3B-PG	2.00	139.69	132.83

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	ATP	C5'-O5'-PA-O2A
3	B	801	ATP	C5'-O5'-PA-O2A
3	B	802	ATP	PB-O3B-PG-O3G
3	B	802	ATP	C5'-O5'-PA-O2A
3	D	801	ATP	PB-O3B-PG-O2G
3	D	801	ATP	C5'-O5'-PA-O1A
3	D	801	ATP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
3	D	802	ATP	PB-O3B-PG-O2G
3	D	802	ATP	PB-O3B-PG-O3G
3	D	802	ATP	C5'-O5'-PA-O2A
3	E	801	ATP	C5'-O5'-PA-O1A
3	E	801	ATP	C5'-O5'-PA-O2A
3	E	802	ATP	PB-O3B-PG-O2G
3	F	802	ATP	PB-O3B-PG-O3G
3	F	802	ATP	C5'-O5'-PA-O2A
3	C	801	ATP	C5'-O5'-PA-O2A
3	C	802	ATP	PB-O3B-PG-O2G
3	C	802	ATP	C5'-O5'-PA-O2A
3	A	801	ATP	O4'-C4'-C5'-O5'
3	A	802	ATP	O4'-C4'-C5'-O5'
3	A	802	ATP	C3'-C4'-C5'-O5'
3	A	801	ATP	C3'-C4'-C5'-O5'
3	A	801	ATP	C5'-O5'-PA-O3A
3	B	801	ATP	C5'-O5'-PA-O3A
3	B	802	ATP	C5'-O5'-PA-O3A
3	D	801	ATP	C5'-O5'-PA-O3A
3	D	802	ATP	C5'-O5'-PA-O3A
3	E	801	ATP	C5'-O5'-PA-O3A
3	F	802	ATP	C5'-O5'-PA-O3A
3	C	801	ATP	C5'-O5'-PA-O3A
3	C	802	ATP	C5'-O5'-PA-O3A
3	D	802	ATP	PA-O3A-PB-O1B
3	A	801	ATP	C5'-O5'-PA-O1A
3	B	801	ATP	C5'-O5'-PA-O1A
3	B	802	ATP	C5'-O5'-PA-O1A
3	D	802	ATP	C5'-O5'-PA-O1A
3	F	802	ATP	C5'-O5'-PA-O1A
3	C	801	ATP	C5'-O5'-PA-O1A
3	C	802	ATP	C5'-O5'-PA-O1A
3	D	802	ATP	O4'-C4'-C5'-O5'
3	D	801	ATP	PB-O3B-PG-O1G
3	A	802	ATP	C4'-C5'-O5'-PA
3	D	801	ATP	C4'-C5'-O5'-PA
3	E	802	ATP	C4'-C5'-O5'-PA
3	E	801	ATP	PB-O3B-PG-O1G
3	E	802	ATP	PB-O3B-PG-O1G
3	C	802	ATP	PB-O3B-PG-O1G
3	B	802	ATP	PB-O3B-PG-O2G
3	F	802	ATP	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
3	D	802	ATP	C3'-C4'-C5'-O5'
3	A	801	ATP	PB-O3A-PA-O2A
3	E	802	ATP	C5'-O5'-PA-O1A
3	B	802	ATP	PB-O3B-PG-O1G

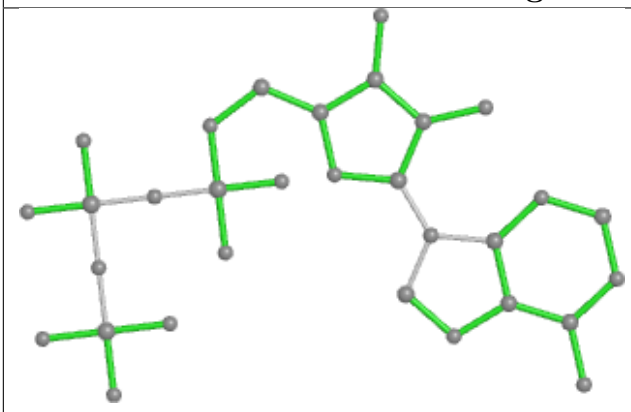
There are no ring outliers.

7 monomers are involved in 16 short contacts:

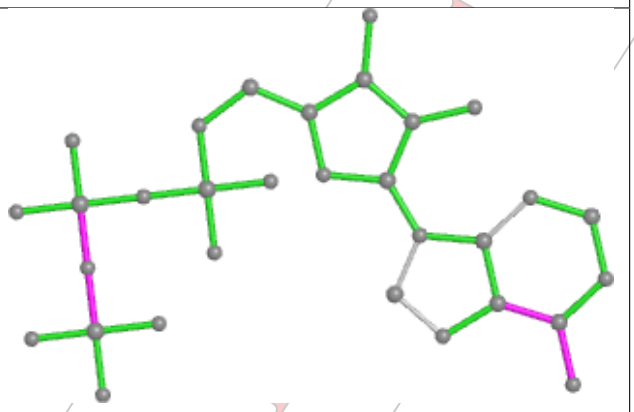
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	802	ATP	4	0
3	D	801	ATP	1	0
3	A	802	ATP	2	0
3	C	801	ATP	1	0
3	A	801	ATP	3	0
3	D	802	ATP	2	0
3	C	802	ATP	3	0

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.

