



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 02:21 AM UTC

PDB ID : 8OO7 / pdb_00008oo7
EMDB ID : EMD-17006
Title : CryoEM Structure INO80core Hexasome complex composite model state1
Authors : Zhang, M.; Jungblut, A.; Hoffmann, T.; Eustermann, S.
Deposited on : 2023-04-04
Resolution : 2.80 Å(reported)
Based on initial models : 8AV6, 7OHC, 6FML, 3I62

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

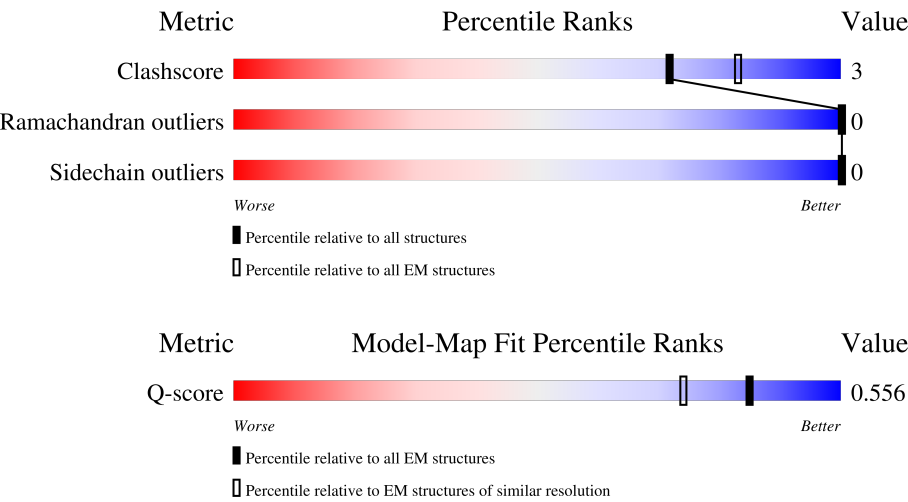
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 Å.

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



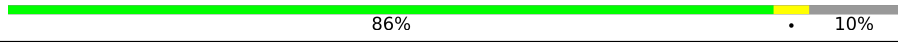
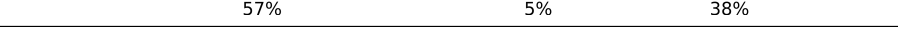
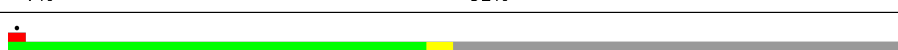
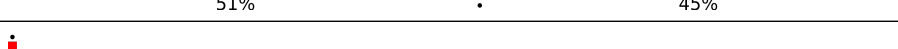
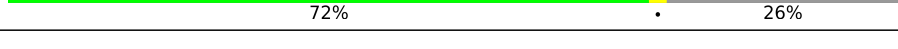
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	462	
1	B	462	
1	C	462	
2	D	488	

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Mol	Chain	Length	Quality of chain
2	E	488	
2	F	488	
3	G	1134	
4	H	492	
5	I	219	
6	J	769	
7	K	226	
8	L	226	
9	M	135	
9	Q	135	
10	N	102	
10	R	102	
11	O	129	
12	P	125	

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 41024 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 RuvB-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	449	Total	C	N	O	S	0	0
			3432	2154	610	653	15		
1	B	438	Total	C	N	O	S	0	0
			3352	2103	597	637	15		
1	C	459	Total	C	N	O	S	0	0
			3511	2199	627	670	15		

- Molecule 2 is a protein called RuvB-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	441	Total	C	N	O	S	0	0
			3401	2129	597	660	15		
2	E	443	Total	C	N	O	S	0	0
			3414	2136	600	663	15		
2	F	439	Total	C	N	O	S	0	0
			3394	2125	596	658	15		

- Molecule 3 is a protein called Chromatin-remodeling ATPase Ino80.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	704	Total	C	N	O	S	0	0
			5736	3657	1020	1024	35		

- Molecule 4 is a protein called Ino eighty subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	38	Total	C	N	O	S	0	0
			283	181	51	48	3		

- Molecule 5 is a protein called Chromatin-remodeling complex subunit IES6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	109	Total	C	N	O	S	0	0
			873	546	167	156	4		

- Molecule 6 is a protein called Actin-related protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	644	Total	C	N	O	S	0	0
			4545	2863	820	846	16		

- Molecule 7 is a DNA chain called DNA Strand 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	113	Total	C	N	O	P	0	0
			2306	1093	422	678	113		

- Molecule 8 is a DNA chain called DNA Strand 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	113	Total	C	N	O	P	0	0
			2327	1100	436	678	113		

- Molecule 9 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	74	Total	C	N	O	S	0	0
			602	381	113	104	4		
9	Q	98	Total	C	N	O	S	0	0
			810	511	157	138	4		

- Molecule 10 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	75	Total	C	N	O	S	0	0
			602	378	120	103	1		
10	R	80	Total	C	N	O	S	0	0
			638	401	125	111	1		

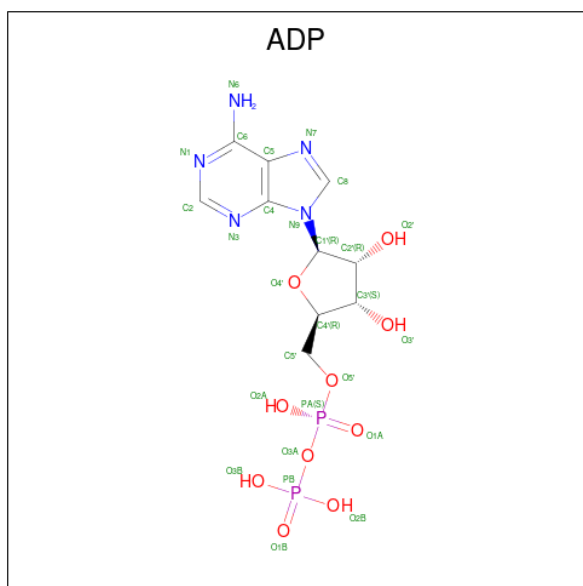
- Molecule 11 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	O	109	Total	C	N	O	0	0
			842	531	167	144		

- Molecule 12 is a protein called Histone H2B.

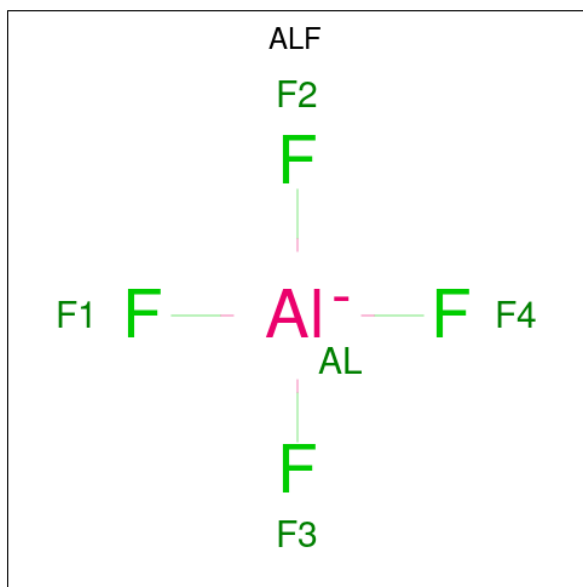
Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	93	Total	C	N	O	S	0	0
			729	458	131	138	2		

- Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	G	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 14 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4) (labeled as "Ligand of Interest" by depositor).

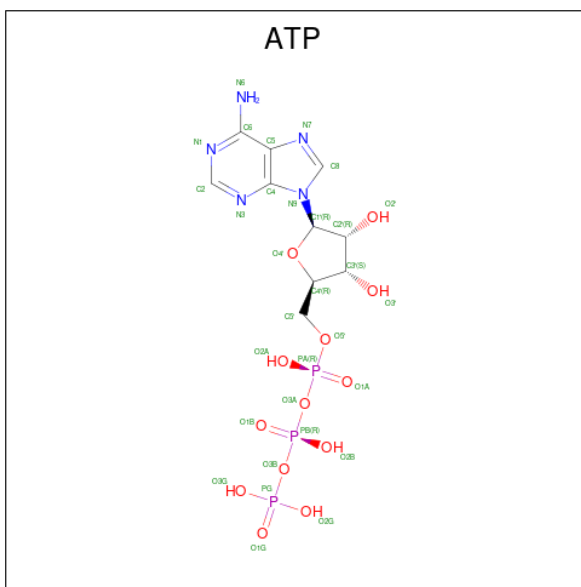


Mol	Chain	Residues	Atoms			AltConf
14	G	1	Total	Al	F	0
			5	1	4	

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
15	G	1	Total	Mg	0
			1	1	
15	J	1	Total	Mg	0
			1	1	

- Molecule 16 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

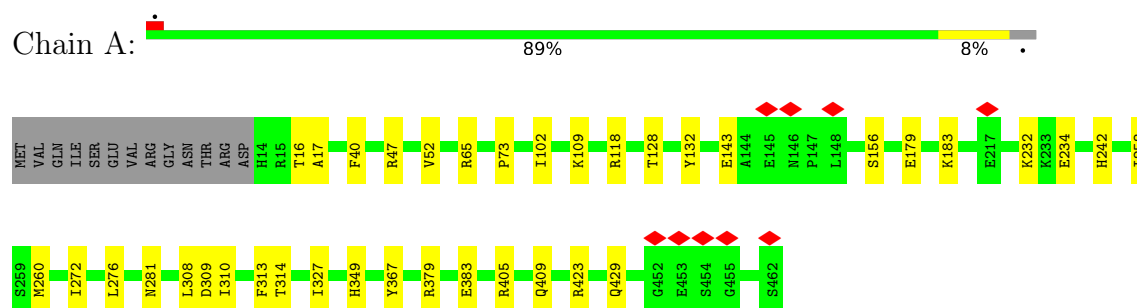


Mol	Chain	Residues	Atoms					AltConf
16	J	1	Total 31	C 10	N 5	O 13	P 3	0

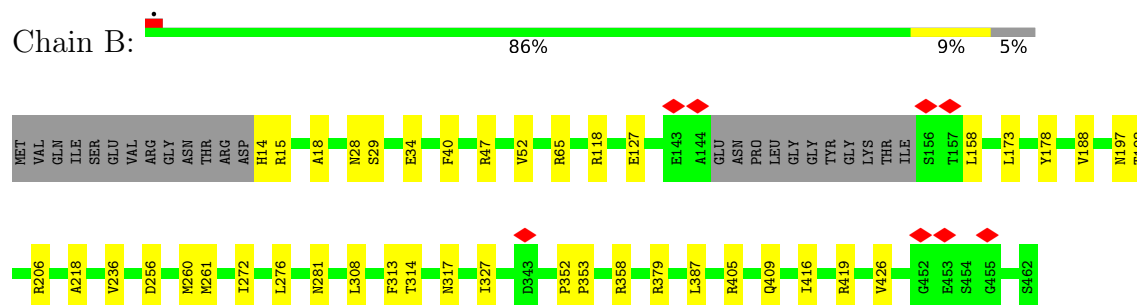
3 Residue-property plots [i](#)

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

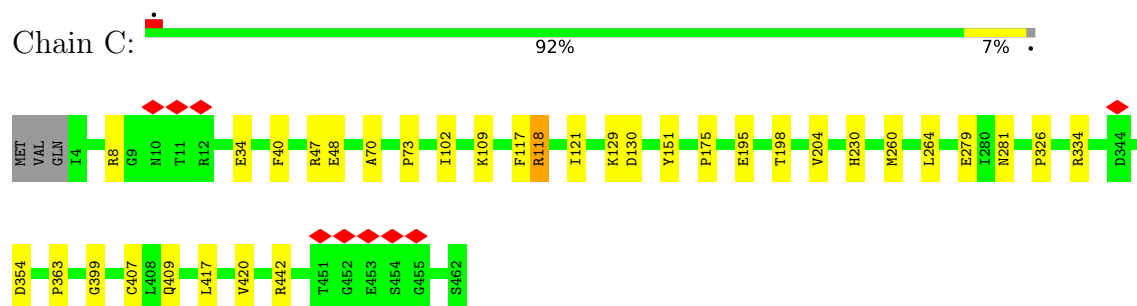
- Molecule 1: RuvB-like protein 1



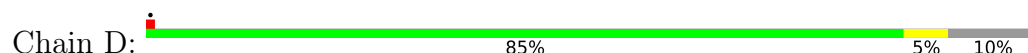
- Molecule 1: RuvB-like protein 1

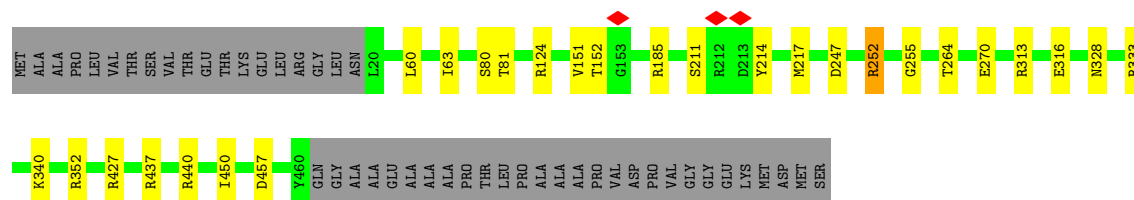


- Molecule 1: RuvB-like protein 1

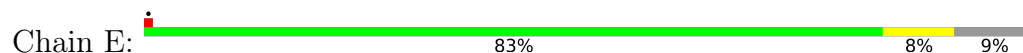


- Molecule 2: RuvB-like protein 2

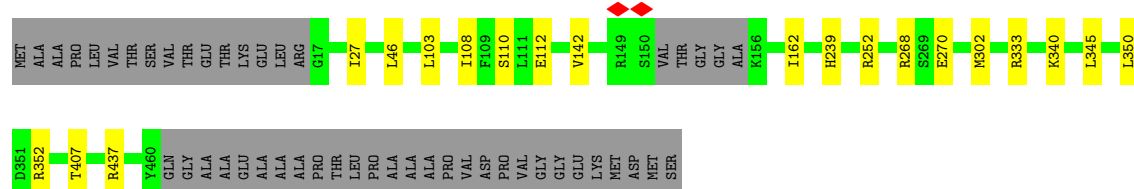
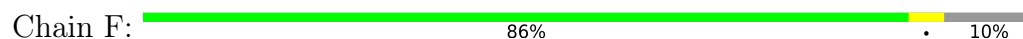




