



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:42 AM UTC

PDB ID : 7CH9 / pdb_00007ch9
EMDB ID : EMD-30372
Title : Cryo-EM structure of P.aeruginosa MlaFEED
Authors : Zhou, C.; Shi, H.; Zhang, M.; Huang, Y.
Deposited on : 2020-07-05
Resolution : 3.50 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:

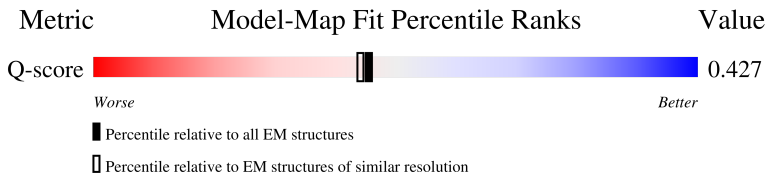
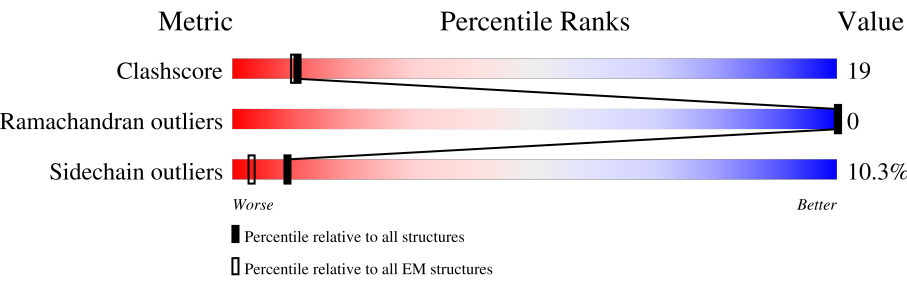
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.50 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	7% 64% 29% • •
1	B	157	• 55% 36% • 6%
1	C	157	8% 53% 36% 6% 6%
1	D	157	• 59% 31% • 6%

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Mol	Chain	Length	Quality of chain
1	E	157	
1	F	157	
2	G	265	
2	H	265	
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	301	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15978 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
			1088	690	181	216	1		
1	B	148	Total	C	N	O	S	0	0
			1068	680	176	211	1		
1	C	148	Total	C	N	O	S	0	0
			1079	685	179	214	1		
1	D	148	Total	C	N	O	S	0	0
			1083	689	177	216	1		
1	E	149	Total	C	N	O	S	0	0
			1090	693	179	217	1		
1	F	148	Total	C	N	O	S	0	0
			1070	679	176	214	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
			1928	1262	317	340	9		
2	H	257	Total	C	N	O	S	0	0
			1908	1251	312	336	9		

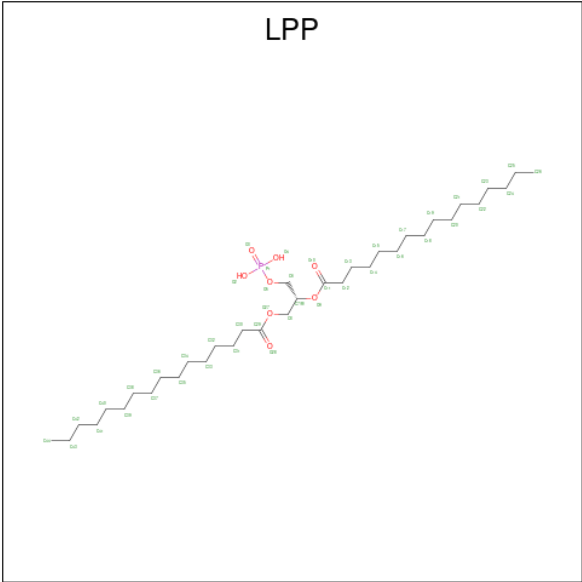
- Molecule 3 is a protein called Probable ATP-binding component of ABC transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	262	Total	C	N	O	S	0	0
			2015	1287	356	364	8		
3	J	262	Total	C	N	O	S	0	0
			1991	1270	352	361	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
			721	448	132	139	2		
4	L	98	Total	C	N	O	S	0	0
			721	448	132	139	2		

- Molecule 5 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (CCD ID: LPP) (formula: C₃₅H₆₉O₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C			0
			13	13			
5	B	1	Total	C			0
			13	13			
5	B	1	Total	C			0
			13	13			
5	C	1	Total	C			0
			13	13			
5	C	1	Total	C			0
			13	13			
5	E	1	Total	C			0
			13	13			
5	F	1	Total	C			0
			13	13			
5	G	1	Total	C	O	P	0
			37	28	8	1	
5	G	1	Total	C	O	P	0
			44	35	8	1	

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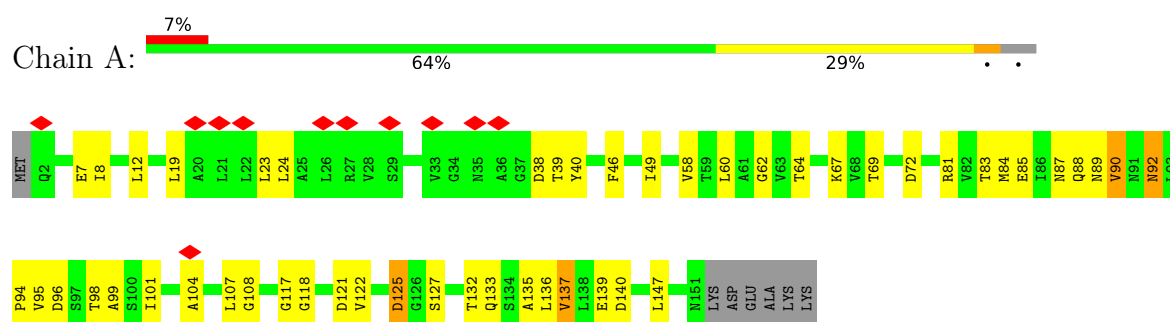
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Mol	Chain	Residues	Atoms				AltConf
5	H	1	Total	C	O	P	0
			44	35	8	1	

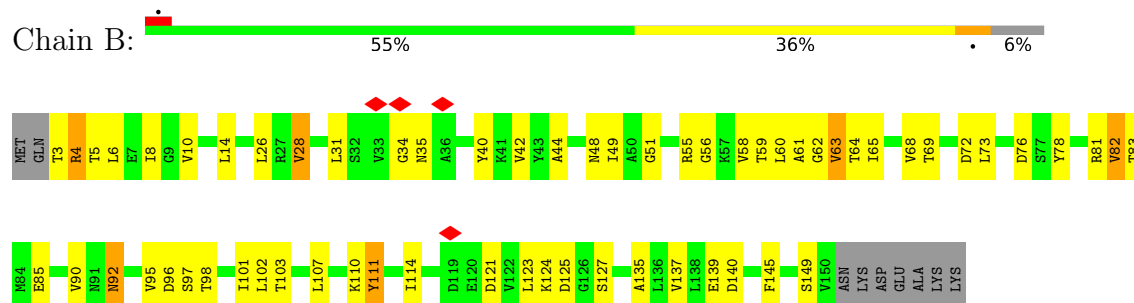
3 Residue-property plots [i](#)

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.

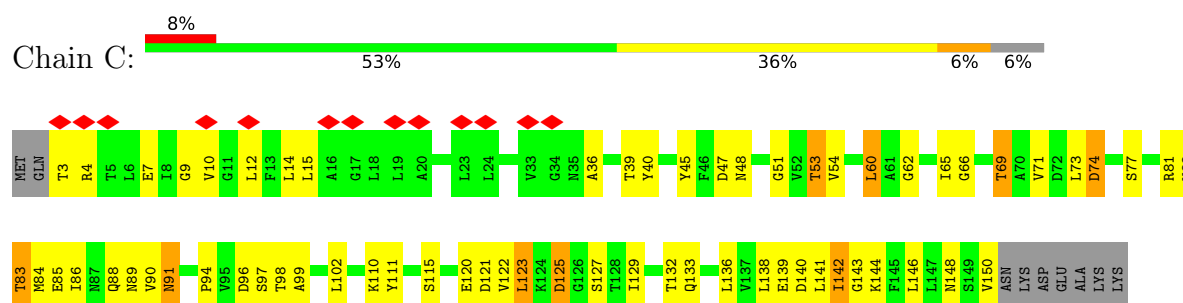
- Molecule 1: MlaD domain-containing protein



- Molecule 1: MlaD domain-containing protein

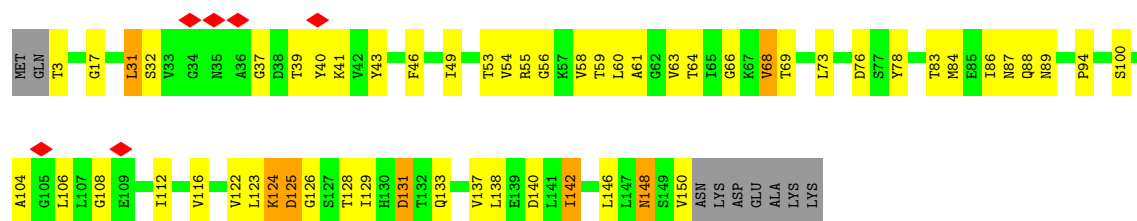


- Molecule 1: MlaD domain-containing protein

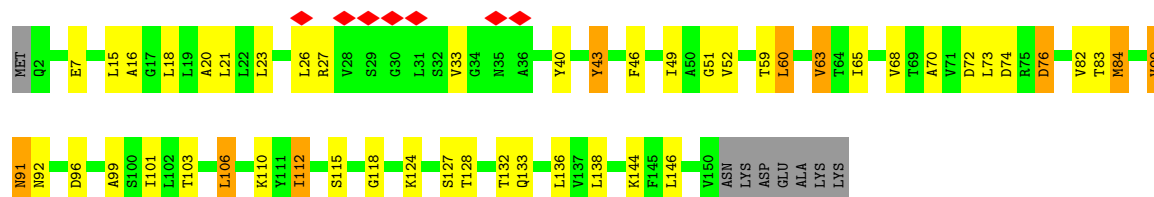


- Molecule 1: MlaD domain-containing protein

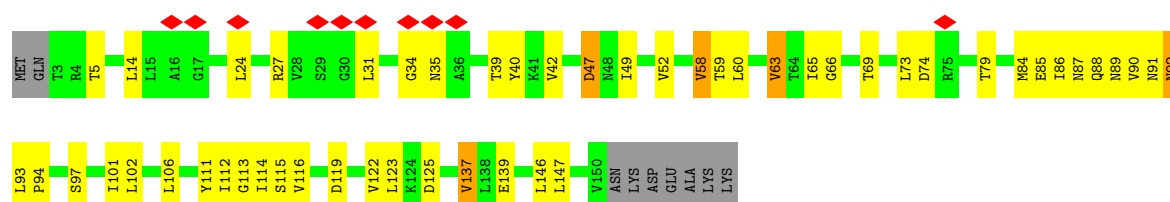




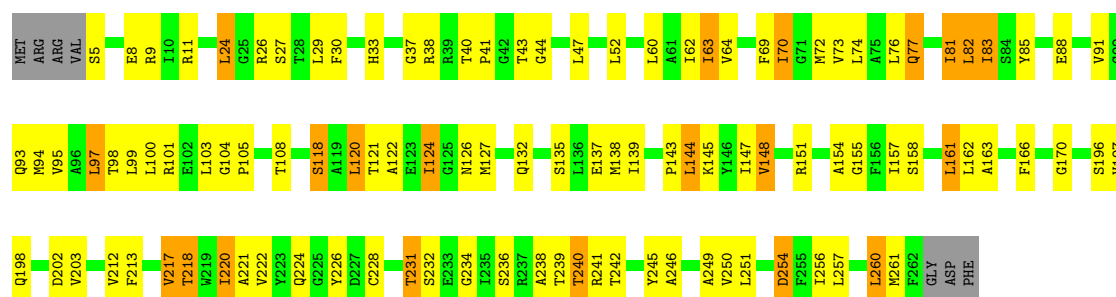
- Molecule 1: MlaD domain-containing protein



- Molecule 1: MlaD domain-containing protein

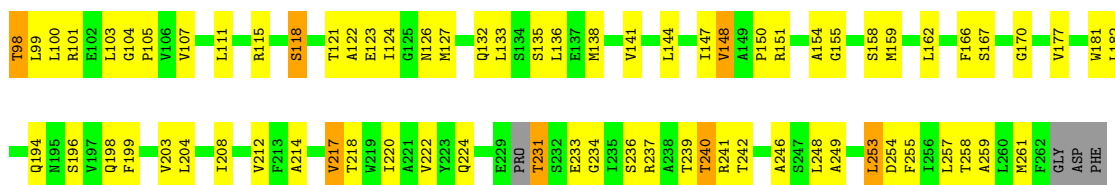


- Molecule 2: Probable permease of ABC transporter



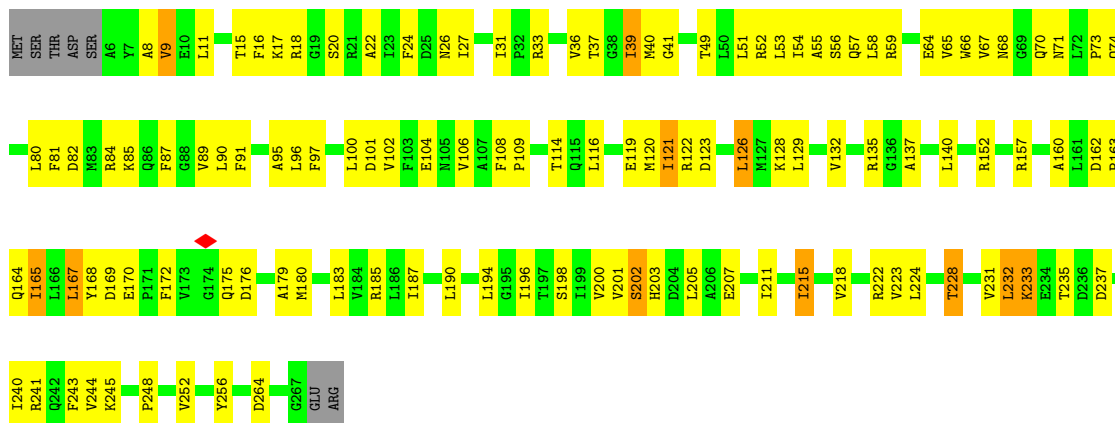
- Molecule 2: Probable permease of ABC transporter





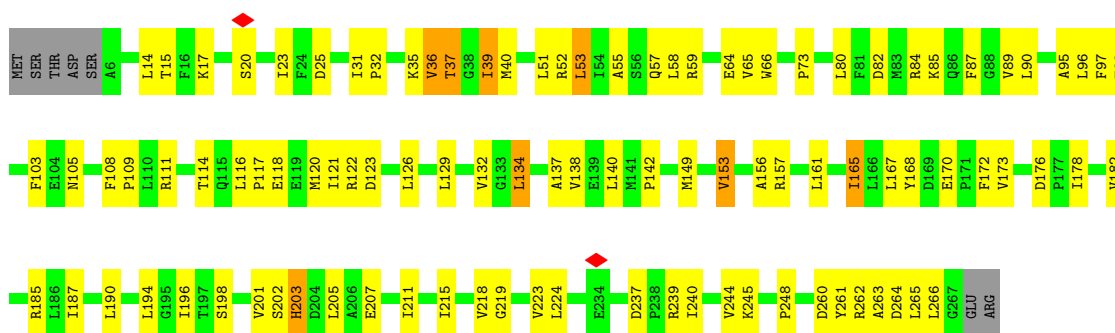
- Molecule 3: Probable ATP-binding component of ABC transporter