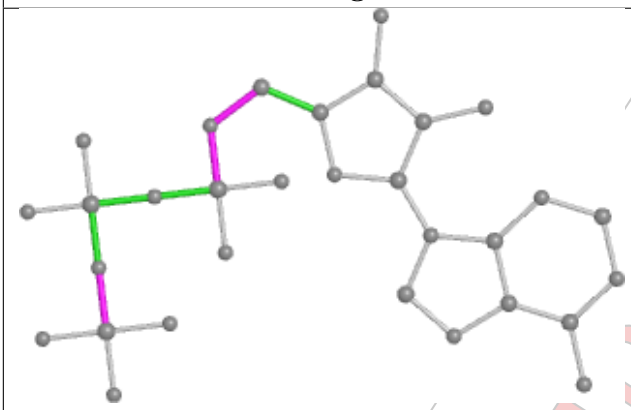
Ligand ATP E 802



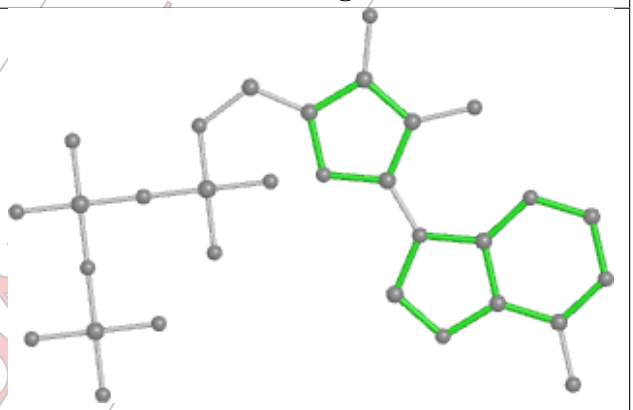
Bond lengths



Bond angles

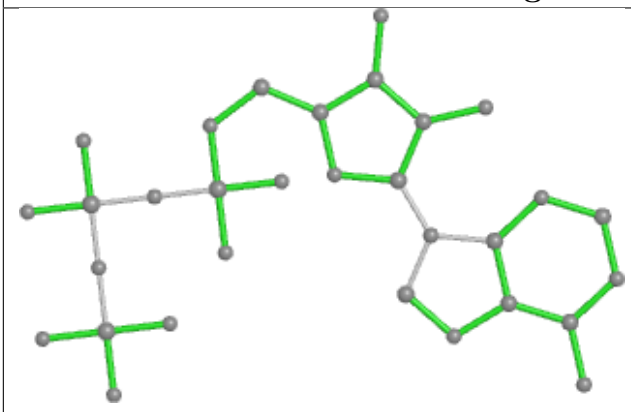


Torsions

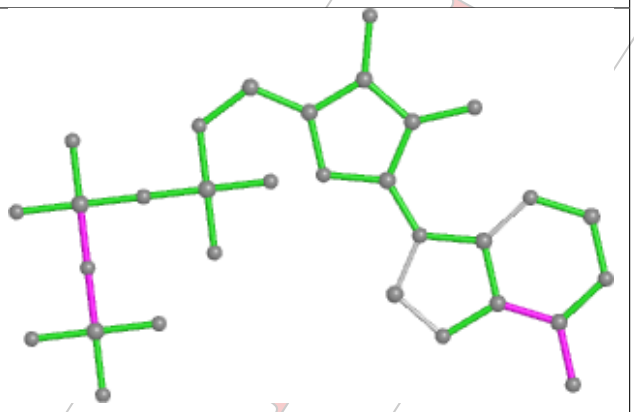


Rings

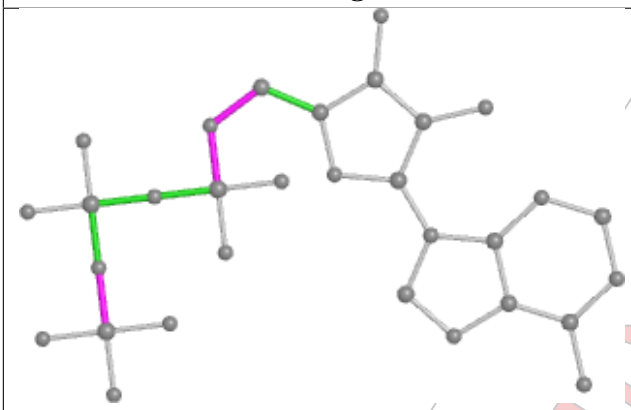
Ligand ATP D 801



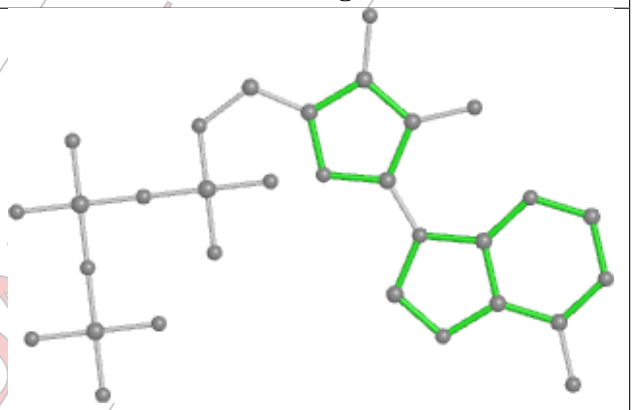
Bond lengths



Bond angles

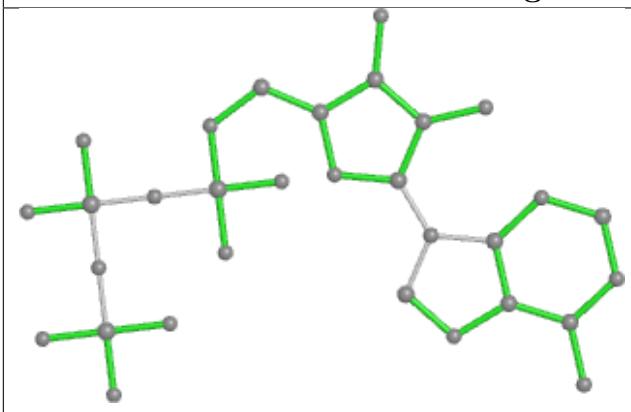


Torsions

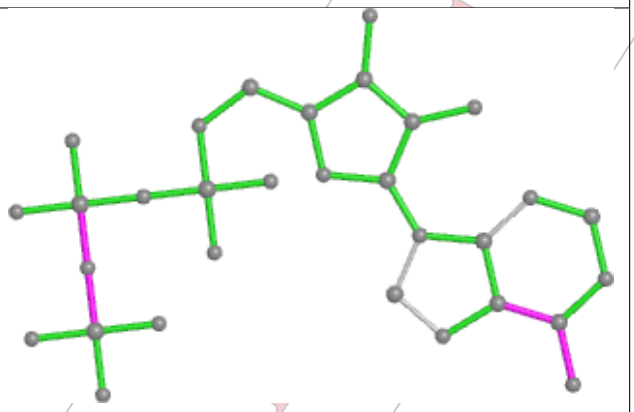


Rings

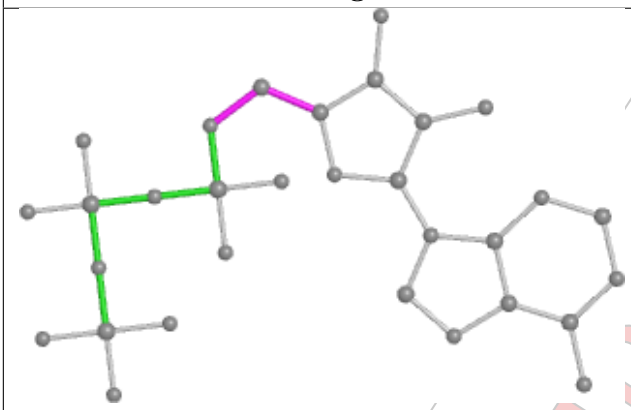
Ligand ATP A 802



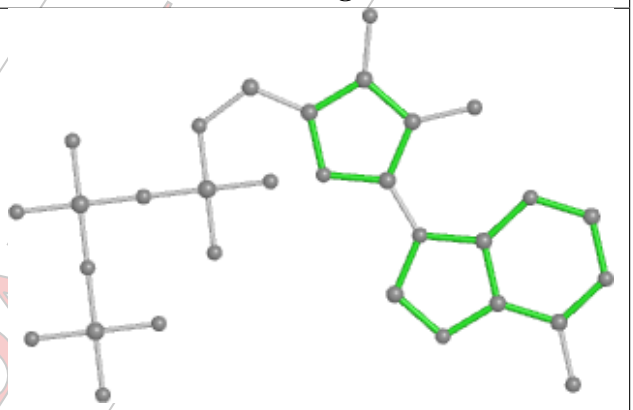
Bond lengths



Bond angles

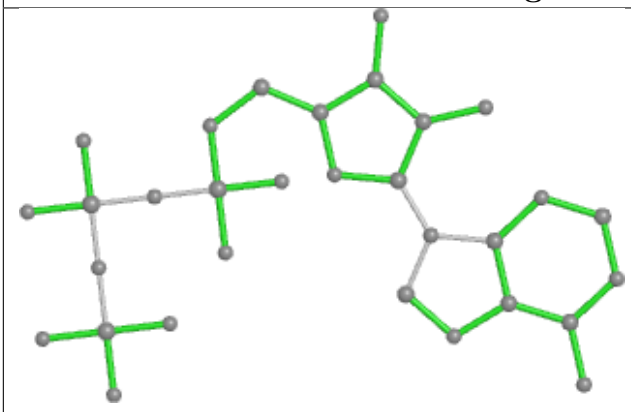


Torsions

