



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 07:03 PM JST

PDB ID : 7CHA
EMDB ID : EMD-30373
Title : Cryo-EM structure of P.aeruginosa MlaFEED with AMPPNP
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.dev43
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 : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

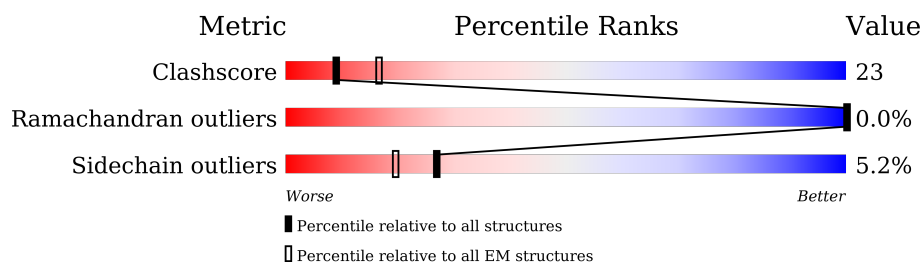
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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>64%</div> <div>52%</div> <div>40%</div> <div>6%</div> </div>
1	B	157	<div> <div>57%</div> <div>48%</div> <div>45%</div> <div>7%</div> </div>
1	C	157	<div> <div>71%</div> <div>54%</div> <div>39%</div> <div>7%</div> </div>
1	D	157	<div> <div>66%</div> <div>49%</div> <div>45%</div> <div>6%</div> </div>
1	E	157	<div> <div>73%</div> <div>47%</div> <div>47%</div> <div>5%</div> </div>
1	F	157	<div> <div>64%</div> <div>52%</div> <div>39%</div> <div>8%</div> </div>
2	G	265	<div> <div>19%</div> <div>60%</div> <div>36%</div> <div>• •</div> </div>
2	H	265	<div> <div>19%</div> <div>60%</div> <div>36%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
3	I	269	<div><div></div><div>21%</div><div>58%</div><div>38%</div><div></div><div></div></div>
3	J	269	<div><div></div><div>23%</div><div>55%</div><div>41%</div><div></div><div></div></div>
4	K	102	<div><div></div><div>31%</div><div>67%</div><div>54%</div><div>10%</div><div></div></div>
4	L	102	<div><div></div><div>30%</div><div>63%</div><div>54%</div><div>11%</div><div></div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16231 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	147	Total	C	N	O	S	0	0
			1085	689	180	215	1		
1	B	146	Total	C	N	O	S	0	0
			1076	684	178	213	1		
1	C	146	Total	C	N	O	S	0	0
			1076	684	178	213	1		
1	D	147	Total	C	N	O	S	0	0
			1082	687	179	215	1		
1	E	149	Total	C	N	O	S	0	0
			1098	697	182	218	1		
1	F	145	Total	C	N	O	S	0	0
			1068	680	176	211	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
			1939	1270	317	343	9		
2	H	258	Total	C	N	O	S	0	0
			1939	1270	317	343	9		

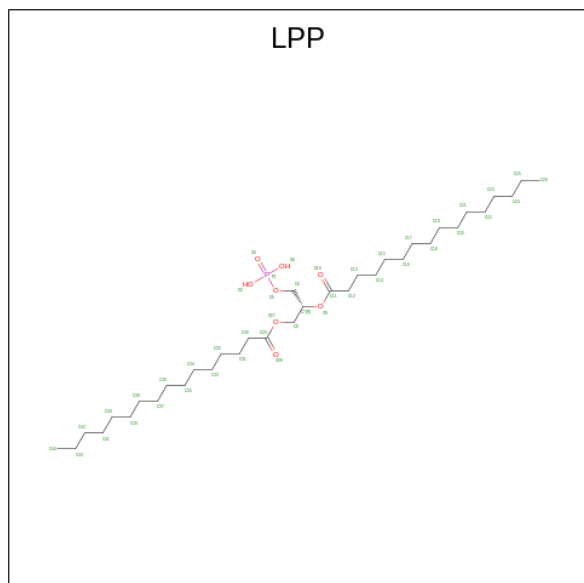
- Molecule 3 is a protein called Probable ATP-binding component of ABC transporter, *P.aeruginosa* Mla F.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	262	Total	C	N	O	S	0	0
			2028	1296	359	365	8		
3	J	262	Total	C	N	O	S	0	0
			2028	1296	359	365	8		

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

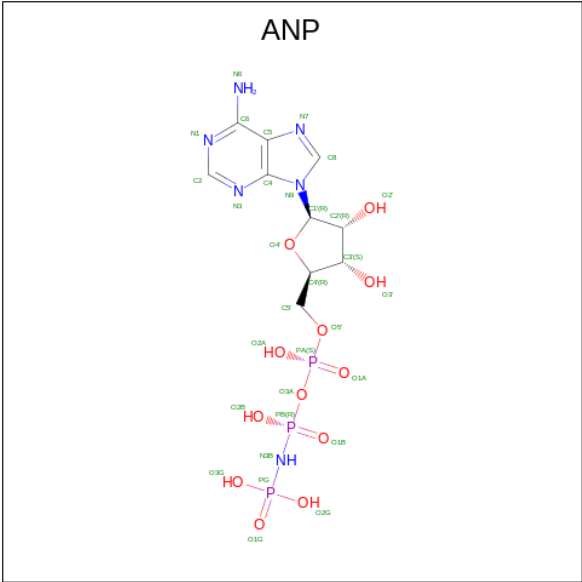
Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	98	Total	C	N	O	S	0	0
			721	448	132	139	2		
4	L	98	Total	C	N	O	S	0	0
			721	448	132	139	2		

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



Mol	Chain	Residues	Atoms				AltConf
5	G	1	Total	C	O	P	0
			176	140	32	4	
5	G	1	Total	C	O	P	0
			176	140	32	4	
5	G	1	Total	C	O	P	0
			176	140	32	4	
5	G	1	Total	C	O	P	0
			176	140	32	4	
5	H	1	Total	C	O	P	0
			132	105	24	3	
5	H	1	Total	C	O	P	0
			132	105	24	3	
5	H	1	Total	C	O	P	0
			132	105	24	3	

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

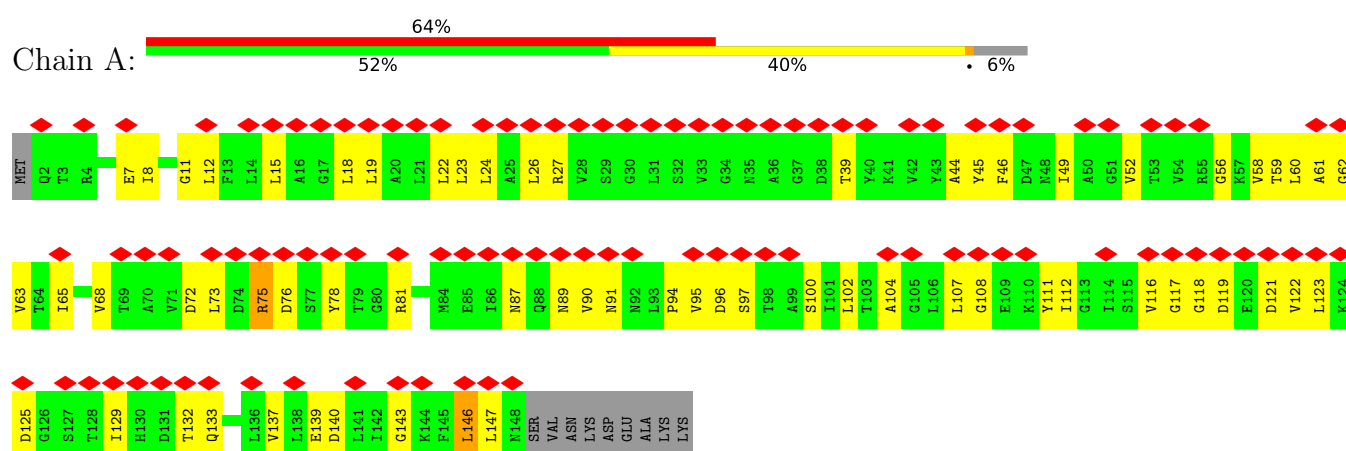


Mol	Chain	Residues	Atoms					AltConf
6	I	1	Total	C	N	O	P	0
			31	10	6	12	3	
6	J	1	Total	C	N	O	P	0
			31	10	6	12	3	

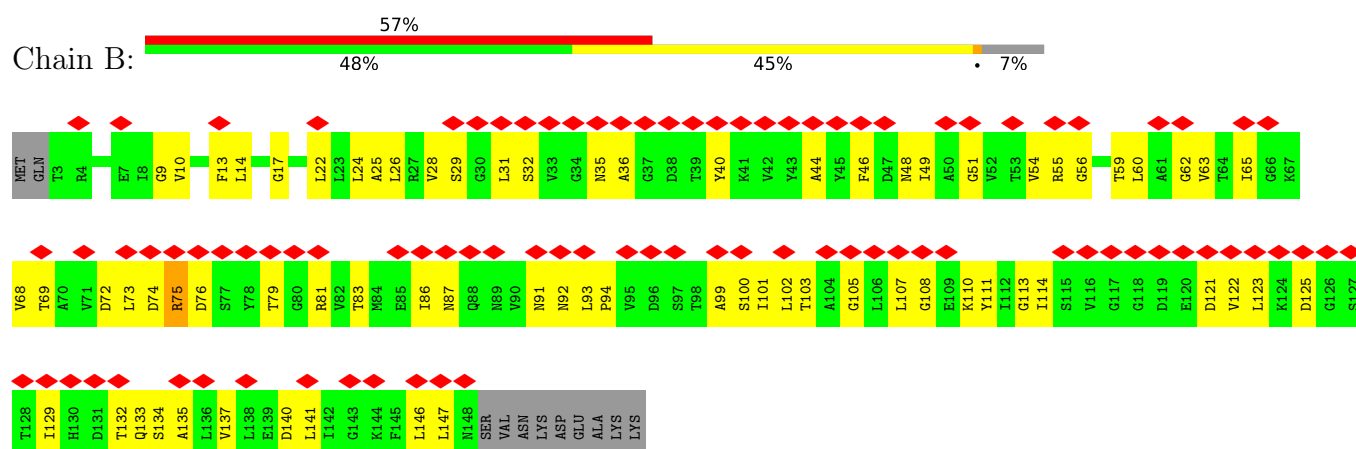
3 Residue-property plots

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.

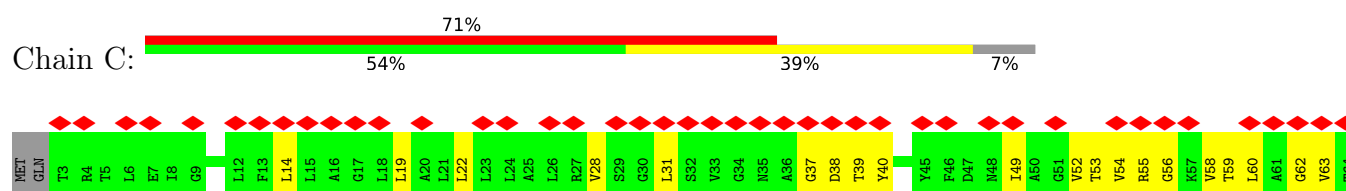
• Molecule 1: MlaD domain-containing protein

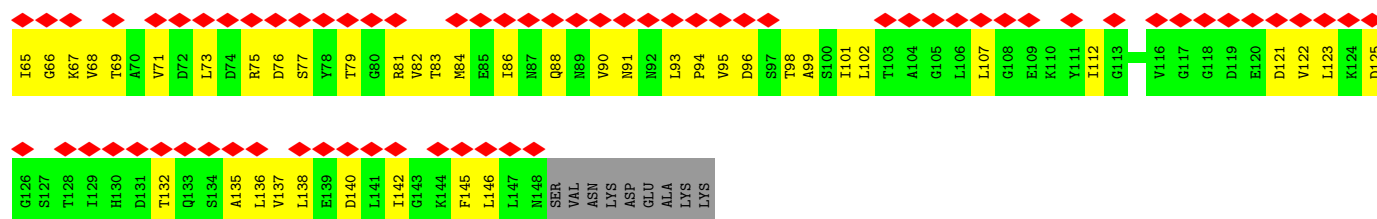


• Molecule 1: MlaD domain-containing protein

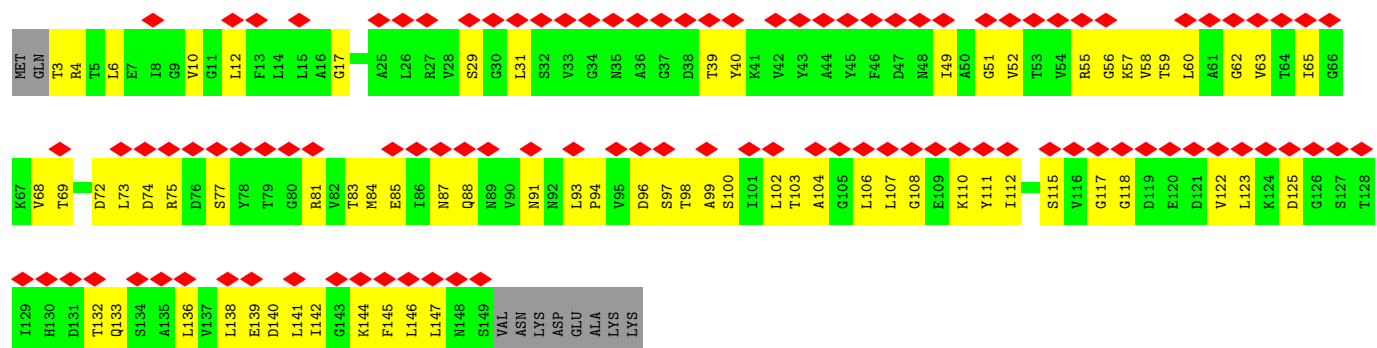


• Molecule 1: MlaD domain-containing protein

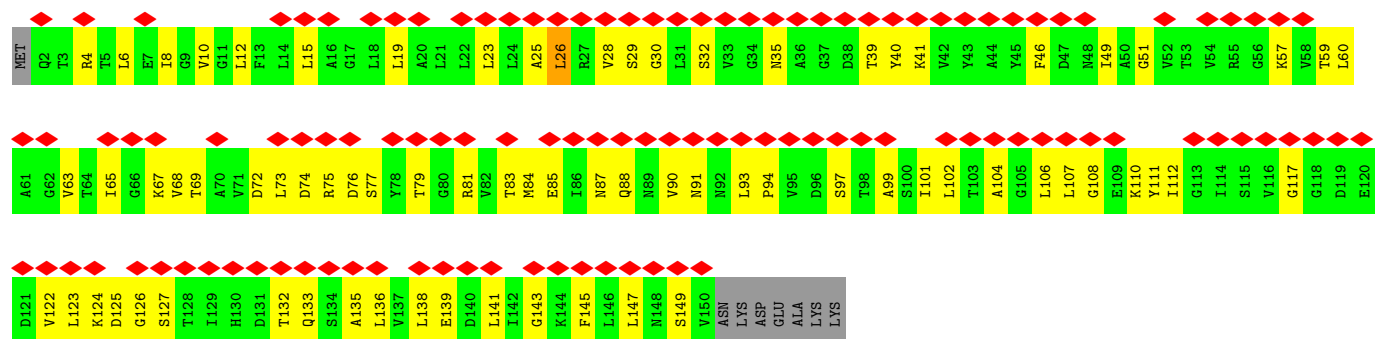
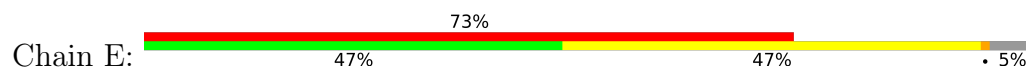




• Molecule 1: MlaD domain-containing protein



• Molecule 1: MlaD domain-containing protein

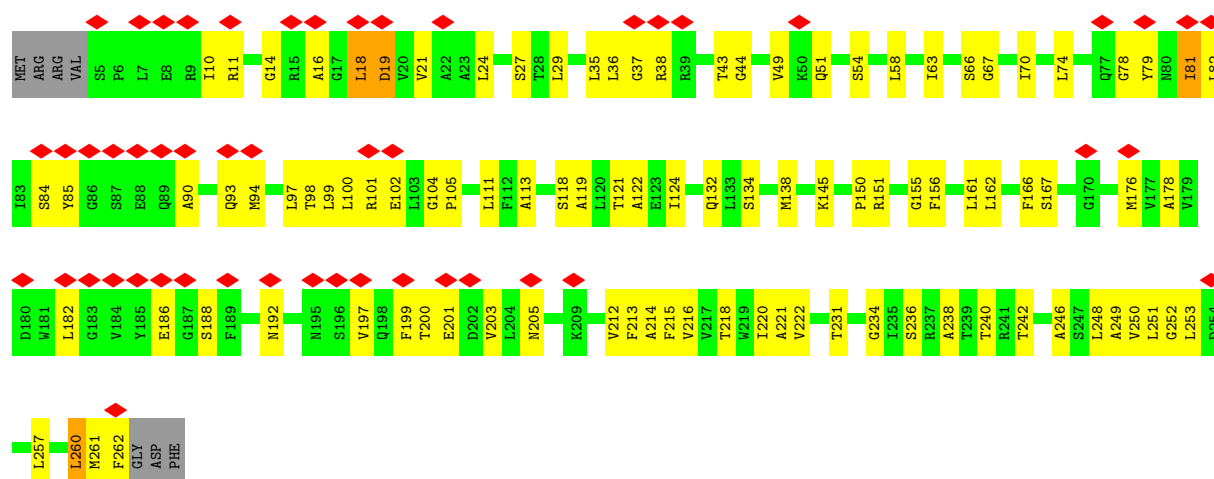


• Molecule 1: MlaD domain-containing protein

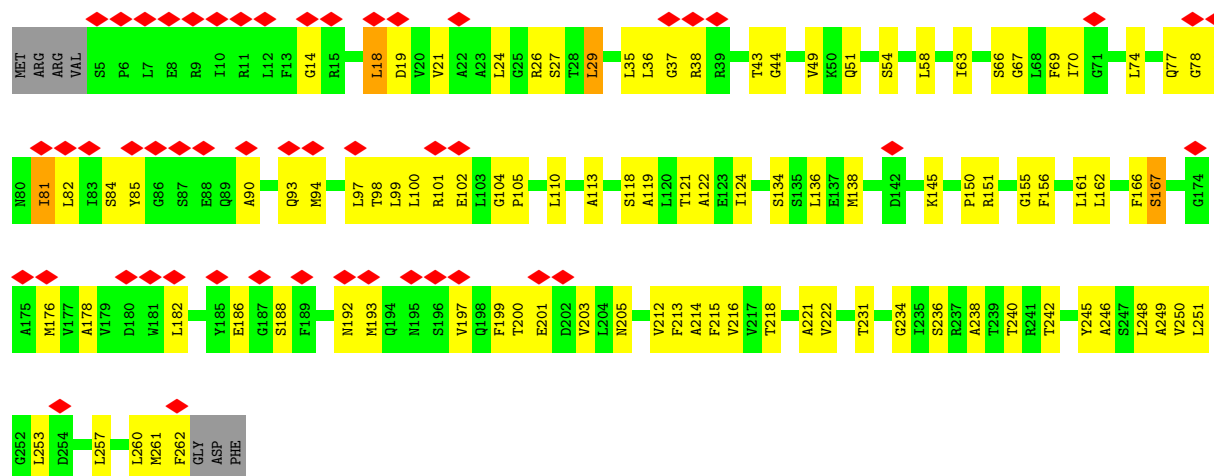




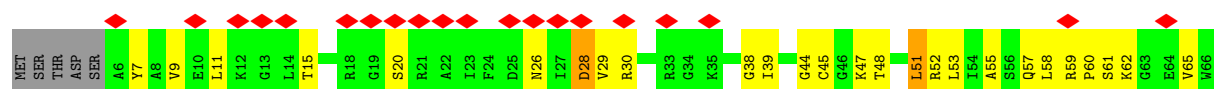
- Molecule 2: Probable permease of ABC transporter

