



Full wwPDB EM Validation Report ⓘ

Mar 20, 2024 – 06:37 AM JST

PDB ID : 7BTE
EMDB ID : EMD-30177
Title : Lifeact-F-actin complex
Authors : Kumari, A.; Ragunath, V.K.; Sirajuddin, M.
Deposited on : 2020-04-01
Resolution : 4.20 Å (reported)
Based on initial model : 5ONV

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:

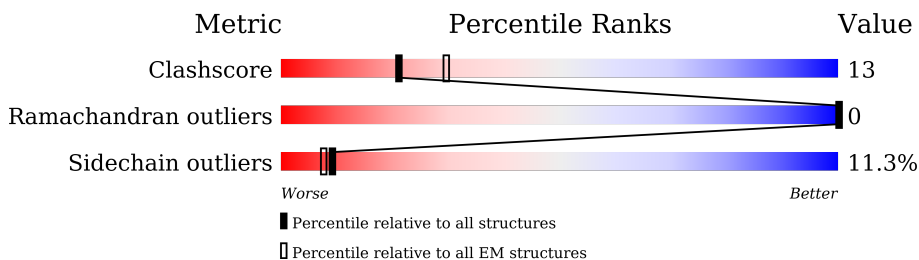
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 4.20 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	377	65% (green), 29% (yellow), 2% (orange), 2% (grey)
1	C	377	64% (green), 29% (yellow), 2% (orange), 2% (grey)
1	E	377	63% (green), 32% (yellow), 2% (orange), 2% (grey)
1	G	377	65% (green), 30% (yellow), 2% (orange), 2% (grey)
1	I	377	68% (green), 27% (yellow), 2% (orange), 2% (grey)
2	L	17	12% (red), 29% (green), 24% (yellow), 29% (orange), 18% (grey)
2	M	17	12% (red), 24% (green), 41% (yellow), 24% (orange), 12% (grey)
2	N	17	53% (green), 29% (yellow), 6% (orange), 12% (grey)

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14814 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	370	2865	1816	487	541	21	0	0
1	C	370	2873	1819	487	546	21	0	0
1	E	370	2876	1821	487	547	21	0	0
1	G	370	2867	1817	487	542	21	0	0
1	I	370	2870	1815	487	547	21	0	0

- Molecule 2 is a protein called Lifeact.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	L	14	102	67	16	18	1	0	0
2	M	15	111	73	18	19	1	0	0
2	N	15	110	73	18	18	1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

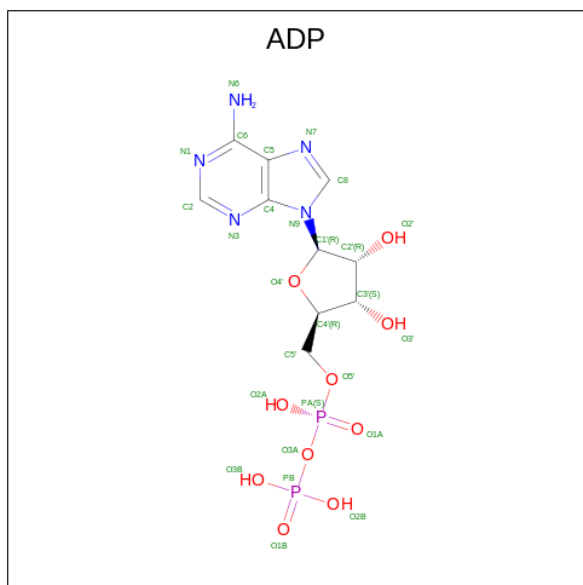
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mg	0
			1	1	
3	C	1	Total	Mg	0
			1	1	
3	E	1	Total	Mg	0
			1	1	
3	G	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
3	I	1	1	1	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

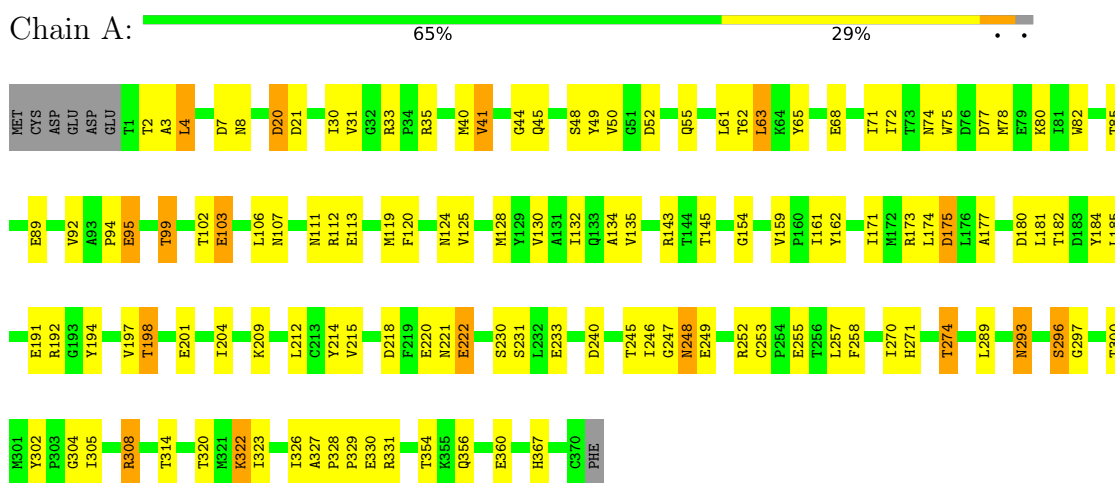


Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		
4	A	1	Total	27	10	5	10	2	0
4	C	1	Total	27	10	5	10	2	0
4	E	1	Total	27	10	5	10	2	0
4	G	1	Total	27	10	5	10	2	0
4	I	1	Total	27	10	5	10	2	0

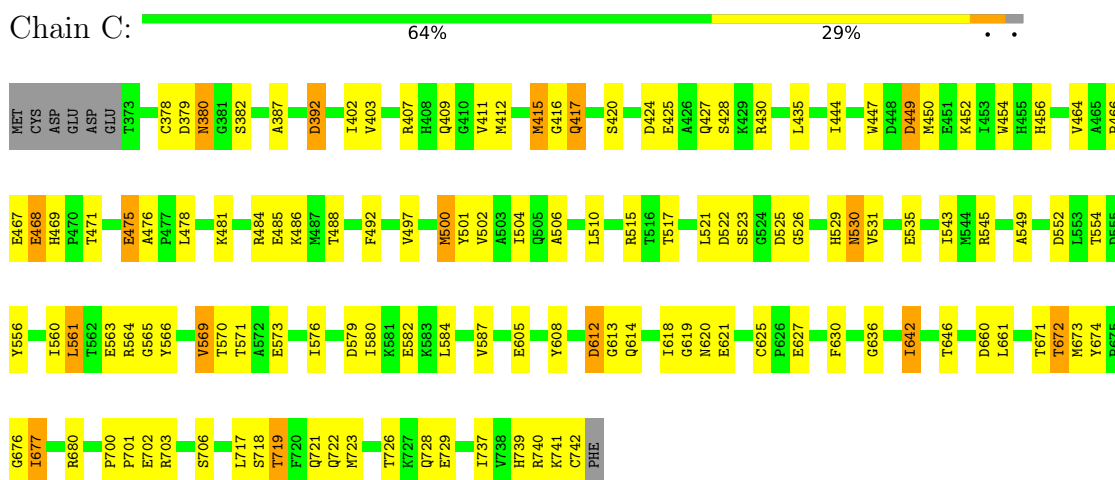
3 Residue-property plots

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

- Molecule 1: Actin, alpha skeletal muscle

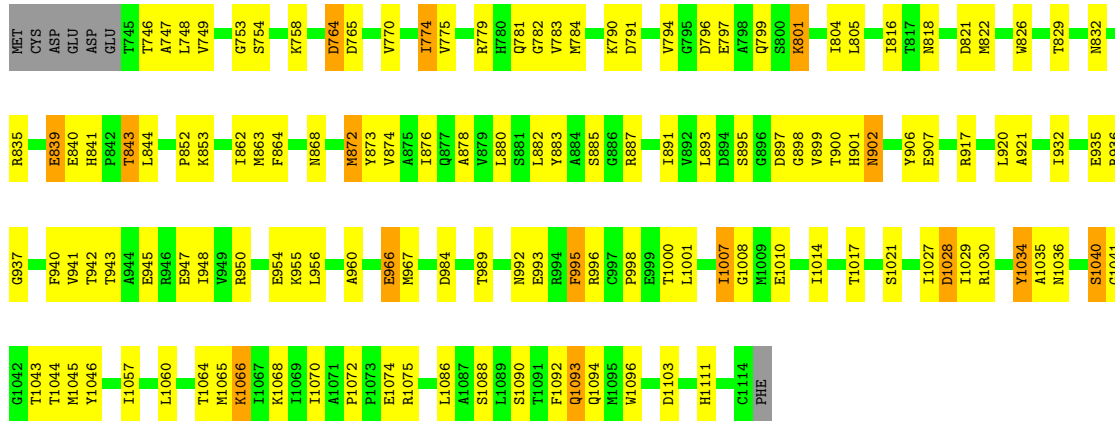


- Molecule 1: Actin, alpha skeletal muscle

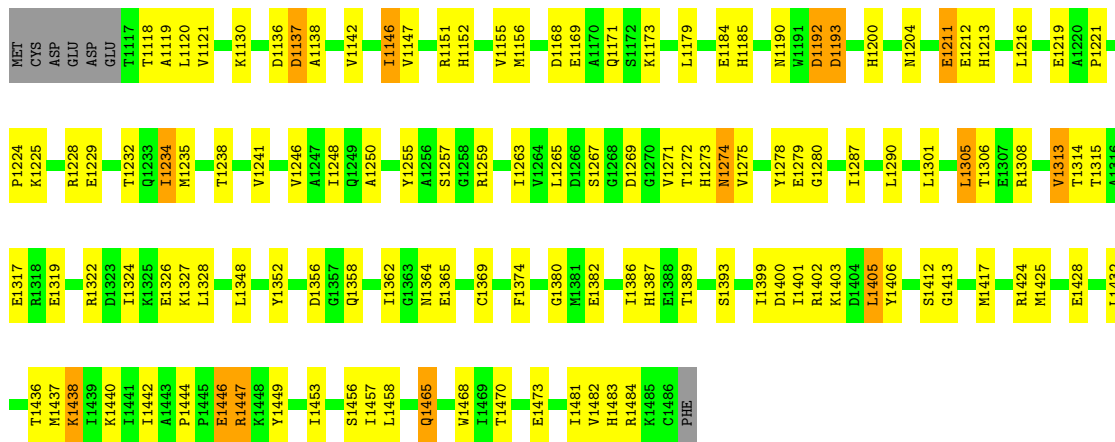


- Molecule 1: Actin, alpha skeletal muscle





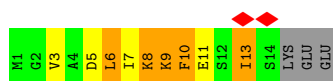
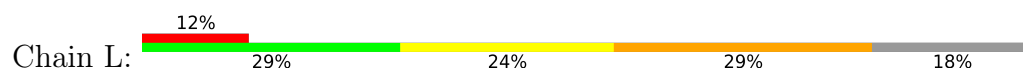
• Molecule 1: Actin, alpha skeletal muscle



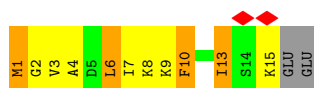
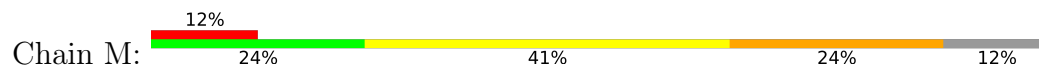
• Molecule 1: Actin, alpha skeletal muscle



• Molecule 2: Lifeact



- Molecule 2: Lifact



- Molecule 2: Lifact



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-166.9°, rise=27.44 Å, axial sym=C1	Depositor
Number of segments used	297584	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; GCTF for CTF correction	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	49.2	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	Not provided	
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.258	Depositor
Minimum map value	-0.096	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.0471	Depositor
Map size (Å)	353.28, 353.28, 353.28	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	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: MG, ADP

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	0.37	0/2927	0.46	0/3968
1	C	0.37	0/2935	0.46	0/3979
1	E	0.37	0/2938	0.45	0/3982
1	G	0.36	0/2929	0.44	0/3970
1	I	0.34	0/2932	0.44	0/3974
2	L	0.28	0/102	0.60	0/134
2	M	0.28	0/111	0.45	0/145
2	N	0.27	0/110	0.33	0/144
All	All	0.36	0/14984	0.45	0/20296

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	2865	0	2826	69	0
1	C	2873	0	2837	81	0
1	E	2876	0	2839	85	0
1	G	2867	0	2828	83	0
1	I	2870	0	2821	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	102	0	112	8	0
2	M	111	0	125	14	0
2	N	110	0	122	3	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	A	27	0	12	1	0
4	C	27	0	12	3	0
4	E	27	0	12	3	0
4	G	27	0	12	4	0
4	I	27	0	12	1	0
All	All	14814	0	14570	387	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 13.