Chain I: 52% 41%



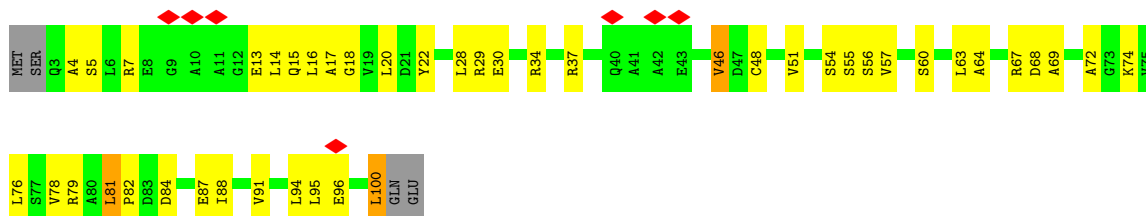
- Molecule 3: Probable ATP-binding component of ABC transporter

Chain J: 60% 34%

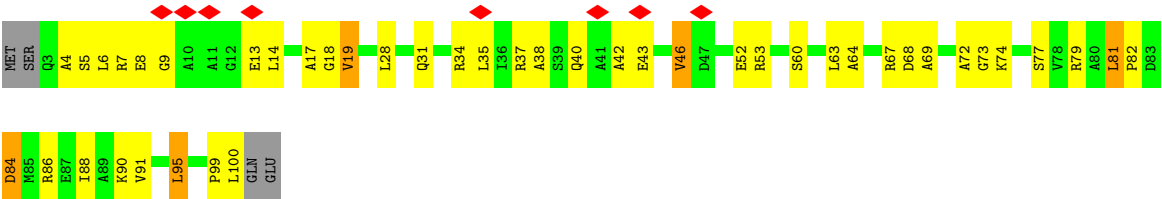


- Molecule 4: STAS domain-containing protein

Chain K: 7% 53% 40%



- Molecule 4: STAS domain-containing protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	622774	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	32.895	Depositor
Minimum map value	-18.727	Depositor
Average map value	-0.005	Depositor
Map value standard deviation	1.035	Depositor
Recommended contour level	3.94	Depositor
Map size ($\text{\AA}$)	256.0, 256.0, 256.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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

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	0.18	0/1096	0.47	0/1490
1	B	0.18	0/1077	0.42	0/1466
1	C	0.22	0/1087	0.44	0/1477
1	D	0.25	0/1092	0.46	0/1485
1	E	0.18	0/1099	0.43	0/1494
1	F	0.19	0/1078	0.48	0/1467
2	G	0.34	0/1965	0.54	0/2675
2	H	0.37	0/1943	0.57	0/2644
3	I	0.21	0/2052	0.45	0/2780
3	J	0.20	0/2026	0.44	0/2746
4	K	0.15	0/725	0.44	0/976
4	L	0.17	0/725	0.52	0/976
All	All	0.25	0/15965	0.48	0/21676

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	1088	0	1119	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1068	0	1084	40	0
1	C	1079	0	1119	53	0
1	D	1083	0	1119	42	0
1	E	1090	0	1122	42	0
1	F	1070	0	1096	39	0
2	G	1928	0	2002	100	0
2	H	1908	0	1975	92	0
3	I	2015	0	2070	89	0
3	J	1991	0	2039	76	0
4	K	721	0	759	36	0
4	L	721	0	759	31	0
5	A	13	0	22	0	0
5	B	26	0	44	3	0
5	C	26	0	44	7	0
5	E	13	0	22	6	0
5	F	13	0	22	1	0
5	G	81	0	114	28	0
5	H	44	0	67	1	0
All	All	15978	0	16598	605	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 19.