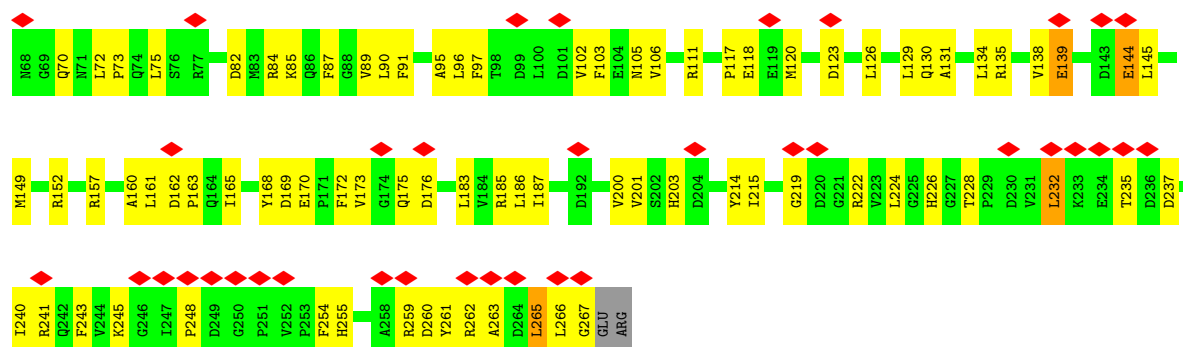


- Molecule 2: Probable permease of ABC transporter

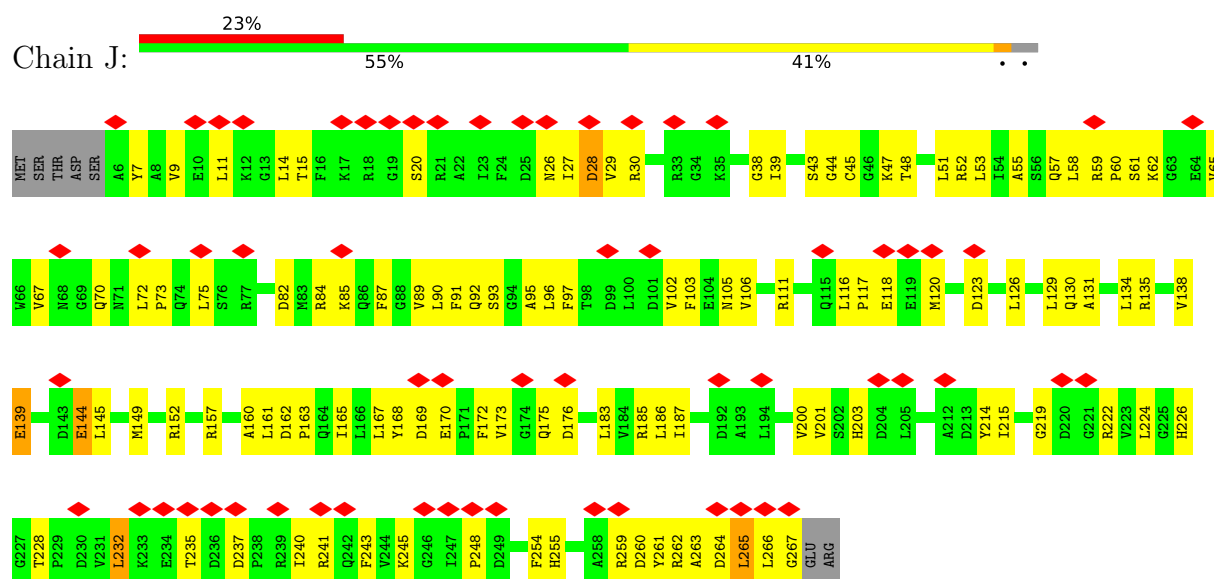


- Molecule 3: Probable ATP-binding component of ABC transporter, *P.aeruginosa* Mla F

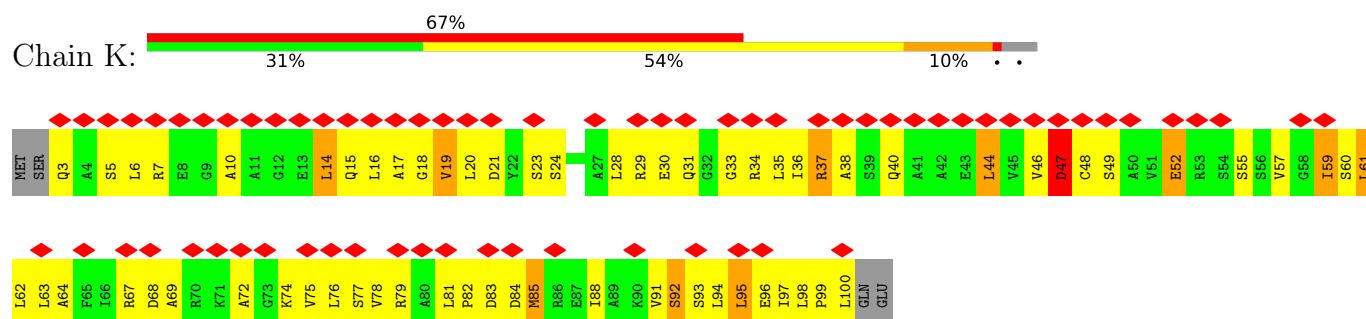




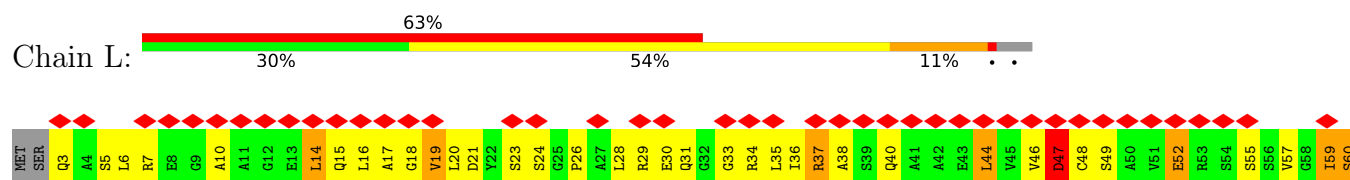
- Molecule 3: Probable ATP-binding component of ABC transporter, *P.aeruginosa* Mla F

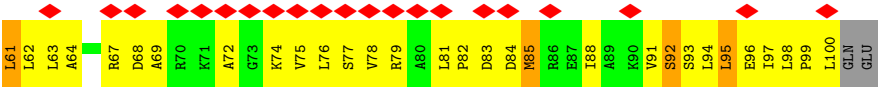


- Molecule 4: STAS domain-containing protein



- 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	419046	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	0.132	Depositor
Minimum map value	-0.072	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0299	Depositor
Map size (\AA)	266.24, 266.24, 266.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.34	0/1094	0.53	0/1486
1	B	0.32	0/1085	0.55	0/1474
1	C	0.31	0/1085	0.56	0/1474
1	D	0.33	0/1091	0.55	0/1482
1	E	0.32	0/1107	0.58	1/1504 (0.1%)
1	F	0.35	0/1077	0.51	0/1463
2	G	0.51	0/1977	0.58	0/2691
2	H	0.51	0/1977	0.58	0/2691
3	I	0.47	0/2066	0.54	0/2798
3	J	0.47	0/2066	0.54	0/2798
4	K	0.39	0/725	0.66	2/976 (0.2%)
4	L	0.39	0/725	0.66	2/976 (0.2%)
All	All	0.42	0/16075	0.57	5/21813 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	2
4	K	0	1
4	L	0	1
All	All	0	4

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	47	ASP	CB-CG-OD1	5.71	123.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	47	ASP	CB-CG-OD1	5.65	123.38	118.30
1	E	26	LEU	CA-CB-CG	5.20	127.25	115.30
4	L	14	LEU	CA-CB-CG	-5.07	103.64	115.30
4	K	14	LEU	CA-CB-CG	-5.07	103.64	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	32	SER	Peptide
1	F	39	THR	Peptide
4	K	92	SER	Peptide
4	L	92	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1085	0	1124	60	0
1	B	1076	0	1116	64	0
1	C	1076	0	1116	49	0
1	D	1082	0	1121	61	0
1	E	1098	0	1138	58	0
1	F	1068	0	1110	59	0
2	G	1939	0	2013	80	0
2	H	1939	0	2013	86	0
3	I	2028	0	2084	92	0
3	J	2028	0	2084	97	0
4	K	721	0	759	66	0
4	L	721	0	759	65	0
5	G	176	0	258	21	0
5	H	132	0	199	27	0
6	I	31	0	12	5	0
6	J	31	0	12	4	0
All	All	16231	0	16918	765	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 23.