All (387) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:GLY:H	1:A:177:ALA:HB3	1.42	0.85
1:C:587:VAL:HB	1:C:676:GLY:HA3	1.65	0.77
1:E:902:ASN:OD1	1:E:902:ASN:N	2.21	0.74
1:E:775:VAL:HG21	1:E:821:ASP:HB2	1.70	0.74
1:C:449:ASP:OD1	1:C:449:ASP:N	2.20	0.72
1:A:20:ASP:OD1	1:A:20:ASP:N	2.22	0.72
1:I:1642:GLY:HA2	1:I:1665:ALA:HB3	1.72	0.72
1:E:1090:SER:O	1:E:1093:GLN:NE2	2.23	0.72
1:A:248:ASN:HD21	1:A:252:ARG:HH11	1.34	0.72
1:C:484:ARG:NH1	1:C:742:CYS:SG	2.63	0.72
1:G:1274:ASN:OD1	1:G:1274:ASN:N	2.23	0.71
1:A:175:ASP:OD1	1:A:175:ASP:N	2.20	0.70
1:C:504:ILE:HG22	1:C:506:ALA:H	1.57	0.70
1:E:1028:ASP:OD1	1:E:1028:ASP:N	2.19	0.70
1:E:885:SER:OG	1:E:887:ARG:NH1	2.25	0.70
1:I:1604:THR:HG21	1:I:1854:VAL:HG11	1.74	0.70
1:I:1528:MET:O	1:I:1533:GLN:NE2	2.25	0.69
1:C:530:ASN:N	1:C:530:ASN:OD1	2.23	0.69
1:C:402:ILE:HD12	1:C:435:LEU:HD22	1.73	0.69
1:A:132:ILE:HG22	1:A:134:ALA:H	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1044:THR:O	1:E:1075:ARG:NE	2.24	0.68
1:C:392:ASP:OD1	1:C:392:ASP:N	2.19	0.67
1:G:1136:ASP:OD1	1:G:1137:ASP:N	2.28	0.67
1:G:1200:HIS:HD2	1:G:1204:ASN:HD22	1.42	0.67
1:G:1278:TYR:HD2	1:G:1401:ILE:HG23	1.58	0.67
1:A:30:ILE:HD12	1:A:63:LEU:HD22	1.76	0.67
1:C:702:GLU:N	1:C:702:GLU:OE1	2.27	0.67
1:E:936:ARG:NH1	1:E:993:GLU:OE2	2.28	0.67
1:G:1308:ARG:NH1	1:G:1365:GLU:OE2	2.27	0.67
2:L:7:ILE:HG13	2:L:10:PHE:HB3	1.75	0.67
1:A:330:GLU:OE1	1:A:330:GLU:N	2.28	0.67
1:G:1137:ASP:N	1:G:1137:ASP:OD1	2.27	0.67
1:C:605:GLU:OE1	1:C:605:GLU:N	2.28	0.66
1:C:526:GLY:H	1:C:549:ALA:HB3	1.58	0.66
1:G:1212:GLU:O	1:G:1213:HIS:ND1	2.29	0.66
1:A:35:ARG:NH1	1:C:636:GLY:O	2.29	0.66
1:C:672:THR:O	1:C:672:THR:OG1	2.11	0.66
1:C:584:LEU:HD13	1:C:618:ILE:HD11	1.78	0.65
1:I:1600:ARG:NH1	1:I:1858:CYS:SG	2.69	0.65
1:G:1147:VAL:HG21	1:G:1193:ASP:HB2	1.79	0.65
1:G:1257:SER:OG	1:G:1259:ARG:NH1	2.29	0.65
1:G:1399:ILE:HG12	1:G:1402:ARG:HH12	1.61	0.65
1:I:1583:GLU:HA	1:I:1613:VAL:HA	1.78	0.65
2:M:3:VAL:HG22	2:M:7:ILE:HB	1.80	0.64
1:A:233:GLU:N	1:A:233:GLU:OE1	2.30	0.64
1:A:215:VAL:HB	1:A:304:GLY:HA3	1.80	0.64
1:E:764:ASP:OD1	1:E:764:ASP:N	2.31	0.63
1:C:674:TYR:HB2	1:C:677:ILE:HG22	1.80	0.63
2:M:3:VAL:O	2:M:8:LYS:N	2.31	0.63
1:C:380:ASN:OD1	1:C:454:TRP:NE1	2.31	0.62
1:E:937:GLY:HA2	1:G:1224:PRO:HG3	1.81	0.62
1:A:322:LYS:NZ	1:A:322:LYS:O	2.32	0.62
1:C:468:GLU:O	1:C:469:HIS:ND1	2.32	0.62
1:G:1130:LYS:NZ	4:G:1502:ADP:O3B	2.32	0.62
1:C:506:ALA:HB2	1:C:529:HIS:HE1	1.65	0.61
1:E:832:ASN:O	1:E:835:ARG:NH1	2.34	0.61
1:C:564:ARG:NH1	1:C:621:GLU:OE2	2.33	0.61
1:I:1591:GLU:OE2	1:I:1599:ASN:ND2	2.33	0.61
1:A:180:ASP:O	1:A:184:TYR:N	2.22	0.61
1:C:522:ASP:OD1	1:C:523:SER:N	2.33	0.61
1:E:876:ILE:HG22	1:E:878:ALA:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1017:THR:O	1:E:1021:SER:N	2.33	0.60
1:E:932:ILE:HD11	1:E:996:ARG:HH21	1.66	0.60
1:I:1761:THR:O	1:I:1765:SER:N	2.34	0.60
1:G:1211:GLU:HA	1:G:1241:VAL:HA	1.83	0.60
1:G:1389:THR:O	1:G:1393:SER:N	2.34	0.60
1:C:420:SER:OG	1:C:452:LYS:NZ	2.34	0.60
1:I:1492:LEU:HB2	1:I:1587:THR:HG22	1.84	0.60
1:A:106:LEU:O	1:A:173:ARG:NH1	2.36	0.59
1:A:300:THR:O	1:A:331:ARG:NE	2.36	0.59
1:G:1313:VAL:N	1:G:1317:GLU:OE1	2.30	0.59
1:C:569:VAL:N	1:C:573:GLU:OE1	2.34	0.59
1:G:1151:ARG:NH1	1:I:1752:GLY:O	2.35	0.59
1:G:1248:ILE:HG22	1:G:1250:ALA:H	1.68	0.59
1:G:1301:LEU:HD13	1:G:1369:CYS:HB2	1.84	0.59
1:A:52:ASP:HA	1:A:55:GLN:HB3	1.85	0.59
1:A:198:THR:N	1:A:201:GLU:OE1	2.36	0.59
1:I:1680:ARG:NH1	1:I:1737:GLU:OE2	2.32	0.59
1:E:942:THR:N	1:E:945:GLU:OE1	2.36	0.59
1:I:1540:ASP:HA	1:I:1543:GLN:HB3	1.84	0.59
1:G:1470:THR:N	1:G:1473:GLU:OE1	2.34	0.59
1:I:1594:LEU:O	1:I:1661:ARG:NH1	2.25	0.59
1:C:563:GLU:HG3	1:E:853:LYS:HG2	1.84	0.58
1:E:901:HIS:O	1:E:901:HIS:ND1	2.36	0.58
1:C:447:TRP:CE2	1:C:486:LYS:HD2	2.39	0.58
1:C:416:GLY:HA2	2:L:13:ILE:HG23	1.84	0.58
1:A:296:SER:OG	1:A:297:GLY:N	2.35	0.58
1:G:1273:HIS:O	1:G:1273:HIS:ND1	2.32	0.58
1:I:1647:VAL:HA	1:I:1659:ILE:HG22	1.85	0.58
1:I:1844:GLN:NE2	1:I:1848:GLU:OE1	2.29	0.58
1:E:779:ARG:NH1	1:G:1380:GLY:O	2.37	0.57
1:I:1815:ALA:HB1	1:I:1819:ARG:HH12	1.69	0.57
1:E:748:LEU:HB2	1:E:843:THR:HG23	1.86	0.57
2:M:2:GLY:O	2:M:8:LYS:NZ	2.26	0.57
1:E:872:MET:HG2	1:E:873:TYR:N	2.18	0.57
1:G:1192:ASP:OD1	1:G:1192:ASP:N	2.37	0.57
1:G:1374:PHE:CE2	1:G:1424:ARG:HG2	2.39	0.57
1:I:1646:ASN:N	1:I:1646:ASN:OD1	2.37	0.57
1:E:887:ARG:HD3	1:E:1036:ASN:HD22	1.69	0.57
1:E:1040:SER:OG	1:E:1041:GLY:N	2.37	0.57
2:L:9:LYS:HG2	2:L:9:LYS:O	2.03	0.57
1:E:897:ASP:HB2	4:E:1202:ADP:H4'	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:SER:HB2	1:C:525:ASP:O	2.04	0.57
1:E:941:VAL:N	1:E:945:GLU:OE1	2.36	0.57
1:I:1669:LEU:HD11	1:I:1745:LEU:HD21	1.86	0.56
1:E:782:GLY:HA2	1:I:1653:TYR:HA	1.86	0.56
1:G:1412:SER:OG	1:G:1413:GLY:N	2.38	0.56
1:I:1518:ILE:HD12	1:I:1551:LEU:HD22	1.87	0.56
1:I:1543:GLN:HE22	1:I:1691:GLU:HG3	1.70	0.56
1:E:784:MET:HB2	1:I:1652:GLY:HA2	1.87	0.56
1:G:1193:ASP:N	1:G:1193:ASP:OD1	2.37	0.56
1:I:1508:ASP:OD1	1:I:1509:ASP:N	2.38	0.56
1:I:1770:ASP:O	1:I:1774:ARG:NE	2.38	0.56
1:A:212:LEU:HD13	1:A:246:ILE:HD11	1.88	0.56
1:E:954:GLU:HB2	4:E:1202:ADP:C5	2.41	0.56
1:G:1146:ILE:HD12	1:G:1179:LEU:HD22	1.88	0.56
2:M:9:LYS:NZ	2:M:10:PHE:O	2.39	0.56
1:E:906:TYR:HD1	1:E:1029:ILE:HG23	1.69	0.55
2:L:8:LYS:O	2:L:9:LYS:HD3	2.06	0.55
2:M:1:MET:SD	2:M:1:MET:N	2.69	0.55
1:E:818:ASN:ND2	1:E:821:ASP:OD2	2.39	0.55
1:E:893:LEU:HD21	1:E:1014:ILE:HD12	1.88	0.55
1:A:192:ARG:NH1	1:A:249:GLU:OE2	2.39	0.55
1:E:853:LYS:HD2	1:E:1111:HIS:CE1	2.42	0.55
1:C:407:ARG:NH1	1:E:1008:GLY:O	2.40	0.54
1:E:960:ALA:HB2	1:E:995:PHE:HD2	1.70	0.54
1:G:1267:SER:HG	1:G:1272:THR:HG1	1.55	0.54
1:C:552:ASP:O	1:C:556:TYR:N	2.24	0.54
1:G:1232:THR:HG21	1:G:1482:VAL:HG21	1.89	0.54
2:M:4:ALA:HA	2:M:8:LYS:HB2	1.88	0.54
1:G:1324:ILE:HG23	1:G:1328:LEU:HD12	1.88	0.54
1:A:356:GLN:NE2	1:A:360:GLU:OE1	2.40	0.54
1:E:883:TYR:CE2	1:E:1086:LEU:HD12	2.43	0.54
1:C:475:GLU:OE2	1:C:484:ARG:NH2	2.41	0.54
1:A:233:GLU:HA	1:A:247:GLY:HA2	1.90	0.54
1:C:582:GLU:HG2	4:C:802:ADP:C5	2.43	0.54
1:I:1650:TYR:HD1	1:I:1773:ILE:HG23	1.72	0.54
1:A:35:ARG:HD3	1:A:62:THR:HG23	1.90	0.54
1:G:1319:GLU:OE2	1:G:1322:ARG:NE	2.34	0.54
1:C:630:PHE:HD2	1:C:680:ARG:HH11	1.54	0.53
1:G:1184:GLU:OE2	1:G:1185:HIS:ND1	2.40	0.53
1:C:722:GLN:OE1	1:C:722:GLN:N	2.40	0.53
1:I:1644:THR:HB	1:I:1662:LEU:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:VAL:O	1:C:412:MET:HG2	2.08	0.53
1:E:935:GLU:HG3	1:G:1225:LYS:HG3	1.90	0.53
2:L:6:LEU:HD13	2:L:6:LEU:H	1.73	0.53
1:G:1265:LEU:HD21	1:G:1386:ILE:HD12	1.90	0.53
1:G:1446:GLU:CD	1:G:1446:GLU:H	2.12	0.52
1:I:1684:PHE:HA	1:I:1689:GLU:HG2	1.91	0.52
1:E:936:ARG:NE	1:E:989:THR:O	2.41	0.52
1:C:717:LEU:HD22	1:C:718:SER:H	1.73	0.52
1:E:782:GLY:HA3	1:I:1653:TYR:HD1	1.75	0.52
1:E:1072:PRO:O	1:E:1075:ARG:NH1	2.42	0.52
1:G:1221:PRO:HD2	1:G:1273:HIS:CD2	2.45	0.52
1:I:1788:THR:O	1:I:1819:ARG:NE	2.43	0.52
2:L:6:LEU:O	2:L:8:LYS:NZ	2.29	0.52
1:C:570:THR:N	1:C:573:GLU:OE1	2.42	0.52
1:C:723:MET:SD	1:C:723:MET:N	2.83	0.52
1:G:1328:LEU:HD13	1:G:1362:ILE:HD11	1.90	0.52
1:E:749:VAL:HG22	1:E:844:LEU:HD23	1.92	0.52
1:I:1565:ASP:OD1	1:I:1565:ASP:N	2.42	0.52
2:M:6:LEU:O	2:M:10:PHE:HA	2.10	0.52
1:I:1721:GLU:HA	1:I:1735:GLY:HA2	1.92	0.52
1:A:145:THR:OG1	1:A:162:TYR:O	2.28	0.51
1:E:967:MET:HA	1:E:995:PHE:HZ	1.75	0.51
1:G:1440:LYS:HE3	1:G:1442:ILE:HD11	1.92	0.51
1:G:1453:ILE:O	1:G:1456:SER:OG	2.27	0.51
2:L:3:VAL:HG13	2:L:5:ASP:H	1.75	0.51
1:G:1314:THR:N	1:G:1317:GLU:OE1	2.43	0.51
1:E:758:LYS:HG2	1:E:770:VAL:HG12	1.92	0.51
1:G:1444:PRO:O	1:G:1447:ARG:NH1	2.43	0.51
1:C:415:MET:HB3	1:C:417:GLN:HG3	1.91	0.51
1:C:485:GLU:OE2	1:C:739:HIS:NE2	2.41	0.51
1:C:565:GLY:HA2	1:E:852:PRO:HG3	1.93	0.51
1:C:605:GLU:HA	1:C:619:GLY:HA2	1.92	0.51
1:C:412:MET:HG3	1:G:1280:GLY:HA2	1.93	0.51
1:G:1465:GLN:HA	1:G:1468:TRP:HE1	1.74	0.51
1:I:1541:GLU:O	1:I:1544:SER:OG	2.25	0.51
2:N:10:PHE:HA	2:N:13:ILE:HG22	1.93	0.51
1:I:1686:THR:N	1:I:1689:GLU:OE2	2.45	0.50
1:I:1842:THR:N	1:I:1845:GLU:OE1	2.44	0.50
1:G:1269:ASP:HB2	4:G:1502:ADP:H4'	1.94	0.50
1:I:1689:GLU:N	1:I:1689:GLU:OE1	2.45	0.50
1:I:1706:ASP:O	1:I:1710:GLU:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1725:GLU:HB2	1:I:1731:VAL:HG12	1.94	0.50
1:E:796:ASP:HA	1:E:799:GLN:HB3	1.93	0.50
1:I:1543:GLN:OE1	1:I:1546:ARG:NE	2.45	0.50
1:G:1275:VAL:HG13	1:G:1287:ILE:HD12	1.93	0.50
1:I:1509:ASP:N	1:I:1509:ASP:OD1	2.41	0.50
1:C:726:THR:HB	1:C:729:GLU:HG3	1.93	0.49
1:E:765:ASP:N	1:E:765:ASP:OD1	2.43	0.49
1:I:1581:ALA:HB3	1:I:1584:GLU:HB2	1.93	0.49
1:A:191:GLU:HB2	1:C:481:LYS:HG2	1.94	0.49
1:C:488:THR:OG1	1:C:500:MET:SD	2.64	0.49
1:E:754:SER:HB2	1:E:897:ASP:O	2.13	0.49
1:A:31:VAL:HG21	1:A:77:ASP:HB2	1.93	0.49
1:A:95:GLU:HB3	1:A:124:ASN:O	2.12	0.49
1:C:403:VAL:HG21	1:C:449:ASP:HB3	1.94	0.49
1:I:1641:ASP:N	1:I:1641:ASP:OD1	2.44	0.49
1:A:8:ASN:OD1	1:A:82:TRP:NE1	2.44	0.49
1:I:1561:THR:OG1	1:I:1562:ASN:N	2.45	0.49
1:E:783:VAL:O	1:E:784:MET:HG2	2.12	0.49
1:E:826:TRP:HA	1:E:829:THR:HG22	1.93	0.49
2:L:10:PHE:HD1	2:L:11:GLU:H	1.60	0.48