All (605) 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:85:TYR:CE1	5:G:301:LPP:HC81	1.55	1.40
2:G:85:TYR:CZ	5:G:301:LPP:HC81	1.84	1.13
2:G:85:TYR:CE1	5:G:301:LPP:C8	2.48	0.97
2:H:99:LEU:HD11	2:H:170:GLY:HA3	1.51	0.92
1:C:139:GLU:HA	1:C:142:ILE:HD11	1.52	0.92
5:C:201:LPP:C43	1:D:106:LEU:HD13	2.04	0.87
1:C:146:LEU:HD21	5:C:202:LPP:H372	1.55	0.85
5:G:301:LPP:H381	2:H:98:THR:HB	1.60	0.83
4:L:6:LEU:HB3	4:L:31:GLN:HE21	1.42	0.83
1:C:139:GLU:O	1:C:142:ILE:HD12	1.78	0.83
1:B:137:VAL:HG13	1:B:139:GLU:H	1.43	0.82
3:J:51:LEU:HD11	3:J:167:LEU:HB3	1.60	0.81
2:G:122:ALA:HB1	2:H:236:SER:HB3	1.61	0.81
2:G:81:ILE:HG13	5:G:301:LPP:H341	1.62	0.81
2:G:85:TYR:CZ	5:G:301:LPP:C8	2.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:51:LEU:HD11	3:I:167:LEU:HB3	1.62	0.80
1:D:142:ILE:HD11	1:E:136:LEU:HD13	1.62	0.80
5:G:301:LPP:O2	2:H:87:SER:HB3	1.81	0.79
5:G:301:LPP:H312	5:G:301:LPP:C14	2.13	0.79
2:H:104:GLY:HA2	2:H:166:PHE:HE2	1.47	0.79
4:K:95:LEU:HG	4:K:96:GLU:HG2	1.64	0.79
1:E:76:ASP:N	1:E:76:ASP:OD1	2.16	0.79
5:G:301:LPP:O2	2:H:87:SER:CB	2.32	0.78
1:B:63:VAL:HG11	1:F:73:LEU:HB2	1.67	0.77
1:E:84:MET:SD	1:E:84:MET:N	2.58	0.76
1:E:103:THR:HG22	1:E:110:LYS:HG2	1.68	0.76
1:D:142:ILE:HD11	1:E:136:LEU:CD1	2.16	0.75
2:G:236:SER:HB3	2:H:122:ALA:HB1	1.68	0.75
3:J:224:LEU:HB3	3:J:240:ILE:HD11	1.67	0.75
5:G:301:LPP:O28	2:H:93:GLN:OE1	2.03	0.75
2:G:231:THR:HG23	2:G:234:GLY:H	1.51	0.74
1:C:123:LEU:HD12	1:C:125:ASP:H	1.53	0.73
1:D:138:LEU:HD11	1:E:106:LEU:HA	1.66	0.73
1:B:102:LEU:HB2	1:B:111:TYR:HE1	1.54	0.73
1:E:51:GLY:HA3	1:E:110:LYS:HD3	1.69	0.73
5:G:301:LPP:H312	5:G:301:LPP:H142	1.70	0.73
2:G:103:LEU:HD12	2:H:103:LEU:HD12	1.71	0.72
2:G:63:ILE:HG21	2:G:162:LEU:HD22	1.71	0.72
3:I:36:VAL:HG13	3:I:198:SER:HB2	1.71	0.71
1:D:142:ILE:C	1:D:142:ILE:HD12	2.15	0.71
1:A:49:ILE:H	1:C:62:GLY:HA3	1.56	0.71
1:E:99:ALA:HB1	1:E:112:ILE:HD11	1.73	0.71
3:I:135:ARG:HH12	3:J:261:TYR:HA	1.56	0.70
2:G:220:ILE:HG22	5:G:302:LPP:H131	1.74	0.69
5:C:201:LPP:C43	1:D:106:LEU:CD1	2.70	0.69
3:I:264:ASP:O	3:J:122:ARG:NH1	2.26	0.69
1:D:104:ALA:HB3	1:D:108:GLY:HA3	1.74	0.68
5:C:202:LPP:H331	5:E:201:LPP:H332	1.73	0.68
3:J:237:ASP:HB3	3:J:240:ILE:HB	1.76	0.67
2:G:33:HIS:O	2:G:145:LYS:NZ	2.28	0.67
3:J:51:LEU:HD13	3:J:201:VAL:HG21	1.75	0.67
4:K:81:LEU:HD22	4:K:82:PRO:HD2	1.76	0.67
2:H:93:GLN:HG3	2:H:196:SER:OG	1.94	0.67
1:B:95:VAL:HG12	1:B:123:LEU:HD12	1.76	0.66
3:J:57:GLN:O	3:J:57:GLN:NE2	2.28	0.66
1:B:56:GLY:H	1:B:68:VAL:HG12	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:15:THR:HB	3:I:26:ASN:H	1.61	0.66
1:E:23:LEU:HA	1:E:26:LEU:HD22	1.78	0.66
4:L:34:ARG:HA	4:L:37:ARG:HE	1.59	0.66
3:I:190:LEU:HD13	3:I:194:LEU:HD13	1.78	0.66
5:G:301:LPP:H312	5:G:301:LPP:H141	1.77	0.65
1:B:72:ASP:OD2	1:B:81:ARG:NH2	2.29	0.65
4:K:34:ARG:HG3	4:K:37:ARG:HH21	1.62	0.65
3:J:40:MET:HE1	3:J:205:LEU:HA	1.79	0.65
1:F:137:VAL:HG22	1:F:139:GLU:H	1.62	0.65
3:I:55:ALA:O	3:I:84:ARG:NH2	2.30	0.65
1:C:98:THR:HG23	1:C:132:THR:HA	1.79	0.65
3:I:224:LEU:HB3	3:I:240:ILE:HD11	1.79	0.65
2:G:40:THR:OG1	2:G:43:THR:OG1	2.14	0.64
2:H:99:LEU:HD23	2:H:99:LEU:O	1.98	0.64
2:G:37:GLY:H	2:G:145:LYS:HZ2	1.43	0.64
1:A:67:LYS:N	1:A:85:GLU:OE2	2.30	0.64
3:J:15:THR:HG23	3:J:25:ASP:HA	1.79	0.64
1:F:90:VAL:HG22	1:F:93:LEU:HD11	1.79	0.64
2:H:59:SER:HB2	2:H:115:ARG:HD2	1.80	0.64
1:B:10:VAL:HG11	2:H:49:VAL:HG13	1.79	0.64
2:H:81:ILE:HG13	2:H:82:LEU:HD23	1.80	0.64
1:E:73:LEU:HD21	1:F:60:LEU:HD23	1.78	0.63
5:G:301:LPP:H362	2:H:98:THR:HG22	1.80	0.63
2:H:99:LEU:HD21	2:H:167:SER:HA	1.80	0.63
2:H:177:VAL:HG23	2:H:181:TRP:HE3	1.63	0.63
3:I:91:PHE:HA	3:I:169:ASP:HB3	1.80	0.63
3:I:39:ILE:HG12	3:I:201:VAL:HG22	1.79	0.63
4:L:84:ASP:OD1	4:L:84:ASP:N	2.31	0.63
3:J:97:PHE:H	3:J:105:ASN:HD21	1.45	0.63
3:I:40:MET:HB2	3:I:203:HIS:HA	1.80	0.63
4:K:79:ARG:NH2	4:K:100:LEU:O	2.32	0.63
1:D:68:VAL:HA	1:D:84:MET:HA	1.82	0.62
2:G:155:GLY:HA3	2:G:218:THR:HG21	1.81	0.62
3:I:228:THR:HG22	3:I:231:VAL:HG13	1.80	0.62
2:G:74:LEU:HD12	2:G:99:LEU:HD12	1.80	0.62
2:G:104:GLY:HA2	2:G:166:PHE:HE2	1.65	0.62
3:J:31:ILE:HG23	3:J:37:THR:HG21	1.82	0.62
1:D:40:TYR:HD1	1:D:41:LYS:H	1.46	0.61
3:J:59:ARG:NH1	3:J:73:PRO:O	2.32	0.61
5:C:202:LPP:H341	5:E:201:LPP:H352	1.81	0.61
1:A:7:GLU:OE1	2:H:26:ARG:NH2	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:ARG:NH1	2:G:198:GLN:OE1	2.34	0.61
1:E:49:ILE:HD11	1:F:63:VAL:HB	1.83	0.61
2:H:104:GLY:HA2	2:H:166:PHE:CE2	2.32	0.61
1:D:148:ASN:OD1	1:D:148:ASN:N	2.34	0.60
1:E:7:GLU:OE2	2:G:26:ARG:NH2	2.33	0.60
1:D:94:PRO:HA	1:D:122:VAL:HA	1.83	0.60
3:I:106:VAL:HG21	3:I:129:LEU:HD21	1.83	0.60
1:A:107:LEU:HB2	1:B:107:LEU:HD21	1.81	0.60
4:L:4:ALA:HB1	4:L:28:LEU:HD11	1.83	0.60
3:I:185:ARG:HE	3:J:248:PRO:HG2	1.66	0.60
1:F:146:LEU:HD23	1:F:147:LEU:HD23	1.84	0.60
3:I:17:LYS:HD3	3:I:20:SER:HA	1.82	0.60
1:C:97:SER:OG	1:C:115:SER:O	2.14	0.60
1:C:138:LEU:O	1:C:142:ILE:HG13	2.02	0.60
3:I:57:GLN:O	3:I:57:GLN:NE2	2.34	0.59
3:J:170:GLU:HA	3:J:202:SER:HB2	1.84	0.59
1:F:31:LEU:HB3	1:F:35:ASN:HB3	1.83	0.59
2:H:38:ARG:HG3	2:H:39:ARG:H	1.68	0.59
2:G:70:ILE:HG21	2:G:166:PHE:CZ	2.37	0.59
1:C:51:GLY:H	1:C:110:LYS:HE2	1.68	0.59
3:I:95:ALA:O	3:I:157:ARG:NH2	2.33	0.59
1:F:58:VAL:HG22	1:F:66:GLY:H	1.67	0.59
1:A:96:ASP:CG	1:A:118:GLY:H	2.11	0.59
1:A:94:PRO:HA	1:A:122:VAL:HA	1.85	0.59
1:D:39:THR:HG22	1:D:88:GLN:HB2	1.83	0.59
3:I:27:ILE:HG22	3:I:222:ARG:HA	1.85	0.58
1:F:87:ASN:HB3	1:F:90:VAL:HG12	1.85	0.58
2:G:70:ILE:HG21	2:G:166:PHE:HZ	1.69	0.58
2:G:213:PHE:O	2:G:217:VAL:N	2.36	0.58
2:G:240:THR:OG1	2:H:118:SER:OG	2.21	0.58
2:H:100:LEU:HD21	2:H:203:VAL:HA	1.85	0.58
4:K:78:VAL:HG21	4:K:81:LEU:HD23	1.85	0.58
1:E:43:TYR:HD1	1:E:83:THR:HG23	1.68	0.58
1:C:88:GLN:O	1:C:91:ASN:ND2	2.37	0.58
1:F:97:SER:HA	1:F:115:SER:O	2.02	0.58
2:H:121:THR:HG21	2:H:242:THR:HG21	1.85	0.58
2:H:224:GLN:HE21	2:H:241:ARG:HH11	1.49	0.58
2:G:121:THR:OG1	2:G:221:ALA:O	2.16	0.58
2:H:133:LEU:HD11	2:H:147:ILE:HG21	1.86	0.57
1:D:56:GLY:H	1:D:68:VAL:HG13	1.68	0.57
3:I:175:GLN:HE21	3:I:180:MET:HE2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:69:PHE:O	2:G:73:VAL:HG23	2.04	0.57
1:C:69:THR:HB	1:C:83:THR:HG23	1.85	0.57
1:E:146:LEU:CD2	5:E:201:LPP:H382	2.33	0.57
2:G:213:PHE:CZ	2:G:254:ASP:HB2	2.40	0.57
2:H:233:GLU:OE2	2:H:237:ARG:NH1	2.38	0.57
3:I:119:GLU:OE2	4:K:29:ARG:NH1	2.38	0.57
1:C:73:LEU:HB2	1:D:63:VAL:HG11	1.87	0.56
1:E:91:ASN:N	1:E:91:ASN:OD1	2.38	0.56
5:G:301:LPP:H191	2:H:98:THR:HG21	1.87	0.56
1:B:96:ASP:OD1	1:B:96:ASP:N	2.36	0.56
2:G:74:LEU:HD13	2:G:98:THR:HG23	1.87	0.56
2:H:97:LEU:O	2:H:101:ARG:N	2.28	0.56
1:B:102:LEU:HB2	1:B:111:TYR:CE1	2.39	0.56
1:D:43:TYR:HB2	1:D:128:THR:HG22	1.88	0.56
2:G:120:LEU:O	2:G:124:ILE:HG23	2.05	0.56
3:J:224:LEU:HD21	3:J:239:ARG:HD3	1.85	0.56
4:K:84:ASP:OD1	4:K:84:ASP:N	2.39	0.56
4:L:79:ARG:NH2	4:L:100:LEU:O	2.31	0.56
4:L:31:GLN:HA	4:L:35:LEU:HD13	1.87	0.56
1:F:87:ASN:OD1	1:F:88:GLN:N	2.38	0.56
2:G:105:PRO:HA	2:G:108:THR:HG22	1.88	0.56
3:J:32:PRO:HG2	3:J:35:LYS:HB2	1.86	0.56
3:J:244:VAL:HG23	3:J:245:LYS:HD2	1.88	0.56
2:G:224:GLN:HE22	2:G:241:ARG:HH11	1.52	0.55
1:E:146:LEU:HD22	5:E:201:LPP:H382	1.88	0.55
2:G:81:ILE:HG21	5:G:301:LPP:H332	1.89	0.55
3:I:11:LEU:HD11	3:I:54:ILE:HG22	1.88	0.55
4:K:16:LEU:HD12	4:K:20:LEU:HD11	1.89	0.55
2:G:81:ILE:HG13	5:G:301:LPP:C34	2.35	0.55
2:G:144:LEU:HA	2:G:148:VAL:HG13	1.88	0.55
1:B:3:THR:OG1	1:B:4:ARG:N	2.39	0.55
1:C:51:GLY:HA3	1:C:110:LYS:HG3	1.87	0.55
1:C:146:LEU:HD13	5:C:201:LPP:H331	1.89	0.55
1:C:139:GLU:O	1:C:142:ILE:CD1	2.51	0.55
3:I:71:ASN:HD21	3:I:74:GLN:HB2	1.72	0.55
4:K:4:ALA:HB3	4:K:28:LEU:HD11	1.89	0.55
3:I:183:LEU:O	3:I:187:ILE:HG23	2.06	0.55
1:C:94:PRO:HA	1:C:122:VAL:HA	1.88	0.54
2:H:83:ILE:HD12	2:H:88:GLU:HG2	1.89	0.54
3:J:168:TYR:CE2	3:J:187:ILE:HG12	2.41	0.54
5:G:301:LPP:O27	5:G:301:LPP:H132	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:87:PHE:HB3	3:J:165:ILE:HG12	1.88	0.54
3:J:40:MET:HE3	3:J:203:HIS:HA	1.89	0.54
4:L:77:SER:HA	4:L:99:PRO:HB2	1.89	0.54
3:I:65:VAL:HG12	3:I:67:VAL:HG23	1.90	0.54
1:E:70:ALA:HB3	1:E:83:THR:HB	1.90	0.54
2:H:127:MET:HB3	2:H:133:LEU:HD13	1.90	0.54
3:J:64:GLU:HG3	3:J:66:TRP:HE1	1.71	0.54
4:L:18:GLY:HA2	4:L:52:GLU:H	1.72	0.54
1:C:66:GLY:HA3	1:C:85:GLU:O	2.08	0.54
2:H:154:ALA:O	2:H:158:SER:HB3	2.07	0.54
3:I:64:GLU:OE2	3:I:66:TRP:NE1	2.41	0.54
3:J:190:LEU:HD13	3:J:194:LEU:HD13	1.89	0.54
1:D:58:VAL:HG22	1:D:66:GLY:C	2.33	0.54
1:C:96:ASP:N	1:C:120:GLU:OE2	2.40	0.54
1:A:92:ASN:HB2	1:B:78:TYR:HE1	1.73	0.53
2:H:70:ILE:HG12	2:H:103:LEU:HD21	1.91	0.53
1:E:46:PHE:HD2	1:E:49:ILE:HG22	1.73	0.53
1:E:65:ILE:HG23	1:E:90:VAL:HG11	1.91	0.53
1:E:132:THR:OG1	1:E:133:GLN:N	2.41	0.53
2:G:70:ILE:HG13	2:G:103:LEU:HD21	1.91	0.53
2:G:101:ARG:NH1	2:H:80:ASN:OD1	2.40	0.53
2:G:118:SER:OG	2:H:240:THR:OG1	2.25	0.53
2:G:220:ILE:HD11	2:G:246:ALA:HA	1.89	0.53
1:A:8:ILE:O	1:A:12:LEU:HG	2.09	0.53
2:H:177:VAL:HG23	2:H:181:TRP:CE3	2.43	0.53
3:I:252:VAL:HG11	3:J:178:ILE:HD12	1.91	0.53
3:J:137:ALA:HB1	3:J:140:LEU:HB2	1.90	0.53
1:F:74:ASP:OD1	1:F:79:THR:N	2.41	0.53
2:G:213:PHE:HZ	2:G:254:ASP:HB2	1.73	0.53
1:B:44:ALA:HB3	1:B:82:VAL:HG13	1.90	0.53
3:J:134:LEU:HD21	3:J:149:MET:HE2	1.90	0.53
1:D:142:ILE:HD12	1:D:142:ILE:O	2.09	0.52
1:E:73:LEU:HB2	1:F:63:VAL:HG11	1.91	0.52
2:H:138:MET:SD	3:J:57:GLN:HB2	2.49	0.52
3:J:176:ASP:N	3:J:176:ASP:OD1	2.38	0.52
1:D:137:VAL:HG23	1:D:140:ASP:HB2	1.89	0.52
3:J:39:ILE:HG12	3:J:201:VAL:HG22	1.90	0.52
1:B:40:TYR:HB3	1:B:125:ASP:HB3	1.91	0.52
2:H:257:LEU:HD12	2:H:261:MET:HE2	1.92	0.52
4:L:68:ASP:O	4:L:72:ALA:N	2.38	0.52
1:D:123:LEU:HG	1:D:125:ASP:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:THR:HG23	1:A:84:MET:HA	1.91	0.52
2:H:63:ILE:HG12	2:H:162:LEU:HD22	1.92	0.52
2:H:68:LEU:O	2:H:72:MET:HG2	2.09	0.52
3:I:170:GLU:HA	3:I:202:SER:HB2	1.92	0.52
3:J:190:LEU:HD12	3:J:196:ILE:HD11	1.92	0.52
3:I:248:PRO:HG2	3:J:185:ARG:HE	1.74	0.52
2:G:249:ALA:HA	5:G:302:LPP:H332	1.91	0.52
3:I:68:ASN:ND2	3:I:164:GLN:OE1	2.42	0.52
3:J:55:ALA:O	3:J:84:ARG:NH2	2.43	0.52
1:D:69:THR:OG1	1:D:83:THR:OG1	2.21	0.51
3:J:114:THR:HB	3:J:116:LEU:HD13	1.92	0.51
1:A:99:ALA:O	1:A:132:THR:OG1	2.20	0.51
4:K:46:VAL:HG13	4:K:78:VAL:HA	1.91	0.51
4:K:84:ASP:O	4:K:88:ILE:HG12	2.09	0.51
1:E:127:SER:OG	1:E:128:THR:N	2.41	0.51
2:H:51:GLN:HG3	2:H:150:PRO:HB2	1.93	0.51
2:G:212:VAL:HG11	2:G:257:LEU:HG	1.92	0.51
5:G:301:LPP:C19	2:H:94:MET:HE3	2.40	0.51
2:H:144:LEU:HA	2:H:148:VAL:HG13	1.93	0.51
1:C:144:LYS:HA	1:C:148:ASN:HD22	1.75	0.51
1:F:5:THR:HG23	2:G:11:ARG:HH11	1.76	0.51
1:A:38:ASP:O	1:A:88:GLN:HG2	2.11	0.51
1:C:74:ASP:OD2	1:C:77:SER:N	2.33	0.51
3:I:100:LEU:HB3	3:I:104:GLU:HB2	1.92	0.51
3:I:122:ARG:NH1	3:J:264:ASP:O	2.42	0.51
1:A:94:PRO:HG2	1:A:117:GLY:H	1.76	0.51
1:A:98:THR:HB	1:A:132:THR:HA	1.92	0.51
3:I:137:ALA:HB1	3:I:140:LEU:HB2	1.93	0.51
3:I:235:THR:HG23	3:I:237:ASP:H	1.74	0.51
3:J:117:PRO:HD2	3:J:120:MET:HE2	1.92	0.51
5:B:201:LPP:H321	5:B:202:LPP:H321	1.93	0.50
1:E:43:TYR:CD1	1:E:83:THR:HG23	2.47	0.50
1:A:62:GLY:HA3	1:B:49:ILE:O	2.11	0.50
1:B:28:VAL:O	2:H:194:GLN:HA	2.12	0.50
2:G:83:ILE:HG12	2:G:88:GLU:HG2	1.94	0.50
1:A:132:THR:OG1	1:A:133:GLN:N	2.45	0.50
1:D:131:ASP:OD1	1:D:131:ASP:N	2.30	0.50
2:G:5:SER:O	2:G:9:ARG:N	2.40	0.50
1:B:97:SER:OG	1:B:98:THR:N	2.44	0.50
3:I:190:LEU:HD12	3:I:196:ILE:HD11	1.94	0.50
3:I:102:VAL:O	3:I:106:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:108:THR:HG21	2:G:163:ALA:HB2	1.94	0.50
1:A:96:ASP:N	1:A:96:ASP:OD1	2.45	0.49
1:C:71:VAL:HG12	1:C:82:VAL:HG23	1.93	0.49
1:D:100:SER:OG	1:D:133:GLN:HB2	2.12	0.49
1:D:46:PHE:HD2	1:D:49:ILE:HG22	1.77	0.49
2:G:137:GLU:HG2	2:G:143:PRO:HD3	1.93	0.49
3:I:194:LEU:HD12	4:K:91:VAL:HG21	1.94	0.49
4:L:28:LEU:HA	4:L:31:GLN:HG2	1.94	0.49
1:B:69:THR:OG1	1:B:83:THR:OG1	2.26	0.49
1:B:60:LEU:HD13	1:B:65:ILE:HG13	1.93	0.49
1:C:3:THR:HG23	1:C:4:ARG:HG3	1.94	0.49
1:F:39:THR:OG1	1:F:85:GLU:HB3	2.12	0.49
4:K:82:PRO:HB2	4:K:84:ASP:OD1	2.13	0.49
3:I:122:ARG:NH2	3:J:264:ASP:OD1	2.45	0.49
3:J:95:ALA:O	3:J:157:ARG:NH2	2.39	0.49
3:J:170:GLU:HG3	3:J:173:VAL:HB	1.95	0.49
4:L:84:ASP:O	4:L:88:ILE:HG12	2.13	0.49
1:A:95:VAL:HG23	1:A:121:ASP:O	2.12	0.49
3:J:96:LEU:HD13	3:J:142:PRO:HB3	1.95	0.49
1:A:72:ASP:OD2	1:A:81:ARG:NE	2.45	0.48
2:G:73:VAL:HG22	2:H:255:PHE:HA	1.94	0.48
1:E:16:ALA:O	1:E:20:ALA:N	2.47	0.48
2:G:231:THR:OG1	2:G:232:SER:N	2.45	0.48
3:J:123:ASP:OD1	4:L:67:ARG:NH1	2.40	0.48
4:L:7:ARG:HD2	4:L:8:GLU:H	1.78	0.48
2:G:213:PHE:HZ	2:G:254:ASP:HA	1.78	0.48
3:I:40:MET:HE2	3:I:40:MET:HB3	1.75	0.48
3:J:96:LEU:HD23	3:J:157:ARG:HH21	1.77	0.48
4:K:64:ALA:HA	4:K:67:ARG:HG2	1.95	0.48
3:I:52:ARG:HB3	3:I:57:GLN:HB3	1.93	0.48
1:A:139:GLU:N	1:A:139:GLU:OE1	2.46	0.48
1:F:122:VAL:HG12	1:F:123:LEU:HD23	1.95	0.48
2:H:217:VAL:HG22	2:H:246:ALA:HB1	1.95	0.48
1:B:62:GLY:HA3	1:F:49:ILE:HG13	1.96	0.48
3:I:59:ARG:NH1	3:I:73:PRO:O	2.47	0.48
1:B:31:LEU:HD11	2:H:199:PHE:CE2	2.49	0.48
1:F:47:ASP:OD1	1:F:47:ASP:N	2.45	0.48
2:G:213:PHE:HZ	2:G:254:ASP:CA	2.27	0.48
3:I:241:ARG:HH21	3:I:245:LYS:HE2	1.77	0.48
1:B:140:ASP:OD1	1:B:140:ASP:N	2.46	0.48
1:A:19:LEU:HD12	1:A:23:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:ARG:HH12	2:H:198:GLN:HA	1.77	0.48
2:G:74:LEU:HB3	2:G:95:VAL:HG12	1.95	0.48
3:I:16:PHE:HE2	3:I:18:ARG:HH11	1.61	0.48
3:J:14:LEU:HD23	3:J:15:THR:N	2.29	0.48
4:L:69:ALA:O	4:L:73:GLY:N	2.47	0.48
1:D:54:VAL:HG13	1:D:55:ARG:HG3	1.96	0.47