All (765) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:GLY:H	1:C:68:VAL:HG12	1.33	0.93
3:J:265:LEU:HD21	4:K:63:LEU:HD21	1.56	0.85
3:J:123:ASP:OD1	4:L:67:ARG:NH1	2.12	0.83
3:J:45:CYS:SG	3:J:47:LYS:NZ	2.54	0.80
1:F:93:LEU:O	1:F:123:LEU:N	2.14	0.80
3:I:45:CYS:SG	3:I:47:LYS:NZ	2.54	0.80
3:J:117:PRO:HG2	4:L:29:ARG:HD3	1.63	0.79
3:I:15:THR:HB	3:I:26:ASN:H	1.46	0.79
1:F:123:LEU:HG	1:F:125:ASP:H	1.45	0.79
3:J:15:THR:HB	3:J:26:ASN:H	1.46	0.77
1:C:31:LEU:HD21	1:C:67:LYS:HE2	1.67	0.76
3:J:59:ARG:NH1	3:J:73:PRO:O	2.19	0.76
4:K:6:LEU:HD11	4:K:14:LEU:HD21	1.67	0.76
1:C:49:ILE:H	1:D:62:GLY:HA3	1.51	0.76
1:D:103:THR:OG1	1:D:110:LYS:NZ	2.18	0.76
3:I:59:ARG:NH1	3:I:73:PRO:O	2.19	0.76
1:B:62:GLY:HA3	1:F:49:ILE:H	1.52	0.75
3:I:172:PHE:HA	3:I:175:GLN:HE22	1.52	0.75
1:B:54:VAL:HG12	1:B:55:ARG:HG3	1.67	0.74
4:L:6:LEU:HD11	4:L:14:LEU:HD21	1.67	0.74
1:B:25:ALA:O	1:B:29:SER:OG	2.03	0.74
3:J:70:GLN:N	3:J:70:GLN:OE1	2.21	0.73
3:J:172:PHE:HA	3:J:175:GLN:HE22	1.52	0.73
2:G:81:ILE:HG23	2:G:82:LEU:HG	1.70	0.73
3:I:135:ARG:NH1	3:J:260:ASP:O	2.20	0.72
3:I:70:GLN:OE1	3:I:70:GLN:N	2.21	0.72
2:H:81:ILE:HG23	2:H:82:LEU:HG	1.70	0.71
3:J:111:ARG:NH2	3:J:118:GLU:OE1	2.24	0.71
3:I:111:ARG:NH2	3:I:118:GLU:OE1	2.24	0.70
2:G:104:GLY:HA2	2:G:166:PHE:HE2	1.56	0.70
3:I:95:ALA:O	3:I:157:ARG:NH2	2.24	0.70
2:H:105:PRO:HB2	2:H:213:PHE:HZ	1.56	0.70
2:G:105:PRO:HB2	2:G:213:PHE:HZ	1.56	0.70
3:I:123:ASP:OD1	4:K:67:ARG:NH1	2.24	0.70
3:J:95:ALA:O	3:J:157:ARG:NH2	2.24	0.70
1:B:100:SER:HB3	1:B:133:GLN:HB2	1.73	0.69
1:D:39:THR:HG22	1:D:87:ASN:HA	1.73	0.69
1:E:49:ILE:H	1:F:62:GLY:HA3	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:SER:HA	2:H:197:VAL:HG21	1.75	0.69
1:C:49:ILE:HD11	1:D:63:VAL:HB	1.75	0.69
1:E:143:GLY:HA2	1:E:147:LEU:HB3	1.74	0.69
2:G:188:SER:O	2:G:192:ASN:ND2	2.26	0.69
1:C:69:THR:HG23	1:C:84:MET:HA	1.75	0.68
1:B:29:SER:HB2	2:H:199:PHE:HB2	1.75	0.68
1:C:99:ALA:O	1:C:132:THR:OG1	2.11	0.68
2:H:104:GLY:HA2	2:H:166:PHE:HE2	1.56	0.68
1:A:59:THR:HA	1:A:65:ILE:HG12	1.76	0.68
1:B:74:ASP:OD1	1:B:79:THR:N	2.23	0.68
2:H:188:SER:O	2:H:192:ASN:ND2	2.26	0.68
4:L:68:ASP:O	4:L:72:ALA:N	2.26	0.68
1:C:138:LEU:HD12	1:D:106:LEU:HD12	1.76	0.67
3:I:117:PRO:HG2	4:K:29:ARG:HD3	1.76	0.67
1:D:58:VAL:HG11	1:D:84:MET:HG3	1.78	0.66
1:D:74:ASP:OD2	1:D:77:SER:OG	2.12	0.66
2:H:21:VAL:HG13	5:H:302:LPP:C44	2.25	0.66
4:K:68:ASP:O	4:K:72:ALA:N	2.26	0.66
1:C:90:VAL:HG12	1:C:93:LEU:HD11	1.77	0.66
4:L:7:ARG:HG3	4:L:15:GLN:HB2	1.78	0.65
3:J:215:ILE:HG23	3:J:232:LEU:HD13	1.78	0.65
1:F:94:PRO:HG3	1:F:118:GLY:H	1.62	0.65
1:E:72:ASP:OD2	1:E:81:ARG:NH2	2.29	0.65
3:I:131:ALA:HB2	4:K:92:SER:HB2	1.79	0.65
3:I:215:ILE:HG23	3:I:232:LEU:HD13	1.78	0.65
4:K:47:ASP:HB2	4:K:79:ARG:HB2	1.79	0.65
4:K:79:ARG:NH2	4:K:100:LEU:O	2.30	0.65
2:H:216:VAL:HG21	2:H:253:LEU:HD22	1.78	0.64
1:B:146:LEU:HG	1:B:147:LEU:H	1.62	0.64
1:D:144:LYS:O	1:D:146:LEU:N	2.27	0.64
4:L:79:ARG:NH2	4:L:100:LEU:O	2.30	0.64
1:C:39:THR:HG22	1:C:88:GLN:HG2	1.80	0.64
1:A:139:GLU:O	1:A:143:GLY:N	2.30	0.64
1:B:91:ASN:OD1	1:F:75:ARG:NH1	2.30	0.64
1:D:10:VAL:HG11	2:G:49:VAL:HG13	1.80	0.64
1:E:106:LEU:HG	1:E:107:LEU:HD12	1.80	0.64
1:B:10:VAL:HG11	2:H:49:VAL:HG13	1.78	0.64
2:G:216:VAL:HG21	2:G:253:LEU:HD22	1.78	0.64
4:K:7:ARG:HG3	4:K:15:GLN:HB2	1.78	0.64
1:A:107:LEU:HB2	1:B:107:LEU:HD11	1.80	0.63
4:L:47:ASP:HB2	4:L:79:ARG:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:155:GLY:HA3	2:G:218:THR:HG21	1.81	0.63
1:B:32:SER:O	1:B:36:ALA:N	2.32	0.63
4:K:33:GLY:O	4:K:37:ARG:HB2	1.99	0.62
4:L:81:LEU:HD12	4:L:82:PRO:HD2	1.81	0.62
1:D:144:LYS:HG3	1:D:145:PHE:H	1.65	0.62
2:G:122:ALA:HB1	2:H:236:SER:HB3	1.81	0.62
2:H:78:GLY:O	2:H:81:ILE:HG22	2.00	0.62
1:A:11:GLY:HA3	5:H:302:LPP:H442	1.82	0.62
1:D:99:ALA:O	1:D:132:THR:OG1	2.14	0.62
5:G:304:LPP:H221	2:H:77:GLN:HG2	1.81	0.62
4:L:33:GLY:O	4:L:37:ARG:HB2	1.99	0.62
1:A:123:LEU:HD13	1:A:125:ASP:HB2	1.81	0.62
4:K:81:LEU:HD12	4:K:82:PRO:HD2	1.81	0.62
2:G:236:SER:HB3	2:H:122:ALA:HB1	1.81	0.61
1:B:51:GLY:HA3	1:B:110:LYS:HD3	1.82	0.61
2:G:121:THR:OG1	2:G:221:ALA:O	2.14	0.61
1:D:144:LYS:HG3	1:D:145:PHE:CD1	2.35	0.61
2:G:101:ARG:NH1	2:G:262:PHE:O	2.33	0.61
1:C:14:LEU:HD21	5:H:302:LPP:H222	1.83	0.61
1:A:63:VAL:HG11	1:B:73:LEU:HB2	1.82	0.61
2:H:155:GLY:HA3	2:H:218:THR:HG21	1.81	0.61
1:B:94:PRO:HA	1:B:122:VAL:HA	1.82	0.61
2:G:78:GLY:O	2:G:81:ILE:HG22	2.00	0.61
2:H:101:ARG:NH1	2:H:262:PHE:O	2.33	0.60
1:A:22:LEU:HD21	5:H:301:LPP:H411	1.84	0.60
1:A:87:ASN:HB2	1:A:90:VAL:HG12	1.83	0.60
5:G:302:LPP:H301	5:G:302:LPP:H142	1.83	0.60
4:K:94:LEU:HB3	4:K:98:LEU:HD23	1.84	0.60
1:E:69:THR:HG23	1:E:84:MET:HA	1.82	0.60
3:I:260:ASP:O	3:J:135:ARG:NH1	2.31	0.60
2:G:74:LEU:HD12	2:G:99:LEU:HD12	1.83	0.59
4:L:94:LEU:HB3	4:L:98:LEU:HD23	1.84	0.59
2:H:74:LEU:HD12	2:H:99:LEU:HD12	1.83	0.59
2:H:138:MET:SD	3:J:57:GLN:HB2	2.42	0.59
3:I:130:GLN:HB2	3:I:135:ARG:HD2	1.84	0.59
2:G:78:GLY:HA2	2:G:81:ILE:HG22	1.84	0.59
1:C:84:MET:SD	1:C:84:MET:N	2.75	0.59
2:H:178:ALA:HA	2:H:182:LEU:HD12	1.85	0.59
4:L:91:VAL:HG13	4:L:92:SER:H	1.67	0.59
1:F:7:GLU:O	1:F:10:VAL:HG12	2.02	0.59
4:K:84:ASP:O	4:K:88:ILE:HG12	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:93:SER:OG	4:K:94:LEU:N	2.35	0.59
2:G:178:ALA:HA	2:G:182:LEU:HD12	1.85	0.59
1:D:97:SER:HB2	1:D:117:GLY:H	1.67	0.59
2:H:78:GLY:HA2	2:H:81:ILE:HG22	1.84	0.59
1:C:71:VAL:HG12	1:C:82:VAL:HG12	1.84	0.58
1:E:40:TYR:N	1:E:88:GLN:OE1	2.36	0.58
3:J:130:GLN:HB2	3:J:135:ARG:HD2	1.84	0.58
4:L:93:SER:OG	4:L:94:LEU:N	2.35	0.58
1:F:9:GLY:HA2	1:F:12:LEU:HD12	1.85	0.58
1:E:59:THR:HA	1:E:65:ILE:HG12	1.85	0.58
1:F:93:LEU:HD12	1:F:94:PRO:HD2	1.84	0.58
3:J:47:LYS:HE3	3:J:203:HIS:CD2	2.38	0.58
4:K:5:SER:H	4:K:17:ALA:HB3	1.69	0.58
1:D:29:SER:OG	2:G:199:PHE:HB2	2.03	0.58
1:F:13:PHE:O	1:F:17:GLY:N	2.36	0.58
1:D:29:SER:HA	2:G:197:VAL:HG11	1.86	0.58
1:D:138:LEU:HD11	1:E:106:LEU:HD12	1.84	0.58
4:K:91:VAL:HG13	4:K:92:SER:H	1.67	0.58
1:D:136:LEU:HB2	1:D:141:LEU:HD11	1.85	0.58
4:L:84:ASP:O	4:L:88:ILE:HG12	2.03	0.58
3:I:47:LYS:HE3	3:I:203:HIS:CD2	2.38	0.58
1:D:59:THR:HA	1:D:65:ILE:HG12	1.85	0.58
2:G:231:THR:HG23	2:G:234:GLY:H	1.69	0.57
1:E:104:ALA:HB3	1:E:108:GLY:HA3	1.85	0.57
2:G:132:GLN:NE2	3:I:97:PHE:HA	2.19	0.57
2:H:121:THR:OG1	2:H:221:ALA:O	2.14	0.57
1:F:3:THR:HB	1:F:6:LEU:HB2	1.86	0.57
1:B:92:ASN:O	1:F:78:TYR:OH	2.21	0.57
3:I:7:TYR:HE2	3:I:30:ARG:HH11	1.53	0.57
1:B:103:THR:HG22	1:B:110:LYS:HG2	1.85	0.57
1:E:32:SER:OG	1:E:35:ASN:ND2	2.38	0.57
4:L:14:LEU:HD22	4:L:37:ARG:NH2	2.20	0.57
3:J:214:TYR:OH	3:J:226:HIS:ND1	2.33	0.57
3:J:7:TYR:HE2	3:J:30:ARG:HH11	1.53	0.57
3:J:131:ALA:HB2	4:L:92:SER:HB2	1.87	0.57
4:K:40:GLN:HB3	4:K:44:LEU:HD11	1.87	0.57
2:G:51:GLN:HG3	2:G:150:PRO:HB2	1.86	0.57
4:L:5:SER:H	4:L:17:ALA:HB3	1.69	0.57
1:D:69:THR:HG23	1:D:84:MET:HA	1.87	0.57
3:I:265:LEU:HD21	4:L:63:LEU:HD21	1.85	0.57
4:K:68:ASP:OD1	4:K:68:ASP:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:94:PRO:HG2	1:F:117:GLY:H	1.70	0.56
2:H:51:GLN:HG3	2:H:150:PRO:HB2	1.86	0.56
3:J:130:GLN:HE21	3:J:135:ARG:HD3	1.69	0.56
4:K:14:LEU:HD22	4:K:37:ARG:NH2	2.20	0.56
2:H:231:THR:HG23	2:H:234:GLY:H	1.69	0.56
4:L:40:GLN:HB3	4:L:44:LEU:HD11	1.87	0.56
4:L:59:ILE:HD12	4:L:85:MET:SD	2.46	0.56
3:I:130:GLN:HE21	3:I:135:ARG:HD3	1.70	0.56
4:L:68:ASP:N	4:L:68:ASP:OD1	2.36	0.56
1:A:11:GLY:CA	5:H:302:LPP:H442	2.36	0.56
1:A:15:LEU:HD22	5:H:302:LPP:H412	1.88	0.56
1:A:73:LEU:HD11	1:C:60:LEU:HD22	1.88	0.56
3:I:185:ARG:HE	3:J:248:PRO:HG2	1.71	0.56
1:B:59:THR:HA	1:B:65:ILE:HG12	1.87	0.56
4:K:34:ARG:HD3	4:K:38:ALA:HB2	1.87	0.56
4:K:59:ILE:HD12	4:K:85:MET:SD	2.46	0.56
4:K:64:ALA:HA	4:K:67:ARG:HH21	1.71	0.56
1:A:121:ASP:N	1:A:121:ASP:OD1	2.39	0.55
1:A:122:VAL:HG12	1:A:123:LEU:HG	1.88	0.55
4:L:34:ARG:HD3	4:L:38:ALA:HB2	1.87	0.55
2:G:105:PRO:HB2	2:G:213:PHE:CZ	2.40	0.55
3:I:70:GLN:HG3	3:I:75:LEU:HD11	1.88	0.55
1:E:99:ALA:HB1	1:E:112:ILE:HD11	1.86	0.55
1:F:39:THR:HG22	1:F:88:GLN:HG2	1.89	0.55
2:G:98:THR:HB	5:G:304:LPP:H212	1.88	0.55
1:A:49:ILE:H	1:C:62:GLY:HA3	1.72	0.55
1:B:99:ALA:O	1:B:132:THR:OG1	2.25	0.55
4:L:6:LEU:HG	4:L:14:LEU:HD11	1.89	0.55
1:A:102:LEU:HB2	1:A:111:TYR:CZ	2.42	0.55
4:K:81:LEU:HD11	4:K:85:MET:HG2	1.88	0.55
1:A:104:ALA:HB3	1:A:108:GLY:HA3	1.89	0.55
5:G:301:LPP:H352	5:H:302:LPP:H342	1.88	0.55
4:L:64:ALA:HA	4:L:67:ARG:HH21	1.71	0.55
4:L:81:LEU:HD11	4:L:85:MET:HG2	1.88	0.55
1:B:63:VAL:HB	1:F:49:ILE:HD11	1.88	0.54
1:B:102:LEU:HB2	1:B:111:TYR:CE2	2.42	0.54
1:F:98:THR:OG1	1:F:132:THR:HA	2.07	0.54
4:K:82:PRO:HG2	4:K:85:MET:HB2	1.89	0.54
1:B:72:ASP:OD2	1:B:81:ARG:NH2	2.40	0.54
4:L:78:VAL:HG22	4:L:99:PRO:O	2.08	0.54
1:A:46:PHE:HD1	1:A:132:THR:HG21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:VAL:HG11	1:C:112:ILE:HD11	1.89	0.54
2:H:21:VAL:O	5:H:302:LPP:H443	2.08	0.54
2:H:37:GLY:H	2:H:145:LYS:NZ	2.06	0.54
4:K:6:LEU:HG	4:K:14:LEU:HD11	1.89	0.54
4:K:63:LEU:HG	4:K:67:ARG:HH12	1.73	0.54
2:G:85:TYR:OH	2:H:93:GLN:NE2	2.41	0.54
4:L:63:LEU:HG	4:L:67:ARG:HH12	1.73	0.54
2:G:93:GLN:NE2	2:H:85:TYR:OH	2.41	0.54
3:J:139:GLU:HA	3:J:139:GLU:OE1	2.08	0.54
4:L:46:VAL:O	4:L:78:VAL:HA	2.07	0.54
5:G:301:LPP:H161	5:G:301:LPP:H332	1.90	0.54
4:K:46:VAL:O	4:K:78:VAL:HA	2.08	0.54
1:F:57:LYS:HD2	1:F:64:THR:HB	1.91	0.54
2:G:54:SER:HA	2:G:58:LEU:HD13	1.89	0.54
3:J:70:GLN:HG3	3:J:75:LEU:HD11	1.88	0.53
4:L:82:PRO:HG2	4:L:85:MET:HB2	1.89	0.53
2:H:54:SER:HA	2:H:58:LEU:HD13	1.89	0.53
1:E:51:GLY:HA3	1:E:110:LYS:HD3	1.90	0.53
1:F:74:ASP:O	1:F:78:TYR:N	2.42	0.53
1:F:132:THR:O	1:F:133:GLN:NE2	2.41	0.53
1:B:63:VAL:HG11	1:F:73:LEU:HB2	1.90	0.53
1:E:39:THR:HG22	1:E:87:ASN:HD22	1.73	0.53
2:G:37:GLY:H	2:G:145:LYS:NZ	2.06	0.53
4:L:48:CYS:HB2	4:L:82:PRO:HD3	1.91	0.53
3:J:261:TYR:HE2	4:K:93:SER:HG	1.55	0.53
1:D:147:LEU:O	1:D:147:LEU:HD12	2.09	0.53
3:I:139:GLU:OE1	3:I:139:GLU:HA	2.08	0.53
3:I:176:ASP:OD2	3:J:43:SER:N	2.40	0.53
4:K:78:VAL:HG22	4:K:99:PRO:O	2.08	0.53
1:D:98:THR:HB	1:D:132:THR:HA	1.91	0.53
3:I:176:ASP:OD1	3:I:176:ASP:N	2.41	0.53
3:I:214:TYR:OH	3:I:226:HIS:ND1	2.33	0.53
3:J:176:ASP:N	3:J:176:ASP:OD1	2.41	0.53
1:B:91:ASN:O	1:B:122:VAL:HG21	2.09	0.52
1:D:17:GLY:HA3	2:G:161:LEU:HD12	1.91	0.52
2:H:105:PRO:HB2	2:H:213:PHE:CZ	2.40	0.52
1:B:102:LEU:HB2	1:B:111:TYR:CZ	2.44	0.52
1:A:96:ASP:CG	1:A:118:GLY:H	2.12	0.52
1:D:31:LEU:HD11	2:G:199:PHE:CG	2.45	0.52
4:K:48:CYS:HB2	4:K:82:PRO:HD3	1.91	0.52
4:K:62:LEU:HD12	4:K:85:MET:HE2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:53:LEU:HD23	3:I:58:LEU:HB3	1.90	0.52
1:D:40:TYR:HB3	1:D:125:ASP:HB3	1.91	0.52
3:I:261:TYR:HA	3:J:135:ARG:CZ	2.39	0.52
1:A:132:THR:O	1:A:133:GLN:NE2	2.42	0.52
5:H:302:LPP:H181	5:H:302:LPP:H371	1.92	0.52
4:K:29:ARG:HB2	4:K:61:LEU:HD11	1.92	0.52
1:A:45:TYR:HE1	1:A:81:ARG:HG3	1.75	0.52
1:A:49:ILE:HD11	1:C:63:VAL:HB	1.91	0.52
1:B:69:THR:OG1	1:B:83:THR:HG23	2.10	0.52
3:J:48:THR:HG22	3:J:52:ARG:HE	1.75	0.52
1:C:94:PRO:HA	1:C:122:VAL:HA	1.91	0.52
2:G:98:THR:OG1	5:G:304:LPP:H241	2.09	0.52
3:J:162:ASP:OD2	4:L:55:SER:HB2	2.10	0.52
1:B:29:SER:HA	2:H:197:VAL:HG11	1.92	0.52
3:I:44:GLY:N	6:I:301:ANP:O2G	2.43	0.52
3:J:103:PHE:HB2	3:J:138:VAL:HG22	1.91	0.52
1:C:82:VAL:HG23	1:C:84:MET:HE1	1.92	0.51
3:I:263:ALA:O	3:I:267:GLY:N	2.34	0.51
3:J:38:GLY:O	3:J:215:ILE:HG13	2.10	0.51
3:J:53:LEU:HD23	3:J:58:LEU:HB3	1.90	0.51
5:G:301:LPP:H421	5:H:301:LPP:H241	1.92	0.51
1:A:73:LEU:HD21	1:A:78:TYR:HA	1.90	0.51
4:L:62:LEU:HD12	4:L:85:MET:HE2	1.93	0.51
3:I:11:LEU:O	3:I:28:ASP:HA	2.11	0.51
3:J:11:LEU:O	3:J:28:ASP:HA	2.11	0.51
3:J:123:ASP:OD1	4:L:67:ARG:CZ	2.58	0.51
1:C:39:THR:HB	1:C:86:ILE:O	2.10	0.51
1:C:137:VAL:HG13	1:C:140:ASP:H	1.74	0.51
3:I:103:PHE:HB2	3:I:138:VAL:HG22	1.91	0.51
3:I:248:PRO:HG2	3:J:185:ARG:HE	1.76	0.51
4:K:37:ARG:HD3	4:K:37:ARG:N	2.26	0.51
1:B:22:LEU:O	1:B:26:LEU:N	2.40	0.51
1:A:96:ASP:N	1:A:119:ASP:OD1	2.35	0.51
1:F:102:LEU:HB2	1:F:111:TYR:CZ	2.46	0.51
2:H:186:GLU:OE1	2:H:186:GLU:N	2.44	0.51
3:I:38:GLY:O	3:I:215:ILE:HG13	2.10	0.51
4:K:63:LEU:HG	4:K:67:ARG:HH22	1.76	0.51
4:L:29:ARG:HB2	4:L:61:LEU:HD11	1.92	0.51
2:H:245:TYR:CE2	5:H:301:LPP:HC62	2.46	0.51
3:J:44:GLY:N	6:J:301:ANP:O2G	2.43	0.51
2:G:186:GLU:N	2:G:186:GLU:OE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:24:SER:O	4:K:28:LEU:HG	2.11	0.51
4:L:63:LEU:HG	4:L:67:ARG:HH22	1.76	0.51
1:D:100:SER:OG	1:D:133:GLN:HB2	2.12	0.50
4:L:24:SER:O	4:L:28:LEU:HG	2.11	0.50
1:D:140:ASP:O	1:D:144:LYS:N	2.43	0.50
1:F:3:THR:HA	1:F:6:LEU:HD13	1.91	0.50
2:G:63:ILE:HD13	2:G:162:LEU:HB3	1.93	0.50
1:F:84:MET:HG2	1:F:86:ILE:HD11	1.92	0.50
4:L:37:ARG:N	4:L:37:ARG:HD3	2.26	0.50
1:D:94:PRO:HG3	1:D:118:GLY:H	1.76	0.50
2:H:21:VAL:HG13	5:H:302:LPP:H443	1.94	0.50
3:J:117:PRO:O	3:J:120:MET:N	2.44	0.50
3:J:97:PHE:H	3:J:105:ASN:HD21	1.59	0.50
1:E:136:LEU:HD21	1:E:141:LEU:HD22	1.92	0.50
3:I:97:PHE:H	3:I:105:ASN:HD21	1.59	0.50
1:F:59:THR:HA	1:F:65:ILE:HG12	1.94	0.50
2:H:63:ILE:HD13	2:H:162:LEU:HB3	1.93	0.50
3:J:9:VAL:HG22	3:J:67:VAL:HG22	1.94	0.50
1:F:55:ARG:HA	1:F:68:VAL:O	2.11	0.50
3:I:117:PRO:O	3:I:120:MET:N	2.44	0.50
3:I:168:TYR:HB2	3:I:200:VAL:HA	1.94	0.50
1:A:44:ALA:HA	1:A:129:ILE:HG22	1.93	0.50
1:D:122:VAL:HG12	1:D:123:LEU:HG	1.93	0.50
1:E:76:ASP:OD1	1:E:77:SER:N	2.42	0.50
2:G:138:MET:SD	3:I:57:GLN:HB2	2.52	0.50
3:I:9:VAL:HG22	3:I:67:VAL:HG22	1.94	0.50
4:K:5:SER:N	4:K:17:ALA:HB3	2.27	0.50
4:L:69:ALA:HB3	4:L:76:LEU:HD22	1.94	0.50
1:B:40:TYR:HB2	1:B:125:ASP:CG	2.32	0.49
1:D:69:THR:OG1	1:D:83:THR:HG23	2.12	0.49
1:E:59:THR:OG1	1:E:60:LEU:N	2.45	0.49
1:E:94:PRO:HG2	1:E:97:SER:HG	1.77	0.49
3:I:91:PHE:HA	3:I:169:ASP:HB3	1.94	0.49
3:I:241:ARG:HH21	3:I:245:LYS:HE3	1.76	0.49
3:J:263:ALA:O	3:J:267:GLY:N	2.34	0.49
1:A:19:LEU:O	1:A:23:LEU:HB2	2.12	0.49
1:B:28:VAL:HG13	2:H:193:MET:HE3	1.93	0.49
5:G:304:LPP:H411	2:H:98:THR:HB	1.94	0.49
2:H:214:ALA:O	2:H:218:THR:HG22	2.12	0.49
2:G:249:ALA:HB2	5:G:302:LPP:H332	1.95	0.49
4:K:21:ASP:CG	4:K:23:SER:HG	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:TYR:CE1	1:A:81:ARG:HG3	2.47	0.49
1:B:105:GLY:O	1:B:108:GLY:N	2.45	0.49
3:I:48:THR:HG22	3:I:52:ARG:HE	1.75	0.49
4:L:5:SER:N	4:L:17:ALA:HB3	2.27	0.49
1:D:84:MET:SD	1:D:84:MET:N	2.86	0.49
1:E:73:LEU:HD12	1:E:79:THR:O	2.12	0.49
1:E:93:LEU:HD12	1:E:94:PRO:HD2	1.94	0.49
1:F:68:VAL:HA	1:F:84:MET:CB	2.43	0.49
1:F:124:LYS:HB2	1:F:127:SER:OG	2.13	0.49
2:G:24:LEU:HA	2:G:27:SER:HB3	1.94	0.49
2:G:43:THR:OG1	2:G:44:GLY:N	2.45	0.49
3:J:168:TYR:HB2	3:J:200:VAL:HA	1.94	0.49
1:A:46:PHE:CD1	1:A:132:THR:HG21	2.48	0.49
1:A:46:PHE:HE1	1:A:132:THR:HG1	1.61	0.49
1:B:59:THR:OG1	1:B:63:VAL:O	2.17	0.49
2:H:24:LEU:HA	2:H:27:SER:HB3	1.94	0.49
3:I:170:GLU:HB3	3:I:173:VAL:HG21	1.94	0.49
1:B:46:PHE:HD2	1:B:49:ILE:HG22	1.78	0.49
2:G:104:GLY:HA2	2:G:166:PHE:CE2	2.43	0.49
2:H:21:VAL:HA	5:H:302:LPP:H422	1.94	0.48
1:E:74:ASP:OD2	1:E:77:SER:OG	2.31	0.48
2:G:214:ALA:O	2:G:218:THR:HG22	2.12	0.48
3:I:261:TYR:HA	3:J:135:ARG:NH1	2.27	0.48
2:G:205:ASN:ND2	2:G:261:MET:SD	2.86	0.48
2:H:205:ASN:ND2	2:H:261:MET:SD	2.86	0.48
3:J:91:PHE:HA	3:J:169:ASP:HB3	1.94	0.48
5:G:301:LPP:HC7	5:H:302:LPP:HC81	1.95	0.48
4:L:78:VAL:O	4:L:79:ARG:HD2	2.14	0.48
1:C:76:ASP:OD1	1:C:77:SER:N	2.43	0.48
1:C:95:VAL:HG23	1:C:121:ASP:O	2.14	0.48
1:F:69:THR:H	1:F:84:MET:HA	1.79	0.48
4:K:72:ALA:HB1	4:K:74:LYS:HZ3	1.78	0.48
1:A:75:ARG:NH1	1:A:76:ASP:HB2	2.28	0.48
1:C:59:THR:HA	1:C:65:ILE:HG12	1.96	0.48
1:F:30:GLY:O	1:F:32:SER:N	2.44	0.48
5:G:304:LPP:H361	2:H:94:MET:HG2	1.94	0.48
3:I:254:PHE:HD2	3:I:255:HIS:CD2	2.32	0.48
3:J:170:GLU:HB3	3:J:173:VAL:HG21	1.94	0.48
3:J:224:LEU:HB3	3:J:240:ILE:HD11	1.95	0.48
3:J:241:ARG:HH21	3:J:245:LYS:HE3	1.76	0.48
3:J:254:PHE:HD2	3:J:255:HIS:CD2	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:LEU:HB3	1:E:145:PHE:HZ	1.77	0.48
2:G:238:ALA:O	2:G:242:THR:HG22	2.13	0.48
3:I:45:CYS:SG	3:I:47:LYS:HG3	2.54	0.48
3:I:224:LEU:HB3	3:I:240:ILE:HD11	1.95	0.48
3:J:45:CYS:SG	3:J:47:LYS:HG3	2.54	0.48
1:C:142:ILE:O	1:C:146:LEU:HB2	2.14	0.48
2:G:79:TYR:HB2	2:G:182:LEU:HD13	1.96	0.48
6:J:301:ANP:H5'1	6:J:301:ANP:H8	1.96	0.48
1:B:122:VAL:HG13	1:B:123:LEU:H	1.78	0.48
1:C:137:VAL:HG21	1:D:102:LEU:HD13	1.96	0.48
2:G:156:PHE:CE1	2:G:215:PHE:HA	2.49	0.48
2:H:43:THR:OG1	2:H:44:GLY:N	2.45	0.48
5:G:303:LPP:H321	5:H:303:LPP:H362	1.96	0.48
2:H:138:MET:HG2	3:J:89:VAL:HG21	1.95	0.48
3:J:39:ILE:HG12	3:J:201:VAL:HG22	1.96	0.48
4:K:78:VAL:O	4:K:79:ARG:HD2	2.14	0.48
1:B:17:GLY:HA3	2:H:161:LEU:HD12	1.94	0.47
2:G:138:MET:HG2	3:I:89:VAL:HG21	1.94	0.47
2:H:156:PHE:CE1	2:H:215:PHE:HA	2.49	0.47
4:K:69:ALA:HB3	4:K:76:LEU:HD22	1.94	0.47
1:D:56:GLY:H	1:D:68:VAL:HG12	1.79	0.47
1:E:23:LEU:HA	1:E:26:LEU:HG	1.96	0.47
1:F:102:LEU:HB2	1:F:111:TYR:CE2	2.48	0.47
