



Full wwPDB EM Validation Report ⓘ

Nov 8, 2022 – 07:04 AM EST

PDB ID : 6MAT
EMDB ID : EMD-9063
Title : Cryo-EM structure of the essential ribosome assembly AAA-ATPase Rix7
Authors : Lo, Y.H.; Sobhany, M.; Hsu, A.L.; Ford, B.L.; Krahn, J.M.; Borgnia, M.J.; Stanley, R.E.
Deposited on : 2018-08-28
Resolution : 4.50 Å(reported)
Based on initial model : 5FTK

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

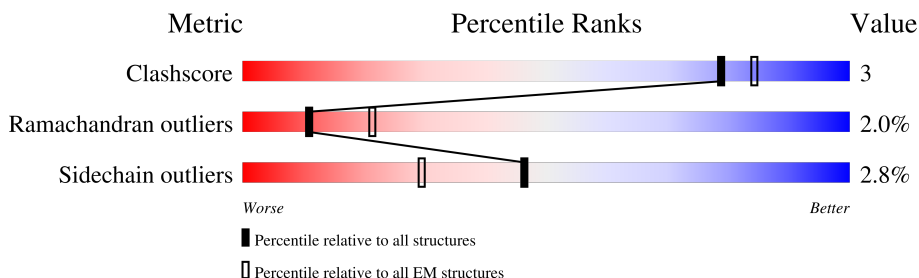
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	813	<div> <div>14%</div> <div>64%</div> <div>6%</div> <div>29%</div> </div>
1	B	813	<div> <div>10%</div> <div>64%</div> <div>6%</div> <div>29%</div> </div>
1	C	813	<div> <div>10%</div> <div>64%</div> <div>6%</div> <div>29%</div> </div>
1	D	813	<div> <div>10%</div> <div>63%</div> <div>7%</div> <div>29%</div> </div>
1	E	813	<div> <div>22%</div> <div>64%</div> <div>5%</div> <div>30%</div> </div>
1	F	813	<div> <div>34%</div> <div>63%</div> <div>6%</div> <div>30%</div> </div>
2	G	27	<div> <div>33%</div> <div>100%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27030 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 Rix7 mutant.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	578	Total	C	N	O	S	0	0
			4454	2788	795	850	21		
1	B	578	Total	C	N	O	S	0	0
			4454	2788	795	850	21		
1	C	578	Total	C	N	O	S	0	0
			4454	2788	795	850	21		
1	D	578	Total	C	N	O	S	0	0
			4454	2788	795	850	21		
1	E	568	Total	C	N	O	S	0	0
			4369	2734	781	834	20		
1	F	568	Total	C	N	O	S	0	0
			4369	2734	781	834	20		

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	303	GLN	GLU	engineered mutation	UNP G0RZG1
A	602	GLN	GLU	engineered mutation	UNP G0RZG1
A	803	ALA	-	expression tag	UNP G0RZG1
A	804	ALA	-	expression tag	UNP G0RZG1
A	805	ALA	-	expression tag	UNP G0RZG1
A	806	LEU	-	expression tag	UNP G0RZG1
A	807	GLU	-	expression tag	UNP G0RZG1
A	808	HIS	-	expression tag	UNP G0RZG1
A	809	HIS	-	expression tag	UNP G0RZG1
A	810	HIS	-	expression tag	UNP G0RZG1
A	811	HIS	-	expression tag	UNP G0RZG1
A	812	HIS	-	expression tag	UNP G0RZG1
A	813	HIS	-	expression tag	UNP G0RZG1
B	303	GLN	GLU	engineered mutation	UNP G0RZG1
B	602	GLN	GLU	engineered mutation	UNP G0RZG1
B	803	ALA	-	expression tag	UNP G0RZG1
B	804	ALA	-	expression tag	UNP G0RZG1
B	805	ALA	-	expression tag	UNP G0RZG1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	806	LEU	-	expression tag	UNP G0RZG1
B	807	GLU	-	expression tag	UNP G0RZG1
B	808	HIS	-	expression tag	UNP G0RZG1
B	809	HIS	-	expression tag	UNP G0RZG1
B	810	HIS	-	expression tag	UNP G0RZG1
B	811	HIS	-	expression tag	UNP G0RZG1
B	812	HIS	-	expression tag	UNP G0RZG1
B	813	HIS	-	expression tag	UNP G0RZG1
C	303	GLN	GLU	engineered mutation	UNP G0RZG1
C	602	GLN	GLU	engineered mutation	UNP G0RZG1
C	803	ALA	-	expression tag	UNP G0RZG1
C	804	ALA	-	expression tag	UNP G0RZG1
C	805	ALA	-	expression tag	UNP G0RZG1
C	806	LEU	-	expression tag	UNP G0RZG1
C	807	GLU	-	expression tag	UNP G0RZG1
C	808	HIS	-	expression tag	UNP G0RZG1
C	809	HIS	-	expression tag	UNP G0RZG1
C	810	HIS	-	expression tag	UNP G0RZG1
C	811	HIS	-	expression tag	UNP G0RZG1
C	812	HIS	-	expression tag	UNP G0RZG1
C	813	HIS	-	expression tag	UNP G0RZG1
D	303	GLN	GLU	engineered mutation	UNP G0RZG1
D	602	GLN	GLU	engineered mutation	UNP G0RZG1
D	803	ALA	-	expression tag	UNP G0RZG1
D	804	ALA	-	expression tag	UNP G0RZG1
D	805	ALA	-	expression tag	UNP G0RZG1
D	806	LEU	-	expression tag	UNP G0RZG1
D	807	GLU	-	expression tag	UNP G0RZG1
D	808	HIS	-	expression tag	UNP G0RZG1
D	809	HIS	-	expression tag	UNP G0RZG1
D	810	HIS	-	expression tag	UNP G0RZG1
D	811	HIS	-	expression tag	UNP G0RZG1
D	812	HIS	-	expression tag	UNP G0RZG1
D	813	HIS	-	expression tag	UNP G0RZG1
E	303	GLN	GLU	engineered mutation	UNP G0RZG1
E	602	GLN	GLU	engineered mutation	UNP G0RZG1
E	803	ALA	-	expression tag	UNP G0RZG1
E	804	ALA	-	expression tag	UNP G0RZG1
E	805	ALA	-	expression tag	UNP G0RZG1
E	806	LEU	-	expression tag	UNP G0RZG1
E	807	GLU	-	expression tag	UNP G0RZG1
E	808	HIS	-	expression tag	UNP G0RZG1

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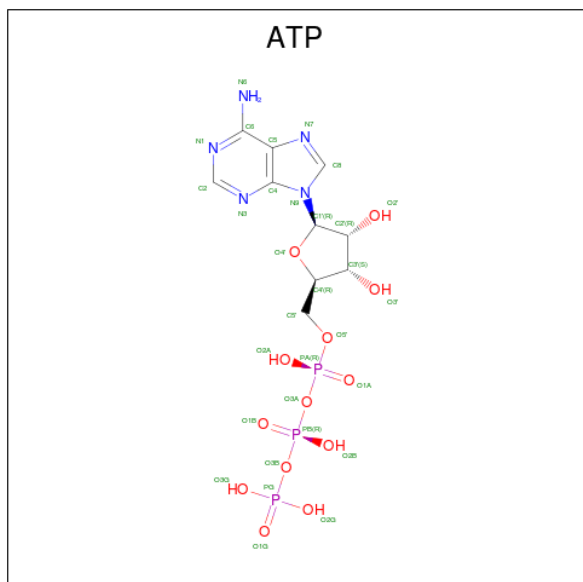
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Chain	Residue	Modelled	Actual	Comment	Reference
E	809	HIS	-	expression tag	UNP G0RZG1
E	810	HIS	-	expression tag	UNP G0RZG1
E	811	HIS	-	expression tag	UNP G0RZG1
E	812	HIS	-	expression tag	UNP G0RZG1
E	813	HIS	-	expression tag	UNP G0RZG1
F	303	GLN	GLU	engineered mutation	UNP G0RZG1
F	602	GLN	GLU	engineered mutation	UNP G0RZG1
F	803	ALA	-	expression tag	UNP G0RZG1
F	804	ALA	-	expression tag	UNP G0RZG1
F	805	ALA	-	expression tag	UNP G0RZG1
F	806	LEU	-	expression tag	UNP G0RZG1
F	807	GLU	-	expression tag	UNP G0RZG1
F	808	HIS	-	expression tag	UNP G0RZG1
F	809	HIS	-	expression tag	UNP G0RZG1
F	810	HIS	-	expression tag	UNP G0RZG1
F	811	HIS	-	expression tag	UNP G0RZG1
F	812	HIS	-	expression tag	UNP G0RZG1
F	813	HIS	-	expression tag	UNP G0RZG1

- Molecule 2 is a protein called unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	G	27	Total	C	N	O	0	0
			135	81	27	27		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

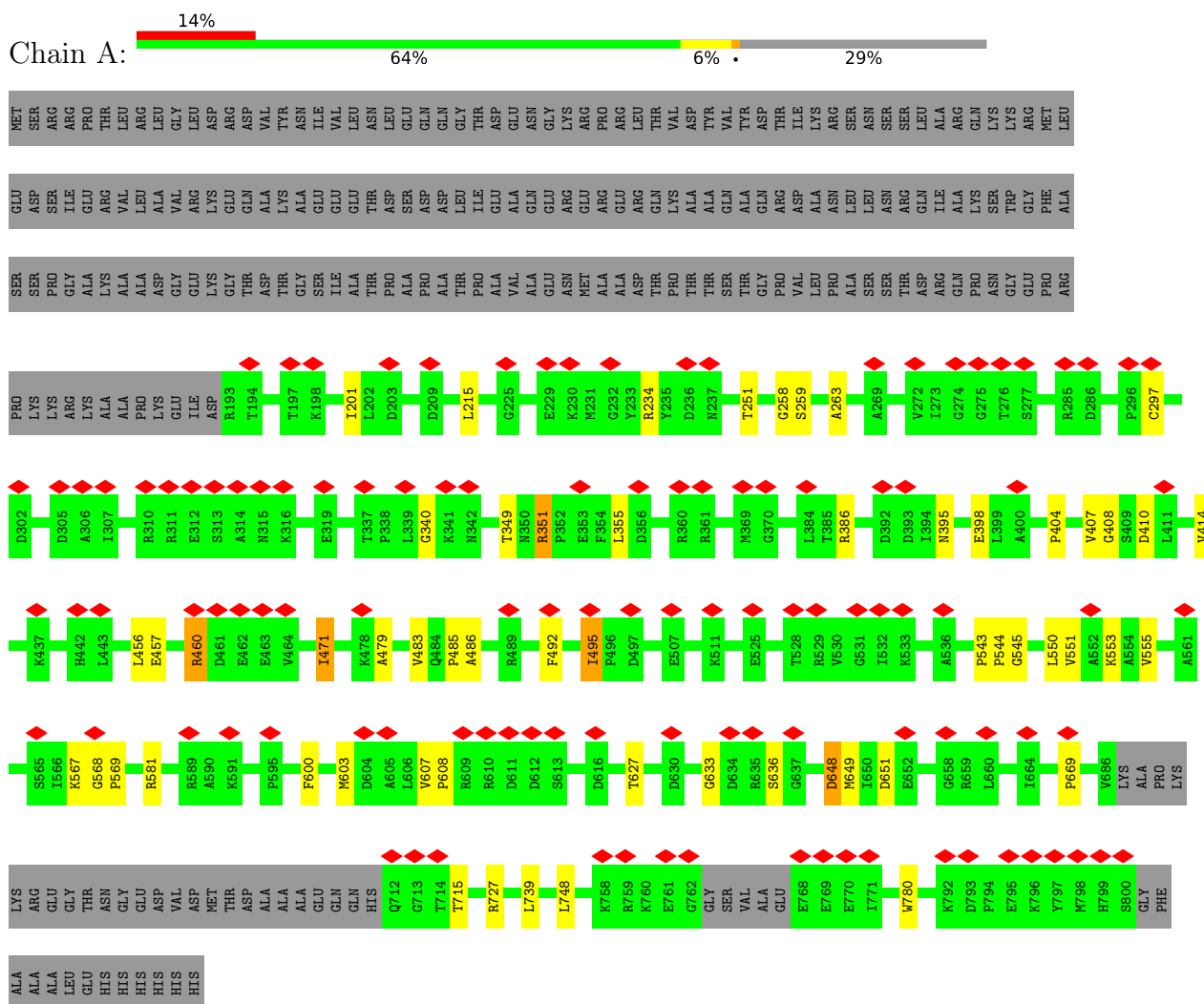


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	A	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	B	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	B	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	C	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	C	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	D	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	D	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	F	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	F	1	Total	C	N	O	P	0
			62	20	10	26	6	

