



Full wwPDB EM Validation Report ⓘ

May 19, 2024 – 09:58 PM JST

PDB ID : 7CH8
EMDB ID : EMD-30371
Title : Cryo-EM structure of P.aeruginosa MlaFEED with ADP-V
Authors : Zhou, C.; Shi, H.; Zhang, M.; Huang, Y.
Deposited on : 2020-07-05
Resolution : 3.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

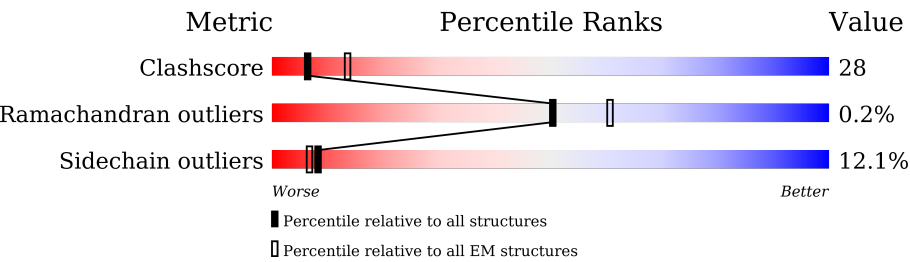
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	157	<div><div>92%</div><div><div>46%</div><div>48%</div><div>• •</div></div></div>
1	B	157	<div><div>78%</div><div><div>69%</div><div>24%</div><div>• 6%</div></div></div>
1	C	157	<div><div>89%</div><div><div>63%</div><div>30%</div><div>• 6%</div></div></div>
1	D	157	<div><div>76%</div><div><div>69%</div><div>25%</div><div>6%</div></div></div>
1	E	157	<div><div>81%</div><div><div>61%</div><div>27%</div><div>7%</div><div>5%</div></div></div>
1	F	157	<div><div>83%</div><div><div>58%</div><div>35%</div><div>• 6%</div></div></div>
2	G	265	<div><div>17%</div><div><div>49%</div><div>42%</div><div>6%</div><div>•</div></div></div>
2	H	265	<div><div>15%</div><div><div>51%</div><div>38%</div><div>8%</div><div>•</div></div></div>

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Mol	Chain	Length	Quality of chain
3	I	269	
3	J	269	
4	K	102	
4	L	102	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	LPP	G	303	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 16213 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 MlaD domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	150	Total	C	N	O	S	0	0
			1103	698	184	220	1		
1	B	148	Total	C	N	O	S	0	0
			1089	692	180	216	1		
1	C	148	Total	C	N	O	S	0	0
			1089	692	180	216	1		
1	D	148	Total	C	N	O	S	0	0
			1089	692	180	216	1		
1	E	149	Total	C	N	O	S	0	0
			1098	697	182	218	1		
1	F	148	Total	C	N	O	S	0	0
			1083	690	180	212	1		

- Molecule 2 is a protein called Probable permease of ABC transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	258	Total	C	N	O	S	0	0
			1932	1265	317	341	9		
2	H	258	Total	C	N	O	S	0	0
			1932	1264	317	342	9		

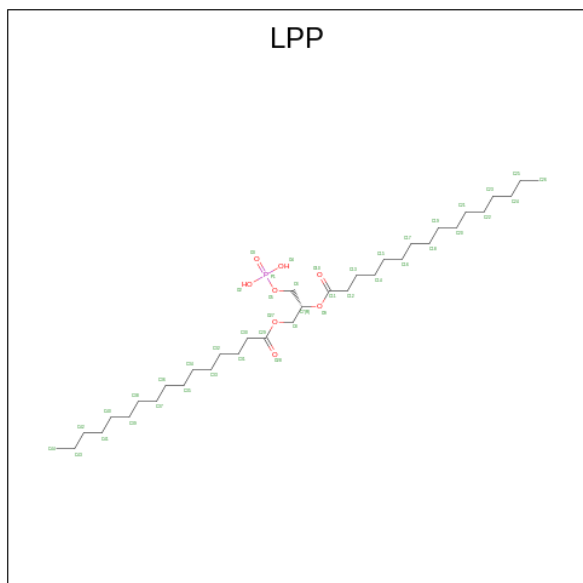
- Molecule 3 is a protein called Probable ATP-binding component of ABC transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	259	Total	C	N	O	S	0	0
			1978	1266	349	356	7		
3	J	261	Total	C	N	O	S	0	0
			1996	1278	354	356	8		

- Molecule 4 is a protein called STAS domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	98	Total	C	N	O	S	0	0
			715	442	132	139	2		
4	L	97	Total	C	N	O	S	0	0
			707	439	128	138	2		

- Molecule 5 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (three-letter code: LPP) (formula: $C_{35}H_{69}O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
5	F	1	Total	C	O	P	0
			44	35	8	1	
5	G	1	Total	C	O	P	0
			44	35	8	1	
5	G	1	Total	C	O	P	0
			44	35	8	1	
5	G	1	Total	C	O	P	0
			38	29	8	1	
5	H	1	Total	C	O	P	0
			44	35	8	1	
5	H	1	Total	C	O	P	0
			44	35	8	1	
5	H	1	Total	C	O	P	0
			36	27	8	1	
5	H	1	Total	C	O	P	0
			44	35	8	1	

- Molecule 6 is ADP METAVANADATE (three-letter code: AD9) (formula: $C_{10}H_{16}N_5O_{13}P_2V$)

[illegible]

Mol	Chain	Residues	Atoms						AltConf
6	I	1	Total 31	C 10	N 5	O 13	P 2	V 1	0
6	J	1	Total 31	C 10	N 5	O 13	P 2	V 1	0

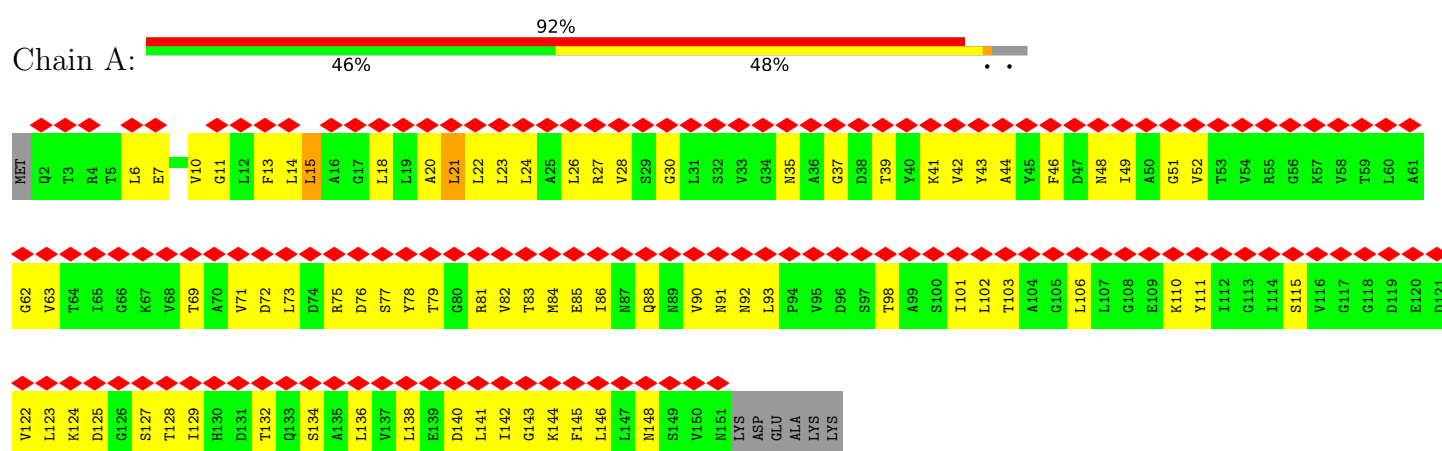
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
7	I	1	Total 1	Mg 1	0
7	J	1	Total 1	Mg 1	0

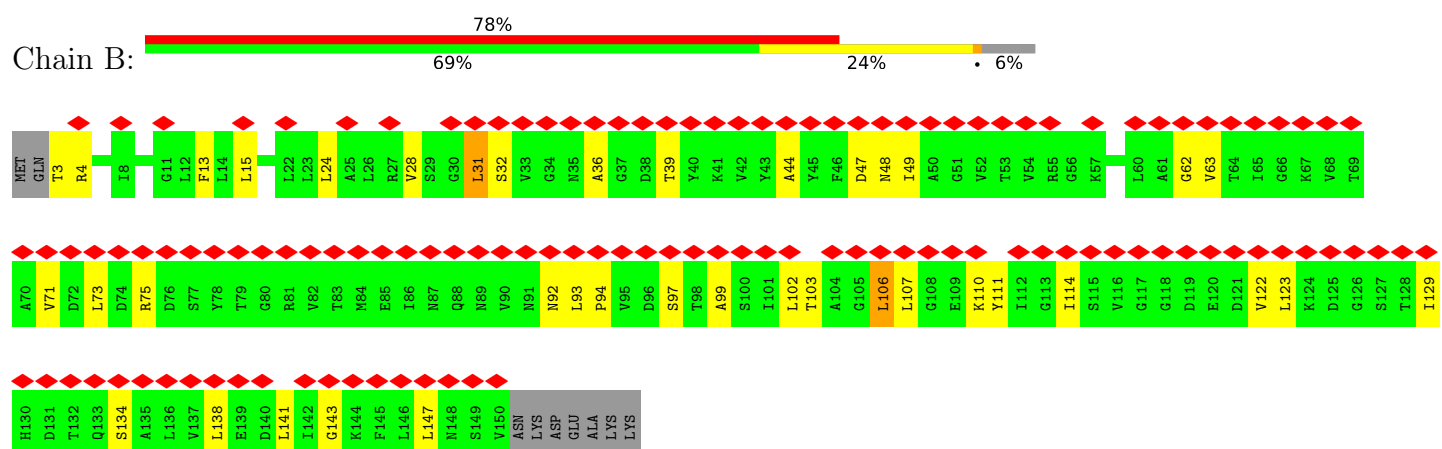
3 Residue-property plots

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

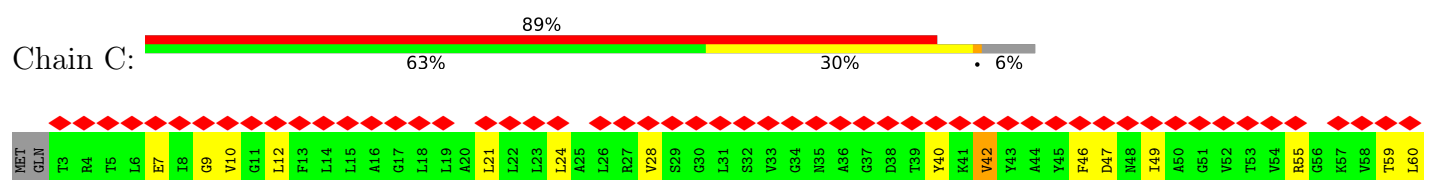
• Molecule 1: MlaD domain-containing protein



• Molecule 1: MlaD domain-containing protein

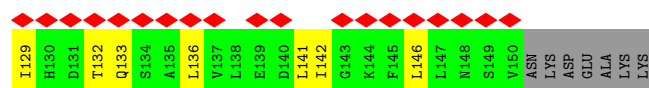
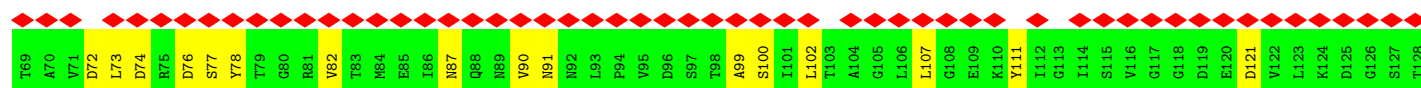
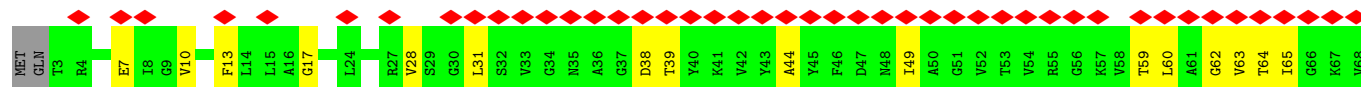
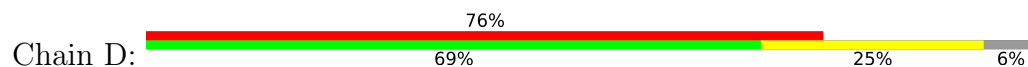


• Molecule 1: MlaD domain-containing protein

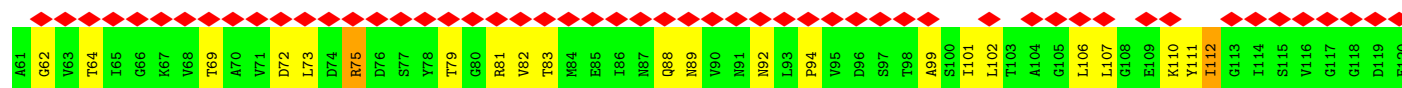
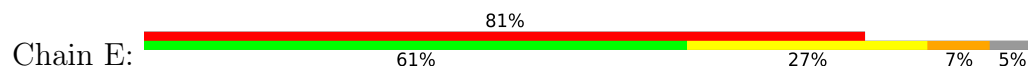




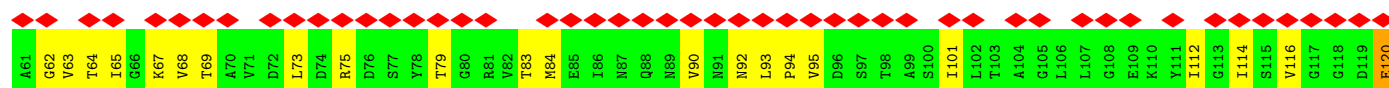
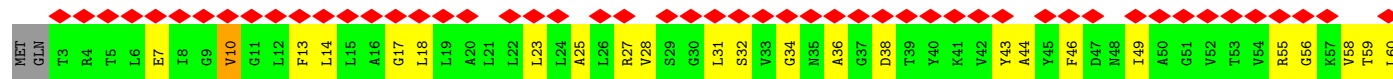
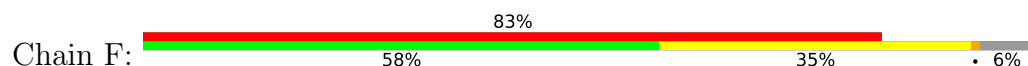
• Molecule 1: MlaD domain-containing protein



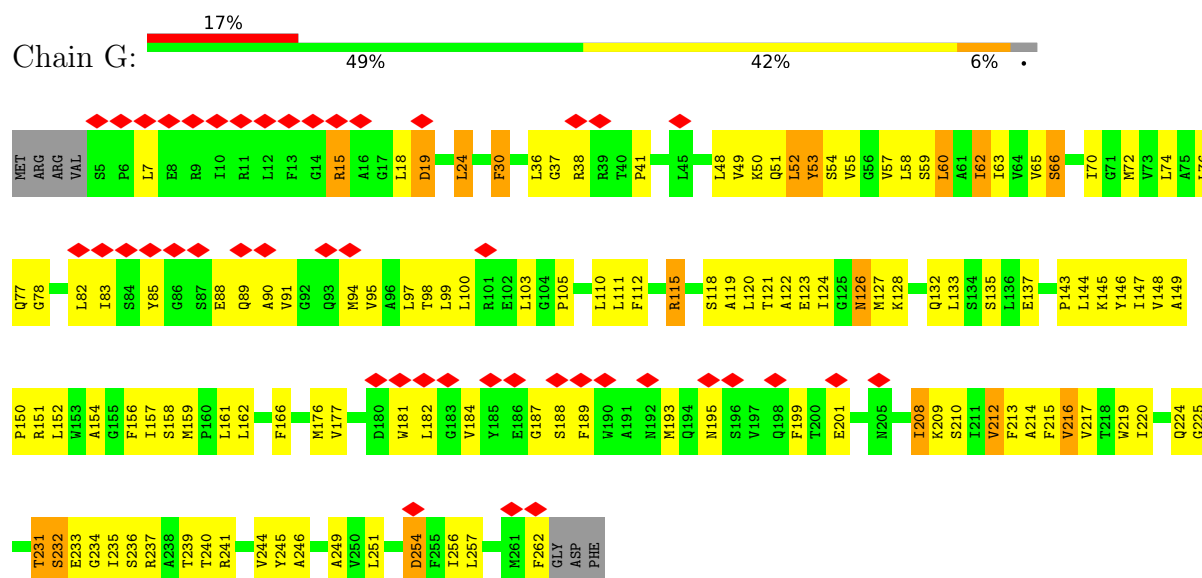
• Molecule 1: MlaD domain-containing protein



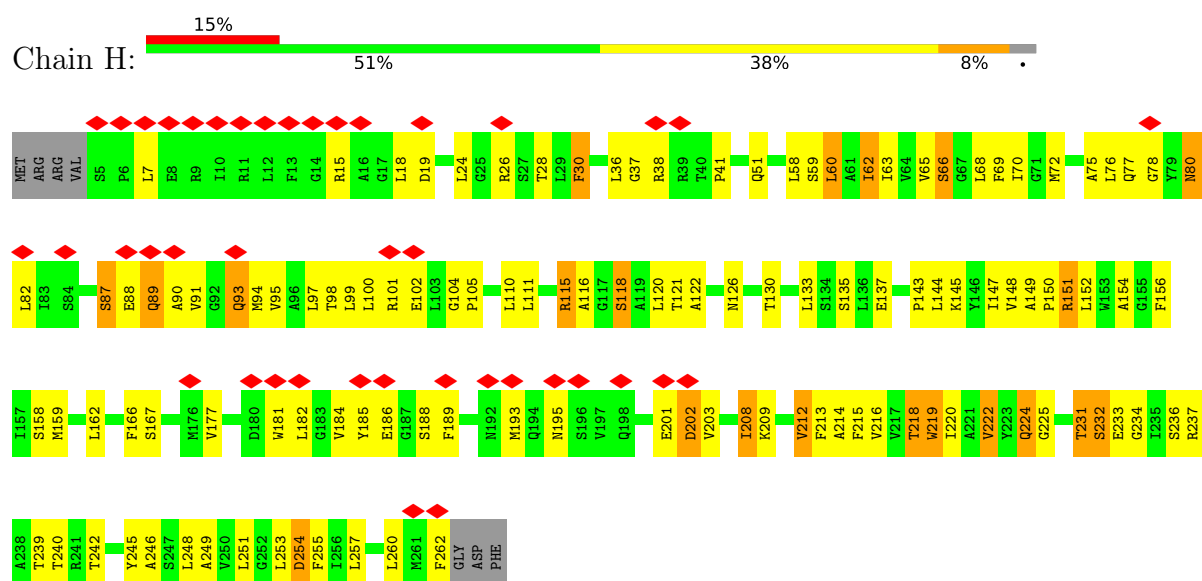
• Molecule 1: MlaD domain-containing protein



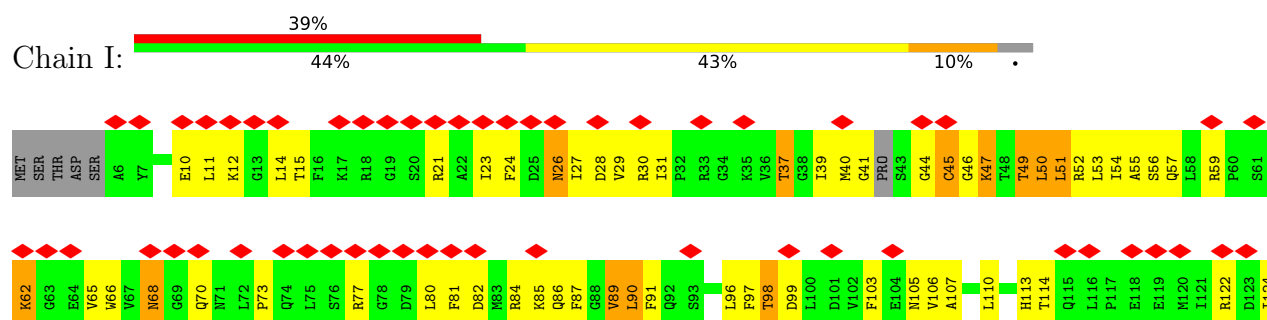
• Molecule 2: Probable permease of ABC transporter



• Molecule 2: Probable permease of ABC transporter



• Molecule 3: Probable ATP-binding component of ABC transporter



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	560624	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.100	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0238	Depositor
Map size (Å)	256.0, 256.0, 256.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LPP, MG, AD9

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	0.30	0/1112	0.52	0/1511
1	B	0.26	0/1098	0.47	0/1492
1	C	0.27	0/1098	0.51	0/1492
1	D	0.25	0/1098	0.48	0/1492
1	E	0.32	0/1107	0.54	0/1504
1	F	0.29	0/1092	0.53	0/1484
2	G	0.40	0/1970	0.52	0/2682
2	H	0.41	0/1969	0.52	0/2680
3	I	0.40	0/2010	0.51	0/2717
3	J	0.37	0/2032	0.50	0/2751
4	K	0.34	0/719	0.49	0/968
4	L	0.41	0/711	0.52	0/958
All	All	0.35	0/16016	0.51	0/21731

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1103	0	1135	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1089	0	1130	34	0
1	C	1089	0	1130	42	0
1	D	1089	0	1130	36	0
1	E	1098	0	1138	47	0
1	F	1083	0	1126	43	0
2	G	1932	0	2000	174	0
2	H	1932	0	2006	149	0
3	I	1978	0	2025	176	0
3	J	1996	0	2053	150	0
4	K	715	0	741	65	0
4	L	707	0	737	73	0
5	F	44	0	67	2	0
5	G	126	0	183	46	0
5	H	168	0	246	27	0
6	I	31	0	14	7	0
6	J	31	0	14	2	0
7	I	1	0	0	0	0
7	J	1	0	0	0	0
All	All	16213	0	16875	943	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 28.

