



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:46 PM UTC

PDB ID : 6JQ0 / pdb_00006jq0
EMDB ID : EMD-9872
Title : CryoEM structure of Abo1 Walker B (E372Q) mutant hexamer - ATP complex
Authors : Cho, C.; Jang, J.; Song, J.J.
Deposited on : 2019-03-28
Resolution : 3.54 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

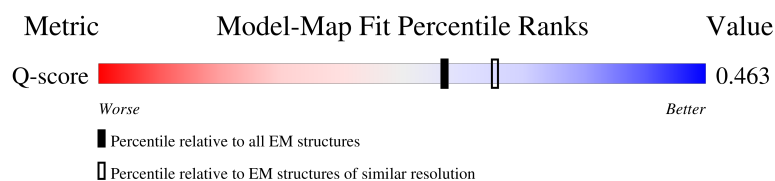
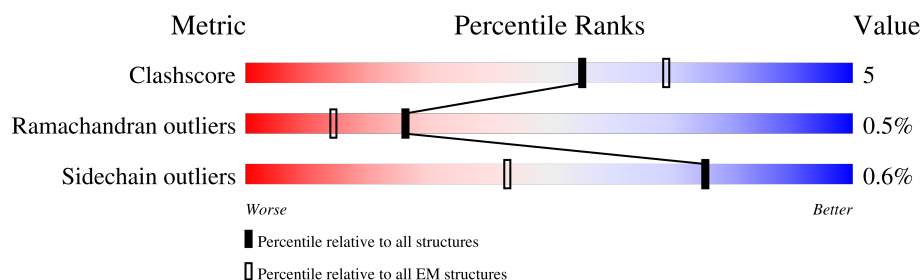
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.54 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	12891 (3.04 - 4.04)

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	1198	
1	B	1198	
1	C	1198	
1	D	1198	

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Mol	Chain	Length	Quality of chain
1	E	1198	41%7%52%
1	F	1198	7%38%6%56%
2	G	14	7%100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26917 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 Uncharacterized AAA domain-containing protein C31G5.19.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	516	Total	C	N	O	S	0	0
			4144	2659	699	764	22		
1	B	571	Total	C	N	O	S	0	0
			4587	2936	784	845	22		
1	C	569	Total	C	N	O	S	0	0
			4574	2929	783	840	22		
1	D	566	Total	C	N	O	S	0	0
			4547	2915	776	834	22		
1	E	577	Total	C	N	O	S	0	0
			4628	2963	790	853	22		
1	F	524	Total	C	N	O	S	0	0
			4185	2680	724	760	21		

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP O14114
A	-6	ALA	-	expression tag	UNP O14114
A	-5	MET	-	expression tag	UNP O14114
A	-4	GLY	-	expression tag	UNP O14114
A	-3	SER	-	expression tag	UNP O14114
A	-2	GLY	-	expression tag	UNP O14114
A	-1	ILE	-	expression tag	UNP O14114
A	0	GLN	-	expression tag	UNP O14114
A	372	GLN	GLU	engineered mutation	UNP O14114
B	-7	GLY	-	expression tag	UNP O14114
B	-6	ALA	-	expression tag	UNP O14114
B	-5	MET	-	expression tag	UNP O14114
B	-4	GLY	-	expression tag	UNP O14114
B	-3	SER	-	expression tag	UNP O14114
B	-2	GLY	-	expression tag	UNP O14114
B	-1	ILE	-	expression tag	UNP O14114
B	0	GLN	-	expression tag	UNP O14114
B	372	GLN	GLU	engineered mutation	UNP O14114

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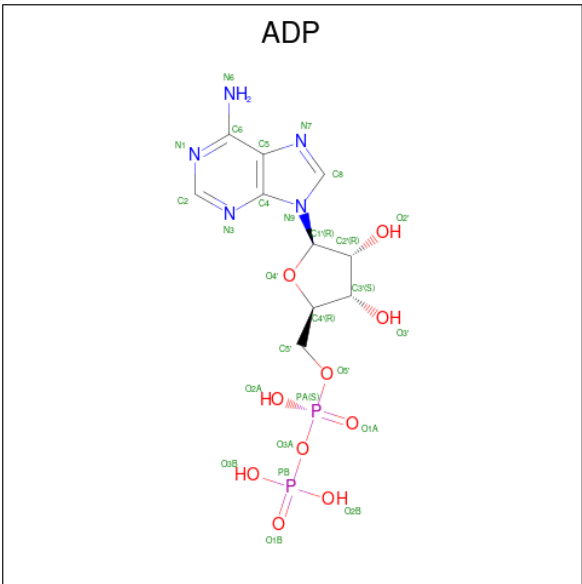
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	GLY	-	expression tag	UNP O14114
C	-6	ALA	-	expression tag	UNP O14114
C	-5	MET	-	expression tag	UNP O14114
C	-4	GLY	-	expression tag	UNP O14114
C	-3	SER	-	expression tag	UNP O14114
C	-2	GLY	-	expression tag	UNP O14114
C	-1	ILE	-	expression tag	UNP O14114
C	0	GLN	-	expression tag	UNP O14114
C	372	GLN	GLU	engineered mutation	UNP O14114
D	-7	GLY	-	expression tag	UNP O14114
D	-6	ALA	-	expression tag	UNP O14114
D	-5	MET	-	expression tag	UNP O14114
D	-4	GLY	-	expression tag	UNP O14114
D	-3	SER	-	expression tag	UNP O14114
D	-2	GLY	-	expression tag	UNP O14114
D	-1	ILE	-	expression tag	UNP O14114
D	0	GLN	-	expression tag	UNP O14114
D	372	GLN	GLU	engineered mutation	UNP O14114
E	-7	GLY	-	expression tag	UNP O14114
E	-6	ALA	-	expression tag	UNP O14114
E	-5	MET	-	expression tag	UNP O14114
E	-4	GLY	-	expression tag	UNP O14114
E	-3	SER	-	expression tag	UNP O14114
E	-2	GLY	-	expression tag	UNP O14114
E	-1	ILE	-	expression tag	UNP O14114
E	0	GLN	-	expression tag	UNP O14114
E	372	GLN	GLU	engineered mutation	UNP O14114
F	-7	GLY	-	expression tag	UNP O14114
F	-6	ALA	-	expression tag	UNP O14114
F	-5	MET	-	expression tag	UNP O14114
F	-4	GLY	-	expression tag	UNP O14114
F	-3	SER	-	expression tag	UNP O14114
F	-2	GLY	-	expression tag	UNP O14114
F	-1	ILE	-	expression tag	UNP O14114
F	0	GLN	-	expression tag	UNP O14114
F	372	GLN	GLU	engineered mutation	UNP O14114

- Molecule 2 is a protein called unknown substrate.