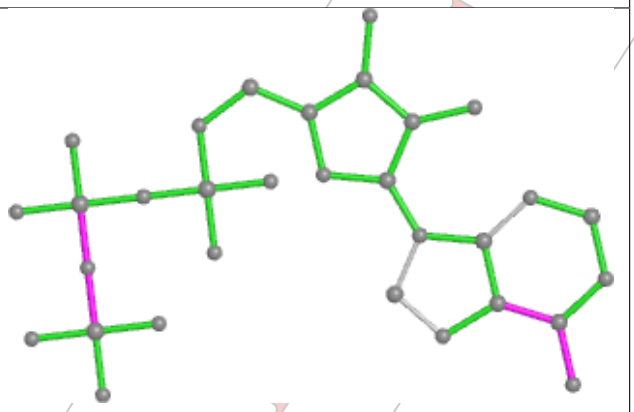


Rings

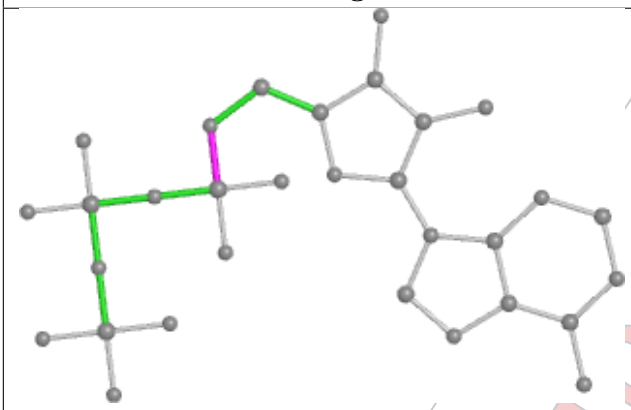
Ligand ATP C 801



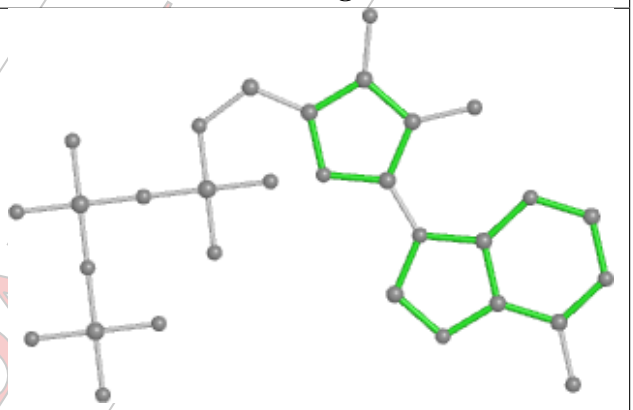
Bond lengths



Bond angles

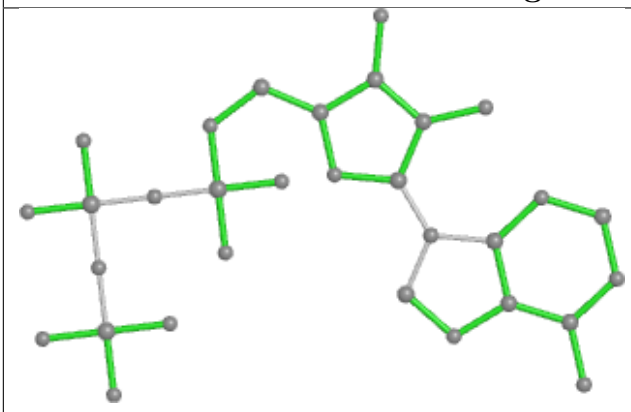


Torsions

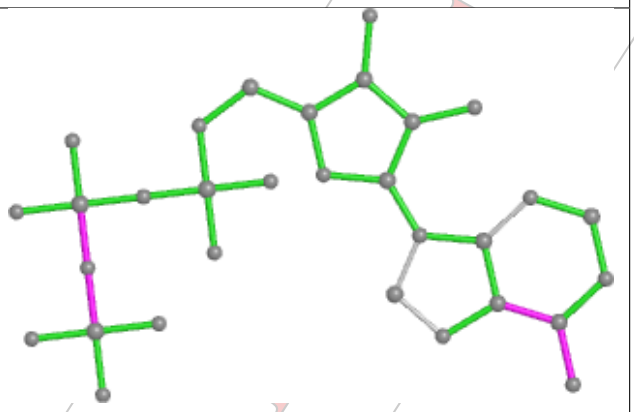


Rings

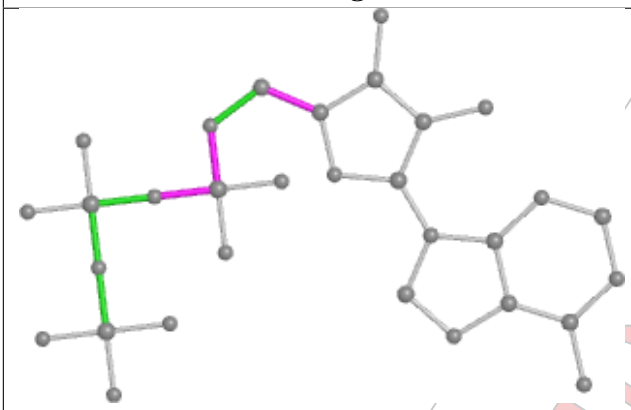
Ligand ATP A 801



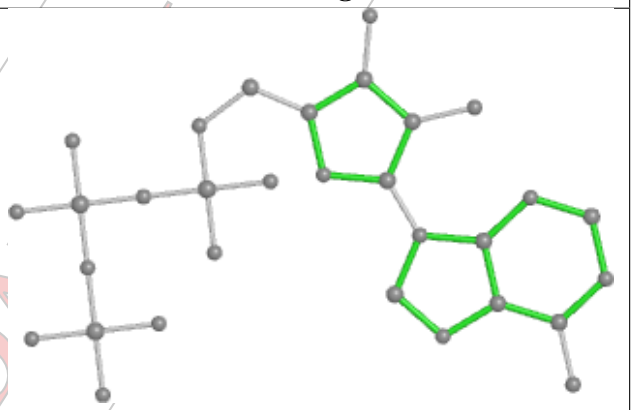
Bond lengths



Bond angles

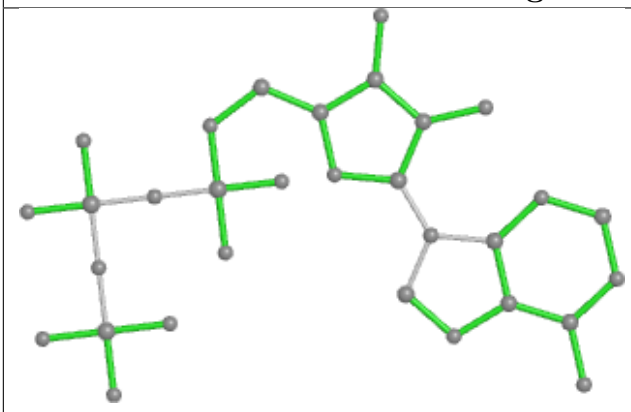


Torsions

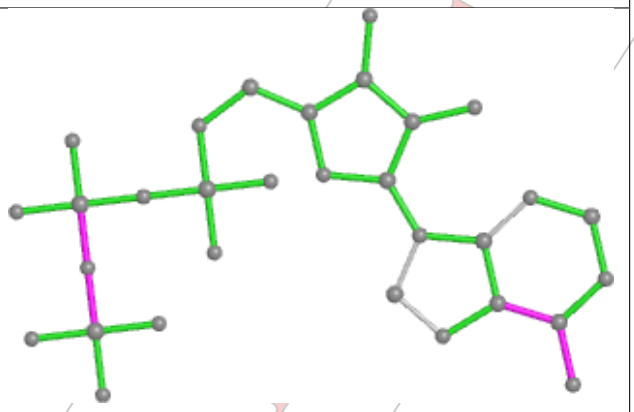


Rings

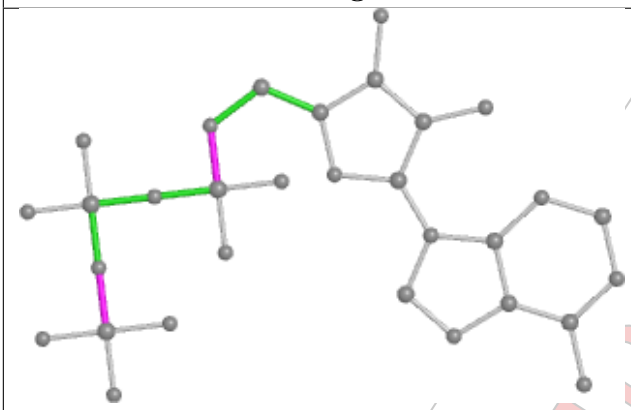
Ligand ATP F 802



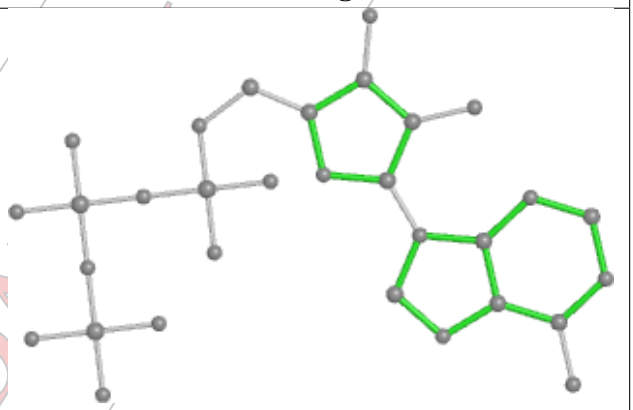
Bond lengths



Bond angles