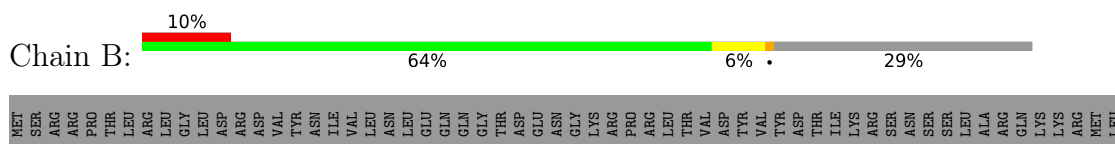
3 Residue-property plots

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: Rix7 mutant

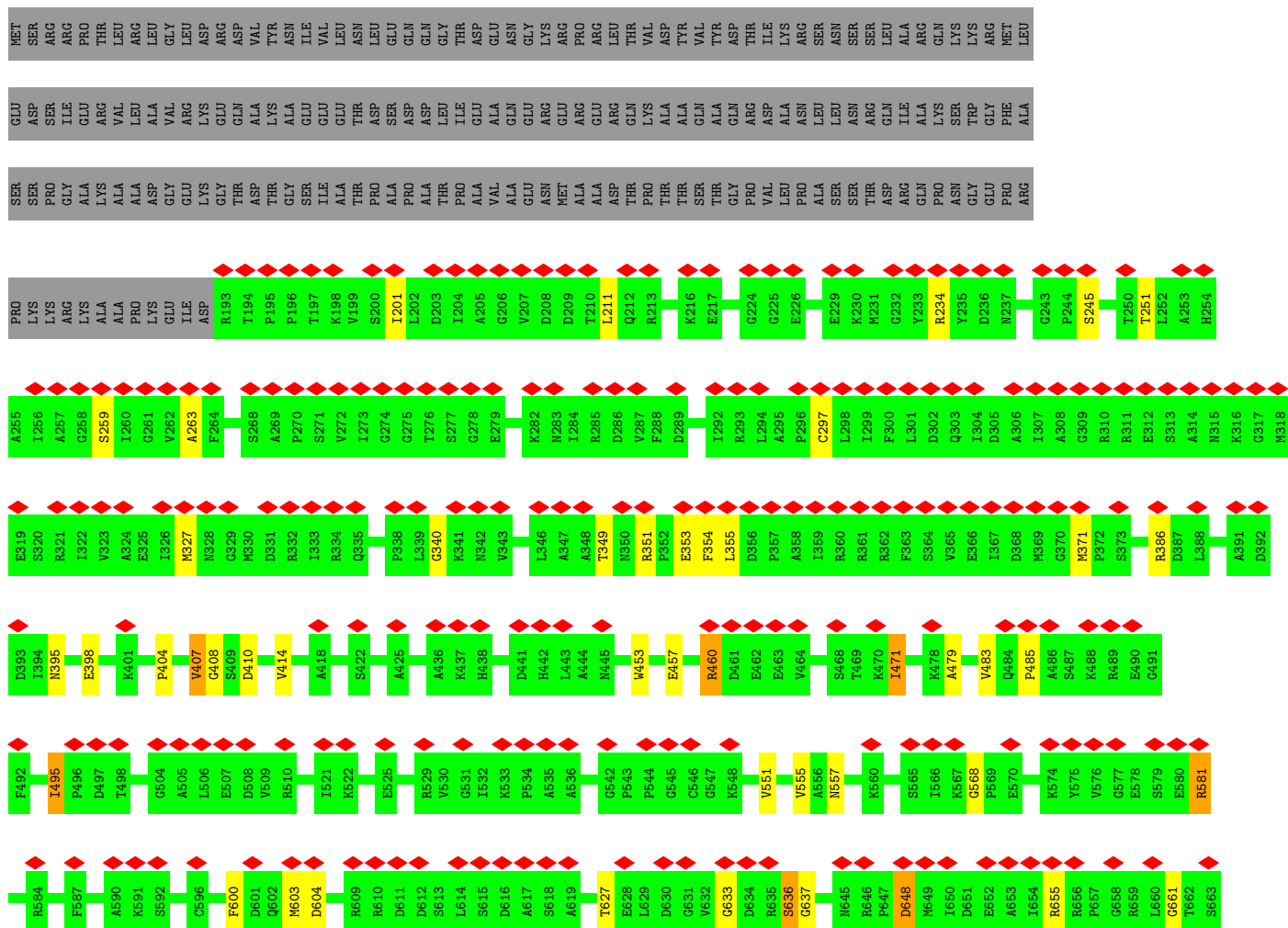


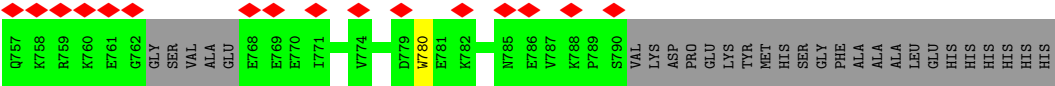
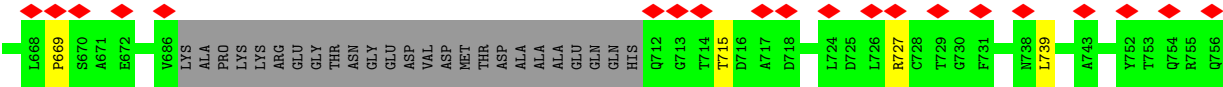
• Molecule 1: Rix7 mutant



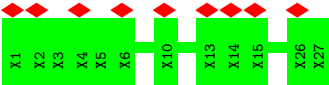


- Molecule 1: Rix7 mutant





• Molecule 2: unknown protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	64386	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	-1200	Depositor
Maximum defocus (nm)	-2700	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.311	Depositor
Minimum map value	-0.148	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.0796	Depositor
Map size (Å)	266.88, 266.88, 266.88	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	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: 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	0.60	0/4527	0.71	0/6120
1	B	0.59	0/4527	0.71	1/6120 (0.0%)
1	C	0.59	0/4527	0.71	0/6120
1	D	0.59	0/4527	0.71	0/6120
1	E	0.61	0/4439	0.72	2/6002 (0.0%)
1	F	0.63	0/4439	0.71	0/6002
All	All	0.60	0/26986	0.71	3/36484 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	568	GLY	N-CA-C	5.83	127.67	113.10
1	B	631	GLY	N-CA-C	5.77	127.53	113.10
1	E	577	GLY	N-CA-C	5.15	125.98	113.10

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	4454	0	4506	29	0
1	B	4454	0	4506	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4454	0	4506	30	0
1	D	4454	0	4506	32	0
1	E	4369	0	4424	23	0
1	F	4369	0	4424	24	0
2	G	135	0	32	0	0
3	A	62	0	24	8	0
3	B	62	0	24	6	0
3	C	62	0	24	2	0
3	D	62	0	24	2	0
3	E	31	0	12	1	0
3	F	62	0	24	2	0
All	All	27030	0	27036	152	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 (152) 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:F:245:SER:O	1:F:407:VAL:HG11	1.86	0.76
1:A:351:ARG:HH22	1:B:311:ARG:HB2	1.52	0.74
1:B:607:VAL:HG12	1:B:651:ASP:H	1.52	0.72
1:E:544:PRO:HB3	1:E:645:ASN:ND2	2.06	0.71
1:C:607:VAL:HG12	1:C:651:ASP:H	1.56	0.70
1:D:404:PRO:HB3	1:D:595:PRO:HD2	1.75	0.68
1:C:495:ILE:H	1:C:495:ILE:HD13	1.59	0.67
1:D:495:ILE:HD13	1:D:495:ILE:H	1.60	0.67
1:E:495:ILE:H	1:E:495:ILE:HD13	1.58	0.66
1:D:607:VAL:HG12	1:D:651:ASP:H	1.61	0.66
1:F:495:ILE:H	1:F:495:ILE:HD13	1.58	0.66
1:B:495:ILE:H	1:B:495:ILE:HD13	1.60	0.65
3:A:901:ATP:H5'1	1:B:656:ARG:HH12	1.60	0.65
1:A:495:ILE:H	1:A:495:ILE:HD13	1.61	0.63
1:B:607:VAL:HG13	1:B:654:ILE:HD13	1.80	0.63
1:D:567:LYS:HD3	1:E:627:THR:HG23	1.80	0.62
1:A:251:THR:HG21	3:A:902:ATP:H3'	1.81	0.62
1:C:251:THR:HG21	3:C:902:ATP:H3'	1.82	0.62
1:D:251:THR:HG21	3:D:902:ATP:H3'	1.83	0.60
1:F:251:THR:HG21	3:F:902:ATP:H3'	1.84	0.60
1:E:251:THR:HG21	3:E:901:ATP:H3'	1.82	0.59
1:D:607:VAL:HG13	1:D:654:ILE:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:607:VAL:HG13	1:C:654:ILE:HD13	1.85	0.59
1:B:251:THR:HG21	3:B:902:ATP:H3'	1.84	0.59
1:F:655:ARG:O	1:F:661:GLY:HA2	2.02	0.58
1:E:479:ALA:O	1:E:483:VAL:HG23	2.03	0.58
1:A:607:VAL:HG12	1:A:651:ASP:H	1.69	0.58
1:A:479:ALA:O	1:A:483:VAL:HG23	2.03	0.58
1:D:488:LYS:NZ	1:E:360:ARG:HH22	2.02	0.57
1:F:353:GLU:HG2	1:F:581:ARG:HG2	1.87	0.56
1:A:351:ARG:NH2	1:B:311:ARG:HB2	2.21	0.56
3:A:901:ATP:H5'1	1:B:656:ARG:NH1	2.21	0.56
1:A:550:LEU:HD11	3:A:901:ATP:H2'	1.88	0.55
1:E:607:VAL:HG13	1:E:654:ILE:HD13	1.87	0.55
1:F:471:ILE:H	1:F:471:ILE:HD13	1.70	0.55
1:A:407:VAL:HG12	1:A:408:GLY:H	1.73	0.54
1:C:479:ALA:O	1:C:483:VAL:HG23	2.08	0.54
1:F:479:ALA:O	1:F:483:VAL:HG23	2.07	0.54
1:B:479:ALA:O	1:B:483:VAL:HG23	2.07	0.54
1:A:258:GLY:O	1:F:460:ARG:NH2	2.41	0.53
1:D:407:VAL:HG12	1:D:408:GLY:H	1.74	0.53
1:E:471:ILE:H	1:E:471:ILE:HD13	1.73	0.53
1:D:479:ALA:O	1:D:483:VAL:HG23	2.08	0.53
1:A:395:ASN:HD22	1:A:398:GLU:HG3	1.72	0.53
1:B:407:VAL:HG12	1:B:408:GLY:H	1.72	0.53
1:E:453:TRP:NE1	1:F:211:LEU:HG	2.24	0.53
1:E:414:VAL:HG22	1:E:483:VAL:HG21	1.91	0.52
1:A:471:ILE:H	1:A:471:ILE:HD13	1.74	0.52
1:C:407:VAL:HG12	1:C:408:GLY:H	1.74	0.52
1:B:395:ASN:HD22	1:B:398:GLU:HG3	1.75	0.52
1:E:607:VAL:HG12	1:E:651:ASP:H	1.74	0.52
1:D:656:ARG:HH21	1:D:659:ARG:HG3	1.75	0.52
1:D:471:ILE:HD13	1:D:471:ILE:H	1.74	0.51
1:F:395:ASN:HD22	1:F:398:GLU:HG3	1.75	0.51
1:C:567:LYS:HD3	1:D:627:THR:HG23	1.93	0.51
1:C:551:VAL:O	1:C:555:VAL:HG23	2.11	0.51
1:D:395:ASN:HD22	1:D:398:GLU:HG3	1.76	0.51
1:E:546:CYS:SG	1:E:732:SER:HB2	2.51	0.51
1:B:550:LEU:HD11	3:B:901:ATP:H2'	1.92	0.51
1:C:373:SER:H	1:C:376:ALA:HB3	1.76	0.50
1:C:471:ILE:HD13	1:C:471:ILE:H	1.76	0.50
1:D:550:LEU:HD11	3:D:901:ATP:H2'	1.92	0.50
1:F:410:ASP:O	1:F:414:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:ASN:HD22	1:C:398:GLU:HG3	1.76	0.50
1:E:407:VAL:HG12	1:E:408:GLY:H	1.78	0.49
1:C:748:LEU:HD21	1:D:530:VAL:HG11	1.93	0.49
1:C:550:LEU:HD11	3:C:901:ATP:H2'	1.94	0.49
1:D:490:GLU:HG2	1:D:491:GLY:H	1.77	0.49
1:B:646:ARG:HH12	1:C:611:ASP:HA	1.78	0.48
1:A:201:ILE:H	1:A:201:ILE:HD12	1.78	0.48
1:B:551:VAL:O	1:B:555:VAL:HG23	2.14	0.48
1:E:263:ALA:HB3	1:E:297:CYS:SG	2.53	0.48
1:B:263:ALA:HB3	1:B:297:CYS:SG	2.53	0.48
1:F:263:ALA:HB3	1:F:297:CYS:SG	2.53	0.48
1:A:263:ALA:HB3	1:A:297:CYS:SG	2.53	0.48
1:E:206:GLY:HA2	1:E:379:GLN:NE2	2.29	0.48
1:E:635:ARG:HD3	1:E:635:ARG:H	1.79	0.48
1:B:656:ARG:HH21	1:B:659:ARG:HG3	1.77	0.48
1:F:407:VAL:HG12	1:F:408:GLY:H	1.78	0.48
3:A:901:ATP:C5'	1:B:656:ARG:HH12	2.26	0.48
1:A:553:LYS:HZ1	1:B:632:VAL:HA	1.77	0.48
1:B:471:ILE:H	1:B:471:ILE:HD13	1.77	0.47
1:B:270:PRO:HG2	1:C:325:GLU:HG2	1.96	0.47
1:F:600:PHE:HB3	1:F:603:MET:SD	2.54	0.47
1:B:373:SER:H	1:B:376:ALA:HB3	1.80	0.47
1:E:544:PRO:HB3	1:E:645:ASN:HD21	1.80	0.47
1:B:632:VAL:HG12	1:B:633:GLY:H	1.81	0.46
1:E:395:ASN:HD22	1:E:398:GLU:HG3	1.80	0.46
1:A:456:LEU:HD13	1:B:219:TRP:NE1	2.31	0.46
1:A:600:PHE:HB3	1:A:603:MET:SD	2.56	0.45
1:C:201:ILE:HD12	1:C:201:ILE:H	1.82	0.45
1:C:263:ALA:HB3	1:C:297:CYS:SG	2.57	0.45
1:D:263:ALA:HB3	1:D:297:CYS:SG	2.57	0.45
1:E:410:ASP:O	1:E:414:VAL:HG23	2.16	0.45
3:A:901:ATP:PG	1:B:659:ARG:NH2	2.90	0.45
1:B:567:LYS:HD3	1:C:627:THR:HG23	1.98	0.45
1:D:551:VAL:O	1:D:555:VAL:HG23	2.16	0.45
1:E:201:ILE:HD12	1:E:201:ILE:H	1.81	0.45
3:B:901:ATP:PG	1:C:659:ARG:NH2	2.90	0.44
1:B:456:LEU:HD13	1:C:219:TRP:NE1	2.32	0.44
1:F:495:ILE:HB	1:F:557:ASN:HD22	1.82	0.44
1:C:456:LEU:HD13	1:D:219:TRP:NE1	2.33	0.44
1:A:351:ARG:HH22	1:B:311:ARG:CB	2.24	0.44
1:C:656:ARG:HH21	1:C:659:ARG:HG3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:ILE:HG13	1:E:321:ARG:HD3	1.99	0.44
1:A:608:PRO:HB3	1:A:649:MET:HB3	2.00	0.43
1:D:485:PRO:C	1:D:487:SER:H	2.22	0.43
1:B:410:ASP:O	1:B:414:VAL:HG23	2.18	0.43
1:A:259:SER:HB2	1:F:457:GLU:HG2	2.00	0.43
1:F:414:VAL:HG22	1:F:483:VAL:HG21	2.01	0.43
1:A:567:LYS:HD3	1:B:627:THR:HG23	1.99	0.43
1:B:600:PHE:HB3	1:B:603:MET:SD	2.59	0.43
1:D:201:ILE:H	1:D:201:ILE:HD12	1.83	0.43
1:D:373:SER:H	1:D:376:ALA:HB3	1.82	0.43
1:A:215:LEU:HB2	1:F:453:TRP:CZ2	2.54	0.43
1:C:607:VAL:HG11	1:C:650:ILE:HG23	2.01	0.43
1:C:270:PRO:HG2	1:D:325:GLU:HG2	2.01	0.43
1:A:748:LEU:HD21	1:B:530:VAL:HG11	2.00	0.42
1:A:545:GLY:HA3	1:B:656:ARG:HD2	2.00	0.42
1:E:457:GLU:HG2	1:F:259:SER:HB2	2.02	0.42
1:B:457:GLU:O	1:B:460:ARG:HG2	2.20	0.42
1:E:547:GLY:O	1:E:551:VAL:HG23	2.20	0.42
1:A:551:VAL:O	1:A:555:VAL:HG23	2.18	0.42
1:D:476:PHE:O	1:D:480:VAL:HG23	2.20	0.42
1:A:543:PRO:HA	1:A:544:PRO:HD3	1.94	0.42
1:A:349:THR:HG21	1:A:355:LEU:HD11	2.02	0.41
1:C:600:PHE:HB3	1:C:603:MET:SD	2.59	0.41
1:A:410:ASP:O	1:A:414:VAL:HG23	2.20	0.41
1:D:600:PHE:HB3	1:D:603:MET:SD	2.60	0.41
1:B:201:ILE:HD12	1:B:201:ILE:H	1.84	0.41
1:D:371:MET:HA	1:D:372:PRO:HD3	1.85	0.41
1:B:632:VAL:HG12	1:B:633:GLY:N	2.35	0.41
1:D:648:ASP:HB3	1:D:800:SER:HB3	2.03	0.41
3:A:901:ATP:O3G	1:B:659:ARG:NH2	2.50	0.41
1:B:646:ARG:NH1	1:C:610:ARG:O	2.54	0.41
3:B:901:ATP:PG	1:C:659:ARG:HH22	2.44	0.41
1:A:457:GLU:O	1:A:460:ARG:HG2	2.21	0.41
1:F:349:THR:HG21	1:F:355:LEU:HD11	2.02	0.41
3:A:901:ATP:PG	1:B:659:ARG:HH22	2.44	0.41
1:D:349:THR:HG21	1:D:355:LEU:HD11	2.03	0.41
1:F:551:VAL:O	1:F:555:VAL:HG23	2.20	0.41
1:F:636:SER:HB3	1:F:637:GLY:H	1.71	0.41
1:D:410:ASP:O	1:D:414:VAL:HG23	2.21	0.40
1:D:543:PRO:HA	1:D:544:PRO:HD3	1.93	0.40
1:C:410:ASP:O	1:C:414:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:490:GLU:HG3	1:C:589:ARG:HD3	2.04	0.40
1:D:457:GLU:O	1:D:460:ARG:HG2	2.21	0.40
1:F:201:ILE:H	1:F:201:ILE:HD12	1.85	0.40
1:A:351:ARG:NH2	1:B:311:ARG:NE	2.70	0.40
3:B:901:ATP:O1G	1:C:659:ARG:NH2	2.49	0.40
1:F:251:THR:CG2	3:F:902:ATP:H3'	2.51	0.40
1:B:251:THR:CG2	3:B:902:ATP:H3'	2.51	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	572/813 (70%)	521 (91%)	38 (7%)	13 (2%)	6	37
1	B	572/813 (70%)	527 (92%)	32 (6%)	13 (2%)	6	37
1	C	572/813 (70%)	521 (91%)	38 (7%)	13 (2%)	6	37
1	D	572/813 (70%)	528 (92%)	35 (6%)	9 (2%)	9	45
1	E	562/813 (69%)	513 (91%)	39 (7%)	10 (2%)	8	42
1	F	562/813 (69%)	516 (92%)	35 (6%)	11 (2%)	7	40
All	All	3412/4878 (70%)	3126 (92%)	217 (6%)	69 (2%)	11	40