All (943) 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)
2:G:159:MET:HG2	2:G:214:ALA:CB	1.61	1.30
2:H:144:LEU:HA	2:H:148:VAL:CG1	1.61	1.30
3:J:45:CYS:SG	3:J:218:VAL:HG12	1.70	1.29
2:G:144:LEU:HA	2:G:148:VAL:CG1	1.62	1.28
2:H:144:LEU:O	2:H:148:VAL:HG13	1.31	1.26
3:I:40:MET:CE	3:I:205:LEU:HA	1.63	1.25
2:G:220:ILE:CG2	5:G:302:LPP:H132	1.67	1.24
2:G:144:LEU:O	2:G:148:VAL:HG13	1.40	1.19
4:L:81:LEU:HD12	4:L:82:PRO:HD2	1.16	1.16
4:K:88:ILE:O	4:K:91:VAL:HG23	1.43	1.15
2:H:214:ALA:O	2:H:218:THR:HG22	1.46	1.14
3:J:262:ARG:CA	4:K:97:ILE:HD12	1.77	1.14
2:G:122:ALA:HB1	2:H:236:SER:HB3	1.31	1.13
2:G:220:ILE:HG22	5:G:302:LPP:H132	1.12	1.11
3:I:40:MET:HE1	3:I:205:LEU:CB	1.77	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:166:LEU:CD1	3:I:196:ILE:HD12	1.82	1.10
5:G:303:LPP:H392	5:G:303:LPP:H191	1.21	1.09
3:J:262:ARG:HA	4:K:97:ILE:HD12	1.11	1.08
2:G:105:PRO:HB2	2:G:213:PHE:HZ	1.18	1.08
3:I:166:LEU:HD11	3:I:196:ILE:CD1	1.84	1.08
2:H:99:LEU:CD2	2:H:167:SER:HA	1.83	1.07
1:F:7:GLU:O	1:F:10:VAL:HG23	1.54	1.07
2:H:213:PHE:HZ	2:H:254:ASP:HB2	1.17	1.07
3:I:40:MET:HE1	3:I:205:LEU:CA	1.86	1.05
2:H:99:LEU:HD21	2:H:167:SER:HA	1.08	1.05
2:G:159:MET:HG2	2:G:214:ALA:HB2	1.36	1.04
2:G:144:LEU:HA	2:G:148:VAL:HG12	1.37	1.04
4:K:82:PRO:HG2	4:K:85:MET:HG3	1.06	1.04
3:J:262:ARG:HB2	4:K:97:ILE:CD1	1.85	1.04
2:G:105:PRO:HB2	2:G:213:PHE:CZ	1.92	1.04
2:H:144:LEU:HA	2:H:148:VAL:HG12	1.35	1.03
3:I:40:MET:HE1	3:I:205:LEU:HA	1.40	1.03
2:G:159:MET:CG	2:G:214:ALA:CB	2.36	1.03
2:H:144:LEU:CA	2:H:148:VAL:CG1	2.38	1.01
4:K:82:PRO:CG	4:K:85:MET:HG3	1.89	1.01
3:I:40:MET:CE	3:I:205:LEU:CA	2.38	1.01
2:G:58:LEU:HD22	5:G:301:LPP:HC61	1.41	0.99
2:G:159:MET:HG2	2:G:214:ALA:HB1	1.43	0.99
3:I:167:LEU:H	3:I:167:LEU:HD22	1.28	0.99
3:I:40:MET:HE2	3:I:205:LEU:HA	1.41	0.98
2:G:144:LEU:CA	2:G:148:VAL:CG1	2.41	0.98
3:I:166:LEU:HD11	3:I:196:ILE:HD12	0.99	0.97
3:J:130:GLN:HG2	4:L:93:SER:OG	1.63	0.97
1:A:14:LEU:CD1	2:H:28:THR:HG21	1.95	0.96
2:H:144:LEU:HA	2:H:148:VAL:HG11	1.44	0.96
2:G:159:MET:CG	2:G:214:ALA:HB2	1.94	0.96
3:I:261:TYR:HA	3:J:135:ARG:HH12	1.29	0.95
3:J:256:TYR:CG	3:J:257:PRO:HD2	2.01	0.95
3:J:45:CYS:SG	3:J:218:VAL:CG1	2.53	0.95
1:A:14:LEU:HD11	2:H:28:THR:HG21	1.47	0.95
2:G:144:LEU:HA	2:G:148:VAL:HG11	1.46	0.95
2:H:213:PHE:CZ	2:H:254:ASP:HB2	2.03	0.94
3:I:40:MET:HE1	3:I:205:LEU:CD1	1.97	0.94
2:H:90:ALA:HB1	2:H:93:GLN:NE2	1.83	0.94
4:K:82:PRO:HG2	4:K:85:MET:CG	1.97	0.94
5:G:303:LPP:H402	5:G:303:LPP:H211	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:208:ILE:O	2:G:212:VAL:HG12	1.69	0.92
3:J:175:GLN:CB	3:J:180:MET:CE	2.49	0.91
3:I:89:VAL:HG13	3:I:167:LEU:CD2	2.00	0.91
5:G:303:LPP:H402	5:G:303:LPP:C21	2.00	0.91
3:I:52:ARG:HG2	3:I:57:GLN:OE1	1.69	0.91
2:G:220:ILE:HG22	5:G:302:LPP:C13	2.00	0.91
3:I:89:VAL:HG13	3:I:167:LEU:HD21	1.49	0.91
1:A:22:LEU:HD21	5:H:301:LPP:H432	1.53	0.90
2:G:159:MET:CG	2:G:214:ALA:HB1	2.01	0.89
2:G:105:PRO:CB	2:G:213:PHE:HZ	1.83	0.89
4:L:47:ASP:HA	4:L:79:ARG:O	1.71	0.88
2:H:144:LEU:O	2:H:148:VAL:CG1	2.21	0.88
2:H:121:THR:HG23	2:H:225:GLY:N	1.88	0.88
3:J:175:GLN:CB	3:J:180:MET:HE1	2.04	0.88
2:H:214:ALA:O	2:H:218:THR:CG2	2.20	0.87
2:H:208:ILE:O	2:H:212:VAL:HG12	1.74	0.87
1:C:107:LEU:HD21	1:D:107:LEU:HD13	1.54	0.87
3:J:171:PRO:HG3	3:J:200:VAL:HG13	1.55	0.87
4:L:81:LEU:CD1	4:L:82:PRO:HD2	2.05	0.87
4:K:88:ILE:O	4:K:91:VAL:CG2	2.21	0.86
3:I:166:LEU:HD22	3:I:197:THR:O	1.75	0.86
2:G:112:PHE:HD2	2:G:217:VAL:HG11	1.38	0.85
2:G:94:MET:HA	5:G:303:LPP:H152	1.58	0.84
3:I:50:LEU:HD12	3:I:50:LEU:O	1.77	0.84
2:G:50:LYS:HD2	2:G:50:LYS:O	1.77	0.84
5:G:303:LPP:H402	5:G:303:LPP:C22	2.08	0.83
3:I:40:MET:HE1	3:I:205:LEU:HD12	1.59	0.83
1:A:14:LEU:HD11	2:H:28:THR:CG2	2.08	0.83
3:I:90:LEU:HD23	3:I:168:TYR:HD2	1.43	0.83
3:J:262:ARG:CB	4:K:97:ILE:CD1	2.56	0.83
3:J:256:TYR:CD1	3:J:257:PRO:HD2	2.14	0.83
3:I:47:LYS:NZ	3:I:203:HIS:ND1	2.27	0.82
3:J:130:GLN:CG	4:L:93:SER:OG	2.27	0.82
3:I:89:VAL:CG1	3:I:167:LEU:HD23	2.09	0.82
3:J:262:ARG:HB2	4:K:97:ILE:HD13	1.58	0.82
4:K:95:LEU:HD23	4:K:95:LEU:H	1.43	0.81
3:I:89:VAL:HG12	3:I:167:LEU:HD23	1.60	0.81
3:I:41:GLY:C	3:I:243:PHE:CZ	2.54	0.80
3:I:40:MET:HE1	3:I:205:LEU:HB2	1.61	0.80
4:L:77:SER:HA	4:L:99:PRO:HG2	1.63	0.80
2:H:144:LEU:C	2:H:148:VAL:HG13	2.01	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:136:GLY:HA2	3:J:258:ALA:HB2	1.64	0.79
3:J:262:ARG:CA	4:K:97:ILE:CD1	2.59	0.79
4:L:78:VAL:HG22	4:L:99:PRO:O	1.83	0.79
3:I:89:VAL:CG1	3:I:167:LEU:CD2	2.60	0.79
5:G:303:LPP:H211	5:G:303:LPP:C40	2.13	0.79
3:I:40:MET:CE	3:I:205:LEU:CB	2.59	0.79
3:I:47:LYS:NZ	3:I:203:HIS:CE1	2.52	0.78
3:J:262:ARG:CB	4:K:97:ILE:HD12	2.13	0.78
1:A:14:LEU:CD1	2:H:28:THR:CG2	2.61	0.78
3:J:261:TYR:CB	4:K:93:SER:OG	2.31	0.78
2:G:220:ILE:HG21	5:G:302:LPP:H132	1.64	0.78
4:K:5:SER:H	4:K:17:ALA:HB3	1.48	0.78
4:L:81:LEU:HD12	4:L:82:PRO:CD	2.09	0.78
4:L:82:PRO:HG2	4:L:85:MET:HB2	1.66	0.78
4:L:5:SER:H	4:L:17:ALA:HB3	1.48	0.77
2:G:159:MET:CE	2:G:213:PHE:HE1	1.97	0.77
2:H:224:GLN:NE2	2:H:224:GLN:HA	1.98	0.77
3:I:203:HIS:CD2	3:I:203:HIS:H	2.01	0.77
4:L:94:LEU:HA	4:L:97:ILE:HG13	1.66	0.77
1:B:92:ASN:HD21	1:F:75:ARG:HE	1.29	0.77
2:G:48:LEU:HD23	2:G:52:LEU:HD22	1.66	0.77
3:J:50:LEU:HD12	3:J:50:LEU:O	1.84	0.77
2:G:151:ARG:HG3	2:G:151:ARG:HH21	1.49	0.77
3:I:166:LEU:HD22	3:I:166:LEU:N	2.00	0.77
2:G:78:GLY:HA3	2:G:94:MET:SD	2.25	0.77
5:G:303:LPP:H171	2:H:81:ILE:HG21	1.66	0.76
3:I:155:LEU:O	3:I:155:LEU:HD12	1.85	0.76
3:I:122:ARG:HG2	3:I:126:LEU:HD23	1.68	0.76
3:I:177:PRO:HG3	3:J:243:PHE:CZ	2.21	0.76
3:J:142:PRO:HA	3:J:145:LEU:HD12	1.67	0.76
1:E:23:LEU:HG	1:E:26:LEU:HG	1.68	0.76
5:G:302:LPP:H401	2:H:69:PHE:HE1	1.51	0.76
3:I:142:PRO:HA	3:I:145:LEU:HD12	1.67	0.75
1:F:10:VAL:HG11	2:G:18:LEU:HG	1.69	0.75
5:G:303:LPP:H121	2:H:81:ILE:HD11	1.68	0.75
3:I:166:LEU:HD22	3:I:166:LEU:H	1.51	0.75
2:G:30:PHE:CZ	2:G:148:VAL:HG21	2.21	0.75
2:G:144:LEU:O	2:G:148:VAL:CG1	2.28	0.75
4:K:95:LEU:HD23	4:K:95:LEU:N	2.02	0.75
2:G:156:PHE:CE1	2:G:215:PHE:CD1	2.75	0.75
5:G:303:LPP:H331	5:G:303:LPP:O10	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:VAL:HG11	2:H:18:LEU:HG	1.70	0.74
3:I:167:LEU:HD22	3:I:167:LEU:N	2.03	0.74
3:J:124:ILE:HD11	4:L:57:VAL:HA	1.68	0.74
3:J:55:ALA:O	3:J:84:ARG:NH2	2.21	0.73
2:G:144:LEU:CA	2:G:148:VAL:HG12	2.15	0.73
2:H:120:LEU:HD11	2:H:151:ARG:HG3	1.70	0.73
3:I:55:ALA:O	3:I:84:ARG:NH2	2.21	0.73
3:I:40:MET:CE	3:I:205:LEU:HD12	2.17	0.73
1:D:39:THR:HG22	1:D:87:ASN:HA	1.70	0.73
1:F:55:ARG:HG2	1:F:67:LYS:HD3	1.69	0.72
2:G:144:LEU:C	2:G:148:VAL:HG13	2.09	0.72
1:E:22:LEU:HD12	2:G:256:ILE:HD11	1.71	0.72
3:I:265:LEU:HG	4:L:94:LEU:HD11	1.70	0.72
1:E:8:ILE:HD13	2:G:18:LEU:HD22	1.71	0.72
2:G:74:LEU:HD11	2:G:103:LEU:HD22	1.72	0.72
3:I:40:MET:CE	3:I:205:LEU:HB2	2.19	0.72
2:G:236:SER:HB3	2:H:122:ALA:HB1	1.73	0.71
1:D:78:TYR:HB3	1:E:60:LEU:HD21	1.72	0.71
2:H:144:LEU:C	2:H:148:VAL:CG1	2.57	0.71
3:J:172:PHE:CZ	3:J:200:VAL:HG11	2.25	0.71
3:I:47:LYS:HZ1	3:I:203:HIS:CE1	2.06	0.71
4:K:81:LEU:HD12	4:K:82:PRO:HD2	1.73	0.71
3:I:40:MET:HE1	3:I:205:LEU:CG	2.21	0.70
2:G:52:LEU:HD21	2:G:157:ILE:HD11	1.73	0.70
2:H:144:LEU:CA	2:H:148:VAL:HG12	2.13	0.70
5:G:303:LPP:H392	5:G:303:LPP:C19	2.12	0.70
3:J:262:ARG:NH1	4:K:97:ILE:HA	2.06	0.70
5:G:302:LPP:H401	2:H:69:PHE:CE1	2.25	0.70
2:G:65:VAL:HG21	5:G:301:LPP:H351	1.73	0.70
1:E:27:ARG:NH1	1:E:27:ARG:HG2	2.07	0.69
3:I:90:LEU:C	3:I:90:LEU:HD12	2.13	0.69
3:J:175:GLN:CB	3:J:180:MET:HE2	2.21	0.69
2:G:231:THR:HG23	2:G:234:GLY:H	1.58	0.69
1:F:43:TYR:HB2	1:F:128:THR:HG23	1.75	0.68
3:J:15:THR:HB	3:J:26:ASN:H	1.57	0.68
1:B:63:VAL:HB	1:F:49:ILE:HD11	1.76	0.68
1:C:75:ARG:HH11	1:C:75:ARG:HA	1.58	0.68
3:I:15:THR:HB	3:I:26:ASN:H	1.57	0.68
6:I:301:AD9:O1G	6:I:301:AD9:VG	1.51	0.68
3:J:166:LEU:HG	3:J:168:TYR:CE1	2.27	0.68
1:E:23:LEU:HA	1:E:26:LEU:HG	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:265:LEU:HG	4:L:94:LEU:CD1	2.24	0.68
3:J:31:ILE:HG23	3:J:37:THR:HG21	1.75	0.68
5:F:201:LPP:H201	5:H:304:LPP:H212	1.76	0.68
2:H:231:THR:HG23	2:H:234:GLY:H	1.58	0.68
3:I:136:GLY:CA	3:J:258:ALA:HB2	2.23	0.68
2:H:59:SER:HB2	2:H:115:ARG:HD2	1.76	0.68
1:E:27:ARG:HG2	1:E:27:ARG:HH11	1.58	0.68
3:I:191:ASN:ND2	3:I:196:ILE:O	2.27	0.68
2:G:59:SER:HB2	2:G:115:ARG:HD2	1.76	0.67
3:I:41:GLY:C	3:I:243:PHE:HZ	1.96	0.67
2:G:144:LEU:C	2:G:148:VAL:CG1	2.63	0.67
2:H:51:GLN:HA	2:H:51:GLN:OE1	1.94	0.67
4:L:84:ASP:OD1	4:L:84:ASP:N	2.27	0.67
1:B:32:SER:O	1:B:36:ALA:N	2.27	0.67
1:A:14:LEU:HD12	2:H:28:THR:HG21	1.76	0.67
3:J:95:ALA:O	3:J:157:ARG:NH2	2.28	0.67
4:K:30:GLU:OE1	4:K:34:ARG:NH2	2.28	0.67
3:I:31:ILE:HG23	3:I:37:THR:HG21	1.75	0.67
1:A:122:VAL:HG12	1:A:123:LEU:HB2	1.76	0.67
2:G:216:VAL:HG11	2:G:249:ALA:HB1	1.77	0.67
6:J:301:AD9:VG	6:J:301:AD9:O1G	1.51	0.67
2:H:99:LEU:CD2	2:H:167:SER:CA	2.68	0.67
1:D:146:LEU:HD21	1:E:145:PHE:HB2	1.76	0.66
2:G:156:PHE:CE1	2:G:215:PHE:HD1	2.11	0.66
2:G:98:THR:HG21	5:G:303:LPP:H381	1.78	0.66
3:I:40:MET:CE	3:I:205:LEU:CD1	2.70	0.66
2:G:112:PHE:CD2	2:G:217:VAL:HG11	2.26	0.66
3:J:262:ARG:HH11	4:K:97:ILE:HG23	1.59	0.66
1:A:11:GLY:O	1:A:15:LEU:HB2	1.95	0.66
1:A:71:VAL:HG12	1:A:82:VAL:HG12	1.77	0.66
3:I:140:LEU:HD23	3:I:144:GLU:HB3	1.78	0.66
4:L:30:GLU:OE1	4:L:34:ARG:NH2	2.28	0.66
3:J:191:ASN:ND2	3:J:196:ILE:O	2.27	0.66
4:L:48:CYS:HB2	4:L:82:PRO:HD3	1.78	0.66
2:G:30:PHE:CE1	2:G:148:VAL:HG21	2.31	0.66
1:C:49:ILE:H	1:D:62:GLY:HA3	1.62	0.65
1:E:72:ASP:OD2	1:E:81:ARG:NH2	2.30	0.65
4:L:63:LEU:O	4:L:63:LEU:HD23	1.96	0.65
1:D:107:LEU:HD21	1:E:107:LEU:HD13	1.79	0.65
2:H:121:THR:CG2	2:H:225:GLY:N	2.59	0.65
3:J:262:ARG:HD3	4:K:97:ILE:HG23	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:37:ARG:HA	4:L:40:GLN:HG2	1.79	0.65
5:H:301:LPP:H361	5:H:302:LPP:H392	1.80	0.64
3:J:263:ALA:HA	3:J:266:LEU:HB2	1.78	0.64
2:G:48:LEU:CD2	2:G:52:LEU:HD22	2.28	0.64
4:K:88:ILE:C	4:K:91:VAL:HG23	2.17	0.64
2:H:82:LEU:HB3	2:H:87:SER:O	1.98	0.64
3:J:45:CYS:SG	3:J:45:CYS:O	2.55	0.64
5:H:301:LPP:H331	5:H:302:LPP:H401	1.80	0.64
4:K:37:ARG:HA	4:K:40:GLN:HG2	1.79	0.64
3:I:127:MET:HE1	4:K:59:ILE:HG22	1.80	0.64
3:I:175:GLN:HA	3:J:203:HIS:CE1	2.33	0.64
3:J:140:LEU:HD23	3:J:144:GLU:HB3	1.78	0.64
1:D:7:GLU:HG2	2:G:49:VAL:HG11	1.79	0.63
2:G:74:LEU:HD12	2:G:99:LEU:HD12	1.78	0.63
2:H:99:LEU:HD21	2:H:167:SER:CA	2.04	0.63
3:I:51:LEU:HD11	3:I:201:VAL:HG21	1.79	0.63
3:J:23:ILE:HG21	3:J:49:THR:HG21	1.80	0.63
2:H:220:ILE:HD11	2:H:246:ALA:HA	1.79	0.63
1:C:69:THR:HG23	1:C:84:MET:HA	1.80	0.63
4:K:48:CYS:HB2	4:K:82:PRO:HD3	1.80	0.63
1:C:94:PRO:HA	1:C:122:VAL:HA	1.80	0.63
3:I:39:ILE:HG22	3:I:216:TYR:HB2	1.80	0.63
1:F:65:ILE:HD12	1:F:90:VAL:HG21	1.81	0.63
4:L:48:CYS:CB	4:L:82:PRO:HD3	2.28	0.63
2:H:90:ALA:HB1	2:H:93:GLN:HE21	1.60	0.62
2:H:100:LEU:HD11	2:H:203:VAL:HA	1.80	0.62
5:H:304:LPP:HC81	5:H:304:LPP:C12	2.27	0.62
3:I:90:LEU:HD22	3:I:155:LEU:HB2	1.80	0.62
3:J:261:TYR:HA	3:J:264:ASP:HB2	1.81	0.62
1:C:123:LEU:HG	1:C:125:ASP:H	1.64	0.62
2:H:99:LEU:O	2:H:104:GLY:HA3	1.99	0.62
4:L:94:LEU:N	4:L:94:LEU:HD23	2.13	0.62
2:G:159:MET:HB3	2:G:214:ALA:HB1	1.82	0.62
1:F:23:LEU:O	1:F:27:ARG:HB2	2.00	0.62
3:J:166:LEU:HD11	3:J:168:TYR:OH	2.00	0.62
4:L:94:LEU:HA	4:L:97:ILE:CG1	2.29	0.62
2:H:30:PHE:CZ	2:H:148:VAL:HG21	2.35	0.61
1:C:75:ARG:HH21	1:D:91:ASN:H	1.46	0.61
1:E:94:PRO:HA	1:E:122:VAL:HA	1.82	0.61
2:G:159:MET:HG3	2:G:214:ALA:HB2	1.80	0.61
1:A:78:TYR:HB3	1:C:60:LEU:HD21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:63:ILE:HG12	2:H:162:LEU:HD22	1.83	0.61
3:I:151:ARG:HH21	3:I:151:ARG:CG	2.13	0.61
1:A:39:THR:HB	1:A:85:GLU:HB2	1.81	0.61
2:G:112:PHE:HD2	2:G:217:VAL:CG1	2.12	0.61
1:B:24:LEU:HD13	2:H:100:LEU:HD13	1.83	0.61
3:J:107:ALA:HB2	3:J:125:VAL:HG21	1.83	0.61
1:B:28:VAL:HG13	2:H:193:MET:HE3	1.82	0.61
3:J:17:LYS:HD2	3:J:20:SER:HA	1.81	0.61
2:G:159:MET:CB	2:G:214:ALA:HB1	2.29	0.61
1:E:27:ARG:HH11	1:E:27:ARG:CG	2.13	0.60
2:G:65:VAL:CG2	5:G:301:LPP:H201	2.30	0.60
2:G:159:MET:CE	2:G:213:PHE:CE1	2.83	0.60
2:G:89:GLN:CD	2:G:89:GLN:H	2.05	0.60
3:I:40:MET:HE2	3:I:205:LEU:CA	2.15	0.60
3:I:47:LYS:HZ2	3:I:203:HIS:CE1	2.20	0.60
3:J:172:PHE:HZ	3:J:200:VAL:HG11	1.66	0.60
1:A:144:LYS:HA	1:A:148:ASN:HD22	1.65	0.60
3:I:172:PHE:CZ	3:I:200:VAL:HG11	2.36	0.60
3:J:130:GLN:HG2	4:L:93:SER:HG	1.66	0.60
1:E:106:LEU:HG	1:E:107:LEU:HD12	1.83	0.60
2:H:212:VAL:HG11	2:H:257:LEU:HG	1.84	0.60
1:F:32:SER:O	1:F:34:GLY:N	2.35	0.59
3:J:59:ARG:NH1	3:J:73:PRO:O	2.35	0.59
2:G:63:ILE:HG12	2:G:162:LEU:HD22	1.83	0.59
3:J:168:TYR:HB3	3:J:171:PRO:HB3	1.82	0.59
3:I:177:PRO:CG	3:J:243:PHE:CZ	2.84	0.59
2:G:122:ALA:HB1	2:H:236:SER:CB	2.19	0.59
2:H:220:ILE:HG22	5:H:301:LPP:H301	1.84	0.59
3:I:12:LYS:HD3	3:I:66:TRP:HD1	1.68	0.59
3:J:45:CYS:HG	3:J:218:VAL:HG12	1.60	0.59
3:J:85:LYS:HZ2	3:J:113:HIS:HB3	1.67	0.59
2:G:127:MET:SD	2:G:147:ILE:HD12	2.43	0.59
3:I:46:GLY:HA2	6:I:301:AD9:PB	2.42	0.59
3:J:170:GLU:HB3	3:J:173:VAL:CG2	2.33	0.59
3:I:85:LYS:HZ2	3:I:113:HIS:HB3	1.67	0.59
2:G:210:SER:O	2:G:214:ALA:CB	2.50	0.59
1:F:124:LYS:HD3	1:F:127:SER:HB3	1.84	0.59
3:I:59:ARG:NH1	3:I:73:PRO:O	2.35	0.59
2:H:100:LEU:HD23	2:H:202:ASP:HB3	1.85	0.59
3:J:172:PHE:HE1	3:J:202:SER:HG	1.51	0.58
1:D:74:ASP:OD2	1:D:77:SER:OG	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:151:ARG:HH21	2:G:151:ARG:CG	2.14	0.58
3:I:167:LEU:HB3	3:I:199:ILE:HB	1.84	0.58
3:I:265:LEU:CD2	4:L:94:LEU:HD21	2.32	0.58
3:I:68:ASN:OD1	3:I:86:GLN:NE2	2.36	0.58
1:B:62:GLY:HA3	1:F:49:ILE:H	1.68	0.58
3:I:142:PRO:O	3:I:150:LYS:HE2	2.03	0.58
3:J:12:LYS:HD3	3:J:66:TRP:HD1	1.68	0.58
4:K:54:SER:N	4:K:84:ASP:OD2	2.35	0.58
1:A:106:LEU:HD12	1:B:138:LEU:CD1	2.32	0.58
3:I:179:ALA:O	3:I:182:VAL:HG12	2.04	0.58
1:A:103:THR:HG22	1:A:110:LYS:HG2	1.84	0.58
3:I:151:ARG:NH2	3:I:151:ARG:HG3	2.17	0.58
4:K:84:ASP:HA	4:K:87:GLU:HG3	1.86	0.58
5:H:304:LPP:HC81	5:H:304:LPP:C13	2.33	0.58
1:F:7:GLU:O	1:F:10:VAL:CG2	2.40	0.58
4:L:77:SER:HA	4:L:99:PRO:CG	2.33	0.58