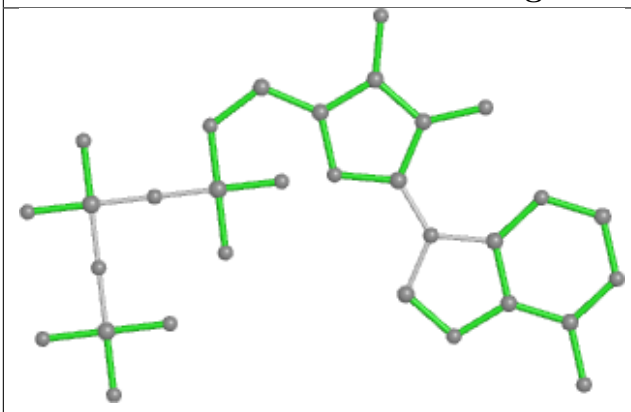


Torsions

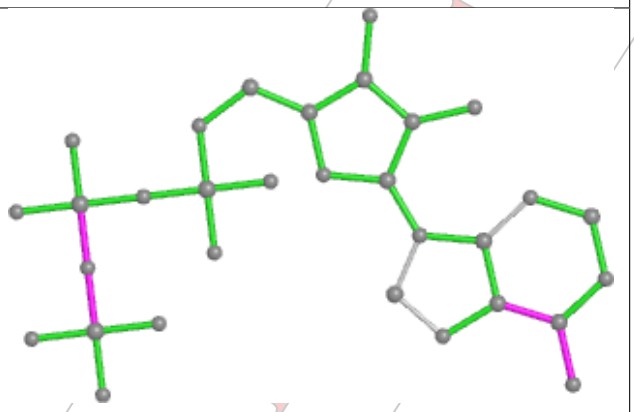


Rings

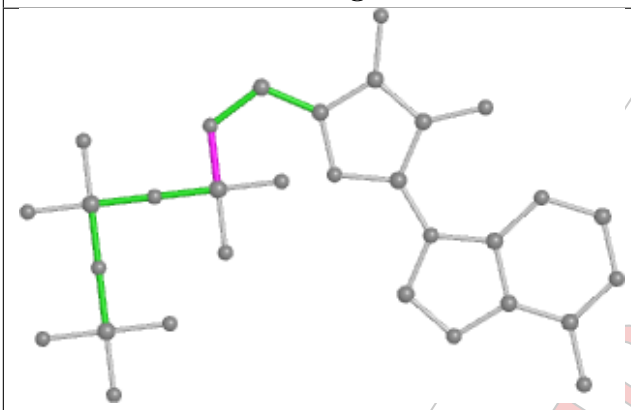
Ligand ATP B 801



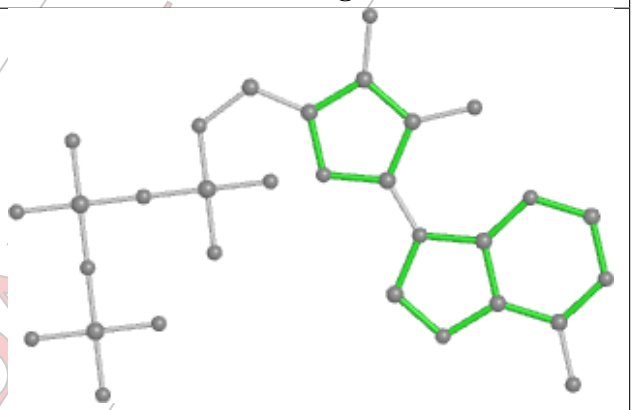
Bond lengths



Bond angles

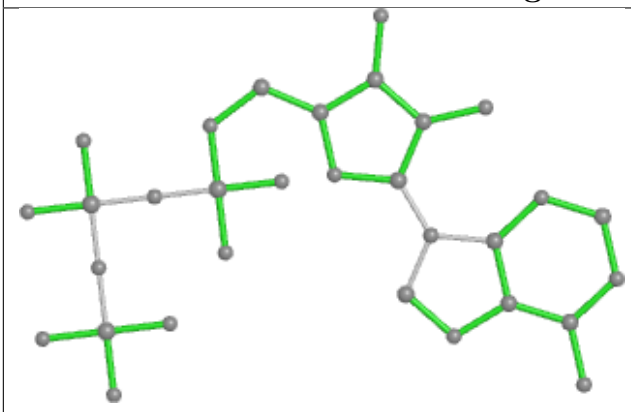


Torsions

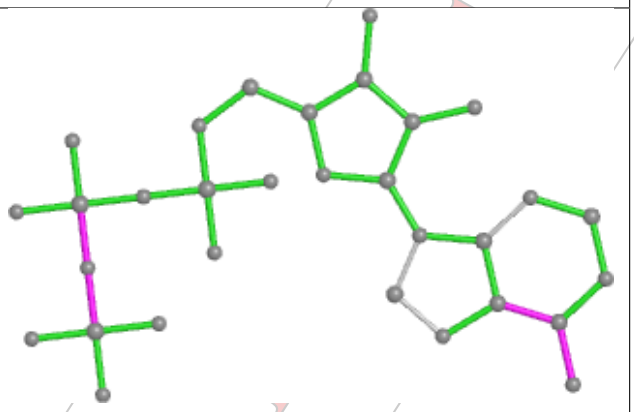


Rings

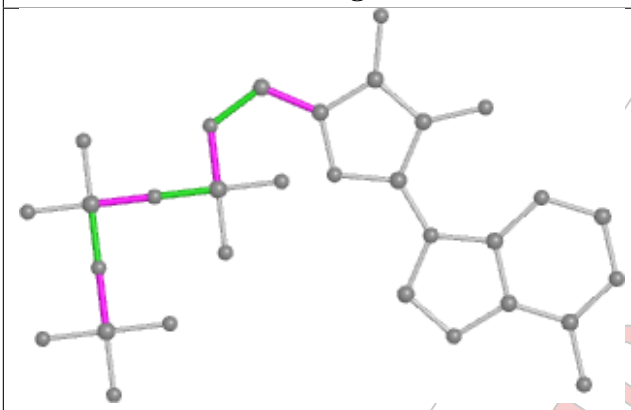
Ligand ATP D 802



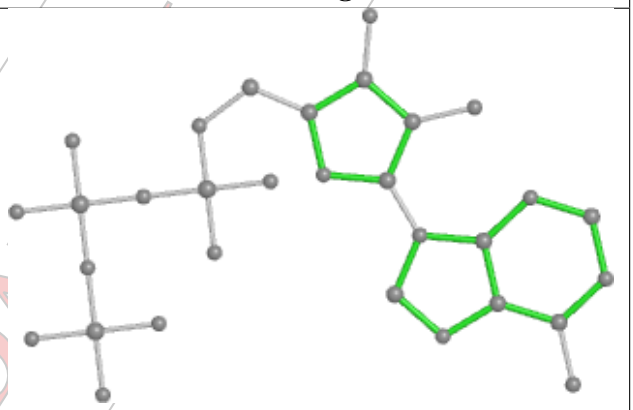
Bond lengths



Bond angles

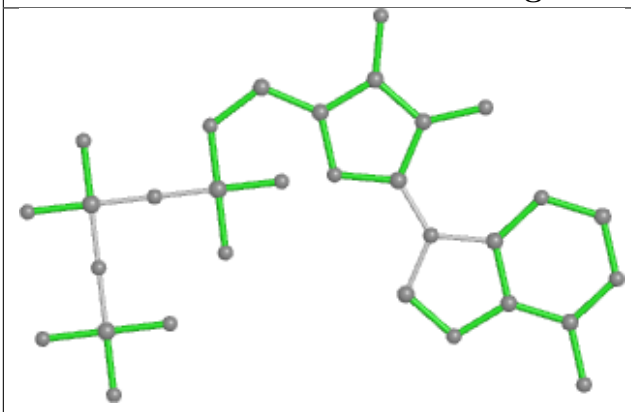


Torsions

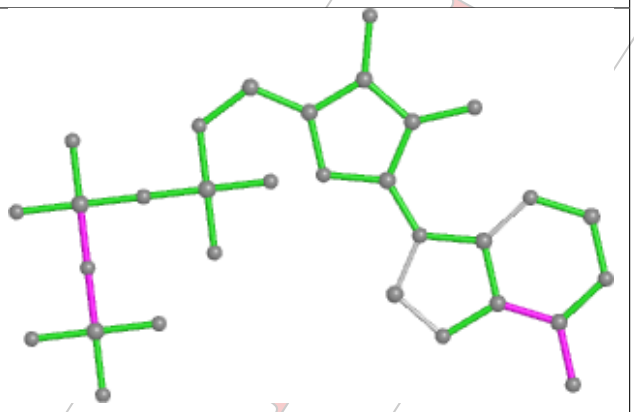


Rings

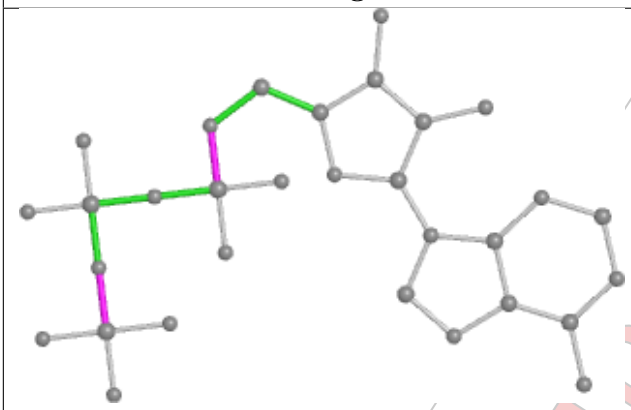
Ligand ATP C 802



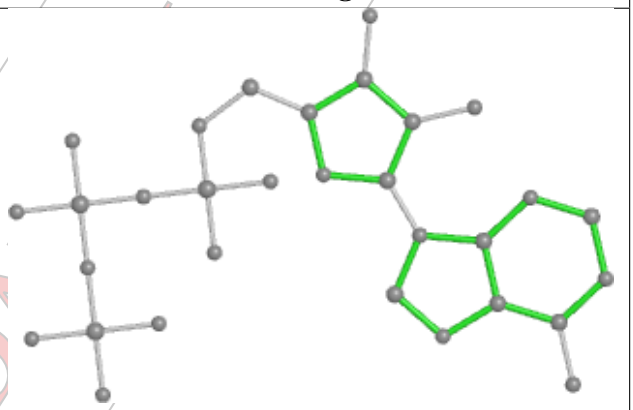