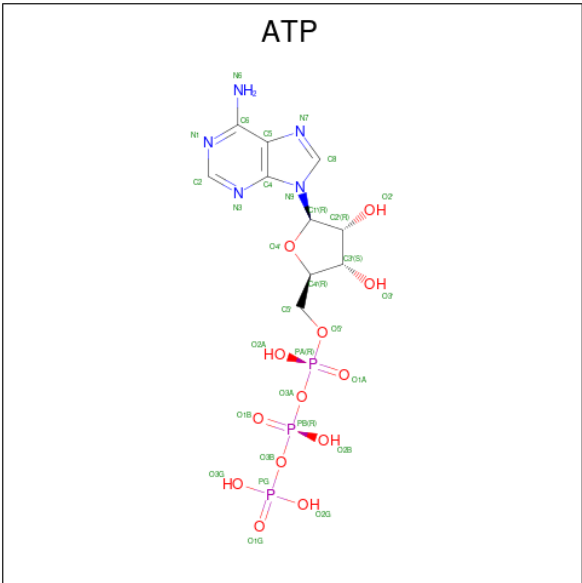
Mol	Chain	Residues	Atoms				AltConf	Trace
2	G	14	Total	C	N	O	0	0
			70	42	14	14		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

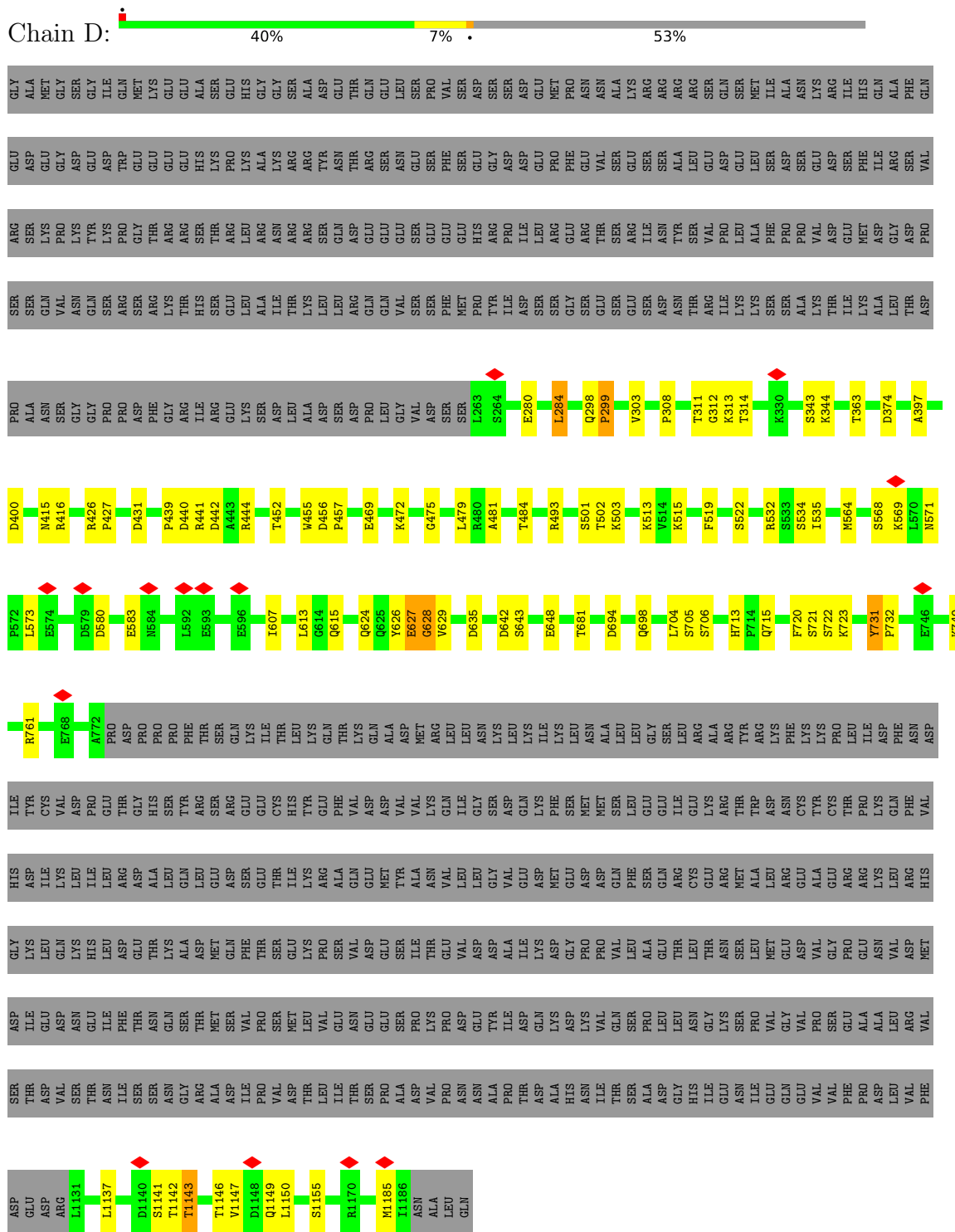
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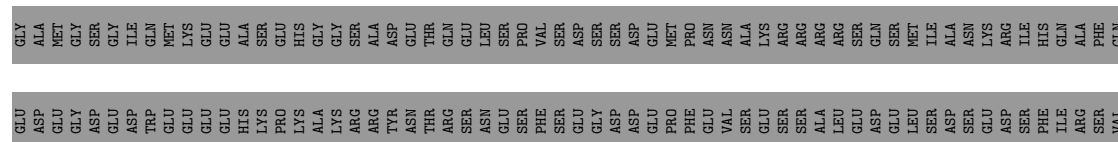
Mol	Chain	Residues	Atoms					AltConf
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	F	1	Total	C	N	O	P	0
			31	10	5	13	3	



- Molecule 1: Uncharacterized AAA domain-containing protein C31G5.19



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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	99421	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 ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	33.699	Depositor
Minimum map value	-21.482	Depositor
Average map value	-0.030	Depositor
Map value standard deviation	1.233	Depositor
Recommended contour level	5.5	Depositor
Map size (Å)	380.8, 380.8, 380.8	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.26	0/4236	0.58	0/5731
1	B	0.33	0/4691	0.68	4/6351 (0.1%)
1	C	0.35	0/4678	0.60	2/6334 (0.0%)
1	D	0.35	0/4651	0.65	1/6298 (0.0%)
1	E	0.32	0/4734	0.66	6/6411 (0.1%)
1	F	0.27	0/4278	0.66	0/5788
All	All	0.32	0/27268	0.64	13/36913 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	8
1	C	0	2
1	D	0	10
1	E	0	4
1	F	0	8
All	All	0	35

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	505	LEU	CA-C-N	6.29	133.55	121.54
1	B	505	LEU	C-N-CA	6.29	133.55	121.54
1	E	284	LEU	CA-CB-CG	5.77	136.50	116.30
1	E	297	MET	CA-C-N	5.50	135.22	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	297	MET	C-N-CA	5.50	135.22	121.80
1	B	615	GLN	CA-C-N	5.36	135.93	126.45
1	B	615	GLN	C-N-CA	5.36	135.93	126.45
1	C	1131	LEU	CA-C-N	5.34	126.76	120.09
1	C	1131	LEU	C-N-CA	5.34	126.76	120.09
1	E	437	PRO	CA-C-O	-5.31	117.29	121.38
1	D	628	GLY	N-CA-C	5.23	125.58	113.18
1	E	615	GLN	CA-C-N	5.03	135.36	126.45
1	E	615	GLN	C-N-CA	5.03	135.36	126.45