2:G:14:GLY:O	2:G:18:LEU:HG	2.14	0.47
1:C:93:LEU:O	1:C:123:LEU:HG	2.14	0.47
1:E:23:LEU:HD21	2:G:260:LEU:HG	1.97	0.47
1:F:94:PRO:HG2	1:F:97:SER:HB2	1.96	0.47
2:H:14:GLY:O	2:H:18:LEU:HG	2.14	0.47
3:I:241:ARG:HB2	3:I:245:LYS:HZ1	1.79	0.47
4:L:21:ASP:CG	4:L:23:SER:HG	2.17	0.47
1:C:93:LEU:HD12	1:C:93:LEU:H	1.79	0.47
1:E:29:SER:OG	1:E:30:GLY:N	2.46	0.47
1:E:138:LEU:HD22	1:F:106:LEU:HG	1.97	0.47
1:F:39:THR:HB	1:F:86:ILE:O	2.15	0.47
2:H:238:ALA:O	2:H:242:THR:HG22	2.13	0.47
3:J:120:MET:HG2	4:L:60:SER:OG	2.14	0.47
1:A:97:SER:OG	1:A:117:GLY:N	2.46	0.47
1:D:73:LEU:HD11	1:E:60:LEU:HD23	1.97	0.47
1:F:137:VAL:HG12	1:F:140:ASP:H	1.80	0.47
2:G:251:LEU:HD22	2:H:66:SER:OG	2.15	0.47
5:G:304:LPP:H401	5:G:304:LPP:H371	1.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:VAL:HA	1:A:112:ILE:HG23	1.97	0.47
1:C:107:LEU:HD11	1:D:107:LEU:HD13	1.97	0.47
2:G:66:SER:OG	2:H:251:LEU:HD22	2.14	0.47
4:L:52:GLU:OE1	4:L:52:GLU:HA	2.15	0.47
4:L:55:SER:OG	4:L:57:VAL:HG12	2.15	0.47
2:H:94:MET:O	2:H:98:THR:HG22	2.15	0.47
2:H:249:ALA:HA	5:H:301:LPP:H161	1.96	0.47
4:K:52:GLU:HA	4:K:52:GLU:OE1	2.15	0.47
1:C:98:THR:OG1	1:C:132:THR:HA	2.15	0.47
3:I:39:ILE:HG12	3:I:201:VAL:HG22	1.96	0.47
6:I:301:ANP:H8	6:I:301:ANP:H5'1	1.96	0.47
3:J:47:LYS:HE2	3:J:47:LYS:HB2	1.75	0.47
1:A:62:GLY:HA3	1:B:49:ILE:HG13	1.96	0.46
1:B:44:ALA:HA	1:B:129:ILE:HG22	1.97	0.46
1:B:51:GLY:CA	1:B:110:LYS:HD3	2.44	0.46
1:D:102:LEU:HB2	1:D:111:TYR:CE2	2.49	0.46
1:D:144:LYS:HG3	1:D:145:PHE:HD1	1.80	0.46
1:E:67:LYS:N	1:E:85:GLU:OE2	2.44	0.46
2:H:97:LEU:O	2:H:101:ARG:HG2	2.15	0.46
3:I:160:ALA:O	3:I:161:LEU:HB2	2.15	0.46
1:E:25:ALA:HB1	1:E:28:VAL:HG12	1.97	0.46
1:A:89:ASN:OD1	1:A:90:VAL:N	2.48	0.46
1:E:102:LEU:HB2	1:E:111:TYR:CZ	2.51	0.46
2:H:79:TYR:HB2	2:H:182:LEU:HD13	1.96	0.46
4:K:3:GLN:NE2	4:K:19:VAL:O	2.49	0.46
4:K:55:SER:OG	4:K:57:VAL:HG12	2.15	0.46
1:A:15:LEU:HD22	5:H:302:LPP:H392	1.98	0.46
2:G:231:THR:O	2:G:234:GLY:N	2.49	0.46
4:L:3:GLN:NE2	4:L:19:VAL:O	2.49	0.46
1:A:12:LEU:HA	5:H:302:LPP:H432	1.97	0.46
1:C:138:LEU:O	1:C:142:ILE:HG12	2.16	0.46
1:D:72:ASP:OD2	1:D:81:ARG:NH2	2.49	0.46
1:D:94:PRO:HB2	1:D:96:ASP:OD1	2.16	0.46
2:G:90:ALA:O	2:G:93:GLN:HG2	2.15	0.46
2:G:97:LEU:O	2:G:101:ARG:HG2	2.15	0.46
1:B:141:LEU:HD13	1:F:142:ILE:HD11	1.96	0.46
2:G:94:MET:O	2:G:98:THR:HG22	2.15	0.46
5:G:304:LPP:H263	5:G:304:LPP:H232	1.66	0.46
1:B:103:THR:CG2	1:B:110:LYS:HG2	2.45	0.46
2:H:21:VAL:C	5:H:302:LPP:H443	2.36	0.46
3:I:47:LYS:HB2	3:I:47:LYS:HE2	1.75	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:123:ASP:OD1	4:K:67:ARG:CZ	2.63	0.46
3:J:11:LEU:HG	3:J:65:VAL:HG12	1.98	0.46
3:J:160:ALA:O	3:J:161:LEU:HB2	2.15	0.46
1:A:49:ILE:HB	1:A:52:VAL:CG2	2.46	0.46
1:E:65:ILE:HG23	1:E:90:VAL:HG21	1.97	0.46
4:L:10:ALA:H	4:L:40:GLN:CD	2.20	0.46
4:L:18:GLY:O	4:L:52:GLU:N	2.45	0.46
1:B:9:GLY:O	1:B:13:PHE:HD2	1.99	0.46
1:B:75:ARG:HD3	1:B:75:ARG:H	1.80	0.46
1:E:93:LEU:HB3	1:E:123:LEU:HD11	1.97	0.46
1:F:84:MET:SD	1:F:84:MET:N	2.89	0.46
2:G:81:ILE:CG2	2:G:82:LEU:HG	2.45	0.46
2:G:253:LEU:HD12	5:G:302:LPP:H362	1.98	0.46
2:H:104:GLY:HA2	2:H:166:PHE:CE2	2.43	0.46
3:J:183:LEU:O	3:J:187:ILE:HG23	2.16	0.46
1:B:60:LEU:HD13	1:B:65:ILE:HG13	1.98	0.45
1:F:76:ASP:OD1	1:F:77:SER:N	2.45	0.45
4:K:37:ARG:NH1	4:K:44:LEU:HG	2.31	0.45
1:A:24:LEU:O	1:A:26:LEU:HG	2.16	0.45
2:G:100:LEU:HD21	2:G:203:VAL:HG22	1.99	0.45
2:H:29:LEU:HD13	2:H:29:LEU:HA	1.81	0.45
2:H:231:THR:O	2:H:234:GLY:N	2.49	0.45
1:F:59:THR:O	1:F:113:GLY:HA2	2.16	0.45
2:H:100:LEU:HD21	2:H:203:VAL:HG22	1.99	0.45
2:H:100:LEU:HD21	2:H:203:VAL:HA	1.97	0.45
4:L:63:LEU:HG	4:L:67:ARG:NH1	2.30	0.45
1:E:91:ASN:N	1:E:91:ASN:OD1	2.49	0.45
1:E:93:LEU:N	1:E:122:VAL:HG13	2.30	0.45
3:I:48:THR:O	3:I:52:ARG:HG3	2.17	0.45
3:J:15:THR:O	3:J:61:SER:OG	2.24	0.45
4:K:63:LEU:HG	4:K:67:ARG:NH1	2.30	0.45
1:A:56:GLY:H	1:A:68:VAL:HG12	1.82	0.45
1:C:37:GLY:N	1:C:38:ASP:HA	2.32	0.45
2:G:70:ILE:HG21	2:G:166:PHE:CZ	2.52	0.45
5:G:303:LPP:H402	5:G:303:LPP:H431	1.59	0.45
2:H:21:VAL:HG22	5:H:302:LPP:H411	1.99	0.45
2:H:70:ILE:HG21	2:H:166:PHE:CZ	2.52	0.45
3:I:135:ARG:NH1	3:J:264:ASP:HB3	2.30	0.45
3:J:240:ILE:O	3:J:243:PHE:N	2.50	0.45
1:B:59:THR:O	1:B:113:GLY:HA2	2.17	0.45
2:G:212:VAL:HG11	2:G:257:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:90:ALA:O	2:H:93:GLN:HG2	2.15	0.45
3:I:15:THR:O	3:I:61:SER:OG	2.24	0.45
3:I:240:ILE:O	3:I:243:PHE:N	2.50	0.45
1:D:104:ALA:HB3	1:D:108:GLY:HA3	1.99	0.45
1:E:40:TYR:HD2	1:E:125:ASP:HB3	1.80	0.45
1:E:124:LYS:HB3	1:E:127:SER:HB3	1.99	0.45
3:I:183:LEU:O	3:I:187:ILE:HG23	2.16	0.45
4:K:18:GLY:O	4:K:52:GLU:N	2.46	0.45
1:D:58:VAL:HG12	1:D:112:ILE:HD11	1.99	0.45
2:G:100:LEU:HD21	2:G:203:VAL:HA	1.97	0.45
3:J:59:ARG:HD2	3:J:60:PRO:HD2	1.99	0.45
3:J:126:LEU:HD23	3:J:126:LEU:HA	1.73	0.45
3:J:241:ARG:HB2	3:J:245:LYS:HZ1	1.82	0.45
4:K:63:LEU:HG	4:K:67:ARG:NH2	2.32	0.45
4:L:37:ARG:NH1	4:L:44:LEU:HG	2.31	0.45
1:A:8:ILE:O	5:H:302:LPP:H441	2.17	0.45
1:C:58:VAL:HG22	1:C:66:GLY:O	2.17	0.45
1:D:56:GLY:N	1:D:68:VAL:HG12	2.32	0.45
2:G:124:ILE:HD13	2:G:222:VAL:HG23	1.98	0.45
3:I:260:ASP:OD2	3:I:263:ALA:N	2.42	0.45
1:B:76:ASP:OD2	1:B:76:ASP:N	2.48	0.44
1:F:27:ARG:HG2	1:F:30:GLY:HA2	1.99	0.44
2:H:35:LEU:HD23	2:H:35:LEU:HA	1.80	0.44
3:I:260:ASP:CG	3:I:262:ARG:H	2.21	0.44
3:J:48:THR:O	3:J:52:ARG:HG3	2.17	0.44
1:C:94:PRO:HB2	1:C:96:ASP:OD1	2.16	0.44
3:I:11:LEU:HG	3:I:65:VAL:HG12	1.98	0.44
1:A:100:SER:OG	1:A:133:GLN:HB2	2.17	0.44
1:A:137:VAL:HG23	1:A:140:ASP:H	1.83	0.44
1:D:91:ASN:OD1	1:D:91:ASN:N	2.49	0.44
5:H:302:LPP:H371	5:H:302:LPP:H341	1.61	0.44
3:I:45:CYS:N	6:I:301:ANP:O1B	2.49	0.44
3:J:45:CYS:N	6:J:301:ANP:O1B	2.49	0.44
3:J:260:ASP:CG	3:J:262:ARG:H	2.21	0.44
4:L:63:LEU:HG	4:L:67:ARG:NH2	2.32	0.44
1:C:40:TYR:N	1:C:88:GLN:OE1	2.51	0.44
1:F:60:LEU:HD12	1:F:114:ILE:HB	1.98	0.44
3:I:82:ASP:HA	3:I:85:LYS:NZ	2.33	0.44
1:C:54:VAL:HG12	1:C:55:ARG:HG3	1.98	0.44
1:F:132:THR:OG1	1:F:133:GLN:N	2.51	0.44
3:I:59:ARG:HD2	3:I:60:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:72:ALA:HB1	4:L:74:LYS:HZ3	1.83	0.44
4:L:97:ILE:O	4:L:99:PRO:HD3	2.17	0.44
1:E:132:THR:OG1	1:E:133:GLN:N	2.50	0.44
2:G:113:ALA:HB1	2:G:246:ALA:HB1	1.99	0.44
2:G:118:SER:O	2:G:121:THR:N	2.51	0.44
2:H:118:SER:O	2:H:121:THR:N	2.51	0.44
4:K:61:LEU:HD13	4:K:61:LEU:HA	1.67	0.44
1:B:46:PHE:CD2	1:B:101:ILE:HD11	2.53	0.44
1:B:101:ILE:HG21	1:B:110:LYS:HE3	2.00	0.44
1:B:137:VAL:HG23	1:B:140:ASP:H	1.83	0.44
1:C:73:LEU:HD21	1:D:60:LEU:HD23	2.00	0.44
1:D:93:LEU:HG	1:D:123:LEU:HD23	1.99	0.44
2:G:250:VAL:HG12	2:G:251:LEU:HD12	2.00	0.44
2:H:51:GLN:O	2:H:54:SER:N	2.50	0.44
3:J:260:ASP:OD2	3:J:263:ALA:N	2.42	0.44
1:F:59:THR:HG1	1:F:60:LEU:H	1.65	0.44
1:F:74:ASP:HB2	1:F:76:ASP:OD1	2.18	0.44
2:G:51:GLN:O	2:G:54:SER:N	2.50	0.44
2:H:113:ALA:HB1	2:H:246:ALA:HB1	1.99	0.44
2:H:136:LEU:HD23	2:H:136:LEU:HA	1.83	0.44
3:I:186:LEU:HD23	3:I:186:LEU:HA	1.71	0.44
1:A:146:LEU:HD12	1:C:145:PHE:HD2	1.83	0.44
1:E:145:PHE:O	1:E:149:SER:OG	2.36	0.44
2:G:119:ALA:HB2	2:H:240:THR:HG21	1.99	0.44
2:H:124:ILE:HD13	2:H:222:VAL:HG23	1.98	0.43
3:J:186:LEU:HA	3:J:186:LEU:HD23	1.71	0.43
4:K:91:VAL:HG13	4:K:92:SER:N	2.33	0.43
1:C:67:LYS:O	1:C:84:MET:HB2	2.18	0.43
2:G:220:ILE:HG22	5:G:302:LPP:O10	2.18	0.43
3:J:82:ASP:HA	3:J:85:LYS:NZ	2.33	0.43
4:K:97:ILE:O	4:K:99:PRO:HD3	2.17	0.43
4:L:46:VAL:HG23	4:L:78:VAL:HG12	2.00	0.43
1:D:55:ARG:HE	1:D:55:ARG:HB3	1.62	0.43
5:G:304:LPP:H201	5:G:304:LPP:H231	1.45	0.43
5:H:302:LPP:H181	5:H:302:LPP:H341	2.01	0.43
3:I:149:MET:HA	3:I:152:ARG:HD3	2.01	0.43
3:J:90:LEU:HD23	3:J:168:TYR:CD1	2.54	0.43
4:K:31:GLN:O	4:K:35:LEU:HB2	2.18	0.43
4:L:47:ASP:C	4:L:47:ASP:OD1	2.57	0.43
1:B:22:LEU:O	1:B:25:ALA:N	2.51	0.43
1:F:59:THR:HA	1:F:65:ILE:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:303:LPP:H221	5:H:303:LPP:H181	1.99	0.43
3:I:55:ALA:O	3:I:84:ARG:NH2	2.51	0.43
3:J:87:PHE:HA	3:J:165:ILE:O	2.18	0.43
1:A:7:GLU:OE2	2:H:26:ARG:HB2	2.18	0.43
1:A:11:GLY:C	5:H:302:LPP:H442	2.38	0.43
1:C:53:THR:HG22	1:C:54:VAL:N	2.34	0.43
1:E:69:THR:OG1	1:E:83:THR:HG23	2.19	0.43
2:H:212:VAL:HG11	2:H:257:LEU:HG	1.99	0.43
3:I:259:ARG:HG3	3:I:260:ASP:H	1.84	0.43
4:L:31:GLN:O	4:L:35:LEU:HB2	2.18	0.43
1:C:91:ASN:OD1	1:C:91:ASN:N	2.52	0.43
3:J:55:ALA:O	3:J:84:ARG:NH2	2.51	0.43
1:B:24:LEU:HD11	2:H:167:SER:HB3	2.00	0.43
6:I:301:ANP:O2A	6:I:301:ANP:O1G	2.37	0.43
1:E:97:SER:OG	1:E:117:GLY:N	2.36	0.43
3:I:51:LEU:HD12	3:I:51:LEU:HA	1.84	0.43
3:I:219:GLY:HA3	3:I:224:LEU:HD11	2.01	0.43
3:I:235:THR:HG23	3:I:237:ASP:H	1.84	0.43
4:K:48:CYS:SG	4:K:62:LEU:HD11	2.59	0.43
1:A:49:ILE:O	1:A:52:VAL:HG22	2.19	0.43
1:A:95:VAL:HG23	1:A:121:ASP:O	2.19	0.43
1:B:56:GLY:O	1:B:68:VAL:HG12	2.18	0.43
1:F:97:SER:OG	1:F:115:SER:O	2.33	0.43
2:G:145:LYS:HB2	2:G:145:LYS:HE2	1.86	0.43
2:G:240:THR:HG21	2:H:119:ALA:HB2	2.01	0.43
2:H:138:MET:HG3	3:J:55:ALA:HB1	2.00	0.43
3:J:144:GLU:OE1	3:J:144:GLU:HA	2.19	0.43
4:L:31:GLN:O	4:L:36:ILE:HG12	2.19	0.43
1:B:101:ILE:HD13	1:B:135:ALA:N	2.34	0.43
1:C:73:LEU:HD12	1:C:79:THR:O	2.19	0.43
2:G:67:GLY:HA2	2:G:166:PHE:CE1	2.54	0.43
3:I:90:LEU:HD23	3:I:168:TYR:CD1	2.54	0.43
4:K:47:ASP:OD1	4:K:47:ASP:C	2.57	0.43
1:E:12:LEU:HD23	1:E:12:LEU:HA	1.83	0.42
1:F:69:THR:N	1:F:83:THR:O	2.51	0.42
2:G:101:ARG:HE	2:G:101:ARG:HB2	1.64	0.42
3:I:7:TYR:CD2	3:I:30:ARG:HB3	2.54	0.42
3:I:84:ARG:HD3	3:I:87:PHE:HZ	1.84	0.42
3:I:126:LEU:HA	3:I:126:LEU:HD23	1.73	0.42
3:I:185:ARG:NE	3:J:248:PRO:HG2	2.32	0.42
3:I:261:TYR:HE2	4:L:93:SER:HG	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:ILE:HG22	1:B:87:ASN:O	2.19	0.42
1:E:94:PRO:HA	1:E:122:VAL:HA	2.01	0.42
2:G:248:LEU:HA	2:G:248:LEU:HD12	1.75	0.42
2:H:78:GLY:HA2	2:H:81:ILE:CG2	2.49	0.42
2:H:145:LYS:HB2	2:H:145:LYS:HE2	1.85	0.42
2:H:250:VAL:HG12	2:H:251:LEU:HD12	2.00	0.42
3:I:144:GLU:HA	3:I:144:GLU:OE1	2.19	0.42
3:I:261:TYR:CZ	3:J:130:GLN:HG2	2.54	0.42
3:J:84:ARG:HD3	3:J:87:PHE:HZ	1.84	0.42
3:J:102:VAL:O	3:J:106:VAL:HG23	2.19	0.42
3:J:261:TYR:HE2	4:K:94:LEU:H	1.66	0.42
4:K:46:VAL:HG23	4:K:78:VAL:HG12	2.00	0.42
4:K:95:LEU:HG	4:K:96:GLU:N	2.34	0.42
1:A:56:GLY:H	1:A:68:VAL:CG1	2.32	0.42
1:A:59:THR:OG1	1:A:60:LEU:N	2.52	0.42
3:J:149:MET:HA	3:J:152:ARG:HD3	2.01	0.42
1:F:8:ILE:HG12	2:G:11:ARG:HA	2.00	0.42
3:I:87:PHE:HA	3:I:165:ILE:O	2.18	0.42
4:L:18:GLY:C	4:L:52:GLU:H	2.23	0.42
4:L:48:CYS:SG	4:L:62:LEU:HD11	2.59	0.42
1:A:94:PRO:HG2	1:A:97:SER:OG	2.19	0.42
1:C:123:LEU:HB3	1:C:125:ASP:H	1.85	0.42
1:F:141:LEU:HD23	1:F:141:LEU:HA	1.82	0.42
3:J:219:GLY:HA3	3:J:224:LEU:HD11	2.01	0.42
1:A:18:LEU:HA	1:A:22:LEU:HD13	2.01	0.42
1:D:49:ILE:HB	1:D:52:VAL:HB	2.00	0.42
3:J:117:PRO:HD2	3:J:120:MET:HE2	2.00	0.42
3:J:259:ARG:HG3	3:J:260:ASP:H	1.84	0.42
6:J:301:ANP:O2A	6:J:301:ANP:O1G	2.37	0.42
4:K:31:GLN:O	4:K:36:ILE:HG12	2.19	0.42
1:A:60:LEU:HD11	1:A:116:VAL:HG12	2.02	0.42
1:B:103:THR:N	1:F:139:GLU:OE1	2.51	0.42
1:E:19:LEU:HD12	1:E:19:LEU:HA	1.91	0.42
1:E:67:LYS:HG3	1:E:68:VAL:O	2.20	0.42
1:F:119:ASP:HB3	1:F:121:ASP:OD1	2.20	0.42
2:H:67:GLY:HA2	2:H:166:PHE:CE1	2.54	0.42
4:K:14:LEU:HB3	4:K:46:VAL:HG12	2.01	0.42
1:A:94:PRO:HB3	1:A:119:ASP:O	2.20	0.42
1:A:139:GLU:HG3	1:C:102:LEU:HD23	2.01	0.42
1:D:138:LEU:O	1:D:142:ILE:HG12	2.19	0.42
1:E:46:PHE:HD1	1:E:132:THR:HG21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:LYS:HB2	1:F:144:LYS:HE2	1.77	0.42
3:J:92:GLN:O	3:J:93:SER:OG	2.31	0.42
4:L:14:LEU:HB3	4:L:46:VAL:HG12	2.01	0.42
1:C:101:ILE:HB	1:C:135:ALA:HB2	2.01	0.42
1:D:132:THR:OG1	1:D:133:GLN:N	2.53	0.42
1:E:8:ILE:HG12	2:G:21:VAL:HG12	2.02	0.42
1:E:39:THR:HG22	1:E:87:ASN:HA	2.01	0.42
1:E:99:ALA:O	1:E:132:THR:OG1	2.27	0.42
1:F:60:LEU:HB3	1:F:65:ILE:HD11	2.01	0.42
2:G:111:LEU:HD23	2:G:111:LEU:HA	1.87	0.42
3:I:102:VAL:O	3:I:106:VAL:HG23	2.19	0.42
3:J:96:LEU:HB3	3:J:105:ASN:ND2	2.35	0.42
1:A:39:THR:HG22	1:A:87:ASN:HD22	1.85	0.41
1:B:121:ASP:OD2	1:B:122:VAL:N	2.53	0.41
2:G:252:GLY:HA3	5:G:302:LPP:H361	2.02	0.41
4:K:10:ALA:H	4:K:40:GLN:CD	2.20	0.41
4:L:95:LEU:HG	4:L:96:GLU:N	2.34	0.41
1:A:72:ASP:OD2	1:A:81:ARG:NH2	2.53	0.41
1:B:31:LEU:HD11	2:H:199:PHE:CE2	2.55	0.41
1:B:132:THR:OG1	1:B:133:GLN:N	2.52	0.41
1:D:6:LEU:O	1:D:10:VAL:HG12	2.20	0.41
1:D:40:TYR:N	1:D:88:GLN:OE1	2.53	0.41
1:D:51:GLY:O	1:D:110:LYS:HB2	2.20	0.41
1:F:9:GLY:O	1:F:12:LEU:HB2	2.20	0.41
3:I:15:THR:HG23	3:I:61:SER:OG	2.20	0.41
3:J:59:ARG:HD2	3:J:59:ARG:HA	1.78	0.41
1:D:57:LYS:O	1:D:111:TYR:HB2	2.20	0.41
3:I:162:ASP:OD2	4:K:55:SER:HB2	2.21	0.41
3:J:84:ARG:HA	3:J:87:PHE:CE2	2.55	0.41
1:B:48:ASN:N	1:B:134:SER:OG	2.52	0.41
1:C:28:VAL:O	1:C:31:LEU:HA	2.20	0.41
1:D:49:ILE:HD11	1:E:63:VAL:HB	2.01	0.41
3:J:145:LEU:HG	3:J:149:MET:HG3	2.02	0.41
3:J:235:THR:HG23	3:J:237:ASP:H	1.84	0.41
1:E:41:LYS:O	1:E:126:GLY:N	2.53	0.41
1:E:101:ILE:HD13	1:E:135:ALA:HB2	2.03	0.41
5:G:303:LPP:H151	5:G:303:LPP:H182	1.59	0.41
2:H:242:THR:OG1	2:H:242:THR:O	2.31	0.41
2:H:248:LEU:HA	2:H:248:LEU:HD12	1.75	0.41
3:I:129:LEU:HD23	3:I:129:LEU:HA	1.76	0.41
3:J:7:TYR:CD2	3:J:30:ARG:HB3	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:15:THR:HG23	3:J:61:SER:OG	2.20	0.41
3:J:116:LEU:CD2	4:L:26:PRO:HG3	2.50	0.41
1:A:91:ASN:OD1	1:A:91:ASN:N	2.54	0.41
1:B:93:LEU:O	1:B:122:VAL:HG23	2.20	0.41
2:G:242:THR:O	2:G:242:THR:OG1	2.31	0.41
2:H:69:PHE:CZ	5:H:303:LPP:H201	2.56	0.41
3:I:145:LEU:HG	3:I:149:MET:HG3	2.02	0.41
4:K:18:GLY:C	4:K:52:GLU:H	2.23	0.41
4:L:74:LYS:H	4:L:74:LYS:HG2	1.73	0.41
1:A:132:THR:OG1	1:A:133:GLN:N	2.54	0.41
1:E:51:GLY:O	1:E:110:LYS:HB2	2.21	0.41
2:G:70:ILE:HD12	2:G:70:ILE:HA	1.90	0.41
2:H:151:ARG:HA	2:H:151:ARG:HD3	1.82	0.41
4:L:16:LEU:HD22	4:L:20:LEU:HD21	2.02	0.41
1:B:60:LEU:HD11	1:B:114:ILE:HD12	2.02	0.41
1:D:12:LEU:HD23	1:D:12:LEU:HA	1.88	0.41
1:F:72:ASP:OD2	1:F:73:LEU:N	2.53	0.41
3:I:84:ARG:HA	3:I:87:PHE:CE2	2.55	0.41
3:J:149:MET:H	3:J:149:MET:HG2	1.58	0.41
4:K:16:LEU:HD22	4:K:20:LEU:HD21	2.02	0.41
1:B:14:LEU:HD23	1:B:14:LEU:HA	1.77	0.41
1:B:60:LEU:HG	1:B:114:ILE:O	2.21	0.41
1:C:19:LEU:O	1:C:22:LEU:HB3	2.21	0.41
1:D:59:THR:OG1	1:D:60:LEU:N	2.53	0.41
1:D:139:GLU:CD	1:E:102:LEU:HA	2.40	0.41
1:E:6:LEU:O	1:E:10:VAL:HG23	2.20	0.41
1:E:59:THR:HG1	1:E:60:LEU:H	1.68	0.41
1:F:15:LEU:HD11	2:G:10:ILE:HD12	2.02	0.41
2:G:151:ARG:HA	2:G:151:ARG:HD3	1.82	0.41
3:I:96:LEU:HB3	3:I:105:ASN:ND2	2.35	0.41
3:J:262:ARG:O	3:J:266:LEU:HB2	2.20	0.41
4:L:18:GLY:HA2	4:L:52:GLU:H	1.86	0.41
1:C:81:ARG:NH1	1:C:83:THR:OG1	2.53	0.41
4:K:18:GLY:HA2	4:K:52:GLU:H	1.86	0.41
4:K:98:LEU:HD13	4:K:98:LEU:HA	1.90	0.41
1:A:91:ASN:O	1:A:122:VAL:HG11	2.21	0.40
1:C:136:LEU:H	1:C:136:LEU:HD23	1.85	0.40
2:H:69:PHE:HZ	5:H:303:LPP:H201	1.86	0.40
3:J:14:LEU:O	3:J:27:ILE:HG12	2.22	0.40
3:J:75:LEU:HD23	3:J:75:LEU:HA	1.89	0.40
1:A:61:ALA:O	1:B:48:ASN:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:THR:OG1	1:D:4:ARG:N	2.52	0.40
1:E:15:LEU:HA	1:E:15:LEU:HD23	1.78	0.40
3:I:48:THR:N	6:I:301:ANP:O2B	2.55	0.40
3:I:84:ARG:HD3	3:I:87:PHE:CZ	2.56	0.40
3:I:129:LEU:HB3	3:I:135:ARG:HA	2.03	0.40
4:K:94:LEU:HA	4:K:94:LEU:HD23	1.79	0.40
1:A:143:GLY:HA2	1:A:147:LEU:HD12	2.04	0.40
1:D:98:THR:OG1	1:D:115:SER:HB3	2.21	0.40
2:H:110:LEU:HD23	2:H:110:LEU:HA	1.86	0.40
3:I:183:LEU:HD12	3:I:183:LEU:HA	1.86	0.40
3:J:89:VAL:HG22	3:J:167:LEU:HB2	2.03	0.40
3:J:129:LEU:HB3	3:J:135:ARG:HA	2.03	0.40
3:J:160:ALA:O	3:J:163:PRO:HD3	2.21	0.40
1:E:4:ARG:NH1	1:F:4:ARG:HH12	2.20	0.40
1:E:57:LYS:O	1:E:111:TYR:HB2	2.21	0.40
2:G:16:ALA:HA	2:G:19:ASP:HB2	2.03	0.40
2:H:81:ILE:CG2	2:H:82:LEU:HG	2.45	0.40
3:I:160:ALA:O	3:I:163:PRO:HD3	2.21	0.40
3:I:262:ARG:O	3:I:266:LEU:HB2	2.20	0.40
4:L:91:VAL:HG13	4:L:92:SER:N	2.33	0.40
1:B:32:SER:O	1:B:35:ASN:N	2.52	0.40
1:C:49:ILE:N	1:D:62:GLY:HA3	2.29	0.40
1:D:69:THR:HG21	1:D:85:GLU:HG2	2.04	0.40
1:E:139:GLU:OE2	1:F:136:LEU:HD22	2.21	0.40
1:F:3:THR:HG22	1:F:6:LEU:HD22	2.04	0.40
1:F:42:VAL:O	1:F:83:THR:HA	2.21	0.40
2:G:10:ILE:HD13	2:G:10:ILE:HA	1.87	0.40
2:G:35:LEU:O	2:G:36:LEU:HD23	2.22	0.40
2:G:78:GLY:HA2	2:G:81:ILE:CG2	2.49	0.40
2:H:35:LEU:O	2:H:36:LEU:HD23	2.22	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	145/157 (92%)	109 (75%)	35 (24%)	1 (1%)	22	60
1	B	144/157 (92%)	117 (81%)	27 (19%)	0	100	100
1	C	144/157 (92%)	121 (84%)	23 (16%)	0	100	100
1	D	145/157 (92%)	123 (85%)	22 (15%)	0	100	100
1	E	147/157 (94%)	122 (83%)	25 (17%)	0	100	100
1	F	143/157 (91%)	125 (87%)	18 (13%)	0	100	100
2	G	256/265 (97%)	229 (90%)	27 (10%)	0	100	100
2	H	256/265 (97%)	229 (90%)	27 (10%)	0	100	100
3	I	260/269 (97%)	228 (88%)	32 (12%)	0	100	100
3	J	260/269 (97%)	228 (88%)	32 (12%)	0	100	100
4	K	96/102 (94%)	79 (82%)	17 (18%)	0	100	100
4	L	96/102 (94%)	79 (82%)	17 (18%)	0	100	100
All	All	2092/2214 (94%)	1789 (86%)	302 (14%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	LEU