2:G:48:LEU:O	2:G:52:LEU:HB2	2.04	0.57
4:K:44:LEU:HD12	4:K:44:LEU:H	1.68	0.57
3:J:201:VAL:HG12	3:J:201:VAL:O	2.02	0.57
1:B:103:THR:OG1	1:B:110:LYS:NZ	2.37	0.57
3:J:68:ASN:OD1	3:J:86:GLN:NE2	2.36	0.57
3:J:170:GLU:HB3	3:J:173:VAL:HG22	1.86	0.57
4:L:62:LEU:HD11	4:L:85:MET:SD	2.43	0.57
3:I:265:LEU:HD21	4:L:94:LEU:HD21	1.85	0.57
3:J:224:LEU:HB2	3:J:240:ILE:HD11	1.86	0.57
2:G:209:LYS:HG2	2:G:213:PHE:HE2	1.69	0.57
1:C:65:ILE:HG23	1:C:90:VAL:HG21	1.86	0.57
2:H:30:PHE:HZ	2:H:222:VAL:HG13	1.69	0.57
2:H:90:ALA:HB1	2:H:93:GLN:HE22	1.63	0.57
3:I:50:LEU:HD12	3:I:50:LEU:C	2.24	0.57
4:L:44:LEU:H	4:L:44:LEU:HD12	1.68	0.57
1:D:65:ILE:HG23	1:D:90:VAL:HG11	1.86	0.57
1:E:38:ASP:O	1:E:88:GLN:HB2	2.04	0.57
2:G:66:SER:HB2	2:H:251:LEU:HD22	1.87	0.57
3:I:177:PRO:HG3	3:J:243:PHE:CE1	2.39	0.57
3:J:23:ILE:O	3:J:221:GLY:HA2	2.03	0.57
3:I:230:ASP:OD1	3:I:230:ASP:N	2.37	0.57
2:G:220:ILE:HD11	2:G:246:ALA:HA	1.86	0.56
2:H:154:ALA:O	2:H:158:SER:HB3	2.05	0.56
3:I:179:ALA:O	3:I:182:VAL:CG1	2.53	0.56
1:A:48:ASN:N	1:A:134:SER:OG	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:105:PRO:C	2:G:213:PHE:CZ	2.79	0.56
2:G:159:MET:HE1	2:G:213:PHE:HE1	1.71	0.56
3:I:46:GLY:HA2	6:I:301:AD9:O1B	2.06	0.56
3:J:90:LEU:HD22	3:J:155:LEU:HB2	1.87	0.56
2:H:89:GLN:CD	2:H:89:GLN:H	2.08	0.56
1:E:23:LEU:HD23	1:E:26:LEU:HB2	1.87	0.56
4:L:31:GLN:HA	4:L:35:LEU:HD12	1.87	0.56
3:I:11:LEU:HD11	3:I:54:ILE:HG22	1.87	0.56
4:L:66:ILE:HG23	4:L:76:LEU:HD21	1.87	0.56
1:E:99:ALA:HB1	1:E:112:ILE:HD11	1.87	0.56
3:I:265:LEU:CG	4:L:94:LEU:HD11	2.36	0.56
4:K:90:LYS:O	4:K:90:LYS:HG2	2.06	0.56
3:I:224:LEU:HB2	3:I:240:ILE:HD11	1.86	0.56
4:K:31:GLN:HA	4:K:35:LEU:HD12	1.87	0.56
4:K:66:ILE:HG23	4:K:76:LEU:HD21	1.87	0.56
1:A:14:LEU:HD12	2:H:28:THR:CG2	2.33	0.55
1:A:106:LEU:HD12	1:B:138:LEU:HD12	1.88	0.55
2:H:65:VAL:HG21	5:H:304:LPP:H172	1.88	0.55
3:I:168:TYR:CD1	3:I:168:TYR:N	2.73	0.55
3:J:11:LEU:HD11	3:J:54:ILE:HG22	1.87	0.55
4:K:47:ASP:HB3	4:K:79:ARG:HB2	1.89	0.55
1:A:49:ILE:HG13	1:C:62:GLY:HA3	1.88	0.55
1:E:24:LEU:HD11	2:H:181:TRP:CH2	2.42	0.55
1:E:49:ILE:HD11	1:F:63:VAL:HB	1.88	0.55
2:G:55:VAL:HG22	2:G:120:LEU:HD13	1.88	0.55
2:H:89:GLN:OE1	2:H:89:GLN:N	2.35	0.55
3:I:127:MET:HE1	4:K:59:ILE:CG2	2.36	0.55
1:A:46:PHE:HD2	1:A:49:ILE:HG22	1.71	0.55
5:G:303:LPP:H362	5:G:303:LPP:H162	1.87	0.55
2:G:209:LYS:O	2:G:213:PHE:CD2	2.60	0.55
3:J:51:LEU:HD11	3:J:167:LEU:HB3	1.88	0.55
3:I:264:ASP:OD1	3:J:122:ARG:NH2	2.39	0.55
4:L:90:LYS:HA	4:L:95:LEU:HD23	1.89	0.55
2:G:209:LYS:HG2	2:G:213:PHE:CE2	2.42	0.55
1:C:59:THR:HA	1:C:65:ILE:HG13	1.89	0.55
1:C:104:ALA:HB3	1:C:108:GLY:HA3	1.89	0.55
3:I:106:VAL:HG21	3:I:129:LEU:HD21	1.88	0.55
2:H:51:GLN:HG2	2:H:150:PRO:HB2	1.88	0.54
3:J:87:PHE:HB3	3:J:165:ILE:HG12	1.89	0.54
1:C:99:ALA:O	1:C:132:THR:OG1	2.24	0.54
1:D:49:ILE:H	1:E:62:GLY:HA3	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:212:VAL:HG11	2:G:257:LEU:HG	1.89	0.54
3:J:39:ILE:HD12	3:J:50:LEU:HD23	1.89	0.54
2:G:82:LEU:HD21	5:G:303:LPP:H332	1.88	0.54
2:G:159:MET:HG2	2:G:214:ALA:CA	2.33	0.54
5:H:304:LPP:C12	5:H:304:LPP:C8	2.86	0.54
3:I:45:CYS:CB	3:I:218:VAL:O	2.55	0.54
3:J:40:MET:CE	3:J:243:PHE:HE1	2.19	0.54
1:A:15:LEU:HD21	5:H:302:LPP:H361	1.88	0.54
4:L:66:ILE:HG12	4:L:76:LEU:HD11	1.90	0.54
3:J:256:TYR:CD2	3:J:257:PRO:HD2	2.43	0.54
1:F:58:VAL:HB	1:F:112:ILE:HD11	1.89	0.54
1:A:49:ILE:H	1:C:62:GLY:HA3	1.73	0.54
1:A:72:ASP:OD2	1:A:81:ARG:NH2	2.41	0.54
2:G:105:PRO:O	2:G:213:PHE:CZ	2.60	0.54
3:I:243:PHE:CZ	3:J:177:PRO:HD2	2.42	0.54
1:F:59:THR:HB	1:F:64:THR:HA	1.91	0.53
1:A:44:ALA:HA	1:A:129:ILE:HG22	1.90	0.53
1:A:44:ALA:HB3	1:A:82:VAL:HG23	1.90	0.53
3:I:87:PHE:HB3	3:I:165:ILE:HG12	1.89	0.53
3:J:124:ILE:HG12	4:L:60:SER:HB2	1.90	0.53
1:F:44:ALA:HA	1:F:129:ILE:HG22	1.89	0.53
3:I:14:LEU:HD12	3:I:27:ILE:HD11	1.91	0.53
3:I:110:LEU:O	3:I:114:THR:OG1	2.20	0.53
3:I:167:LEU:N	3:I:167:LEU:HD13	2.23	0.53
3:J:131:ALA:HB1	4:L:91:VAL:HG23	1.90	0.53
1:A:41:LYS:HA	1:A:84:MET:O	2.09	0.53
1:C:21:LEU:HD23	1:C:24:LEU:HD21	1.90	0.53
3:I:23:ILE:O	3:I:221:GLY:HA2	2.08	0.53
3:I:166:LEU:CD2	3:I:197:THR:O	2.54	0.53
1:C:69:THR:OG1	1:C:83:THR:HG23	2.09	0.52
2:G:209:LYS:HA	2:G:212:VAL:CG1	2.39	0.52
4:K:66:ILE:HG12	4:K:76:LEU:HD11	1.90	0.52
1:C:60:LEU:HB3	1:C:65:ILE:HD11	1.90	0.52
1:F:95:VAL:HG23	1:F:121:ASP:O	2.09	0.52
2:G:128:LYS:HB2	2:G:133:LEU:HD12	1.91	0.52
3:J:230:ASP:OD1	3:J:230:ASP:N	2.37	0.52
2:H:75:ALA:HA	2:H:95:VAL:HG21	1.91	0.52
2:G:62:ILE:HD12	2:H:248:LEU:CD1	2.40	0.52
2:G:232:SER:HB2	2:H:232:SER:HB2	1.91	0.52
3:J:39:ILE:HG12	3:J:201:VAL:HG22	1.90	0.52
3:I:187:ILE:HD11	3:I:211:ILE:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:155:LEU:O	3:I:159:ILE:HG23	2.10	0.52
1:B:47:ASP:HB2	1:B:134:SER:HB2	1.92	0.52
1:F:43:TYR:CD1	1:F:83:THR:HG22	2.44	0.52
2:H:121:THR:HG21	2:H:224:GLN:HB3	1.90	0.52
2:H:209:LYS:O	2:H:212:VAL:HG13	2.10	0.52
2:G:112:PHE:CD2	2:G:217:VAL:CG1	2.89	0.52
3:I:90:LEU:HD23	3:I:168:TYR:CD2	2.34	0.52
1:A:106:LEU:HD23	1:B:107:LEU:HD21	1.92	0.52
2:G:52:LEU:CD2	2:G:157:ILE:HD11	2.39	0.52
3:J:194:LEU:HB3	3:J:196:ILE:HG23	1.92	0.52
2:G:59:SER:O	2:G:59:SER:OG	2.27	0.51
2:H:30:PHE:CE1	2:H:148:VAL:HG21	2.45	0.51
2:G:30:PHE:CZ	2:G:148:VAL:CG2	2.93	0.51
3:J:14:LEU:HD12	3:J:27:ILE:HD11	1.91	0.51
1:F:120:GLU:OE1	1:F:120:GLU:HA	2.07	0.51
3:I:39:ILE:HG13	3:I:39:ILE:O	2.10	0.51
3:I:261:TYR:HA	3:J:135:ARG:NH1	2.12	0.51
3:I:166:LEU:HD11	3:I:196:ILE:CG1	2.41	0.51
6:I:301:AD9:H2'	6:I:301:AD9:N3	2.26	0.51
4:K:52:GLU:OE2	4:K:53:ARG:N	2.44	0.51
1:A:73:LEU:HD22	1:A:79:THR:O	2.11	0.51
3:I:219:GLY:HA3	3:I:224:LEU:HD11	1.93	0.51
4:L:64:ALA:HA	4:L:67:ARG:HH21	1.74	0.51
2:G:98:THR:HG22	5:G:303:LPP:H182	1.93	0.51
3:J:187:ILE:HD11	3:J:211:ILE:HG12	1.92	0.51
3:J:235:THR:HG23	3:J:237:ASP:H	1.76	0.51
3:I:194:LEU:HB3	3:I:196:ILE:HG23	1.92	0.51
1:A:63:VAL:HG11	1:B:73:LEU:HB2	1.93	0.50
1:C:69:THR:CG2	1:C:85:GLU:HG3	2.41	0.50
3:I:151:ARG:CG	3:I:151:ARG:NH2	2.73	0.50
3:I:235:THR:HG23	3:I:237:ASP:H	1.76	0.50
3:J:219:GLY:HA3	3:J:224:LEU:HD11	1.93	0.50
2:H:94:MET:HA	5:H:303:LPP:H162	1.93	0.50
3:I:52:ARG:O	3:I:56:SER:N	2.44	0.50
3:I:172:PHE:CD1	3:I:172:PHE:N	2.79	0.50
4:K:14:LEU:HD22	4:K:37:ARG:NH1	2.26	0.50
2:G:219:TRP:CZ3	5:G:302:LPP:H152	2.46	0.50
2:H:209:LYS:HA	2:H:212:VAL:CG1	2.41	0.50
3:I:166:LEU:N	3:I:166:LEU:CD2	2.73	0.50
4:L:52:GLU:OE2	4:L:53:ARG:N	2.44	0.50
1:B:93:LEU:HD23	1:B:123:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:ARG:HH21	1:D:91:ASN:N	2.10	0.50
2:G:145:LYS:O	2:G:149:ALA:HB3	2.12	0.50
3:J:171:PRO:HD2	3:J:202:SER:HB3	1.94	0.50
4:K:84:ASP:OD1	4:K:84:ASP:N	2.44	0.50
3:I:151:ARG:HH21	3:I:151:ARG:HG3	1.73	0.50
5:G:302:LPP:H412	5:H:304:LPP:H262	1.94	0.50
3:I:174:GLY:HA2	3:J:173:VAL:HG12	1.93	0.50
1:A:69:THR:OG1	1:A:83:THR:HG23	2.11	0.50
1:A:75:ARG:HH12	1:C:92:ASN:H	1.59	0.50
2:H:121:THR:HG23	2:H:225:GLY:H	1.73	0.50
3:J:87:PHE:HA	3:J:165:ILE:O	2.12	0.50
3:J:116:LEU:HB2	3:J:121:ILE:HG13	1.93	0.50
4:L:14:LEU:HD22	4:L:37:ARG:NH1	2.26	0.50
4:L:58:GLY:HA3	4:L:85:MET:CE	2.42	0.50
1:D:121:ASP:OD1	1:D:121:ASP:N	2.44	0.50
3:J:262:ARG:HA	4:K:97:ILE:CD1	2.06	0.50
2:G:210:SER:O	2:G:214:ALA:HB3	2.12	0.49
2:H:94:MET:HB2	5:H:303:LPP:H151	1.94	0.49
2:H:144:LEU:CA	2:H:148:VAL:HG11	2.23	0.49
3:I:51:LEU:HD21	3:I:201:VAL:HG21	1.94	0.49
3:J:217:ILE:HD11	3:J:232:LEU:HD21	1.94	0.49
4:L:14:LEU:HB3	4:L:46:VAL:HB	1.94	0.49
1:B:99:ALA:HB2	1:B:114:ILE:HG23	1.93	0.49
2:G:77:GLN:NE2	2:H:262:PHE:O	2.46	0.49
2:G:105:PRO:HB2	2:G:213:PHE:CE2	2.42	0.49
2:H:59:SER:O	2:H:59:SER:OG	2.27	0.49
2:H:62:ILE:HD11	2:H:111:LEU:HD22	1.94	0.49
2:H:76:LEU:HD12	2:H:182:LEU:HD11	1.93	0.49
1:A:6:LEU:O	1:A:10:VAL:HG23	2.13	0.49
2:G:151:ARG:CG	2:G:151:ARG:NH2	2.73	0.49
2:H:145:LYS:O	2:H:149:ALA:HB3	2.12	0.49
3:I:49:THR:N	6:I:301:AD9:O1A	2.46	0.49
1:F:60:LEU:H	1:F:65:ILE:HG12	1.77	0.49
2:G:105:PRO:O	2:G:213:PHE:CE1	2.65	0.49
4:K:32:GLY:HA2	4:K:36:ILE:HB	1.94	0.49
1:D:44:ALA:HB3	1:D:82:VAL:HG22	1.95	0.49
2:G:76:LEU:HD12	2:G:182:LEU:HD11	1.93	0.49
3:J:265:LEU:O	4:K:67:ARG:NH1	2.46	0.49
1:D:10:VAL:CG2	2:G:53:TYR:HB2	2.43	0.49
3:I:14:LEU:HD11	3:I:53:LEU:HD13	1.95	0.49
1:A:20:ALA:HA	1:A:24:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:PHE:HD1	1:F:132:THR:HG21	1.78	0.49
2:G:62:ILE:HD11	2:G:111:LEU:HD22	1.94	0.49
2:G:154:ALA:O	2:G:158:SER:HB3	2.12	0.49
2:G:156:PHE:CZ	2:G:215:PHE:CD1	3.01	0.49
2:G:159:MET:HE1	2:G:213:PHE:CE1	2.46	0.49
3:I:166:LEU:O	3:I:166:LEU:HD23	2.13	0.49
4:K:28:LEU:HD23	4:K:31:GLN:HE21	1.78	0.49
2:H:121:THR:CG2	2:H:225:GLY:CA	2.90	0.49
1:A:138:LEU:HD21	1:C:106:LEU:HD12	1.93	0.49
1:E:69:THR:OG1	1:E:83:THR:HG23	2.13	0.49
1:E:89:ASN:N	1:E:89:ASN:OD1	2.45	0.49
2:G:144:LEU:CA	2:G:148:VAL:HG11	2.27	0.49
2:H:70:ILE:HG21	2:H:166:PHE:CZ	2.48	0.49
2:H:75:ALA:HA	2:H:95:VAL:CG2	2.43	0.49
4:L:58:GLY:HA3	4:L:85:MET:HE2	1.95	0.49
1:D:17:GLY:HA3	2:G:161:LEU:HD12	1.95	0.48
2:G:65:VAL:HG23	5:G:301:LPP:H201	1.95	0.48
4:K:83:ASP:O	4:K:87:GLU:HG3	2.12	0.48
1:A:62:GLY:HA3	1:B:49:ILE:HG13	1.95	0.48
1:B:143:GLY:HA2	1:B:147:LEU:HD13	1.94	0.48
1:D:28:VAL:HG13	2:G:193:MET:HE3	1.95	0.48
2:H:51:GLN:HG3	2:H:151:ARG:HD3	1.96	0.48
3:I:262:ARG:HD3	4:L:97:ILE:HG23	1.94	0.48
4:L:28:LEU:HD23	4:L:31:GLN:HE21	1.77	0.48
4:L:32:GLY:HA2	4:L:36:ILE:HB	1.94	0.48
1:B:106:LEU:HD23	1:B:107:LEU:HG	1.95	0.48
2:G:145:LYS:HA	2:G:149:ALA:HB2	1.94	0.48
2:H:88:GLU:OE1	2:H:88:GLU:HA	2.13	0.48
3:I:85:LYS:HG3	3:I:113:HIS:CD2	2.48	0.48
3:J:10:GLU:HG2	3:J:30:ARG:HG2	1.95	0.48
3:J:96:LEU:HB3	3:J:105:ASN:HD21	1.78	0.48
1:B:49:ILE:HD13	1:B:71:VAL:HG21	1.95	0.48
2:G:58:LEU:O	5:G:301:LPP:HC82	2.13	0.48
2:G:70:ILE:HG21	2:G:166:PHE:CZ	2.48	0.48
3:I:183:LEU:O	3:I:187:ILE:HG23	2.13	0.48
4:K:10:ALA:H	4:K:40:GLN:NE2	2.12	0.48
4:K:14:LEU:HB3	4:K:46:VAL:HB	1.94	0.48
1:D:13:PHE:CD2	2:G:60:LEU:HG	2.48	0.48
2:G:105:PRO:CA	2:G:213:PHE:HZ	2.26	0.48
3:I:217:ILE:HD11	3:I:232:LEU:HD21	1.94	0.48
3:J:45:CYS:HG	3:J:218:VAL:CG1	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:103:PHE:CE1	3:J:122:ARG:HG3	2.47	0.48
1:E:46:PHE:CD2	1:E:101:ILE:HD11	2.48	0.48
2:G:137:GLU:HG2	2:G:143:PRO:HD3	1.96	0.48
3:I:80:LEU:O	3:I:84:ARG:HG2	2.14	0.48
3:J:131:ALA:HB1	4:L:91:VAL:CG2	2.44	0.48
3:I:87:PHE:HA	3:I:165:ILE:O	2.12	0.48
3:I:107:ALA:HB2	3:I:125:VAL:HG21	1.94	0.48
3:J:85:LYS:HG3	3:J:113:HIS:CD2	2.48	0.48
4:L:10:ALA:H	4:L:40:GLN:NE2	2.12	0.48
1:C:28:VAL:HG21	2:G:176:MET:HG3	1.96	0.48
2:H:75:ALA:CA	2:H:95:VAL:HG21	2.44	0.48
2:H:100:LEU:CD2	2:H:202:ASP:HB3	2.43	0.48
2:H:177:VAL:O	2:H:181:TRP:HB2	2.14	0.48
3:J:80:LEU:O	3:J:84:ARG:HG2	2.14	0.48
3:J:126:LEU:HD12	3:J:135:ARG:HE	1.79	0.48
1:E:44:ALA:HA	1:E:129:ILE:HG22	1.95	0.48
2:G:177:VAL:O	2:G:181:TRP:HB2	2.14	0.48
1:A:136:LEU:HD12	1:A:141:LEU:HD12	1.95	0.48
1:B:102:LEU:HB2	1:B:111:TYR:CE1	2.49	0.48
4:L:78:VAL:CG2	4:L:99:PRO:O	2.59	0.48
1:A:46:PHE:HD1	1:A:132:THR:HG21	1.78	0.47
2:G:105:PRO:C	2:G:213:PHE:HZ	2.16	0.47
2:G:251:LEU:HD22	2:H:66:SER:HB2	1.96	0.47
2:H:99:LEU:O	2:H:104:GLY:CA	2.62	0.47
2:H:212:VAL:HG22	2:H:253:LEU:HD23	1.96	0.47
2:G:132:GLN:NE2	3:I:98:THR:H	2.11	0.47
2:H:37:GLY:H	2:H:145:LYS:NZ	2.12	0.47
2:H:245:TYR:CE2	5:H:301:LPP:HC62	2.49	0.47
3:I:91:PHE:HD1	3:I:169:ASP:OD2	1.97	0.47
3:I:96:LEU:HB3	3:I:105:ASN:HD21	1.78	0.47
1:B:92:ASN:ND2	1:F:75:ARG:HB3	2.29	0.47
2:G:51:GLN:OE1	2:G:51:GLN:HA	2.13	0.47
2:H:30:PHE:CZ	2:H:222:VAL:HG13	2.47	0.47
4:K:32:GLY:O	4:K:37:ARG:HG2	2.15	0.47
2:G:240:THR:HG1	2:H:118:SER:HG	1.57	0.47
2:H:233:GLU:HG3	2:H:237:ARG:HH11	1.79	0.47
3:I:10:GLU:HG2	3:I:30:ARG:HG2	1.96	0.47
3:I:122:ARG:HG2	3:I:126:LEU:CD2	2.43	0.47
3:I:262:ARG:HA	4:L:97:ILE:HD12	1.95	0.47
4:L:32:GLY:O	4:L:37:ARG:HG2	2.14	0.47
1:E:49:ILE:H	1:F:62:GLY:HA3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:ARG:HB2	1:F:92:ASN:ND2	2.30	0.47
1:E:130:HIS:CD2	1:E:130:HIS:H	2.33	0.47
2:G:37:GLY:H	2:G:145:LYS:NZ	2.12	0.47
2:G:105:PRO:CB	2:G:213:PHE:CZ	2.70	0.47
5:G:302:LPP:H412	5:H:304:LPP:C26	2.45	0.47
2:H:137:GLU:HG2	2:H:143:PRO:HD3	1.96	0.47
2:H:220:ILE:HD11	2:H:246:ALA:CA	2.45	0.47
3:J:40:MET:HE2	3:J:243:PHE:HE1	1.79	0.47
3:J:89:VAL:HG13	3:J:167:LEU:HD23	1.96	0.47
3:J:171:PRO:O	3:J:183:LEU:CD2	2.63	0.47
2:G:78:GLY:O	2:G:82:LEU:HG	2.15	0.47
2:G:233:GLU:HG3	2:G:237:ARG:HH11	1.79	0.47
3:J:102:VAL:HG13	3:J:153:VAL:HG21	1.96	0.47
3:J:127:MET:HE1	4:L:59:ILE:HG22	1.96	0.47
1:F:31:LEU:HD23	1:F:31:LEU:H	1.80	0.47
2:G:209:LYS:O	2:G:212:VAL:HG13	2.14	0.47
5:G:301:LPP:O28	5:G:301:LPP:HC7	2.15	0.47
2:H:98:THR:HG22	5:H:303:LPP:C22	2.44	0.47
3:I:165:ILE:HB	3:I:197:THR:HB	1.96	0.47
3:J:165:ILE:HB	3:J:197:THR:HB	1.96	0.47
1:E:44:ALA:HB3	1:E:82:VAL:HG13	1.97	0.46
3:I:15:THR:HG21	3:I:62:LYS:HE3	1.97	0.46
3:J:15:THR:HG21	3:J:62:LYS:HE3	1.97	0.46
1:E:59:THR:OG1	1:E:60:LEU:N	2.47	0.46
1:F:46:PHE:HD2	1:F:49:ILE:HG22	1.80	0.46
2:G:97:LEU:HD23	5:G:303:LPP:H172	1.97	0.46
4:K:91:VAL:HB	4:K:92:SER:H	1.64	0.46
4:L:69:ALA:HB3	4:L:76:LEU:HD22	1.97	0.46
2:G:132:GLN:NE2	3:I:97:PHE:HA	2.30	0.46
2:G:149:ALA:HB3	2:G:150:PRO:HD3	1.96	0.46
2:G:209:LYS:O	2:G:213:PHE:CE2	2.69	0.46
3:J:190:LEU:O	3:J:194:LEU:HB2	2.16	0.46
2:H:151:ARG:HG2	2:H:151:ARG:NH1	2.31	0.46
3:I:11:LEU:HG	3:I:65:VAL:HG12	1.98	0.46
1:B:99:ALA:HA	1:B:114:ILE:HA	1.96	0.46
1:F:101:ILE:HA	1:F:112:ILE:HG22	1.97	0.46
2:G:244:VAL:HG11	5:H:304:LPP:H121	1.97	0.46
3:I:190:LEU:O	3:I:194:LEU:HB2	2.16	0.46
4:L:10:ALA:H	4:L:40:GLN:CD	2.18	0.46
4:L:10:ALA:N	4:L:40:GLN:OE1	2.47	0.46
1:A:88:GLN:O	1:A:91:ASN:ND2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:60:SER:O	4:L:64:ALA:N	2.48	0.46
2:H:116:ALA:O	2:H:120:LEU:HB2	2.16	0.46
3:J:262:ARG:HH11	4:K:97:ILE:HA	1.79	0.46
5:G:303:LPP:H401	2:H:98:THR:HG21	1.97	0.46
1:B:122:VAL:HG12	1:B:123:LEU:HB2	1.98	0.46
3:I:238:PRO:HA	3:I:241:ARG:HG2	1.98	0.46
3:J:175:GLN:CB	3:J:180:MET:HB2	2.45	0.46
4:K:10:ALA:H	4:K:40:GLN:CD	2.18	0.46