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1132	THR	Peptide
1	A	438	LEU	Peptide
1	A	662	THR	Peptide
1	B	312	GLY	Peptide
1	B	499	TYR	Peptide
1	B	507	ILE	Peptide
1	B	509	PRO	Peptide
1	B	615	GLN	Peptide
1	B	662	THR	Peptide
1	B	751	SER	Peptide
1	B	761	ARG	Peptide
1	C	430	PHE	Peptide
1	C	456	ASP	Peptide
1	D	284	LEU	Peptide
1	D	298	GLN	Peptide
1	D	299	PRO	Peptide
1	D	363	THR	Peptide
1	D	455	TRP	Peptide
1	D	626	TYR	Peptide
1	D	627	GLU	Peptide
1	D	720	PHE	Peptide
1	D	731	TYR	Peptide
1	D	732	PRO	Peptide
1	E	284	LEU	Peptide
1	E	298	GLN	Peptide
1	E	453	ARG	Peptide
1	E	660	ARG	Peptide
1	F	363	THR	Peptide

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Mol	Chain	Res	Type	Group
1	F	406	GLY	Peptide
1	F	456	ASP	Peptide
1	F	614	GLY	Peptide
1	F	662	THR	Peptide
1	F	719	TRP	Peptide
1	F	731	TYR	Peptide
1	F	732	PRO	Peptide

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	4144	0	4187	46	0
1	B	4587	0	4658	61	0
1	C	4574	0	4648	42	0
1	D	4547	0	4625	56	0
1	E	4628	0	4700	52	0
1	F	4185	0	4278	37	0
2	G	70	0	19	0	0
3	A	27	0	9	0	0
4	B	31	0	11	2	0
4	C	31	0	11	0	0
4	D	31	0	9	2	0
4	E	31	0	9	1	0
4	F	31	0	10	2	0
All	All	26917	0	27174	271	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 5.