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	636	SER
1	A	669	PRO
1	B	490	GLU
1	B	631	GLY
1	B	669	PRO

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Mol	Chain	Res	Type
1	C	669	PRO
1	D	669	PRO
1	E	544	PRO
1	A	404	PRO
1	A	460	ARG
1	A	485	PRO
1	A	486	ALA
1	A	568	GLY
1	A	648	ASP
1	A	715	THR
1	B	404	PRO
1	B	460	ARG
1	B	568	GLY
1	B	632	VAL
1	B	648	ASP
1	B	715	THR
1	C	404	PRO
1	C	460	ARG
1	C	568	GLY
1	C	636	SER
1	C	648	ASP
1	C	715	THR
1	D	404	PRO
1	D	460	ARG
1	D	648	ASP
1	D	715	THR
1	E	404	PRO
1	E	460	ARG
1	E	493	SER
1	E	568	GLY
1	E	715	THR
1	F	404	PRO
1	F	460	ARG
1	F	568	GLY
1	F	648	ASP
1	F	669	PRO
1	F	715	THR
1	A	340	GLY
1	A	386	ARG
1	A	633	GLY
1	B	340	GLY
1	B	386	ARG

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Mol	Chain	Res	Type
1	C	340	GLY
1	C	386	ARG
1	C	491	GLY
1	C	569	PRO
1	D	340	GLY
1	D	386	ARG
1	E	340	GLY
1	E	648	ASP
1	F	340	GLY
1	F	386	ARG
1	F	633	GLY
1	F	636	SER
1	B	569	PRO
1	E	386	ARG
1	F	485	PRO
1	A	569	PRO
1	E	789	PRO
1	D	270	PRO
1	D	569	PRO
1	B	270	PRO
1	C	270	PRO
1	C	632	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	481/671 (72%)	470 (98%)	11 (2%)	50	70
1	B	481/671 (72%)	468 (97%)	13 (3%)	44	66
1	C	481/671 (72%)	468 (97%)	13 (3%)	44	66
1	D	481/671 (72%)	468 (97%)	13 (3%)	44	66
1	E	471/671 (70%)	457 (97%)	14 (3%)	41	63
1	F	471/671 (70%)	456 (97%)	15 (3%)	39	62
All	All	2866/4026 (71%)	2787 (97%)	79 (3%)	46	65

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	234	ARG
1	A	351	ARG
1	A	471	ILE
1	A	492	PHE
1	A	495	ILE
1	A	581	ARG
1	A	627	THR
1	A	648	ASP
1	A	727	ARG
1	A	739	LEU
1	A	780	TRP
1	B	234	ARG
1	B	351	ARG
1	B	471	ILE
1	B	495	ILE
1	B	580	GLU
1	B	581	ARG
1	B	604	ASP
1	B	627	THR
1	B	648	ASP
1	B	656	ARG
1	B	727	ARG
1	B	739	LEU
1	B	780	TRP
1	C	234	ARG
1	C	351	ARG
1	C	471	ILE
1	C	495	ILE
1	C	581	ARG
1	C	604	ASP
1	C	624	THR
1	C	627	THR
1	C	648	ASP
1	C	656	ARG
1	C	727	ARG
1	C	739	LEU
1	C	780	TRP
1	D	234	ARG
1	D	351	ARG
1	D	471	ILE
1	D	492	PHE
1	D	495	ILE

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Mol	Chain	Res	Type
1	D	581	ARG
1	D	604	ASP
1	D	624	THR
1	D	627	THR
1	D	648	ASP
1	D	727	ARG
1	D	739	LEU
1	D	780	TRP
1	E	234	ARG
1	E	351	ARG
1	E	407	VAL
1	E	471	ILE
1	E	484	GLN
1	E	495	ILE
1	E	581	ARG
1	E	624	THR
1	E	627	THR
1	E	635	ARG
1	E	648	ASP
1	E	727	ARG
1	E	739	LEU
1	E	780	TRP
1	F	234	ARG
1	F	327	MET
1	F	351	ARG
1	F	354	PHE
1	F	371	MET
1	F	407	VAL
1	F	471	ILE
1	F	495	ILE
1	F	581	ARG
1	F	604	ASP
1	F	627	THR
1	F	648	ASP
1	F	727	ARG
1	F	739	LEU
1	F	780	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	336	ASN

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Mol	Chain	Res	Type
1	A	395	ASN
1	A	445	ASN
1	A	502	HIS
1	A	785	ASN
1	B	336	ASN
1	B	395	ASN
1	B	445	ASN
1	B	502	HIS
1	B	785	ASN
1	C	336	ASN
1	C	395	ASN
1	C	445	ASN
1	C	484	GLN
1	C	502	HIS
1	C	785	ASN
1	D	254	HIS
1	D	336	ASN
1	D	395	ASN
1	D	445	ASN
1	D	502	HIS
1	D	785	ASN
1	E	254	HIS
1	E	336	ASN
1	E	379	GLN
1	E	395	ASN
1	E	445	ASN
1	E	557	ASN
1	E	785	ASN
1	F	254	HIS
1	F	336	ASN
1	F	395	ASN
1	F	445	ASN
1	F	557	ASN
1	F	585	GLN
1	F	785	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	ATP	B	901	-	26,33,33	0.96	2 (7%)	31,52,52	1.65	8 (25%)
3	ATP	A	901	-	26,33,33	0.98	1 (3%)	31,52,52	1.58	6 (19%)
3	ATP	D	901	-	26,33,33	0.99	3 (11%)	31,52,52	1.56	8 (25%)
3	ATP	C	901	-	26,33,33	0.99	2 (7%)	31,52,52	1.61	8 (25%)
3	ATP	F	901	-	26,33,33	0.95	1 (3%)	31,52,52	1.62	5 (16%)
3	ATP	E	901	-	26,33,33	0.97	2 (7%)	31,52,52	1.57	5 (16%)
3	ATP	C	902	-	26,33,33	1.05	3 (11%)	31,52,52	1.59	5 (16%)
3	ATP	F	902	-	26,33,33	0.99	1 (3%)	31,52,52	1.51	5 (16%)
3	ATP	D	902	-	26,33,33	1.04	3 (11%)	31,52,52	1.62	6 (19%)
3	ATP	A	902	-	26,33,33	1.05	3 (11%)	31,52,52	1.64	6 (19%)
3	ATP	B	902	-	26,33,33	1.12	3 (11%)	31,52,52	1.55	6 (19%)

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
3	ATP	B	901	-	-	4/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	901	-	-	5/18/38/38	0/3/3/3
3	ATP	D	901	-	-	4/18/38/38	0/3/3/3
3	ATP	C	901	-	-	4/18/38/38	0/3/3/3
3	ATP	F	901	-	-	2/18/38/38	0/3/3/3
3	ATP	E	901	-	-	3/18/38/38	0/3/3/3
3	ATP	C	902	-	-	3/18/38/38	0/3/3/3
3	ATP	F	902	-	-	3/18/38/38	0/3/3/3
3	ATP	D	902	-	-	3/18/38/38	0/3/3/3
3	ATP	A	902	-	-	3/18/38/38	0/3/3/3
3	ATP	B	902	-	-	3/18/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	ATP	C5-C4	2.76	1.48	1.40
3	C	901	ATP	C5-C4	2.62	1.47	1.40
3	D	901	ATP	C5-C4	2.61	1.47	1.40
3	A	901	ATP	C5-C4	2.59	1.47	1.40
3	C	902	ATP	C5-C4	2.58	1.47	1.40
3	D	902	ATP	C5-C4	2.57	1.47	1.40
3	A	902	ATP	C5-C4	2.56	1.47	1.40
3	B	901	ATP	C5-C4	2.54	1.47	1.40
3	F	901	ATP	C5-C4	2.52	1.47	1.40
3	E	901	ATP	C5-C4	2.51	1.47	1.40
3	F	902	ATP	C5-C4	2.49	1.47	1.40
3	B	902	ATP	C2-N3	2.44	1.36	1.32
3	A	902	ATP	O4'-C1'	2.39	1.44	1.41
3	C	902	ATP	C2-N3	2.34	1.35	1.32
3	D	902	ATP	O4'-C1'	2.28	1.44	1.41
3	C	902	ATP	O4'-C1'	2.25	1.44	1.41
3	B	901	ATP	O4'-C1'	2.23	1.44	1.41
3	B	902	ATP	O4'-C1'	2.21	1.44	1.41
3	C	901	ATP	O4'-C1'	2.20	1.44	1.41
3	D	902	ATP	C2-N3	2.20	1.35	1.32
3	D	901	ATP	O4'-C1'	2.15	1.44	1.41
3	A	902	ATP	C2-N3	2.12	1.35	1.32
3	D	901	ATP	C2-N3	2.05	1.35	1.32
3	E	901	ATP	C2-N3	2.02	1.35	1.32

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	902	ATP	PB-O3B-PG	-4.20	118.42	132.83
3	E	901	ATP	PB-O3B-PG	-4.06	118.91	132.83
3	A	902	ATP	PB-O3B-PG	-4.05	118.92	132.83
3	B	902	ATP	PB-O3B-PG	-3.90	119.45	132.83
3	D	902	ATP	PB-O3B-PG	-3.89	119.47	132.83
3	C	902	ATP	PA-O3A-PB	-3.81	119.76	132.83
3	F	902	ATP	PB-O3B-PG	-3.76	119.93	132.83
3	D	901	ATP	PA-O3A-PB	-3.76	119.94	132.83
3	D	902	ATP	PA-O3A-PB	-3.71	120.11	132.83
3	E	901	ATP	PA-O3A-PB	-3.62	120.39	132.83
3	F	901	ATP	PB-O3B-PG	-3.59	120.50	132.83
3	A	902	ATP	PA-O3A-PB	-3.57	120.58	132.83
3	A	901	ATP	PA-O3A-PB	-3.56	120.59	132.83
3	B	901	ATP	PA-O3A-PB	-3.55	120.65	132.83
3	C	901	ATP	C3'-C2'-C1'	3.54	106.31	100.98
3	F	901	ATP	C3'-C2'-C1'	3.53	106.30	100.98
3	C	901	ATP	PA-O3A-PB	-3.50	120.81	132.83
3	D	901	ATP	C3'-C2'-C1'	3.50	106.25	100.98
3	B	901	ATP	C3'-C2'-C1'	3.49	106.24	100.98
3	F	901	ATP	PA-O3A-PB	-3.37	121.25	132.83
3	F	901	ATP	N3-C2-N1	-3.34	123.45	128.68
3	B	902	ATP	PA-O3A-PB	-3.33	121.40	132.83
3	A	902	ATP	N3-C2-N1	-3.26	123.59	128.68
3	A	901	ATP	C3'-C2'-C1'	3.25	105.87	100.98
3	F	902	ATP	PA-O3A-PB	-3.23	121.73	132.83
3	A	902	ATP	C3'-C2'-C1'	3.18	105.77	100.98
3	F	902	ATP	N3-C2-N1	-3.12	123.80	128.68
3	D	902	ATP	N3-C2-N1	-3.10	123.84	128.68
3	E	901	ATP	N3-C2-N1	-3.07	123.88	128.68
3	C	901	ATP	N3-C2-N1	-3.03	123.94	128.68
3	D	902	ATP	C4-C5-N7	-3.02	106.25	109.40
3	A	901	ATP	N3-C2-N1	-3.02	123.96	128.68
3	D	901	ATP	N3-C2-N1	-2.99	124.01	128.68
3	C	902	ATP	N3-C2-N1	-2.94	124.09	128.68
3	B	901	ATP	N3-C2-N1	-2.89	124.16	128.68
3	F	901	ATP	C4-C5-N7	-2.80	106.48	109.40
3	A	902	ATP	C4-C5-N7	-2.75	106.53	109.40
3	B	902	ATP	N3-C2-N1	-2.73	124.41	128.68
3	E	901	ATP	C4-C5-N7	-2.67	106.61	109.40
3	F	902	ATP	C4-C5-N7	-2.67	106.62	109.40
3	E	901	ATP	C3'-C2'-C1'	2.65	104.97	100.98
3	B	902	ATP	C4-C5-N7	-2.63	106.66	109.40
3	C	902	ATP	C4-C5-N7	-2.58	106.71	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	901	ATP	O3G-PG-O2G	2.55	117.40	107.64
3	C	902	ATP	C3'-C2'-C1'	2.55	104.81	100.98
3	D	902	ATP	C3'-C2'-C1'	2.54	104.81	100.98
3	A	901	ATP	PB-O3B-PG	-2.53	124.14	132.83
3	B	902	ATP	C3'-C2'-C1'	2.49	104.73	100.98
3	B	901	ATP	O3B-PG-O1G	-2.49	97.38	111.19
3	B	901	ATP	C4-C5-N7	-2.49	106.81	109.40
3	F	902	ATP	C3'-C2'-C1'	2.48	104.71	100.98
3	B	901	ATP	PB-O3B-PG	-2.43	124.48	132.83
3	B	901	ATP	O2B-PB-O1B	2.42	124.19	112.24
3	C	901	ATP	PB-O3B-PG	-2.37	124.69	132.83
3	A	901	ATP	O2B-PB-O1B	2.36	123.88	112.24
3	D	901	ATP	PB-O3B-PG	-2.34	124.78	132.83
3	A	901	ATP	C4-C5-N7	-2.31	106.99	109.40
3	D	901	ATP	C4-C5-N7	-2.27	107.03	109.40
3	C	901	ATP	O2B-PB-O1B	2.22	123.21	112.24
3	C	901	ATP	C4-C5-N7	-2.19	107.12	109.40
3	A	902	ATP	O4'-C4'-C3'	2.18	109.42	105.11
3	D	901	ATP	O2B-PB-O1B	2.17	122.98	112.24
3	C	901	ATP	O3B-PG-O1G	-2.16	99.18	111.19
3	B	902	ATP	O4'-C4'-C3'	2.15	109.37	105.11
3	D	901	ATP	O3G-PG-O2G	2.14	115.83	107.64
3	D	901	ATP	O3B-PG-O1G	-2.04	99.87	111.19
3	D	902	ATP	O4'-C4'-C3'	2.03	109.13	105.11
3	B	901	ATP	O4'-C4'-C3'	2.03	109.13	105.11