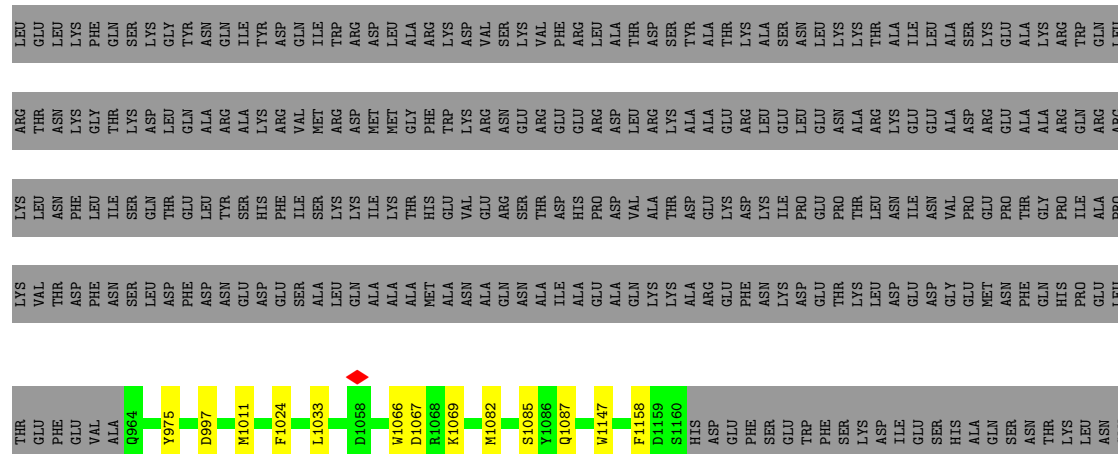
- Molecule 2: RuvB-like protein 2



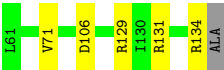
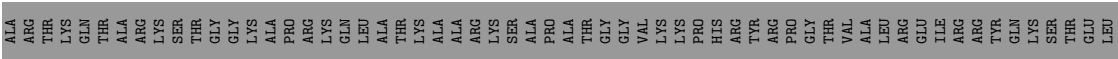
- Molecule 2: RuvB-like protein 2



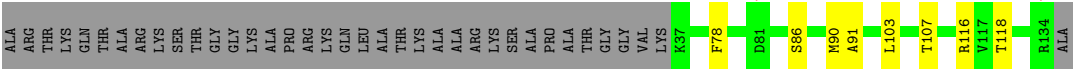
- Molecule 3: Chromatin-remodeling ATPase Ino80



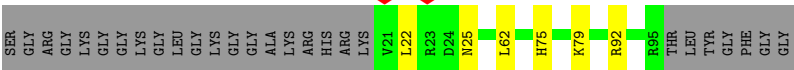




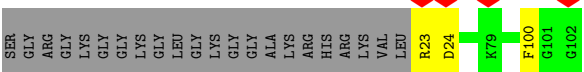
• Molecule 9: Histone H3.1



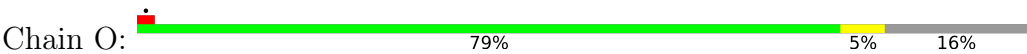
• Molecule 10: Histone H4



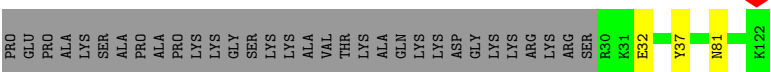
• Molecule 10: Histone H4



• Molecule 11: Histone H2A



• Molecule 12: Histone H2B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	72400	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.36	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	12.627	Depositor
Minimum map value	-4.257	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.266	Depositor
Recommended contour level	0.95	Depositor
Map size (Å)	295.92, 295.92, 295.92	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.14	0/3481	0.44	0/4703
1	B	0.14	0/3398	0.43	0/4589
1	C	0.14	0/3560	0.41	0/4809
2	D	0.13	0/3445	0.40	0/4640
2	E	0.13	0/3457	0.42	0/4654
2	F	0.14	0/3437	0.44	0/4627
3	G	0.15	0/5866	0.47	0/7926
4	H	0.13	0/290	0.44	0/393
5	I	0.14	0/893	0.42	0/1207
6	J	0.14	0/4637	0.43	0/6327
7	K	0.33	0/2584	0.72	0/3983
8	L	0.33	0/2612	0.71	0/4032
9	M	0.15	0/609	0.48	0/816
9	Q	0.14	0/822	0.44	0/1102
10	N	0.15	0/607	0.45	0/813
10	R	0.15	0/645	0.46	0/862
11	O	0.14	0/852	0.43	0/1147
12	P	0.14	0/740	0.44	0/993
All	All	0.18	0/41935	0.48	0/57623

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	C	0	3
2	D	0	1
2	E	0	1
2	F	0	2
6	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	N	0	1
All	All	0	9

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	118	ARG	Sidechain
1	C	334	ARG	Sidechain
1	C	8	ARG	Sidechain
2	D	252	ARG	Sidechain
2	E	313	ARG	Sidechain
2	F	252	ARG	Sidechain
2	F	437	ARG	Sidechain
6	J	626	GLU	Peptide
10	N	92	ARG	Sidechain

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	3432	0	3518	28	0
1	B	3352	0	3438	28	0
1	C	3511	0	3595	24	0
2	D	3401	0	3472	19	0
2	E	3414	0	3482	27	0
2	F	3394	0	3464	11	0
3	G	5736	0	5776	41	0
4	H	283	0	289	3	0
5	I	873	0	868	7	0
6	J	4545	0	3940	18	0
7	K	2306	0	1267	47	0
8	L	2327	0	1267	39	0
9	M	602	0	632	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	Q	810	0	851	6	0
10	N	602	0	651	4	0
10	R	638	0	676	3	0
11	O	842	0	908	5	0
12	P	729	0	751	3	0
13	A	27	0	12	2	0
13	B	27	0	12	1	0
13	C	27	0	12	0	0
13	D	27	0	12	0	0
13	E	27	0	12	2	0
13	F	27	0	12	0	0
13	G	27	0	12	0	0
14	G	5	0	0	0	0
15	G	1	0	0	0	0
15	J	1	0	0	0	0
16	J	31	0	12	1	0
All	All	41024	0	38941	262	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 3.