2:G:77:GLN:OE1	2:H:258:THR:OG1	2.30	0.47
3:I:135:ARG:NH1	3:J:261:TYR:HA	2.26	0.47
2:H:132:GLN:NE2	3:J:97:PHE:HA	2.28	0.47
2:H:132:GLN:HE22	3:J:98:THR:H	1.62	0.47
1:A:89:ASN:OD1	1:A:90:VAL:N	2.47	0.47
4:K:5:SER:H	4:K:17:ALA:HB3	1.79	0.47
3:I:185:ARG:HH11	3:J:248:PRO:HB2	1.79	0.47
5:G:301:LPP:H191	2:H:94:MET:HE3	1.96	0.47
3:I:51:LEU:O	3:I:54:ILE:HG12	2.15	0.47
1:C:39:THR:HA	1:C:86:ILE:O	2.15	0.47
2:G:104:GLY:HA2	2:G:166:PHE:CE2	2.46	0.47
5:G:301:LPP:H322	2:H:94:MET:HG3	1.97	0.47
2:H:74:LEU:CD1	2:H:99:LEU:HB2	2.43	0.47
4:L:5:SER:HB3	4:L:17:ALA:HB2	1.95	0.47
1:E:26:LEU:HD23	1:E:27:ARG:H	1.80	0.47
2:G:24:LEU:HG	5:G:302:LPP:H122	1.96	0.47
2:G:81:ILE:HG22	2:G:82:LEU:CD2	2.45	0.47
5:G:301:LPP:H401	2:H:103:LEU:HB2	1.96	0.47
2:H:93:GLN:NE2	2:H:196:SER:HB2	2.30	0.47
1:B:6:LEU:HD21	2:H:50:LYS:HD3	1.97	0.47
3:I:17:LYS:HB2	3:I:22:ALA:H	1.80	0.47
4:K:37:ARG:HE	4:K:37:ARG:HB3	1.62	0.47
4:K:48:CYS:HB3	4:K:51:VAL:HG21	1.97	0.47
1:A:40:TYR:HB3	1:A:125:ASP:HB3	1.96	0.46
1:E:49:ILE:O	1:E:52:VAL:HG22	2.16	0.46
2:G:239:THR:HG21	2:H:239:THR:HG21	1.96	0.46
2:H:16:ALA:O	2:H:20:VAL:HG23	2.14	0.46
3:I:9:VAL:HG13	3:I:67:VAL:HG22	1.96	0.46
4:K:13:GLU:H	4:K:13:GLU:CD	2.22	0.46
2:G:154:ALA:O	2:G:158:SER:HB3	2.15	0.46
2:G:213:PHE:CZ	2:G:254:ASP:CB	2.98	0.46
2:G:213:PHE:HZ	2:G:254:ASP:CB	2.28	0.46
2:H:104:GLY:N	2:H:105:PRO:HD2	2.30	0.46
2:H:155:GLY:HA3	2:H:218:THR:HG21	1.96	0.46
2:H:224:GLN:HE21	2:H:241:ARG:NH1	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:80:LEU:O	3:I:84:ARG:HG2	2.15	0.46
1:D:69:THR:N	1:D:83:THR:O	2.38	0.46
3:I:71:ASN:HD22	3:I:73:PRO:HD2	1.81	0.46
3:I:170:GLU:HG3	3:I:202:SER:HA	1.97	0.46
3:J:82:ASP:OD1	3:J:85:LYS:NZ	2.30	0.46
3:J:123:ASP:OD2	4:L:67:ARG:NH2	2.49	0.46
3:J:194:LEU:HD11	4:L:91:VAL:HG11	1.96	0.46
1:A:89:ASN:OD1	1:A:90:VAL:HG22	2.15	0.46
1:C:9:GLY:O	1:C:12:LEU:HG	2.15	0.46
1:C:136:LEU:HD13	1:C:141:LEU:HD11	1.96	0.46
1:E:144:LYS:HE2	1:E:144:LYS:HB3	1.66	0.46
3:I:128:LYS:HD3	3:I:128:LYS:HA	1.63	0.46
3:I:215:ILE:HG23	3:I:232:LEU:HD13	1.97	0.46
3:J:52:ARG:HB3	3:J:57:GLN:HB3	1.97	0.46
3:J:90:LEU:HD23	3:J:168:TYR:CD2	2.50	0.46
2:G:81:ILE:HG22	2:G:82:LEU:HD23	1.97	0.46
2:G:81:ILE:CG1	5:G:301:LPP:H341	2.42	0.46
2:H:121:THR:HG21	2:H:239:THR:HA	1.97	0.46
1:A:104:ALA:HB3	1:A:108:GLY:HA3	1.98	0.46
1:C:89:ASN:OD1	1:C:90:VAL:N	2.49	0.46
2:G:62:ILE:HD12	2:H:248:LEU:HD13	1.97	0.46
2:H:208:ILE:O	2:H:212:VAL:HG23	2.16	0.46
1:D:78:TYR:HB3	1:E:60:LEU:HD21	1.97	0.46
1:E:124:LYS:NZ	1:E:124:LYS:O	2.49	0.46
2:H:62:ILE:HG23	2:H:63:ILE:HG23	1.97	0.46
1:B:63:VAL:HG23	1:F:49:ILE:HD11	1.98	0.46
2:G:93:GLN:O	2:G:97:LEU:HB2	2.15	0.46
4:K:7:ARG:NH2	4:K:15:GLN:HG3	2.31	0.46
1:B:72:ASP:OD1	1:B:73:LEU:N	2.49	0.46
1:B:59:THR:HA	1:B:65:ILE:HG12	1.98	0.45
1:D:146:LEU:CD1	5:E:201:LPP:H371	2.46	0.45
2:G:100:LEU:HD11	2:G:203:VAL:HG22	1.98	0.45
3:I:194:LEU:HD22	3:I:196:ILE:HD13	1.98	0.45
4:L:37:ARG:NH2	4:L:38:ALA:HB2	2.31	0.45
1:C:132:THR:OG1	1:C:133:GLN:N	2.47	0.45
2:G:228:CYS:HB3	2:G:238:ALA:HB2	1.98	0.45
2:H:99:LEU:CD1	2:H:170:GLY:HA3	2.34	0.45
3:I:108:PHE:HB3	3:I:109:PRO:HD3	1.98	0.45
3:I:205:LEU:HD22	3:I:244:VAL:HA	1.99	0.45
3:J:80:LEU:O	3:J:84:ARG:HG2	2.17	0.45
1:D:37:GLY:O	1:D:39:THR:HG23	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:43:THR:OG1	2:H:44:GLY:N	2.49	0.45
1:C:102:LEU:HB2	1:C:111:TYR:CE1	2.51	0.45
1:E:40:TYR:HE2	1:E:91:ASN:HB3	1.81	0.45
1:E:49:ILE:HB	1:E:52:VAL:HG21	1.97	0.45
2:G:145:LYS:HB2	2:G:145:LYS:HE2	1.69	0.45
3:I:116:LEU:HB2	3:I:121:ILE:HD13	1.96	0.45
3:J:36:VAL:HG23	3:J:198:SER:HB2	1.97	0.45
3:J:65:VAL:HG22	3:J:73:PRO:HD3	1.98	0.45
1:F:24:LEU:HA	1:F:27:ARG:HB2	1.99	0.45
2:G:38:ARG:H	2:G:145:LYS:HE3	1.82	0.45
5:G:301:LPP:O2	2:H:87:SER:OG	2.34	0.45
3:J:261:TYR:OH	4:K:94:LEU:HB2	2.17	0.45
4:L:14:LEU:HB3	4:L:46:VAL:HA	1.98	0.45
1:F:40:TYR:HB3	1:F:125:ASP:CG	2.41	0.45
3:J:132:VAL:HG11	3:J:156:ALA:HB2	1.99	0.45
1:B:92:ASN:OD1	1:B:92:ASN:N	2.49	0.45
2:G:44:GLY:H	2:G:47:LEU:HD12	1.82	0.45
3:I:101:ASP:OD1	3:I:104:GLU:HG2	2.16	0.45
4:K:4:ALA:HB1	4:K:17:ALA:HB3	1.99	0.45
4:K:34:ARG:HG3	4:K:37:ARG:NH2	2.29	0.45
1:C:40:TYR:HB2	1:C:125:ASP:CG	2.42	0.45
1:F:49:ILE:O	1:F:52:VAL:HG12	2.16	0.45
2:H:159:MET:HG2	2:H:214:ALA:HB2	1.99	0.45
3:I:176:ASP:OD1	3:I:179:ALA:N	2.32	0.45
3:J:40:MET:HB3	3:J:202:SER:O	2.17	0.45
3:J:98:THR:HA	3:J:142:PRO:HG2	1.98	0.45
4:L:81:LEU:HD22	4:L:82:PRO:HD2	1.98	0.45
2:G:197:VAL:O	2:G:202:ASP:HB2	2.16	0.45
3:I:120:MET:HG3	4:K:60:SER:OG	2.17	0.45
1:C:91:ASN:O	1:C:122:VAL:HG11	2.17	0.45
1:C:139:GLU:O	1:C:143:GLY:N	2.49	0.45
2:G:74:LEU:CD1	2:G:99:LEU:HB2	2.47	0.45
4:L:86:ARG:HH22	4:L:95:LEU:HG	1.81	0.45
2:H:249:ALA:O	2:H:253:LEU:HB2	2.17	0.44
3:I:126:LEU:HD13	3:I:126:LEU:HA	1.77	0.44
3:J:17:LYS:HD3	3:J:20:SER:HA	1.99	0.44
2:G:254:ASP:OD1	2:H:73:VAL:HG21	2.17	0.44
2:H:78:GLY:HA3	2:H:94:MET:SD	2.57	0.44
1:A:23:LEU:HG	1:A:24:LEU:H	1.82	0.44
1:D:31:LEU:HD22	1:D:31:LEU:HA	1.69	0.44
2:H:30:PHE:HZ	2:H:222:VAL:HG12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:93:GLN:HE21	2:H:196:SER:HB2	1.83	0.44
3:I:180:MET:SD	3:I:207:GLU:HG3	2.58	0.44
1:F:49:ILE:HB	1:F:52:VAL:CG1	2.46	0.44
4:K:68:ASP:O	4:K:72:ALA:N	2.40	0.44
1:C:36:ALA:O	1:C:39:THR:OG1	2.30	0.44
1:C:47:ASP:OD1	1:C:47:ASP:N	2.50	0.44
1:F:89:ASN:OD1	1:F:90:VAL:N	2.51	0.44
2:G:8:GLU:HA	2:G:11:ARG:HB3	1.99	0.44
2:G:37:GLY:H	2:G:145:LYS:NZ	2.15	0.44
3:I:160:ALA:O	3:I:163:PRO:HD3	2.18	0.44
1:B:76:ASP:OD1	1:B:76:ASP:N	2.39	0.44
1:E:59:THR:OG1	1:E:60:LEU:N	2.50	0.44
1:D:32:SER:O	1:D:32:SER:OG	2.36	0.44
1:F:35:ASN:O	1:F:87:ASN:ND2	2.51	0.44
3:J:207:GLU:O	3:J:211:ILE:HG22	2.18	0.44
2:G:124:ILE:HD11	2:G:226:TYR:HB2	2.00	0.43
2:H:123:GLU:OE2	2:H:151:ARG:NH1	2.50	0.43
3:J:108:PHE:HB3	3:J:109:PRO:HD3	1.98	0.43
3:J:265:LEU:HD21	4:K:63:LEU:HG	1.99	0.43
4:K:54:SER:OG	4:K:55:SER:N	2.49	0.43
1:C:39:THR:HB	1:C:85:GLU:HB3	1.99	0.43
1:A:137:VAL:HG23	1:A:140:ASP:HB3	2.01	0.43
1:B:101:ILE:HG12	1:B:135:ALA:HA	2.01	0.43
2:G:238:ALA:O	2:G:242:THR:HG22	2.18	0.43
2:H:35:LEU:HD23	2:H:35:LEU:HA	1.86	0.43
1:B:26:LEU:HD13	1:B:34:GLY:HA2	2.00	0.43
1:C:53:THR:HG22	1:C:54:VAL:H	1.83	0.43
1:F:94:PRO:HG3	1:F:116:VAL:HG13	2.00	0.43
2:G:127:MET:HE1	2:G:151:ARG:HH22	1.84	0.43
3:I:70:GLN:OE1	3:I:70:GLN:N	2.45	0.43
1:A:69:THR:HG1	1:A:83:THR:C	2.25	0.43
1:A:139:GLU:HG3	1:C:136:LEU:HD23	1.98	0.43
1:D:53:THR:OG1	1:D:54:VAL:N	2.51	0.43
1:E:146:LEU:HD11	5:E:201:LPP:H331	2.00	0.43
3:I:51:LEU:HD13	3:I:201:VAL:HG21	2.01	0.43
3:I:90:LEU:HD23	3:I:168:TYR:CD2	2.54	0.43
3:J:129:LEU:HD22	3:J:134:LEU:O	2.19	0.43
1:F:59:THR:O	1:F:113:GLY:HA2	2.19	0.43
2:G:52:LEU:HD12	2:G:52:LEU:HA	1.84	0.43
2:H:147:ILE:O	2:H:151:ARG:HG2	2.19	0.43
4:L:9:GLY:HA2	4:L:40:GLN:HE22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ILE:HG13	1:C:62:GLY:HA3	2.01	0.43
1:C:48:ASN:HA	1:D:61:ALA:O	2.19	0.43
2:G:69:PHE:CZ	5:H:301:LPP:H211	2.54	0.43
2:G:257:LEU:HD12	2:G:261:MET:HE2	2.00	0.43
2:H:204:LEU:O	2:H:208:ILE:HG22	2.18	0.43
3:J:219:GLY:HA3	3:J:224:LEU:HD22	2.00	0.43
4:K:69:ALA:HB2	4:K:76:LEU:HD23	1.99	0.43
4:L:19:VAL:HA	4:L:53:ARG:O	2.19	0.43
1:B:124:LYS:HE2	1:B:127:SER:HB3	1.99	0.43
2:H:79:TYR:CG	2:H:182:LEU:HD13	2.54	0.43
3:I:243:PHE:HA	3:J:178:ILE:HG22	2.00	0.43
4:K:87:GLU:O	4:K:91:VAL:HG23	2.18	0.43
4:L:60:SER:O	4:L:64:ALA:N	2.51	0.43
1:D:17:GLY:C	2:G:161:LEU:HD12	2.44	0.43
2:G:76:LEU:HD21	2:H:259:ALA:HA	2.00	0.43
2:H:136:LEU:HD22	2:H:141:VAL:HB	2.01	0.43
3:I:123:ASP:OD1	4:K:67:ARG:NH1	2.50	0.43
4:K:18:GLY:HA2	4:K:51:VAL:HA	2.01	0.43
4:K:30:GLU:HA	4:K:34:ARG:NH2	2.34	0.43
4:L:6:LEU:HD11	4:L:14:LEU:HG	2.00	0.43
1:B:4:ARG:HA	1:B:4:ARG:HD3	1.69	0.43
1:C:99:ALA:O	1:C:132:THR:OG1	2.16	0.43
1:E:21:LEU:HD23	2:G:256:ILE:HG21	2.00	0.43
3:I:237:ASP:HB3	3:I:240:ILE:HB	2.01	0.43
2:G:99:LEU:HD21	2:G:170:GLY:HA3	2.01	0.42
5:B:202:LPP:H322	5:B:202:LPP:H351	1.46	0.42
1:C:4:ARG:HA	1:C:7:GLU:HB2	2.01	0.42
3:I:233:LYS:HE3	3:I:233:LYS:HB2	1.86	0.42
4:K:29:ARG:HD2	4:K:30:GLU:OE2	2.19	0.42
1:D:124:LYS:NZ	1:D:126:GLY:HA3	2.35	0.42
3:I:8:ALA:HB3	3:I:31:ILE:HG22	2.01	0.42
1:C:138:LEU:HD23	1:C:138:LEU:HA	1.82	0.42
1:D:73:LEU:HB2	1:E:63:VAL:HG11	2.01	0.42
1:F:39:THR:OG1	1:F:40:TYR:N	2.52	0.42
3:J:109:PRO:HG2	3:J:157:ARG:HG3	2.01	0.42
1:C:138:LEU:HD11	1:D:106:LEU:HD12	2.01	0.42
1:D:59:THR:OG1	1:D:60:LEU:N	2.53	0.42
1:F:65:ILE:HG23	1:F:90:VAL:HG11	2.01	0.42
2:G:127:MET:SD	2:G:147:ILE:HD12	2.60	0.42
2:G:157:ILE:O	2:G:161:LEU:HD23	2.20	0.42
3:I:162:ASP:OD2	4:K:56:SER:OG	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:THR:HG21	1:B:85:GLU:HG2	2.01	0.42
2:G:74:LEU:HD12	2:G:99:LEU:CD1	2.46	0.42
2:G:85:TYR:OH	5:G:301:LPP:C8	2.67	0.42
1:A:46:PHE:HD2	1:A:49:ILE:HG22	1.84	0.42
1:A:87:ASN:HB2	1:A:89:ASN:OD1	2.19	0.42
1:B:35:ASN:OD1	1:B:35:ASN:N	2.51	0.42
1:F:101:ILE:HG13	1:F:112:ILE:HG22	2.02	0.42
2:H:220:ILE:HD11	2:H:246:ALA:HA	2.02	0.42
3:I:235:THR:HG21	3:I:240:ILE:HB	2.01	0.42
3:J:262:ARG:HD2	3:J:266:LEU:HD23	2.02	0.42
1:A:101:ILE:H	1:A:101:ILE:HD12	1.84	0.42
1:C:146:LEU:HD12	1:C:146:LEU:HA	1.93	0.42
3:I:33:ARG:H	3:I:33:ARG:HG2	1.67	0.42
3:I:168:TYR:HB2	3:I:200:VAL:HA	2.02	0.42
3:J:96:LEU:HD11	3:J:153:VAL:CG1	2.50	0.42
1:C:60:LEU:N	1:C:65:ILE:HG12	2.35	0.42
1:C:146:LEU:HD13	5:C:201:LPP:C33	2.50	0.42
3:J:111:ARG:NE	3:J:118:GLU:OE2	2.40	0.42
1:D:142:ILE:C	1:D:142:ILE:CD1	2.85	0.42
1:F:34:GLY:O	1:F:87:ASN:ND2	2.53	0.42
2:G:77:GLN:NE2	2:G:77:GLN:HA	2.29	0.42
2:G:147:ILE:HD13	2:G:147:ILE:HA	1.87	0.42
2:H:115:ARG:HD3	2:H:115:ARG:C	2.45	0.42
3:I:132:VAL:HG21	3:I:152:ARG:O	2.19	0.42
1:B:48:ASN:OD1	1:B:49:ILE:N	2.53	0.41
1:E:46:PHE:CD2	1:E:101:ILE:HD11	2.55	0.41
2:H:7:LEU:HD12	2:H:7:LEU:HA	1.87	0.41
3:I:87:PHE:HA	3:I:165:ILE:O	2.20	0.41
3:I:96:LEU:HD23	3:I:157:ARG:HH21	1.85	0.41
1:C:82:VAL:HG13	1:C:84:MET:HE1	2.02	0.41
1:D:76:ASP:OD1	1:D:76:ASP:N	2.51	0.41
1:F:92:ASN:N	1:F:92:ASN:OD1	2.51	0.41
3:I:49:THR:O	3:I:53:LEU:HG	2.20	0.41
3:I:187:ILE:HD11	3:I:211:ILE:HG12	2.02	0.41
3:I:241:ARG:HA	3:I:244:VAL:HG22	2.02	0.41
1:B:61:ALA:O	1:F:49:ILE:N	2.47	0.41
1:B:137:VAL:HG13	1:B:139:GLU:N	2.23	0.41
1:C:144:LYS:HA	1:C:148:ASN:ND2	2.36	0.41
1:D:87:ASN:OD1	1:D:89:ASN:ND2	2.53	0.41
1:F:42:VAL:HG12	1:F:84:MET:HG2	2.02	0.41
2:H:135:SER:O	2:H:135:SER:OG	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:14:LEU:O	4:K:46:VAL:HA	2.20	0.41
4:L:74:LYS:H	4:L:74:LYS:HG2	1.59	0.41
1:E:23:LEU:HD21	2:G:260:LEU:HB2	2.02	0.41
2:G:72:MET:HE2	2:G:72:MET:HB3	1.78	0.41
2:H:97:LEU:HD13	2:H:97:LEU:HA	1.75	0.41
2:H:231:THR:HG23	2:H:234:GLY:H	1.85	0.41
3:I:114:THR:HG22	4:K:22:TYR:CD2	2.55	0.41
3:J:87:PHE:HA	3:J:165:ILE:O	2.19	0.41
1:C:45:TYR:HE1	1:C:81:ARG:HD3	1.84	0.41
1:C:140:ASP:N	1:C:140:ASP:OD1	2.53	0.41
1:E:15:LEU:HD23	1:E:18:LEU:HD23	2.02	0.41
2:G:81:ILE:HD13	2:G:81:ILE:HA	1.78	0.41
3:J:103:PHE:HB2	3:J:138:VAL:O	2.20	0.41
3:J:123:ASP:HB2	4:L:60:SER:OG	2.21	0.41
4:L:42:ALA:O	4:L:43:GLU:HG3	2.20	0.41
4:L:90:LYS:HE3	4:L:90:LYS:HB2	1.66	0.41
5:B:202:LPP:H371	5:B:202:LPP:H342	1.44	0.41
1:D:49:ILE:HD11	1:E:63:VAL:HB	2.03	0.41
3:I:41:GLY:HA3	3:I:218:VAL:O	2.21	0.41
3:J:260:ASP:HB3	3:J:263:ALA:HB3	2.02	0.41
1:A:58:VAL:HG21	1:A:84:MET:HB2	2.02	0.41
1:B:145:PHE:HA	1:B:149:SER:OG	2.20	0.41
1:C:14:LEU:HD23	1:C:15:LEU:HD22	2.02	0.41
1:E:138:LEU:HD12	1:F:106:LEU:HG	2.03	0.41
1:A:101:ILE:HD13	1:A:135:ALA:HB2	2.02	0.41
1:F:94:PRO:HB2	1:F:119:ASP:OD1	2.20	0.41
1:F:146:LEU:HD12	5:F:201:LPP:H341	2.01	0.41
2:G:103:LEU:CD1	2:H:103:LEU:HD12	2.47	0.41
2:H:121:THR:HA	2:H:124:ILE:HG22	2.03	0.41
3:J:120:MET:HG3	4:L:60:SER:OG	2.21	0.41
4:L:86:ARG:HH12	4:L:95:LEU:HG	1.86	0.41
1:C:88:GLN:HG3	1:C:91:ASN:HD22	1.85	0.41
2:G:41:PRO:HG2	3:I:81:PHE:CE1	2.56	0.41
2:H:47:LEU:O	2:H:51:GLN:HG2	2.21	0.41
3:I:132:VAL:HG22	3:I:152:ARG:HB3	2.02	0.41
1:B:51:GLY:H	1:B:110:LYS:HD3	1.86	0.40
2:H:138:MET:HG2	3:J:89:VAL:HG21	2.02	0.40
3:I:82:ASP:HA	3:I:85:LYS:NZ	2.35	0.40
2:G:132:GLN:HG3	3:I:97:PHE:HD1	1.85	0.40
2:G:135:SER:O	2:G:139:ILE:HG13	2.22	0.40
2:G:138:MET:O	3:I:84:ARG:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:245:TYR:CD2	5:G:302:LPP:HC82	2.56	0.40
2:G:250:VAL:O	2:G:254:ASP:HB3	2.20	0.40
3:J:53:LEU:HD12	3:J:53:LEU:HA	1.79	0.40
1:C:121:ASP:OD1	1:C:121:ASP:N	2.54	0.40
2:G:162:LEU:HD23	2:G:162:LEU:HA	1.84	0.40
3:I:24:PHE:CG	3:I:27:ILE:HD13	2.56	0.40
3:I:256:TYR:CD1	3:J:149:MET:HE1	2.56	0.40
1:A:39:THR:HB	1:A:85:GLU:HB2	2.04	0.40
1:E:96:ASP:OD2	1:E:118:GLY:N	2.34	0.40
1:C:65:ILE:HG22	1:C:86:ILE:HG13	2.04	0.40
1:E:49:ILE:HB	1:E:52:VAL:CG2	2.51	0.40
1:F:40:TYR:HB3	1:F:125:ASP:OD1	2.22	0.40
1:F:102:LEU:HB2	1:F:111:TYR:CE1	2.57	0.40
2:G:220:ILE:HD11	2:G:246:ALA:CA	2.52	0.40
2:H:127:MET:SD	2:H:147:ILE:HD12	2.62	0.40
4:K:74:LYS:H	4:K:74:LYS:HG2	1.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	126 (85%)	22 (15%)	0	100	100
1	B	146/157 (93%)	130 (89%)	16 (11%)	0	100	100
1	C	146/157 (93%)	126 (86%)	20 (14%)	0	100	100
1	D	146/157 (93%)	133 (91%)	13 (9%)	0	100	100
1	E	147/157 (94%)	129 (88%)	18 (12%)	0	100	100
1	F	146/157 (93%)	122 (84%)	24 (16%)	0	100	100
2	G	256/265 (97%)	240 (94%)	16 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	253/265 (96%)	236 (93%)	17 (7%)	0	100	100
3	I	260/269 (97%)	244 (94%)	16 (6%)	0	100	100
3	J	260/269 (97%)	242 (93%)	18 (7%)	0	100	100
4	K	96/102 (94%)	87 (91%)	9 (9%)	0	100	100
4	L	96/102 (94%)	84 (88%)	12 (12%)	0	100	100
All	All	2100/2214 (95%)	1899 (90%)	201 (10%)	0	100	100