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	ATP	PB-O3B-PG-O2G
3	A	901	ATP	PB-O3B-PG-O3G
3	B	901	ATP	PB-O3B-PG-O2G
3	C	901	ATP	PB-O3B-PG-O2G
3	D	901	ATP	PB-O3B-PG-O2G
3	F	901	ATP	C5'-O5'-PA-O1A
3	F	901	ATP	C5'-O5'-PA-O3A
3	C	902	ATP	O4'-C4'-C5'-O5'
3	D	902	ATP	O4'-C4'-C5'-O5'
3	A	901	ATP	PA-O3A-PB-O1B
3	B	901	ATP	PA-O3A-PB-O1B
3	C	901	ATP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
3	D	901	ATP	PA-O3A-PB-O1B
3	A	902	ATP	O4'-C4'-C5'-O5'
3	B	902	ATP	O4'-C4'-C5'-O5'
3	F	902	ATP	O4'-C4'-C5'-O5'
3	E	901	ATP	O4'-C4'-C5'-O5'
3	A	901	ATP	PA-O3A-PB-O2B
3	B	901	ATP	PA-O3A-PB-O2B
3	C	901	ATP	PA-O3A-PB-O2B
3	C	902	ATP	PA-O3A-PB-O1B
3	D	901	ATP	PA-O3A-PB-O2B
3	F	902	ATP	PA-O3A-PB-O1B
3	A	902	ATP	PA-O3A-PB-O1B
3	B	902	ATP	PA-O3A-PB-O1B
3	C	902	ATP	PA-O3A-PB-O2B
3	D	902	ATP	PA-O3A-PB-O1B
3	E	901	ATP	PA-O3A-PB-O1B
3	F	902	ATP	PA-O3A-PB-O2B
3	A	901	ATP	PB-O3B-PG-O1G
3	A	902	ATP	PA-O3A-PB-O2B
3	B	902	ATP	PA-O3A-PB-O2B
3	D	902	ATP	PA-O3A-PB-O2B
3	E	901	ATP	PA-O3A-PB-O2B
3	B	901	ATP	PB-O3B-PG-O1G
3	C	901	ATP	PB-O3B-PG-O1G
3	D	901	ATP	PB-O3B-PG-O1G

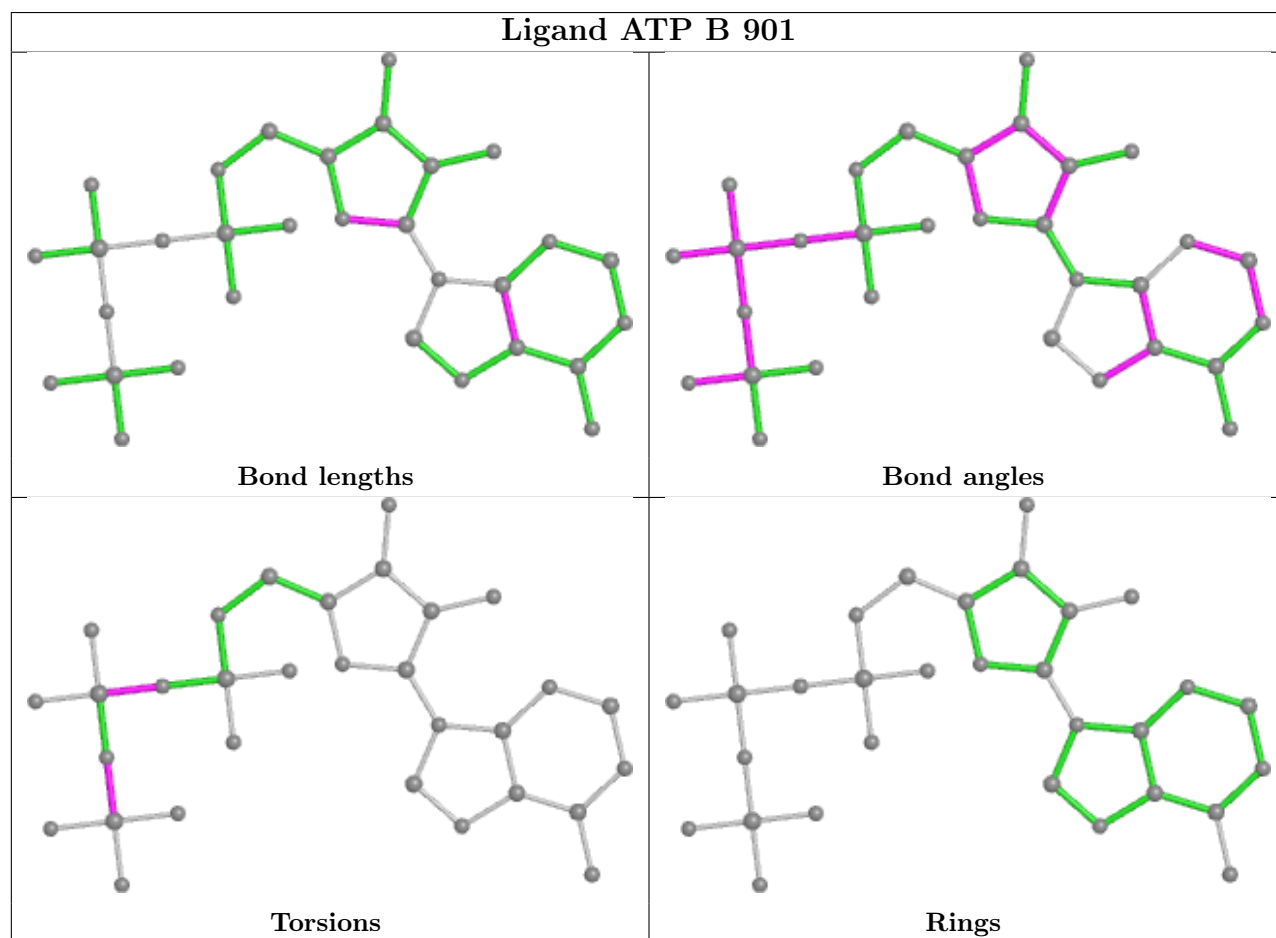
There are no ring outliers.

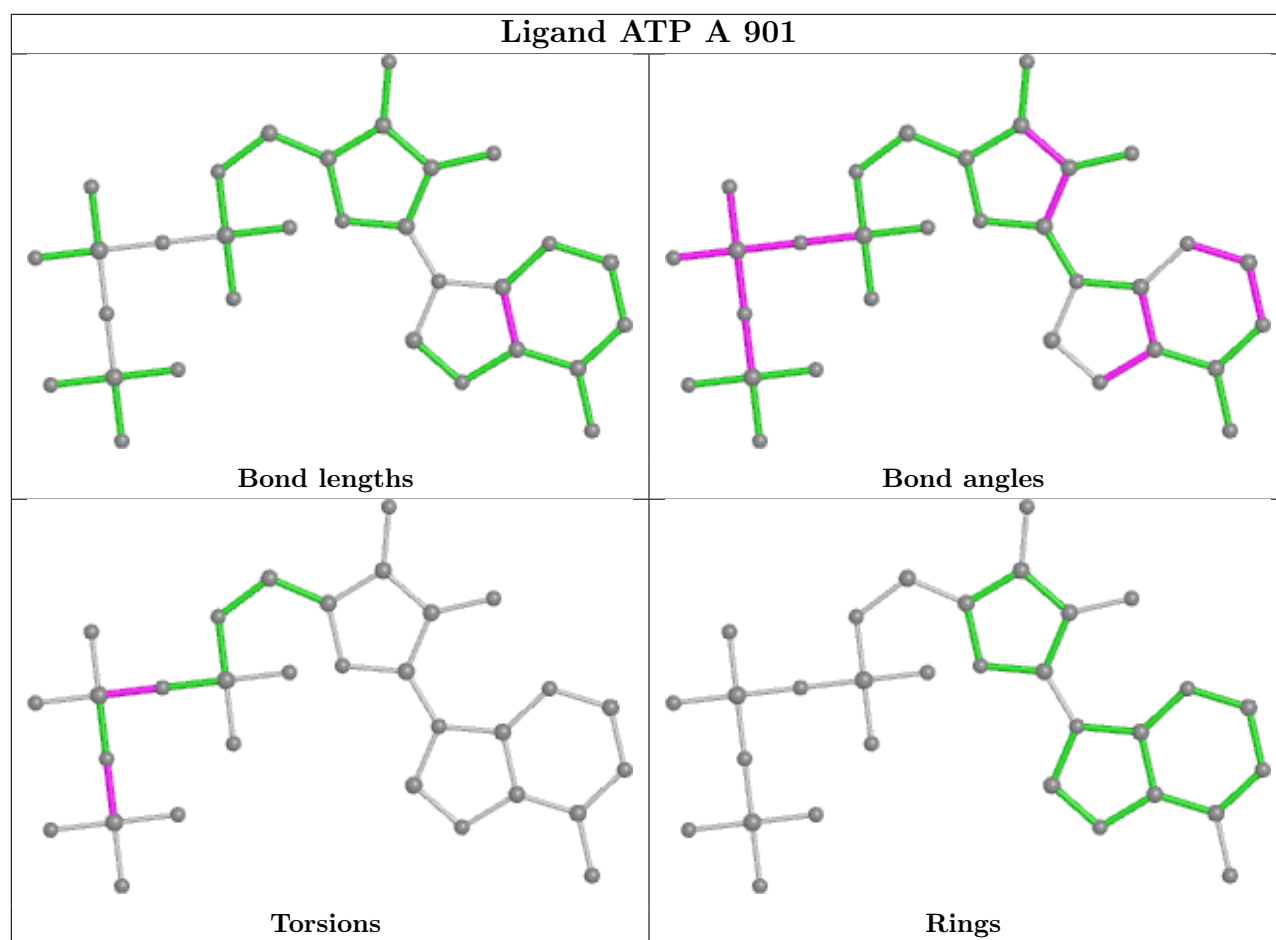
10 monomers are involved in 21 short contacts:

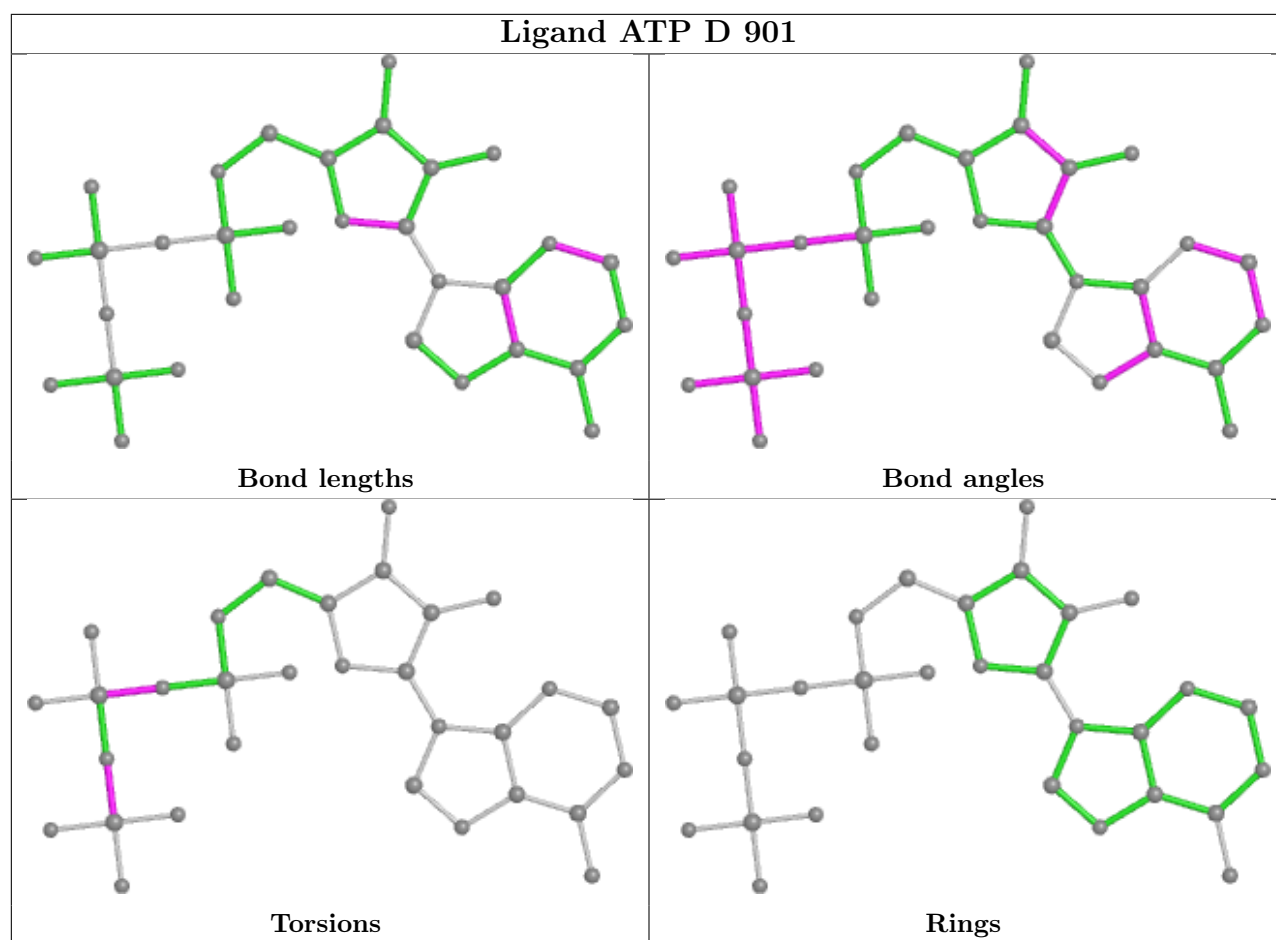
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	901	ATP	4	0
3	A	901	ATP	7	0
3	D	901	ATP	1	0
3	C	901	ATP	1	0
3	E	901	ATP	1	0
3	C	902	ATP	1	0
3	F	902	ATP	2	0
3	D	902	ATP	1	0
3	A	902	ATP	1	0
3	B	902	ATP	2	0