All (271) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:LEU:HD21	1:A:732:PRO:HD3	1.72	0.70
1:E:752:PRO:HB3	1:E:1168:TRP:HE1	1.58	0.68
1:D:613:LEU:HD12	1:D:731:TYR:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:LYS:N	4:B:1201:ATP:O1A	2.24	0.66
1:F:455:TRP:HB3	1:F:458:PRO:HA	1.79	0.65
1:B:380:ARG:HH22	1:C:415:ASN:HD22	1.46	0.64
1:B:335:MET:SD	1:B:335:MET:N	2.72	0.62
1:C:550:ASN:HA	1:C:553:PHE:HB3	1.80	0.62
1:D:1185:MET:SD	1:D:1185:MET:N	2.75	0.60
1:D:1146:THR:H	1:D:1149:GLN:HE21	1.49	0.60
1:A:646:SER:HB3	1:A:649:THR:HG22	1.84	0.60
1:F:610:ARG:HA	1:F:708:PRO:HD3	1.84	0.60
1:C:294:ARG:NH2	1:D:456:ASP:OD1	2.36	0.59
1:A:638:THR:HA	1:A:641:GLN:HE22	1.66	0.59
1:D:1147:VAL:HA	1:D:1150:LEU:HB2	1.85	0.59
1:A:350:GLU:HB3	1:A:354:ARG:HH12	1.68	0.59
1:D:427:PRO:HG2	1:E:478:ASP:HB3	1.84	0.59
1:F:478:ASP:OD1	1:F:478:ASP:N	2.35	0.58
1:D:457:PRO:HG3	1:D:513:LYS:HD2	1.85	0.58
1:D:493:ARG:HH12	1:D:515:LYS:HG3	1.67	0.58
1:B:294:ARG:NH2	1:C:456:ASP:OD1	2.37	0.58
1:C:705:SER:OG	1:C:706:SER:N	2.37	0.58
1:D:580:ASP:OD1	1:D:580:ASP:N	2.37	0.58
1:B:555:ASP:OD1	1:B:555:ASP:N	2.34	0.58
1:C:444:ARG:NH1	1:C:471:SER:O	2.37	0.58
1:A:429:ARG:NH1	4:B:1201:ATP:O2G	2.34	0.58
1:A:308:PRO:O	1:A:313:LYS:NZ	2.37	0.57
1:B:400:ASP:OD1	1:B:426:ARG:NH1	2.37	0.57
1:C:529:SER:HA	1:C:532:ARG:HD2	1.86	0.57
1:B:427:PRO:HA	1:B:431:ASP:HB3	1.87	0.57
1:E:440:ASP:OD1	1:E:440:ASP:N	2.36	0.57
1:C:502:THR:HG23	1:C:503:LYS:HG3	1.87	0.56
1:F:615:GLN:HB2	1:F:704:LEU:HD22	1.88	0.56
1:E:705:SER:OG	1:E:706:SER:N	2.38	0.56
1:F:313:LYS:NZ	1:F:414:THR:O	2.38	0.56
1:F:448:ILE:HD13	1:F:479:LEU:HD12	1.87	0.56
1:A:426:ARG:NH2	1:A:427:PRO:O	2.39	0.56
1:B:440:ASP:OD1	1:B:440:ASP:N	2.36	0.56
1:B:546:LYS:NZ	1:B:550:ASN:OD1	2.38	0.56
1:E:426:ARG:NH1	4:F:1201:ATP:O2G	2.39	0.55
1:E:380:ARG:HH22	1:F:415:ASN:HD22	1.52	0.55
1:F:613:LEU:HD12	1:F:731:TYR:HB3	1.89	0.55
1:B:290:GLU:OE2	1:C:504:ARG:NH1	2.40	0.55
1:C:1129:ASP:OD1	1:C:1129:ASP:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:442:ASP:OD1	1:D:442:ASP:N	2.40	0.55
1:D:427:PRO:HA	1:D:431:ASP:HB3	1.88	0.55
1:B:1176:GLU:HA	1:B:1179:ARG:HG3	1.88	0.55
1:E:557:GLU:OE2	1:E:625:GLN:NE2	2.40	0.54
1:C:425:ARG:O	1:D:532:ARG:NH1	2.40	0.54
1:A:1147:VAL:HA	1:A:1150:LEU:HD12	1.89	0.54
1:D:635:ASP:OD1	1:D:635:ASP:N	2.38	0.54
1:E:314:THR:OG1	4:E:1201:ATP:O2A	2.26	0.54
1:F:555:ASP:OD1	1:F:555:ASP:N	2.41	0.54
1:E:277:GLN:OE1	1:E:432:ARG:NH1	2.41	0.54
1:E:583:GLU:OE2	1:E:589:GLN:NE2	2.41	0.54
1:B:697:ASP:OD1	1:B:697:ASP:N	2.39	0.53
1:C:380:ARG:HH22	1:D:415:ASN:HD22	1.56	0.53
1:E:615:GLN:HB2	1:E:704:LEU:HD12	1.89	0.53
1:F:334:TYR:HB2	1:F:368:ILE:HG13	1.90	0.53
1:A:694:ASP:OD1	1:A:694:ASP:N	2.41	0.53
1:F:604:ARG:HB3	1:F:720:PHE:HD1	1.74	0.53
1:F:444:ARG:NH2	1:F:468:ALA:O	2.43	0.52
1:C:1170:ARG:HH21	1:C:1173:VAL:HG11	1.73	0.52
1:E:444:ARG:HA	1:E:447:ILE:HG22	1.90	0.52
1:C:444:ARG:HA	1:C:447:ILE:HG22	1.89	0.52
1:C:508:ASP:OD1	1:C:508:ASP:N	2.40	0.52
1:C:1146:THR:H	1:C:1149:GLN:HE21	1.57	0.52
1:E:576:VAL:HG21	1:F:493:ARG:HA	1.92	0.52
1:B:1146:THR:H	1:B:1149:GLN:HE21	1.56	0.52
1:E:694:ASP:OD1	1:E:694:ASP:N	2.40	0.52
1:F:329:LYS:HB3	1:F:330:LYS:HG2	1.92	0.52
1:E:429:ARG:NH2	4:F:1201:ATP:O2G	2.41	0.52
1:F:267:SER:HA	1:F:450:ILE:HD11	1.90	0.52
1:A:332:SER:OG	1:A:333:PHE:N	2.44	0.51
1:A:433:GLU:OE2	1:B:532:ARG:NH1	2.43	0.51
1:C:494:THR:HG21	1:C:512:ILE:HG12	1.92	0.51
1:D:439:PRO:HD2	1:D:475:GLY:HA2	1.92	0.51
1:D:343:SER:OG	1:D:344:LYS:N	2.42	0.51
1:A:665:ILE:HG12	1:A:700:LEU:HD21	1.93	0.51
1:A:558:LYS:O	1:A:562:LYS:NZ	2.41	0.51
1:A:739:ALA:HA	1:A:742:GLN:HB2	1.92	0.51
1:D:308:PRO:O	1:D:313:LYS:NZ	2.43	0.51
1:D:568:SER:OG	1:D:569:LYS:N	2.44	0.51
1:E:501:SER:OG	1:E:502:THR:N	2.44	0.51
1:A:604:ARG:NH2	1:A:719:TRP:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1159:GLN:NE2	1:A:1176:GLU:OE2	2.37	0.51
1:B:713:HIS:O	1:B:715:GLN:N	2.39	0.51
1:D:583:GLU:HG2	1:E:517:LYS:HD3	1.92	0.51
1:B:355:LEU:HA	1:B:358:GLU:HB2	1.93	0.50
1:A:1159:GLN:O	1:A:1163:ASN:ND2	2.44	0.50
1:D:705:SER:OG	1:D:706:SER:N	2.43	0.50
1:B:722:SER:OG	1:B:723:LYS:N	2.45	0.50
1:D:722:SER:OG	1:D:723:LYS:N	2.45	0.50
1:B:426:ARG:NH2	1:B:427:PRO:O	2.44	0.50
1:D:314:THR:OG1	4:D:1201:ATP:O2A	2.29	0.50
1:B:751:SER:O	1:B:753:THR:N	2.45	0.50
1:D:519:PHE:O	1:D:522:SER:OG	2.29	0.50
1:D:534:SER:OG	1:D:535:ILE:N	2.44	0.50
1:C:440:ASP:OD1	1:C:440:ASP:N	2.37	0.49
1:A:723:LYS:NZ	1:B:1183:GLU:O	2.37	0.49
1:D:615:GLN:HB2	1:D:704:LEU:HD23	1.94	0.49
1:D:713:HIS:HD2	1:D:715:GLN:H	1.59	0.49
1:E:454:ASN:HD22	1:E:459:VAL:HG12	1.77	0.49
1:B:585:ASP:HB3	1:B:587:GLU:HG2	1.92	0.49
1:B:1146:THR:HG23	1:B:1149:GLN:HE21	1.77	0.49
1:C:664:SER:HB2	1:C:699:ILE:HG22	1.93	0.49
1:B:571:ASN:ND2	1:B:574:GLU:OE1	2.43	0.49
1:A:380:ARG:HD2	1:B:416:ARG:HE	1.77	0.49
1:C:399:MET:HE2	1:C:410:ILE:HD13	1.93	0.49
1:D:501:SER:OG	1:D:502:THR:N	2.45	0.49
1:F:444:ARG:HA	1:F:447:ILE:HG22	1.94	0.49
1:A:374:ASP:N	1:A:374:ASP:OD1	2.45	0.49
1:C:635:ASP:OD1	1:C:635:ASP:N	2.40	0.49
1:A:404:SER:OG	1:A:405:ARG:N	2.45	0.48
1:C:603:PRO:HB2	1:C:700:LEU:HD23	1.95	0.48
1:B:509:PRO:O	1:B:511:THR:N	2.40	0.48
1:B:1140:ASP:OD1	1:B:1140:ASP:N	2.46	0.48
1:D:441:ARG:NH2	1:D:469:GLU:OE2	2.46	0.48
1:D:642:ASP:OD1	1:D:642:ASP:N	2.46	0.48
1:E:587:GLU:HA	1:E:590:GLN:HG2	1.96	0.48
1:B:1141:SER:O	1:B:1141:SER:OG	2.31	0.48
1:C:585:ASP:OD1	1:C:585:ASP:N	2.46	0.48
1:F:1176:GLU:OE2	1:F:1179:ARG:NH2	2.47	0.48
1:B:497:GLN:HA	1:B:500:ARG:HD3	1.95	0.48
1:B:1146:THR:OG1	1:B:1148:ASP:OD1	2.32	0.48
1:A:646:SER:OG	1:A:647:ILE:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:ASP:HB2	1:B:627:GLU:HG3	1.96	0.47
1:A:324:CYS:SG	1:A:325:SER:N	2.86	0.47
1:E:1146:THR:OG1	1:E:1148:ASP:OD1	2.32	0.47
1:E:571:ASN:OD1	1:E:571:ASN:N	2.47	0.47
1:E:294:ARG:HH11	1:F:510:LYS:HG2	1.78	0.47
1:B:301:ARG:NH1	1:B:406:GLY:O	2.47	0.47
1:D:571:ASN:N	1:D:571:ASN:OD1	2.47	0.47
1:A:613:LEU:HG	1:A:1147:VAL:HG21	1.95	0.47
1:D:452:THR:O	1:D:452:THR:OG1	2.29	0.47
1:C:1146:THR:HG23	1:C:1149:GLN:HE21	1.79	0.47
1:F:734:ARG:NH1	1:F:735:ASP:OD1	2.47	0.47
1:E:1169:ASN:O	1:E:1172:SER:OG	2.32	0.47
1:C:635:ASP:HB3	1:C:669:PRO:HD2	1.97	0.46
1:D:1142:THR:OG1	1:D:1143:THR:N	2.45	0.46