2:G:210:SER:O	2:G:214:ALA:HB2	2.16	0.46
2:H:260:LEU:HD23	2:H:260:LEU:HA	1.69	0.46
6:J:301:AD9:H5'2	6:J:301:AD9:O1B	2.15	0.46
4:L:78:VAL:HG22	4:L:99:PRO:HD2	1.98	0.46
3:J:238:PRO:HA	3:J:241:ARG:HG2	1.98	0.45
2:G:82:LEU:CD2	5:G:303:LPP:H332	2.46	0.45
2:H:147:ILE:HG23	2:H:151:ARG:NH2	2.32	0.45
3:I:242:GLN:HA	3:I:247:ILE:HG21	1.98	0.45
3:J:70:GLN:OE1	3:J:70:GLN:N	2.45	0.45
3:J:242:GLN:HA	3:J:247:ILE:HG21	1.98	0.45
1:C:100:SER:OG	1:C:133:GLN:HB2	2.17	0.45
4:K:69:ALA:HB3	4:K:76:LEU:HD22	1.97	0.45
4:L:8:GLU:HB2	4:L:15:GLN:HB2	1.98	0.45
1:A:92:ASN:ND2	1:B:75:ARG:O	2.49	0.45
1:C:9:GLY:O	1:C:12:LEU:HG	2.15	0.45
5:F:201:LPP:H331	5:H:304:LPP:H351	1.99	0.45
2:G:119:ALA:HB2	2:H:240:THR:HG21	1.97	0.45
3:I:21:ARG:NH1	6:I:301:AD9:H1'	2.32	0.45
3:I:143:ASP:N	3:I:143:ASP:OD1	2.50	0.45
3:I:259:ARG:HG3	3:I:264:ASP:HB2	1.99	0.45
1:A:43:TYR:HB2	1:A:128:THR:HB	1.98	0.45
1:D:78:TYR:HE1	1:E:92:ASN:HB2	1.82	0.45
1:E:59:THR:HB	1:E:64:THR:HA	1.99	0.45
5:G:301:LPP:H202	5:G:301:LPP:H172	1.42	0.45
1:B:31:LEU:HD23	1:B:31:LEU:HA	1.87	0.45
1:C:55:ARG:CD	2:G:187:GLY:HA3	2.47	0.45
1:D:59:THR:OG1	1:D:60:LEU:N	2.50	0.45
1:D:91:ASN:N	1:D:91:ASN:OD1	2.49	0.45
2:G:41:PRO:HG2	3:I:81:PHE:CZ	2.51	0.45
2:G:98:THR:HG22	5:G:303:LPP:C19	2.46	0.45
3:J:114:THR:CG2	4:L:22:TYR:HB2	2.47	0.45
1:C:137:VAL:HG21	1:D:102:LEU:HD13	1.97	0.45
1:F:94:PRO:HD2	1:F:116:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:53:TYR:CD1	2:G:53:TYR:C	2.89	0.45
2:H:78:GLY:HA2	2:H:81:ILE:HG23	1.97	0.45
3:I:46:GLY:HA2	6:I:301:AD9:O2B	2.17	0.45
4:L:20:LEU:HB2	4:L:54:SER:OG	2.17	0.45
2:H:219:TRP:O	2:H:219:TRP:CD1	2.70	0.45
3:J:11:LEU:HG	3:J:65:VAL:HG12	1.97	0.45
4:K:94:LEU:H	4:K:95:LEU:HD23	1.81	0.45
2:G:189:PHE:O	2:G:193:MET:HB2	2.17	0.45
3:I:103:PHE:HB2	3:I:138:VAL:HG22	1.98	0.45
4:L:54:SER:N	4:L:84:ASP:OD2	2.49	0.45
4:L:67:ARG:HB3	4:L:67:ARG:CZ	2.47	0.45
1:B:48:ASN:N	1:B:134:SER:OG	2.50	0.45
1:E:2:GLN:O	1:E:5:THR:OG1	2.23	0.45
2:G:121:THR:HG23	2:G:225:GLY:N	2.32	0.45
3:J:143:ASP:OD1	3:J:143:ASP:N	2.50	0.45
1:A:73:LEU:HD12	1:A:75:ARG:HH21	1.82	0.44
1:D:76:ASP:OD1	1:D:76:ASP:N	2.34	0.44
2:H:126:ASN:O	2:H:130:THR:HG22	2.17	0.44
2:H:189:PHE:O	2:H:193:MET:HB2	2.17	0.44
3:I:14:LEU:HD11	3:I:53:LEU:CD1	2.47	0.44
3:J:40:MET:SD	3:J:215:ILE:HD11	2.57	0.44
3:J:183:LEU:O	3:J:187:ILE:HG23	2.16	0.44
4:L:21:ASP:O	4:L:57:VAL:HG11	2.16	0.44
1:A:124:LYS:NZ	1:A:127:SER:HB3	2.32	0.44
1:A:145:PHE:HD1	1:A:146:LEU:HD12	1.83	0.44
1:D:100:SER:OG	1:D:133:GLN:HB2	2.16	0.44
2:G:98:THR:HG22	5:G:303:LPP:C18	2.47	0.44
2:H:121:THR:HG22	2:H:225:GLY:CA	2.47	0.44
5:H:304:LPP:H392	5:H:304:LPP:H361	1.87	0.44
4:K:20:LEU:HB2	4:K:54:SER:OG	2.17	0.44
1:A:102:LEU:HB2	1:A:111:TYR:CZ	2.52	0.44
1:F:69:THR:OG1	1:F:83:THR:O	2.34	0.44
2:H:99:LEU:O	2:H:104:GLY:N	2.49	0.44
1:F:56:GLY:HA2	2:H:185:TYR:OH	2.17	0.44
2:G:38:ARG:HG3	3:I:77:ARG:HH12	1.83	0.44
2:H:41:PRO:HG2	3:J:81:PHE:CZ	2.52	0.44
2:H:151:ARG:HD3	2:H:151:ARG:HA	1.82	0.44
3:J:11:LEU:O	3:J:28:ASP:HA	2.18	0.44
3:J:262:ARG:C	3:J:262:ARG:CD	2.85	0.44
2:G:62:ILE:HD12	2:H:248:LEU:HD13	1.99	0.44
2:G:224:GLN:NE2	2:G:241:ARG:HE	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:303:LPP:C12	2:H:81:ILE:HD11	2.45	0.44
2:H:152:LEU:HG	2:H:222:VAL:HG11	1.99	0.44
3:I:137:ALA:HB2	3:J:256:TYR:CE2	2.52	0.44
4:K:37:ARG:HA	4:K:37:ARG:HD2	1.77	0.44
3:I:11:LEU:HD22	3:I:29:VAL:HG22	1.99	0.44
3:I:96:LEU:HD23	3:I:157:ARG:HH21	1.83	0.44
3:I:192:ASP:OD1	3:I:193:ALA:N	2.51	0.44
3:J:192:ASP:OD1	3:J:193:ALA:N	2.51	0.44
3:J:266:LEU:HD12	4:K:70:ARG:HD2	1.99	0.44
1:A:140:ASP:O	1:A:144:LYS:HG2	2.17	0.44
1:B:13:PHE:CD2	2:H:60:LEU:HG	2.53	0.44
1:B:24:LEU:HD13	2:H:100:LEU:CD1	2.45	0.44
2:H:121:THR:OG1	2:H:242:THR:HG21	2.17	0.44
3:I:31:ILE:HD12	3:I:37:THR:HG21	1.99	0.44
3:I:203:HIS:O	3:I:205:LEU:N	2.51	0.44
3:I:237:ASP:HB3	3:I:240:ILE:HB	2.00	0.44
1:F:139:GLU:O	1:F:142:ILE:HG13	2.17	0.44
2:G:98:THR:HG22	5:G:303:LPP:H191	2.00	0.44
3:J:11:LEU:HD22	3:J:29:VAL:HG22	1.99	0.44
3:J:31:ILE:HD12	3:J:37:THR:HG21	1.99	0.44
3:J:149:MET:O	3:J:153:VAL:HG12	2.18	0.44
4:L:53:ARG:HA	4:L:84:ASP:OD2	2.18	0.44
1:E:15:LEU:HD23	1:E:15:LEU:HA	1.81	0.44
3:I:243:PHE:HA	3:J:178:ILE:HG23	2.00	0.44
3:J:96:LEU:HD23	3:J:157:ARG:HH21	1.83	0.44
3:J:103:PHE:HB2	3:J:138:VAL:HG22	1.98	0.44
1:E:73:LEU:HD22	1:E:79:THR:O	2.18	0.43
1:F:95:VAL:HG21	1:F:121:ASP:OD2	2.18	0.43
2:H:149:ALA:N	2:H:150:PRO:HD2	2.33	0.43
4:K:8:GLU:HB2	4:K:15:GLN:HB2	1.98	0.43
4:K:10:ALA:N	4:K:40:GLN:OE1	2.47	0.43
1:B:94:PRO:HA	1:B:122:VAL:HA	2.01	0.43
1:E:51:GLY:O	1:E:110:LYS:HB2	2.17	0.43
3:I:90:LEU:C	3:I:90:LEU:CD1	2.85	0.43
3:I:224:LEU:CB	3:I:240:ILE:HD11	2.49	0.43
3:J:261:TYR:CB	4:K:93:SER:CB	2.95	0.43
1:A:76:ASP:OD1	1:A:77:SER:N	2.47	0.43
2:G:98:THR:HG22	5:G:303:LPP:H161	1.99	0.43
2:H:145:LYS:HA	2:H:149:ALA:HB2	2.00	0.43
3:I:11:LEU:HB2	3:I:29:VAL:HG22	2.01	0.43
3:I:39:ILE:CG1	3:I:201:VAL:HG22	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:237:ASP:HB3	3:J:240:ILE:HB	2.00	0.43
4:K:90:LYS:HB2	4:K:90:LYS:HE2	1.72	0.43
4:L:95:LEU:HD12	4:L:96:GLU:H	1.84	0.43
4:L:96:GLU:H	4:L:96:GLU:HG3	1.67	0.43
1:A:28:VAL:HG22	1:A:30:GLY:H	1.83	0.43
1:F:73:LEU:HD22	1:F:79:THR:O	2.19	0.43
3:J:262:ARG:HH11	4:K:97:ILE:CG2	2.29	0.43
1:A:18:LEU:CB	5:H:302:LPP:H391	2.48	0.43
1:D:136:LEU:HD12	1:D:141:LEU:HD12	1.99	0.43
1:F:58:VAL:HG11	1:F:84:MET:HB2	1.99	0.43
2:G:209:LYS:HD3	2:G:254:ASP:OD1	2.19	0.43
1:D:59:THR:HG1	1:D:63:VAL:C	2.17	0.43
5:G:301:LPP:H391	5:G:301:LPP:H422	1.70	0.43
3:I:40:MET:SD	3:I:205:LEU:HD13	2.58	0.43
3:I:51:LEU:HD23	3:I:169:ASP:HB2	2.01	0.43
4:K:82:PRO:CG	4:K:85:MET:CG	2.77	0.43
1:B:63:VAL:HG11	1:F:73:LEU:HB2	2.01	0.43
1:C:46:PHE:CD2	1:C:101:ILE:HD11	2.53	0.43
2:G:126:ASN:HA	2:G:235:ILE:HD13	2.00	0.43
2:H:93:GLN:HE21	2:H:93:GLN:HB3	1.50	0.43
3:I:11:LEU:O	3:I:28:ASP:HA	2.18	0.43
3:I:169:ASP:HA	3:I:201:VAL:HB	1.99	0.43
1:A:49:ILE:HB	1:A:52:VAL:CG2	2.48	0.43
1:D:99:ALA:HB2	1:D:129:ILE:HD13	2.01	0.43
1:D:99:ALA:O	1:D:132:THR:OG1	2.29	0.43
2:G:15:ARG:O	2:G:19:ASP:HB2	2.19	0.43
3:J:11:LEU:HB2	3:J:29:VAL:HG22	2.00	0.43
4:L:64:ALA:HA	4:L:67:ARG:NH2	2.34	0.43
1:A:42:VAL:HG13	1:A:86:ILE:HD13	2.00	0.43
1:A:98:THR:HG22	1:A:115:SER:OG	2.19	0.43
1:B:24:LEU:HA	1:B:28:VAL:HB	2.01	0.43
1:C:7:GLU:O	1:C:10:VAL:HG12	2.19	0.43
2:G:58:LEU:HD22	5:G:301:LPP:C6	2.30	0.43
2:G:83:ILE:HA	2:G:88:GLU:OE1	2.19	0.43
3:I:151:ARG:HH21	3:I:151:ARG:HB2	1.83	0.43
3:I:260:ASP:HB3	3:I:263:ALA:HB3	2.01	0.43
3:J:40:MET:HE1	3:J:243:PHE:HE1	1.84	0.43
3:J:194:LEU:HD11	4:L:91:VAL:HG11	2.01	0.43
1:A:73:LEU:HB2	1:C:63:VAL:HG11	2.01	0.42
1:C:102:LEU:HB2	1:C:111:TYR:CE1	2.54	0.42
1:C:139:GLU:O	1:C:142:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:PHE:O	1:F:17:GLY:N	2.52	0.42
5:H:301:LPP:C36	5:H:302:LPP:H392	2.46	0.42
1:B:44:ALA:HA	1:B:129:ILE:HG22	2.00	0.42
1:E:27:ARG:H	1:E:27:ARG:HG3	1.46	0.42
2:G:90:ALA:CB	5:G:303:LPP:HC61	2.49	0.42
2:G:236:SER:HA	2:G:239:THR:HG22	2.01	0.42
3:J:262:ARG:HD2	3:J:262:ARG:O	2.19	0.42
1:B:36:ALA:O	1:B:39:THR:HG23	2.19	0.42
1:D:10:VAL:HG23	2:G:53:TYR:HB2	1.99	0.42
1:F:56:GLY:HA3	1:F:68:VAL:HB	2.01	0.42
1:F:93:LEU:HD11	1:F:114:ILE:HG21	2.01	0.42
2:G:50:LYS:HD2	2:G:50:LYS:C	2.33	0.42
2:G:135:SER:O	2:G:135:SER:OG	2.38	0.42
2:H:121:THR:HG23	2:H:225:GLY:CA	2.48	0.42
2:H:209:LYS:HD3	2:H:254:ASP:OD1	2.19	0.42
3:I:265:LEU:HD23	4:L:94:LEU:CD2	2.49	0.42
3:J:207:GLU:O	3:J:211:ILE:HG13	2.19	0.42
1:A:46:PHE:CD2	1:A:101:ILE:HD11	2.55	0.42
1:C:71:VAL:HG12	1:C:82:VAL:HG23	2.01	0.42
1:D:72:ASP:OD1	1:D:73:LEU:N	2.52	0.42
1:E:21:LEU:HD12	1:E:21:LEU:O	2.19	0.42
2:H:133:LEU:HD22	2:H:143:PRO:HB2	2.02	0.42
2:H:151:ARG:HG2	2:H:151:ARG:HH11	1.84	0.42
3:I:207:GLU:O	3:I:211:ILE:HG13	2.20	0.42
1:A:14:LEU:HB3	5:H:302:LPP:H412	2.01	0.42
1:E:22:LEU:HD12	2:G:256:ILE:CD1	2.47	0.42
2:G:65:VAL:HG22	5:G:301:LPP:H201	2.02	0.42
2:G:122:ALA:CB	2:H:236:SER:HB3	2.23	0.42
4:K:68:ASP:O	4:K:72:ALA:N	2.45	0.42
2:G:152:LEU:HD22	2:G:156:PHE:CZ	2.55	0.42
2:H:51:GLN:CG	2:H:150:PRO:HB2	2.49	0.42
2:H:159:MET:HG2	2:H:214:ALA:HB2	2.01	0.42
1:C:69:THR:HG22	1:C:85:GLU:HG3	2.01	0.42
1:C:90:VAL:HG12	1:C:93:LEU:HD21	2.01	0.42
1:F:14:LEU:O	1:F:18:LEU:N	2.52	0.42
2:G:209:LYS:HE3	2:G:209:LYS:HB2	1.86	0.42
2:H:100:LEU:HD21	2:H:203:VAL:HG23	2.01	0.42
2:H:209:LYS:HE3	2:H:209:LYS:HB2	1.86	0.42
2:H:236:SER:HA	2:H:239:THR:HG22	2.01	0.42
3:I:177:PRO:HG2	3:J:243:PHE:CE2	2.54	0.42
3:J:179:ALA:O	3:J:182:VAL:CG1	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:86:ARG:O	4:K:90:LYS:N	2.52	0.42
4:L:58:GLY:C	4:L:85:MET:HE1	2.40	0.42
1:A:48:ASN:H	1:A:134:SER:HG	1.67	0.42
1:A:75:ARG:NH1	1:C:91:ASN:H	2.18	0.42
1:F:55:ARG:HD3	2:H:186:GLU:OE1	2.19	0.42
2:G:38:ARG:HG3	3:I:77:ARG:HH22	1.85	0.42
3:I:70:GLN:OE1	3:I:70:GLN:N	2.45	0.42
3:J:127:MET:HE3	3:J:127:MET:HB3	1.70	0.42
3:J:224:LEU:CB	3:J:240:ILE:HD11	2.48	0.42
3:J:262:ARG:NH1	4:K:97:ILE:O	2.51	0.42
4:L:90:LYS:HE3	4:L:90:LYS:HB2	1.82	0.42
1:A:35:ASN:O	1:A:37:GLY:N	2.52	0.42
2:G:110:LEU:HD23	2:H:110:LEU:HD23	2.01	0.42
5:G:303:LPP:H391	5:G:303:LPP:H361	1.69	0.42
2:H:58:LEU:HD23	2:H:58:LEU:HA	1.89	0.42
3:I:203:HIS:O	3:J:177:PRO:HG3	2.20	0.42
3:I:265:LEU:CD2	4:L:94:LEU:HD11	2.50	0.42
3:I:265:LEU:HD23	4:L:94:LEU:HD21	2.01	0.42
3:J:96:LEU:HD11	3:J:153:VAL:HG13	2.01	0.42
3:J:203:HIS:CD2	3:J:203:HIS:H	2.38	0.42
1:C:75:ARG:NE	1:D:90:VAL:HA	2.35	0.41
3:I:167:LEU:CD2	3:I:167:LEU:N	2.73	0.41
3:J:171:PRO:CG	3:J:200:VAL:HG13	2.39	0.41
1:A:90:VAL:HG12	1:A:93:LEU:HD21	2.01	0.41
1:E:23:LEU:HA	1:E:26:LEU:CG	2.48	0.41
1:E:24:LEU:CD1	2:H:181:TRP:CH2	3.03	0.41
2:G:53:TYR:HA	2:G:57:VAL:HB	2.02	0.41
2:H:38:ARG:HG3	3:J:77:ARG:HH12	1.85	0.41
2:H:145:LYS:HB2	2:H:145:LYS:HE2	1.87	0.41
3:I:24:PHE:HE2	3:I:50:LEU:HB2	1.84	0.41
3:I:44:GLY:C	3:I:46:GLY:N	2.73	0.41
1:E:40:TYR:HB2	1:E:125:ASP:CG	2.41	0.41
1:F:25:ALA:O	1:F:28:VAL:HG23	2.21	0.41
4:K:95:LEU:N	4:K:95:LEU:CD2	2.73	0.41
1:E:6:LEU:O	1:E:10:VAL:HG23	2.21	0.41
2:G:18:LEU:HD23	2:G:18:LEU:HA	1.86	0.41
2:G:133:LEU:HD22	2:G:143:PRO:HB2	2.02	0.41
3:I:137:ALA:N	3:J:256:TYR:CD2	2.88	0.41
1:D:31:LEU:HD21	2:G:199:PHE:HB3	2.01	0.41
2:G:126:ASN:ND2	2:G:126:ASN:C	2.73	0.41
2:H:135:SER:O	2:H:135:SER:OG	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:152:LEU:HD22	2:H:156:PHE:CZ	2.55	0.41
3:I:51:LEU:HD12	3:I:51:LEU:HA	1.88	0.41
1:A:138:LEU:HD23	1:A:138:LEU:HA	1.84	0.41
2:G:245:TYR:CD2	5:G:302:LPP:HC7	2.56	0.41
3:J:41:GLY:O	3:J:243:PHE:CZ	2.74	0.41
1:A:7:GLU:OE1	2:H:26:ARG:NH2	2.54	0.41
1:A:92:ASN:N	1:A:92:ASN:OD1	2.53	0.41
1:A:142:ILE:HG13	1:A:143:GLY:N	2.36	0.41
1:C:49:ILE:HG13	1:D:62:GLY:HA3	2.01	0.41
2:G:72:MET:O	2:G:76:LEU:HB2	2.21	0.41
2:H:68:LEU:O	2:H:72:MET:HG2	2.21	0.41
2:H:80:ASN:ND2	2:H:80:ASN:C	2.73	0.41
2:H:121:THR:HG22	2:H:225:GLY:HA2	2.01	0.41
3:J:41:GLY:C	3:J:243:PHE:CE2	2.94	0.41
3:J:214:TYR:CE1	3:J:227:GLY:HA2	2.56	0.41
4:L:10:ALA:H	4:L:40:GLN:HE22	1.68	0.41
1:A:14:LEU:HD23	1:A:14:LEU:HA	1.90	0.41
2:G:72:MET:HA	2:G:177:VAL:HG11	2.03	0.41
2:H:102:GLU:O	2:H:105:PRO:HG2	2.21	0.41
2:H:156:PHE:CE1	2:H:215:PHE:HA	2.55	0.41
3:I:177:PRO:HD3	3:J:203:HIS:HB2	2.03	0.41
3:J:40:MET:HE2	3:J:40:MET:HB2	2.00	0.41
4:L:95:LEU:H	4:L:95:LEU:HG	1.53	0.41
1:A:21:LEU:N	1:A:21:LEU:CD2	2.84	0.41
1:A:49:ILE:HB	1:A:52:VAL:HG22	2.02	0.41
1:A:51:GLY:HA3	1:A:110:LYS:HD3	2.02	0.41
1:B:3:THR:OG1	1:B:4:ARG:N	2.53	0.41
1:B:141:LEU:HD12	1:B:141:LEU:HA	1.90	0.41
1:C:47:ASP:N	1:C:47:ASP:OD1	2.54	0.41
1:D:102:LEU:HB2	1:D:111:TYR:CZ	2.56	0.41
1:E:14:LEU:HD22	2:G:24:LEU:HD21	2.02	0.41
1:E:29:SER:OG	1:E:31:LEU:O	2.37	0.41
1:F:36:ALA:O	1:F:38:ASP:N	2.54	0.41
2:G:85:TYR:CZ	5:H:303:LPP:H121	2.56	0.41
3:I:128:LYS:HA	3:I:128:LYS:HD3	1.80	0.41
1:C:42:VAL:HG12	1:C:84:MET:HG2	2.03	0.41
2:G:262:PHE:O	2:H:77:GLN:NE2	2.54	0.41
2:H:94:MET:HG2	5:H:303:LPP:H172	2.03	0.41
2:H:249:ALA:HA	5:H:301:LPP:H161	2.02	0.41
3:I:124:ILE:HA	3:I:127:MET:HG2	2.03	0.41
4:K:29:ARG:NE	4:K:34:ARG:HH12	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:ARG:NE	2:G:187:GLY:HA3	2.36	0.40
2:G:72:MET:HG3	2:H:255:PHE:CD1	2.56	0.40
2:G:146:TYR:HD1	2:G:147:ILE:HG12	1.86	0.40
2:G:224:GLN:OE1	5:G:302:LPP:HC61	2.21	0.40
3:I:50:LEU:O	3:I:53:LEU:HB2	2.21	0.40
1:A:69:THR:OG1	1:A:83:THR:O	2.27	0.40
1:D:132:THR:OG1	1:D:133:GLN:N	2.54	0.40
1:E:46:PHE:HD1	1:E:132:THR:HG21	1.86	0.40
1:F:56:GLY:O	1:F:67:LYS:NZ	2.46	0.40
3:I:39:ILE:HG13	3:I:201:VAL:HG22	2.02	0.40
2:G:98:THR:CG2	5:G:303:LPP:H161	2.52	0.40
2:G:220:ILE:HD11	2:G:246:ALA:CA	2.51	0.40
5:H:303:LPP:P1	5:H:303:LPP:O9	2.79	0.40
3:J:117:PRO:HD2	3:J:120:MET:HE3	2.02	0.40
3:J:172:PHE:CZ	3:J:200:VAL:CG1	3.01	0.40
4:K:61:LEU:HD13	4:K:61:LEU:HA	1.93	0.40
1:A:26:LEU:HB3	1:A:27:ARG:H	1.67	0.40
1:A:51:GLY:O	1:A:110:LYS:HB2	2.22	0.40
1:A:110:LYS:HB3	1:A:110:LYS:HE3	1.93	0.40
1:C:74:ASP:OD1	1:C:74:ASP:N	2.55	0.40
1:E:59:THR:HG1	1:E:60:LEU:N	2.20	0.40
1:E:102:LEU:HB2	1:E:111:TYR:CZ	2.56	0.40
3:I:214:TYR:CE1	3:I:227:GLY:HA2	2.56	0.40
1:A:23:LEU:HB3	1:A:24:LEU:H	1.59	0.40
1:D:142:ILE:HD11	1:E:136:LEU:HD22	2.03	0.40
2:H:98:THR:HG22	5:H:303:LPP:H202	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	148/157 (94%)	125 (84%)	23 (16%)	0	100	100
1	B	146/157 (93%)	133 (91%)	13 (9%)	0	100	100
1	C	146/157 (93%)	128 (88%)	18 (12%)	0	100	100
1	D	146/157 (93%)	129 (88%)	17 (12%)	0	100	100
1	E	147/157 (94%)	128 (87%)	18 (12%)	1 (1%)	22	60
1	F	146/157 (93%)	122 (84%)	24 (16%)	0	100	100
2	G	256/265 (97%)	238 (93%)	18 (7%)	0	100	100
2	H	256/265 (97%)	244 (95%)	12 (5%)	0	100	100
3	I	251/269 (93%)	231 (92%)	18 (7%)	2 (1%)	19	57
3	J	257/269 (96%)	239 (93%)	17 (7%)	1 (0%)	34	71
4	K	96/102 (94%)	83 (86%)	12 (12%)	1 (1%)	15	52
4	L	95/102 (93%)	85 (90%)	10 (10%)	0	100	100
All	All	2090/2214 (94%)	1885 (90%)	200 (10%)	5 (0%)	50	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	38	ASP
3	I	204	ASP
3	I	45	CYS
4	K	91	VAL
3	J	173	VAL