There are no Ramachandran outliers to report.

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	117/127 (92%)	108 (92%)	9 (8%)	12	37
1	B	112/127 (88%)	96 (86%)	16 (14%)	3	18
1	C	117/127 (92%)	104 (89%)	13 (11%)	6	25
1	D	118/127 (93%)	104 (88%)	14 (12%)	5	23
1	E	118/127 (93%)	102 (86%)	16 (14%)	3	19
1	F	115/127 (91%)	105 (91%)	10 (9%)	9	33
2	G	201/209 (96%)	169 (84%)	32 (16%)	2	14
2	H	197/209 (94%)	180 (91%)	17 (9%)	10	33
3	I	215/224 (96%)	198 (92%)	17 (8%)	11	36
3	J	211/224 (94%)	193 (92%)	18 (8%)	10	34
4	K	76/80 (95%)	72 (95%)	4 (5%)	20	47
4	L	76/80 (95%)	69 (91%)	7 (9%)	8	32
All	All	1673/1788 (94%)	1500 (90%)	173 (10%)	9	28

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LEU
1	A	64	THR
1	A	90	VAL
1	A	92	ASN
1	A	125	ASP
1	A	127	SER
1	A	136	LEU
1	A	137	VAL
1	A	147	LEU
1	B	4	ARG
1	B	5	THR
1	B	8	ILE
1	B	14	LEU
1	B	28	VAL
1	B	42	VAL
1	B	58	VAL
1	B	63	VAL
1	B	64	THR
1	B	82	VAL
1	B	90	VAL
1	B	92	ASN
1	B	103	THR
1	B	111	TYR
1	B	114	ILE
1	B	121	ASP
1	C	10	VAL
1	C	53	THR
1	C	60	LEU
1	C	69	THR
1	C	74	ASP
1	C	83	THR
1	C	91	ASN
1	C	123	LEU
1	C	125	ASP
1	C	127	SER
1	C	129	ILE
1	C	142	ILE
1	C	150	VAL
1	D	3	THR
1	D	31	LEU
1	D	64	THR
1	D	68	VAL
1	D	86	ILE

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Mol	Chain	Res	Type
1	D	112	ILE
1	D	116	VAL
1	D	124	LYS
1	D	125	ASP
1	D	129	ILE
1	D	131	ASP
1	D	142	ILE
1	D	148	ASN
1	D	150	VAL
1	E	33	VAL
1	E	43	TYR
1	E	60	LEU
1	E	63	VAL
1	E	68	VAL
1	E	72	ASP
1	E	74	ASP
1	E	76	ASP
1	E	82	VAL
1	E	84	MET
1	E	90	VAL
1	E	91	ASN
1	E	92	ASN
1	E	106	LEU
1	E	112	ILE
1	E	115	SER
1	F	14	LEU
1	F	47	ASP
1	F	58	VAL
1	F	63	VAL
1	F	69	THR
1	F	86	ILE
1	F	91	ASN
1	F	92	ASN
1	F	114	ILE
1	F	137	VAL
2	G	24	LEU
2	G	27	SER
2	G	29	LEU
2	G	30	PHE
2	G	60	LEU
2	G	63	ILE
2	G	64	VAL

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Mol	Chain	Res	Type
2	G	70	ILE
2	G	77	GLN
2	G	81	ILE
2	G	82	LEU
2	G	83	ILE
2	G	91	VAL
2	G	94	MET
2	G	97	LEU
2	G	118	SER
2	G	120	LEU
2	G	124	ILE
2	G	126	ASN
2	G	144	LEU
2	G	148	VAL
2	G	161	LEU
2	G	196	SER
2	G	217	VAL
2	G	218	THR
2	G	220	ILE
2	G	222	VAL
2	G	231	THR
2	G	240	THR
2	G	251	LEU
2	G	254	ASP
2	G	260	LEU
2	H	27	SER
2	H	82	LEU
2	H	87	SER
2	H	91	VAL
2	H	94	MET
2	H	97	LEU
2	H	98	THR
2	H	107	VAL
2	H	111	LEU
2	H	118	SER
2	H	126	ASN
2	H	148	VAL
2	H	217	VAL
2	H	231	THR
2	H	240	THR
2	H	253	LEU
2	H	254	ASP

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Mol	Chain	Res	Type
3	I	9	VAL
3	I	37	THR
3	I	39	ILE
3	I	56	SER
3	I	58	LEU
3	I	89	VAL
3	I	121	ILE
3	I	126	LEU
3	I	165	ILE
3	I	167	LEU
3	I	172	PHE
3	I	202	SER
3	I	215	ILE
3	I	223	VAL
3	I	228	THR
3	I	232	LEU
3	I	233	LYS
3	J	23	ILE
3	J	36	VAL
3	J	37	THR
3	J	39	ILE
3	J	53	LEU
3	J	58	LEU
3	J	121	ILE
3	J	126	LEU
3	J	134	LEU
3	J	153	VAL
3	J	161	LEU
3	J	165	ILE
3	J	172	PHE
3	J	182	VAL
3	J	203	HIS
3	J	215	ILE
3	J	218	VAL
3	J	223	VAL
4	K	46	VAL
4	K	57	VAL
4	K	81	LEU
4	K	100	LEU
4	L	13	GLU
4	L	19	VAL
4	L	46	VAL