1:C:330:LYS:HD2	1:C:330:LYS:HA	1.74	0.46
1:B:427:PRO:HG2	1:C:478:ASP:HA	1.97	0.46
1:A:414:THR:OG1	1:A:415:ASN:N	2.49	0.46
1:B:497:GLN:HB3	1:B:766:LEU:HD22	1.98	0.46
1:A:623:LEU:HD21	1:A:631:VAL:HG11	1.98	0.46
1:B:481:ALA:HA	1:B:484:THR:HG22	1.98	0.46
1:C:580:ASP:OD2	1:D:761:ARG:NH2	2.48	0.46
1:C:493:ARG:NH1	1:C:518:ASP:OD2	2.48	0.46
1:E:1175:ASP:OD1	1:E:1175:ASP:N	2.44	0.46
1:B:502:THR:HG23	1:B:503:LYS:HG3	1.96	0.46
1:C:643:SER:O	1:C:643:SER:OG	2.32	0.46
1:E:582:LYS:HA	1:E:582:LYS:HD3	1.78	0.46
1:A:440:ASP:O	1:A:444:ARG:N	2.49	0.46
1:B:499:TYR:O	1:B:501:SER:N	2.49	0.46
1:B:709:LEU:HD11	1:B:728:SER:HB3	1.98	0.46
1:D:627:GLU:O	1:D:629:VAL:N	2.46	0.46
1:A:741:PHE:O	1:A:745:LEU:N	2.41	0.45
1:B:583:GLU:HG2	1:C:517:LYS:HD3	1.98	0.45
1:E:688:SER:O	1:E:688:SER:OG	2.32	0.45
1:F:1172:SER:O	1:F:1172:SER:OG	2.34	0.45
1:D:1137:LEU:O	1:D:1141:SER:OG	2.30	0.45
1:F:645:GLN:HE21	1:F:649:THR:HG23	1.81	0.45
1:B:529:SER:HA	1:B:532:ARG:HD2	1.98	0.45
1:E:329:LYS:HA	1:E:330:LYS:HA	1.80	0.45
1:B:444:ARG:NH1	1:B:471:SER:OG	2.50	0.45
1:A:400:ASP:OD2	1:A:426:ARG:NH1	2.46	0.45
1:D:374:ASP:OD2	1:D:416:ARG:NE	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:367:ILE:HG22	1:E:409:ILE:HB	1.99	0.45
1:A:427:PRO:HA	1:A:431:ASP:HB3	1.99	0.45
1:A:399:MET:O	1:A:405:ARG:NH2	2.50	0.44
1:B:712:LEU:HD23	1:B:712:LEU:HA	1.87	0.44
1:D:280:GLU:OE2	1:E:499:TYR:OH	2.30	0.44
1:D:694:ASP:N	1:D:694:ASP:OD1	2.45	0.44
1:F:450:ILE:HG23	1:F:451:HIS:HD2	1.81	0.44
1:D:481:ALA:HA	1:D:484:THR:HG22	2.00	0.44
1:F:329:LYS:HA	1:F:330:LYS:HA	1.82	0.44
1:E:675:LEU:HD22	1:E:713:HIS:HE1	1.82	0.44
1:A:613:LEU:O	1:A:615:GLN:NE2	2.50	0.44
1:E:706:SER:OG	1:E:707:SER:N	2.35	0.44
1:B:641:GLN:H	1:B:641:GLN:HG3	1.70	0.44
1:C:636:MET:HE3	1:C:636:MET:HB2	1.87	0.44
1:E:478:ASP:OD1	1:E:478:ASP:N	2.36	0.44
1:A:269:GLY:HA3	1:A:447:ILE:HD12	2.00	0.44
1:B:509:PRO:HG2	1:B:510:LYS:HG2	2.00	0.44
1:E:472:LYS:HD2	1:E:472:LYS:HA	1.77	0.44
1:E:579:ASP:HB2	1:F:764:ARG:HB3	2.00	0.44
1:E:1146:THR:OG1	1:E:1149:GLN:OE1	2.26	0.44
1:E:1136:GLN:NE2	1:E:1140:ASP:OD2	2.50	0.43
1:A:607:ILE:HG22	1:A:727:TYR:HB3	1.99	0.43
1:B:501:SER:OG	1:B:502:THR:N	2.50	0.43
1:D:312:GLY:N	4:D:1201:ATP:O1A	2.51	0.43
1:E:479:LEU:HD23	1:E:479:LEU:HA	1.80	0.43
1:F:539:LYS:HB2	1:F:539:LYS:HE3	1.78	0.43
1:B:560:LEU:HD23	1:B:560:LEU:HA	1.90	0.43
1:C:769:LEU:HD23	1:C:769:LEU:HA	1.84	0.43
1:A:579:ASP:HB2	1:B:762:LYS:HB2	2.00	0.43
1:A:598:LEU:HD12	1:A:598:LEU:HA	1.90	0.43
1:B:303:VAL:HA	1:B:432:ARG:HB2	2.00	0.43
1:E:613:LEU:HD11	1:E:731:TYR:HA	2.00	0.43
1:A:590:GLN:O	1:A:594:THR:OG1	2.36	0.43
1:B:646:SER:OG	1:B:647:ILE:N	2.52	0.43
1:D:648:GLU:OE2	1:D:681:THR:OG1	2.31	0.43
1:E:1170:ARG:HH11	1:E:1173:VAL:HG11	1.84	0.43
1:C:336:ARG:NH1	1:C:341:CYS:SG	2.92	0.42
1:C:459:VAL:HA	1:C:460:PRO:HD3	1.91	0.42
1:B:424:LEU:HD12	1:B:429:ARG:HD3	2.01	0.42
1:D:400:ASP:OD2	1:D:426:ARG:NH1	2.49	0.42
1:E:541:LEU:HD23	1:E:541:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:SER:HA	1:A:537:PRO:HD3	1.92	0.42
1:F:1143:THR:OG1	1:F:1144:GLY:N	2.52	0.42
1:A:373:ILE:HD12	1:A:373:ILE:HA	1.94	0.42
1:D:440:ASP:OD1	1:D:440:ASP:N	2.45	0.42
1:C:1165:LYS:HE2	1:C:1165:LYS:HB3	1.83	0.42
1:D:1155:SER:O	1:D:1155:SER:OG	2.34	0.42
1:E:632:GLN:HE21	1:E:634:PHE:HE1	1.65	0.42
1:F:1131:LEU:HD23	1:F:1131:LEU:HA	1.91	0.42
1:A:307:GLY:HA3	1:A:308:PRO:HD3	1.82	0.42
1:A:665:ILE:HG21	1:A:702:LEU:HD12	2.02	0.42
1:A:1146:THR:O	1:A:1149:GLN:NE2	2.32	0.42
1:B:329:LYS:HD3	1:B:329:LYS:HA	1.75	0.42
1:B:340:ASP:OD1	1:B:340:ASP:N	2.52	0.42
1:D:643:SER:O	1:D:643:SER:OG	2.36	0.42
1:A:583:GLU:HB2	1:B:517:LYS:HB2	2.01	0.42
1:B:635:ASP:OD1	1:B:635:ASP:N	2.44	0.42
1:E:280:GLU:OE2	1:F:499:TYR:OH	2.30	0.42
1:F:523:MET:HE2	1:F:523:MET:HB3	1.91	0.42
1:C:414:THR:OG1	1:C:415:ASN:N	2.52	0.42
1:C:613:LEU:HA	1:C:613:LEU:HD23	1.87	0.41
1:D:479:LEU:HD23	1:D:479:LEU:HA	1.91	0.41
1:B:306:HIS:HA	1:B:313:LYS:HZ1	1.85	0.41
1:E:542:SER:HA	1:E:543:PRO:HD3	1.93	0.41
1:A:1172:SER:O	1:A:1172:SER:OG	2.32	0.41
1:F:441:ARG:NH2	1:F:469:GLU:OE2	2.54	0.41
1:B:1148:ASP:OD1	1:B:1148:ASP:N	2.50	0.41
1:C:326:SER:OG	1:C:327:GLU:OE2	2.33	0.41
1:D:444:ARG:HE	1:D:444:ARG:HB2	1.69	0.41
1:E:417:PRO:O	1:E:425:ARG:NH2	2.54	0.41
1:E:660:ARG:HB3	1:E:661:HIS:H	1.63	0.41
1:D:472:LYS:HG2	1:D:624:GLN:HG3	2.02	0.41
1:D:749:LYS:HD2	1:D:749:LYS:HA	1.89	0.41
1:E:622:ILE:HD11	1:E:702:LEU:HD11	2.02	0.41
1:A:630:HIS:O	1:A:664:SER:OG	2.34	0.41
1:B:400:ASP:OD2	1:B:400:ASP:N	2.53	0.41
1:C:598:LEU:HA	1:C:598:LEU:HD23	1.87	0.41
1:D:564:MET:HE3	1:D:698:GLN:HB3	2.02	0.41
1:E:290:GLU:O	1:E:293:GLN:NE2	2.47	0.41
1:F:647:ILE:O	1:F:650:SER:OG	2.38	0.41
1:A:705:SER:OG	1:A:706:SER:N	2.54	0.41
1:B:370:PHE:HB3	1:B:373:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:593:GLU:OE1	1:B:594:THR:OG1	2.39	0.41
1:B:629:VAL:HG12	1:B:663:PRO:HB2	2.02	0.41
1:C:713:HIS:O	1:C:715:GLN:N	2.54	0.41
1:D:311:THR:O	1:D:311:THR:OG1	2.37	0.41
1:E:464:CYS:HA	1:E:465:SER:HA	1.78	0.41
1:E:639:LEU:HD23	1:E:639:LEU:HA	1.94	0.41
1:E:1170:ARG:HH11	1:E:1173:VAL:HG21	1.86	0.41
1:F:694:ASP:OD1	1:F:694:ASP:N	2.50	0.41
1:C:510:LYS:HA	1:C:510:LYS:HD3	1.79	0.41
1:F:634:PHE:HE1	1:F:654:LEU:HB3	1.86	0.41
1:B:598:LEU:HD23	1:B:598:LEU:HA	1.91	0.40
1:D:573:LEU:HD23	1:D:573:LEU:HA	1.96	0.40
1:D:613:LEU:HA	1:D:1147:VAL:HG12	2.04	0.40
1:F:647:ILE:HD11	1:F:678:LEU:HD22	2.02	0.40
1:B:752:PRO:HG3	1:B:1168:TRP:HE1	1.86	0.40
1:D:503:LYS:HB2	1:D:503:LYS:HE2	1.84	0.40
1:F:706:SER:OG	1:F:707:SER:N	2.40	0.40
1:D:400:ASP:N	1:D:400:ASP:OD1	2.54	0.40
1:F:444:ARG:NH2	1:F:471:SER:O	2.54	0.40
1:F:713:HIS:HA	1:F:714:PRO:HD3	1.95	0.40
1:D:397:ALA:HB2	1:E:372:GLN:HG3	2.04	0.40
1:E:498:LEU:HD23	1:E:498:LEU:HA	1.89	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	508/1198 (42%)	449 (88%)	56 (11%)	3 (1%)	21	55
1	B	567/1198 (47%)	492 (87%)	69 (12%)	6 (1%)	11	44
1	C	565/1198 (47%)	505 (89%)	58 (10%)	2 (0%)	30	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	562/1198 (47%)	475 (84%)	83 (15%)	4 (1%)	18	52
1	E	573/1198 (48%)	491 (86%)	81 (14%)	1 (0%)	43	73
1	F	516/1198 (43%)	434 (84%)	80 (16%)	2 (0%)	30	61
All	All	3291/7188 (46%)	2846 (86%)	427 (13%)	18 (0%)	26	58