5.3.2 Protein sidechains ⓘ

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	120/127 (94%)	116 (97%)	4 (3%)	38	63
1	B	119/127 (94%)	115 (97%)	4 (3%)	37	62
1	C	119/127 (94%)	115 (97%)	4 (3%)	37	62
1	D	119/127 (94%)	117 (98%)	2 (2%)	60	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	120/127 (94%)	108 (90%)	12 (10%)	7	30
1	F	117/127 (92%)	112 (96%)	5 (4%)	29	57
2	G	201/209 (96%)	171 (85%)	30 (15%)	3	18
2	H	202/209 (97%)	167 (83%)	35 (17%)	2	13
3	I	208/224 (93%)	173 (83%)	35 (17%)	2	15
3	J	211/224 (94%)	177 (84%)	34 (16%)	2	16
4	K	74/80 (92%)	56 (76%)	18 (24%)	0	5
4	L	74/80 (92%)	54 (73%)	20 (27%)	0	3
All	All	1684/1788 (94%)	1481 (88%)	203 (12%)	8	24

All (203) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	PHE
1	A	15	LEU
1	A	21	LEU
1	A	125	ASP
1	B	15	LEU
1	B	31	LEU
1	B	97	SER
1	B	106	LEU
1	C	40	TYR
1	C	42	VAL
1	C	124	LYS
1	C	125	ASP
1	D	38	ASP
1	D	64	THR
1	E	19	LEU
1	E	21	LEU
1	E	22	LEU
1	E	23	LEU
1	E	24	LEU
1	E	26	LEU
1	E	27	ARG
1	E	41	LYS
1	E	59	THR
1	E	75	ARG
1	E	112	ILE
1	E	125	ASP

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Mol	Chain	Res	Type
1	F	10	VAL
1	F	120	GLU
1	F	123	LEU
1	F	125	ASP
1	F	136	LEU
2	G	7	LEU
2	G	15	ARG
2	G	19	ASP
2	G	24	LEU
2	G	30	PHE
2	G	36	LEU
2	G	52	LEU
2	G	53	TYR
2	G	54	SER
2	G	60	LEU
2	G	62	ILE
2	G	66	SER
2	G	91	VAL
2	G	95	VAL
2	G	100	LEU
2	G	115	ARG
2	G	118	SER
2	G	123	GLU
2	G	124	ILE
2	G	126	ASN
2	G	184	VAL
2	G	188	SER
2	G	195	ASN
2	G	201	GLU
2	G	208	ILE
2	G	212	VAL
2	G	216	VAL
2	G	231	THR
2	G	232	SER
2	G	254	ASP
2	H	7	LEU
2	H	15	ARG
2	H	19	ASP
2	H	24	LEU
2	H	30	PHE
2	H	36	LEU
2	H	60	LEU

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Mol	Chain	Res	Type
2	H	62	ILE
2	H	66	SER
2	H	80	ASN
2	H	81	ILE
2	H	87	SER
2	H	89	GLN
2	H	91	VAL
2	H	93	GLN
2	H	97	LEU
2	H	101	ARG
2	H	115	ARG
2	H	118	SER
2	H	151	ARG
2	H	184	VAL
2	H	188	SER
2	H	195	ASN
2	H	201	GLU
2	H	202	ASP
2	H	208	ILE
2	H	212	VAL
2	H	216	VAL
2	H	218	THR
2	H	219	TRP
2	H	222	VAL
2	H	224	GLN
2	H	231	THR
2	H	232	SER
2	H	254	ASP
3	I	26	ASN
3	I	37	THR
3	I	47	LYS
3	I	49	THR
3	I	50	LEU
3	I	51	LEU
3	I	62	LYS
3	I	68	ASN
3	I	82	ASP
3	I	89	VAL
3	I	90	LEU
3	I	98	THR
3	I	99	ASP
3	I	126	LEU

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Mol	Chain	Res	Type
3	I	128	LYS
3	I	143	ASP
3	I	149	MET
3	I	151	ARG
3	I	153	VAL
3	I	165	ILE
3	I	166	LEU
3	I	167	LEU
3	I	168	TYR
3	I	169	ASP
3	I	172	PHE
3	I	173	VAL
3	I	178	ILE
3	I	183	LEU
3	I	203	HIS
3	I	222	ARG
3	I	228	THR
3	I	230	ASP
3	I	236	ASP
3	I	244	VAL
3	I	265	LEU
3	J	17	LYS
3	J	26	ASN
3	J	37	THR
3	J	39	ILE
3	J	43	SER
3	J	45	CYS
3	J	49	THR
3	J	51	LEU
3	J	62	LYS
3	J	68	ASN
3	J	82	ASP
3	J	89	VAL
3	J	98	THR
3	J	99	ASP
3	J	120	MET
3	J	124	ILE
3	J	127	MET
3	J	135	ARG
3	J	143	ASP
3	J	165	ILE
3	J	167	LEU

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Mol	Chain	Res	Type
3	J	169	ASP
3	J	172	PHE
3	J	173	VAL
3	J	203	HIS
3	J	222	ARG
3	J	228	THR
3	J	230	ASP
3	J	236	ASP
3	J	244	VAL
3	J	259	ARG
3	J	262	ARG
3	J	265	LEU
3	J	266	LEU
4	K	5	SER
4	K	29	ARG
4	K	34	ARG
4	K	45	VAL
4	K	46	VAL
4	K	47	ASP
4	K	49	SER
4	K	52	GLU
4	K	54	SER
4	K	59	ILE
4	K	61	LEU
4	K	77	SER
4	K	83	ASP
4	K	88	ILE
4	K	91	VAL
4	K	95	LEU
4	K	98	LEU
4	K	100	LEU
4	L	5	SER
4	L	34	ARG
4	L	45	VAL
4	L	46	VAL
4	L	47	ASP
4	L	49	SER
4	L	52	GLU
4	L	54	SER
4	L	61	LEU
4	L	67	ARG
4	L	77	SER

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Mol	Chain	Res	Type
4	L	84	ASP
4	L	87	GLU
4	L	91	VAL
4	L	92	SER
4	L	93	SER
4	L	94	LEU
4	L	95	LEU
4	L	96	GLU
4	L	98	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	B	87	ASN
1	B	92	ASN
1	D	88	GLN
1	E	87	ASN
1	E	92	ASN
1	F	87	ASN
1	F	92	ASN
1	F	148	ASN
2	G	126	ASN
2	G	132	GLN
2	G	224	GLN
2	H	93	GLN
2	H	224	GLN
3	I	26	ASN
3	I	68	ASN
3	I	86	GLN
3	I	175	GLN
3	I	203	HIS
3	J	26	ASN
3	J	68	ASN
3	J	86	GLN
3	J	113	HIS
4	K	31	GLN
4	L	31	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	LPP	H	302	-	43,43,43	0.36	0	47,48,48	0.49	1 (2%)
5	LPP	F	201	-	43,43,43	0.36	0	47,48,48	0.48	1 (2%)
6	AD9	I	301	7	24,33,33	1.28	2 (8%)	26,52,52	1.45	4 (15%)
5	LPP	H	301	-	43,43,43	0.37	0	47,48,48	0.49	1 (2%)
5	LPP	H	303	-	35,35,43	0.40	0	39,40,48	0.52	1 (2%)
5	LPP	G	301	-	43,43,43	0.36	0	47,48,48	0.47	1 (2%)
5	LPP	H	304	-	43,43,43	0.37	0	47,48,48	0.48	1 (2%)
5	LPP	G	303	-	37,37,43	0.39	0	41,42,48	0.51	1 (2%)
5	LPP	G	302	-	43,43,43	0.37	0	47,48,48	0.47	1 (2%)
6	AD9	J	301	7	24,33,33	1.28	2 (8%)	26,52,52	1.46	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LPP	H	302	-	-	23/45/45/45	-
5	LPP	F	201	-	-	25/45/45/45	-
6	AD9	I	301	7	-	4/12/38/38	0/3/3/3
5	LPP	H	301	-	-	25/45/45/45	-
5	LPP	H	303	-	-	25/37/37/45	-
5	LPP	G	301	-	-	29/45/45/45	-
5	LPP	H	304	-	-	26/45/45/45	-
5	LPP	G	303	-	-	27/39/39/45	-
5	LPP	G	302	-	-	19/45/45/45	-
6	AD9	J	301	7	-	5/12/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	301	AD9	O3B-VG	-4.38	1.60	1.80
6	I	301	AD9	O3B-VG	-4.28	1.60	1.80
6	J	301	AD9	C5-C4	2.36	1.47	1.40
6	I	301	AD9	C5-C4	2.35	1.47	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	301	AD9	PA-O3A-PB	-4.39	117.76	132.83
6	I	301	AD9	PA-O3A-PB	-4.15	118.59	132.83
6	I	301	AD9	N3-C2-N1	-3.18	123.70	128.68
6	J	301	AD9	N3-C2-N1	-3.16	123.74	128.68
6	I	301	AD9	C4-C5-N7	-2.43	106.87	109.40
5	H	301	LPP	O2-P1-O3	2.39	120.04	110.68
5	H	304	LPP	O2-P1-O3	2.38	120.00	110.68
5	F	201	LPP	O2-P1-O3	2.37	119.94	110.68
5	H	303	LPP	O2-P1-O3	2.36	119.91	110.68
5	G	303	LPP	O2-P1-O3	2.35	119.90	110.68
5	H	302	LPP	O2-P1-O3	2.35	119.89	110.68
5	G	301	LPP	O2-P1-O3	2.35	119.87	110.68
5	G	302	LPP	O2-P1-O3	2.30	119.69	110.68
6	J	301	AD9	C4-C5-N7	-2.28	107.03	109.40
6	I	301	AD9	C3'-C2'-C1'	2.10	104.13	100.98

There are no chirality outliers.