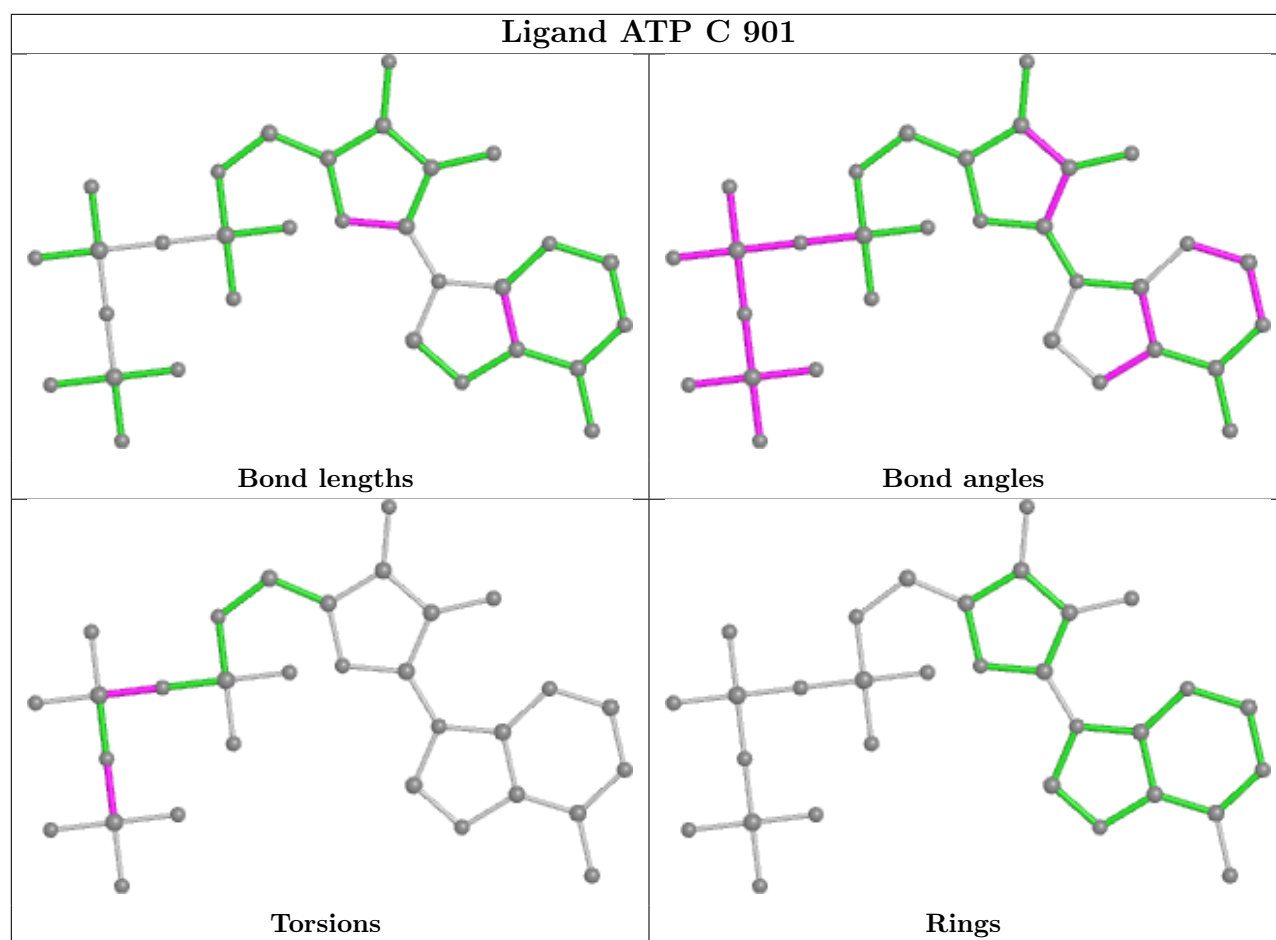
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

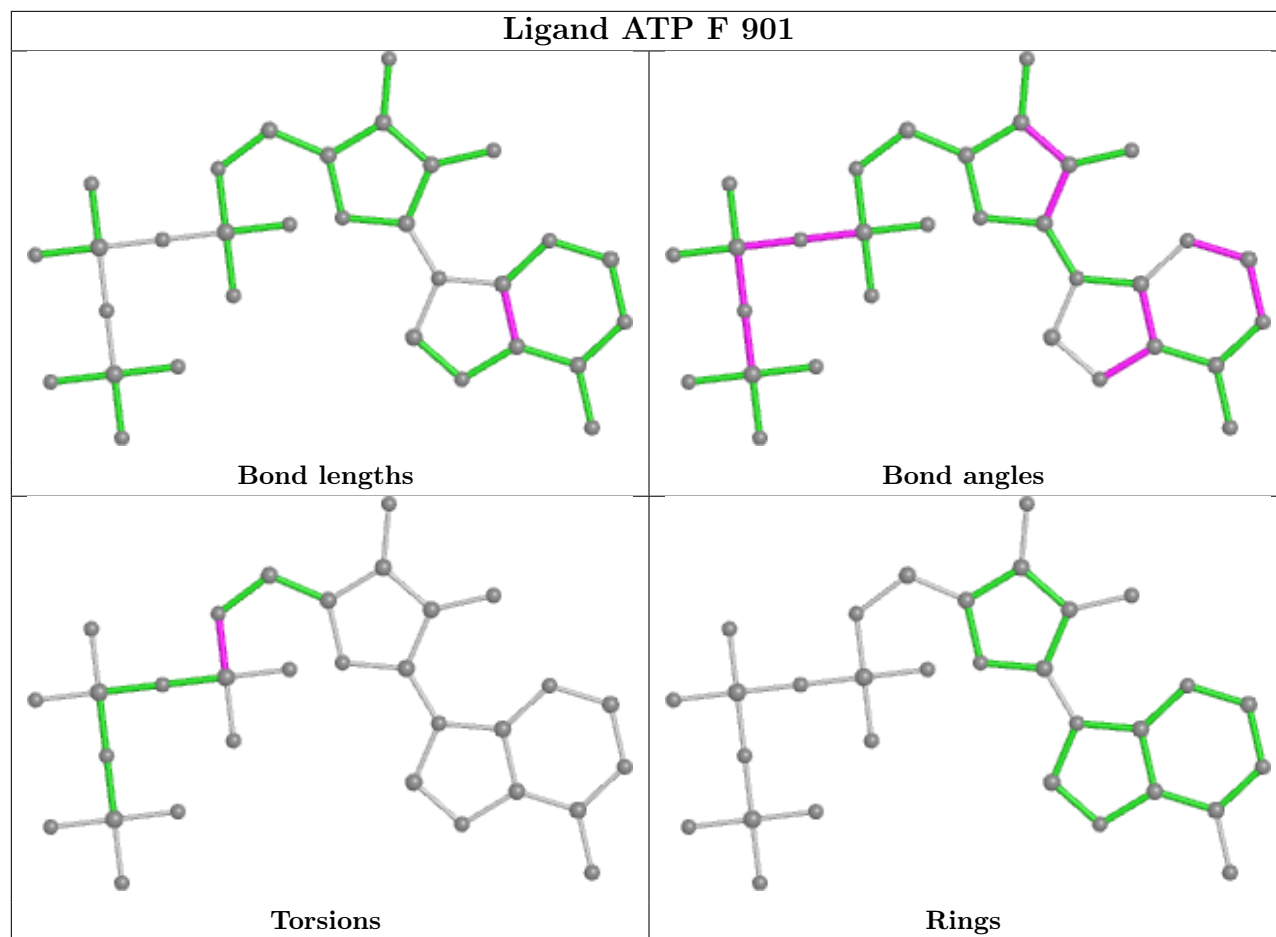
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