Bond lengths



Bond angles

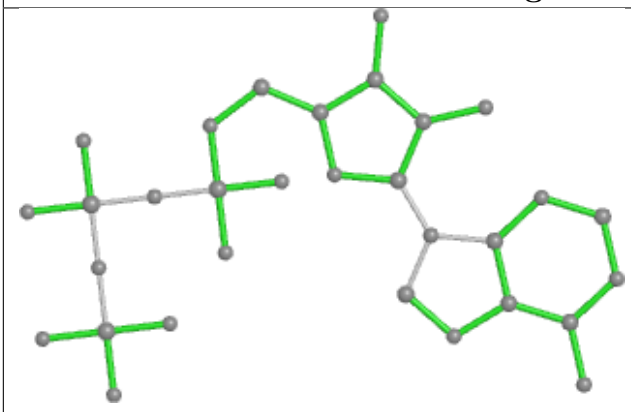


Torsions

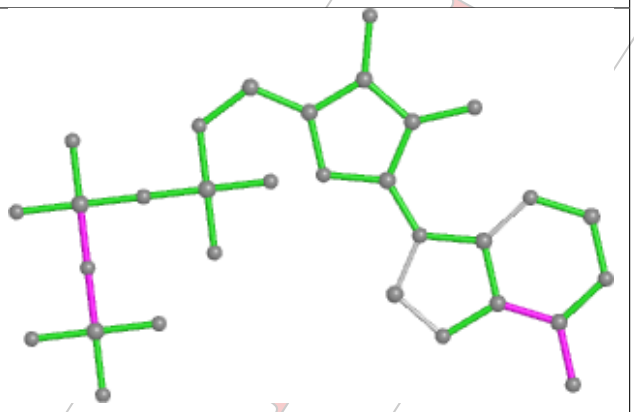


Rings

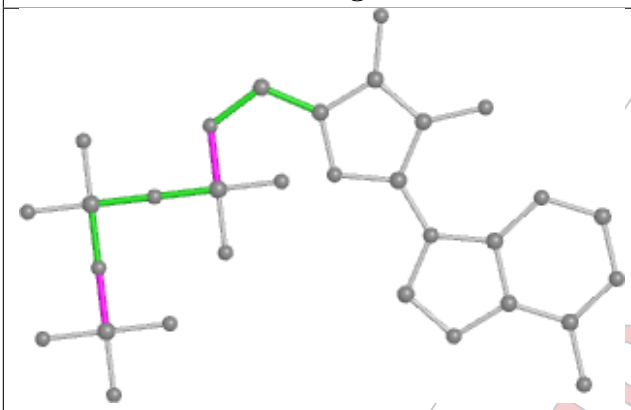
Ligand ATP B 802



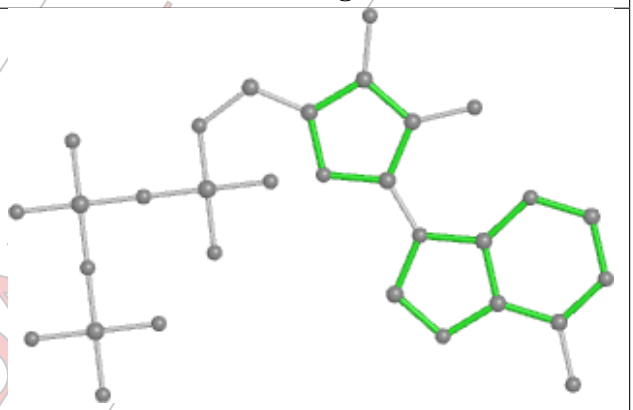
Bond lengths



Bond angles

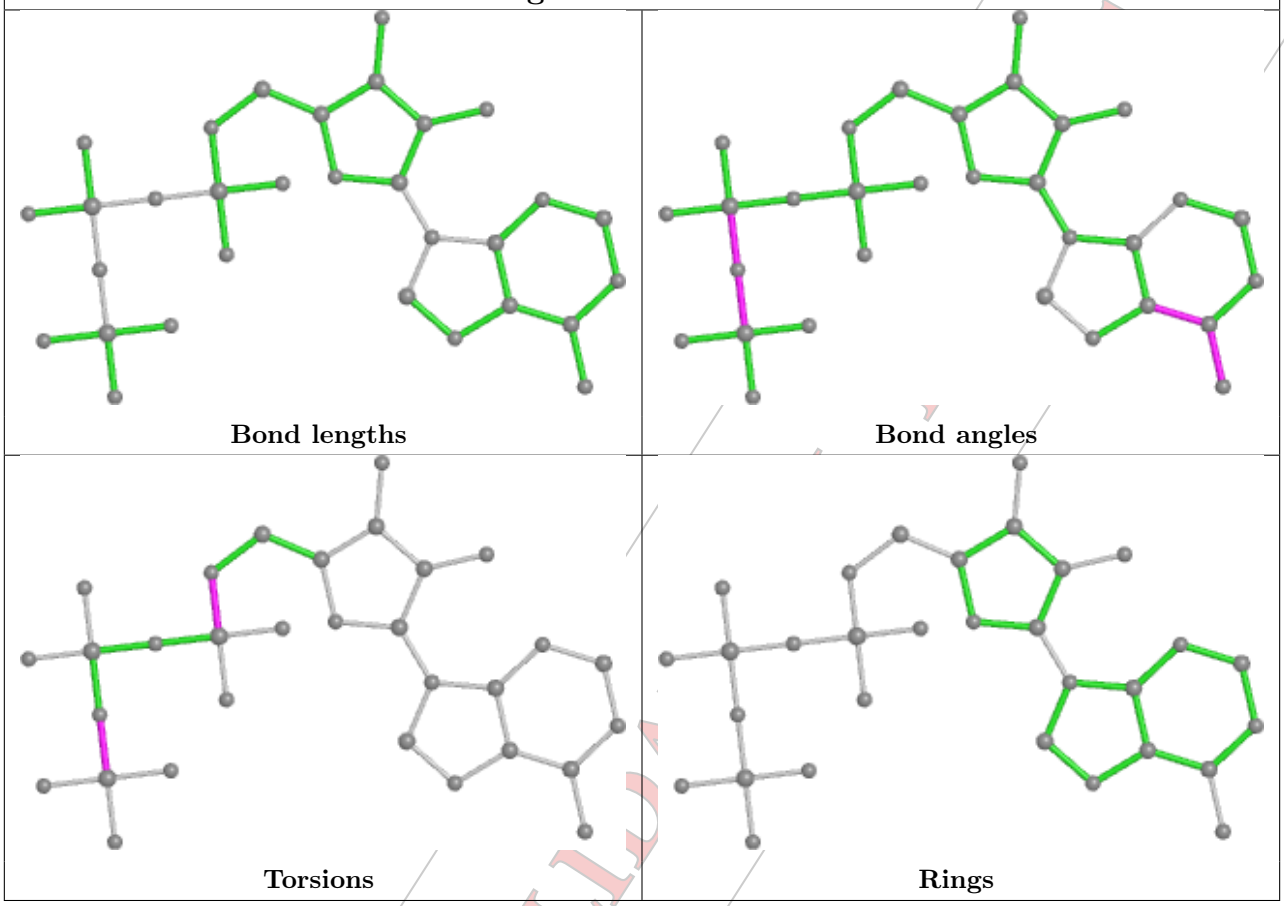


Torsions



Rings

Ligand ATP E 801



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	D	1
1	A	1
1	B	1
1	E	1
1	F	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	185:ASP	C	208:ASP	N	13.57
1	A	185:ASP	C	208:ASP	N	12.99
1	B	185:ASP	C	208:ASP	N	12.64
1	E	185:ASP	C	208:ASP	N	12.51
1	F	185:ASP	C	208:ASP	N	12.34
1	C	185:ASP	C	208:ASP	N	11.66