1:A:314:THR:HG22	1:A:323:ILE:HD13	1.95	0.48
1:E:898:GLY:H	1:E:921:ALA:CB	2.26	0.48
1:I:1818:GLU:OE1	1:I:1818:GLU:N	2.28	0.48
1:G:1190:ASN:ND2	1:G:1193:ASP:OD2	2.47	0.48
1:G:1234:ILE:O	1:G:1238:THR:OG1	2.28	0.48
1:G:1326:GLU:HG2	4:G:1502:ADP:C5	2.49	0.48
1:C:466:PRO:HB2	1:C:497:VAL:HG12	1.96	0.48
1:C:521:LEU:HD21	1:C:642:ILE:HD12	1.94	0.48
1:C:531:VAL:HG22	1:C:543:ILE:HG12	1.94	0.48
1:G:1315:THR:N	1:I:1754:GLU:OE1	2.41	0.48
1:G:1328:LEU:HD11	1:G:1352:TYR:HB2	1.94	0.48
1:I:1582:PRO:HB2	1:I:1611:PHE:HB3	1.96	0.48
1:A:21:ASP:N	1:A:21:ASP:OD1	2.47	0.47
2:M:6:LEU:HG	2:M:7:ILE:HD12	1.95	0.47
1:E:906:TYR:CD2	1:E:907:GLU:HB2	2.50	0.47
1:E:1000:THR:HG21	1:E:1007:ILE:HD11	1.95	0.47
1:I:1498:SER:OG	1:I:1641:ASP:HB2	2.14	0.47
1:A:103:GLU:OE1	1:A:112:ARG:NH2	2.48	0.47
1:I:1616:MET:HG2	1:I:1617:TYR:N	2.30	0.47
1:E:1034:TYR:HD2	1:E:1065:MET:HG2	1.79	0.47
2:N:8:LYS:H	2:N:8:LYS:HZ2	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1521:ARG:HB2	1:I:1550:THR:HG22	1.97	0.47
1:A:143:ARG:HH12	1:A:326:ILE:HG21	1.80	0.46
1:E:821:ASP:N	1:E:821:ASP:OD1	2.48	0.46
1:E:1093:GLN:OE1	1:E:1094:GLN:N	2.48	0.46
1:E:790:LYS:HD2	1:E:790:LYS:HA	1.64	0.46
1:C:560:ILE:O	1:C:563:GLU:HB3	2.16	0.46
1:A:135:VAL:HG12	1:A:161:ILE:HD11	1.97	0.46
1:G:1136:ASP:OD1	1:G:1138:ALA:N	2.48	0.46
1:A:154:GLY:N	1:A:177:ALA:HB3	2.20	0.46
1:C:478:LEU:O	1:C:545:ARG:NH1	2.49	0.46
1:C:444:ILE:HD13	1:C:450:MET:HG2	1.97	0.46
1:C:510:LEU:HD12	1:C:510:LEU:HA	1.75	0.46
1:C:726:THR:HG22	1:C:728:GLN:H	1.80	0.46
1:E:816:ILE:HD13	1:E:822:MET:HG2	1.98	0.46
1:E:956:LEU:HD23	1:E:956:LEU:HA	1.72	0.46
1:A:4:LEU:HB3	1:A:99:THR:HG23	1.96	0.46
1:C:427:GLN:O	1:C:430:ARG:HG3	2.15	0.46
1:C:571:THR:N	1:E:1010:GLU:OE1	2.45	0.46
1:C:703:ARG:HA	1:C:706:SER:HB2	1.97	0.46
1:E:887:ARG:NH1	1:E:1070:ILE:HG21	2.30	0.46
1:I:1523:ARG:HG3	1:I:1524:HIS:ND1	2.31	0.46
1:I:1645:HIS:HA	1:I:1660:MET:O	2.16	0.46
1:I:1700:LEU:HD11	1:I:1724:TYR:HB2	1.97	0.46
1:E:943:THR:N	1:G:1382:GLU:OE1	2.46	0.45
1:A:77:ASP:OD1	1:A:77:ASP:N	2.49	0.45
1:C:424:ASP:HA	1:C:427:GLN:HB3	1.98	0.45
1:A:30:ILE:HG22	1:A:65:TYR:CE1	2.51	0.45
1:A:185:LEU:HD13	1:A:253:CYS:HB2	1.98	0.45
1:E:995:PHE:HD1	1:E:995:PHE:H	1.64	0.45
1:I:1746:PHE:CE2	1:I:1796:ARG:HD2	2.51	0.45
1:A:94:PRO:HB2	1:A:125:VAL:HG12	1.99	0.45
1:I:1698:GLU:HG2	4:I:1902:ADP:C5	2.51	0.45
1:A:41:VAL:HG11	1:E:1092:PHE:HD1	1.81	0.45
1:E:839:GLU:HB3	1:E:868:ASN:O	2.17	0.45
1:G:1200:HIS:CD2	1:G:1204:ASN:HD22	2.29	0.45
1:G:1259:ARG:NH1	1:G:1442:ILE:HG21	2.32	0.45
1:E:746:THR:OG1	1:E:747:ALA:N	2.50	0.45
1:I:1592:ALA:O	1:I:1595:ASN:ND2	2.39	0.45
1:A:230:SER:OG	1:A:231:SER:N	2.49	0.45
1:A:258:PHE:CE2	1:A:308:ARG:HD2	2.52	0.45
1:I:1810:LYS:HE3	1:I:1810:LYS:HB3	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ARG:NE	1:A:245:THR:O	2.50	0.44
1:C:612:ASP:OD1	1:C:613:GLY:N	2.51	0.44
1:A:48:SER:OG	1:A:80:LYS:NZ	2.46	0.44
1:A:82:TRP:HA	1:A:85:THR:HG22	2.00	0.44
1:A:174:LEU:HA	1:A:174:LEU:HD12	1.76	0.44
1:A:201:GLU:O	1:A:204:ILE:N	2.51	0.44
1:E:840:GLU:O	1:E:841:HIS:ND1	2.51	0.44
1:A:72:ILE:HD13	1:A:78:MET:HG2	2.00	0.44
1:G:1403:LYS:HG3	1:G:1437:MET:HE1	2.00	0.44
1:I:1633:THR:OG1	1:I:1650:TYR:O	2.34	0.44
1:I:1680:ARG:NE	1:I:1733:THR:O	2.50	0.44
1:A:270:ILE:O	1:A:274:THR:OG1	2.35	0.44
1:E:1066:LYS:HE3	1:E:1066:LYS:HB3	1.77	0.44
1:G:1399:ILE:HA	1:G:1402:ARG:NH1	2.33	0.44
1:G:1120:LEU:HD23	1:G:1120:LEU:HA	1.80	0.44
1:A:74:ASN:OD1	1:A:75:TRP:N	2.51	0.43
1:A:181:LEU:HD11	1:A:257:LEU:HD21	2.00	0.43
1:A:220:GLU:OE1	1:A:220:GLU:N	2.49	0.43
1:G:1438:LYS:HE3	1:G:1438:LYS:HB3	1.80	0.43
1:A:68:GLU:O	1:A:71:ILE:HG12	2.18	0.43
1:E:796:ASP:OD1	1:E:797:GLU:N	2.51	0.43
1:G:1305:LEU:HD22	1:G:1305:LEU:HA	1.86	0.43
1:I:1777:LEU:HD22	1:I:1777:LEU:HA	1.85	0.43
1:A:293:ASN:N	1:A:293:ASN:OD1	2.52	0.43
1:A:44:GLY:H	2:M:13:ILE:HG13	1.83	0.43
1:C:717:LEU:HD13	1:C:719:THR:N	2.33	0.43
1:E:895:SER:O	1:E:895:SER:OG	2.33	0.43
1:G:1225:LYS:HB3	1:G:1483:HIS:CE1	2.54	0.43
1:G:1267:SER:OG	1:G:1272:THR:OG1	2.24	0.43
1:G:1481:ILE:O	1:G:1484:ARG:HG2	2.18	0.43
1:I:1622:ALA:HB2	1:I:1645:HIS:CE1	2.53	0.43
1:A:214:TYR:OH	1:A:222:GLU:OE2	2.25	0.43
1:C:674:TYR:HE1	4:C:802:ADP:C2	2.35	0.43
1:E:882:LEU:HA	1:E:882:LEU:HD12	1.77	0.43
1:G:1229:GLU:OE2	1:G:1483:HIS:NE2	2.49	0.43
1:E:895:SER:HB2	1:E:900:THR:HG1	1.84	0.43
1:E:998:PRO:HB3	1:E:1046:TYR:CE2	2.54	0.43
1:A:2:THR:OG1	1:A:3:ALA:N	2.52	0.43
1:C:452:LYS:O	1:C:456:HIS:N	2.39	0.43
1:C:506:ALA:HB2	1:C:529:HIS:CE1	2.49	0.43
1:I:1612:ASN:OD1	1:I:1612:ASN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:9:LYS:HD2	2:M:9:LYS:HA	1.64	0.43
1:C:430:ARG:NE	1:G:1400:ASP:OD2	2.52	0.42
1:A:328:PRO:HA	1:A:329:PRO:HD3	1.80	0.42
1:A:159:VAL:HG13	1:A:171:ILE:HG12	2.01	0.42
1:C:468:GLU:H	1:C:468:GLU:HG3	1.60	0.42
1:E:993:GLU:H	1:E:993:GLU:CD	2.23	0.42
1:G:1405:LEU:HD23	1:G:1405:LEU:HA	1.85	0.42
1:I:1723:SER:HA	1:I:1733:THR:HG22	2.02	0.42
1:C:737:ILE:O	1:C:740:ARG:HG2	2.20	0.42
1:G:1151:ARG:HG3	1:G:1152:HIS:ND1	2.35	0.42
1:A:63:LEU:H	1:A:63:LEU:HG	1.37	0.42
1:E:955:LYS:HE2	1:E:955:LYS:HB2	1.87	0.42
1:G:1386:ILE:HG13	1:G:1425:MET:HE1	2.01	0.42
1:A:302:TYR:C	1:A:304:GLY:H	2.22	0.42
1:C:430:ARG:NH2	1:G:1400:ASP:OD1	2.52	0.42
1:C:721:GLN:N	1:C:721:GLN:OE1	2.52	0.42
1:E:895:SER:HB2	1:E:900:THR:OG1	2.18	0.42
1:E:945:GLU:O	1:E:948:ILE:N	2.52	0.42
1:C:526:GLY:N	1:C:549:ALA:HB3	2.30	0.42
1:C:561:LEU:HD23	1:C:561:LEU:HA	1.79	0.42
1:E:1001:LEU:HA	1:E:1001:LEU:HD23	1.75	0.42
1:A:49:TYR:HD1	1:A:61:LEU:HD21	1.84	0.42
1:C:515:ARG:HG2	1:C:517:THR:H	1.85	0.42
1:G:1278:TYR:CD2	1:G:1401:ILE:HG23	2.46	0.42
1:A:255:GLU:OE2	1:A:308:ARG:NH1	2.45	0.42
1:E:753:GLY:HA3	4:E:1202:ADP:O2B	2.19	0.42
1:E:940:PHE:HB3	1:E:945:GLU:HB3	2.02	0.42
1:E:1027:ILE:HG12	1:E:1030:ARG:NH1	2.35	0.42
1:E:1035:ALA:HB2	1:E:1066:LYS:HZ1	1.85	0.42
1:C:674:TYR:HE1	4:C:802:ADP:H2	1.68	0.41
1:G:1168:ASP:HA	1:G:1171:GLN:HB3	2.02	0.41
1:G:1365:GLU:OE1	1:G:1365:GLU:N	2.52	0.41
1:G:1269:ASP:OD1	4:G:1502:ADP:O3'	2.39	0.41
1:I:1699:LYS:O	1:I:1700:LEU:HD23	2.20	0.41
1:A:103:GLU:OE2	1:A:107:ASN:HB2	2.20	0.41
1:C:425:GLU:O	1:C:428:SER:OG	2.35	0.41
1:E:774:ILE:O	1:E:794:VAL:HG23	2.21	0.41
1:E:947:GLU:OE2	1:E:950:ARG:NH2	2.47	0.41
1:G:1121:VAL:HG22	1:G:1216:LEU:HB3	2.02	0.41
1:I:1841:ILE:HG12	1:I:1857:LYS:NZ	2.34	0.41
2:M:2:GLY:C	2:M:8:LYS:HZ3	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLU:OE2	1:A:367:HIS:NE2	2.49	0.41
1:C:580:ILE:HG12	1:C:608:TYR:CD2	2.56	0.41
1:A:218:ASP:OD2	1:A:221:ASN:ND2	2.53	0.41
1:C:717:LEU:HD13	1:C:719:THR:H	1.86	0.41
1:G:1348:LEU:HD13	1:G:1348:LEU:HA	1.88	0.41
2:M:15:LYS:HB3	2:M:15:LYS:HE2	1.75	0.41
1:A:215:VAL:HG11	1:A:258:PHE:HE2	1.86	0.41
1:E:801:LYS:O	1:E:805:LEU:HD13	2.21	0.41
1:G:1142:VAL:HG21	1:G:1449:TYR:HE2	1.85	0.41
1:G:1278:TYR:HD1	1:G:1279:GLU:HB2	1.85	0.41
1:G:1358:GLN:HE21	1:G:1358:GLN:HB3	1.60	0.41
1:I:1540:ASP:O	1:I:1544:SER:N	2.51	0.41
1:I:1778:TYR:HD2	1:I:1809:MET:HG2	1.85	0.41
1:C:415:MET:HG3	1:G:1280:GLY:HA3	2.03	0.41
1:E:932:ILE:HD12	1:E:932:ILE:HA	1.91	0.41
1:G:1118:THR:OG1	1:G:1119:ALA:N	2.54	0.41
1:G:1327:LYS:HE2	1:G:1327:LYS:HB3	1.87	0.41
2:M:9:LYS:O	2:M:10:PHE:C	2.59	0.41
1:C:475:GLU:HG2	1:C:476:ALA:N	2.36	0.40
1:C:501:TYR:HE1	1:C:741:LYS:O	2.05	0.40
1:G:1290:LEU:HD12	1:G:1290:LEU:HA	1.85	0.40
2:N:3:VAL:O	2:N:7:ILE:HG13	2.21	0.40
1:A:159:VAL:HG22	1:A:171:ILE:HG23	2.03	0.40
1:C:467:GLU:OE1	1:C:467:GLU:N	2.35	0.40
1:C:552:ASP:N	1:C:552:ASP:OD1	2.53	0.40
1:C:700:PRO:HA	1:C:701:PRO:HD3	1.81	0.40
1:E:1093:GLN:HA	1:E:1096:TRP:HE1	1.87	0.40
1:G:1255:TYR:HE2	1:G:1458:LEU:HD13	1.87	0.40
1:C:564:ARG:HD3	1:C:566:TYR:HE2	1.86	0.40
1:E:966:GLU:HB3	1:E:995:PHE:CE2	2.57	0.40
1:G:1228:ARG:HE	1:G:1246:VAL:HG21	1.87	0.40
1:I:1564:ASP:O	1:I:1567:GLU:HB3	2.21	0.40
2:M:4:ALA:O	2:M:9:LYS:N	2.52	0.40
1:A:327:ALA:HB1	1:A:331:ARG:NH1	2.36	0.40
1:C:378:CYS:HA	1:C:387:ALA:HA	2.03	0.40
1:E:1057:ILE:O	1:E:1060:LEU:HD23	2.22	0.40
1:G:1387:HIS:HB2	1:G:1428:GLU:HB3	2.04	0.40
1:I:1523:ARG:NH1	1:I:1524:HIS:HE1	2.19	0.40
1:A:209:LYS:NZ	4:A:402:ADP:O2'	2.32	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	368/377 (98%)	318 (86%)	50 (14%)	0	100	100
1	C	368/377 (98%)	317 (86%)	51 (14%)	0	100	100
1	E	368/377 (98%)	323 (88%)	45 (12%)	0	100	100
1	G	368/377 (98%)	328 (89%)	40 (11%)	0	100	100
1	I	368/377 (98%)	329 (89%)	39 (11%)	0	100	100
2	L	12/17 (71%)	6 (50%)	6 (50%)	0	100	100
2	M	13/17 (76%)	7 (54%)	6 (46%)	0	100	100
2	N	13/17 (76%)	12 (92%)	1 (8%)	0	100	100
All	All	1878/1936 (97%)	1640 (87%)	238 (13%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	305/320 (95%)	267 (88%)	38 (12%)	4	22
1	C	309/320 (97%)	274 (89%)	35 (11%)	6	25
1	E	309/320 (97%)	273 (88%)	36 (12%)	5	23
1	G	306/320 (96%)	276 (90%)	30 (10%)	8	29
1	I	307/320 (96%)	279 (91%)	28 (9%)	9	32
2	L	11/15 (73%)	6 (54%)	5 (46%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	12/15 (80%)	8 (67%)	4 (33%)	0	2
2	N	11/15 (73%)	9 (82%)	2 (18%)	1	11
All	All	1570/1645 (95%)	1392 (89%)	178 (11%)	9	25