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	500	ARG
1	B	510	LYS
1	D	628	GLY
1	B	509	PRO
1	D	721	SER
1	D	1143	THR
1	A	431	ASP
1	B	378	PRO
1	C	615	GLN
1	D	299	PRO
1	E	299	PRO
1	F	767	PRO
1	B	537	PRO
1	F	720	PHE
1	A	365	PRO
1	A	364	GLN
1	B	663	PRO
1	C	714	PRO

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	466/1086 (43%)	462 (99%)	4 (1%)	70	76
1	B	517/1086 (48%)	514 (99%)	3 (1%)	78	80
1	C	515/1086 (47%)	513 (100%)	2 (0%)	84	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	512/1086 (47%)	509 (99%)	3 (1%)	78	80
1	E	522/1086 (48%)	519 (99%)	3 (1%)	78	80
1	F	470/1086 (43%)	466 (99%)	4 (1%)	70	76
All	All	3002/6516 (46%)	2983 (99%)	19 (1%)	76	80

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	263	LEU
1	A	1132	THR
1	A	1139	ILE
1	A	1146	THR
1	B	303	VAL
1	B	600	ILE
1	B	613	LEU
1	C	303	VAL
1	C	527	ILE
1	D	284	LEU
1	D	303	VAL
1	D	607	ILE
1	E	303	VAL
1	E	459	VAL
1	E	759	ILE
1	F	346	VAL
1	F	367	ILE
1	F	607	ILE
1	F	1142	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	554	GLN
1	A	561	GLN
1	A	589	GLN
1	A	676	ASN
1	A	715	GLN
1	A	1136	GLN
1	B	590	GLN
1	B	1149	GLN
1	B	1152	HIS

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Mol	Chain	Res	Type
1	C	298	GLN
1	C	415	ASN
1	C	584	ASN
1	C	715	GLN
1	C	742	GLN
1	C	1136	GLN
1	C	1149	GLN
1	D	328	ASN
1	D	352	GLN
1	D	364	GLN
1	D	415	ASN
1	D	454	ASN
1	D	489	ASN
1	D	506	GLN
1	D	584	ASN
1	D	589	GLN
1	D	625	GLN
1	D	676	ASN
1	D	713	HIS
1	D	724	GLN
1	D	1149	GLN
1	D	1152	HIS
1	E	273	ASN
1	E	328	ASN
1	E	407	GLN
1	E	415	ASN
1	E	625	GLN
1	E	653	HIS
1	E	676	ASN
1	E	715	GLN
1	E	1152	HIS
1	F	384	GLN
1	F	561	GLN
1	F	630	HIS
1	F	645	GLN
1	F	713	HIS
1	F	742	GLN
1	F	1152	HIS
1	F	1163	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	ADP	A	1201	-	28,29,29	1.46	6 (21%)	43,45,45	1.95	7 (16%)
4	ATP	F	1201	-	32,33,33	1.33	4 (12%)	48,52,52	1.88	8 (16%)
4	ATP	C	1201	-	32,33,33	1.34	4 (12%)	48,52,52	1.88	8 (16%)
4	ATP	E	1201	-	32,33,33	1.33	4 (12%)	48,52,52	1.88	8 (16%)
4	ATP	D	1201	-	32,33,33	1.34	4 (12%)	48,52,52	1.88	8 (16%)
4	ATP	B	1201	-	32,33,33	1.33	4 (12%)	48,52,52	1.88	8 (16%)