All (208) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	201	LPP	C6-O5-P1-O2
5	F	201	LPP	C6-O5-P1-O3
5	F	201	LPP	C6-O5-P1-O4
5	G	301	LPP	C6-O5-P1-O2
5	G	301	LPP	C6-O5-P1-O3
5	G	301	LPP	C6-O5-P1-O4
5	G	301	LPP	C12-C11-O9-C7
5	G	302	LPP	C6-O5-P1-O2
5	G	302	LPP	C6-O5-P1-O4
5	G	303	LPP	C6-O5-P1-O4
5	G	303	LPP	O10-C11-O9-C7
5	G	303	LPP	C12-C11-O9-C7
5	H	301	LPP	C6-O5-P1-O2
5	H	301	LPP	C6-O5-P1-O4
5	H	303	LPP	C6-O5-P1-O2
5	H	303	LPP	C6-O5-P1-O3
5	H	303	LPP	C6-O5-P1-O4
5	H	303	LPP	C30-C29-O27-C8
5	H	304	LPP	C12-C11-O9-C7
6	I	301	AD9	C5'-O5'-PA-O2A
6	I	301	AD9	C5'-O5'-PA-O3A
6	J	301	AD9	C5'-O5'-PA-O1A
5	H	303	LPP	O28-C29-O27-C8
5	H	304	LPP	O28-C29-O27-C8
5	G	303	LPP	O28-C29-O27-C8
5	G	301	LPP	O10-C11-O9-C7
5	H	304	LPP	O10-C11-O9-C7
5	G	301	LPP	C30-C29-O27-C8
5	G	303	LPP	C30-C29-O27-C8
5	H	304	LPP	C30-C29-O27-C8
5	G	303	LPP	C38-C39-C40-C41
5	F	201	LPP	O28-C29-O27-C8
5	G	301	LPP	O28-C29-O27-C8
5	F	201	LPP	C30-C29-O27-C8
5	G	301	LPP	C17-C18-C19-C20
5	G	303	LPP	C34-C35-C36-C37
5	G	303	LPP	C36-C37-C38-C39
5	H	304	LPP	C15-C16-C17-C18
5	H	303	LPP	C17-C18-C19-C20
5	H	304	LPP	C33-C34-C35-C36
6	I	301	AD9	O4'-C4'-C5'-O5'
5	H	302	LPP	C39-C40-C41-C42
5	H	302	LPP	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
5	H	301	LPP	C12-C11-O9-C7
5	G	301	LPP	C39-C40-C41-C42
5	H	304	LPP	C31-C32-C33-C34
5	H	301	LPP	C29-C30-C31-C32
5	G	302	LPP	C11-C12-C13-C14
5	G	302	LPP	C29-C30-C31-C32
5	H	304	LPP	C11-C12-C13-C14
5	H	302	LPP	C37-C38-C39-C40
5	H	303	LPP	C11-C12-C13-C14
5	H	301	LPP	O10-C11-O9-C7
5	H	304	LPP	C36-C37-C38-C39
5	F	201	LPP	C29-C30-C31-C32
5	G	302	LPP	C35-C36-C37-C38
5	H	302	LPP	C19-C20-C21-C22
5	G	301	LPP	C14-C15-C16-C17
5	G	301	LPP	C37-C38-C39-C40
5	G	302	LPP	C13-C14-C15-C16
5	H	304	LPP	C8-C7-O9-C11
5	H	302	LPP	C20-C21-C22-C23
5	H	303	LPP	C7-C6-O5-P1
5	G	303	LPP	C15-C16-C17-C18
5	F	201	LPP	C14-C15-C16-C17
5	G	301	LPP	C20-C21-C22-C23
5	G	302	LPP	C15-C16-C17-C18
5	H	304	LPP	C35-C36-C37-C38
5	F	201	LPP	C40-C41-C42-C43
5	H	301	LPP	C38-C39-C40-C41
5	G	301	LPP	C29-C30-C31-C32
5	F	201	LPP	C30-C31-C32-C33
5	G	301	LPP	C12-C13-C14-C15
5	H	304	LPP	C21-C22-C23-C24
5	H	304	LPP	C39-C40-C41-C42
5	H	302	LPP	C40-C41-C42-C43
5	G	303	LPP	C14-C15-C16-C17
5	H	304	LPP	C20-C21-C22-C23
5	H	303	LPP	C6-C7-C8-O27
5	G	302	LPP	C34-C35-C36-C37
5	G	301	LPP	C18-C19-C20-C21
5	F	201	LPP	C13-C14-C15-C16
5	F	201	LPP	C18-C19-C20-C21
5	G	302	LPP	C19-C20-C21-C22
5	H	301	LPP	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
5	H	303	LPP	C34-C35-C36-C37
5	F	201	LPP	C20-C21-C22-C23
5	G	303	LPP	C13-C14-C15-C16
5	H	303	LPP	C30-C31-C32-C33
5	G	301	LPP	C34-C35-C36-C37
5	H	301	LPP	C37-C38-C39-C40
5	H	303	LPP	C12-C11-O9-C7
5	H	302	LPP	C18-C19-C20-C21
5	F	201	LPP	C11-C12-C13-C14
5	G	301	LPP	C40-C41-C42-C43
5	G	303	LPP	C12-C13-C14-C15
5	H	304	LPP	C40-C41-C42-C43
5	H	302	LPP	C34-C35-C36-C37
5	H	303	LPP	O10-C11-O9-C7
5	G	301	LPP	C7-C8-O27-C29
5	H	302	LPP	C31-C32-C33-C34
5	H	303	LPP	C16-C17-C18-C19
5	G	303	LPP	O5-C6-C7-C8
5	G	301	LPP	C22-C23-C24-C25
5	H	304	LPP	C23-C24-C25-C26
5	F	201	LPP	C36-C37-C38-C39
5	H	304	LPP	C30-C31-C32-C33
5	G	301	LPP	C21-C22-C23-C24
5	G	301	LPP	C6-C7-C8-O27
5	H	303	LPP	C32-C33-C34-C35
5	H	303	LPP	C33-C34-C35-C36
5	G	301	LPP	C16-C17-C18-C19
5	F	201	LPP	C12-C11-O9-C7
5	F	201	LPP	C38-C39-C40-C41
5	H	301	LPP	C41-C42-C43-C44
5	H	303	LPP	C35-C36-C37-C38
5	F	201	LPP	C23-C24-C25-C26
5	G	303	LPP	C8-C7-O9-C11
5	G	302	LPP	C6-O5-P1-O3
5	G	303	LPP	C6-O5-P1-O3
5	H	302	LPP	C6-O5-P1-O3
5	H	304	LPP	C29-C30-C31-C32
5	G	302	LPP	C30-C29-O27-C8
5	G	301	LPP	C31-C32-C33-C34
5	G	301	LPP	C41-C42-C43-C44
5	G	303	LPP	C19-C20-C21-C22
5	G	303	LPP	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
5	H	301	LPP	C36-C37-C38-C39
5	H	304	LPP	C41-C42-C43-C44
5	H	303	LPP	C29-C30-C31-C32
5	G	301	LPP	C35-C36-C37-C38
5	H	303	LPP	C31-C32-C33-C34
5	H	302	LPP	C36-C37-C38-C39
5	G	301	LPP	C23-C24-C25-C26
5	G	302	LPP	O28-C29-O27-C8
5	H	301	LPP	C34-C35-C36-C37
5	G	302	LPP	C33-C34-C35-C36
5	G	301	LPP	O9-C7-C8-O27
5	F	201	LPP	O10-C11-O9-C7
5	F	201	LPP	C34-C35-C36-C37
5	F	201	LPP	C21-C22-C23-C24
5	G	303	LPP	C30-C31-C32-C33
5	G	301	LPP	O5-C6-C7-C8
5	H	301	LPP	O5-C6-C7-C8
5	G	303	LPP	C6-O5-P1-O2
5	G	303	LPP	C6-C7-C8-O27
5	F	201	LPP	O5-C6-C7-O9
5	H	301	LPP	O5-C6-C7-O9
5	H	301	LPP	C32-C33-C34-C35
5	G	303	LPP	O9-C7-C8-O27
5	H	303	LPP	O9-C7-C8-O27
5	H	304	LPP	O9-C7-C8-O27
6	J	301	AD9	C5'-O5'-PA-O3A
5	G	302	LPP	C41-C42-C43-C44
5	H	302	LPP	C17-C18-C19-C20
5	H	302	LPP	C22-C23-C24-C25
5	F	201	LPP	C7-C6-O5-P1
6	J	301	AD9	C5'-O5'-PA-O2A
5	F	201	LPP	O5-C6-C7-C8
5	H	302	LPP	C41-C42-C43-C44
5	H	304	LPP	C34-C35-C36-C37
5	G	302	LPP	C22-C23-C24-C25
5	H	302	LPP	C12-C13-C14-C15
5	H	301	LPP	C40-C41-C42-C43
5	H	301	LPP	C12-C13-C14-C15
5	H	302	LPP	C32-C33-C34-C35
5	G	301	LPP	C32-C33-C34-C35
5	H	304	LPP	C16-C17-C18-C19
5	H	303	LPP	C37-C38-C39-C40

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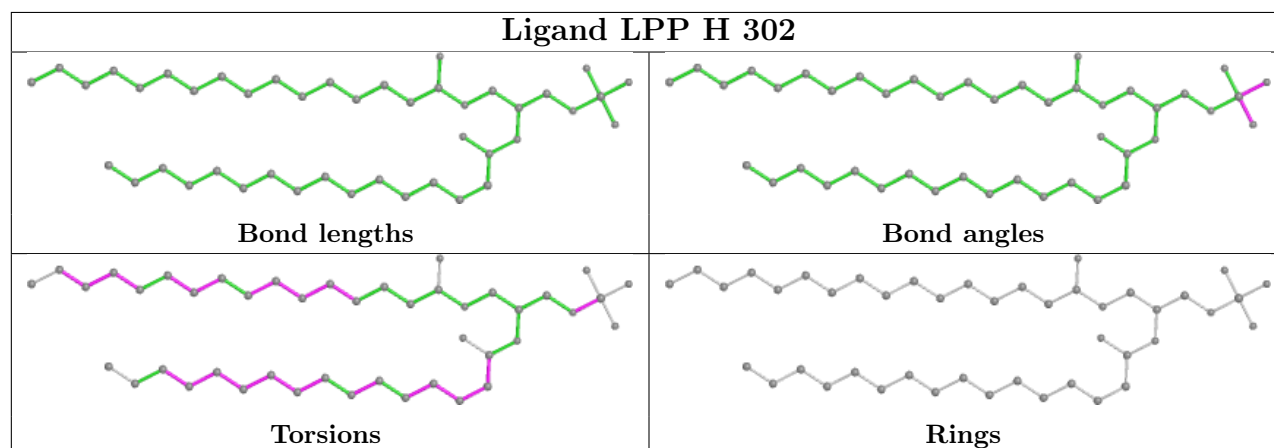
Mol	Chain	Res	Type	Atoms
5	H	303	LPP	C36-C37-C38-C39
5	G	303	LPP	O5-C6-C7-O9
5	H	302	LPP	C21-C22-C23-C24
5	H	304	LPP	C6-C7-C8-O27
5	F	201	LPP	C16-C17-C18-C19
5	H	302	LPP	C33-C34-C35-C36
5	G	302	LPP	C16-C17-C18-C19
5	H	301	LPP	C23-C24-C25-C26
5	H	302	LPP	C13-C14-C15-C16
6	I	301	AD9	C3'-C4'-C5'-O5'
6	J	301	AD9	O4'-C4'-C5'-O5'
5	F	201	LPP	C37-C38-C39-C40
5	H	304	LPP	C38-C39-C40-C41
5	G	303	LPP	C35-C36-C37-C38
5	H	303	LPP	O5-C6-C7-O9
5	H	301	LPP	O27-C29-C30-C31
5	G	302	LPP	O9-C7-C8-O27
5	H	301	LPP	C33-C34-C35-C36
5	H	301	LPP	C16-C17-C18-C19
6	J	301	AD9	C3'-C4'-C5'-O5'
5	H	301	LPP	C14-C15-C16-C17
5	H	304	LPP	C19-C20-C21-C22
5	H	302	LPP	C6-O5-P1-O4
5	H	301	LPP	C6-C7-O9-C11
5	H	301	LPP	C8-C7-O9-C11
5	H	302	LPP	O9-C11-C12-C13
5	H	301	LPP	C6-O5-P1-O3
5	H	304	LPP	C12-C13-C14-C15
5	G	302	LPP	C30-C31-C32-C33
5	H	303	LPP	O5-C6-C7-C8
5	H	301	LPP	O9-C7-C8-O27
5	G	303	LPP	O9-C11-C12-C13
5	G	303	LPP	O27-C29-C30-C31
5	H	303	LPP	C19-C20-C21-C22
5	H	302	LPP	O10-C11-C12-C13
5	H	302	LPP	C15-C16-C17-C18
5	G	303	LPP	O10-C11-C12-C13
5	G	302	LPP	C40-C41-C42-C43
5	G	303	LPP	O28-C29-C30-C31

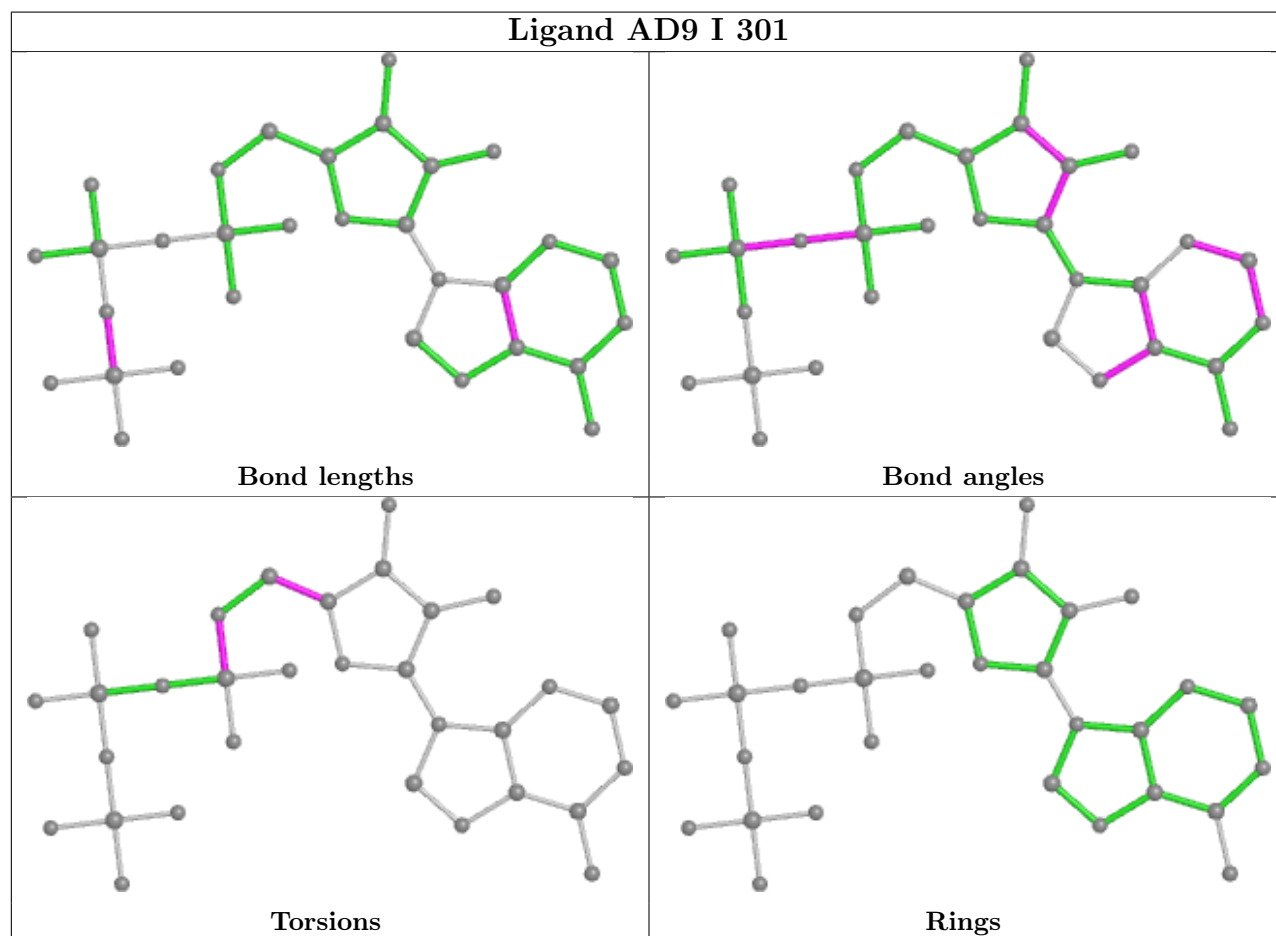
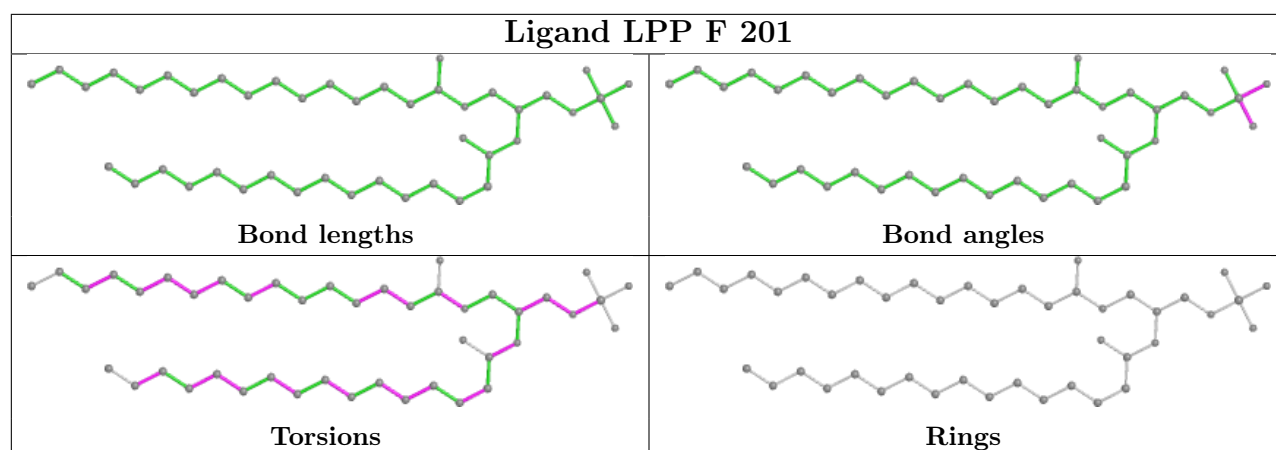
There are no ring outliers.