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	7	ASP
1	A	20	ASP
1	A	33	ARG
1	A	40	MET
1	A	41	VAL
1	A	45	GLN
1	A	50	VAL
1	A	63	LEU
1	A	89	GLU
1	A	92	VAL
1	A	95	GLU
1	A	99	THR
1	A	102	THR
1	A	103	GLU
1	A	111	ASN
1	A	119	MET
1	A	120	PHE
1	A	128	MET
1	A	130	VAL
1	A	175	ASP
1	A	182	THR
1	A	194	TYR
1	A	197	VAL
1	A	198	THR
1	A	222	GLU
1	A	240	ASP
1	A	248	ASN
1	A	271	HIS
1	A	274	THR
1	A	289	LEU
1	A	293	ASN
1	A	296	SER
1	A	305	ILE

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Mol	Chain	Res	Type
1	A	308	ARG
1	A	320	THR
1	A	322	LYS
1	A	354	THR
1	C	379	ASP
1	C	380	ASN
1	C	392	ASP
1	C	409	GLN
1	C	415	MET
1	C	417	GLN
1	C	449	ASP
1	C	464	VAL
1	C	468	GLU
1	C	471	THR
1	C	475	GLU
1	C	492	PHE
1	C	500	MET
1	C	502	VAL
1	C	530	ASN
1	C	535	GLU
1	C	554	THR
1	C	561	LEU
1	C	569	VAL
1	C	576	ILE
1	C	579	ASP
1	C	612	ASP
1	C	614	GLN
1	C	620	ASN
1	C	625	CYS
1	C	627	GLU
1	C	642	ILE
1	C	646	THR
1	C	660	ASP
1	C	661	LEU
1	C	671	THR
1	C	672	THR
1	C	673	MET
1	C	677	ILE
1	C	719	THR
1	E	764	ASP
1	E	774	ILE
1	E	781	GLN

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Mol	Chain	Res	Type
1	E	791	ASP
1	E	801	LYS
1	E	804	ILE
1	E	839	GLU
1	E	843	THR
1	E	862	ILE
1	E	863	MET
1	E	864	PHE
1	E	872	MET
1	E	874	VAL
1	E	880	LEU
1	E	891	ILE
1	E	899	VAL
1	E	902	ASN
1	E	917	ARG
1	E	920	LEU
1	E	966	GLU
1	E	984	ASP
1	E	992	ASN
1	E	995	PHE
1	E	1007	ILE
1	E	1028	ASP
1	E	1034	TYR
1	E	1040	SER
1	E	1043	THR
1	E	1045	MET
1	E	1064	THR
1	E	1066	LYS
1	E	1068	LYS
1	E	1074	GLU
1	E	1088	SER
1	E	1093	GLN
1	E	1103	ASP
1	G	1137	ASP
1	G	1146	ILE
1	G	1155	VAL
1	G	1156	MET
1	G	1169	GLU
1	G	1173	LYS
1	G	1192	ASP
1	G	1193	ASP
1	G	1211	GLU

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Mol	Chain	Res	Type
1	G	1219	GLU
1	G	1234	ILE
1	G	1235	MET
1	G	1263	ILE
1	G	1271	VAL
1	G	1274	ASN
1	G	1305	LEU
1	G	1306	THR
1	G	1313	VAL
1	G	1356	ASP
1	G	1364	ASN
1	G	1405	LEU
1	G	1406	TYR
1	G	1417	MET
1	G	1432	LEU
1	G	1436	THR
1	G	1438	LYS
1	G	1446	GLU
1	G	1447	ARG
1	G	1457	ILE
1	G	1465	GLN
1	I	1493	VAL
1	I	1498	SER
1	I	1524	HIS
1	I	1527	VAL
1	I	1528	MET
1	I	1583	GLU
1	I	1607	MET
1	I	1612	ASN
1	I	1616	MET
1	I	1618	VAL
1	I	1632	THR
1	I	1635	ILE
1	I	1641	ASP
1	I	1646	ASN
1	I	1657	HIS
1	I	1661	ARG
1	I	1678	THR
1	I	1725	GLU
1	I	1728	ASP
1	I	1777	LEU
1	I	1778	TYR