All (262) 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)
7:K:24:DA:H2''	7:K:25:DG:C8	2.18	0.79
8:L:-18:DG:H2''	8:L:-17:DT:C6	2.21	0.75
1:A:102:ILE:HG22	1:A:109:LYS:HB2	1.70	0.73
1:C:102:ILE:HG22	1:C:109:LYS:HB2	1.70	0.73
7:K:-70:DG:H2''	7:K:-69:DA:C8	2.23	0.73
3:G:975:TYR:O	3:G:1201:ARG:NH1	2.22	0.73
8:L:-37:DG:H2''	8:L:-36:DG:C8	2.27	0.70
7:K:8:DC:H2''	7:K:9:DG:C8	2.27	0.69
8:L:3:DC:H2''	8:L:4:DG:C8	2.28	0.68
7:K:15:DT:H2''	7:K:16:DA:C8	2.28	0.68
3:G:1693:LYS:NZ	7:K:34:DT:OP1	2.27	0.68
1:C:442:ARG:NH2	2:D:457:ASP:OD1	2.26	0.67
8:L:-6:DG:H2''	8:L:-5:DG:C8	2.30	0.66
1:B:317:ASN:OD1	1:B:358:ARG:NH1	2.28	0.66
1:B:18:ALA:O	1:B:379:ARG:NH1	2.29	0.66
2:D:124:ARG:NE	2:D:247:ASP:OD2	2.26	0.66
8:L:-17:DT:H2''	8:L:-16:DT:C5	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:GLU:OE2	3:G:1497:ARG:NE	2.26	0.63
5:I:30:ARG:HH22	6:J:133:GLU:HG2	1.63	0.62
7:K:-62:DC:H6	7:K:-62:DC:OP2	1.83	0.62
8:L:5:DT:H2''	8:L:6:DA:C8	2.35	0.61
1:A:258:ILE:HA	1:B:261:MET:HE1	1.83	0.61
5:I:162:SER:HB2	6:J:655:ALA:HA	1.82	0.61
7:K:-27:DC:H4'	7:K:-26:DT:H5'	1.83	0.61
7:K:25:DG:H2''	7:K:26:DG:C8	2.36	0.60
7:K:-47:DT:H2'	7:K:-47:DT:OP2	2.01	0.60
1:C:118:ARG:NH2	1:C:281:ASN:OD1	2.35	0.60
3:G:1608:ARG:NH2	8:L:-28:DC:OP2	2.33	0.60
7:K:-7:DG:H2''	7:K:-6:DT:C6	2.37	0.60
2:F:333:ARG:HA	2:F:340:LYS:HA	1.84	0.59
7:K:25:DG:OP2	7:K:25:DG:H2'	2.03	0.59
7:K:-48:DC:H2''	7:K:-47:DT:C5	2.37	0.59
1:A:409:GLN:HE22	2:D:352:ARG:C	2.09	0.59
5:I:184:THR:HG23	5:I:186:LEU:H	1.67	0.58
6:J:725:ILE:HG13	6:J:726:LEU:H	1.69	0.58
3:G:1583:ASP:OD1	3:G:1598:ARG:NH1	2.31	0.58
8:L:59:DA:H2''	8:L:60:DC:C6	2.38	0.58
7:K:-71:DG:H2''	7:K:-70:DG:C8	2.39	0.58
7:K:-48:DC:H2''	7:K:-47:DT:C6	2.38	0.58
7:K:-46:DC:H4'	7:K:-45:DA:H5'	1.86	0.58
8:L:15:DT:H2''	8:L:16:DA:C8	2.39	0.58
7:K:-36:DT:H2''	7:K:-35:DA:C8	2.39	0.57
1:A:349:HIS:NE2	2:E:438:SER:OG	2.32	0.57
1:A:409:GLN:NE2	2:D:352:ARG:O	2.35	0.57
8:L:-32:DT:H2''	8:L:-31:DA:C8	2.40	0.57
2:E:160:LEU:HD11	2:E:162:ILE:HD11	1.87	0.56
8:L:-39:DT:H2''	8:L:-38:DA:C8	2.41	0.56
7:K:-56:DC:OP2	7:K:-56:DC:H2'	2.06	0.56
1:B:28:ASN:OD1	1:B:29:SER:N	2.39	0.56
7:K:-58:DG:H2''	7:K:-57:DC:C5	2.41	0.56
1:B:272:ILE:HG23	1:B:276:LEU:HD23	1.87	0.56
8:L:-16:DT:H4'	8:L:-15:DA:H5'	1.88	0.56
8:L:35:DT:H2'	8:L:35:DT:OP2	2.06	0.55
3:G:1087:GLN:HG3	8:L:-28:DC:H4'	1.87	0.55
3:G:997:ASP:OD1	3:G:997:ASP:N	2.38	0.55
3:G:1147:TRP:NE1	3:G:1158:PHE:O	2.29	0.54
1:A:272:ILE:HG23	1:A:276:LEU:HD23	1.90	0.54
3:G:1284:PHE:HZ	3:G:1307:THR:HG23	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:MET:HE1	3:G:1394:ALA:HA	1.90	0.53
1:B:40:PHE:CG	1:B:47:ARG:HD3	2.43	0.53
7:K:-68:DG:N2	8:L:69:DT:O2	2.41	0.52
7:K:-35:DA:H2''	7:K:-34:DG:C8	2.44	0.52
8:L:62:DG:H2''	8:L:63:DG:C8	2.44	0.52
3:G:1284:PHE:CZ	3:G:1307:THR:HG23	2.43	0.52
2:E:105:ALA:HB3	2:E:302:MET:HB2	1.92	0.52
1:A:128:THR:HG23	1:A:234:GLU:HG2	1.92	0.52
6:J:249:LYS:NZ	6:J:631:HIS:O	2.41	0.52
7:K:-43:DT:H4'	11:O:14:ALA:HB1	1.91	0.52
8:L:14:DT:H2''	8:L:15:DT:C6	2.44	0.52
7:K:-67:DA:OP2	7:K:-67:DA:H8	1.93	0.52
3:G:1011:MET:HE2	3:G:1024:PHE:HB3	1.91	0.52
8:L:-15:DA:H2''	8:L:-14:DA:C8	2.45	0.52
1:A:183:LYS:NZ	1:A:260:MET:SD	2.72	0.51
7:K:4:DC:H2''	7:K:5:DC:C6	2.46	0.51
7:K:18:DC:H42	8:L:-18:DG:H1	1.58	0.51
1:B:127:GLU:OE2	1:B:197:ASN:ND2	2.40	0.51
7:K:-58:DG:H2''	7:K:-57:DC:C6	2.46	0.51
2:E:137:ILE:HD12	2:E:235:LYS:HD2	1.92	0.51
3:G:1632:GLY:O	3:G:1661:ARG:NH1	2.43	0.51
8:L:-18:DG:H2''	8:L:-17:DT:C5	2.46	0.51
1:A:40:PHE:CG	1:A:47:ARG:HD3	2.45	0.51
6:J:196:ARG:NH1	6:J:763:ASP:OD2	2.38	0.51
1:A:143:GLU:HA	1:A:156:SER:H	1.75	0.51
1:C:198:THR:O	2:D:185:ARG:NH1	2.44	0.51
1:A:118:ARG:NH2	1:A:281:ASN:OD1	2.35	0.50
7:K:25:DG:H4'	7:K:26:DG:H5'	1.93	0.50
1:C:34:GLU:O	1:C:47:ARG:NH2	2.29	0.50
3:G:1328:LYS:O	3:G:1333:ASN:ND2	2.44	0.50
7:K:4:DC:H2''	7:K:5:DC:C5	2.46	0.50
1:A:16:THR:HG21	1:A:383:GLU:HG2	1.94	0.50
1:A:405:ARG:NH2	13:A:501:ADP:O1B	2.39	0.50
1:B:409:GLN:O	2:E:71:ARG:NH1	2.42	0.50
2:D:313:ARG:NH1	2:D:316:GLU:OE2	2.37	0.50
8:L:-11:DC:H2''	8:L:-10:DG:H5'	1.94	0.50
1:B:314:THR:HG21	2:F:302:MET:HG3	1.94	0.50
8:L:-2:DC:H2''	8:L:-1:DA:C8	2.47	0.50
5:I:42:LYS:NZ	5:I:50:GLU:OE1	2.33	0.50
7:K:6:DC:H2''	7:K:7:DC:C5	2.47	0.49
8:L:-25:DC:H1'	8:L:-24:DT:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:41:DC:H2''	8:L:42:DA:C8	2.46	0.49
7:K:-57:DC:H2''	7:K:-56:DC:C5	2.48	0.49
7:K:4:DC:H2''	7:K:5:DC:C4	2.48	0.49
2:E:313:ARG:NH1	2:E:352:ARG:HH22	2.10	0.49
7:K:-36:DT:H2''	7:K:-35:DA:N7	2.28	0.49
2:D:80:SER:O	2:D:81:THR:HG22	2.13	0.48
7:K:33:DC:C6	7:K:34:DT:H72	2.48	0.48
8:L:54:DT:H2''	8:L:55:DC:C5	2.47	0.48
8:L:63:DG:H8	8:L:63:DG:OP2	1.96	0.48
8:L:-16:DT:H2''	8:L:-15:DA:C8	2.47	0.48
2:E:184:GLU:HG3	2:E:201:ILE:HB	1.95	0.48
8:L:-38:DA:H2''	8:L:-37:DG:C8	2.48	0.48
7:K:-16:DT:H2''	7:K:-15:DA:C8	2.49	0.48
2:F:239:HIS:ND1	3:G:1366:THR:HG23	2.28	0.48
3:G:1571:ARG:NH1	3:G:1621:ILE:O	2.47	0.48
1:C:40:PHE:CG	1:C:47:ARG:HD3	2.48	0.48
2:F:103:LEU:HD21	2:F:108:ILE:HD11	1.96	0.48
6:J:102:GLY:N	6:J:104:ASP:OD1	2.47	0.48
1:C:175:PRO:HB2	4:H:459:VAL:HG23	1.96	0.47
2:E:361:TYR:OH	13:E:501:ADP:N7	2.35	0.47
6:J:284:TYR:O	6:J:293:ARG:NH1	2.46	0.47
1:A:179:GLU:CD	3:G:1497:ARG:HE	2.16	0.47
1:A:367:TYR:OH	13:A:501:ADP:N7	2.31	0.47
1:B:256:ASP:HA	3:G:1385:ASP:HB3	1.96	0.47
8:L:5:DT:H2''	8:L:6:DA:N7	2.30	0.47
3:G:1657:GLN:O	3:G:1661:ARG:NH1	2.47	0.47
1:B:387:LEU:HD23	1:B:426:VAL:HB	1.97	0.47
6:J:268:ARG:HD3	16:J:802:ATP:C8	2.49	0.47
7:K:-27:DC:OP2	7:K:-27:DC:H2'	2.14	0.47
1:C:279:GLU:OE1	3:G:1452:LYS:NZ	2.39	0.47
2:D:211:SER:O	2:D:217:MET:HE1	2.14	0.47
2:D:255:GLY:N	3:G:1531:ASP:OD2	2.42	0.47
2:E:400:TYR:OH	2:E:432:PHE:O	2.21	0.47
9:Q:116:ARG:NH1	9:Q:118:THR:O	2.48	0.47
7:K:28:DG:H2''	7:K:29:DA:C8	2.50	0.47
11:O:26:PRO:HG3	12:P:37:TYR:CE2	2.50	0.46
3:G:1566:LYS:HD2	3:G:1594:TYR:CE1	2.50	0.46
1:B:52:VAL:HG11	2:F:407:THR:HG23	1.97	0.46
3:G:1554:LYS:HE2	3:G:1676:LEU:O	2.16	0.46
9:M:71:VAL:HG12	10:N:62:LEU:HD21	1.98	0.46
1:C:195:GLU:OE2	1:C:198:THR:OG1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:42:LYS:HE2	6:J:167:TYR:CZ	2.51	0.46
1:A:65:ARG:HB2	1:A:327:ILE:HD12	1.98	0.46
5:I:30:ARG:NH1	6:J:133:GLU:OE2	2.24	0.46
6:J:274:SER:O	6:J:701:ARG:NH1	2.49	0.46
2:E:212:ARG:NH1	9:Q:78:PHE:O	2.46	0.45
7:K:21:DC:OP2	7:K:21:DC:H6	1.99	0.45
1:B:158:LEU:HD23	1:B:173:LEU:HD22	1.98	0.45
1:A:17:ALA:O	1:A:379:ARG:NH2	2.42	0.45
1:C:73:PRO:HG3	2:D:450:ILE:HD11	1.98	0.45
8:L:14:DT:H2"	8:L:15:DT:C5	2.52	0.45
2:E:142:VAL:HA	2:E:162:ILE:HD13	1.99	0.45
2:F:268:ARG:NH1	2:F:270:GLU:OE2	2.48	0.45
3:G:1566:LYS:HD2	3:G:1594:TYR:HE1	1.80	0.45
1:B:405:ARG:NH2	13:B:501:ADP:O2B	2.44	0.45
10:R:23:ARG:HG3	10:R:24:ASP:H	1.81	0.45
3:G:1437:THR:O	3:G:1443:ARG:NH2	2.49	0.44
1:B:236:VAL:HG13	1:B:236:VAL:O	2.18	0.44
8:L:60:DC:OP2	8:L:60:DC:H6	2.00	0.44
3:G:1265:ARG:HG3	3:G:1682:ILE:HD11	1.99	0.44
8:L:-16:DT:H2"	8:L:-15:DA:N7	2.32	0.44
9:Q:86:SER:O	9:Q:90:MET:HG2	2.18	0.44
6:J:277:TYR:CD1	6:J:641:GLU:HG3	2.53	0.44
6:J:725:ILE:HG13	6:J:726:LEU:N	2.32	0.44
1:B:14:HIS:NE2	2:E:318:ASP:OD2	2.47	0.44
1:A:132:TYR:OH	2:E:185:ARG:NH2	2.47	0.44
3:G:1475:GLU:HG2	3:G:1491:MET:HE1	1.99	0.44
10:N:22:LEU:HB3	10:N:25:ASN:ND2	2.33	0.44
6:J:255:PRO:HB2	6:J:628:HIS:CE1	2.53	0.44
1:B:158:LEU:HD22	1:B:178:TYR:CD1	2.53	0.44
1:B:188:VAL:O	1:B:206:ARG:NH1	2.46	0.43
1:C:121:ILE:HD11	1:C:326:PRO:HD3	2.00	0.43
1:C:129:LYS:NZ	3:G:1408:ASP:OD2	2.42	0.43
7:K:-47:DT:H2"	7:K:-46:DC:C2	2.53	0.43
7:K:-16:DT:H2"	7:K:-15:DA:N7	2.33	0.43
8:L:34:DC:H2"	8:L:35:DT:C5	2.53	0.43
2:E:76:ALA:O	2:E:357:ASN:HA	2.19	0.43
7:K:9:DG:N7	7:K:10:DC:N4	2.67	0.43
11:O:64:GLU:HG3	11:O:65:LEU:N	2.33	0.43
9:Q:91:ALA:HA	10:R:100:PHE:CZ	2.53	0.43
2:E:248:VAL:HG22	2:E:267:ILE:HD11	2.00	0.43
6:J:639:VAL:HB	6:J:640:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:ILE:HD12	1:B:419:ARG:HH21	1.83	0.43
1:C:204:VAL:HG21	3:G:1406:VAL:HG21	2.00	0.43
1:C:417:LEU:HA	1:C:420:VAL:HG22	2.01	0.43
3:G:1066:TRP:CZ2	3:G:1082:MET:HE1	2.53	0.43
1:C:48:GLU:OE1	2:D:427:ARG:NH2	2.39	0.43
2:E:134:GLU:OE1	2:E:234:ARG:NH1	2.49	0.43
2:F:27:ILE:HG23	2:F:46:LEU:HD11	2.00	0.43
4:H:442:ARG:NH2	4:H:464:GLU:OE2	2.51	0.43
1:A:310:ILE:HG23	2:E:302:MET:HE1	2.00	0.43
1:C:399:GLY:N	1:C:407:CYS:SG	2.92	0.43
2:F:345:LEU:HD12	2:F:350:LEU:HD21	2.01	0.43
7:K:-69:DA:OP2	7:K:-69:DA:H8	2.01	0.43
8:L:28:DA:OP1	10:N:79:LYS:N	2.38	0.43
1:A:52:VAL:HG11	2:E:407:THR:HG23	2.01	0.43
1:A:314:THR:HG21	2:E:302:MET:HG3	2.01	0.43
11:O:24:GLN:N	11:O:56:GLU:OE1	2.48	0.43
8:L:-19:DG:H2''	8:L:-18:DG:C8	2.54	0.42
9:M:106:ASP:OD2	9:M:131:ARG:NH1	2.43	0.42
2:E:60:LEU:HA	2:E:63:ILE:HD12	2.00	0.42
1:A:109:LYS:NZ	1:A:309:ASP:OD2	2.49	0.42
1:C:117:PHE:CE2	1:C:326:PRO:HD2	2.54	0.42
7:K:26:DG:OP2	7:K:26:DG:H2'	2.19	0.42
1:B:118:ARG:NH2	1:B:281:ASN:OD1	2.49	0.42
1:C:264:LEU:HD21	3:G:1393:LEU:HD11	2.00	0.42
2:D:214:TYR:O	2:D:217:MET:HE2	2.18	0.42
6:J:62:ASP:OD2	6:J:69:ARG:NH2	2.51	0.42
10:N:75:HIS:HD2	12:P:81:ASN:ND2	2.17	0.42
2:D:151:VAL:O	2:D:152:THR:OG1	2.33	0.42
1:A:423:ARG:NH2	1:A:429:GLN:OE1	2.47	0.42
1:B:14:HIS:CG	1:B:15:ARG:N	2.87	0.42
2:D:60:LEU:HA	2:D:63:ILE:HD12	2.01	0.42
7:K:-47:DT:H2''	7:K:-46:DC:C6	2.54	0.42
8:L:63:DG:H2''	8:L:64:DG:C8	2.54	0.42
1:A:242:HIS:ND1	2:D:270:GLU:OE2	2.53	0.42
1:A:308:LEU:HB2	1:A:313:PHE:CZ	2.54	0.42
7:K:-6:DT:H2''	7:K:-5:DA:C8	2.55	0.42
1:B:308:LEU:HB2	1:B:313:PHE:CZ	2.55	0.42
1:C:354:ASP:OD2	2:D:328:ASN:ND2	2.33	0.42
3:G:1586:GLU:HB2	3:G:1596:TYR:CZ	2.55	0.42
3:G:1660:ASP:O	3:G:1664:ARG:HG3	2.20	0.42
9:Q:91:ALA:HA	10:R:100:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ARG:HB2	1:B:327:ILE:HD12	2.02	0.42
3:G:1475:GLU:CD	3:G:1487:ARG:HE	2.27	0.42
3:G:1575:TYR:HA	3:G:1626:LEU:O	2.20	0.42
1:C:130:ASP:OD1	1:C:230:HIS:HE1	2.02	0.42
7:K:4:DC:H2''	7:K:5:DC:C2	2.55	0.42
1:B:198:THR:HA	3:G:1341:LYS:HD2	2.02	0.41
1:B:352:PRO:HA	1:B:353:PRO:HD3	1.95	0.41
1:C:70:ALA:O	1:C:363:PRO:HA	2.19	0.41
2:D:333:ARG:HA	2:D:340:LYS:HA	2.02	0.41
7:K:5:DC:OP2	7:K:5:DC:H2'	2.20	0.41
2:E:119:LEU:HD21	2:E:311:ILE:HG13	2.02	0.41
3:G:1367:TRP:CD1	3:G:1367:TRP:H	2.38	0.41
1:A:232:LYS:HB2	3:G:1294:PHE:HZ	1.86	0.41
9:M:129:ARG:HA	9:M:134:ARG:HB2	2.02	0.41
9:Q:103:LEU:O	9:Q:107:THR:HG23	2.21	0.41
1:C:151:TYR:CG	4:H:460:ALA:HB1	2.56	0.41
2:E:300:VAL:HG21	2:E:325:MET:SD	2.60	0.41
2:F:110:SER:OG	2:F:112:GLU:HG2	2.20	0.41
2:F:142:VAL:HA	2:F:162:ILE:HD13	2.03	0.41
2:D:437:ARG:HG3	2:D:440:ARG:NH2	2.36	0.41
7:K:-67:DA:OP2	7:K:-67:DA:C8	2.72	0.41
3:G:1033:LEU:HD11	3:G:1085:SER:HB2	2.03	0.41
3:G:1067:ASP:OD1	3:G:1069:LYS:N	2.53	0.41
2:E:126:SER:HB2	2:E:321:PRO:HG3	2.03	0.41
8:L:36:DA:N7	8:L:37:DC:N4	2.69	0.41
1:A:73:PRO:O	2:E:448:ARG:NH2	2.54	0.41
1:B:34:GLU:O	1:B:47:ARG:NH2	2.28	0.41
1:B:260:MET:HE3	1:B:261:MET:HE2	2.03	0.41
2:E:98:VAL:CG1	2:E:293:GLY:HA2	2.50	0.41
6:J:233:TRP:HE1	6:J:238:MET:HG2	1.86	0.41
11:O:32:ARG:HH22	12:P:32:GLU:CD	2.27	0.41
1:B:218:ALA:O	2:E:176:LYS:HE3	2.21	0.40
3:G:1444:ASP:HA	3:G:1447:ASN:ND2	2.36	0.40
8:L:4:DG:H1'	8:L:5:DT:C2	2.56	0.40
1:C:409:GLN:HE22	2:F:352:ARG:C	2.29	0.40
2:D:252:ARG:NH2	2:D:264:THR:HA	2.37	0.40
5:I:162:SER:HB2	6:J:655:ALA:CA	2.49	0.40
7:K:-6:DT:H2''	7:K:-5:DA:N7	2.36	0.40
8:L:11:DC:H2''	8:L:12:DG:C8	2.57	0.40
2:E:47:VAL:O	13:E:501:ADP:N6	2.54	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	447/462 (97%)	436 (98%)	11 (2%)	0	100	100
1	B	434/462 (94%)	418 (96%)	16 (4%)	0	100	100
1	C	457/462 (99%)	449 (98%)	8 (2%)	0	100	100
2	D	439/488 (90%)	435 (99%)	4 (1%)	0	100	100
2	E	439/488 (90%)	431 (98%)	8 (2%)	0	100	100
2	F	435/488 (89%)	427 (98%)	8 (2%)	0	100	100
3	G	698/1134 (62%)	676 (97%)	22 (3%)	0	100	100
4	H	36/492 (7%)	34 (94%)	2 (6%)	0	100	100
5	I	105/219 (48%)	104 (99%)	1 (1%)	0	100	100
6	J	632/769 (82%)	615 (97%)	17 (3%)	0	100	100
9	M	72/135 (53%)	71 (99%)	1 (1%)	0	100	100
9	Q	96/135 (71%)	95 (99%)	1 (1%)	0	100	100
10	N	73/102 (72%)	72 (99%)	1 (1%)	0	100	100
10	R	78/102 (76%)	76 (97%)	2 (3%)	0	100	100
11	O	107/129 (83%)	106 (99%)	1 (1%)	0	100	100
12	P	91/125 (73%)	89 (98%)	2 (2%)	0	100	100
All	All	4639/6192 (75%)	4534 (98%)	105 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/377 (97%)	365 (100%)	0	100	100
1	B	357/377 (95%)	357 (100%)	0	100	100
1	C	374/377 (99%)	374 (100%)	0	100	100
2	D	369/402 (92%)	369 (100%)	0	100	100
2	E	370/402 (92%)	370 (100%)	0	100	100
2	F	369/402 (92%)	369 (100%)	0	100	100
3	G	625/989 (63%)	625 (100%)	0	100	100
4	H	30/398 (8%)	30 (100%)	0	100	100
5	I	93/171 (54%)	93 (100%)	0	100	100
6	J	372/644 (58%)	372 (100%)	0	100	100
9	M	64/110 (58%)	64 (100%)	0	100	100
9	Q	86/110 (78%)	86 (100%)	0	100	100
10	N	63/78 (81%)	63 (100%)	0	100	100
10	R	65/78 (83%)	65 (100%)	0	100	100
11	O	85/98 (87%)	85 (100%)	0	100	100
12	P	80/105 (76%)	80 (100%)	0	100	100
All	All	3767/5118 (74%)	3767 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	86	GLN
1	A	116	ASN
1	A	248	ASN
1	A	458	HIS
1	C	86	GLN
1	C	230	HIS
1	C	263	GLN
1	C	458	HIS
2	D	24	HIS
2	D	394	GLN
2	E	24	HIS
2	F	19	ASN
2	F	244	HIS
2	F	359	HIS