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	118/127 (93%)	116 (98%)	2 (2%)	60	78
1	B	117/127 (92%)	116 (99%)	1 (1%)	78	87
1	C	117/127 (92%)	116 (99%)	1 (1%)	78	87
1	D	118/127 (93%)	117 (99%)	1 (1%)	81	89
1	E	120/127 (94%)	119 (99%)	1 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	116/127 (91%)	116 (100%)	0	100	100
2	G	203/209 (97%)	190 (94%)	13 (6%)	17	47
2	H	203/209 (97%)	190 (94%)	13 (6%)	17	47
3	I	217/224 (97%)	204 (94%)	13 (6%)	19	49
3	J	217/224 (97%)	204 (94%)	13 (6%)	19	49
4	K	76/80 (95%)	61 (80%)	15 (20%)	1	9
4	L	76/80 (95%)	61 (80%)	15 (20%)	1	9
All	All	1698/1788 (95%)	1610 (95%)	88 (5%)	27	53

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ARG
1	A	75	ARG
1	B	75	ARG
1	C	75	ARG
1	D	75	ARG
1	E	75	ARG
2	G	18	LEU
2	G	19	ASP
2	G	29	LEU
2	G	38	ARG
2	G	81	ILE
2	G	84	SER
2	G	102	GLU
2	G	134	SER
2	G	167	SER
2	G	176	MET
2	G	200	THR
2	G	201	GLU
2	G	260	LEU
2	H	18	LEU
2	H	19	ASP
2	H	29	LEU
2	H	38	ARG
2	H	81	ILE
2	H	84	SER
2	H	102	GLU
2	H	134	SER
2	H	167	SER

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Mol	Chain	Res	Type
2	H	176	MET
2	H	200	THR
2	H	201	GLU
2	H	260	LEU
3	I	20	SER
3	I	28	ASP
3	I	29	VAL
3	I	51	LEU
3	I	62	LYS
3	I	72	LEU
3	I	134	LEU
3	I	139	GLU
3	I	144	GLU
3	I	222	ARG
3	I	228	THR
3	I	232	LEU
3	I	265	LEU
3	J	20	SER
3	J	28	ASP
3	J	29	VAL
3	J	51	LEU
3	J	62	LYS
3	J	72	LEU
3	J	134	LEU
3	J	139	GLU
3	J	144	GLU
3	J	222	ARG
3	J	228	THR
3	J	232	LEU
3	J	265	LEU
4	K	19	VAL
4	K	30	GLU
4	K	37	ARG
4	K	44	LEU
4	K	47	ASP
4	K	49	SER
4	K	52	GLU
4	K	59	ILE
4	K	60	SER
4	K	61	LEU
4	K	75	VAL
4	K	77	SER

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Mol	Chain	Res	Type
4	K	83	ASP
4	K	85	MET
4	K	95	LEU
4	L	19	VAL
4	L	30	GLU
4	L	37	ARG
4	L	44	LEU
4	L	47	ASP
4	L	49	SER
4	L	52	GLU
4	L	59	ILE
4	L	60	SER
4	L	61	LEU
4	L	75	VAL
4	L	77	SER
4	L	83	ASP
4	L	85	MET
4	L	95	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	88	GLN
1	A	133	GLN
1	D	148	ASN
1	E	35	ASN
1	E	87	ASN
1	F	87	ASN
1	F	133	GLN
2	G	77	GLN
2	G	93	GLN
2	G	195	ASN
2	G	224	GLN
2	H	77	GLN
2	H	93	GLN
2	H	195	ASN
2	H	224	GLN
3	I	26	ASN
3	I	86	GLN
3	I	105	ASN
3	I	113	HIS

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Mol	Chain	Res	Type
3	I	255	HIS
3	J	26	ASN
3	J	86	GLN
3	J	105	ASN
3	J	113	HIS
3	J	130	GLN
3	J	255	HIS
4	K	3	GLN
4	L	3	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	$\# Z > 2$
6	ANP	J	301	-	29,33,33	1.13	4 (13%)	31,52,52	1.19	4 (12%)
5	LPP	H	302	-	43,43,43	0.89	4 (9%)	47,48,48	1.04	2 (4%)
5	LPP	H	303	-	43,43,43	0.90	4 (9%)	47,48,48	0.93	2 (4%)
6	ANP	I	301	-	29,33,33	1.13	4 (13%)	31,52,52	1.19	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	LPP	G	302	-	43,43,43	0.90	3 (6%)	47,48,48	1.04	2 (4%)
5	LPP	G	304	-	43,43,43	0.90	2 (4%)	47,48,48	1.10	2 (4%)
5	LPP	H	301	-	43,43,43	0.91	4 (9%)	47,48,48	1.01	2 (4%)
5	LPP	G	301	-	43,43,43	0.92	4 (9%)	47,48,48	0.99	2 (4%)
5	LPP	G	303	-	43,43,43	0.89	4 (9%)	47,48,48	0.97	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ANP	J	301	-	-	4/14/38/38	0/3/3/3
5	LPP	H	302	-	-	21/45/45/45	-
5	LPP	H	303	-	-	25/45/45/45	-
6	ANP	I	301	-	-	4/14/38/38	0/3/3/3
5	LPP	G	302	-	-	30/45/45/45	-
5	LPP	G	304	-	-	27/45/45/45	-
5	LPP	H	301	-	-	27/45/45/45	-
5	LPP	G	301	-	-	31/45/45/45	-
5	LPP	G	303	-	-	26/45/45/45	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	301	ANP	PB-O3A	-2.77	1.55	1.59
6	J	301	ANP	PB-O3A	-2.77	1.55	1.59
6	J	301	ANP	PB-O1B	2.74	1.50	1.46
6	I	301	ANP	PB-O1B	2.71	1.50	1.46
5	G	302	LPP	O9-C7	-2.65	1.40	1.46
5	G	304	LPP	O27-C29	2.60	1.40	1.33
5	G	301	LPP	O27-C29	2.58	1.40	1.33
5	G	301	LPP	O9-C7	-2.51	1.40	1.46
5	G	304	LPP	O9-C11	2.50	1.41	1.34
5	H	303	LPP	O9-C7	-2.49	1.40	1.46
5	H	302	LPP	O9-C7	-2.49	1.40	1.46
5	H	303	LPP	O27-C29	2.41	1.40	1.33
5	G	303	LPP	O9-C7	-2.41	1.40	1.46
5	G	302	LPP	O27-C8	-2.37	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	301	LPP	O27-C8	-2.35	1.39	1.45
6	I	301	ANP	PG-N3B	2.35	1.69	1.63
5	H	302	LPP	O27-C29	2.34	1.40	1.33
5	H	301	LPP	O9-C11	2.34	1.40	1.34
6	J	301	ANP	PG-N3B	2.30	1.69	1.63
5	G	303	LPP	O27-C8	-2.29	1.39	1.45
5	G	302	LPP	O27-C29	2.28	1.40	1.33
5	H	303	LPP	O27-C8	-2.24	1.40	1.45
5	G	301	LPP	O9-C11	2.21	1.40	1.34
5	G	303	LPP	O9-C11	2.20	1.40	1.34
5	H	301	LPP	O27-C29	2.17	1.39	1.33
5	H	302	LPP	O27-C8	-2.15	1.40	1.45
5	G	303	LPP	O27-C29	2.14	1.39	1.33
5	H	301	LPP	O9-C7	-2.14	1.41	1.46
5	H	302	LPP	O9-C11	2.10	1.40	1.34
5	H	303	LPP	O9-C11	2.10	1.40	1.34
6	J	301	ANP	PG-O1G	2.04	1.49	1.46
5	G	301	LPP	O27-C8	-2.04	1.40	1.45
6	I	301	ANP	PG-O1G	2.04	1.49	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	304	LPP	O9-C11-C12	5.30	122.93	111.50
5	H	301	LPP	O9-C11-C12	4.48	121.16	111.50
5	H	302	LPP	O9-C11-C12	4.40	120.98	111.50
5	G	301	LPP	O9-C11-C12	4.37	120.92	111.50
5	G	302	LPP	O9-C11-C12	4.23	120.63	111.50
5	G	303	LPP	O9-C11-C12	4.20	120.54	111.50
5	H	303	LPP	O9-C11-C12	4.13	120.40	111.50
6	J	301	ANP	PB-O3A-PA	-3.58	120.00	132.62
6	I	301	ANP	PB-O3A-PA	-3.58	120.02	132.62
5	G	301	LPP	O27-C29-C30	2.96	121.19	111.91
5	H	302	LPP	O27-C29-C30	2.92	121.08	111.91
5	G	302	LPP	O27-C29-C30	2.88	120.94	111.91
5	G	304	LPP	O27-C29-C30	2.74	120.51	111.91
5	H	301	LPP	O27-C29-C30	2.55	119.90	111.91
5	H	303	LPP	O27-C29-C30	2.53	119.84	111.91
5	G	303	LPP	O27-C29-C30	2.51	119.78	111.91
6	J	301	ANP	O3G-PG-O1G	-2.51	107.15	113.45
6	I	301	ANP	O3G-PG-O1G	-2.49	107.19	113.45
6	I	301	ANP	C5-C6-N6	2.12	123.57	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	301	ANP	O2B-PB-O3A	2.11	111.70	104.64
6	I	301	ANP	O2B-PB-O3A	2.11	111.69	104.64
6	J	301	ANP	C5-C6-N6	2.09	123.53	120.35

There are no chirality outliers.