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Mol	Chain	Res	Type
4	L	63	LEU
4	L	81	LEU
4	L	84	ASP
4	L	95	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	130	HIS
1	A	151	ASN
1	B	89	ASN
1	C	91	ASN
1	C	148	ASN
1	E	87	ASN
1	E	88	GLN
1	E	133	GLN
2	G	93	GLN
2	G	192	ASN
2	G	224	GLN
2	H	89	GLN
2	H	132	GLN
2	H	194	GLN
2	H	195	ASN
2	H	224	GLN
3	I	71	ASN
3	I	105	ASN
3	I	203	HIS
3	J	26	ASN
3	J	105	ASN
3	J	255	HIS
4	K	3	GLN
4	K	15	GLN
4	L	3	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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	$\# Z > 2$
5	LPP	C	202	-	12,12,43	0.09	0	11,11,48	0.07	0
5	LPP	B	202	-	12,12,43	0.29	0	11,11,48	0.37	0
5	LPP	A	301	-	12,12,43	0.28	0	11,11,48	0.39	0
5	LPP	F	201	-	12,12,43	0.30	0	11,11,48	0.32	0
5	LPP	G	301	-	36,36,43	0.40	0	39,41,48	0.53	1 (2%)
5	LPP	G	302	-	43,43,43	0.92	4 (9%)	46,48,48	0.87	2 (4%)
5	LPP	H	301	-	43,43,43	0.90	4 (9%)	46,48,48	0.95	2 (4%)
5	LPP	B	201	-	12,12,43	0.28	0	11,11,48	0.39	0
5	LPP	E	201	-	12,12,43	0.10	0	11,11,48	0.07	0
5	LPP	C	201	-	12,12,43	0.09	0	11,11,48	0.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LPP	C	202	-	-	6/10/10/45	-
5	LPP	B	202	-	-	6/10/10/45	-
5	LPP	A	301	-	-	7/10/10/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LPP	F	201	-	-	7/10/10/45	-
5	LPP	G	301	-	-	20/38/38/45	-
5	LPP	G	302	-	-	20/45/45/45	-
5	LPP	H	301	-	-	28/45/45/45	-
5	LPP	B	201	-	-	7/10/10/45	-
5	LPP	E	201	-	-	5/10/10/45	-
5	LPP	C	201	-	-	9/10/10/45	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	302	LPP	O9-C7	-2.81	1.40	1.46
5	G	302	LPP	O27-C29	2.44	1.40	1.33
5	H	301	LPP	O9-C7	-2.38	1.41	1.46
5	H	301	LPP	O27-C8	-2.35	1.39	1.45
5	H	301	LPP	O27-C29	2.27	1.40	1.33
5	H	301	LPP	O9-C11	2.26	1.40	1.34
5	G	302	LPP	O27-C8	-2.18	1.40	1.45
5	G	302	LPP	O9-C11	2.08	1.40	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	301	LPP	O9-C11-C12	4.16	120.47	111.48
5	G	302	LPP	O9-C11-C12	3.38	118.80	111.48
5	G	302	LPP	O27-C29-C30	2.80	120.38	111.83
5	H	301	LPP	O27-C29-C30	2.69	120.03	111.83
5	G	301	LPP	O2-P1-O3	2.34	119.94	110.83

There are no chirality outliers.

All (115) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	301	LPP	C6-O5-P1-O3
5	G	301	LPP	C6-O5-P1-O4
5	G	301	LPP	O10-C11-O9-C7
5	G	302	LPP	C6-O5-P1-O2
5	G	302	LPP	C6-O5-P1-O3
5	G	302	LPP	C6-O5-P1-O4
5	H	301	LPP	C6-O5-P1-O2

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Mol	Chain	Res	Type	Atoms
5	H	301	LPP	C6-O5-P1-O4
5	H	301	LPP	O10-C11-O9-C7
5	G	301	LPP	C12-C11-O9-C7
5	H	301	LPP	C30-C29-O27-C8
5	H	301	LPP	C12-C11-O9-C7
5	H	301	LPP	O28-C29-O27-C8
5	F	201	LPP	C39-C40-C41-C42
5	C	202	LPP	C32-C33-C34-C35
5	G	302	LPP	C30-C29-O27-C8
5	B	202	LPP	C32-C33-C34-C35
5	B	202	LPP	C34-C35-C36-C37
5	G	302	LPP	O28-C29-O27-C8
5	G	302	LPP	C29-C30-C31-C32
5	C	201	LPP	C32-C33-C34-C35
5	F	201	LPP	C35-C36-C37-C38
5	H	301	LPP	C11-C12-C13-C14
5	H	301	LPP	C32-C33-C34-C35
5	B	201	LPP	C35-C36-C37-C38
5	C	201	LPP	C39-C40-C41-C42
5	F	201	LPP	C33-C34-C35-C36
5	G	301	LPP	C36-C37-C38-C39
5	E	201	LPP	C35-C36-C37-C38
5	B	202	LPP	C35-C36-C37-C38
5	B	202	LPP	C33-C34-C35-C36
5	G	302	LPP	C33-C34-C35-C36
5	H	301	LPP	C19-C20-C21-C22
5	G	302	LPP	C40-C41-C42-C43
5	G	301	LPP	C17-C18-C19-C20
5	A	301	LPP	C39-C40-C41-C42
5	G	301	LPP	C14-C15-C16-C17
5	H	301	LPP	C38-C39-C40-C41
5	H	301	LPP	C40-C41-C42-C43
5	A	301	LPP	C35-C36-C37-C38
5	H	301	LPP	C12-C13-C14-C15
5	H	301	LPP	C21-C22-C23-C24
5	C	201	LPP	C34-C35-C36-C37
5	B	201	LPP	C40-C41-C42-C43
5	C	202	LPP	C35-C36-C37-C38
5	H	301	LPP	C20-C21-C22-C23
5	G	302	LPP	O9-C7-C8-O27
5	G	302	LPP	C38-C39-C40-C41
5	B	202	LPP	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
5	G	302	LPP	C22-C23-C24-C25
5	H	301	LPP	C22-C23-C24-C25
5	C	202	LPP	C38-C39-C40-C41
5	E	201	LPP	C40-C41-C42-C43
5	G	302	LPP	C6-C7-C8-O27
5	B	201	LPP	C33-C34-C35-C36
5	G	301	LPP	C33-C34-C35-C36
5	B	201	LPP	C39-C40-C41-C42
5	C	202	LPP	C39-C40-C41-C42
5	G	302	LPP	C34-C35-C36-C37
5	G	301	LPP	C19-C20-C21-C22
5	G	302	LPP	C41-C42-C43-C44
5	H	301	LPP	C35-C36-C37-C38
5	B	201	LPP	C31-C32-C33-C34
5	E	201	LPP	C39-C40-C41-C42
5	G	301	LPP	C32-C33-C34-C35
5	F	201	LPP	C40-C41-C42-C43
5	A	301	LPP	C33-C34-C35-C36
5	B	201	LPP	C32-C33-C34-C35
5	B	202	LPP	C31-C32-C33-C34
5	C	201	LPP	C40-C41-C42-C43
5	H	301	LPP	C41-C42-C43-C44
5	H	301	LPP	O5-C6-C7-C8
5	G	302	LPP	C17-C18-C19-C20
5	C	202	LPP	C40-C41-C42-C43
5	F	201	LPP	C36-C37-C38-C39
5	G	302	LPP	C31-C32-C33-C34
5	E	201	LPP	C37-C38-C39-C40
5	A	301	LPP	C34-C35-C36-C37
5	C	201	LPP	C31-C32-C33-C34
5	F	201	LPP	C34-C35-C36-C37
5	G	301	LPP	O5-C6-C7-O9
5	G	302	LPP	C20-C21-C22-C23
5	H	301	LPP	C29-C30-C31-C32
5	H	301	LPP	C15-C16-C17-C18
5	H	301	LPP	C8-C7-O9-C11
5	G	301	LPP	C18-C19-C20-C21
5	G	301	LPP	C13-C14-C15-C16
5	G	301	LPP	C37-C38-C39-C40
5	G	301	LPP	O5-C6-C7-C8
5	H	301	LPP	C37-C38-C39-C40
5	C	201	LPP	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
5	G	302	LPP	C23-C24-C25-C26
5	G	301	LPP	C35-C36-C37-C38
5	G	302	LPP	C32-C33-C34-C35
5	G	302	LPP	C12-C13-C14-C15
5	E	201	LPP	C31-C32-C33-C34
5	C	201	LPP	C38-C39-C40-C41
5	A	301	LPP	C40-C41-C42-C43
5	H	301	LPP	C13-C14-C15-C16
5	H	301	LPP	O5-C6-C7-O9
5	H	301	LPP	C34-C35-C36-C37
5	A	301	LPP	C38-C39-C40-C41
5	F	201	LPP	C31-C32-C33-C34
5	H	301	LPP	C23-C24-C25-C26
5	H	301	LPP	C33-C34-C35-C36
5	H	301	LPP	C6-O5-P1-O3
5	G	301	LPP	C11-C12-C13-C14
5	C	201	LPP	C37-C38-C39-C40
5	A	301	LPP	C31-C32-C33-C34
5	B	201	LPP	C34-C35-C36-C37
5	G	301	LPP	O27-C29-C30-C31
5	C	201	LPP	C36-C37-C38-C39
5	C	202	LPP	C31-C32-C33-C34
5	G	301	LPP	O28-C29-C30-C31
5	G	301	LPP	C31-C32-C33-C34

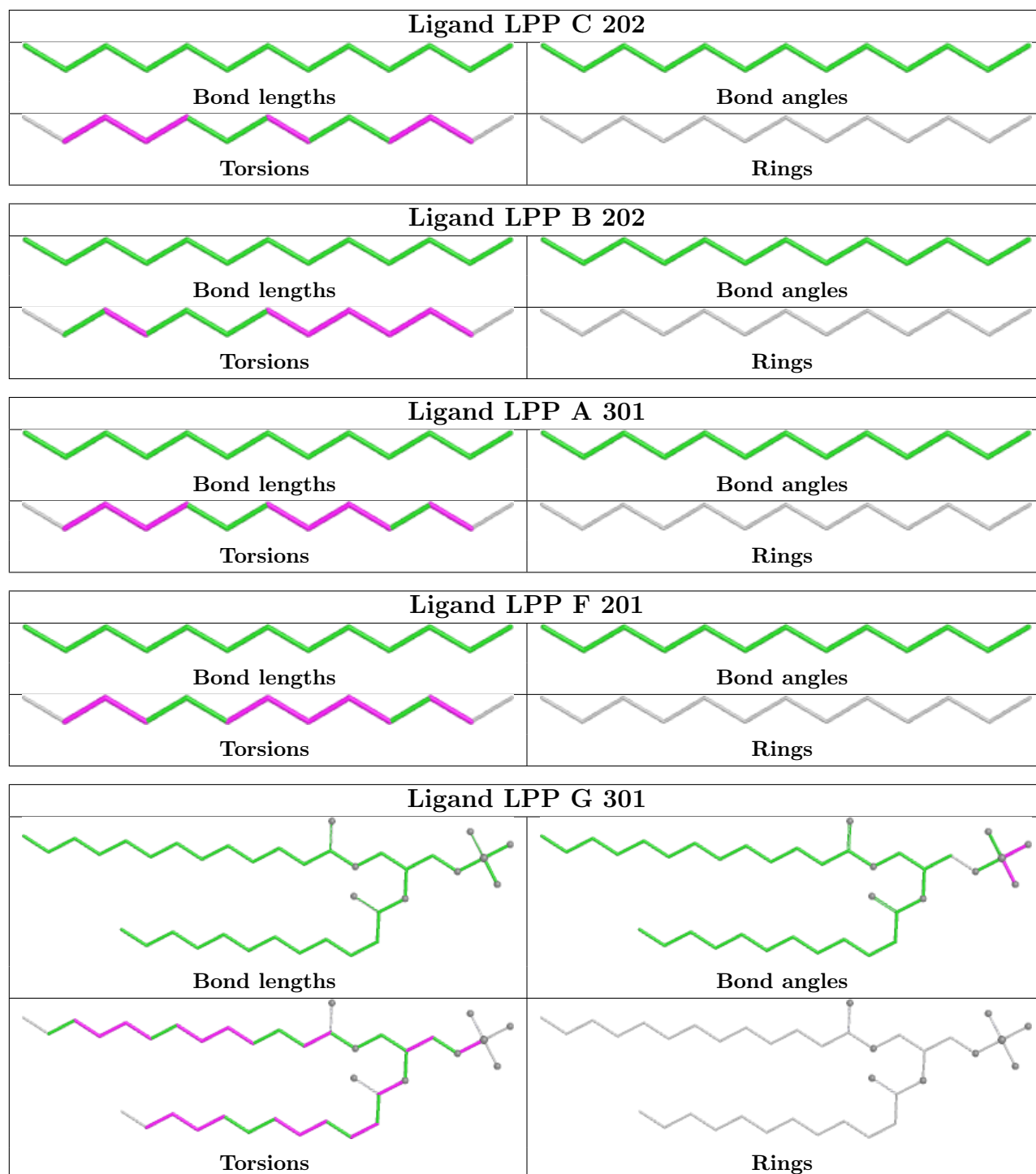
There are no ring outliers.