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Mol	Chain	Res	Type
3	G	969	ASN
3	G	1151	HIS
3	G	1345	HIS
3	G	1577	GLN
4	H	452	ASN
6	J	628	HIS
9	M	113	HIS
11	O	24	GLN
12	P	81	ASN
9	Q	85	GLN
10	R	75	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	$\# Z > 2$
13	ADP	B	501	-	28,29,29	1.38	4 (14%)	43,45,45	1.82	8 (18%)
14	ALF	G	1901	-	4,4,4	1.42	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	ADP	F	501	-	28,29,29	1.40	4 (14%)	43,45,45	1.80	8 (18%)
13	ADP	A	501	-	28,29,29	1.38	4 (14%)	43,45,45	1.77	7 (16%)
13	ADP	G	1902	15	28,29,29	1.38	4 (14%)	43,45,45	1.77	7 (16%)
13	ADP	C	501	-	28,29,29	1.40	4 (14%)	43,45,45	1.78	7 (16%)
16	ATP	J	802	15	32,33,33	0.52	1 (3%)	48,52,52	0.32	0
13	ADP	D	501	-	28,29,29	1.38	4 (14%)	43,45,45	1.79	9 (20%)
13	ADP	E	501	-	28,29,29	1.38	4 (14%)	43,45,45	1.78	9 (20%)

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
13	ADP	B	501	-	-	7/16/32/32	0/3/3/3
13	ADP	F	501	-	-	1/16/32/32	0/3/3/3
13	ADP	A	501	-	-	5/16/32/32	0/3/3/3
13	ADP	G	1902	15	-	2/16/32/32	0/3/3/3
13	ADP	C	501	-	-	1/16/32/32	0/3/3/3
16	ATP	J	802	15	-	4/22/38/38	0/3/3/3
13	ADP	D	501	-	-	1/16/32/32	0/3/3/3
13	ADP	E	501	-	-	6/16/32/32	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F	501	ADP	C5-C4	4.65	1.47	1.39
13	C	501	ADP	C5-C4	4.57	1.47	1.39
13	B	501	ADP	C5-C4	4.55	1.47	1.39
13	G	1902	ADP	C5-C4	4.51	1.47	1.39
13	E	501	ADP	C5-C4	4.50	1.47	1.39
13	D	501	ADP	C5-C4	4.49	1.47	1.39
13	A	501	ADP	C5-C4	4.49	1.47	1.39
13	F	501	ADP	C5-C6	2.74	1.48	1.41
13	C	501	ADP	C5-C6	2.70	1.48	1.41
13	E	501	ADP	C5-C6	2.65	1.48	1.41
13	G	1902	ADP	C5-C6	2.65	1.48	1.41
13	B	501	ADP	C5-C6	2.64	1.48	1.41
13	D	501	ADP	C5-C6	2.58	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	501	ADP	C5-C6	2.57	1.48	1.41
13	A	501	ADP	C5-N7	-2.42	1.34	1.39
13	C	501	ADP	C5-N7	-2.37	1.34	1.39
13	E	501	ADP	C5-N7	-2.36	1.34	1.39
13	E	501	ADP	C8-N7	2.35	1.36	1.31
13	B	501	ADP	C5-N7	-2.33	1.34	1.39
13	D	501	ADP	C5-N7	-2.33	1.34	1.39
13	F	501	ADP	C5-N7	-2.32	1.34	1.39
13	G	1902	ADP	C5-N7	-2.31	1.34	1.39
13	G	1902	ADP	C8-N7	2.29	1.36	1.31
13	B	501	ADP	C8-N7	2.28	1.36	1.31
13	C	501	ADP	C8-N7	2.26	1.36	1.31
13	D	501	ADP	C8-N7	2.25	1.36	1.31
13	F	501	ADP	C8-N7	2.25	1.36	1.31
16	J	802	ATP	PB-O3B	-2.20	1.57	1.59
13	A	501	ADP	C8-N7	2.11	1.35	1.31

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	F	501	ADP	C5-C4-N3	-6.13	118.28	126.72
13	B	501	ADP	C5-C4-N3	-6.01	118.44	126.72
13	C	501	ADP	C5-C4-N3	-6.01	118.44	126.72
13	A	501	ADP	C5-C4-N3	-6.00	118.45	126.72
13	G	1902	ADP	C5-C4-N3	-5.90	118.59	126.72
13	D	501	ADP	C5-C4-N3	-5.88	118.62	126.72
13	E	501	ADP	C5-C4-N3	-5.81	118.72	126.72
13	A	501	ADP	N3-C4-N9	4.87	135.46	127.17
13	B	501	ADP	N3-C4-N9	4.77	135.29	127.17
13	F	501	ADP	N3-C4-N9	4.76	135.26	127.17
13	C	501	ADP	N3-C4-N9	4.71	135.17	127.17
13	D	501	ADP	N3-C4-N9	4.68	135.13	127.17
13	G	1902	ADP	N3-C4-N9	4.59	134.97	127.17
13	E	501	ADP	N3-C4-N9	4.54	134.89	127.17
13	B	501	ADP	C2-N3-C4	3.83	121.19	111.83
13	F	501	ADP	C2-N3-C4	3.78	121.07	111.83
13	C	501	ADP	C2-N3-C4	3.75	120.98	111.83
13	G	1902	ADP	C2-N3-C4	3.71	120.90	111.83
13	D	501	ADP	C2-N3-C4	3.68	120.83	111.83
13	A	501	ADP	C2-N3-C4	3.68	120.81	111.83
13	E	501	ADP	C2-N3-C4	3.64	120.71	111.83
13	F	501	ADP	C4-C5-N7	-3.54	106.54	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	501	ADP	C4-C5-N7	-3.47	106.61	110.58
13	D	501	ADP	C4-C5-N7	-3.43	106.67	110.58
13	E	501	ADP	C4-C5-N7	-3.42	106.67	110.58
13	G	1902	ADP	C4-C5-N7	-3.37	106.73	110.58
13	B	501	ADP	C4-C5-N7	-3.30	106.81	110.58
13	B	501	ADP	N3-C2-N1	-3.30	123.59	128.58
13	A	501	ADP	C4-C5-N7	-3.23	106.89	110.58
13	F	501	ADP	N3-C2-N1	-3.22	123.70	128.58
13	A	501	ADP	N3-C2-N1	-3.21	123.72	128.58
13	D	501	ADP	N3-C2-N1	-3.19	123.75	128.58
13	G	1902	ADP	N3-C2-N1	-3.15	123.81	128.58
13	C	501	ADP	N3-C2-N1	-3.13	123.84	128.58
13	E	501	ADP	N3-C2-N1	-3.12	123.86	128.58
13	D	501	ADP	C4-N9-C8	2.71	108.58	105.74
13	E	501	ADP	C4-N9-C8	2.64	108.51	105.74
13	A	501	ADP	C4-N9-C8	2.61	108.48	105.74
13	D	501	ADP	C5-N7-C8	2.57	107.49	103.45
13	B	501	ADP	C4-N9-C8	2.55	108.42	105.74
13	E	501	ADP	C5-N7-C8	2.51	107.40	103.45
13	F	501	ADP	C5-N7-C8	2.51	107.40	103.45
13	C	501	ADP	C4-N9-C8	2.50	108.36	105.74
13	C	501	ADP	C5-N7-C8	2.50	107.38	103.45
13	G	1902	ADP	C4-N9-C8	2.46	108.33	105.74
13	B	501	ADP	C5-N7-C8	2.42	107.25	103.45
13	A	501	ADP	C5-N7-C8	2.41	107.24	103.45
13	G	1902	ADP	C5-N7-C8	2.36	107.16	103.45
13	F	501	ADP	C4-N9-C8	2.36	108.21	105.74
13	D	501	ADP	N9-C8-N7	-2.06	111.01	113.94
13	B	501	ADP	C3'-C2'-C1'	2.06	105.36	101.46
13	E	501	ADP	N9-C8-N7	-2.04	111.04	113.94
13	E	501	ADP	C6-C5-N7	2.02	135.99	132.09
13	F	501	ADP	C6-C5-N7	2.01	135.96	132.09
13	D	501	ADP	C6-C5-N7	2.00	135.96	132.09

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	501	ADP	PA-O3A-PB-O2B
13	A	501	ADP	PA-O3A-PB-O3B
13	A	501	ADP	C5'-O5'-PA-O1A
13	A	501	ADP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
13	B	501	ADP	PA-O3A-PB-O3B
13	B	501	ADP	C5'-O5'-PA-O2A
13	E	501	ADP	C5'-O5'-PA-O1A
13	E	501	ADP	C5'-O5'-PA-O3A
13	G	1902	ADP	PA-O3A-PB-O2B
13	E	501	ADP	PA-O3A-PB-O1B
16	J	802	ATP	C3'-C4'-C5'-O5'
16	J	802	ATP	PB-O3B-PG-O3G
13	A	501	ADP	C5'-O5'-PA-O2A
13	B	501	ADP	C5'-O5'-PA-O1A
13	B	501	ADP	C5'-O5'-PA-O3A
13	E	501	ADP	C5'-O5'-PA-O2A
13	D	501	ADP	PA-O3A-PB-O1B
13	G	1902	ADP	PA-O3A-PB-O1B
13	E	501	ADP	C4'-C5'-O5'-PA
13	B	501	ADP	C4'-C5'-O5'-PA
13	C	501	ADP	C4'-C5'-O5'-PA
13	B	501	ADP	PA-O3A-PB-O1B
16	J	802	ATP	PB-O3B-PG-O1G
13	B	501	ADP	PA-O3A-PB-O2B
13	E	501	ADP	PA-O3A-PB-O2B
16	J	802	ATP	PB-O3B-PG-O2G
13	F	501	ADP	PB-O3A-PA-O2A

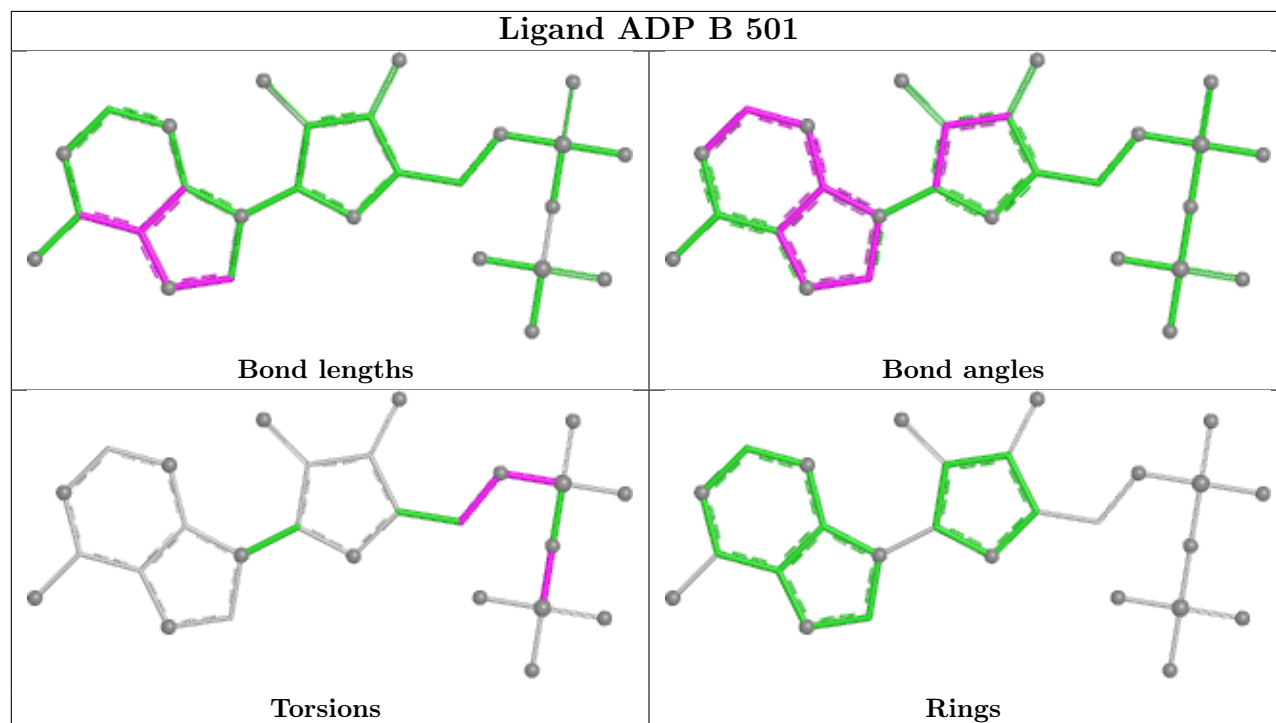
There are no ring outliers.