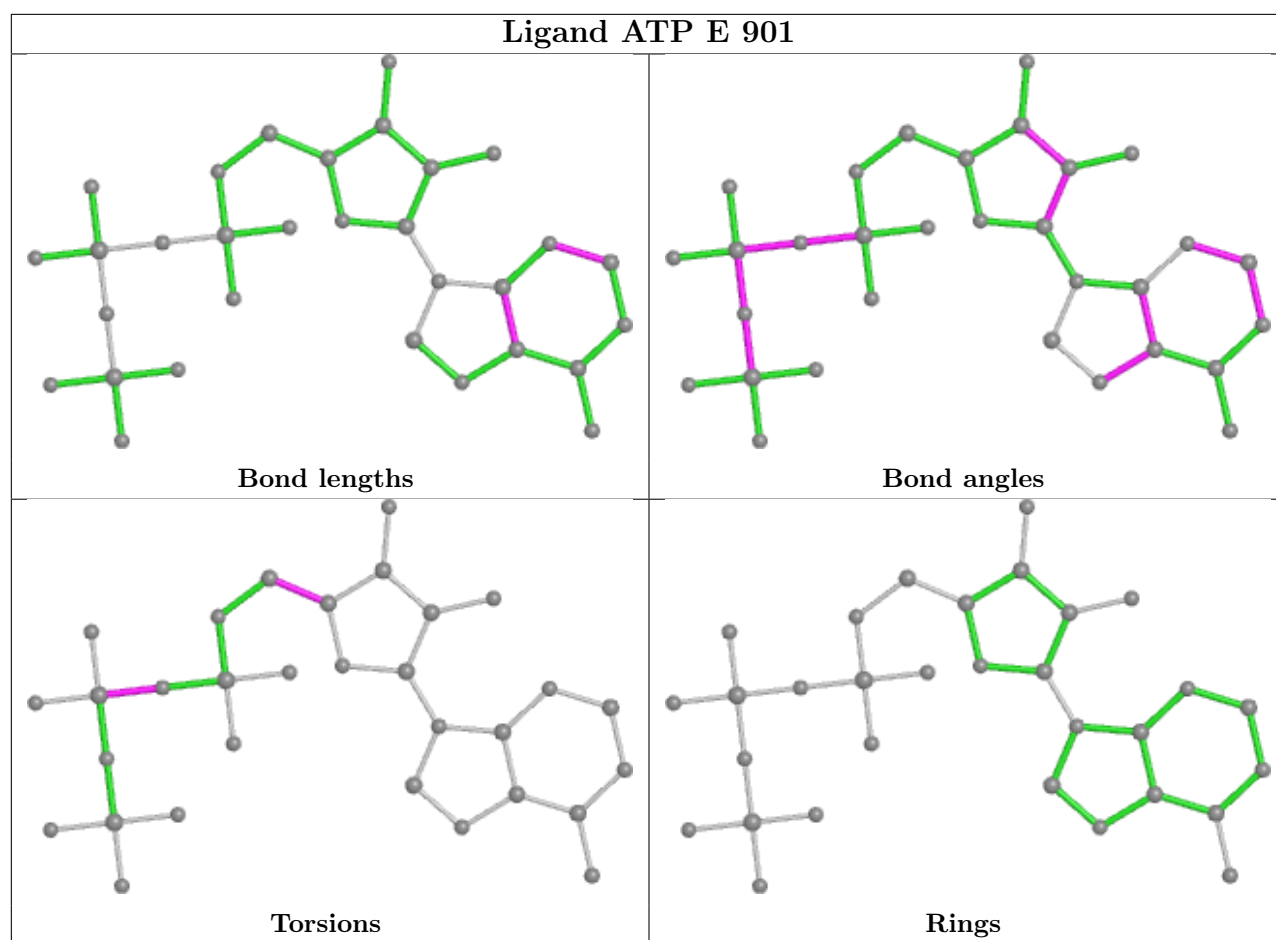


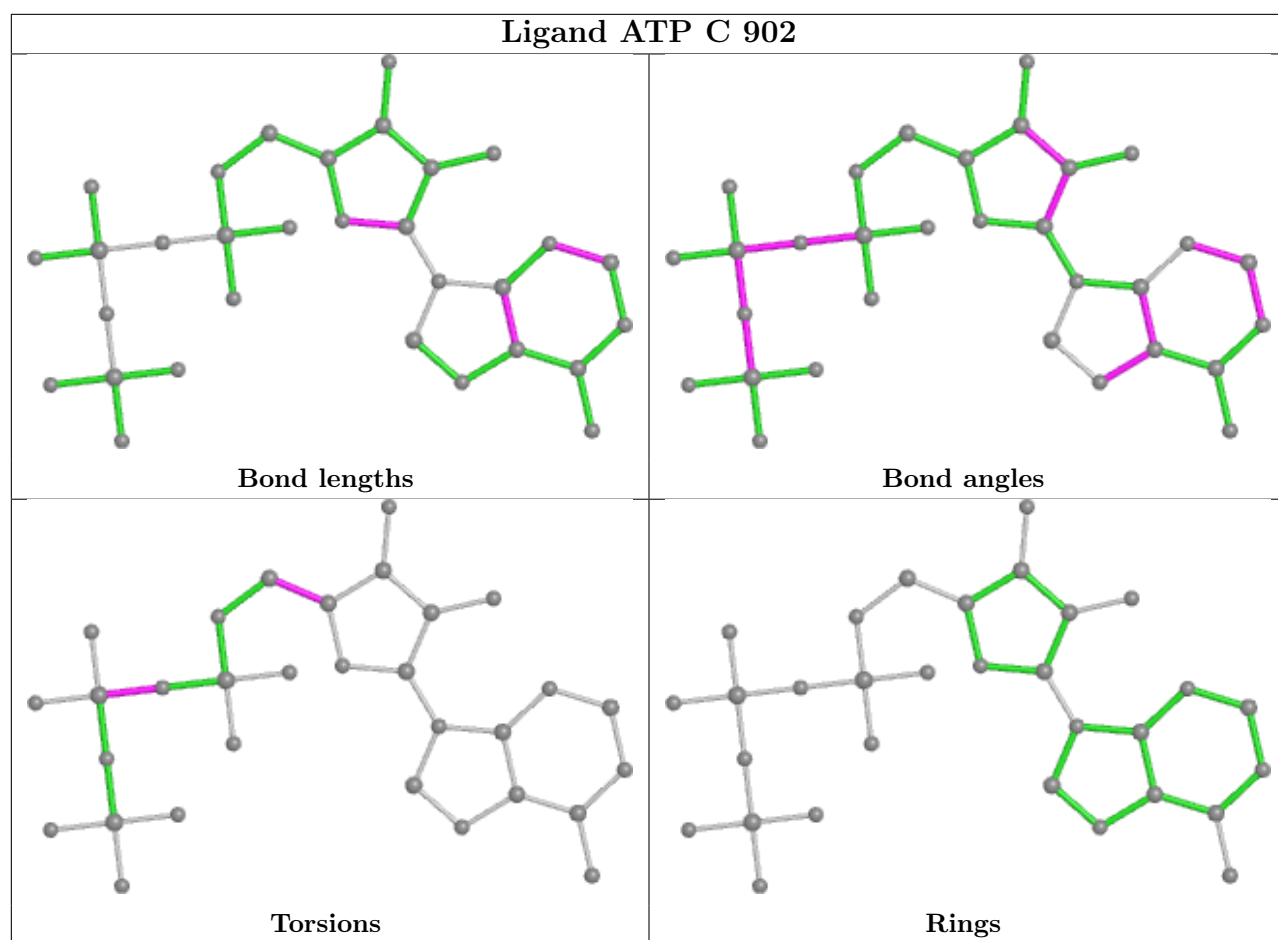


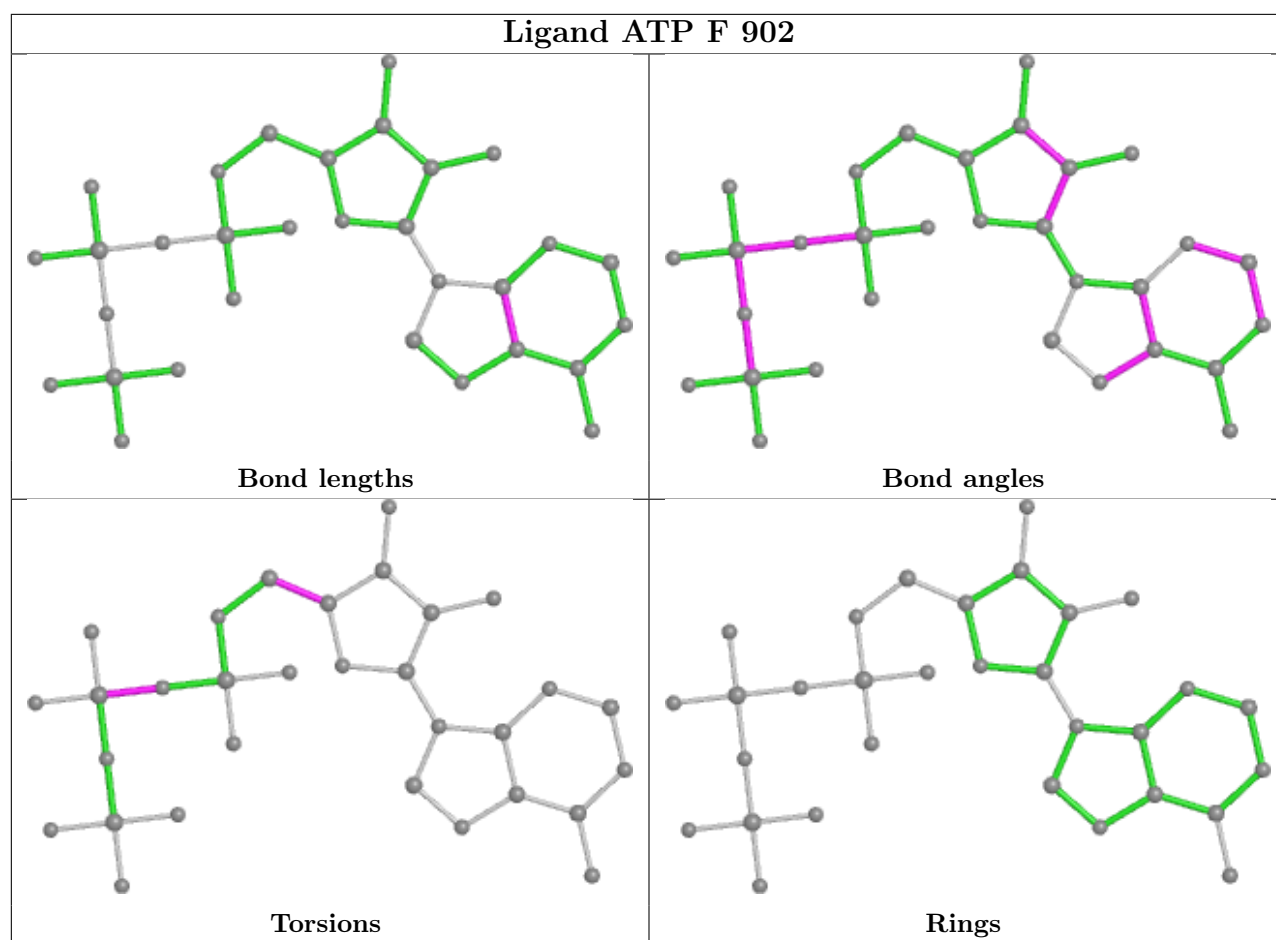


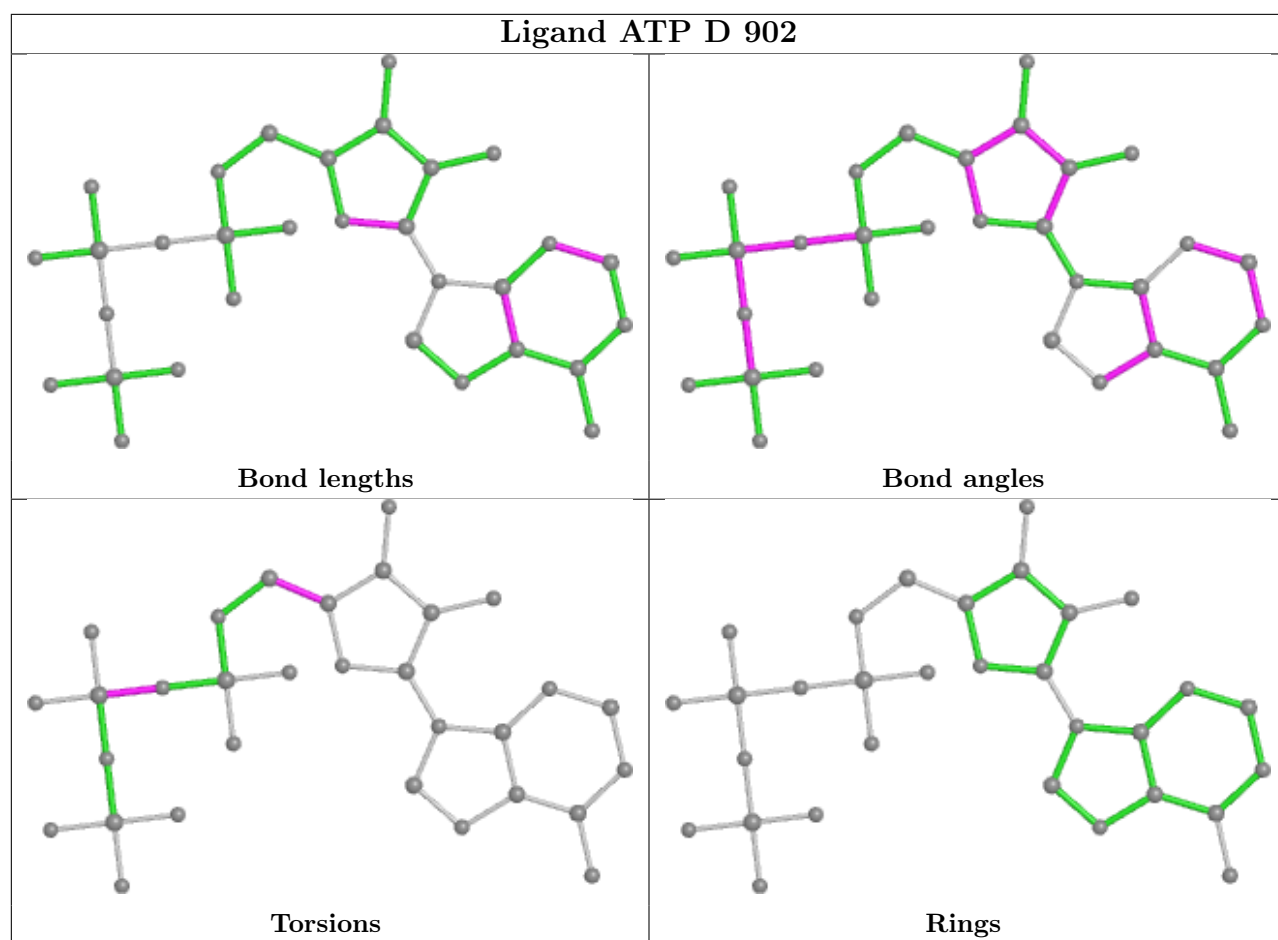


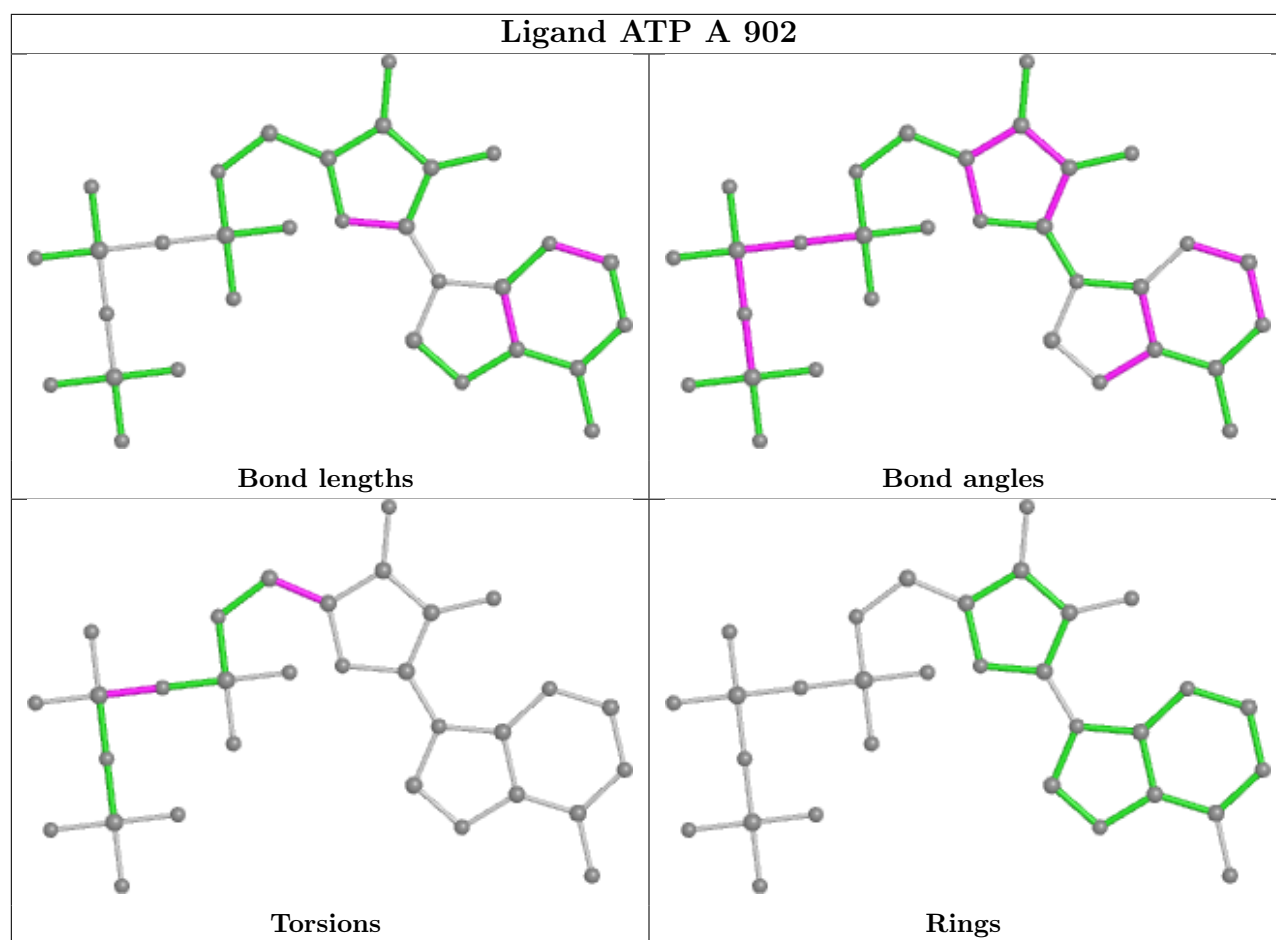


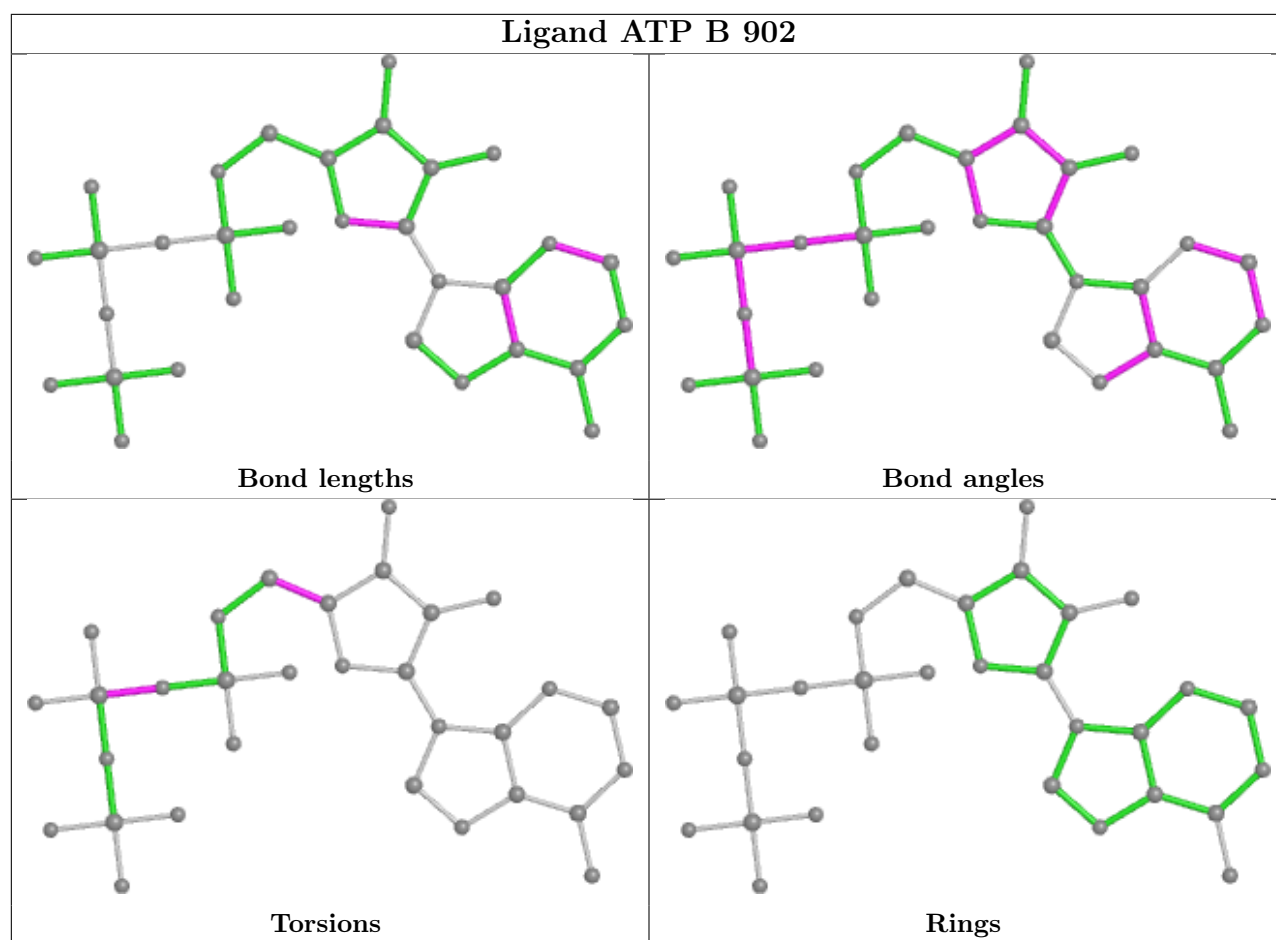












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

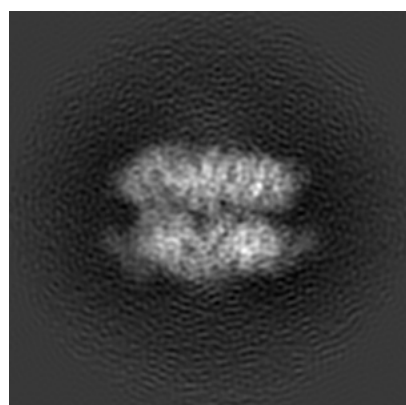
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9063. These allow visual inspection of the internal detail of the map and identification of artifacts.