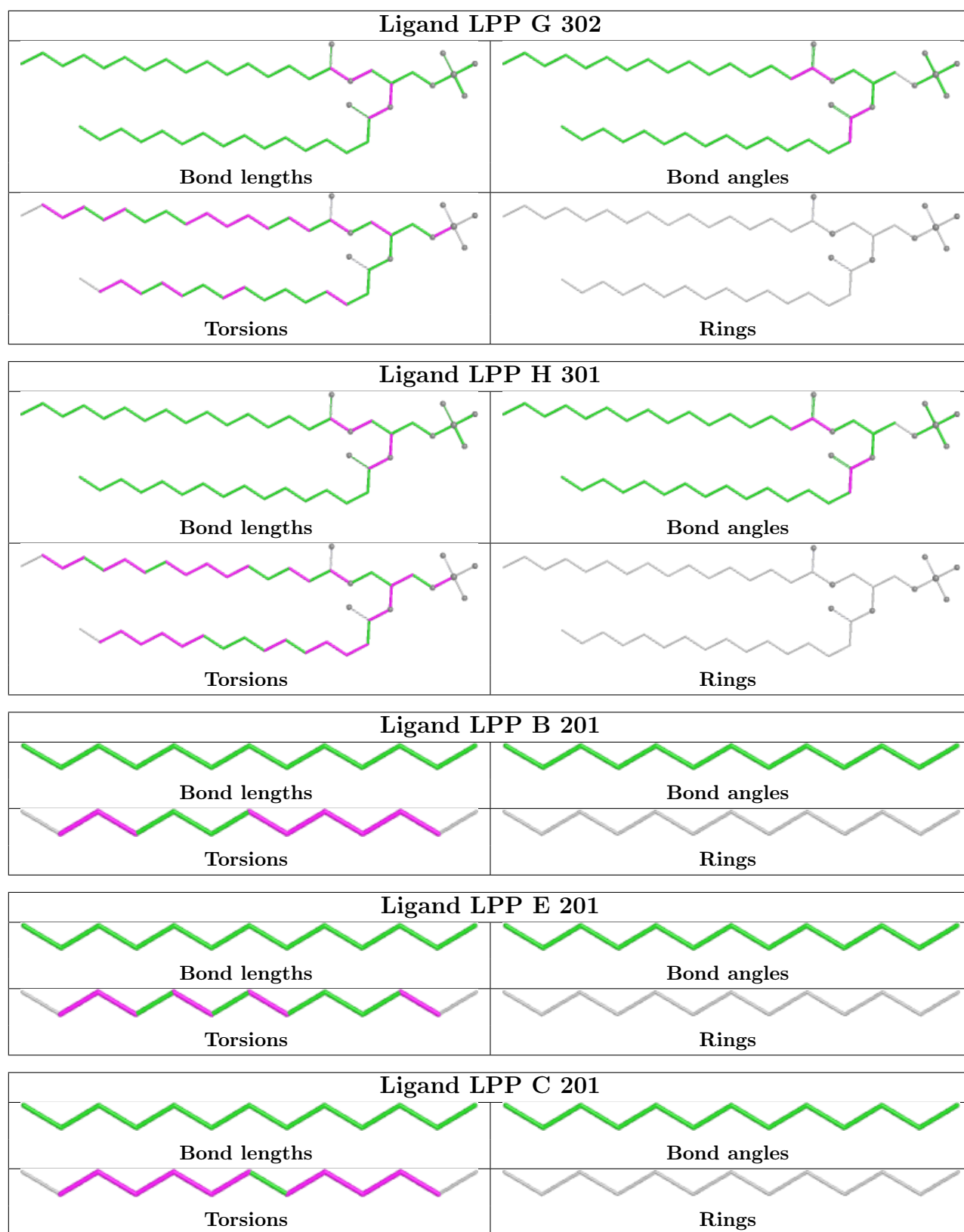
9 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	202	LPP	3	0
5	B	202	LPP	3	0
5	F	201	LPP	1	0
5	G	301	LPP	24	0
5	G	302	LPP	4	0
5	H	301	LPP	1	0
5	B	201	LPP	1	0
5	E	201	LPP	6	0
5	C	201	LPP	4	0

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

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

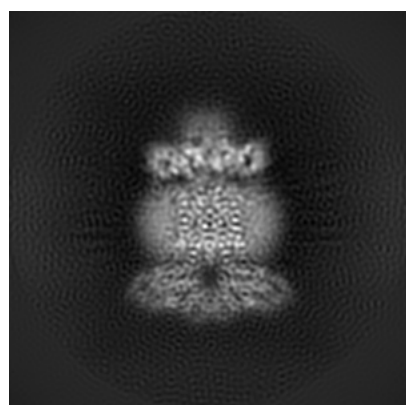
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30372. These allow visual inspection of the internal detail of the map and identification of artifacts.

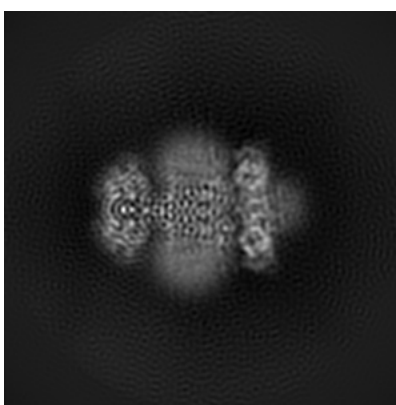
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

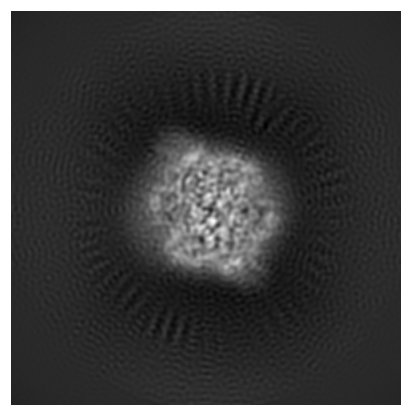
6.1.1 Primary map



X



Y

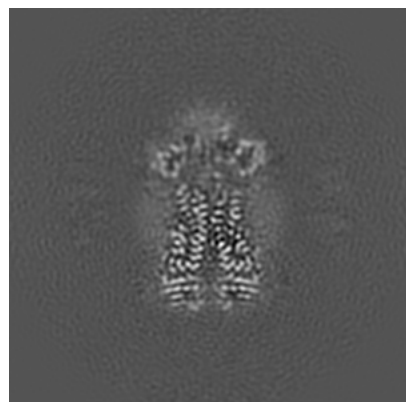


Z

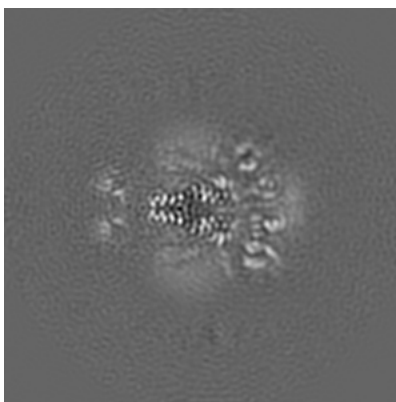
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

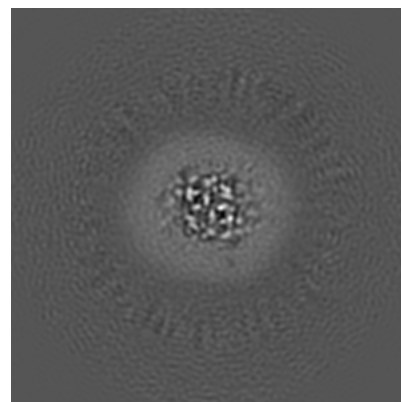
6.2.1 Primary map



X Index: 128



Y Index: 128

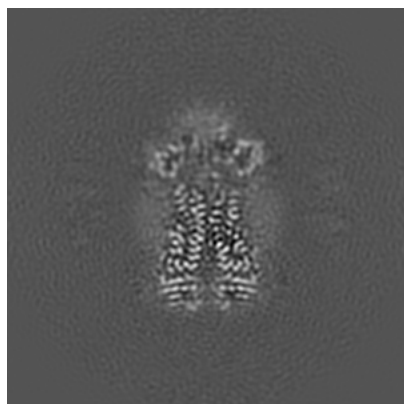


Z Index: 128

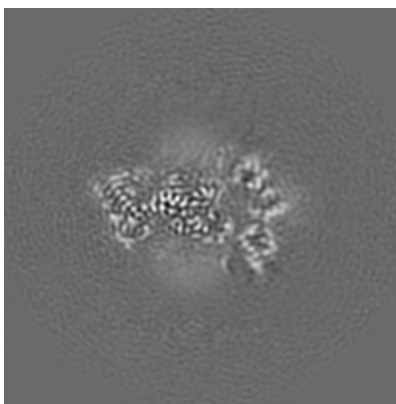
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

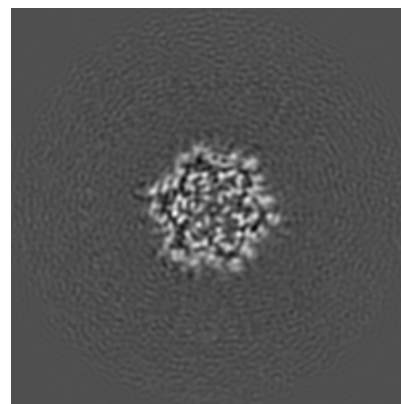
6.3.1 Primary map



X Index: 128



Y Index: 139

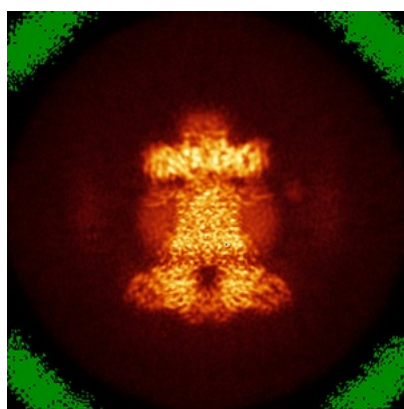


Z Index: 161

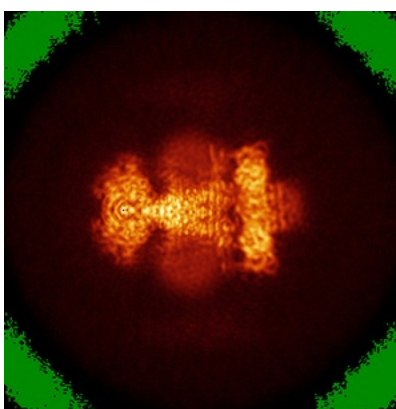
The images above show the largest variance slices of the map in three orthogonal directions.

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

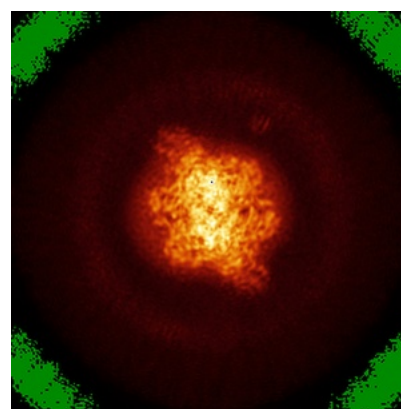
6.4.1 Primary map



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 3.94. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

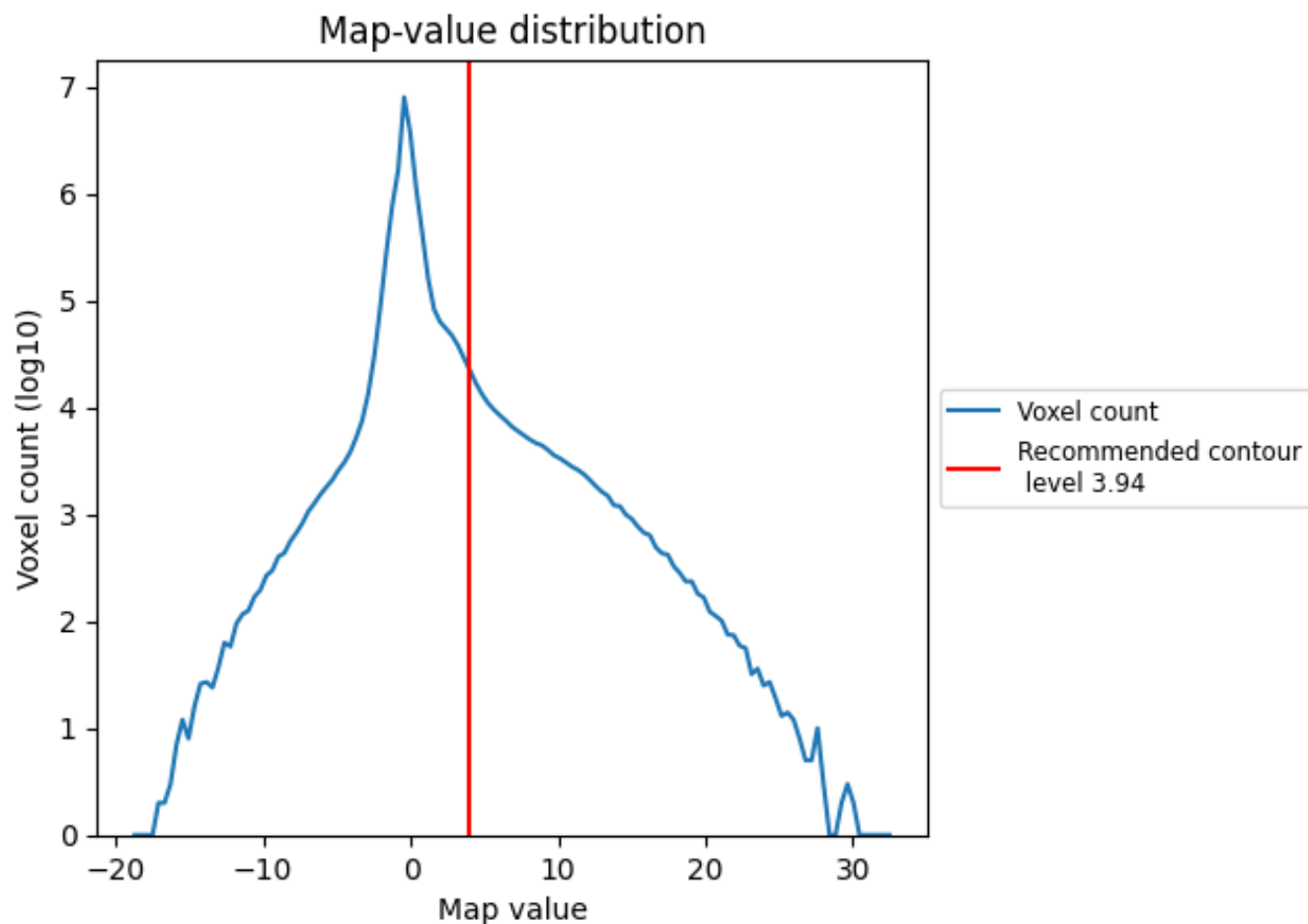
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

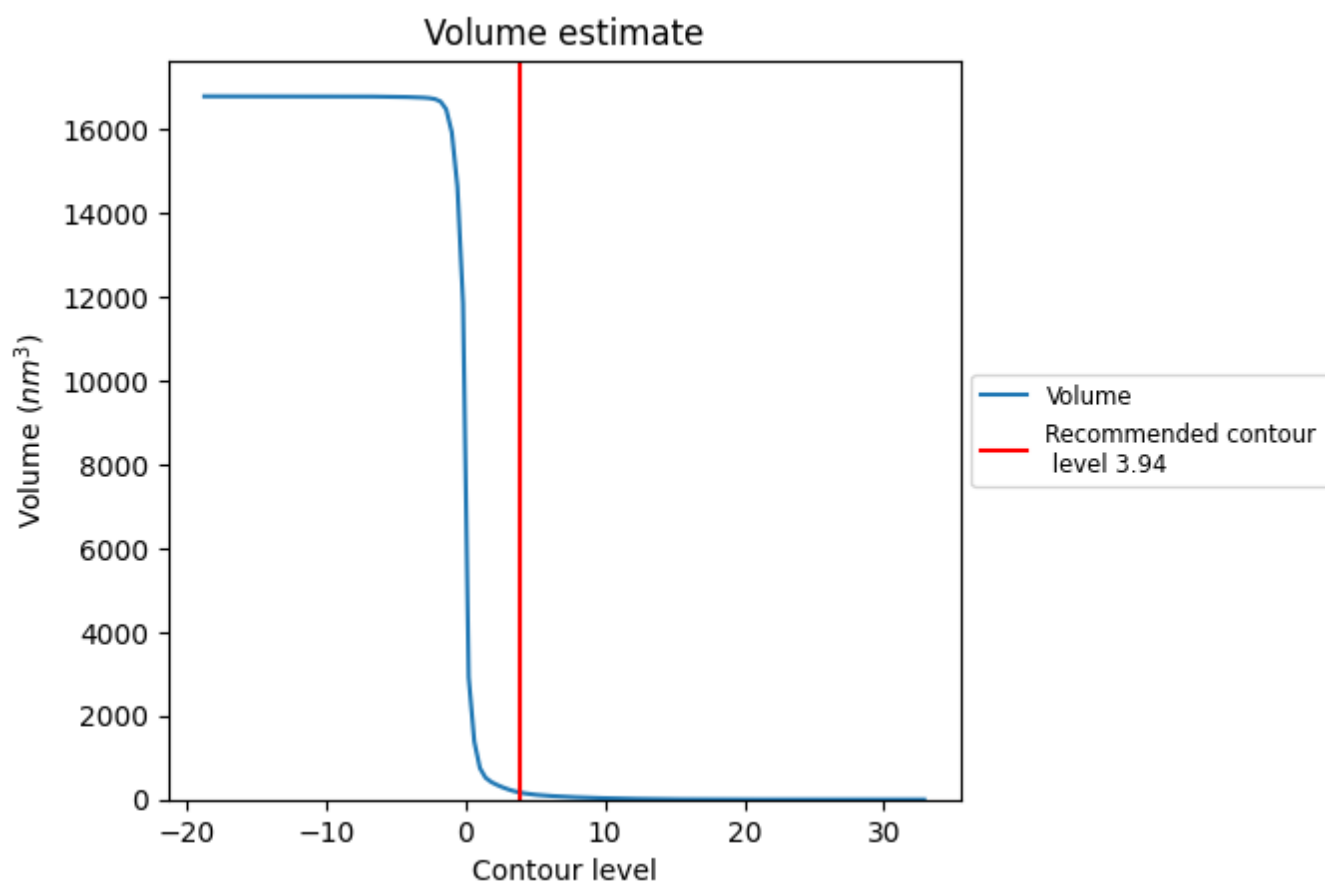
This section contains the results of statistical analysis of the map.