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Mol	Chain	Res	Type
1	I	1787	THR
1	I	1789	MET
1	I	1796	ARG
1	I	1804	LEU
1	I	1808	THR
1	I	1837	GLN
1	I	1855	HIS
2	L	6	LEU
2	L	8	LYS
2	L	9	LYS
2	L	10	PHE
2	L	13	ILE
2	M	1	MET
2	M	6	LEU
2	M	10	PHE
2	M	13	ILE
2	N	5	ASP
2	N	8	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	248	ASN
1	A	271	HIS
1	A	349	GLN
1	A	356	GLN
1	C	483	ASN
1	C	529	HIS
1	C	614	GLN
1	C	620	ASN
1	C	643	HIS
1	E	752	ASN
1	E	986	GLN
1	E	992	ASN
1	E	1015	HIS
1	G	1200	HIS
1	G	1249	GLN
1	G	1358	GLN
1	G	1364	ASN
1	G	1408	ASN
1	I	1533	GLN

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Mol	Chain	Res	Type
1	I	1572	HIS
1	I	1576	ASN
1	I	1599	ASN
1	I	1764	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ADP	I	1902	3	24,29,29	0.91	1 (4%)	29,45,45	1.52	4 (13%)
4	ADP	A	402	3	24,29,29	0.88	1 (4%)	29,45,45	1.54	4 (13%)
4	ADP	C	802	3	24,29,29	0.90	1 (4%)	29,45,45	1.52	4 (13%)
4	ADP	G	1502	3	24,29,29	0.89	1 (4%)	29,45,45	1.50	4 (13%)
4	ADP	E	1202	3	24,29,29	0.90	1 (4%)	29,45,45	1.54	4 (13%)

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
4	ADP	I	1902	3	-	4/12/32/32	0/3/3/3
4	ADP	A	402	3	-	5/12/32/32	0/3/3/3
4	ADP	C	802	3	-	3/12/32/32	0/3/3/3
4	ADP	G	1502	3	-	4/12/32/32	0/3/3/3
4	ADP	E	1202	3	-	4/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	1902	ADP	C5-C4	2.18	1.46	1.40
4	A	402	ADP	C5-C4	2.13	1.46	1.40
4	E	1202	ADP	C5-C4	2.13	1.46	1.40
4	C	802	ADP	C5-C4	2.12	1.46	1.40
4	G	1502	ADP	C5-C4	2.06	1.46	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	402	ADP	PA-O3A-PB	-4.97	115.77	132.83
4	C	802	ADP	PA-O3A-PB	-4.68	116.76	132.83
4	G	1502	ADP	PA-O3A-PB	-4.29	118.11	132.83
4	E	1202	ADP	PA-O3A-PB	-4.27	118.16	132.83
4	I	1902	ADP	PA-O3A-PB	-3.99	119.14	132.83
4	G	1502	ADP	N3-C2-N1	-3.29	123.54	128.68
4	I	1902	ADP	N3-C2-N1	-3.24	123.61	128.68
4	C	802	ADP	C3'-C2'-C1'	3.12	105.68	100.98
4	E	1202	ADP	N3-C2-N1	-3.11	123.82	128.68
4	I	1902	ADP	C3'-C2'-C1'	3.10	105.65	100.98
4	A	402	ADP	N3-C2-N1	-3.08	123.86	128.68
4	E	1202	ADP	C3'-C2'-C1'	3.03	105.55	100.98
4	C	802	ADP	N3-C2-N1	-2.89	124.16	128.68
4	G	1502	ADP	C3'-C2'-C1'	2.73	105.09	100.98
4	A	402	ADP	C3'-C2'-C1'	2.56	104.83	100.98
4	G	1502	ADP	C4-C5-N7	-2.50	106.79	109.40
4	A	402	ADP	C4-C5-N7	-2.47	106.83	109.40
4	E	1202	ADP	C4-C5-N7	-2.45	106.84	109.40
4	C	802	ADP	C4-C5-N7	-2.40	106.90	109.40
4	I	1902	ADP	C4-C5-N7	-2.38	106.92	109.40

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	402	ADP	C5'-O5'-PA-O3A
4	C	802	ADP	C5'-O5'-PA-O1A
4	C	802	ADP	C5'-O5'-PA-O3A
4	E	1202	ADP	C5'-O5'-PA-O1A
4	E	1202	ADP	C3'-C4'-C5'-O5'
4	G	1502	ADP	C5'-O5'-PA-O1A
4	G	1502	ADP	C5'-O5'-PA-O3A
4	I	1902	ADP	C5'-O5'-PA-O3A
4	I	1902	ADP	C3'-C4'-C5'-O5'
4	A	402	ADP	C3'-C4'-C5'-O5'
4	G	1502	ADP	C3'-C4'-C5'-O5'
4	E	1202	ADP	O4'-C4'-C5'-O5'
4	I	1902	ADP	O4'-C4'-C5'-O5'
4	A	402	ADP	O4'-C4'-C5'-O5'
4	G	1502	ADP	O4'-C4'-C5'-O5'
4	A	402	ADP	C5'-O5'-PA-O1A
4	I	1902	ADP	C5'-O5'-PA-O1A
4	A	402	ADP	PA-O3A-PB-O1B
4	C	802	ADP	C3'-C4'-C5'-O5'
4	E	1202	ADP	C5'-O5'-PA-O3A

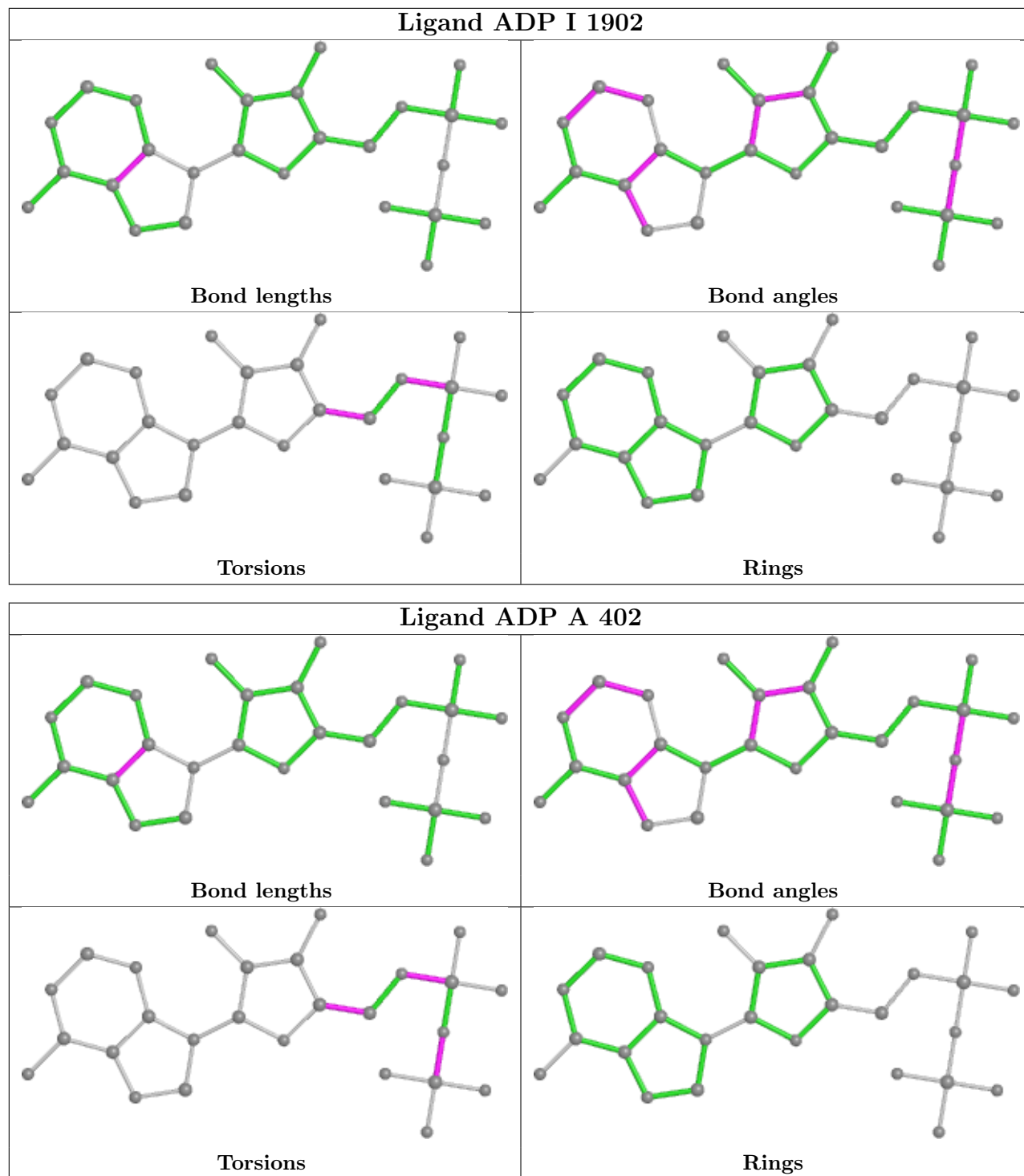
There are no ring outliers.

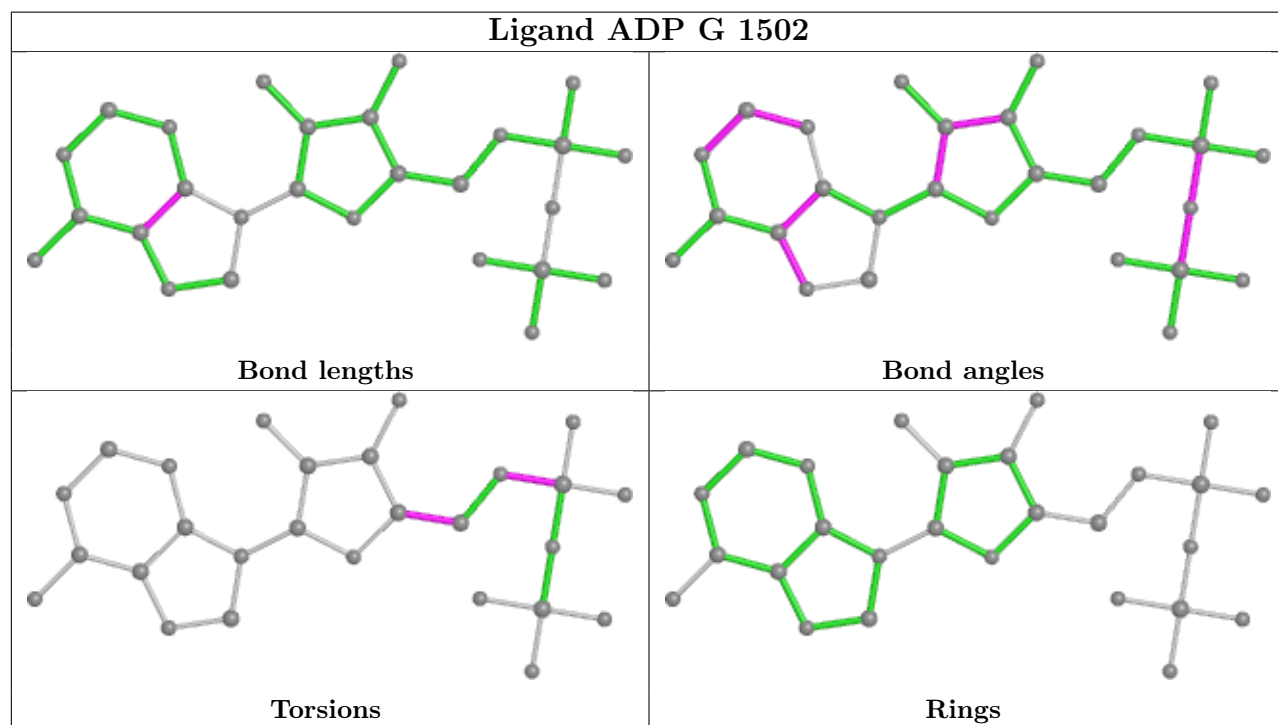
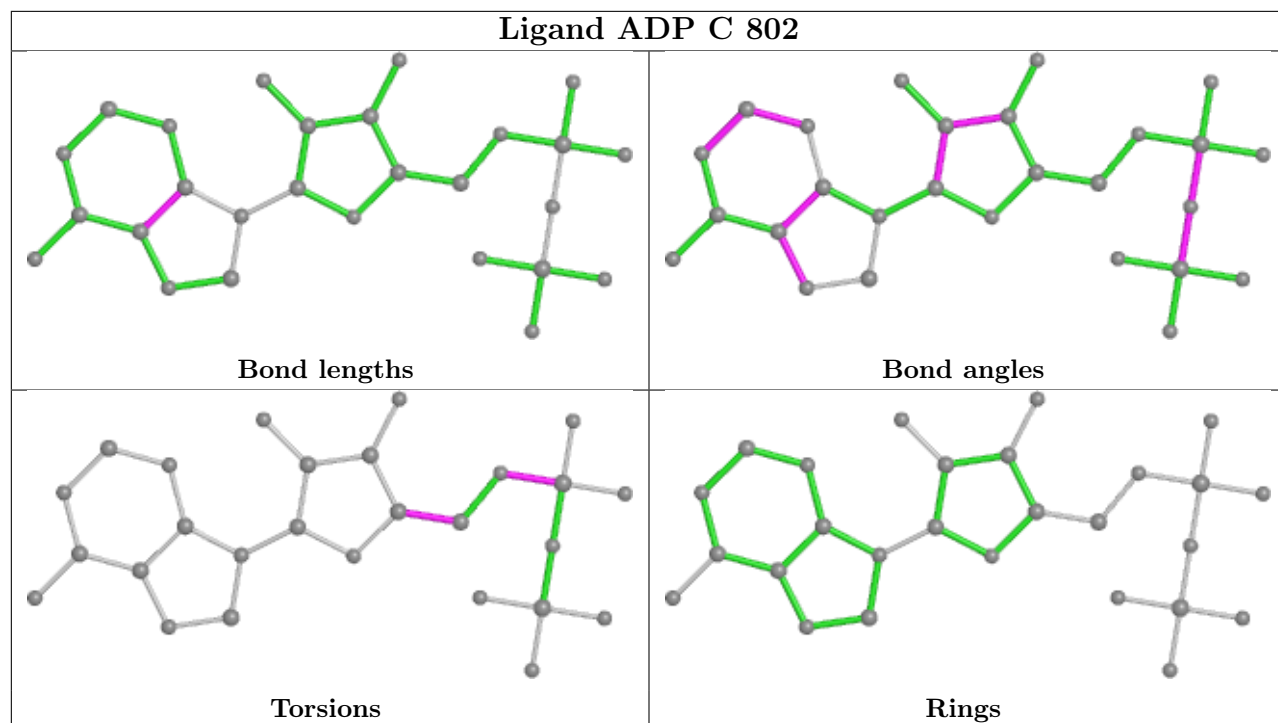
5 monomers are involved in 12 short contacts:

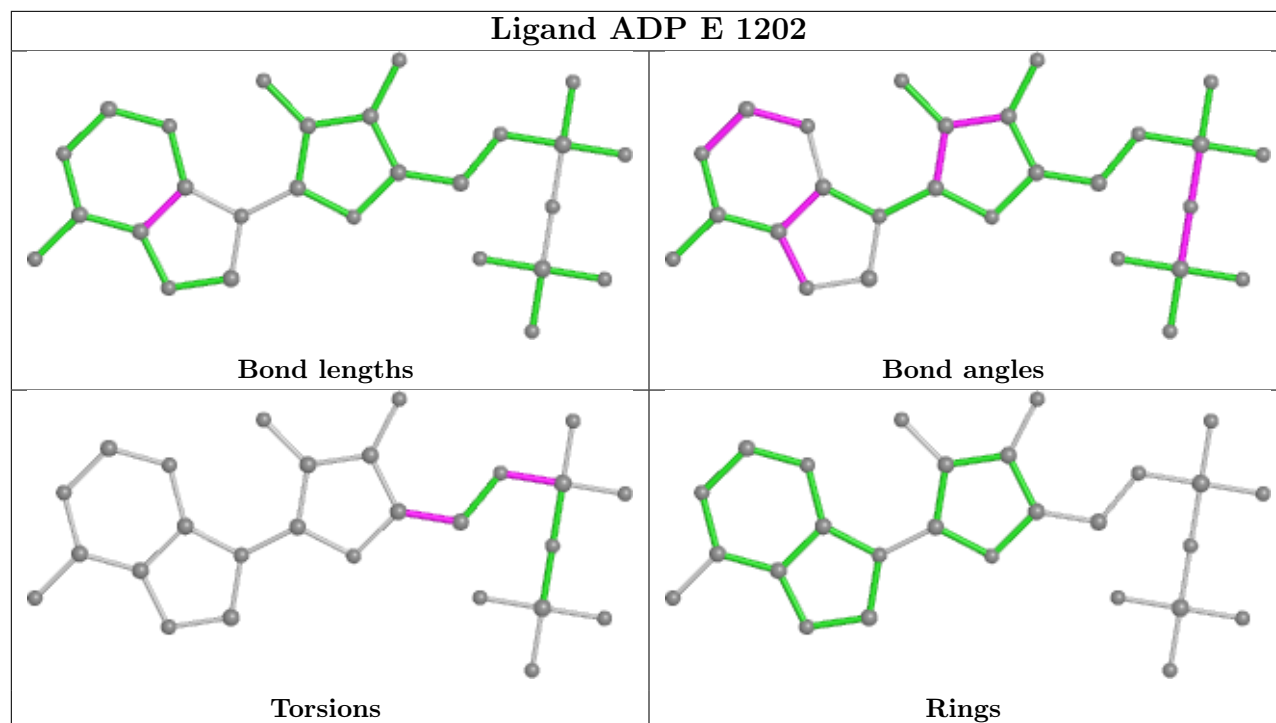
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1902	ADP	1	0
4	A	402	ADP	1	0
4	C	802	ADP	3	0
4	G	1502	ADP	4	0
4	E	1202	ADP	3	0

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

equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

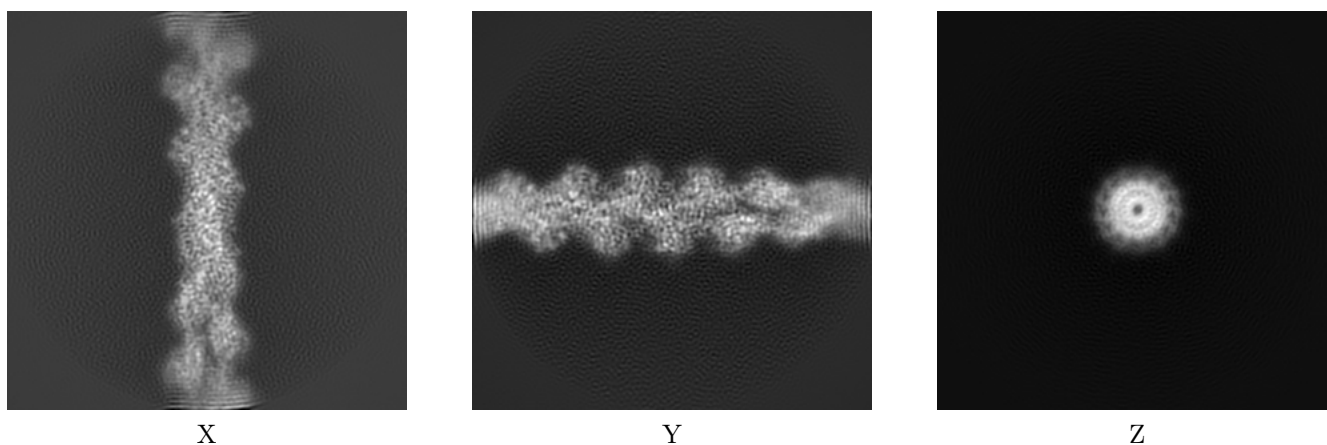
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30177. 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](#)

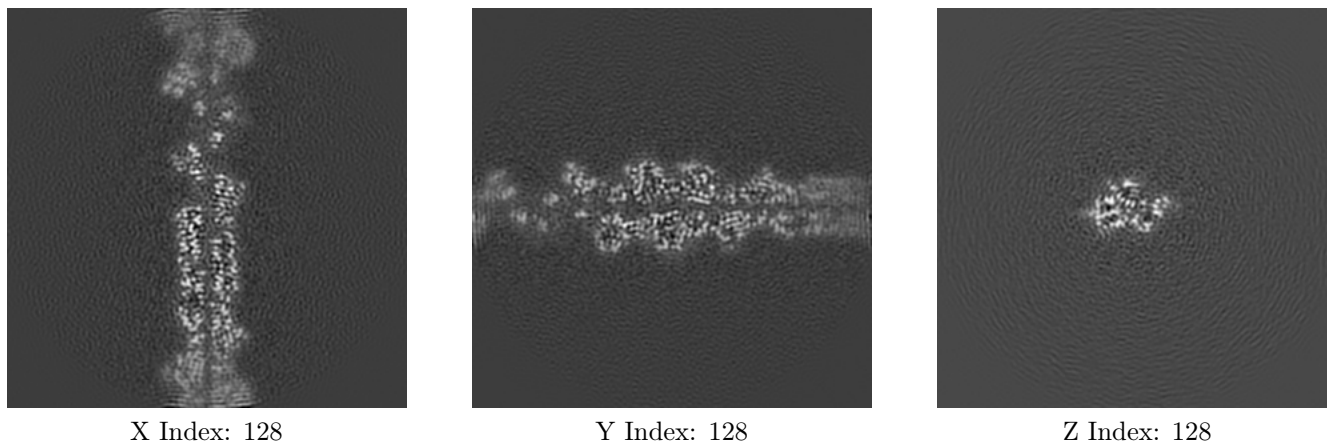
6.1.1 Primary map



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

6.2 Central slices [i](#)

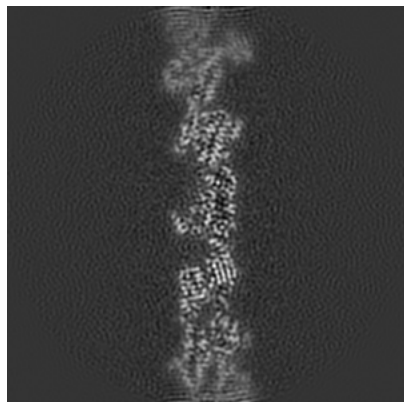
6.2.1 Primary map



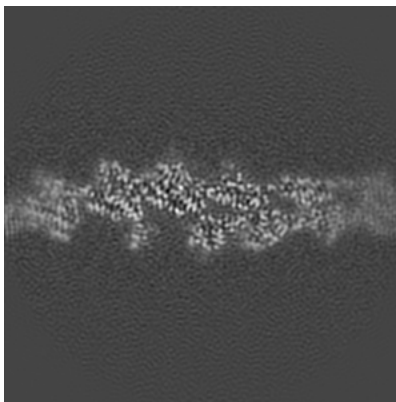
The images above show central slices of the map in three orthogonal directions.

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

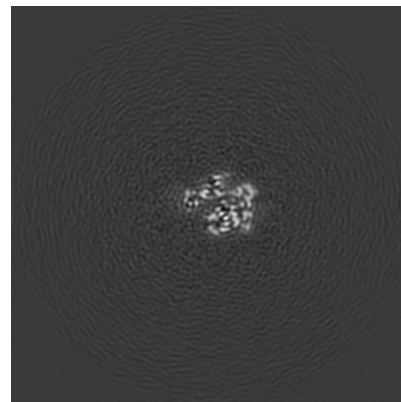
6.3.1 Primary map



X Index: 122



Y Index: 122

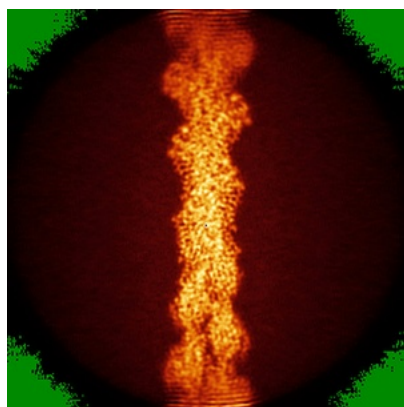


Z Index: 103

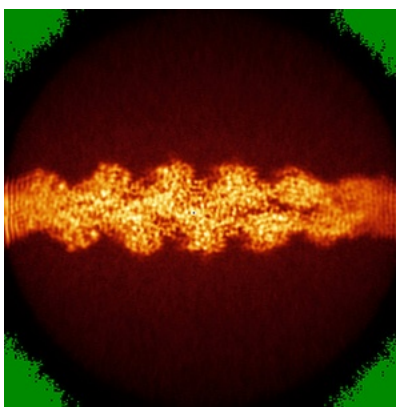
The images above show the largest variance slices of the map in three orthogonal directions.