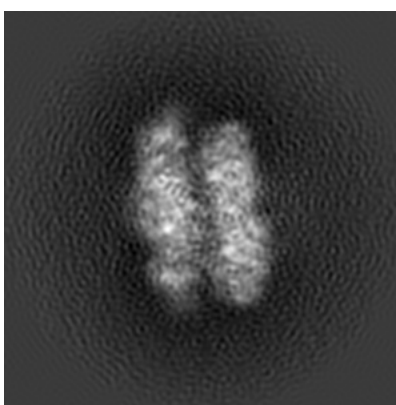
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

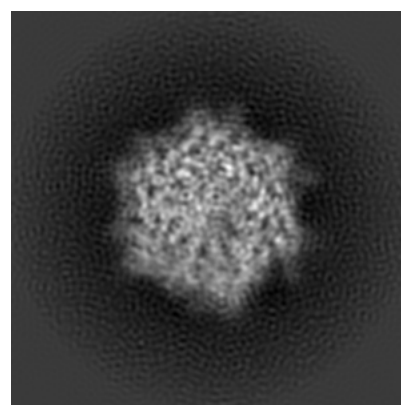
6.1.1 Primary map



X



Y

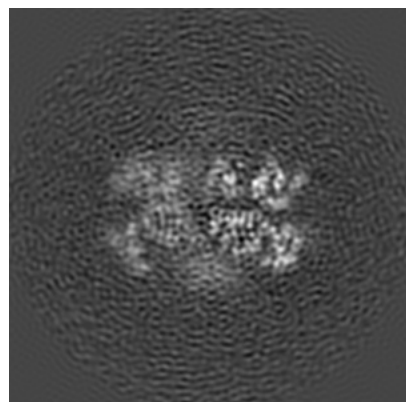


Z

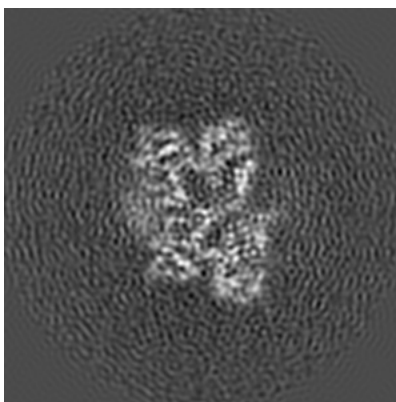
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

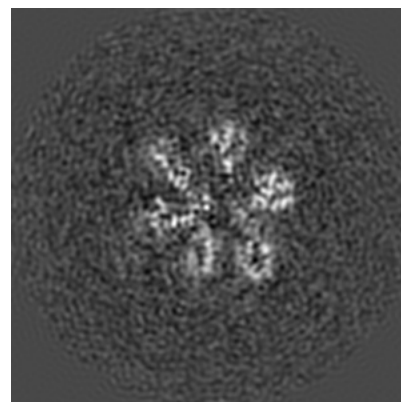
6.2.1 Primary map



X Index: 96



Y Index: 96

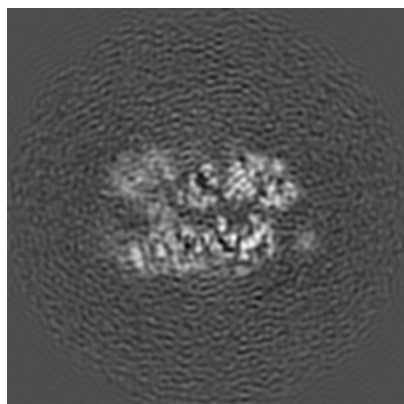


Z Index: 96

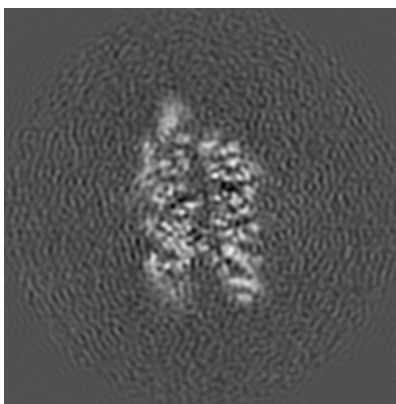
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

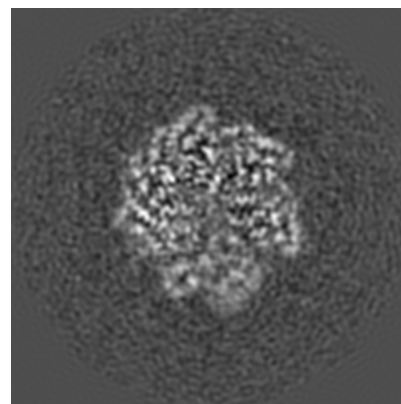
6.3.1 Primary map



X Index: 110



Y Index: 111



Z Index: 109

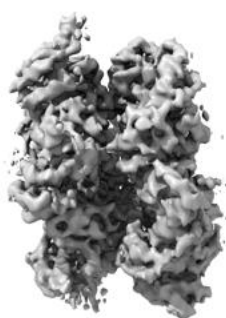
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

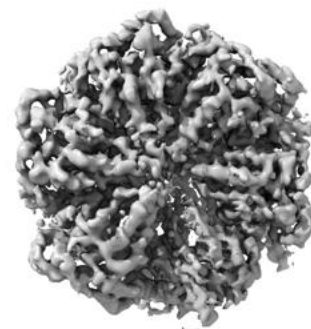
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0796. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

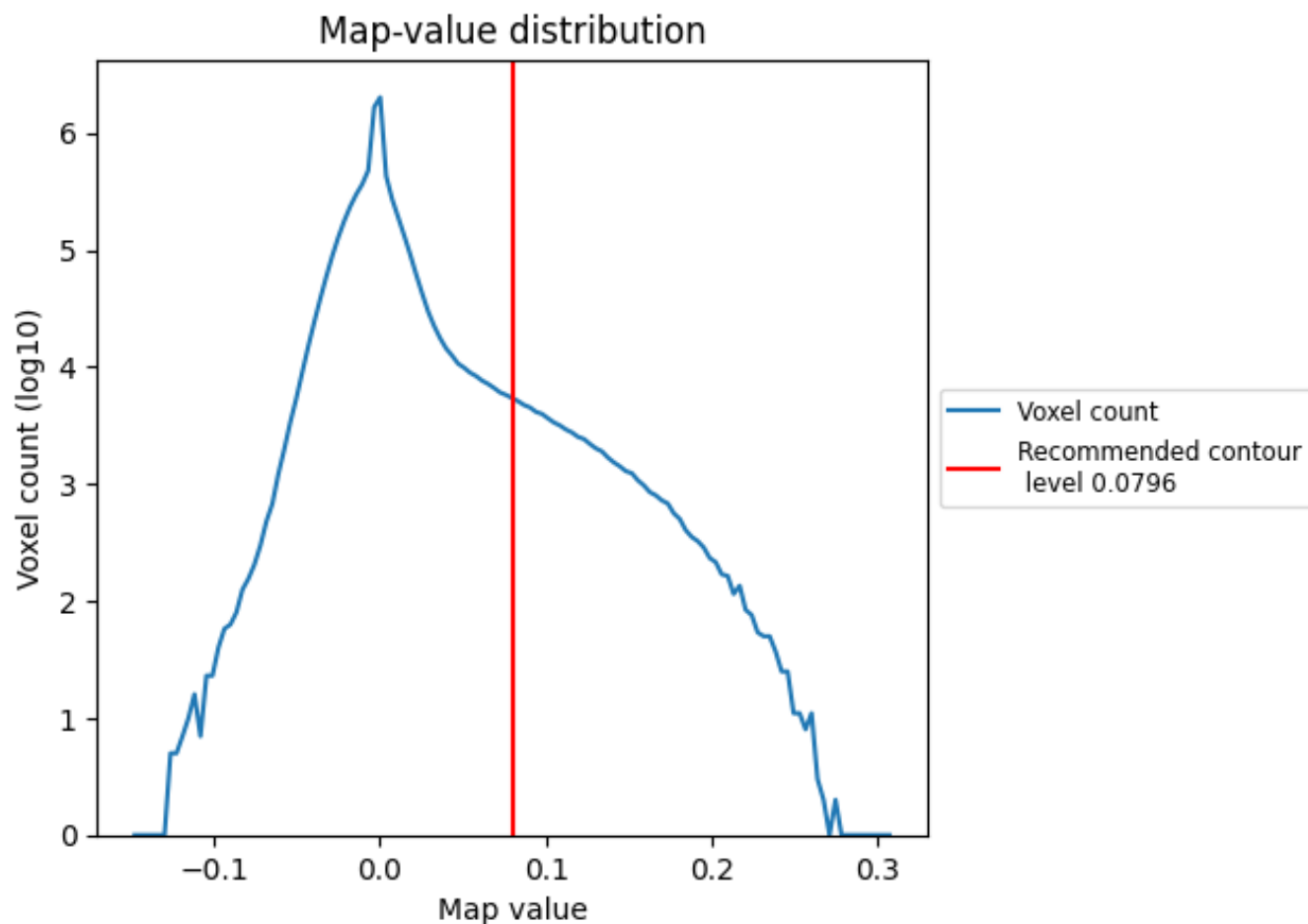
6.5 Mask visualisation

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

7 Map analysis [i](#)

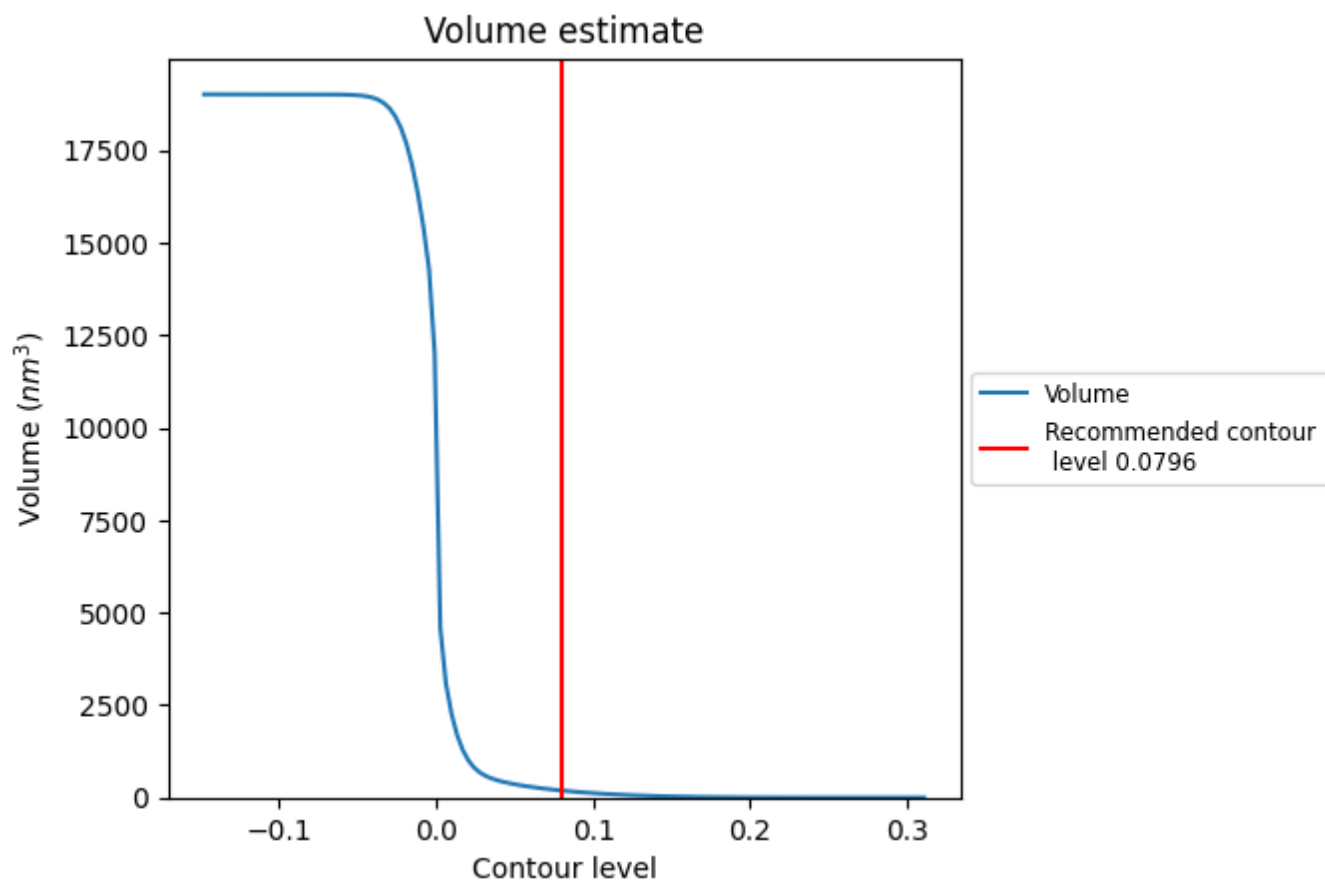
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

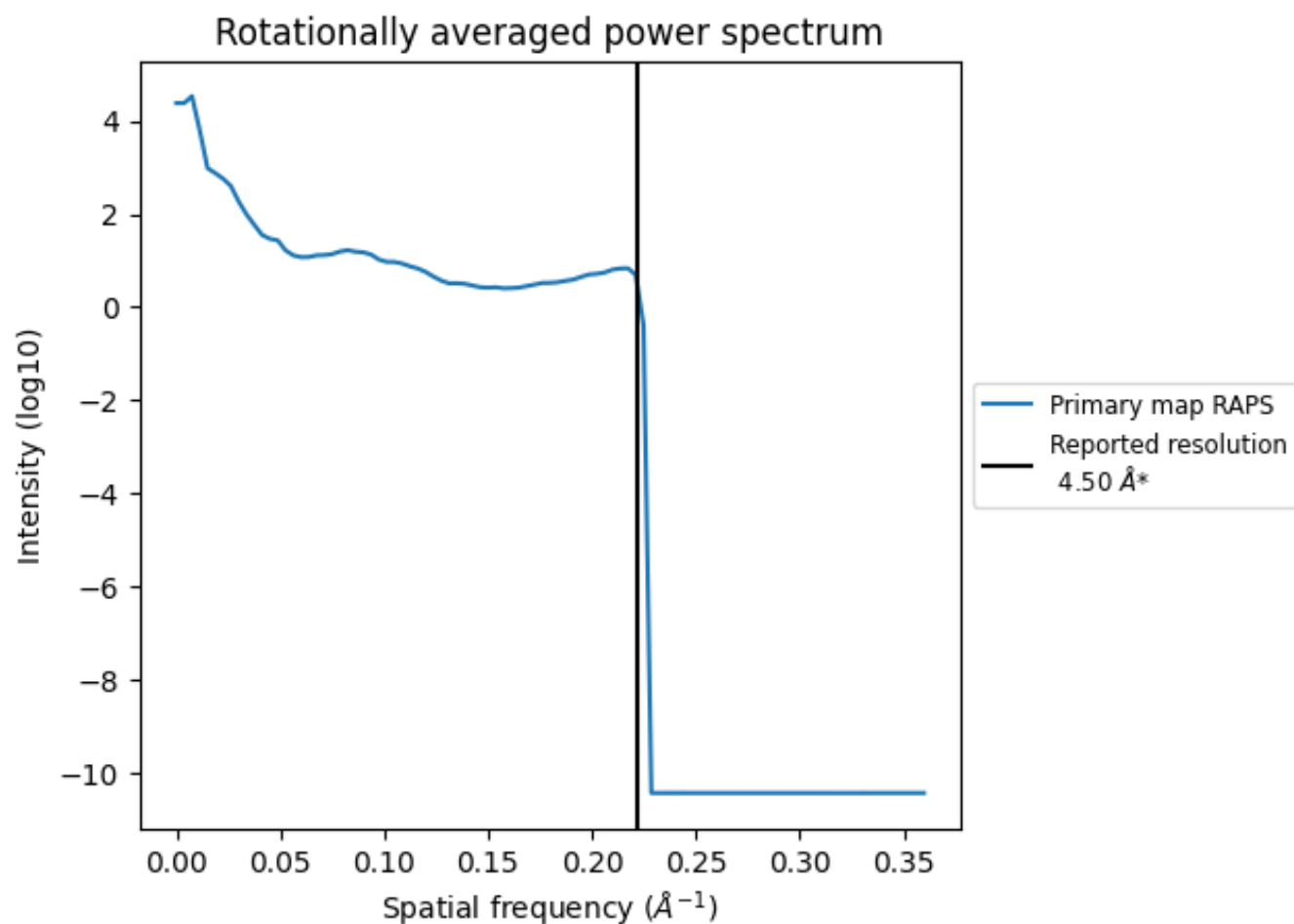
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 191 nm³; this corresponds to an approximate mass of 173 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 ⓘ