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.

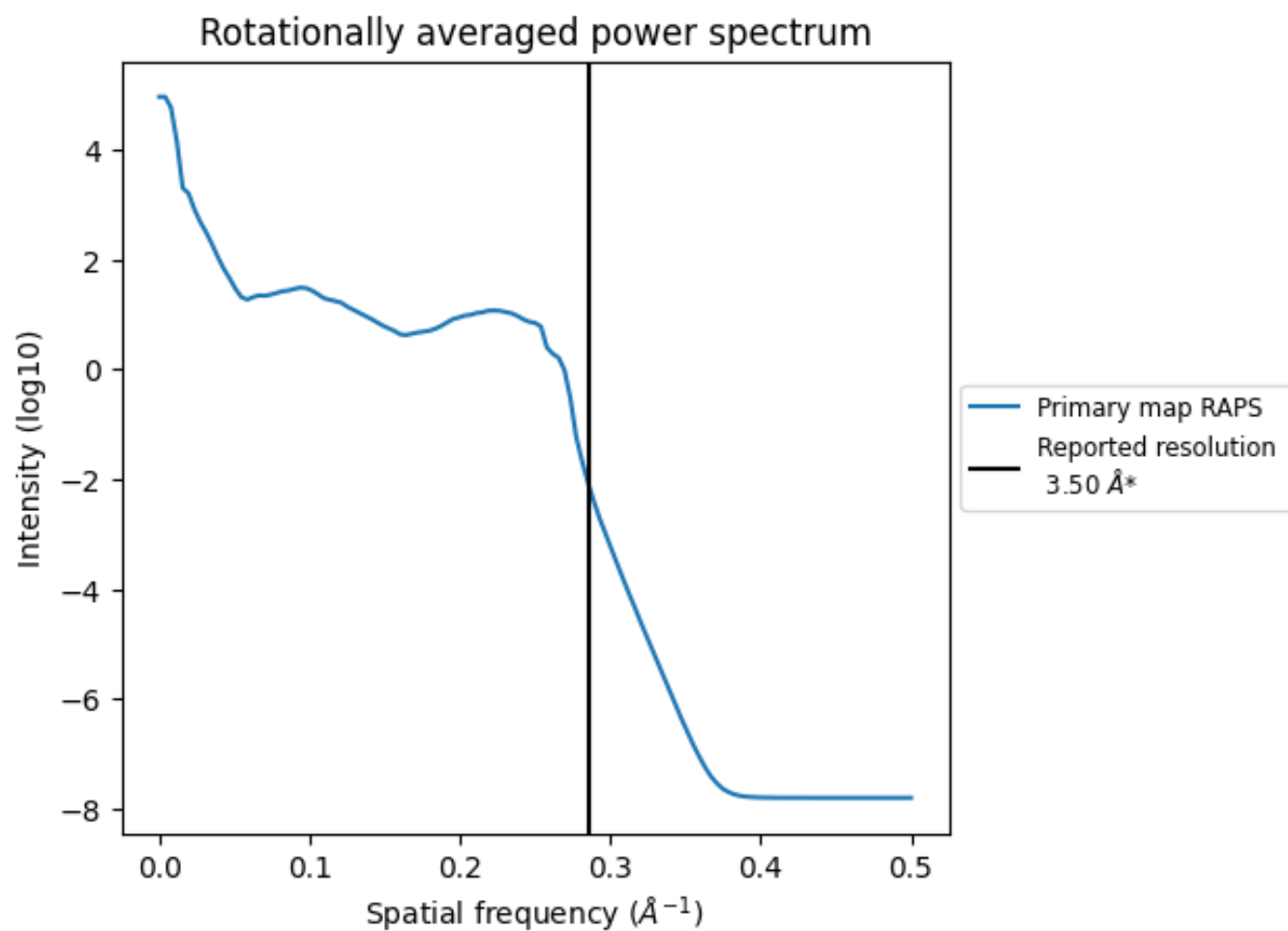
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 166 nm^3 ; this corresponds to an approximate mass of 150 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 ⓘ

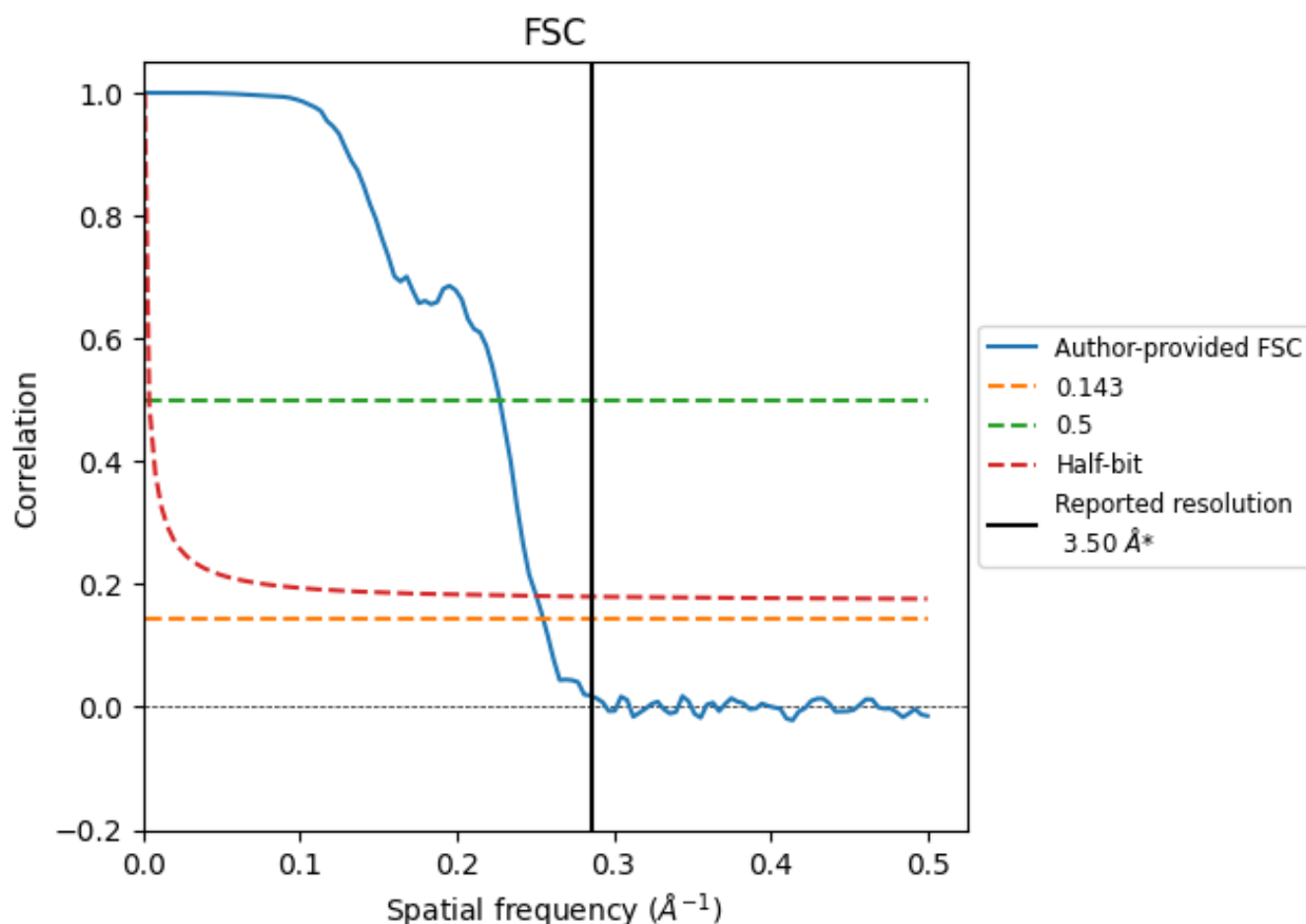


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.92	4.40	3.99
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 3.92 differs from the reported value 3.5 by more than 10 %

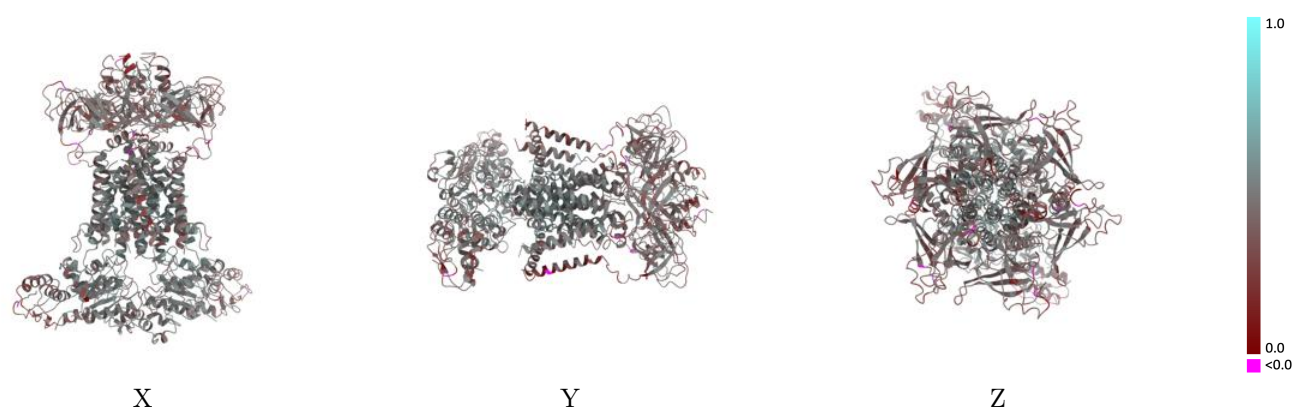
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-30372 and PDB model 7CH9. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

This section was not generated.

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



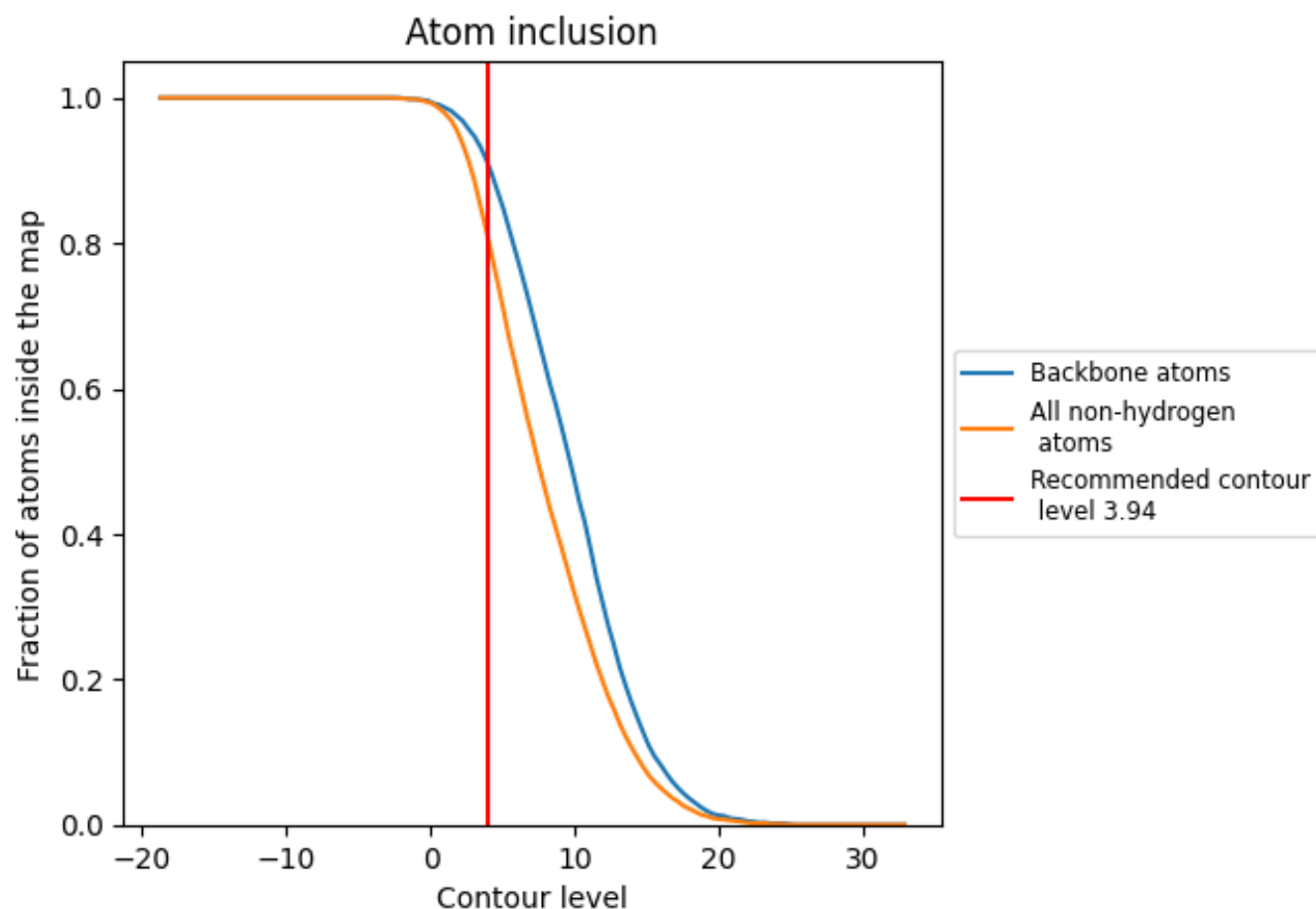
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.94).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 81% 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 (3.94) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8120	0.4270
A	0.7970	0.3840
B	0.8120	0.3900
C	0.7660	0.3540
D	0.8190	0.3940
E	0.8050	0.3810
F	0.7810	0.3770
G	0.8250	0.4800
H	0.8300	0.4820
I	0.8500	0.4710
J	0.8420	0.4660
K	0.7440	0.3720
L	0.7510	0.3870

1.0

0.0

<0.0