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

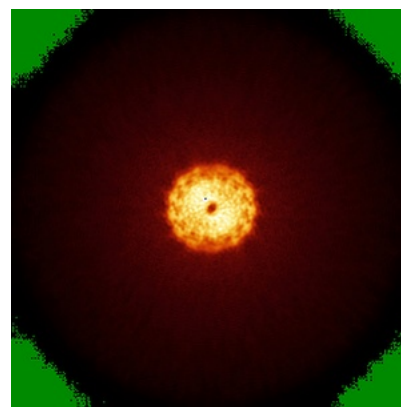
6.4.1 Primary map



X



Y

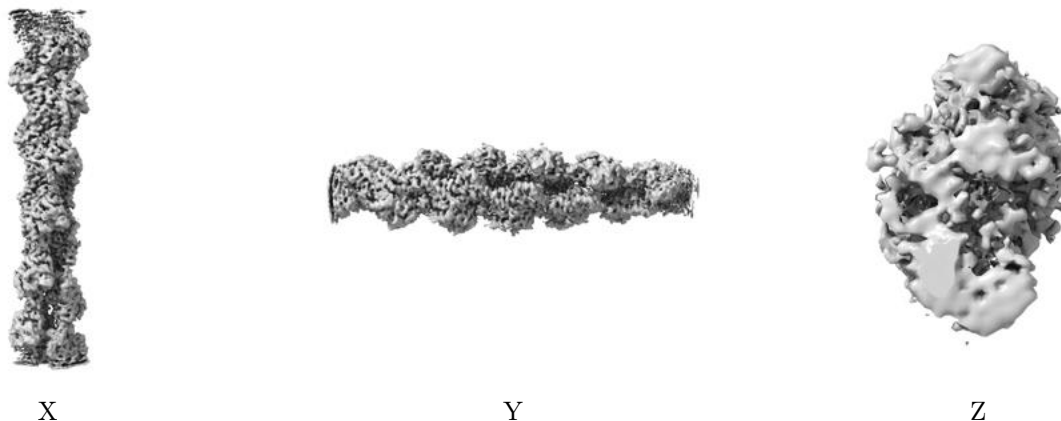


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0471. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

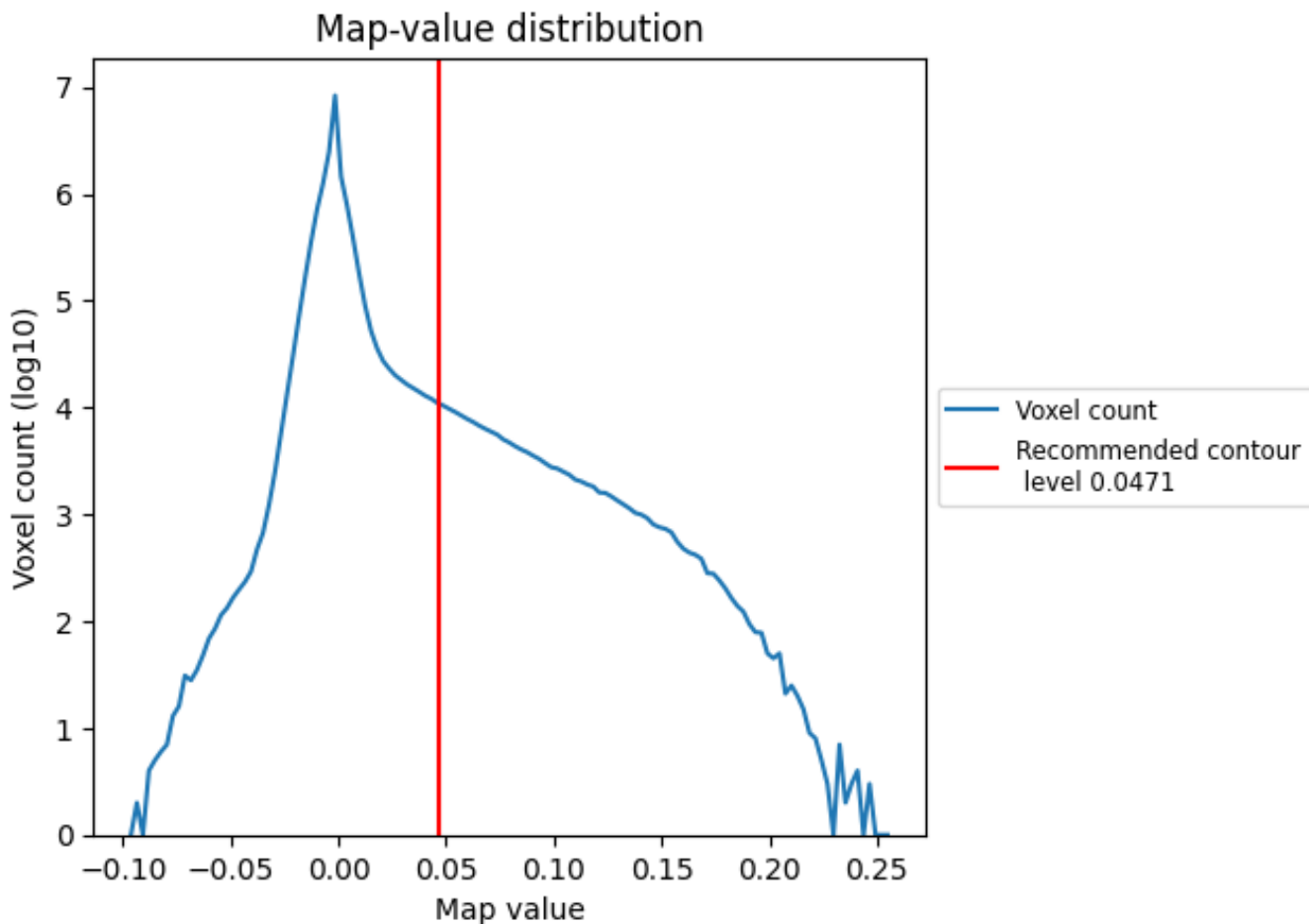
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

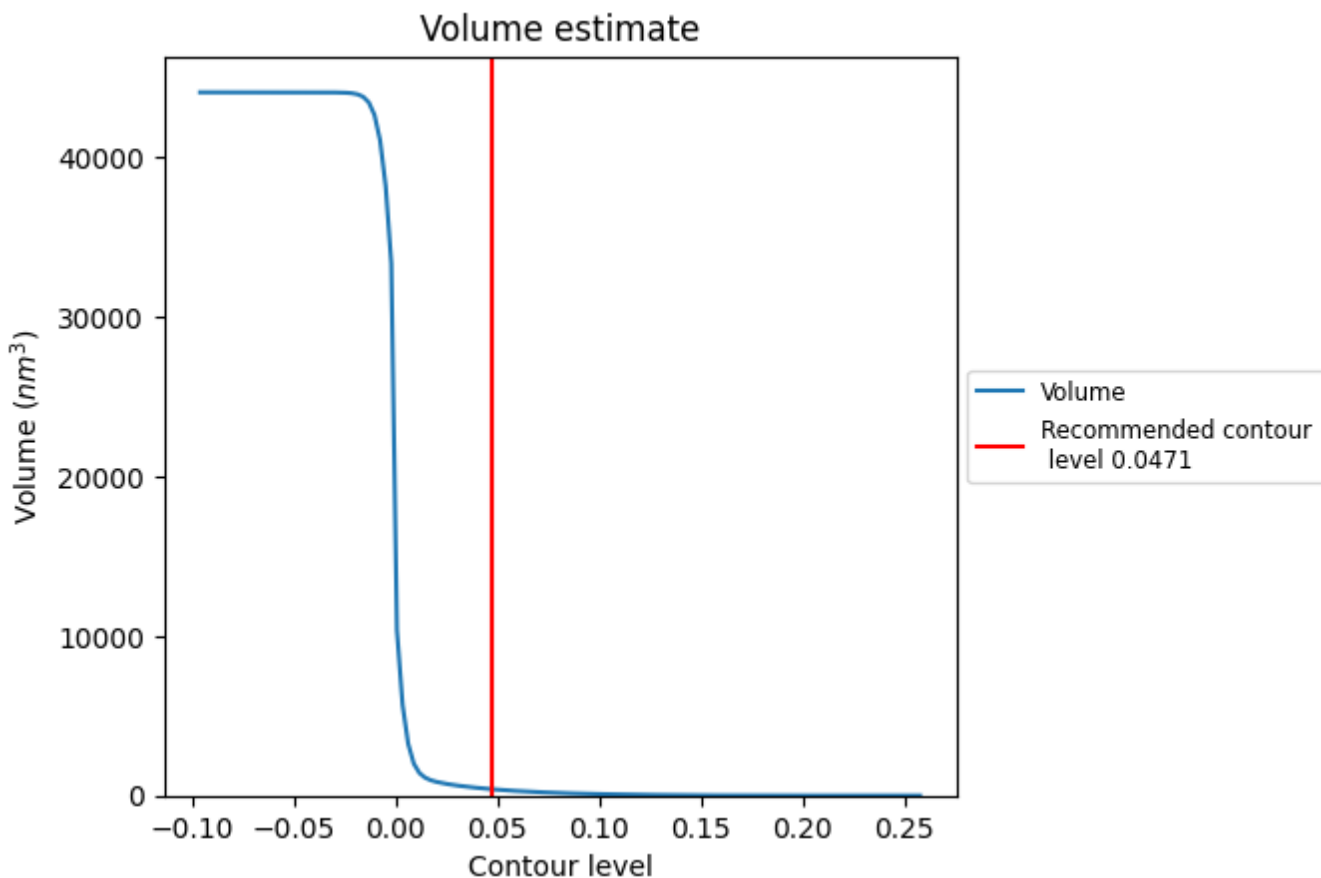
This section contains the results of statistical analysis of the map.

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.

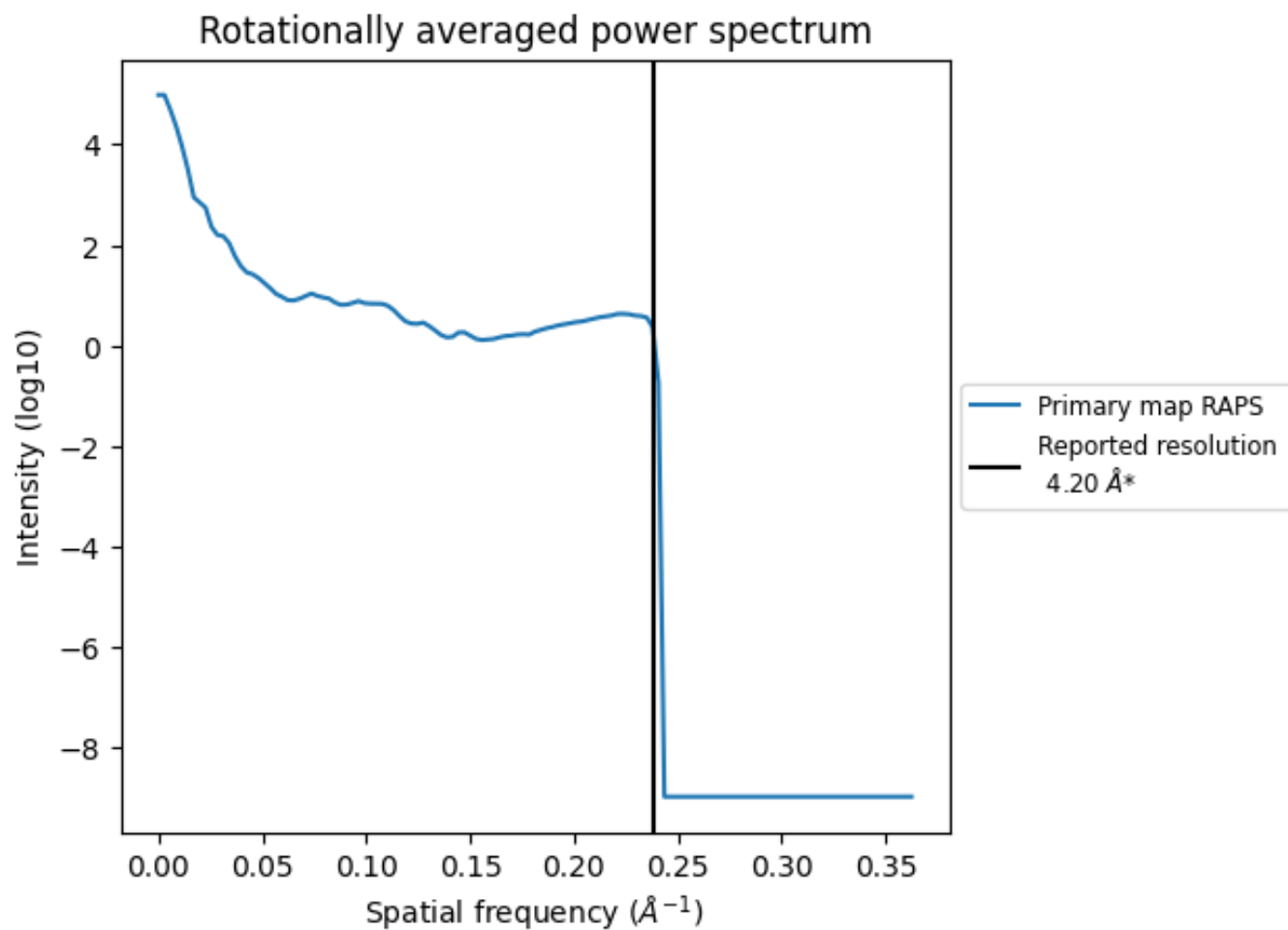
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 400 nm^3 ; this corresponds to an approximate mass of 362 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