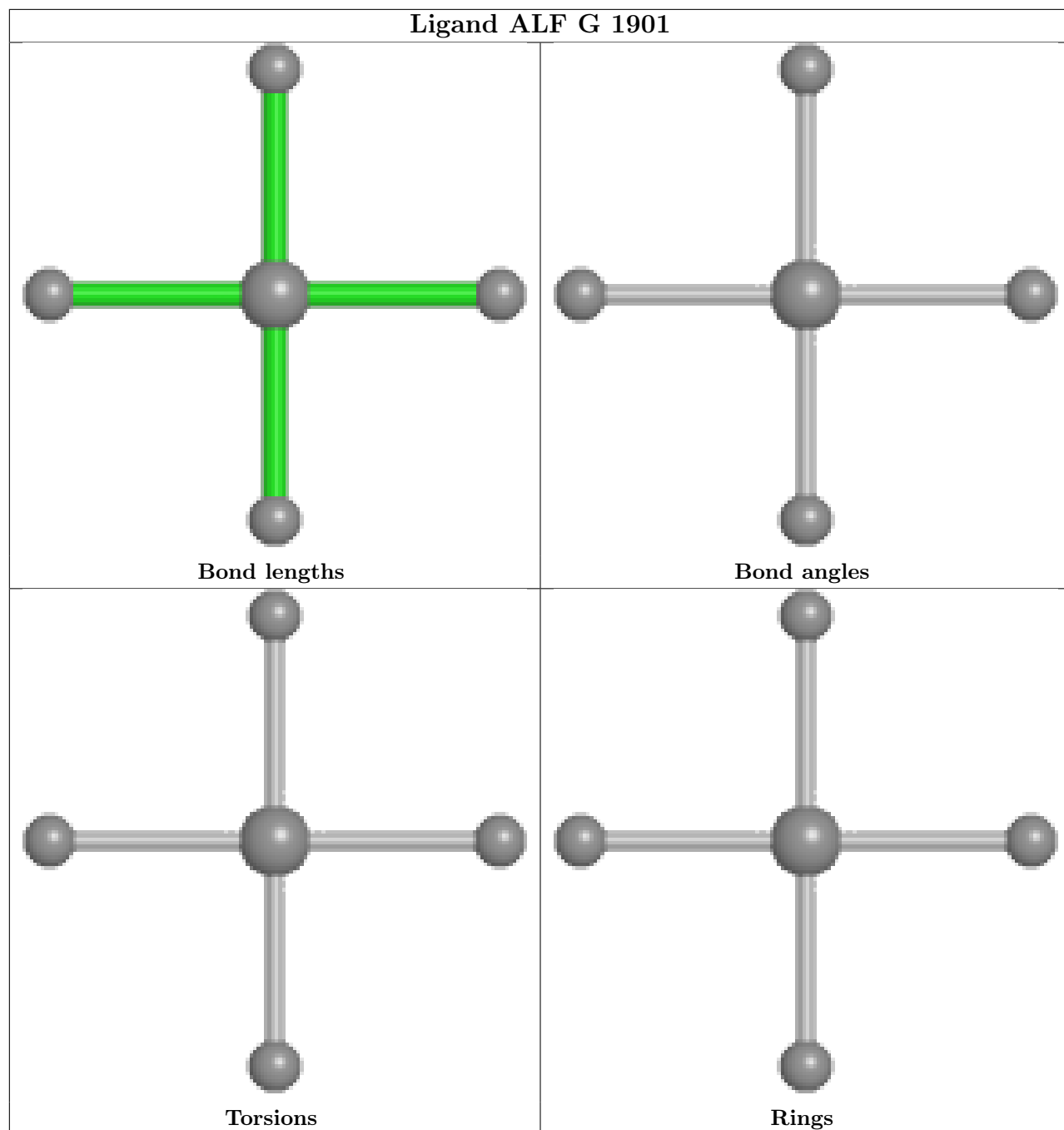
4 monomers are involved in 6 short contacts:

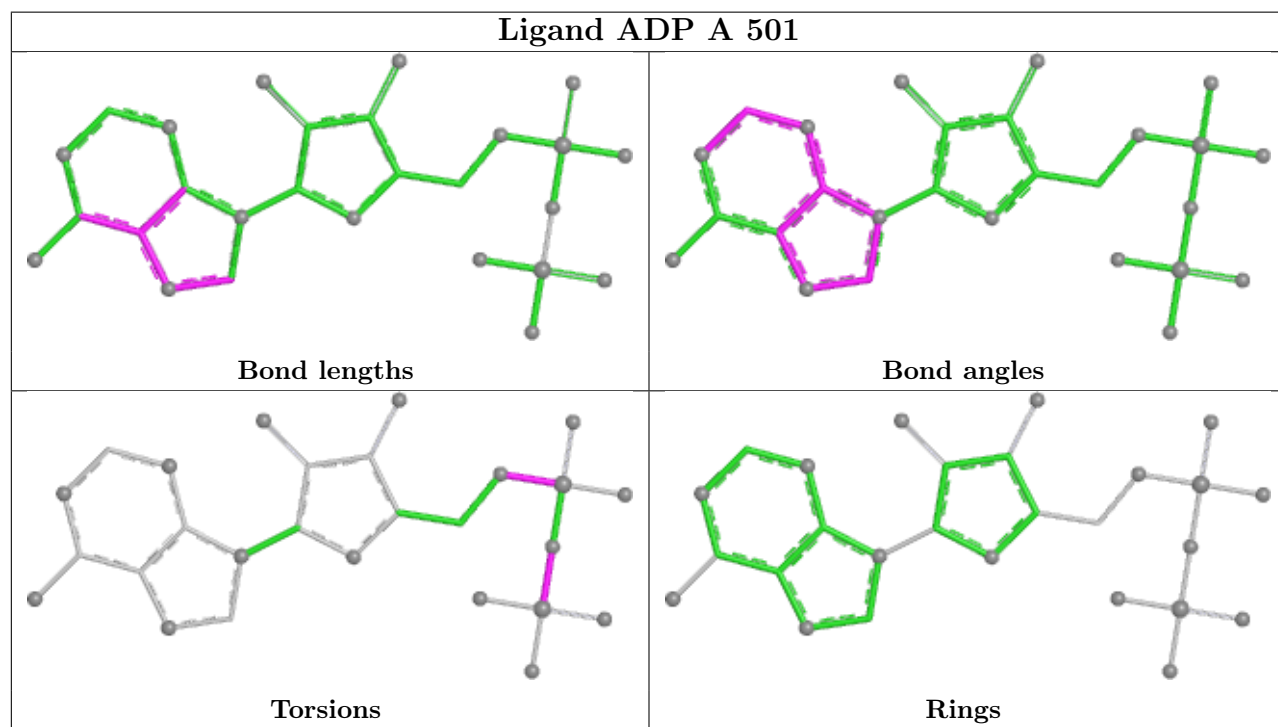
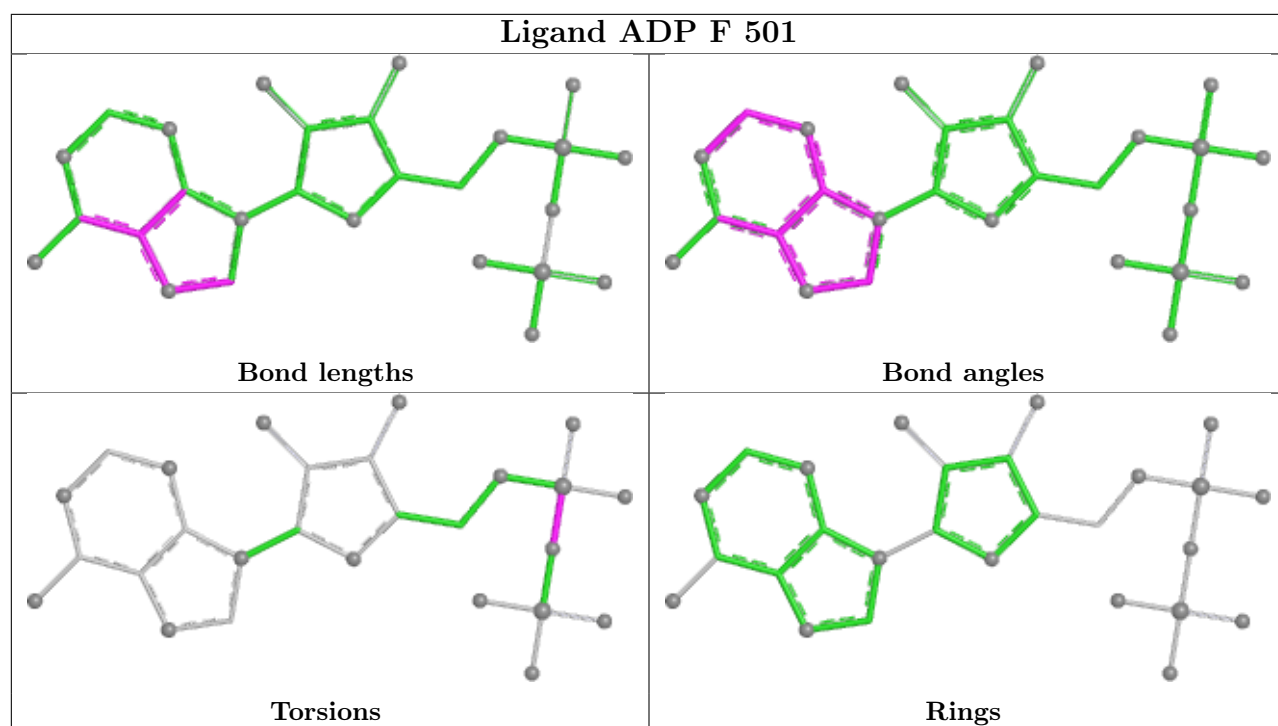
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	501	ADP	1	0
13	A	501	ADP	2	0
16	J	802	ATP	1	0
13	E	501	ADP	2	0