10 monomers are involved in 80 short contacts:

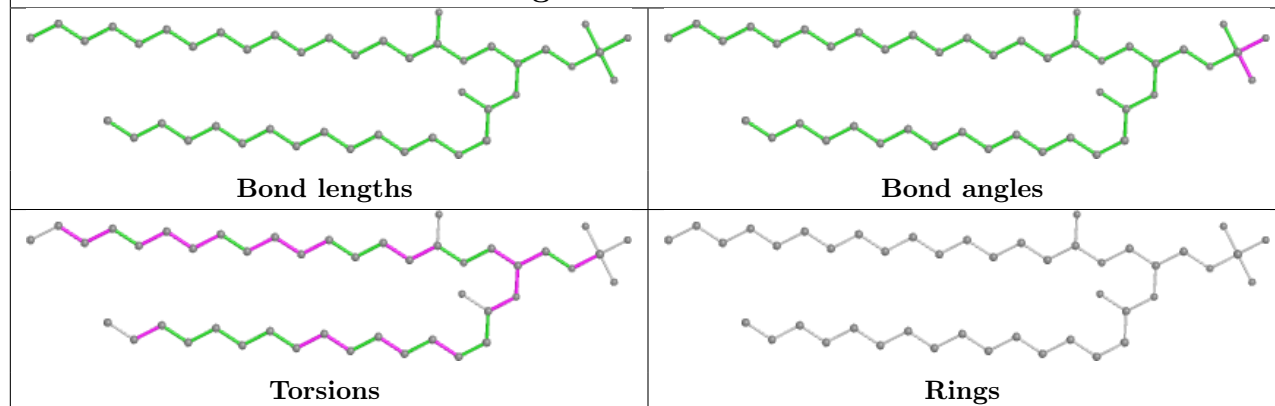
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	302	LPP	6	0
5	F	201	LPP	2	0
6	I	301	AD9	7	0
5	H	301	LPP	7	0
5	H	303	LPP	7	0
5	G	301	LPP	10	0
5	H	304	LPP	10	0
5	G	303	LPP	25	0
5	G	302	LPP	11	0
6	J	301	AD9	2	0

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

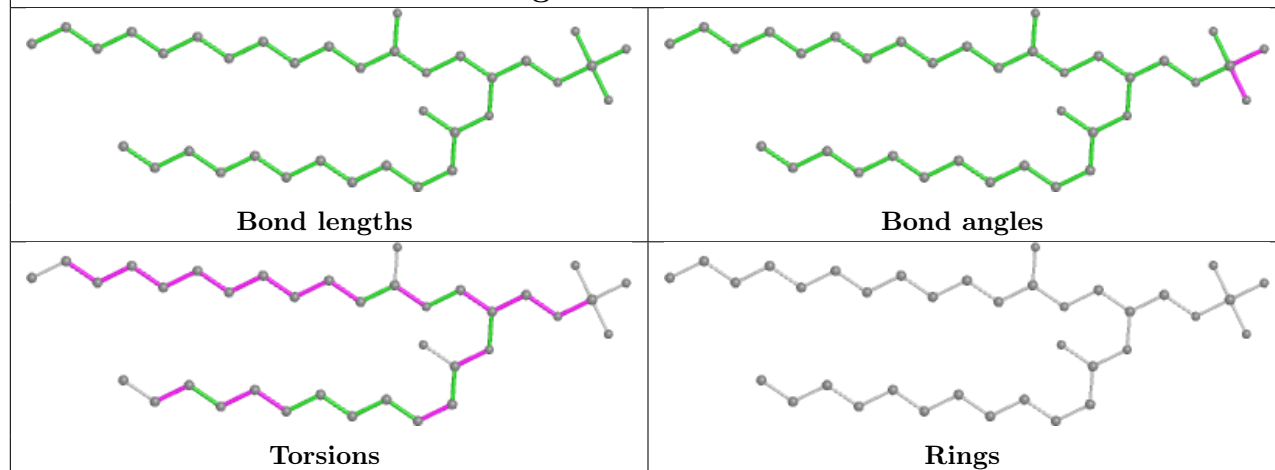




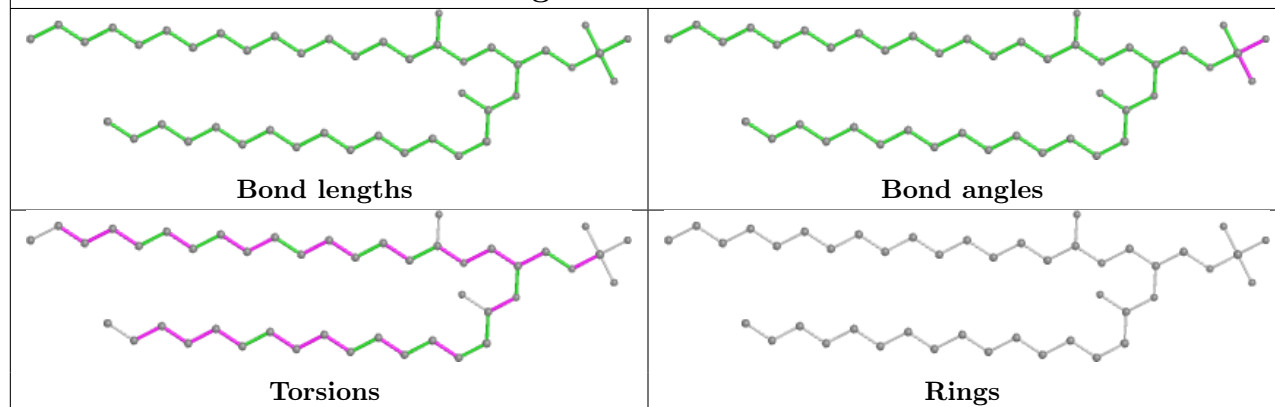
Ligand LPP H 301

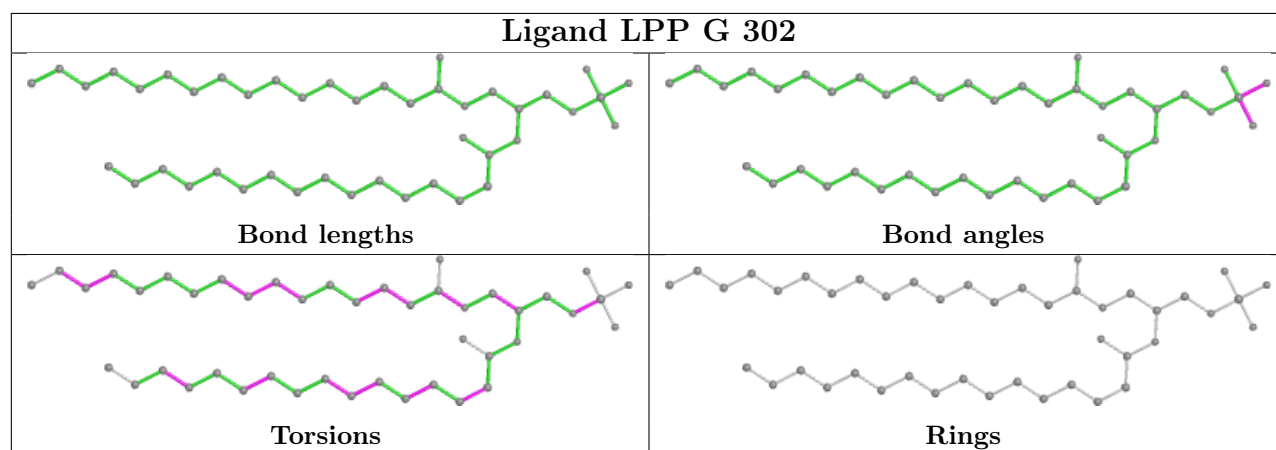
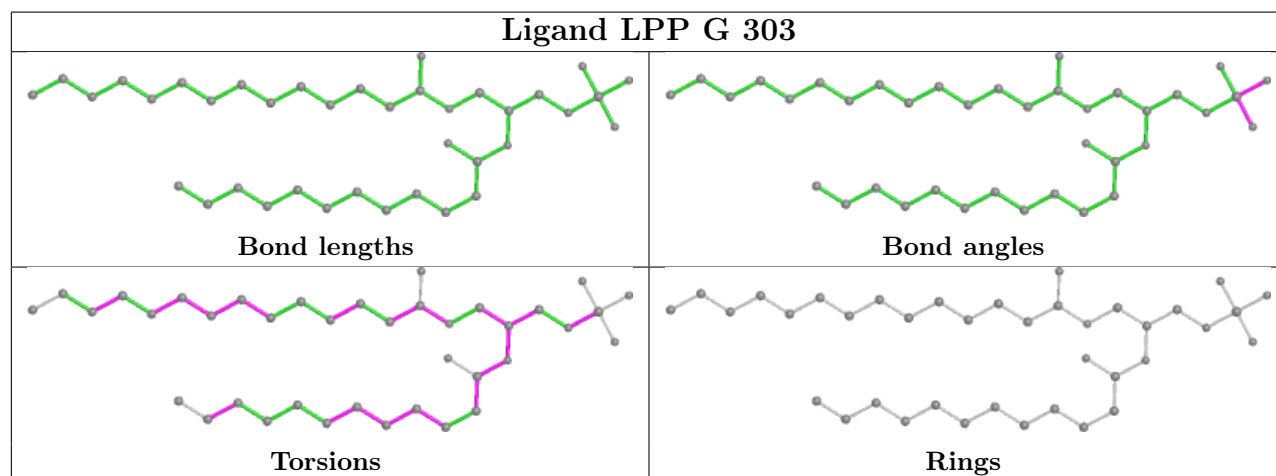
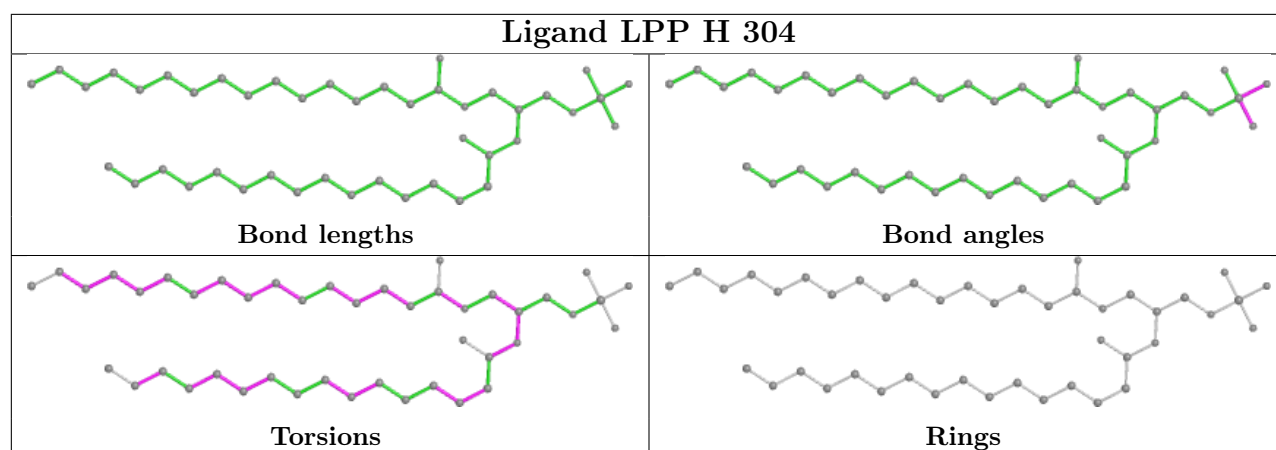


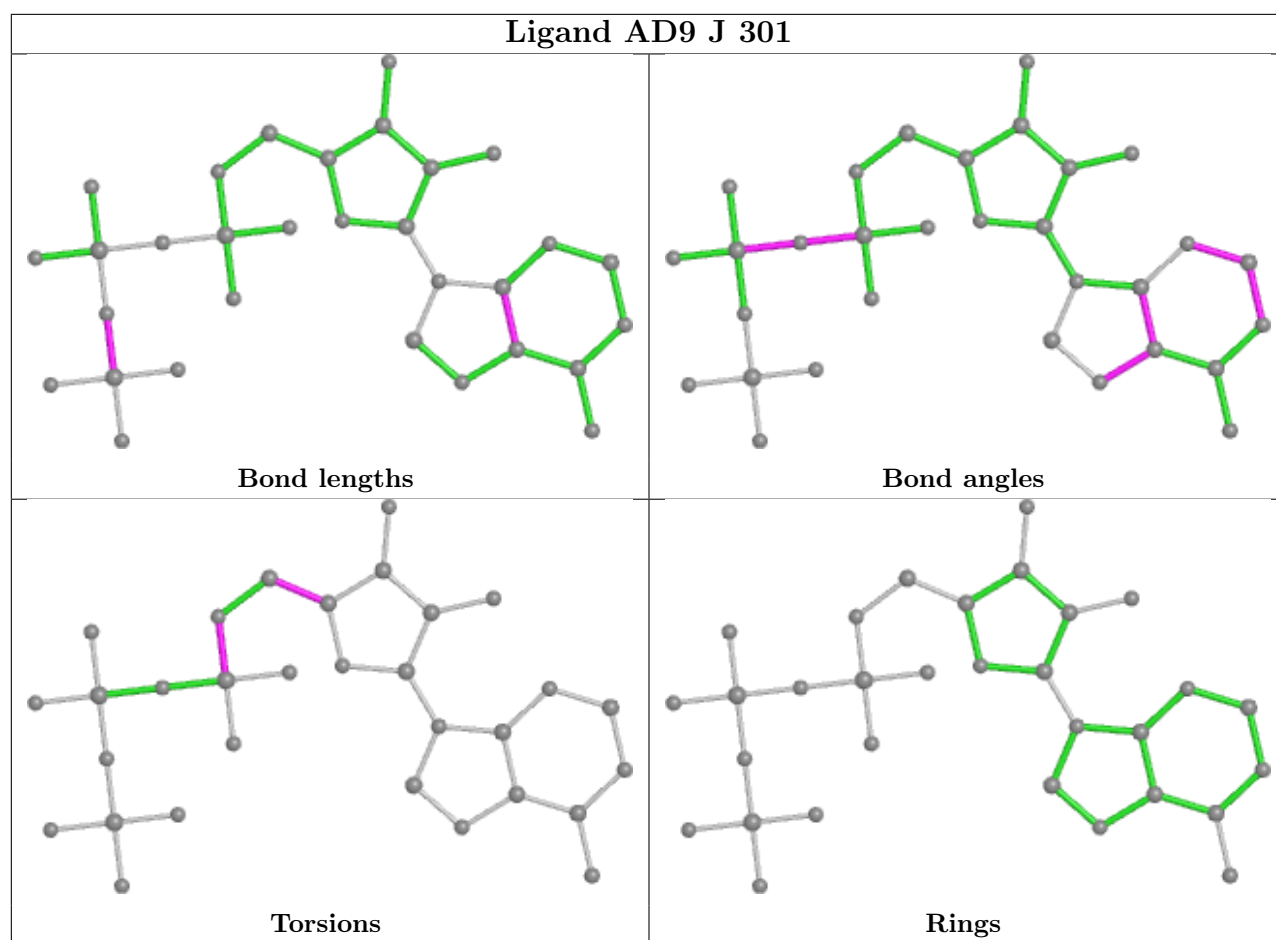
Ligand LPP H 303



Ligand LPP G 301







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

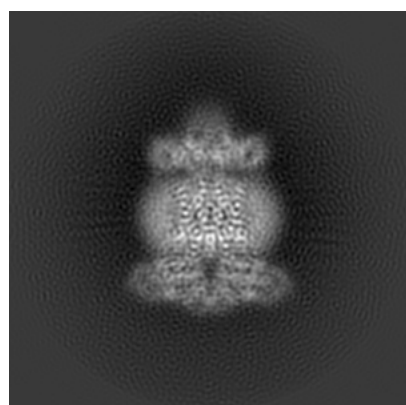
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30371. These allow visual inspection of the internal detail of the map and identification of artifacts.

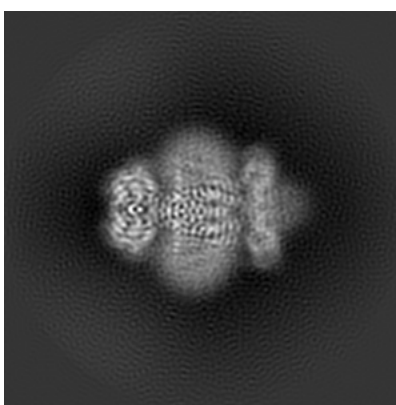
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

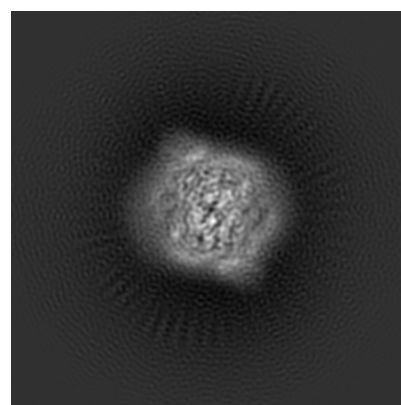
6.1.1 Primary map



X



Y

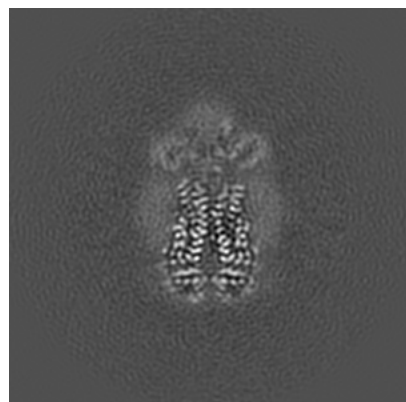


Z

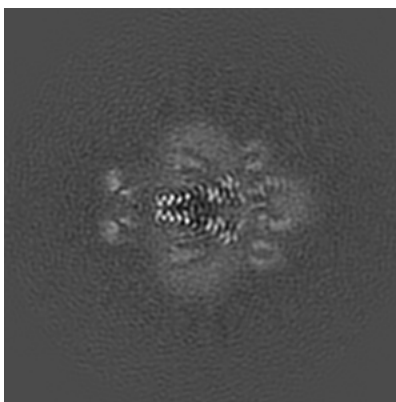
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

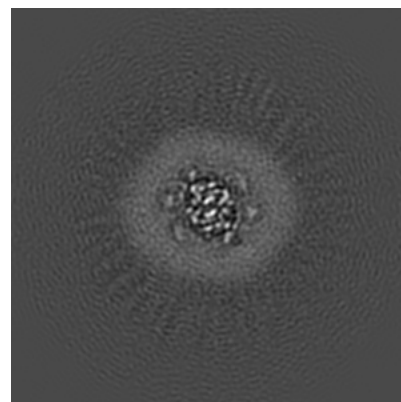
6.2.1 Primary map



X Index: 128



Y Index: 128

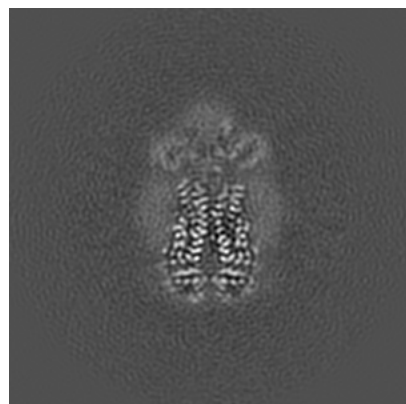


Z Index: 128

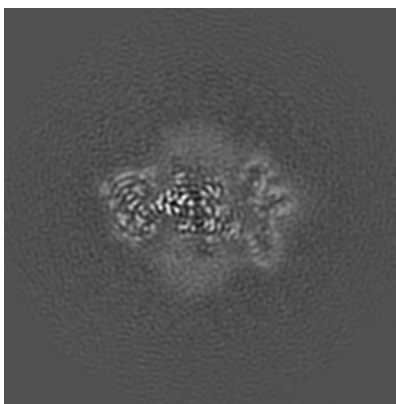
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

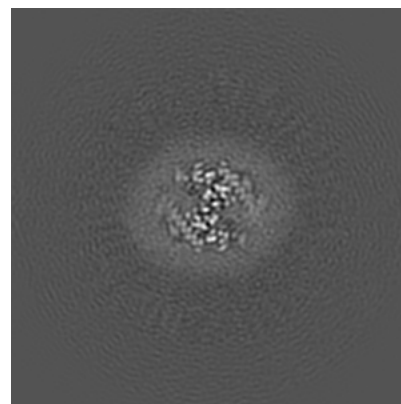
6.3.1 Primary map



X Index: 128



Y Index: 138

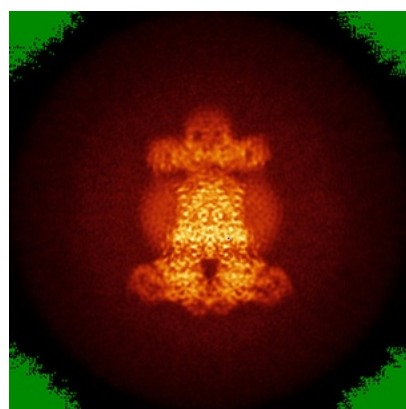


Z Index: 110

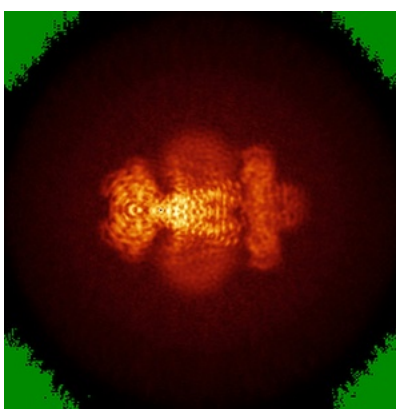
The images above show the largest variance slices of the map in three orthogonal directions.

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

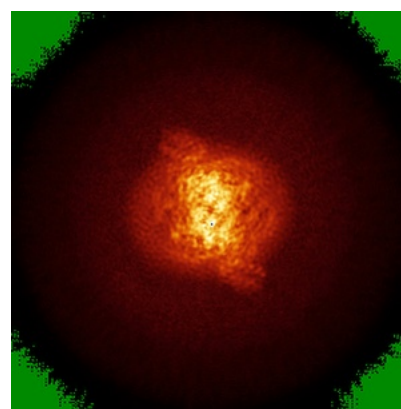
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0238. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

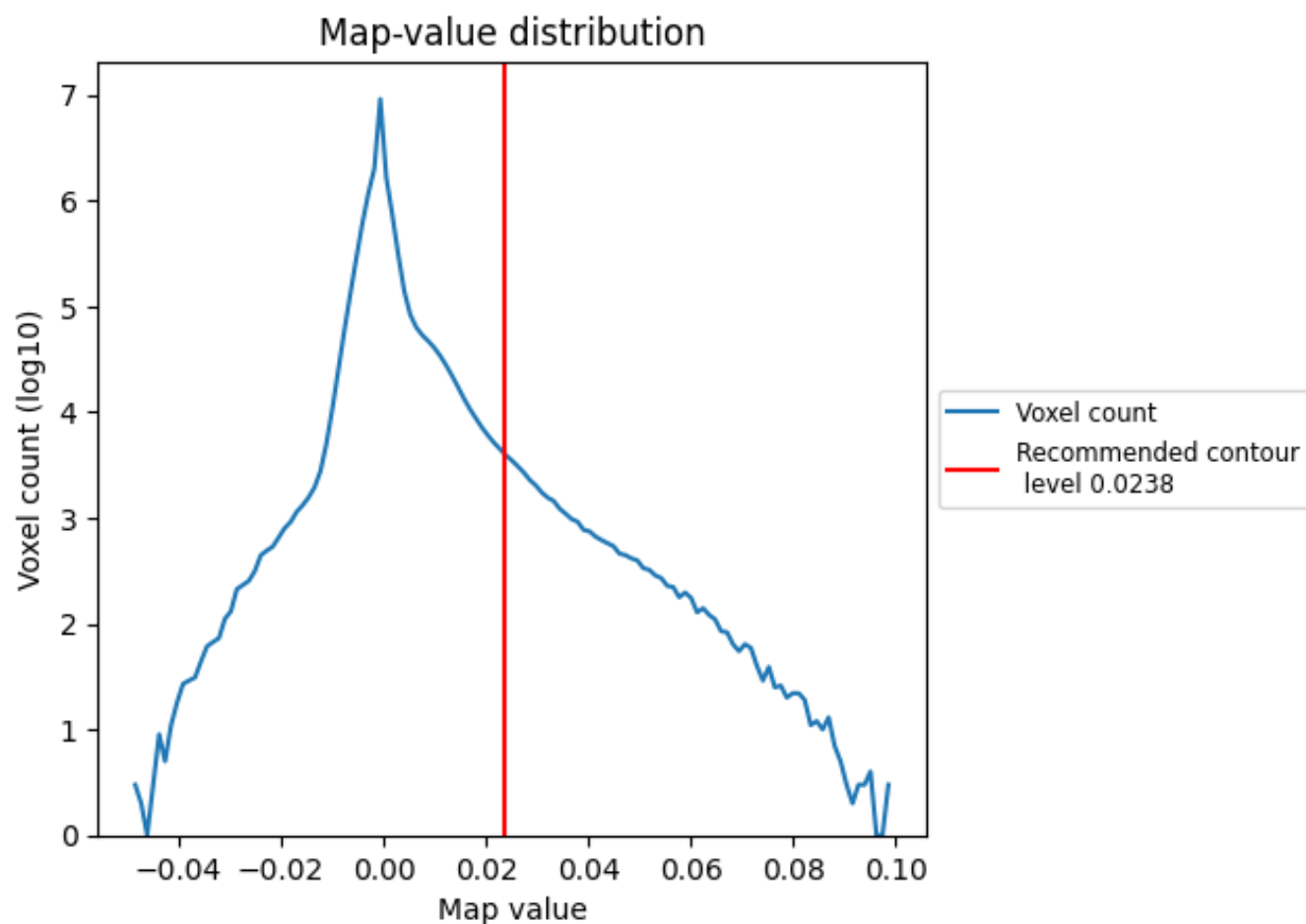
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