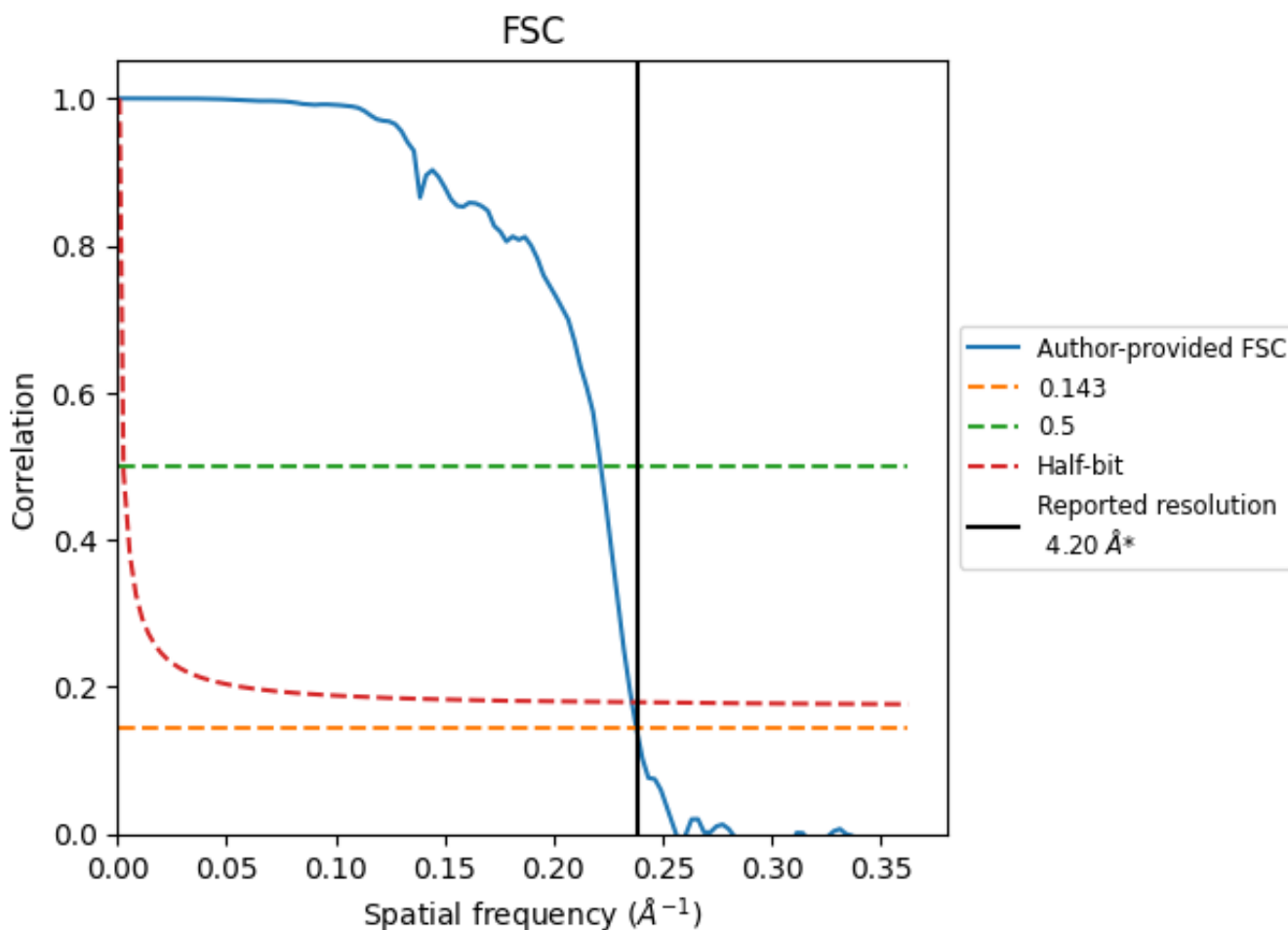


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

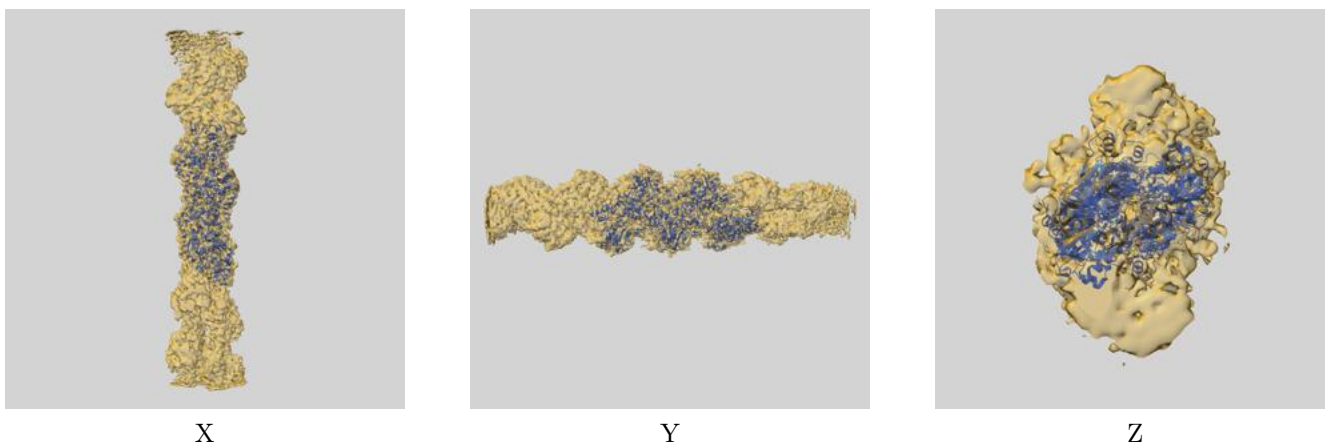
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.20	4.51	4.24
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

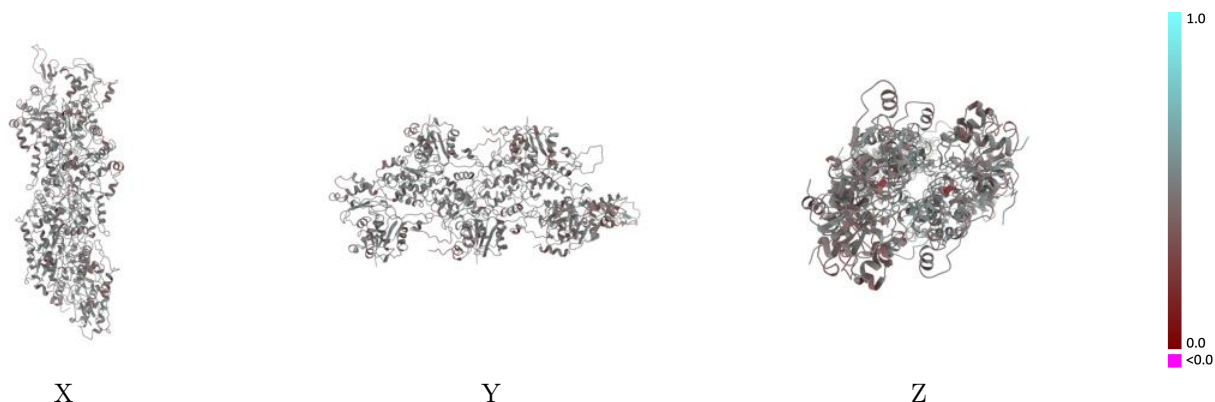
This section contains information regarding the fit between EMDB map EMD-30177 and PDB model 7BTE. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



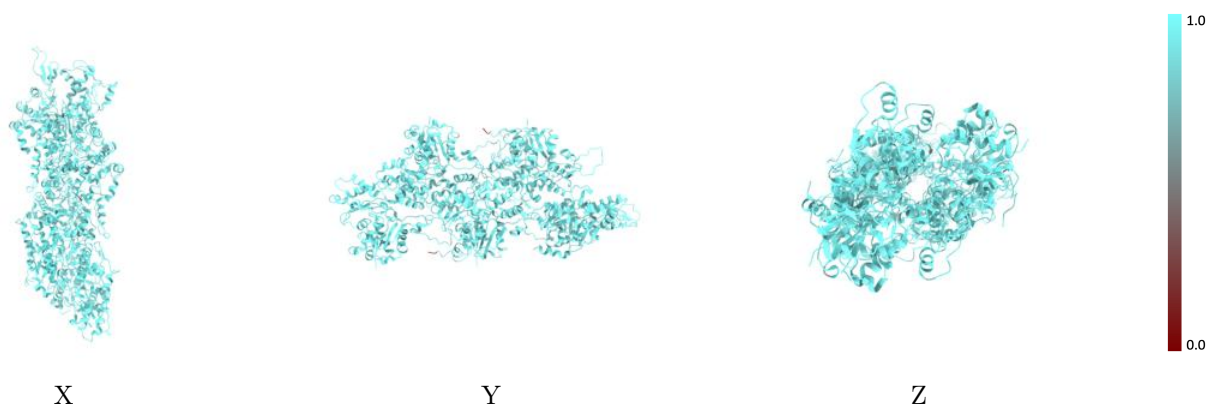
The images above show the 3D surface view of the map at the recommended contour level 0.0471 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



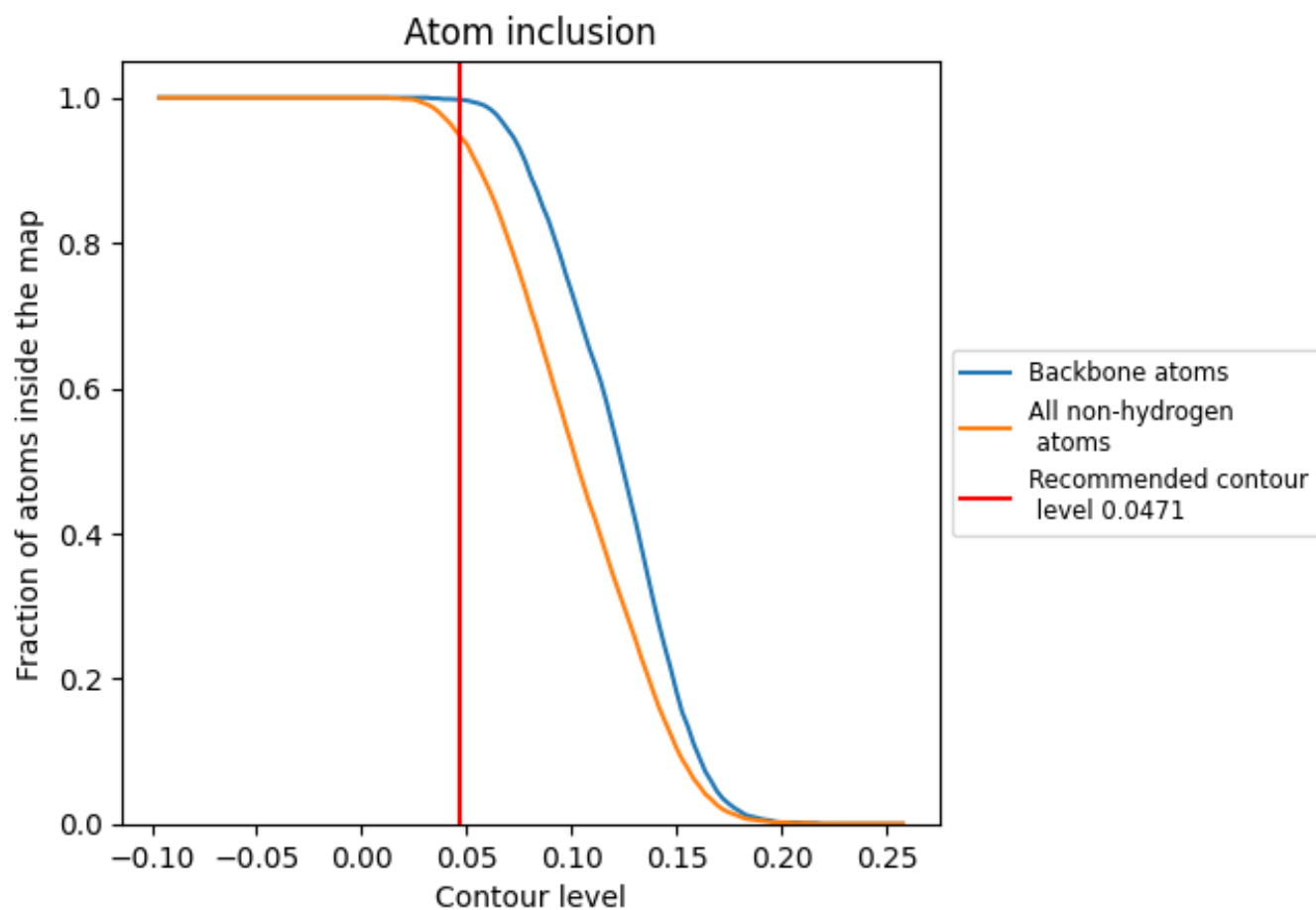
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0471).



















9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 95% 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 (0.0471) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9460	 0.4630
A	 0.9560	 0.4670
C	 0.9590	 0.4720
E	 0.9520	 0.4720
G	 0.9430	 0.4650
I	 0.9310	 0.4480
L	 0.8530	 0.3810
M	 0.7750	 0.3420
N	 0.9270	 0.4330