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	ADP	A	1201	-	-	4/16/32/32	0/3/3/3
4	ATP	F	1201	-	-	0/22/38/38	0/3/3/3
4	ATP	C	1201	-	-	0/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	E	1201	-	-	0/22/38/38	0/3/3/3
4	ATP	D	1201	-	-	0/22/38/38	0/3/3/3
4	ATP	B	1201	-	-	0/22/38/38	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1201	ADP	C5-C4	4.58	1.47	1.39
4	C	1201	ATP	C5-C4	4.47	1.47	1.39
4	D	1201	ATP	C5-C4	4.47	1.47	1.39
4	F	1201	ATP	C5-C4	4.47	1.47	1.39
4	B	1201	ATP	C5-C4	4.47	1.47	1.39
4	E	1201	ATP	C5-C4	4.43	1.47	1.39
4	C	1201	ATP	C5-N7	-3.04	1.33	1.39
4	D	1201	ATP	C5-N7	-3.03	1.33	1.39
4	B	1201	ATP	C5-N7	-3.01	1.33	1.39
4	E	1201	ATP	C5-N7	-2.99	1.33	1.39
4	F	1201	ATP	C5-N7	-2.96	1.33	1.39
3	A	1201	ADP	C5-N7	-2.94	1.33	1.39
3	A	1201	ADP	C5-C6	2.60	1.48	1.41
4	B	1201	ATP	C5-C6	2.21	1.47	1.41
4	D	1201	ATP	C5-C6	2.21	1.47	1.41
4	C	1201	ATP	C5-C6	2.20	1.47	1.41
4	F	1201	ATP	C5-C6	2.20	1.47	1.41
4	F	1201	ATP	C8-N7	2.20	1.35	1.31
4	C	1201	ATP	C8-N7	2.20	1.35	1.31
4	E	1201	ATP	C5-C6	2.19	1.47	1.41
4	E	1201	ATP	C8-N7	2.19	1.35	1.31
4	D	1201	ATP	C8-N7	2.18	1.35	1.31
4	B	1201	ATP	C8-N7	2.18	1.35	1.31
3	A	1201	ADP	C8-N7	2.07	1.35	1.31
3	A	1201	ADP	C8-N9	-2.02	1.34	1.37
3	A	1201	ADP	PA-O3A	2.00	1.61	1.59

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1201	ADP	C5-C4-N3	-6.66	117.54	126.72
4	F	1201	ATP	C5-C4-N3	-5.82	118.71	126.72
4	E	1201	ATP	C5-C4-N3	-5.81	118.72	126.72
4	C	1201	ATP	C5-C4-N3	-5.80	118.73	126.72
4	B	1201	ATP	C5-C4-N3	-5.80	118.73	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1201	ATP	C5-C4-N3	-5.79	118.74	126.72
3	A	1201	ADP	N3-C4-N9	5.12	135.88	127.17
4	E	1201	ATP	N3-C2-N1	-5.10	120.87	128.58
4	F	1201	ATP	N3-C2-N1	-5.09	120.88	128.58
4	C	1201	ATP	N3-C2-N1	-5.08	120.89	128.58
4	B	1201	ATP	N3-C2-N1	-5.08	120.90	128.58
4	D	1201	ATP	N3-C2-N1	-5.06	120.92	128.58
4	D	1201	ATP	N3-C4-N9	4.65	135.08	127.17
4	C	1201	ATP	N3-C4-N9	4.65	135.07	127.17
4	B	1201	ATP	N3-C4-N9	4.64	135.06	127.17
4	E	1201	ATP	N3-C4-N9	4.64	135.05	127.17
4	F	1201	ATP	N3-C4-N9	4.63	135.05	127.17
4	E	1201	ATP	C2-N3-C4	4.31	122.36	111.83
4	B	1201	ATP	C2-N3-C4	4.31	122.35	111.83
4	C	1201	ATP	C2-N3-C4	4.31	122.35	111.83
4	F	1201	ATP	C2-N3-C4	4.31	122.35	111.83
4	D	1201	ATP	C2-N3-C4	4.30	122.32	111.83
3	A	1201	ADP	C2-N3-C4	4.04	121.69	111.83
3	A	1201	ADP	C4-C5-N7	-3.69	106.36	110.58
3	A	1201	ADP	N3-C2-N1	-3.32	123.55	128.58
4	F	1201	ATP	C2-N1-C6	2.90	123.50	118.73
4	C	1201	ATP	C2-N1-C6	2.89	123.48	118.73
4	B	1201	ATP	C2-N1-C6	2.89	123.47	118.73
4	E	1201	ATP	C2-N1-C6	2.89	123.47	118.73
4	D	1201	ATP	C2-N1-C6	2.88	123.45	118.73
4	F	1201	ATP	C3'-C2'-C1'	2.79	106.75	101.46
4	D	1201	ATP	C3'-C2'-C1'	2.78	106.71	101.46
4	B	1201	ATP	C3'-C2'-C1'	2.77	106.70	101.46
4	C	1201	ATP	C3'-C2'-C1'	2.77	106.69	101.46
4	E	1201	ATP	C3'-C2'-C1'	2.76	106.69	101.46
4	F	1201	ATP	C4-C5-N7	-2.76	107.43	110.58
4	E	1201	ATP	C4-C5-N7	-2.74	107.45	110.58
4	B	1201	ATP	C4-C5-N7	-2.73	107.46	110.58
4	D	1201	ATP	C4-C5-N7	-2.72	107.47	110.58
4	C	1201	ATP	C4-C5-N7	-2.72	107.47	110.58
3	A	1201	ADP	C5-N7-C8	2.66	107.64	103.45
3	A	1201	ADP	C3'-C2'-C1'	2.25	105.72	101.46
4	D	1201	ATP	O2B-PB-O1B	2.09	122.18	112.44
4	E	1201	ATP	O2B-PB-O1B	2.08	122.14	112.44
4	B	1201	ATP	O2B-PB-O1B	2.08	122.12	112.44
4	C	1201	ATP	O2B-PB-O1B	2.08	122.10	112.44
4	F	1201	ATP	O2B-PB-O1B	2.08	122.10	112.44

There are no chirality outliers.