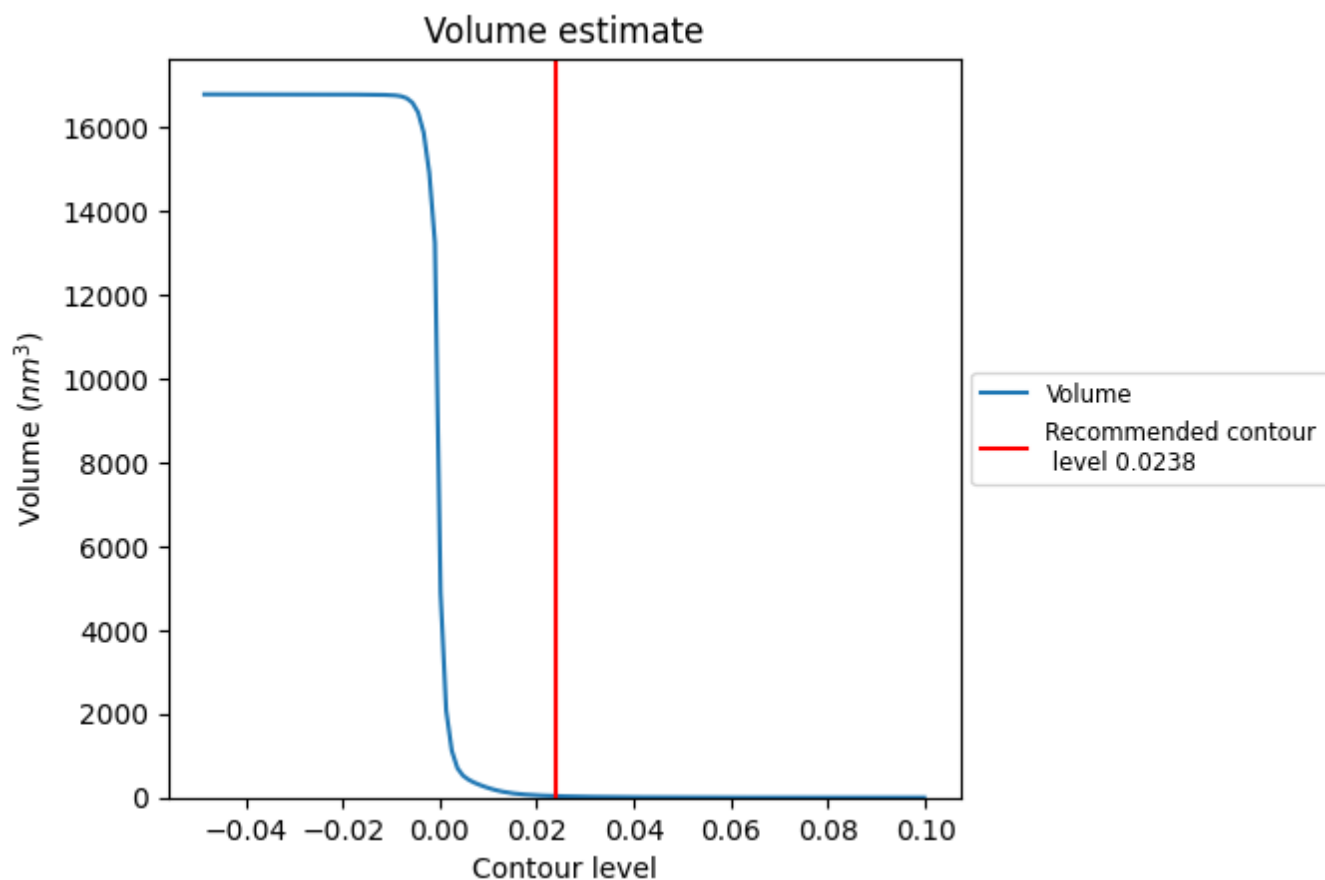
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

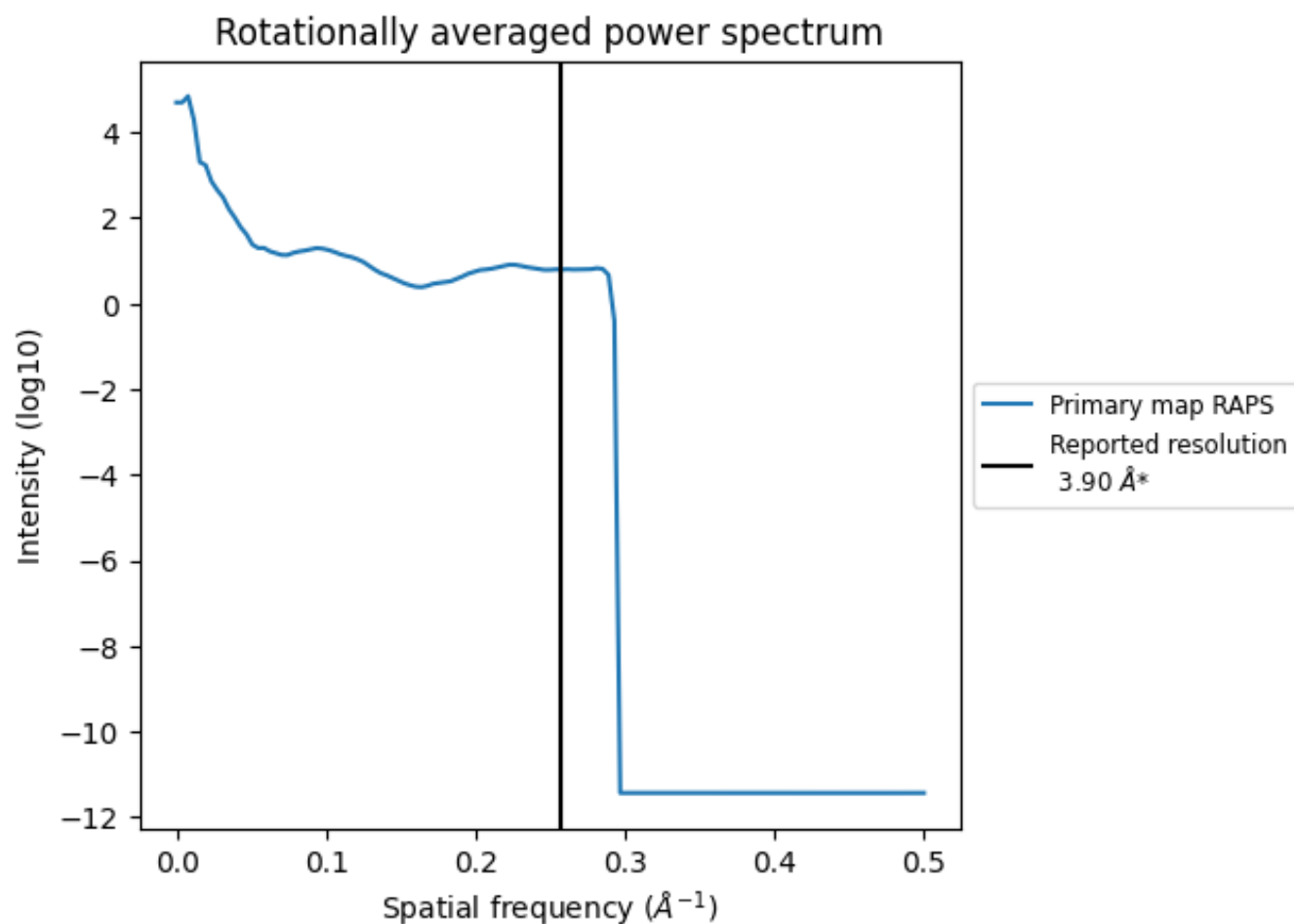
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 36 nm³; this corresponds to an approximate mass of 33 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 ⓘ

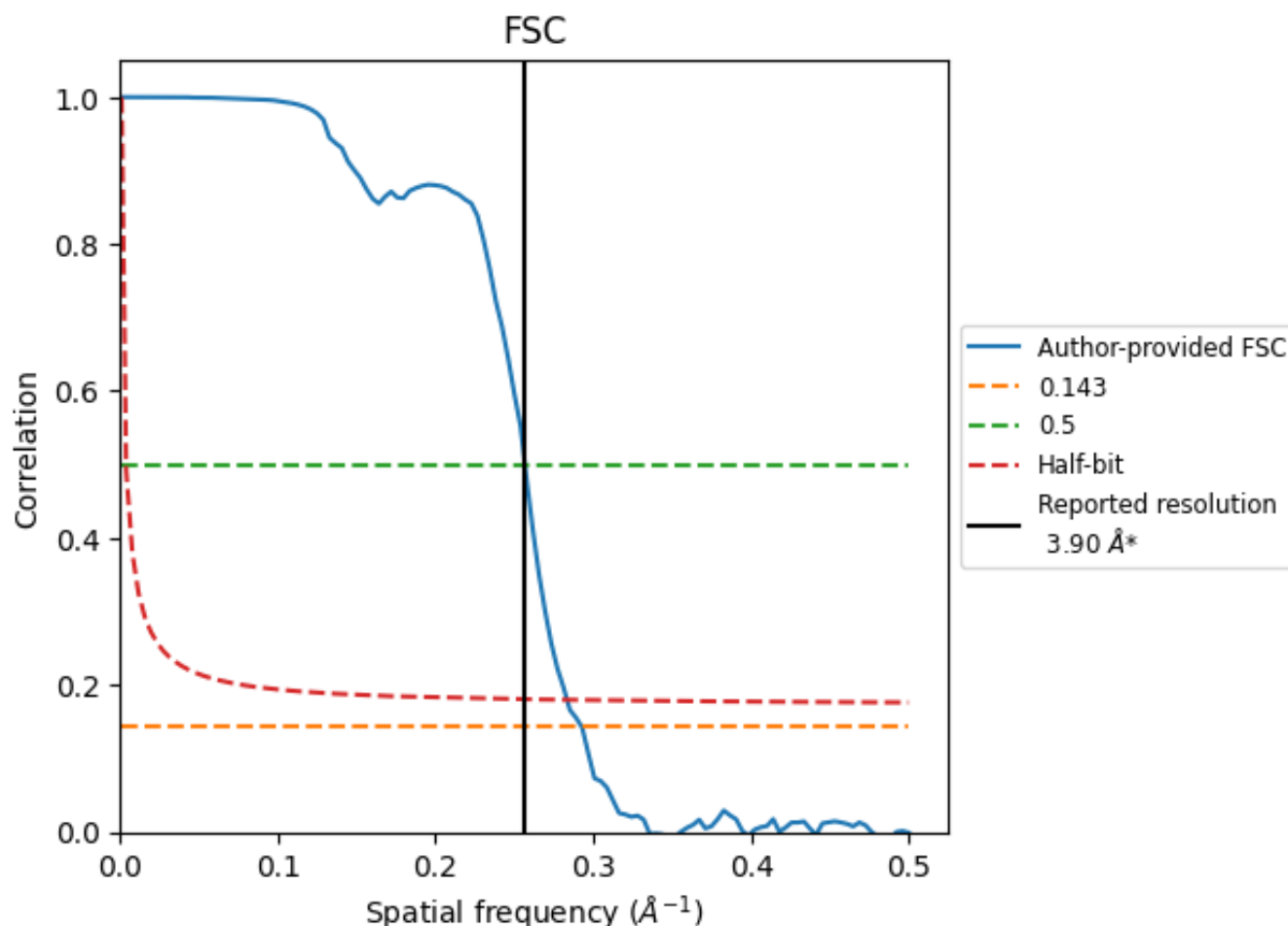


*Reported resolution corresponds to spatial frequency of 0.256 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

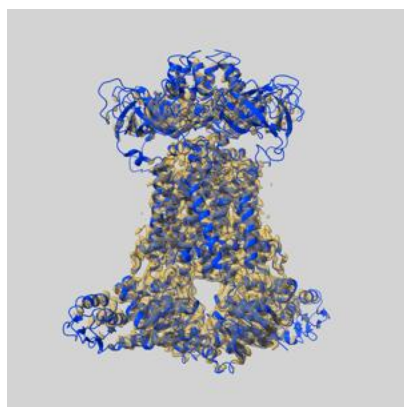
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.42	3.90	3.53
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.42 differs from the reported value 3.9 by more than 10 %

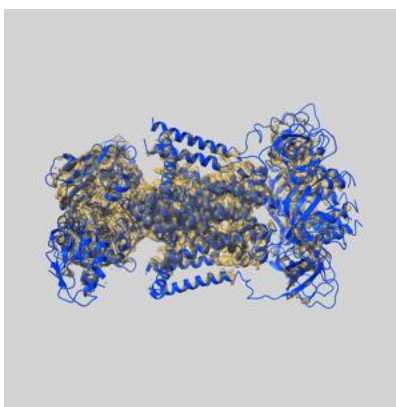
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30371 and PDB model 7CH8. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

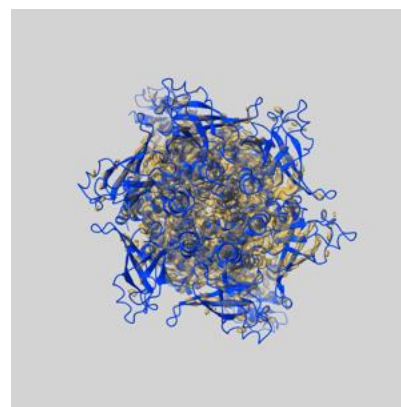
9.1 Map-model overlay [i](#)



X



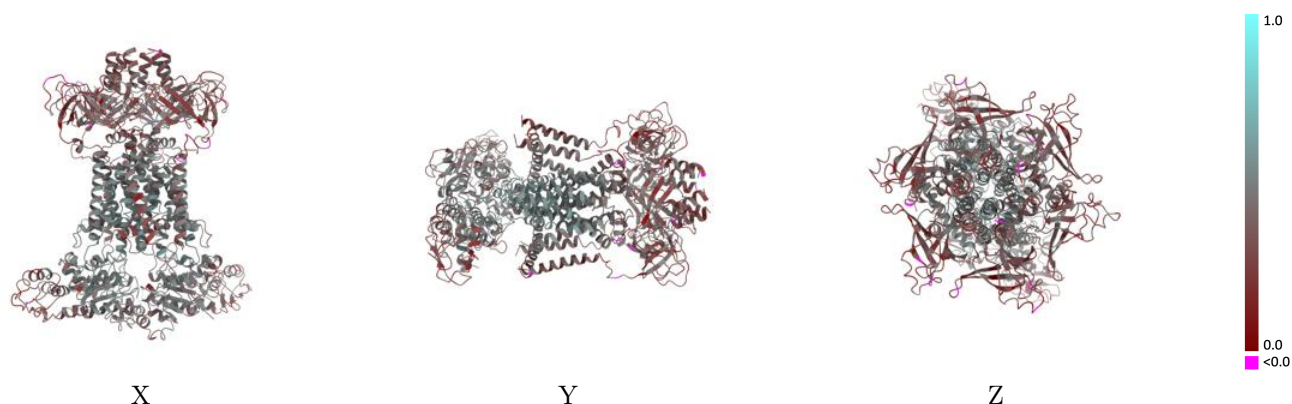
Y



Z

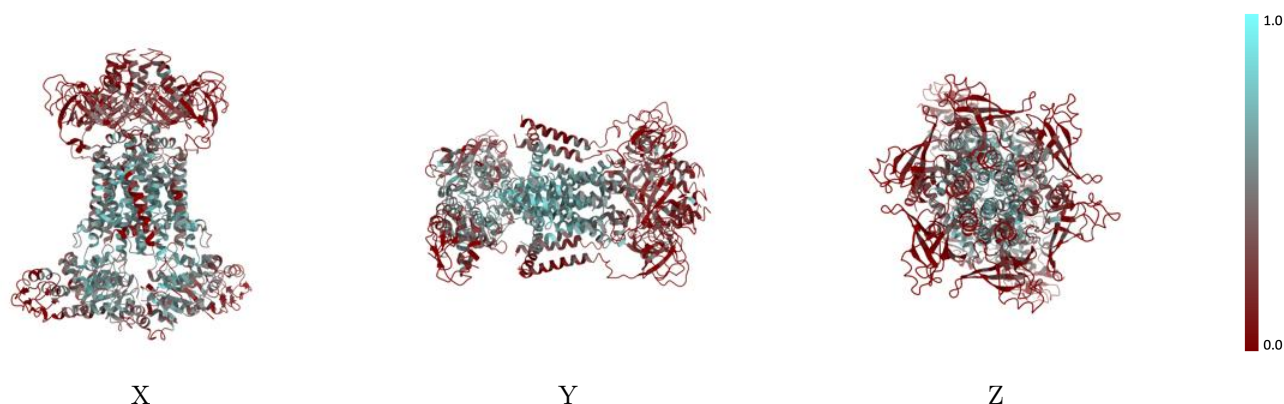
The images above show the 3D surface view of the map at the recommended contour level 0.0238 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



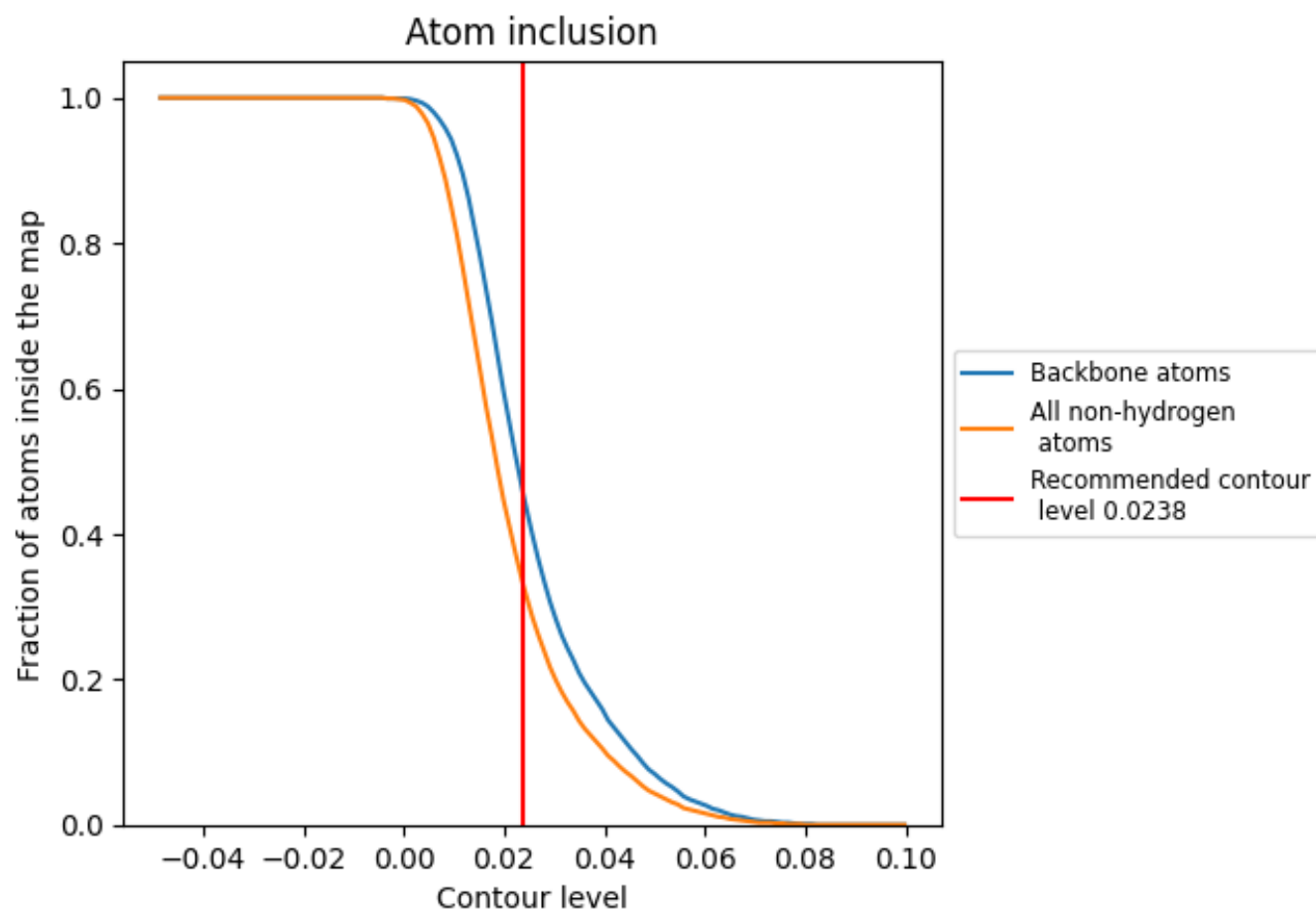
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0238).

9.4 Atom inclusion [i](#)



At the recommended contour level, 46% of all backbone atoms, 33% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0238) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.3300	<div></div> 0.4010
A	<div></div> 0.0900	<div></div> 0.3150
B	<div></div> 0.1770	<div></div> 0.3100
C	<div></div> 0.1150	<div></div> 0.3300
D	<div></div> 0.2050	<div></div> 0.3570
E	<div></div> 0.1740	<div></div> 0.3240
F	<div></div> 0.1420	<div></div> 0.3290
G	<div></div> 0.5550	<div></div> 0.4840
H	<div></div> 0.5500	<div></div> 0.4910
I	<div></div> 0.4600	<div></div> 0.4540
J	<div></div> 0.4610	<div></div> 0.4660
K	<div></div> 0.1440	<div></div> 0.3310
L	<div></div> 0.1550	<div></div> 0.3150