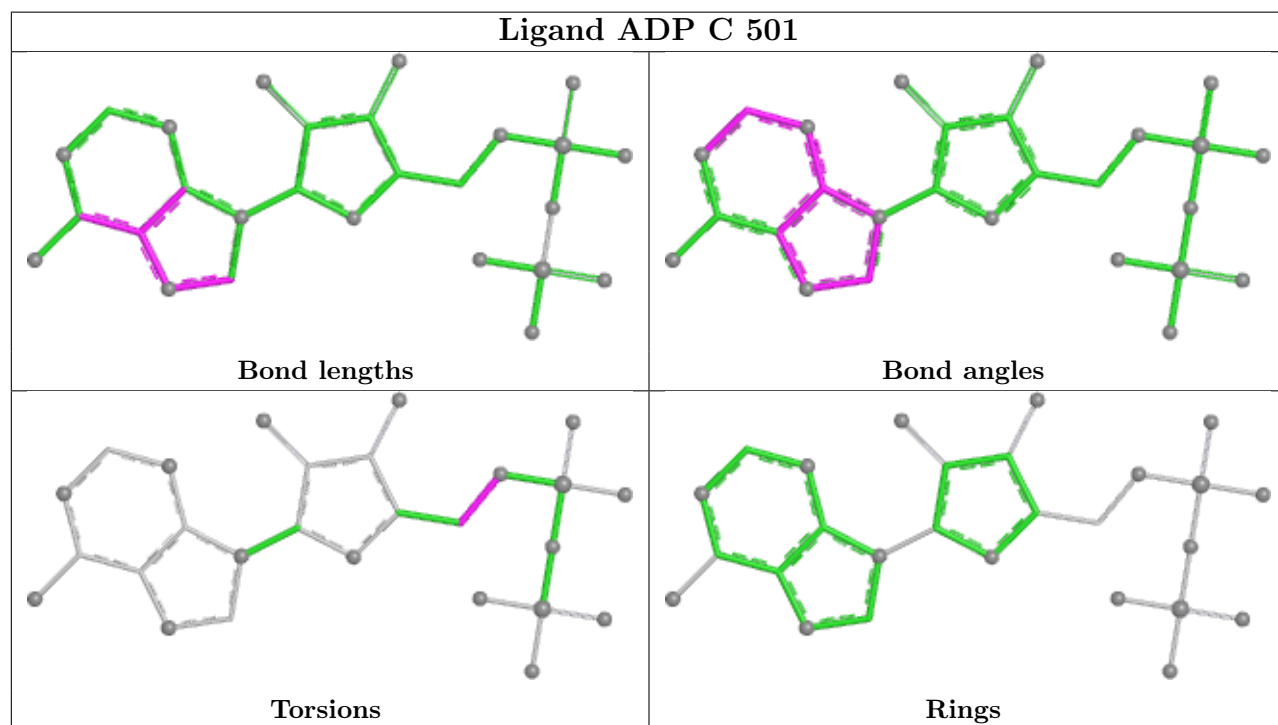
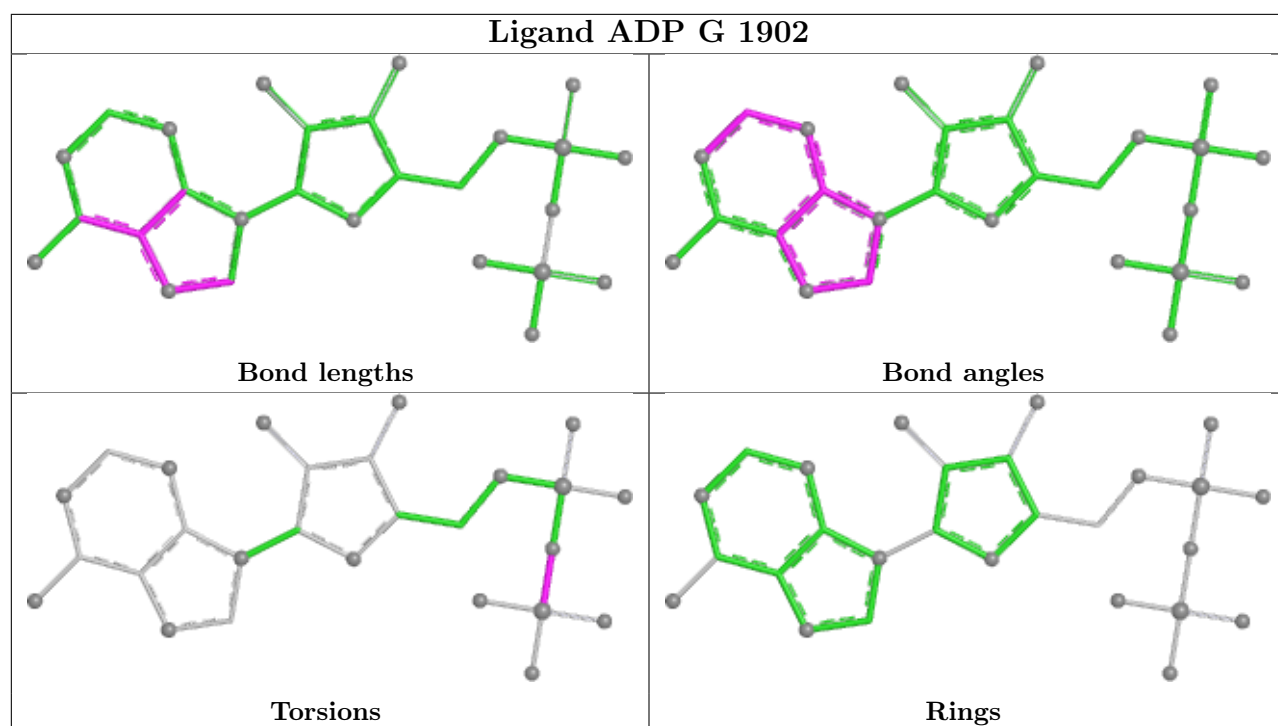
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

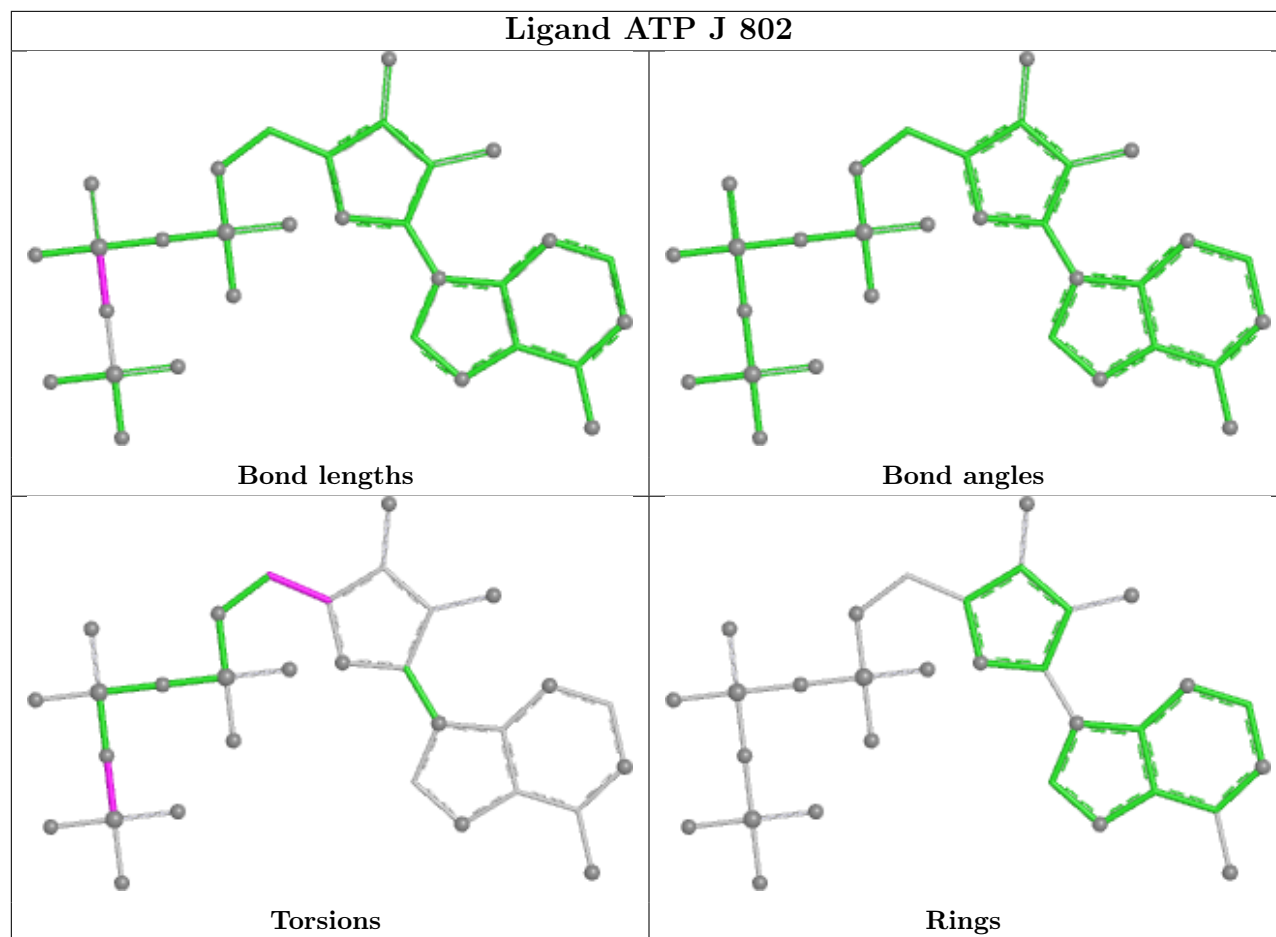




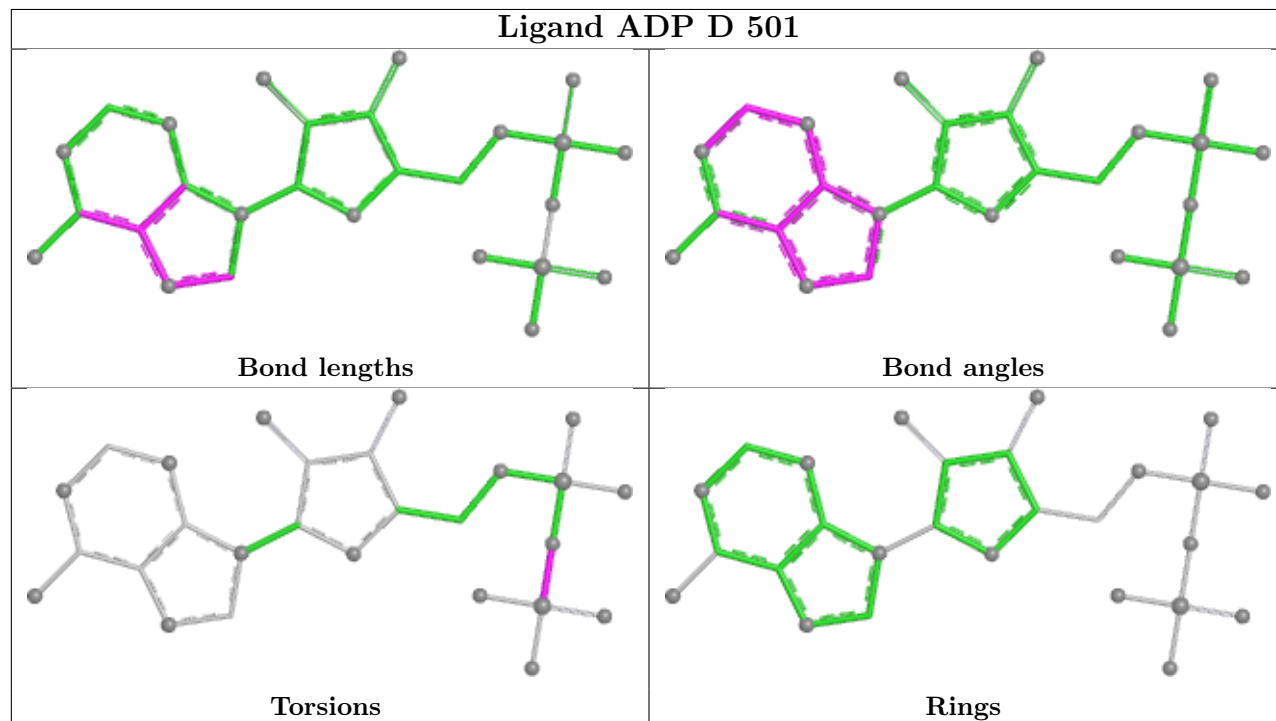


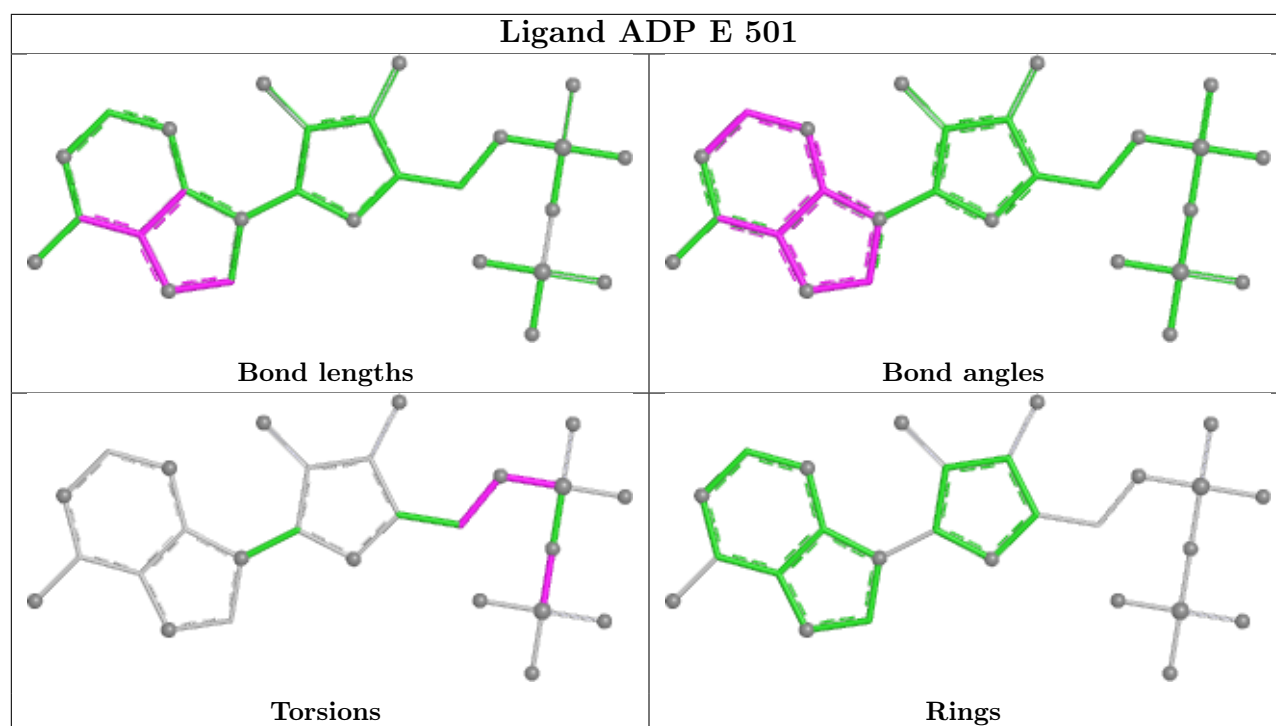


Ligand ATP J 802



Ligand ADP D 501





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.

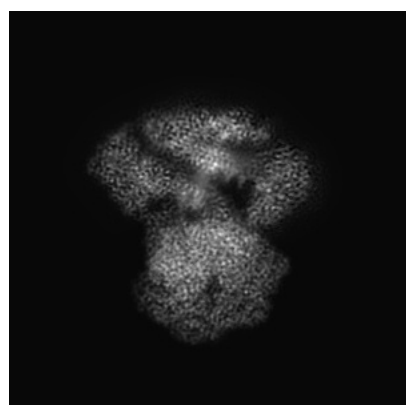
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17006. These allow visual inspection of the internal detail of the map and identification of artifacts.