All (195) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	301	LPP	C6-O5-P1-O2
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-O3
5	H	301	LPP	C6-O5-P1-O2
5	H	301	LPP	C6-O5-P1-O3
5	H	301	LPP	C6-O5-P1-O4
5	H	302	LPP	C6-O5-P1-O2
5	H	303	LPP	C6-O5-P1-O2
5	H	303	LPP	C6-O5-P1-O4
5	H	303	LPP	C12-C11-O9-C7
5	H	303	LPP	C30-C29-O27-C8
6	I	301	ANP	PB-N3B-PG-O1G
6	I	301	ANP	PG-N3B-PB-O1B
6	I	301	ANP	O4'-C4'-C5'-O5'
6	J	301	ANP	PB-N3B-PG-O1G
6	J	301	ANP	PG-N3B-PB-O1B
6	J	301	ANP	O4'-C4'-C5'-O5'
5	H	303	LPP	O28-C29-O27-C8
5	G	301	LPP	O10-C11-O9-C7
5	H	303	LPP	O10-C11-O9-C7
5	G	303	LPP	O28-C29-O27-C8
5	G	303	LPP	C40-C41-C42-C43
5	G	301	LPP	C12-C13-C14-C15
6	I	301	ANP	C3'-C4'-C5'-O5'
6	J	301	ANP	C3'-C4'-C5'-O5'
5	G	303	LPP	C30-C29-O27-C8
5	G	301	LPP	C30-C29-O27-C8
5	H	301	LPP	C30-C29-O27-C8
5	G	302	LPP	O9-C7-C8-O27
5	H	301	LPP	O28-C29-O27-C8
5	H	303	LPP	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
5	G	301	LPP	O28-C29-O27-C8
5	G	303	LPP	C29-C30-C31-C32
5	G	304	LPP	C29-C30-C31-C32
5	G	304	LPP	C20-C21-C22-C23
5	H	301	LPP	C12-C11-O9-C7
5	G	304	LPP	C37-C38-C39-C40
5	G	304	LPP	C30-C29-O27-C8
5	H	301	LPP	O10-C11-O9-C7
5	H	302	LPP	C34-C35-C36-C37
5	H	303	LPP	C17-C18-C19-C20
5	G	302	LPP	C32-C33-C34-C35
5	H	303	LPP	C34-C35-C36-C37
5	G	301	LPP	C33-C34-C35-C36
5	G	301	LPP	C38-C39-C40-C41
5	H	302	LPP	C22-C23-C24-C25
5	H	302	LPP	C38-C39-C40-C41
5	G	304	LPP	C34-C35-C36-C37
5	G	301	LPP	C31-C32-C33-C34
5	H	301	LPP	C33-C34-C35-C36
5	H	303	LPP	C32-C33-C34-C35
5	G	304	LPP	C16-C17-C18-C19
5	G	304	LPP	C21-C22-C23-C24
5	G	304	LPP	C31-C32-C33-C34
5	G	302	LPP	C13-C14-C15-C16
5	G	302	LPP	C38-C39-C40-C41
5	G	303	LPP	C33-C34-C35-C36
5	G	302	LPP	C29-C30-C31-C32
5	G	303	LPP	C37-C38-C39-C40
5	G	304	LPP	C17-C18-C19-C20
5	H	302	LPP	C35-C36-C37-C38
5	G	302	LPP	C34-C35-C36-C37
5	G	304	LPP	C33-C34-C35-C36
5	G	302	LPP	C21-C22-C23-C24
5	G	303	LPP	C22-C23-C24-C25
5	G	304	LPP	C22-C23-C24-C25
5	H	301	LPP	C38-C39-C40-C41
5	G	301	LPP	C34-C35-C36-C37
5	G	301	LPP	C37-C38-C39-C40
5	H	302	LPP	C15-C16-C17-C18
5	H	303	LPP	C16-C17-C18-C19
5	G	304	LPP	O28-C29-O27-C8
5	H	302	LPP	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
5	H	302	LPP	C30-C31-C32-C33
5	G	303	LPP	C21-C22-C23-C24
5	G	304	LPP	C39-C40-C41-C42
5	G	302	LPP	C17-C18-C19-C20
5	H	302	LPP	C32-C33-C34-C35
5	G	302	LPP	C40-C41-C42-C43
5	G	304	LPP	C40-C41-C42-C43
5	G	303	LPP	C36-C37-C38-C39
5	G	303	LPP	C16-C17-C18-C19
5	G	303	LPP	C19-C20-C21-C22
5	G	304	LPP	C32-C33-C34-C35
5	G	301	LPP	C29-C30-C31-C32
5	G	304	LPP	C11-C12-C13-C14
5	H	301	LPP	C31-C32-C33-C34
5	G	302	LPP	C30-C29-O27-C8
5	G	301	LPP	C22-C23-C24-C25
5	G	303	LPP	C11-C12-C13-C14
5	G	304	LPP	C36-C37-C38-C39
5	G	301	LPP	C15-C16-C17-C18
5	H	301	LPP	C30-C31-C32-C33
5	G	302	LPP	C20-C21-C22-C23
5	G	303	LPP	C15-C16-C17-C18
5	G	304	LPP	C30-C31-C32-C33
5	H	302	LPP	C40-C41-C42-C43
5	G	302	LPP	O28-C29-O27-C8
5	H	303	LPP	C38-C39-C40-C41
5	G	302	LPP	C22-C23-C24-C25
5	G	304	LPP	C38-C39-C40-C41
5	G	302	LPP	C11-C12-C13-C14
5	H	303	LPP	C22-C23-C24-C25
5	G	303	LPP	C31-C32-C33-C34
5	G	302	LPP	C31-C32-C33-C34
5	G	304	LPP	C23-C24-C25-C26
5	G	301	LPP	C6-C7-C8-O27
5	G	304	LPP	C6-C7-C8-O27
5	G	303	LPP	C12-C13-C14-C15
5	H	303	LPP	C41-C42-C43-C44
5	G	303	LPP	C41-C42-C43-C44
5	H	302	LPP	C29-C30-C31-C32
5	G	301	LPP	C6-O5-P1-O3
5	H	302	LPP	C6-O5-P1-O3
5	H	303	LPP	C6-O5-P1-O3

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Mol	Chain	Res	Type	Atoms
5	H	303	LPP	O5-C6-C7-O9
5	G	301	LPP	C41-C42-C43-C44
5	H	301	LPP	C17-C18-C19-C20
5	H	301	LPP	C19-C20-C21-C22
5	H	301	LPP	C34-C35-C36-C37
5	G	304	LPP	C41-C42-C43-C44
5	H	302	LPP	C17-C18-C19-C20
5	G	303	LPP	C30-C31-C32-C33
5	G	302	LPP	C35-C36-C37-C38
5	G	301	LPP	C16-C17-C18-C19
5	G	301	LPP	C23-C24-C25-C26
5	H	301	LPP	C12-C13-C14-C15
5	H	303	LPP	C21-C22-C23-C24
5	G	302	LPP	C6-C7-C8-O27
5	G	301	LPP	C19-C20-C21-C22
5	G	304	LPP	O5-C6-C7-O9
5	G	301	LPP	O9-C7-C8-O27
5	G	301	LPP	C32-C33-C34-C35
5	H	302	LPP	C6-O5-P1-O4
5	G	303	LPP	C38-C39-C40-C41
5	G	302	LPP	O5-C6-C7-O9
5	G	304	LPP	O9-C7-C8-O27
5	G	303	LPP	C20-C21-C22-C23
5	H	301	LPP	C20-C21-C22-C23
5	H	301	LPP	C23-C24-C25-C26
5	H	301	LPP	C22-C23-C24-C25
5	G	303	LPP	C17-C18-C19-C20
5	G	302	LPP	O5-C6-C7-C8
5	H	303	LPP	O5-C6-C7-C8
5	H	301	LPP	O5-C6-C7-O9
5	H	301	LPP	C29-C30-C31-C32
5	G	302	LPP	C12-C11-O9-C7
5	G	301	LPP	C39-C40-C41-C42
5	G	304	LPP	C7-C6-O5-P1
5	G	301	LPP	C21-C22-C23-C24
5	G	304	LPP	C13-C14-C15-C16
5	H	301	LPP	C8-C7-O9-C11
5	G	301	LPP	C36-C37-C38-C39
5	G	302	LPP	C6-O5-P1-O3
5	G	303	LPP	C35-C36-C37-C38
5	G	302	LPP	C33-C34-C35-C36
5	H	301	LPP	C41-C42-C43-C44

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

There are no ring outliers.

9 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	301	ANP	4	0
5	H	302	LPP	19	0

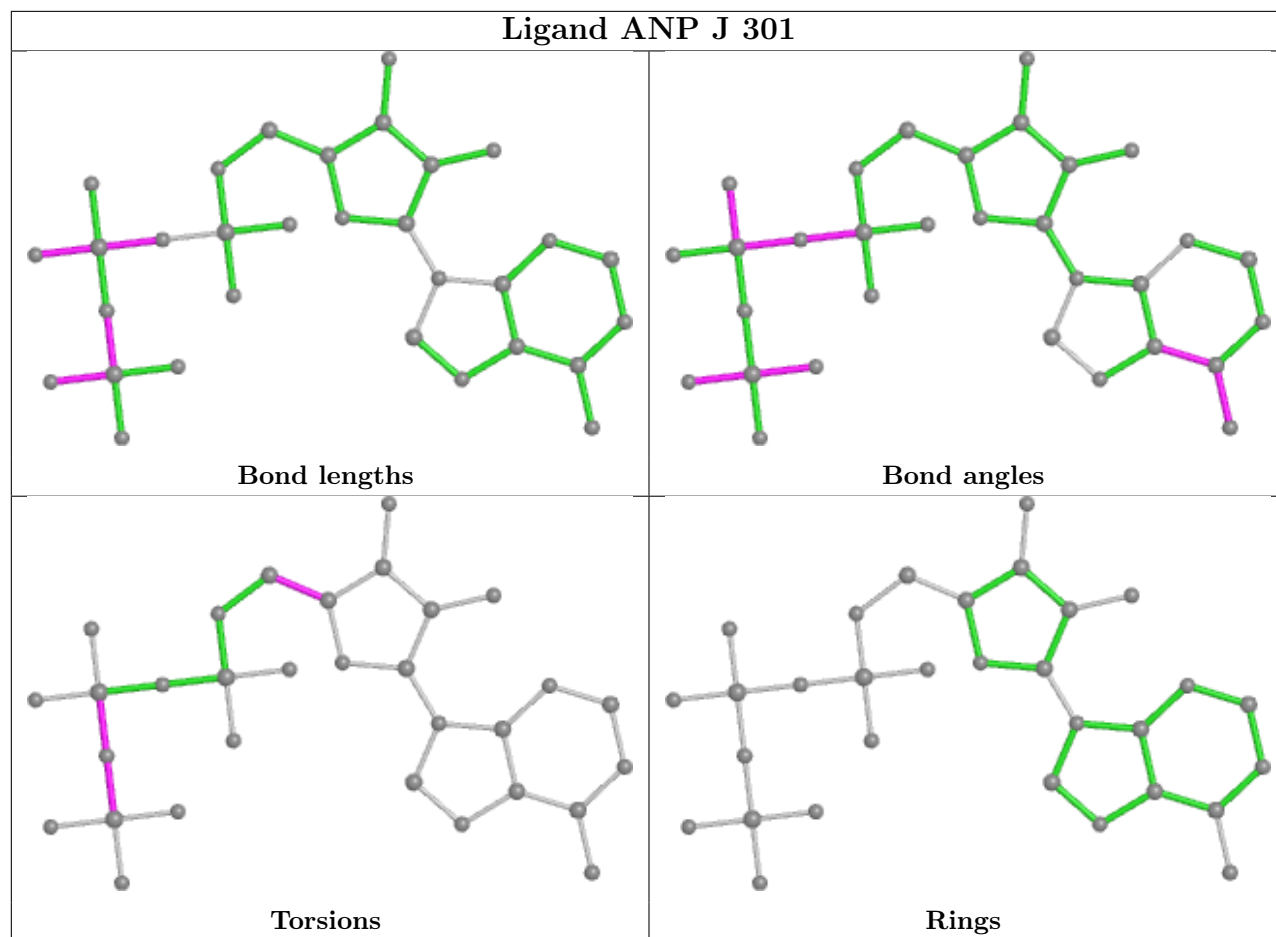
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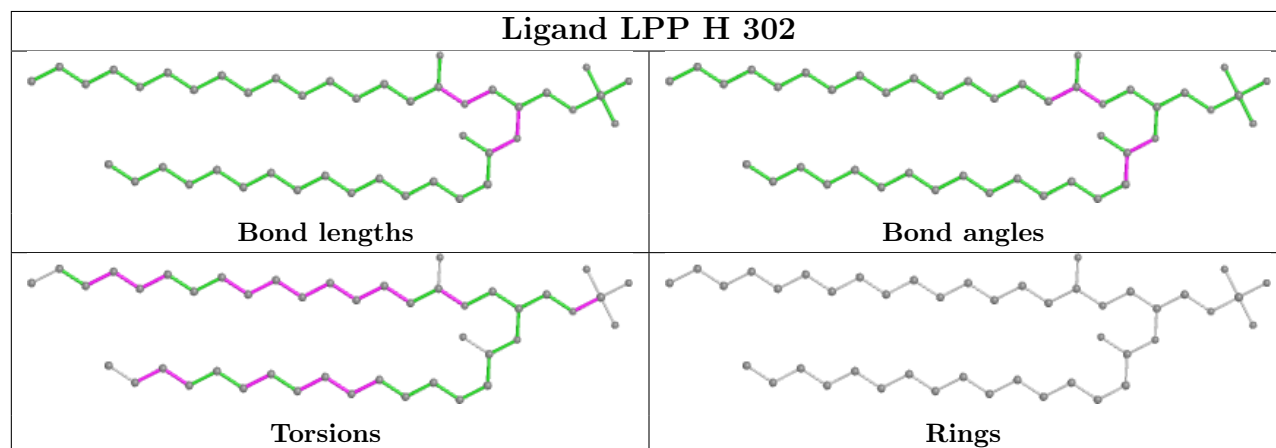
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	303	LPP	4	0
6	I	301	ANP	5	0
5	G	302	LPP	5	0
5	G	304	LPP	8	0
5	H	301	LPP	4	0
5	G	301	LPP	4	0
5	G	303	LPP	4	0

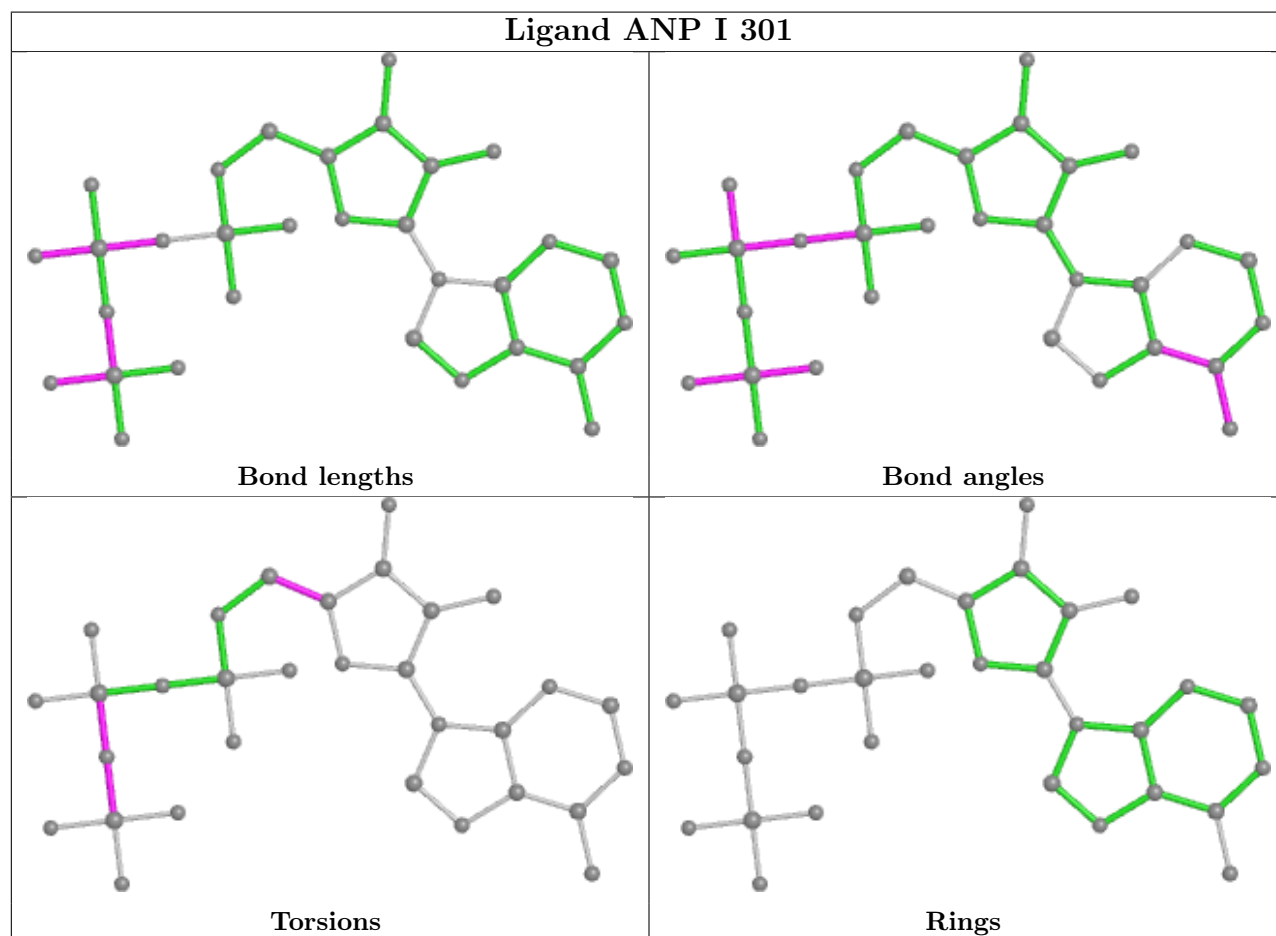
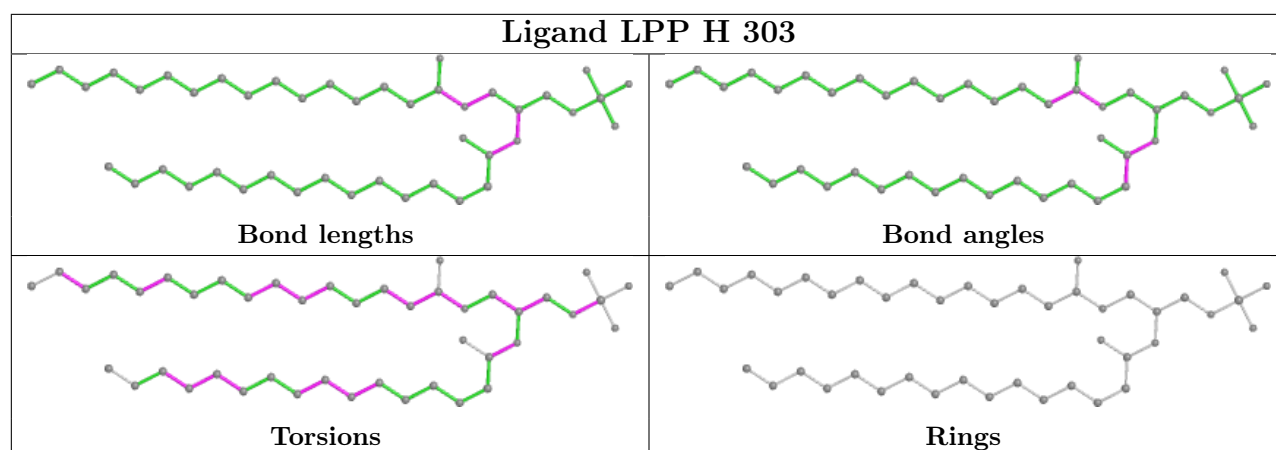
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