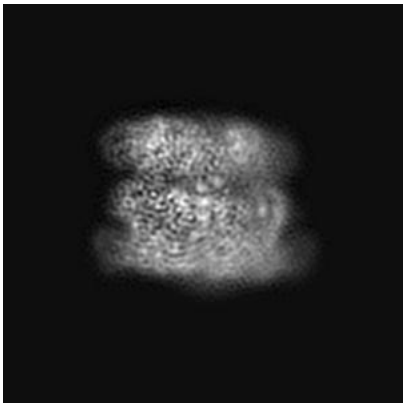
6 Map visualisation

This section contains visualisations of the EMDB entry D_1300026309. These allow visual inspection of the internal detail of the map and identification of artifacts.

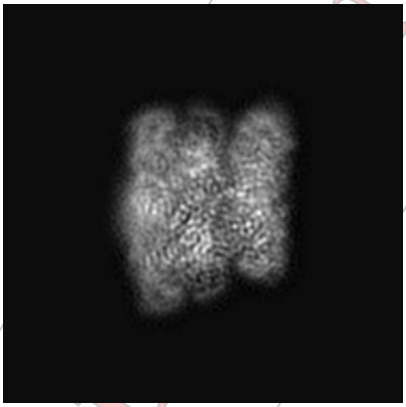
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

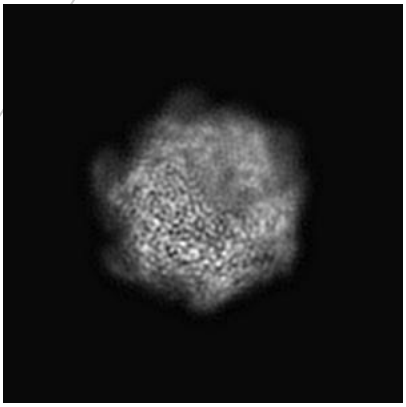
6.1.1 Primary map



X



Y

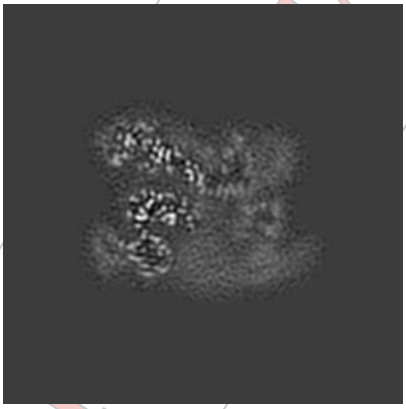


Z

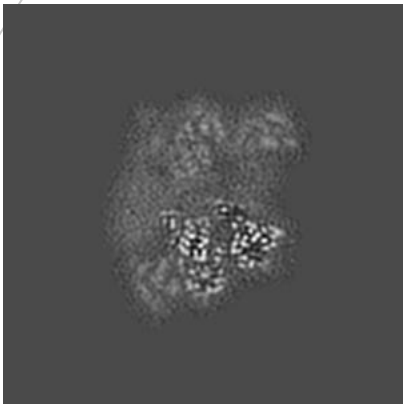
The images above show the map projected in three orthogonal directions.

6.2 Central slices

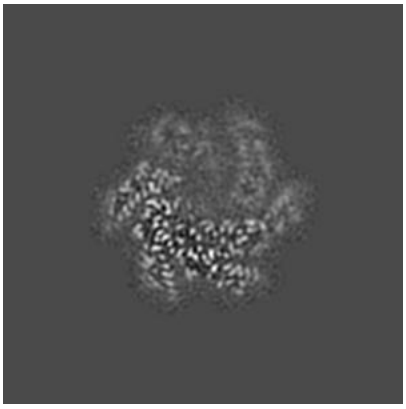
6.2.1 Primary map



X Index: 120



Y Index: 120

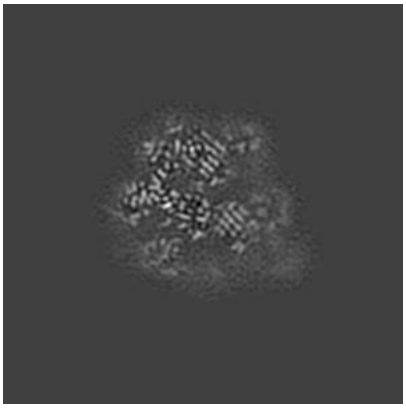


Z Index: 120

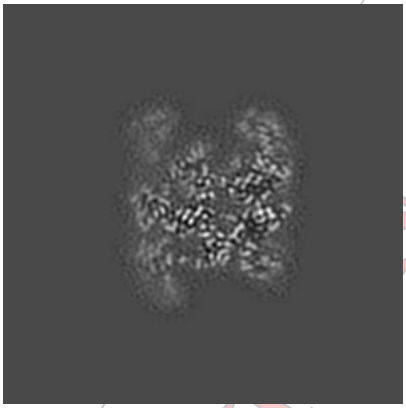
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

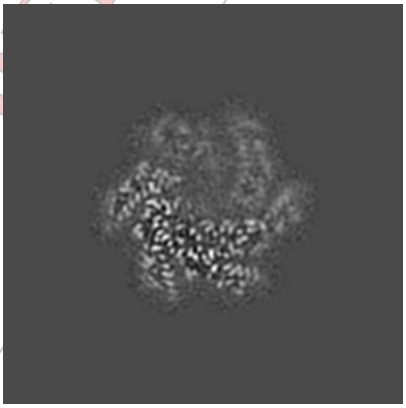
6.3.1 Primary map



X Index: 96



Y Index: 91

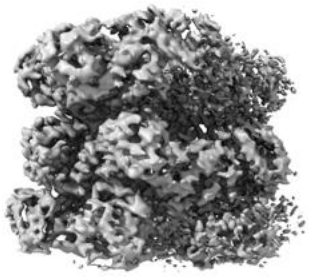


Z Index: 120

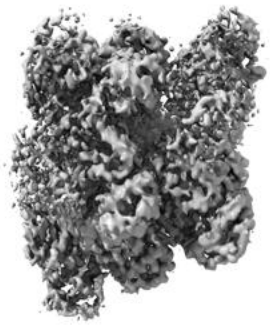
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

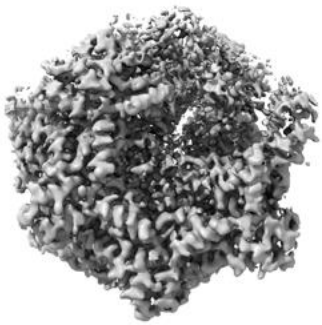
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