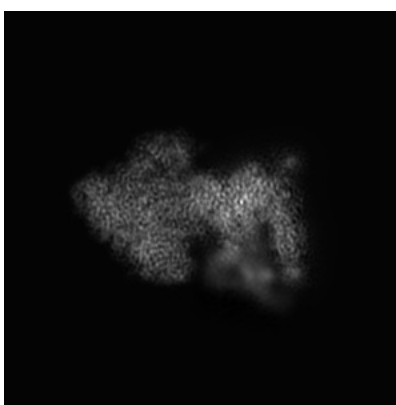
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

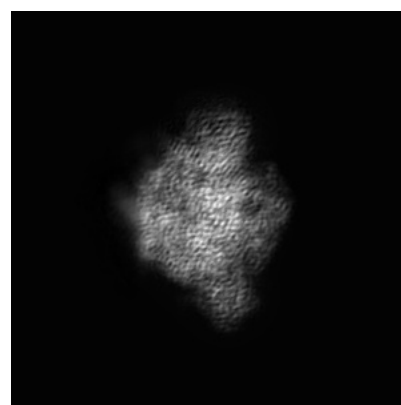
6.1.1 Primary map



X



Y

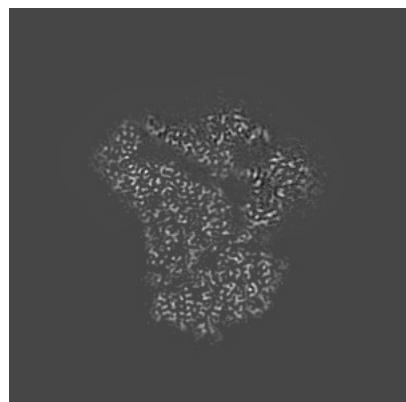


Z

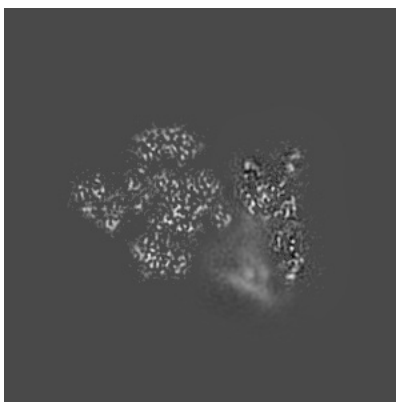
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

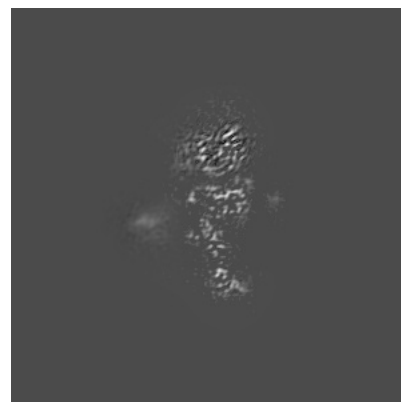
6.2.1 Primary map



X Index: 180



Y Index: 180



Z Index: 180

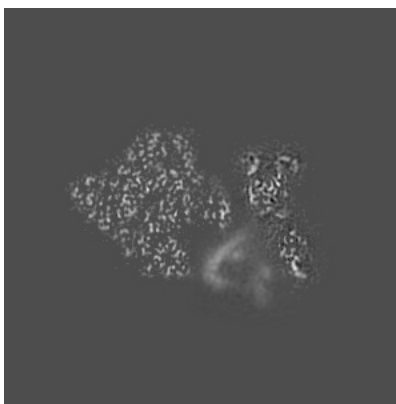
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

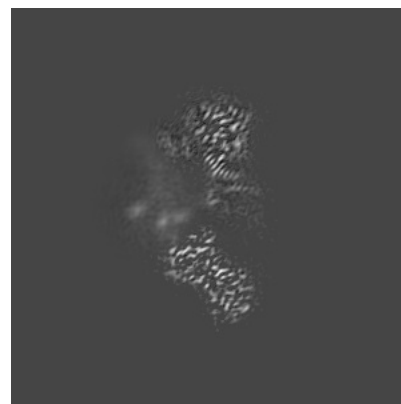
6.3.1 Primary map



X Index: 188



Y Index: 169

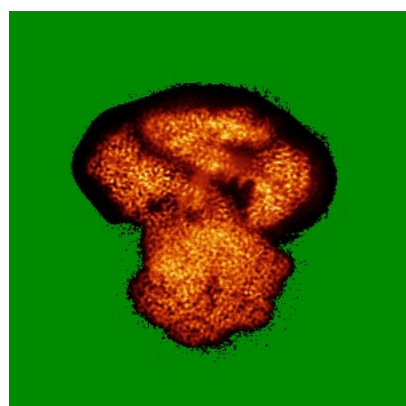


Z Index: 209

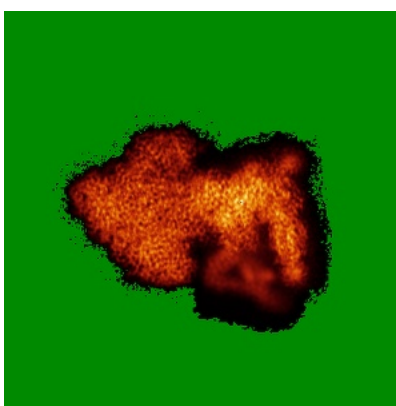
The images above show the largest variance slices of the map in three orthogonal directions.

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

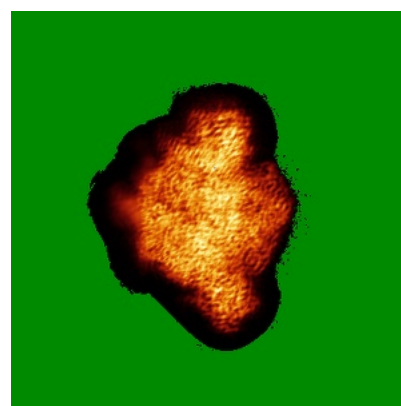
6.4.1 Primary map



X



Y

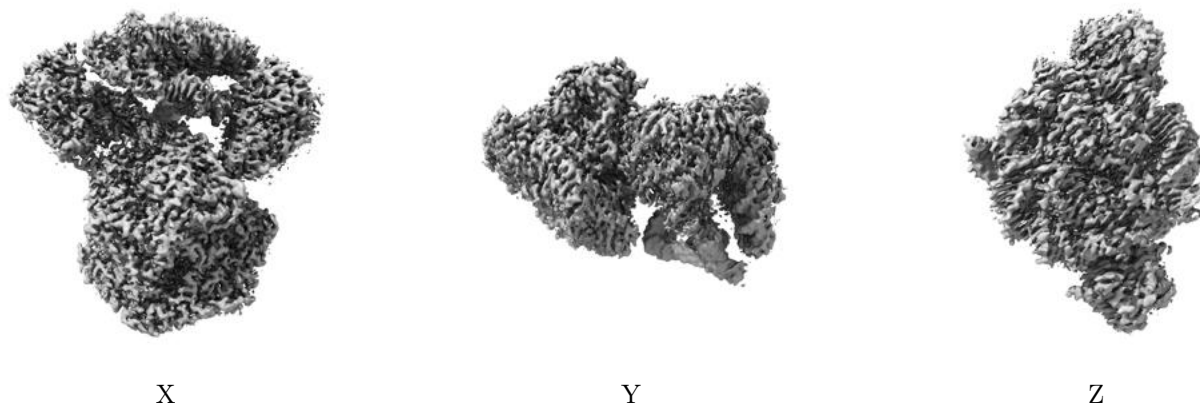


Z

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

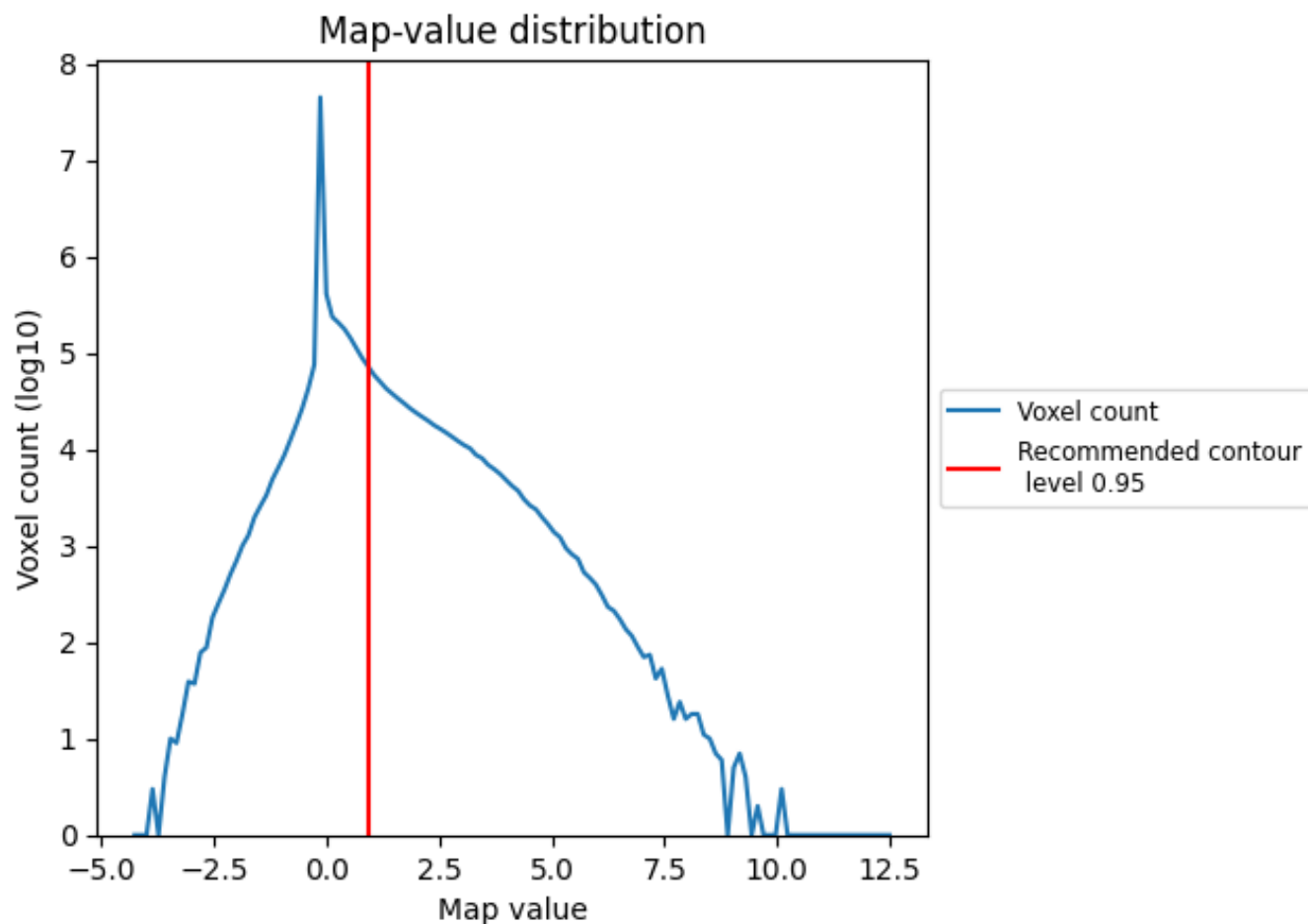
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

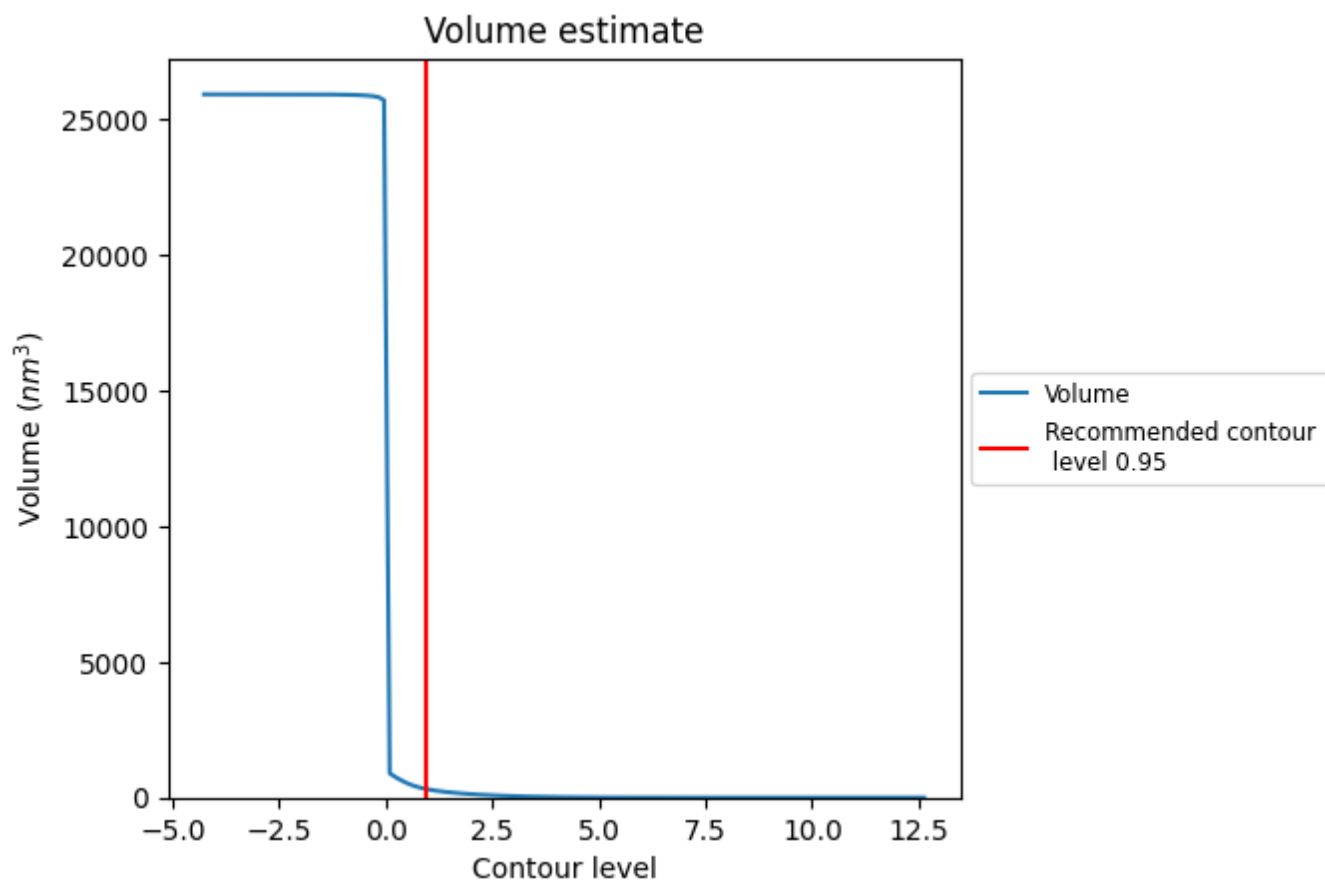
This section contains the results of statistical analysis of the map.