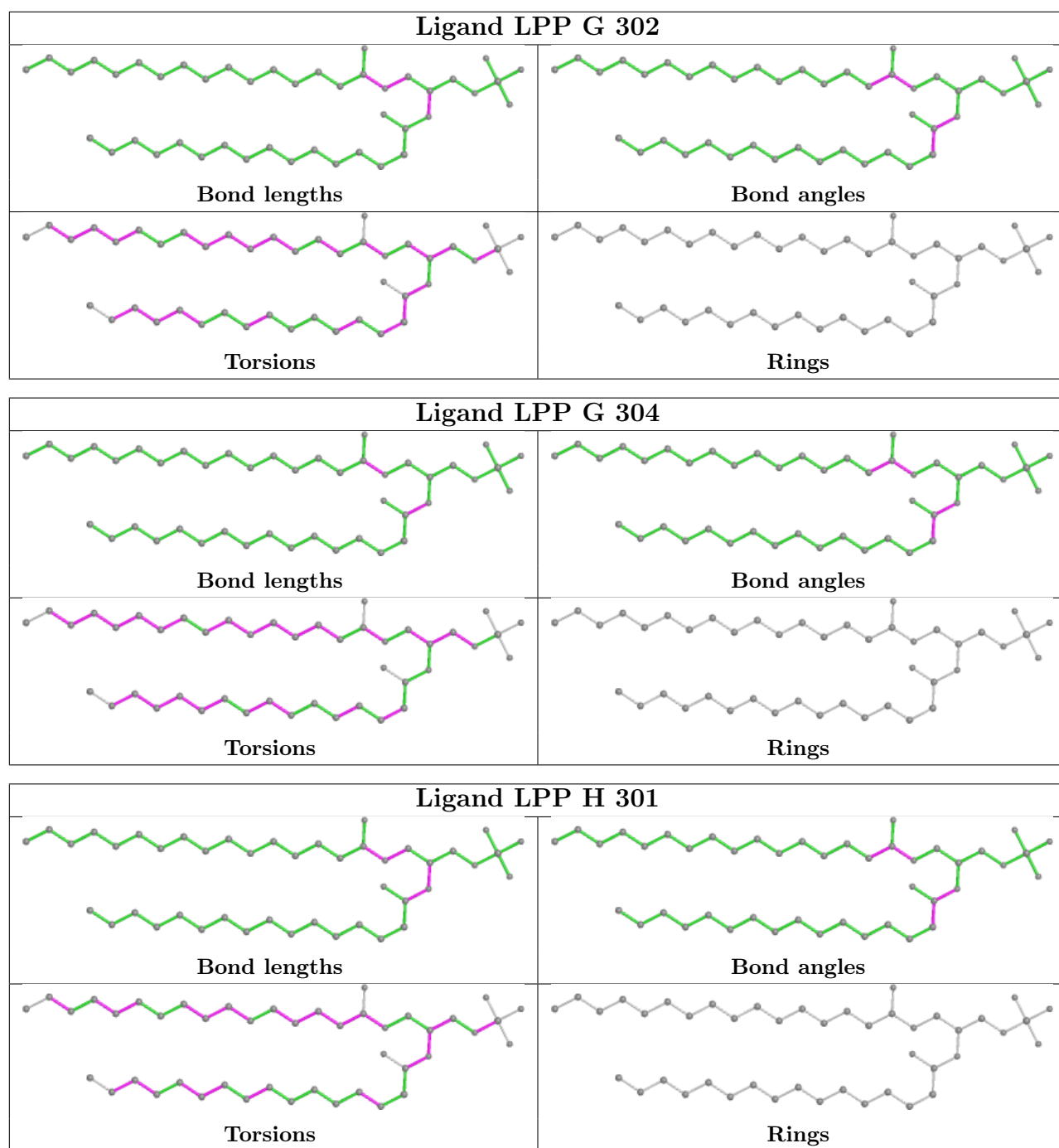
Ligand ANP J 301

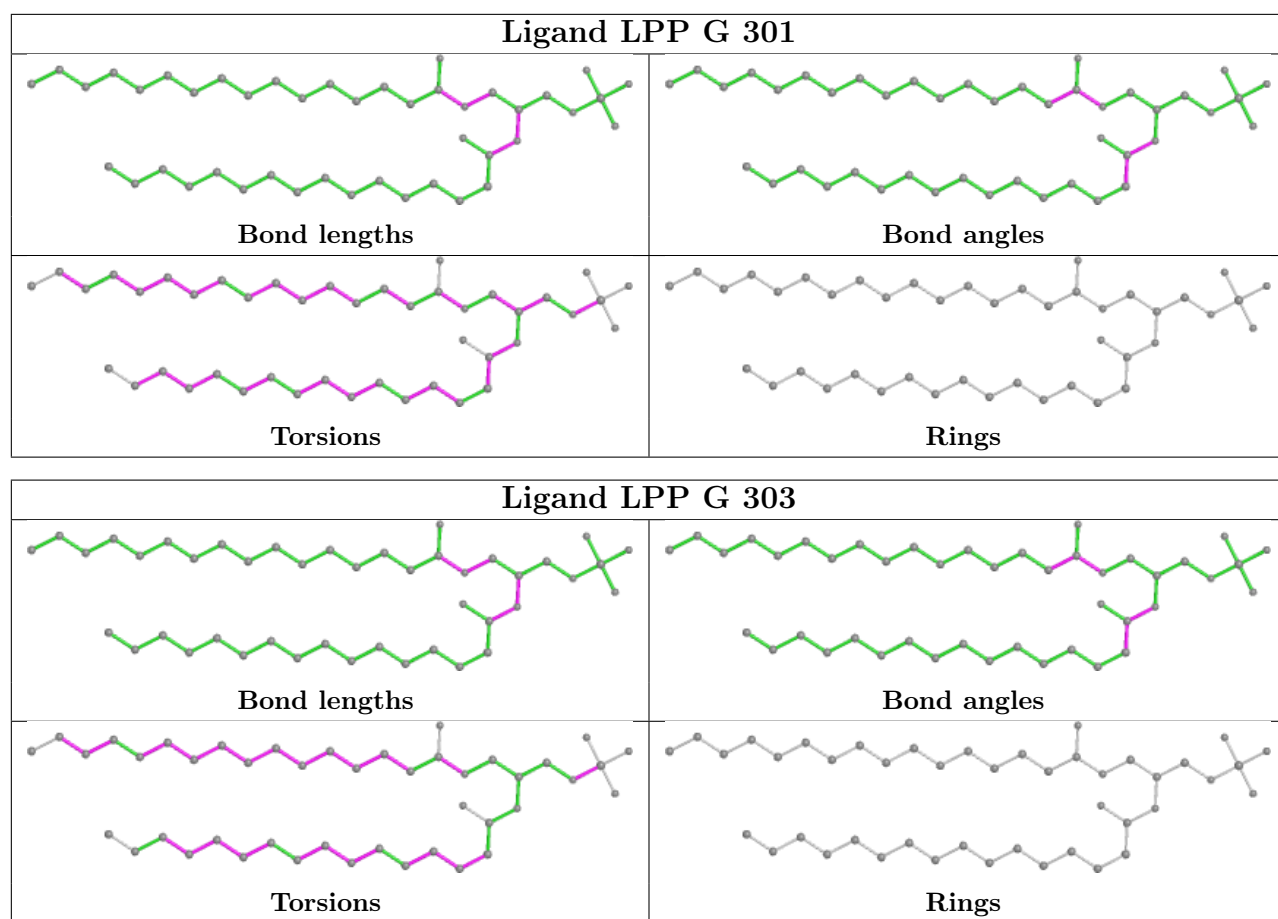


Ligand LPP H 302









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.

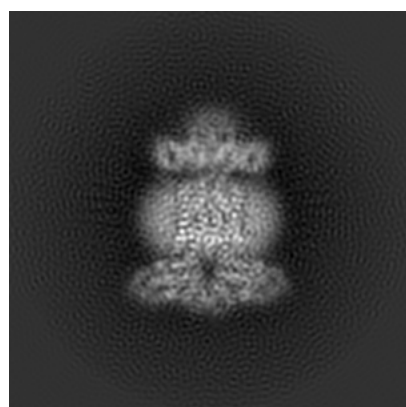
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30373. These allow visual inspection of the internal detail of the map and identification of artifacts.

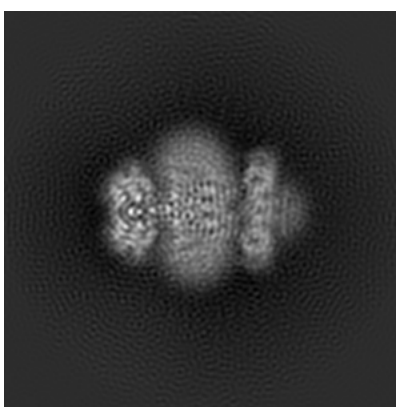
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

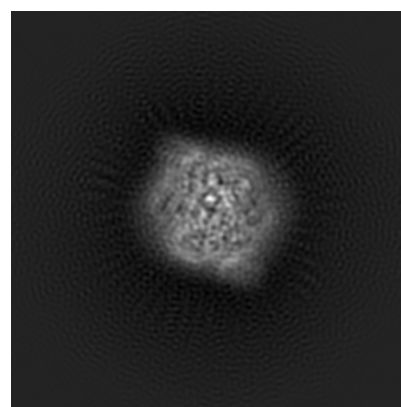
6.1.1 Primary map



X



Y

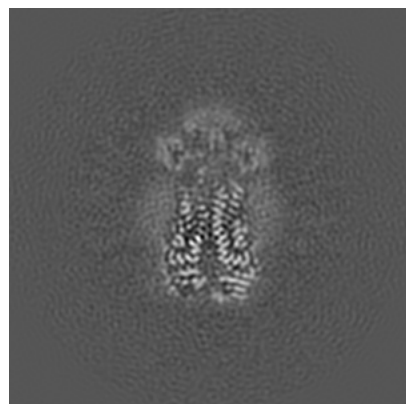


Z

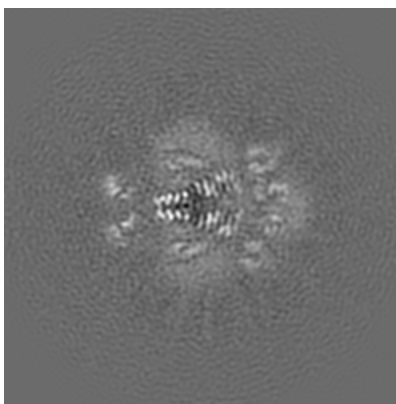
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

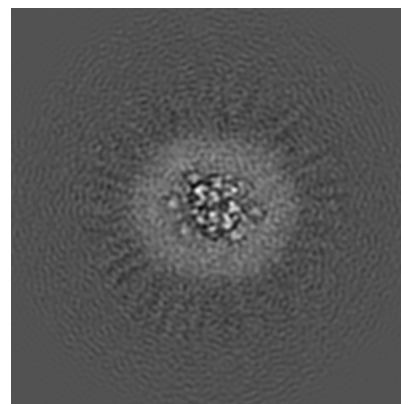
6.2.1 Primary map



X Index: 128



Y Index: 128

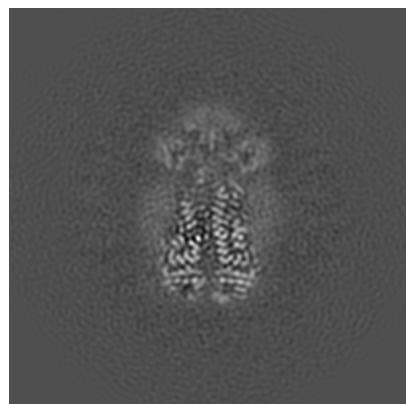


Z Index: 128

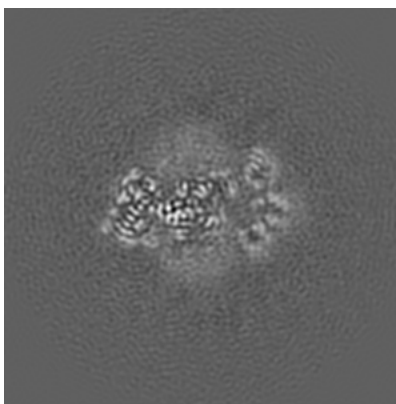
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

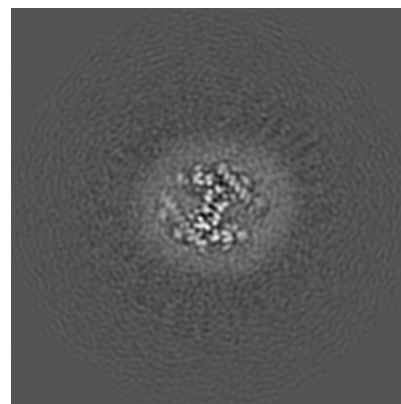
6.3.1 Primary map



X Index: 127



Y Index: 117



Z Index: 110

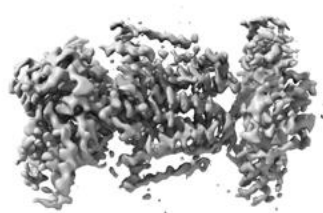
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

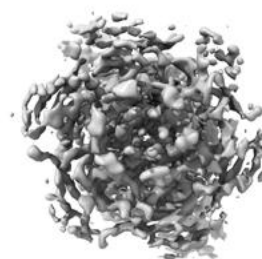
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0299. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

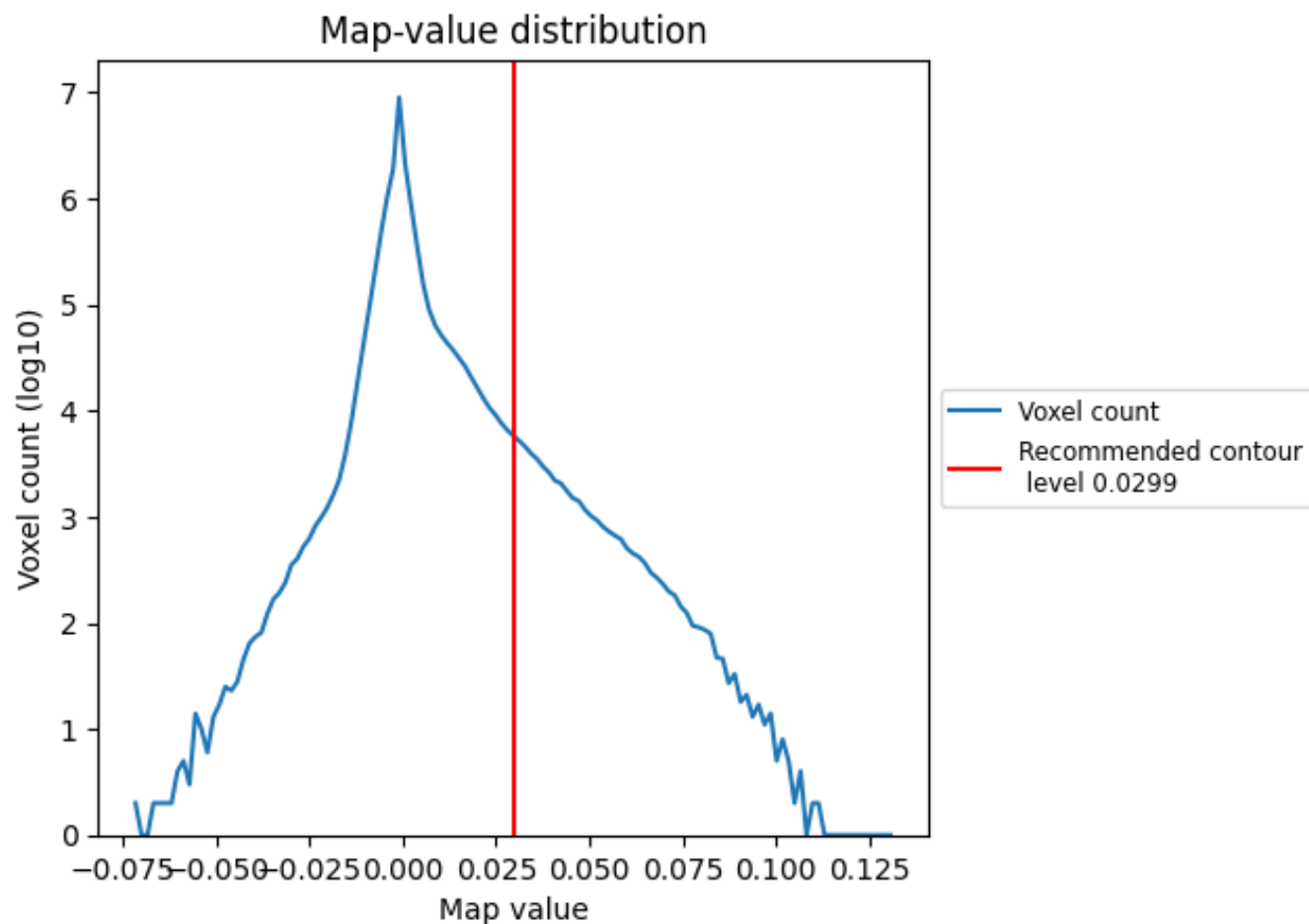
6.5 Mask visualisation

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

7 Map analysis [i](#)

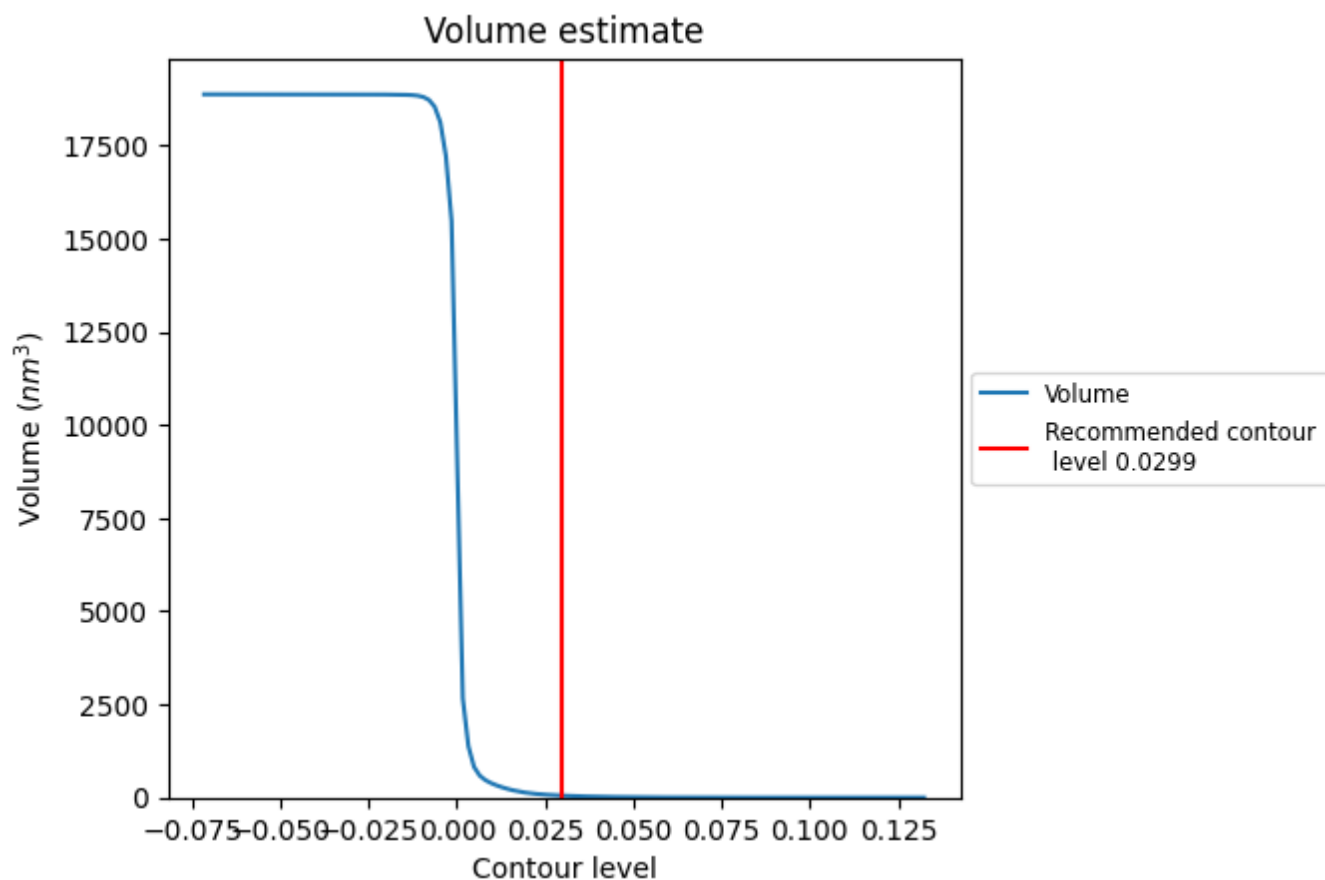
This section contains the results of statistical analysis of the map.