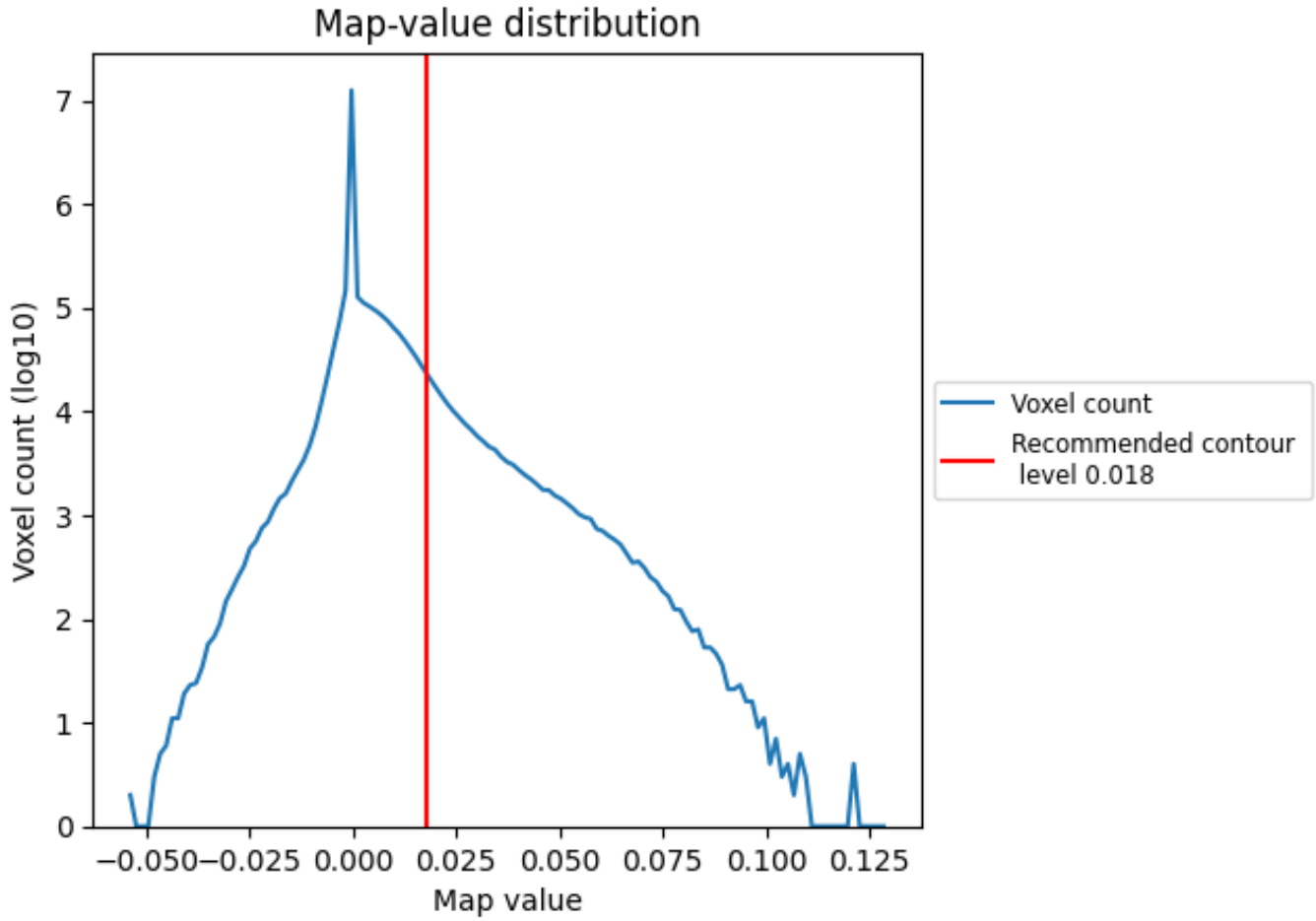
6.5 Mask visualisation (i)

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

7 Map analysis

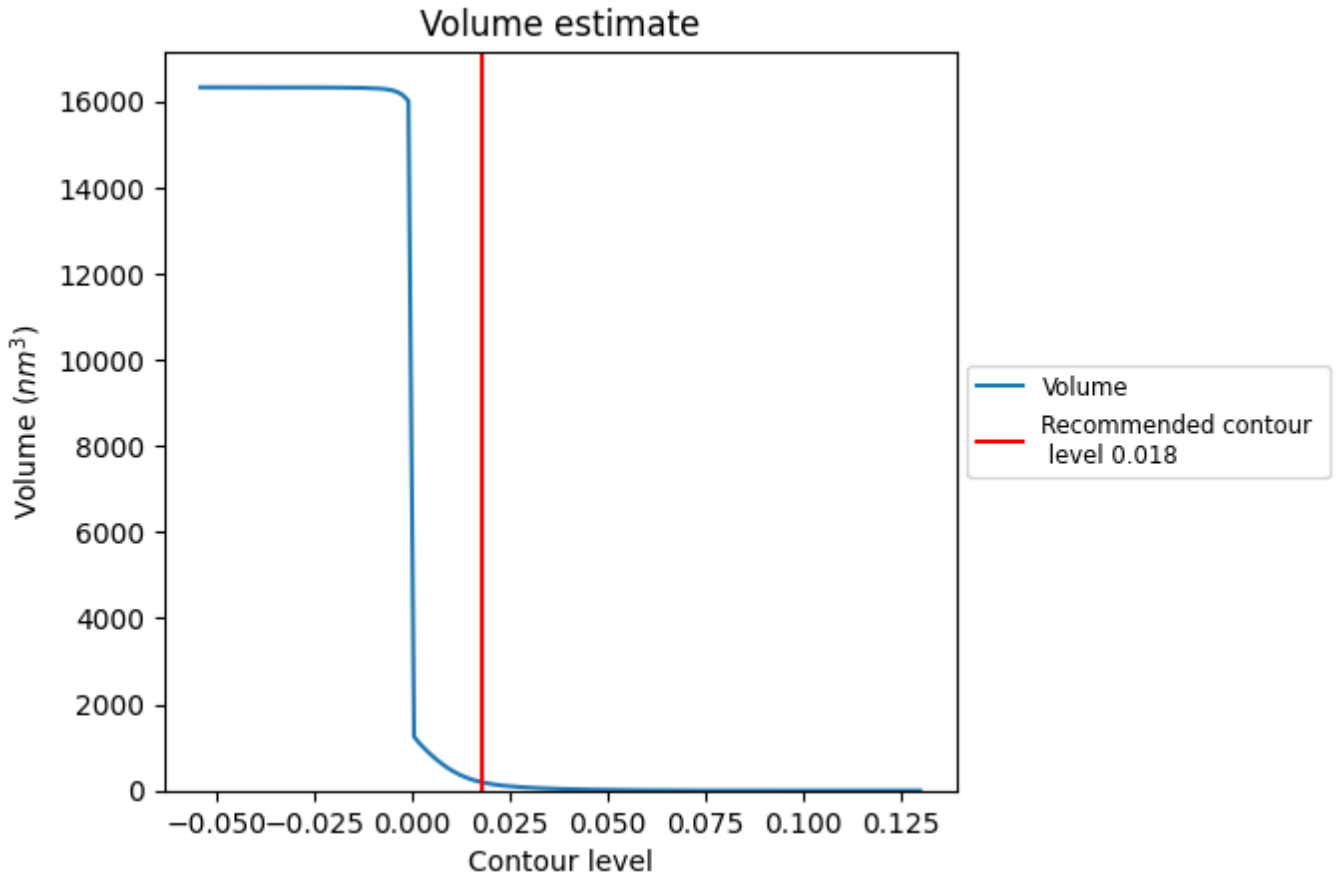
This section contains the results of statistical analysis of the map.

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.