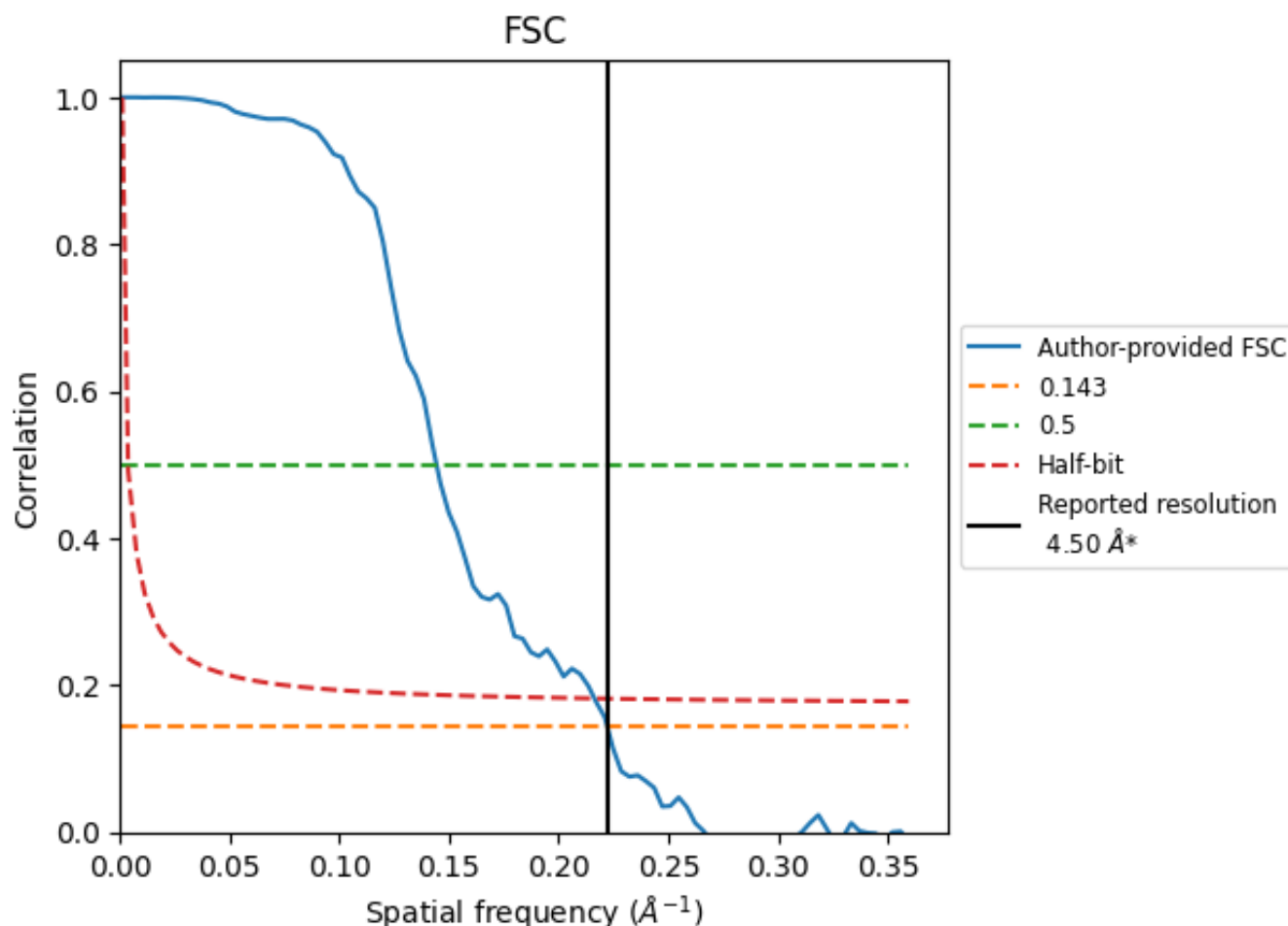


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

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 0.222 Å⁻¹

8.2 Resolution estimates [i](#)

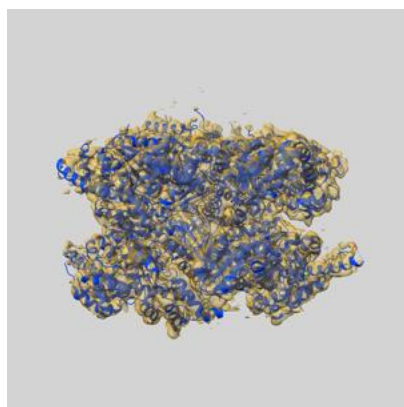
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.50	6.93	4.62
Unmasked-calculated*	-	-	-

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

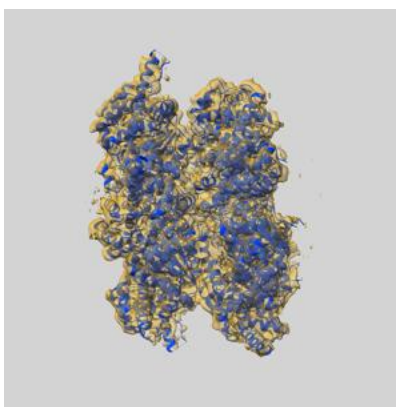
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9063 and PDB model 6MAT. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

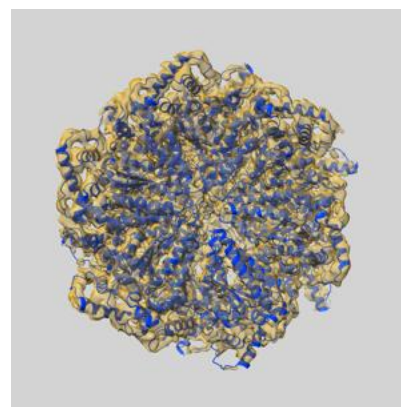
9.1 Map-model overlay [i](#)



X



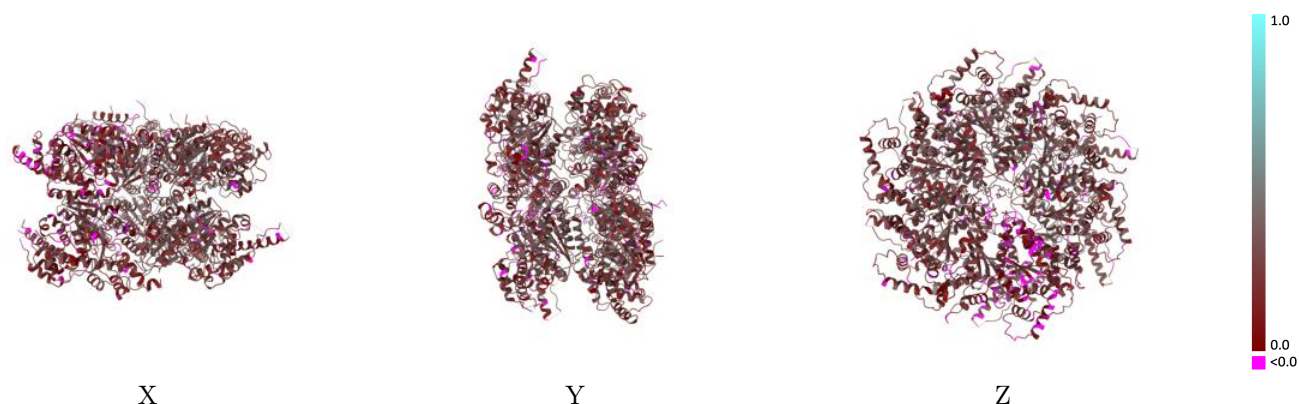
Y



Z

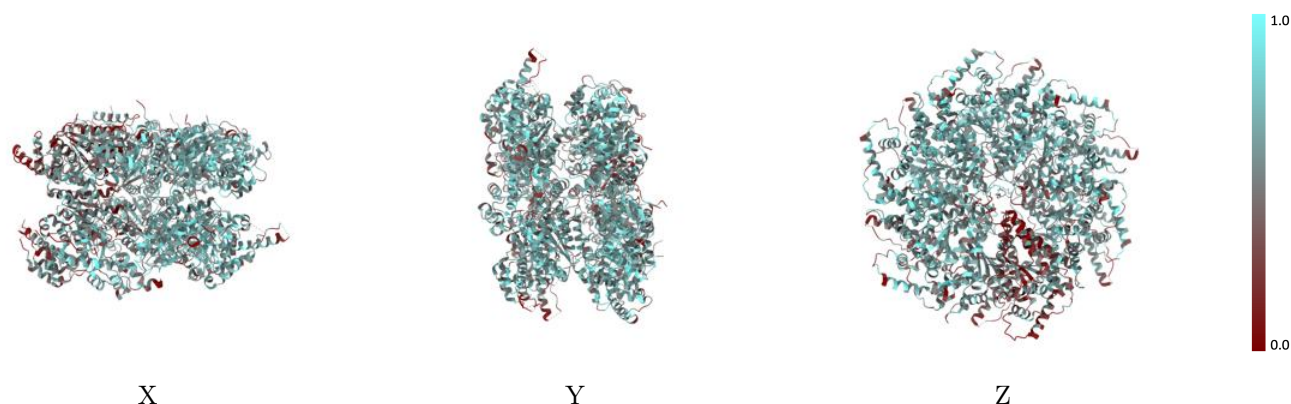
The images above show the 3D surface view of the map at the recommended contour level 0.0796 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



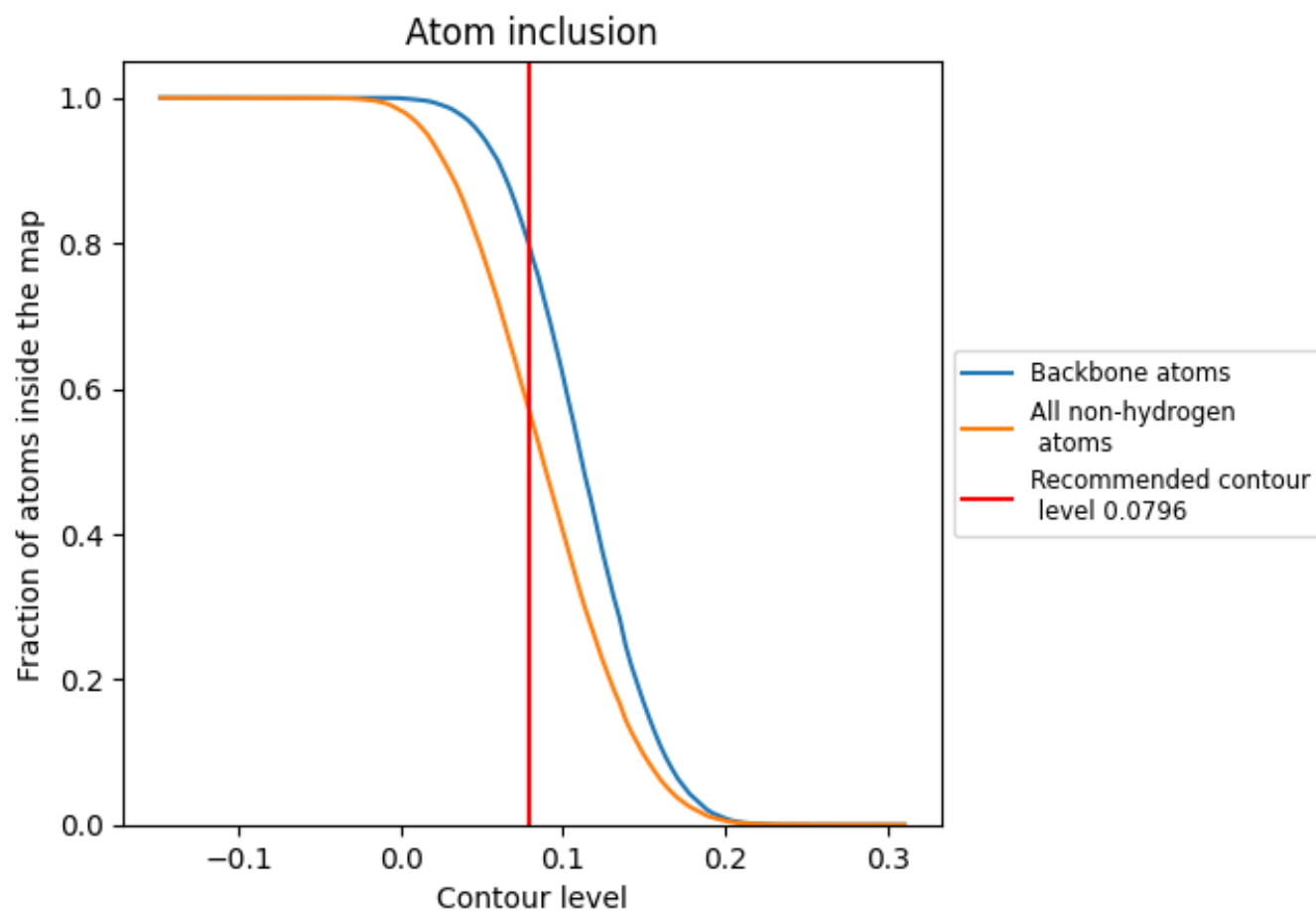
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0796).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 57% 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 (0.0796) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.5684	<div><div></div></div> 0.2300
A	<div><div></div></div> 0.5956	<div><div></div></div> 0.2380
B	<div><div></div></div> 0.6332	<div><div></div></div> 0.2570
C	<div><div></div></div> 0.6286	<div><div></div></div> 0.2560
D	<div><div></div></div> 0.6146	<div><div></div></div> 0.2550
E	<div><div></div></div> 0.5178	<div><div></div></div> 0.2130
F	<div><div></div></div> 0.4153	<div><div></div></div> 0.1560
G	<div><div></div></div> 0.6148	<div><div></div></div> 0.3040

1.0

0.0

<0.0