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.

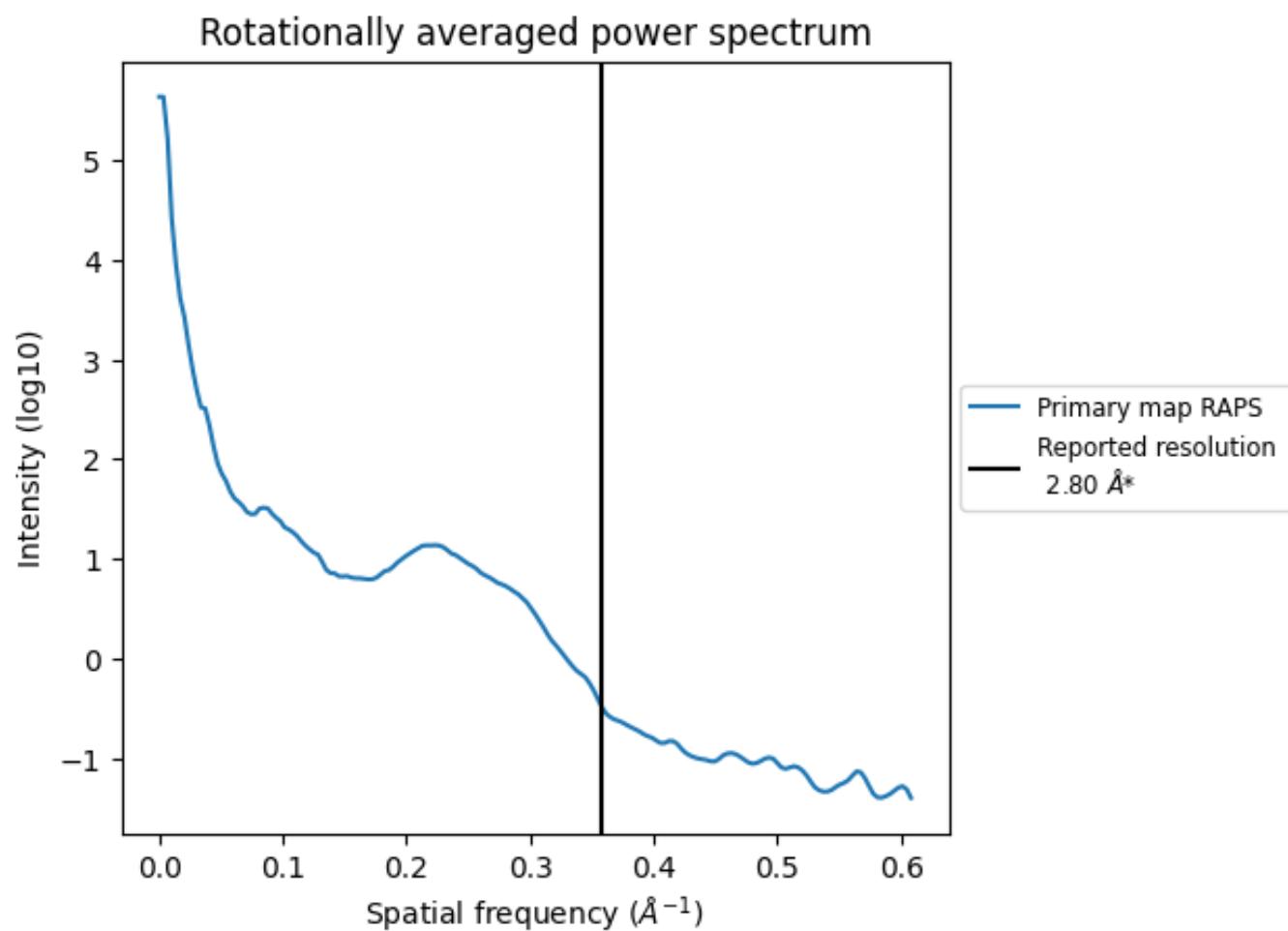
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 316 nm^3 ; this corresponds to an approximate mass of 285 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 0.357 Å⁻¹

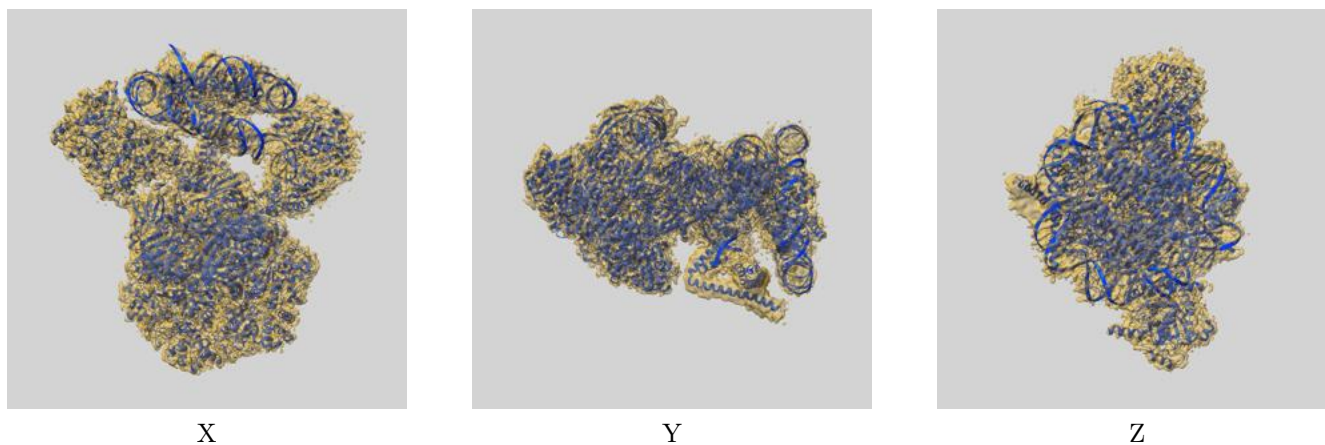
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

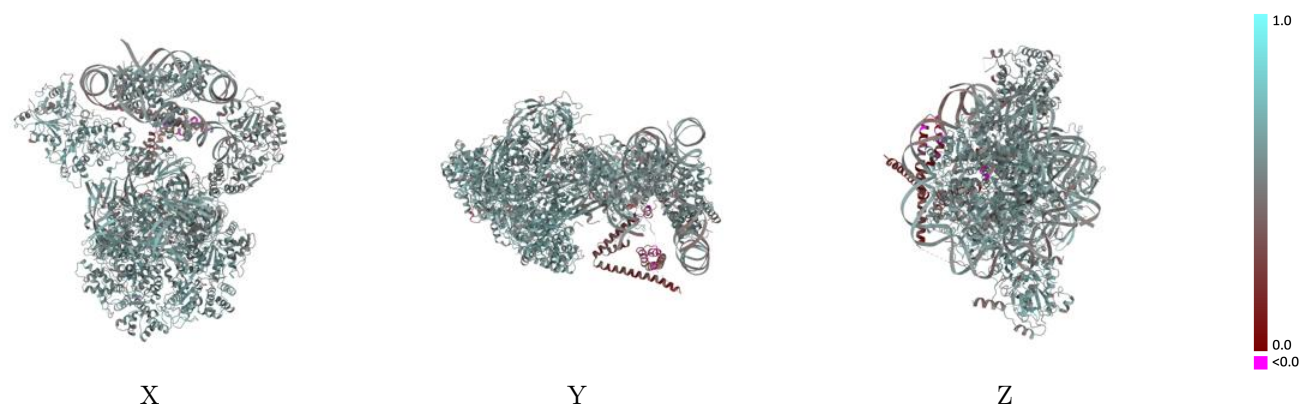
This section contains information regarding the fit between EMDB map EMD-17006 and PDB model 8007. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



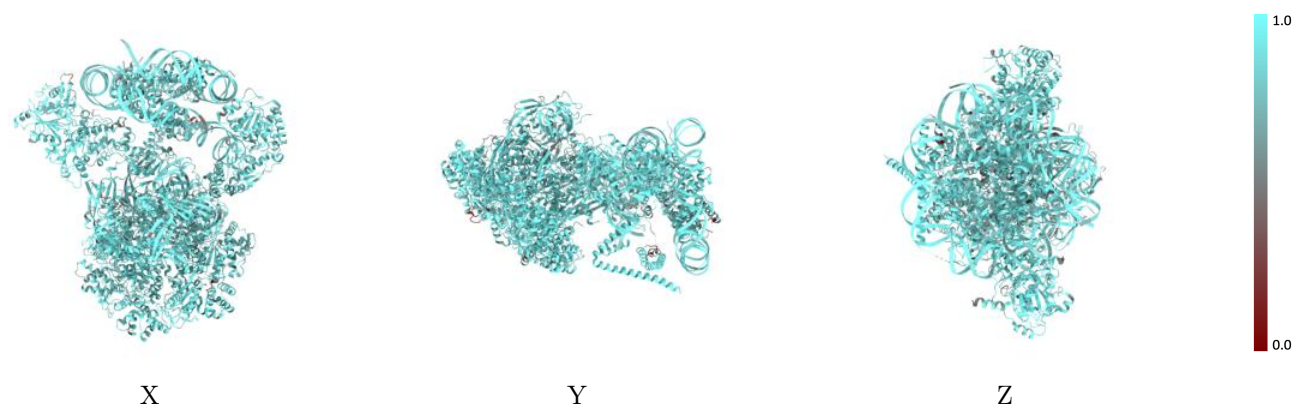
The images above show the 3D surface view of the map at the recommended contour level 0.95 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



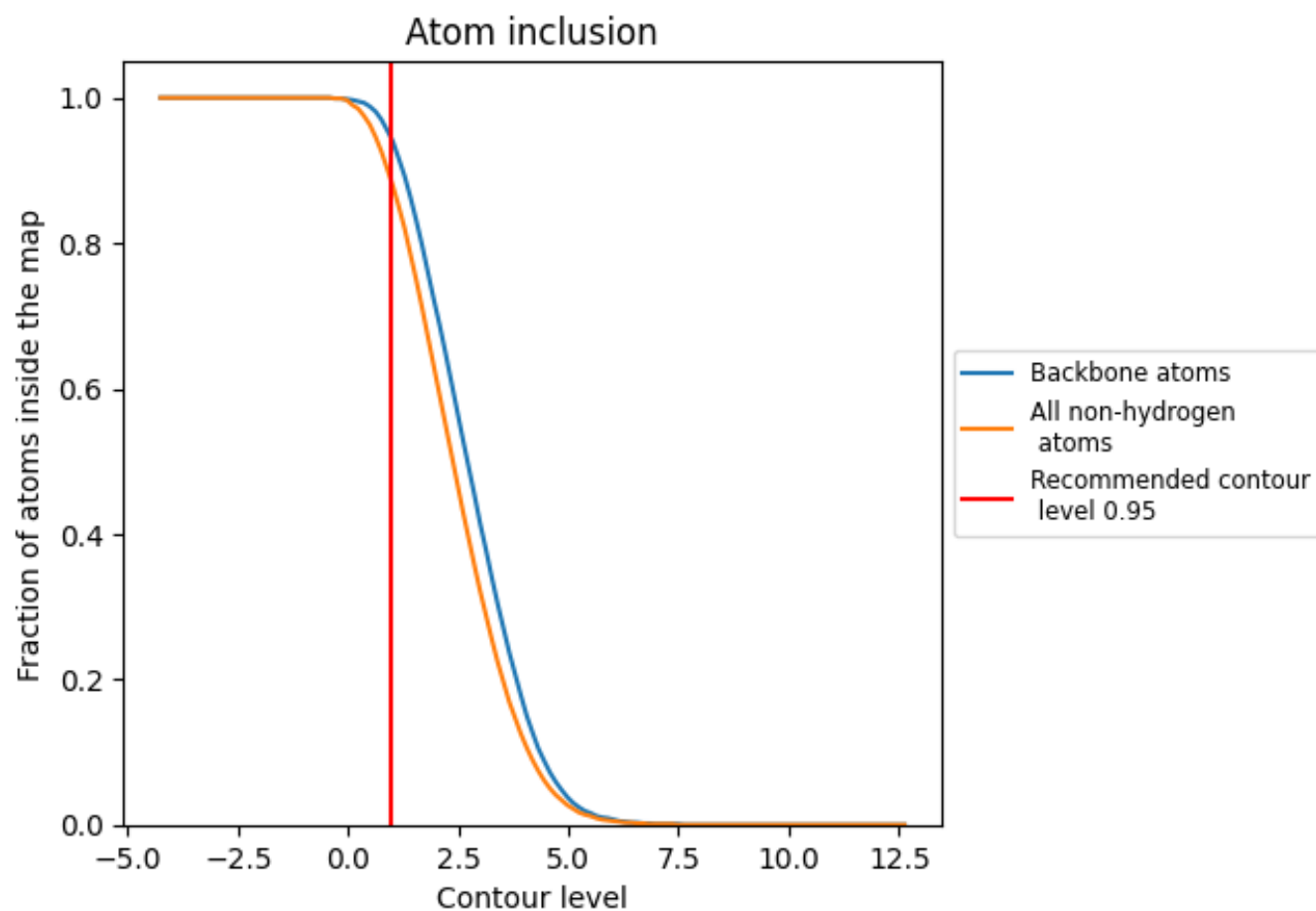
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.95).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 89% 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 (0.95) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8910	 0.5560
A	 0.8950	 0.5810
B	 0.8980	 0.5870
C	 0.8900	 0.5770
D	 0.8800	 0.5710
E	 0.9010	 0.5960
F	 0.8920	 0.5820
G	 0.8930	 0.5470
H	 0.8990	 0.5600
I	 0.8360	 0.5520
J	 0.9250	 0.5040
K	 0.8740	 0.5030
L	 0.8860	 0.5130
M	 0.8710	 0.5520
N	 0.8250	 0.5320
O	 0.8700	 0.5540
P	 0.8650	 0.5430
Q	 0.8730	 0.5530
R	 0.8690	 0.5360