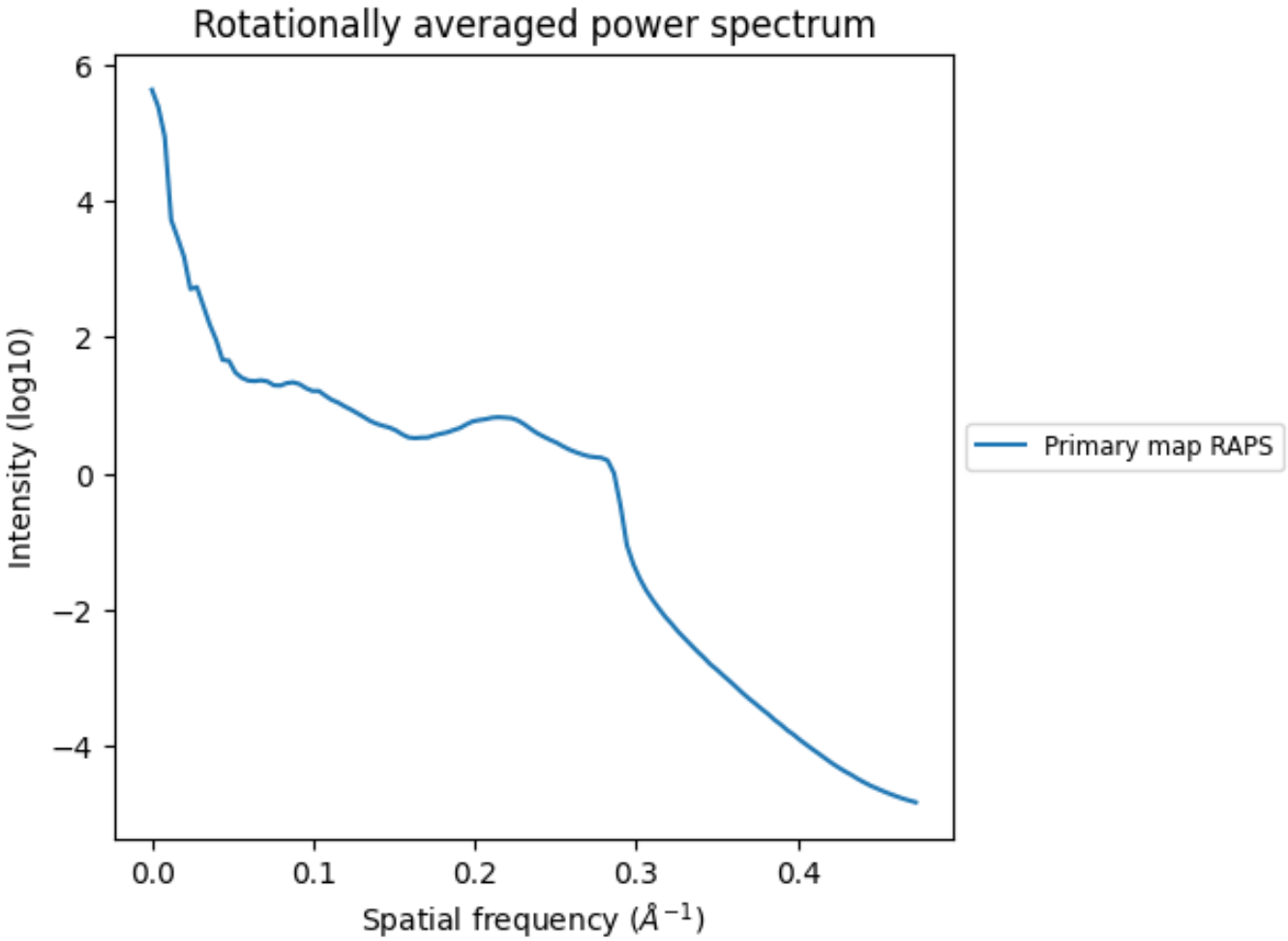
7.2 Volume estimate



The volume at the recommended contour level is 193 nm^3; this corresponds to an approximate mass of 174 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)



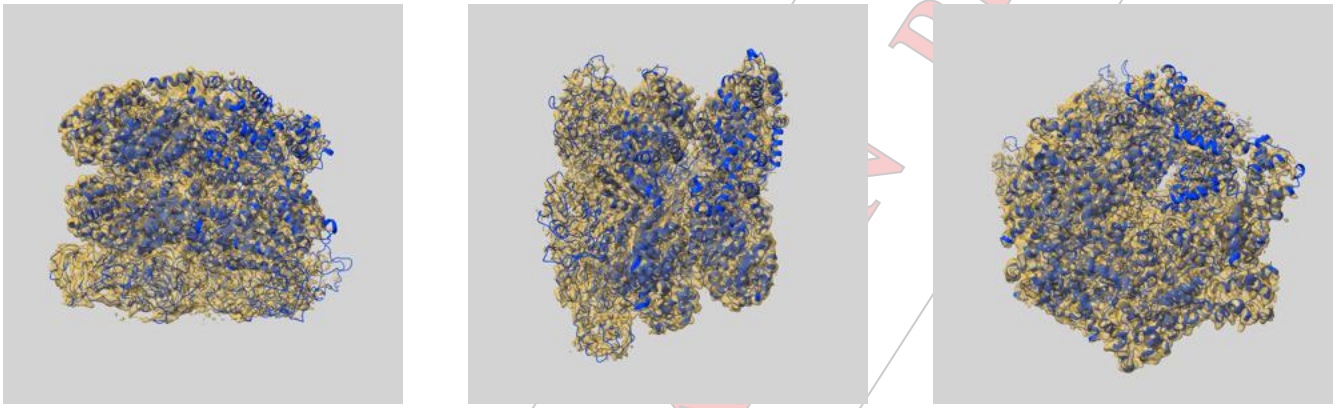
8 Fourier-Shell correlation

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

9 Map-model fit

This section contains information regarding the fit between EMDB map D_1300026309 and PDB model D_1300026309. Per-residue inclusion information can be found in section 3 on page 5.

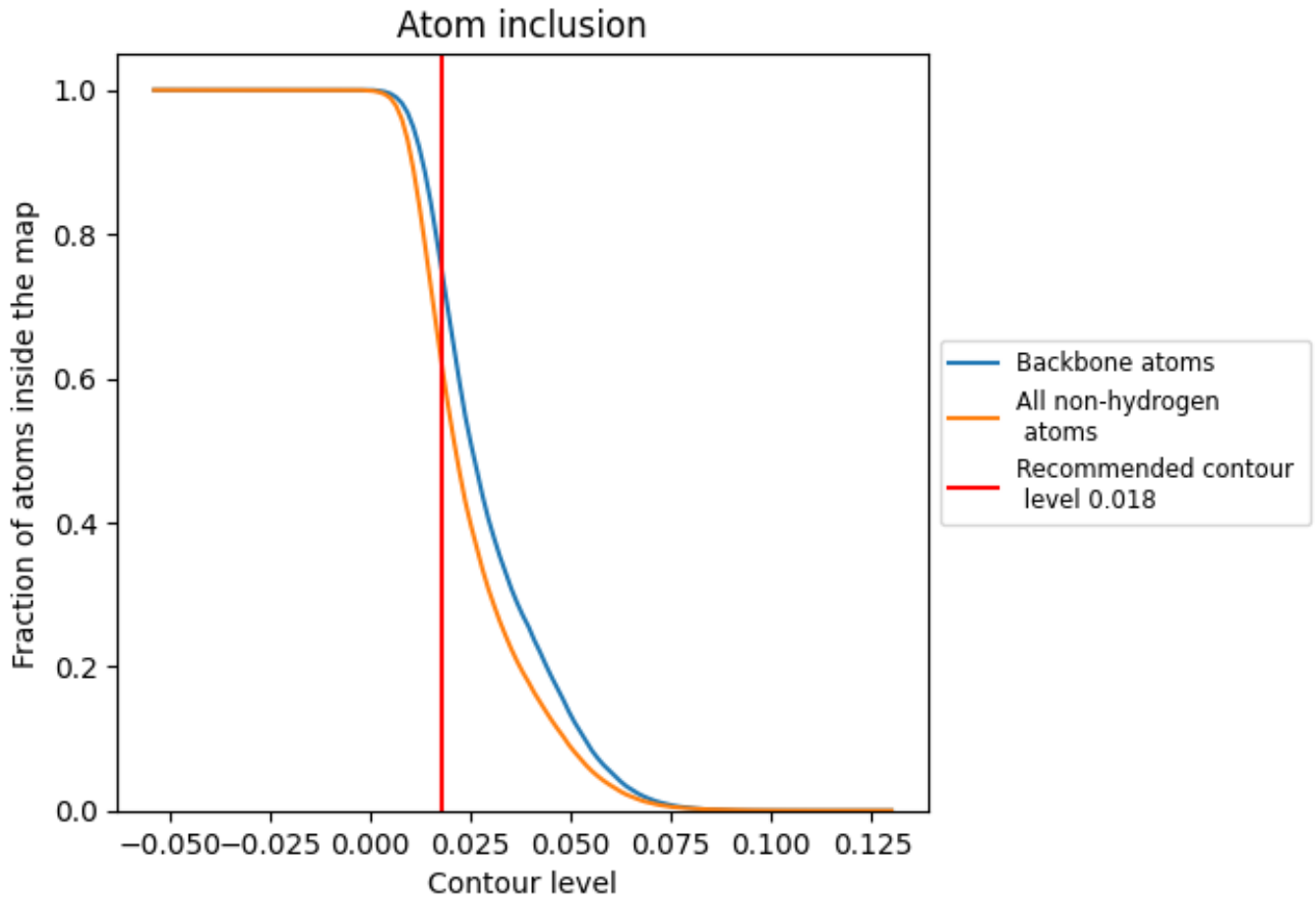
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.018 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 Atom inclusion



At the recommended contour level, 74% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.