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.

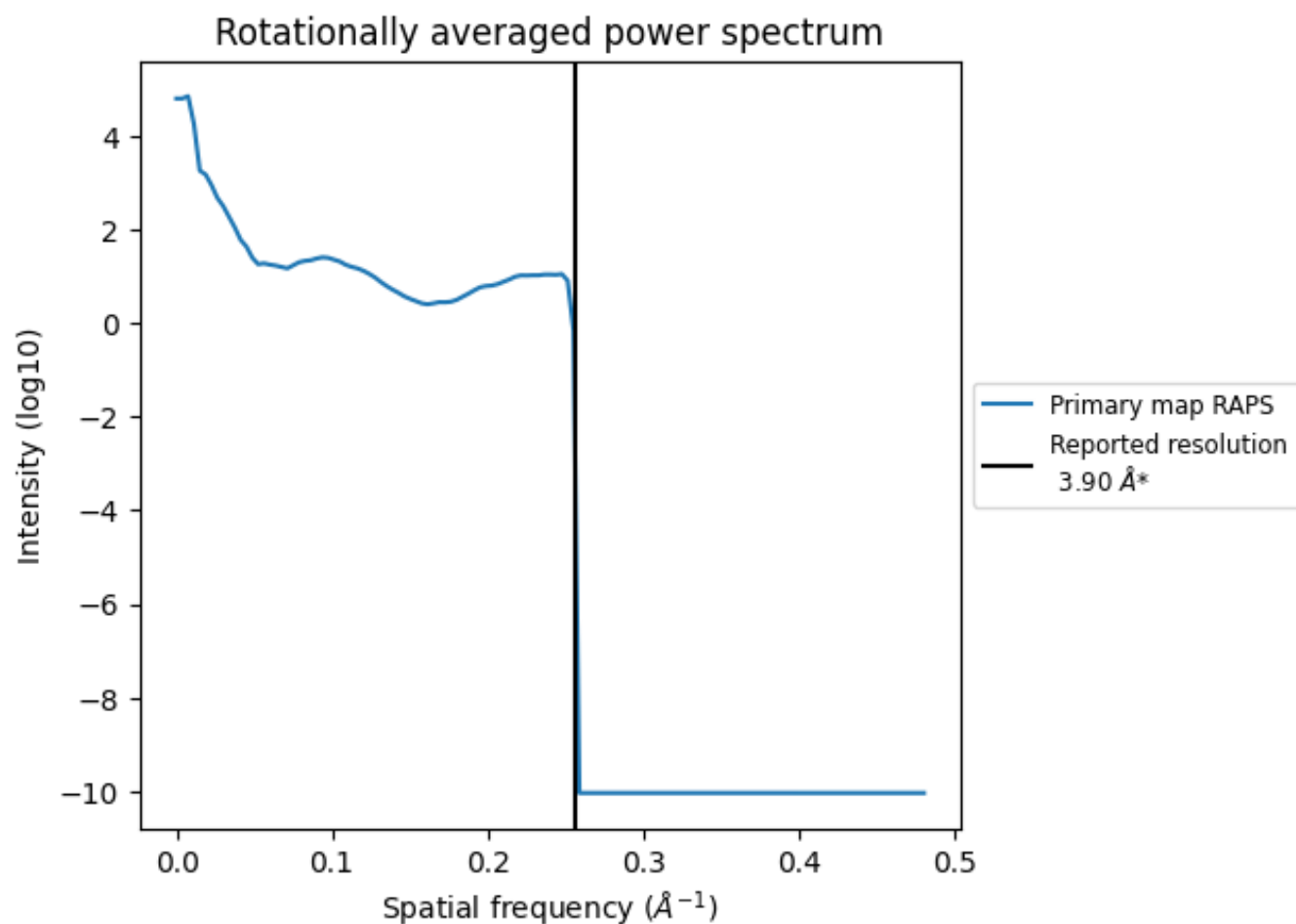
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 52 nm³; this corresponds to an approximate mass of 47 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 ⓘ

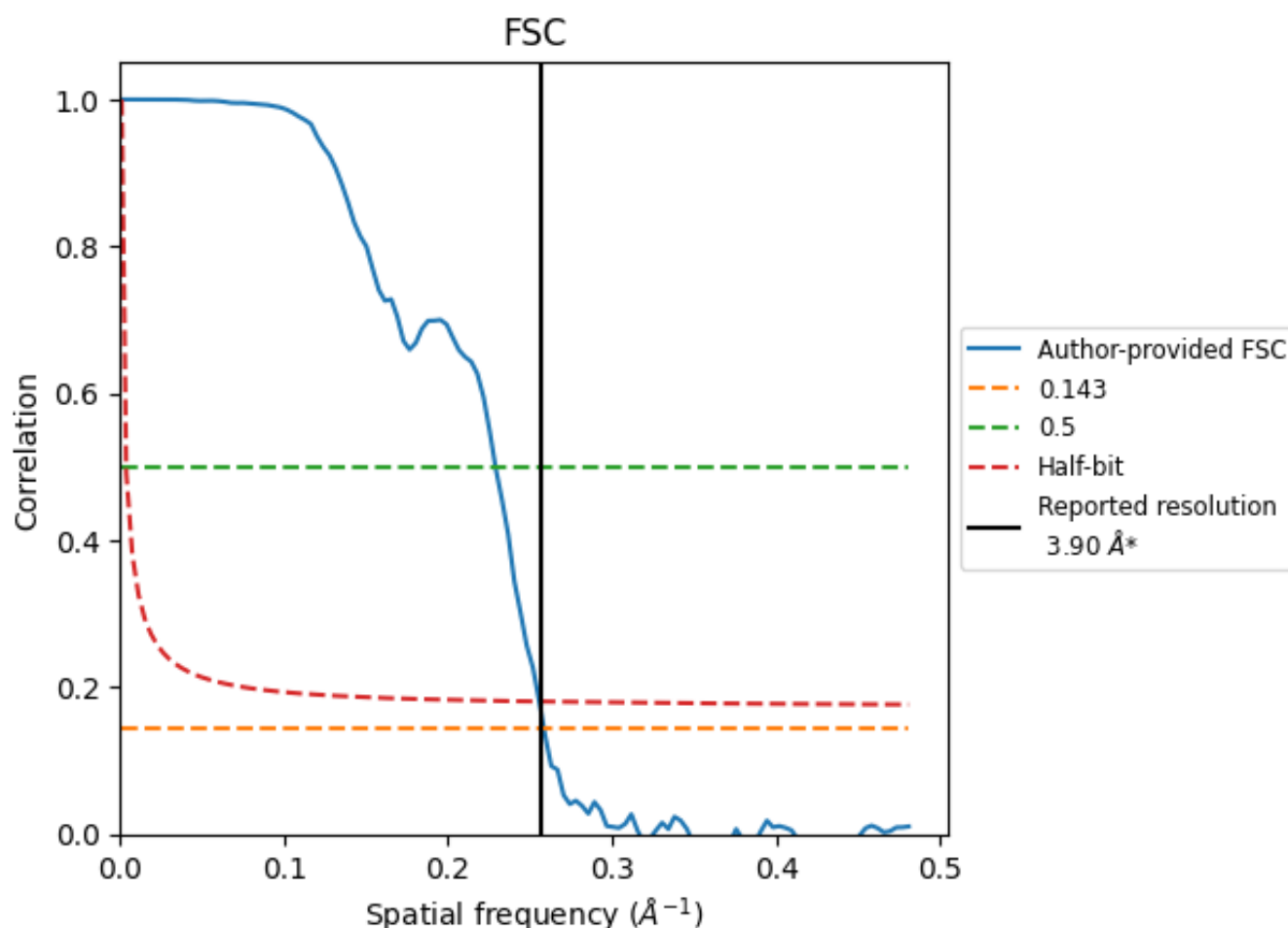


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 \AA^{-1}

8.2 Resolution estimates [i](#)

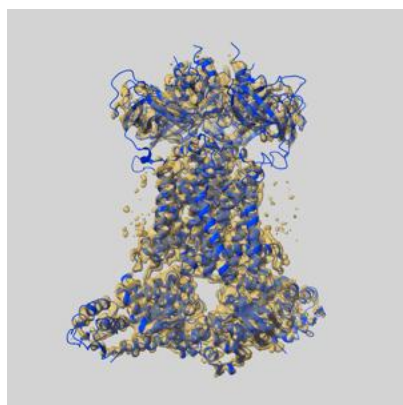
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.87	4.37	3.91
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

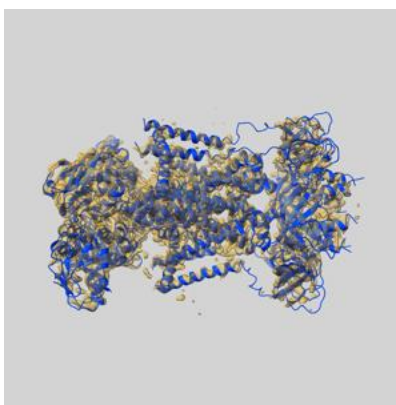
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30373 and PDB model 7CHA. Per-residue inclusion information can be found in section [3](#) on page [7](#).

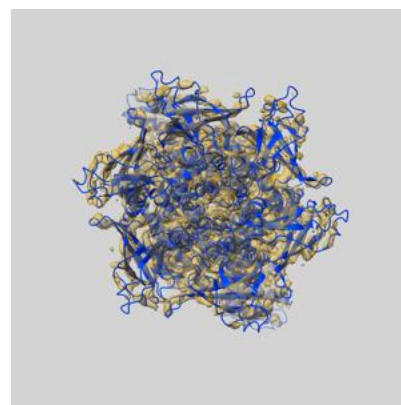
9.1 Map-model overlay [i](#)



X



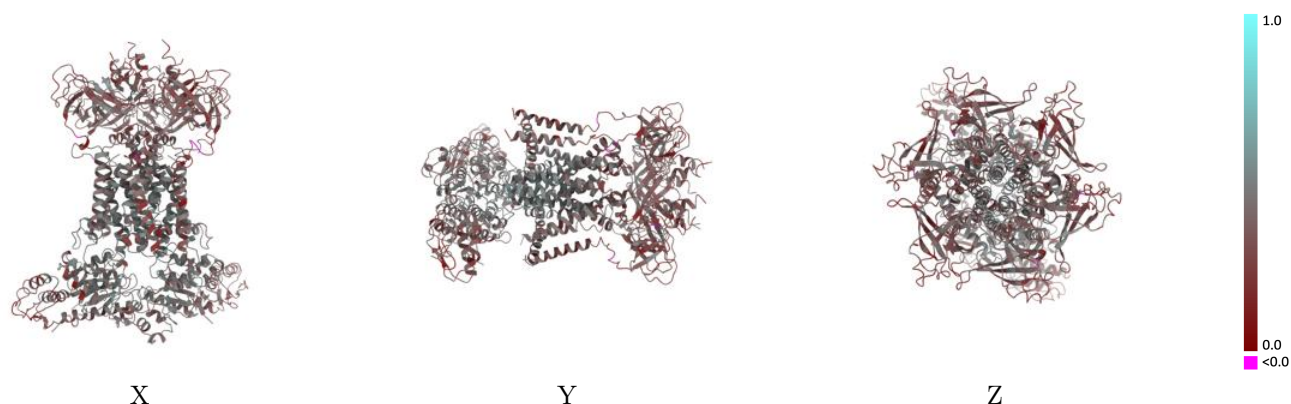
Y



Z

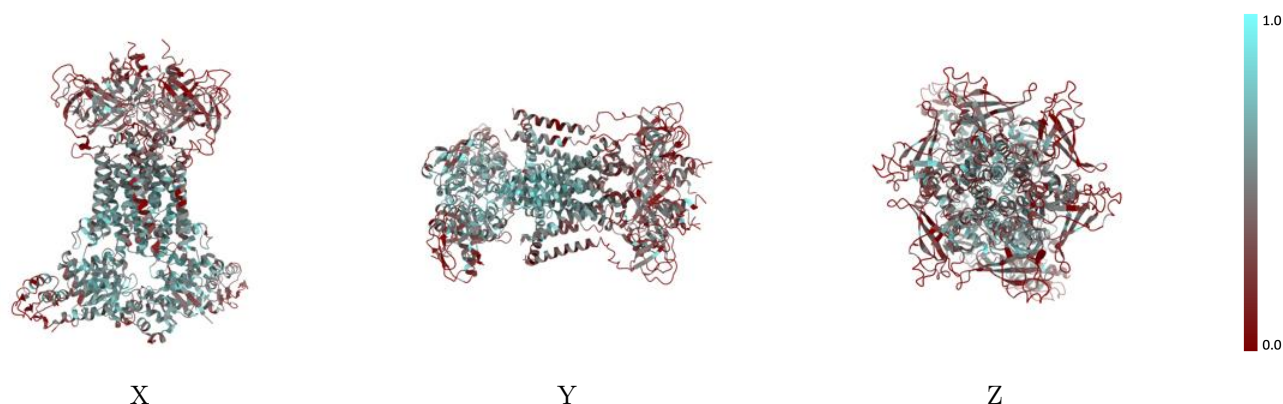
The images above show the 3D surface view of the map at the recommended contour level 0.0299 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



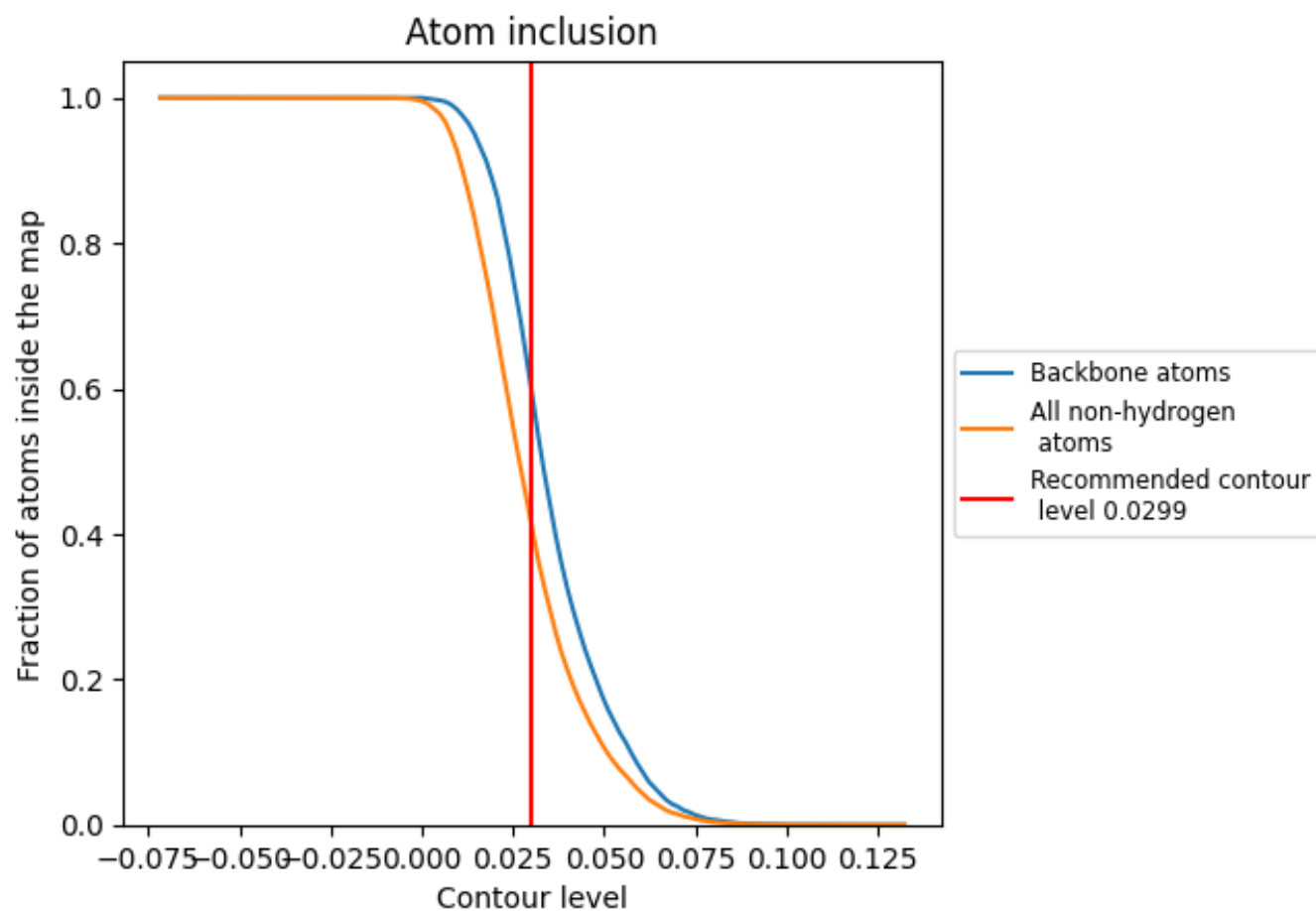
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0299).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 42% 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 (0.0299) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4166	<div></div> 0.3860
A	<div></div> 0.2692	<div></div> 0.3200
B	<div></div> 0.3261	<div></div> 0.3580
C	<div></div> 0.2582	<div></div> 0.3100
D	<div></div> 0.2802	<div></div> 0.3430
E	<div></div> 0.2207	<div></div> 0.3200
F	<div></div> 0.2707	<div></div> 0.3420
G	<div></div> 0.5322	<div></div> 0.4400
H	<div></div> 0.5457	<div></div> 0.4450
I	<div></div> 0.5632	<div></div> 0.4380
J	<div></div> 0.5607	<div></div> 0.4320
K	<div></div> 0.3134	<div></div> 0.3210
L	<div></div> 0.2991	<div></div> 0.3310