All (4) torsion outliers are listed below:

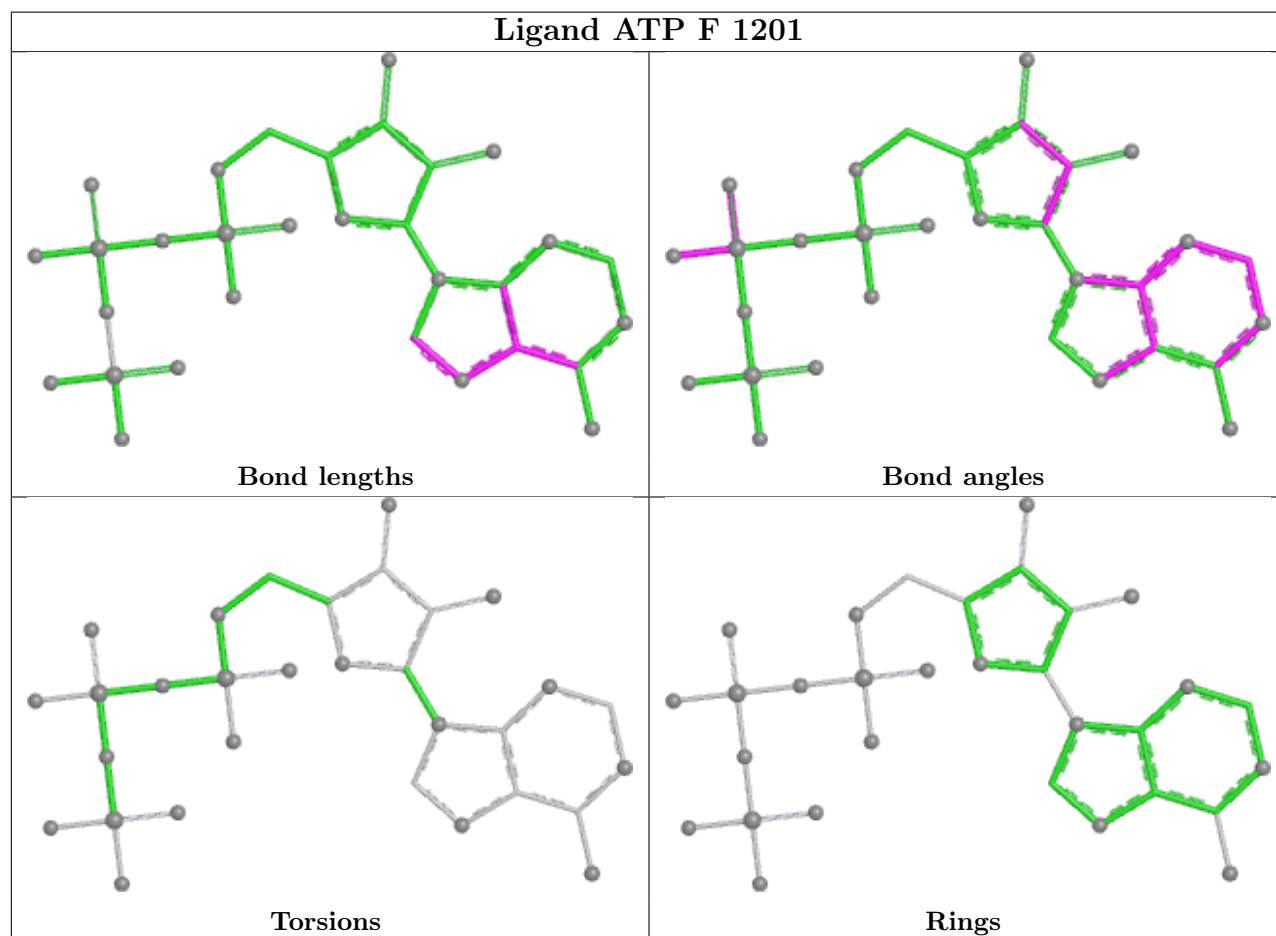
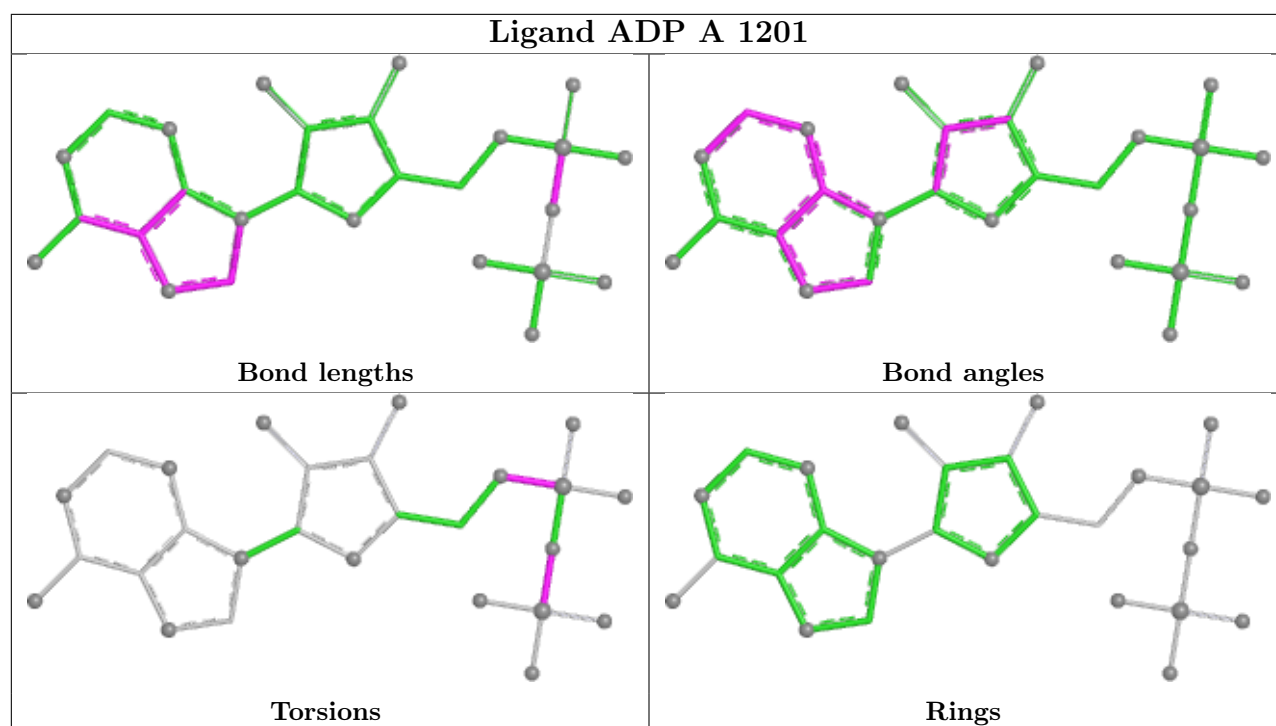
Mol	Chain	Res	Type	Atoms
3	A	1201	ADP	C5'-O5'-PA-O2A
3	A	1201	ADP	PA-O3A-PB-O1B
3	A	1201	ADP	C5'-O5'-PA-O1A
3	A	1201	ADP	C5'-O5'-PA-O3A

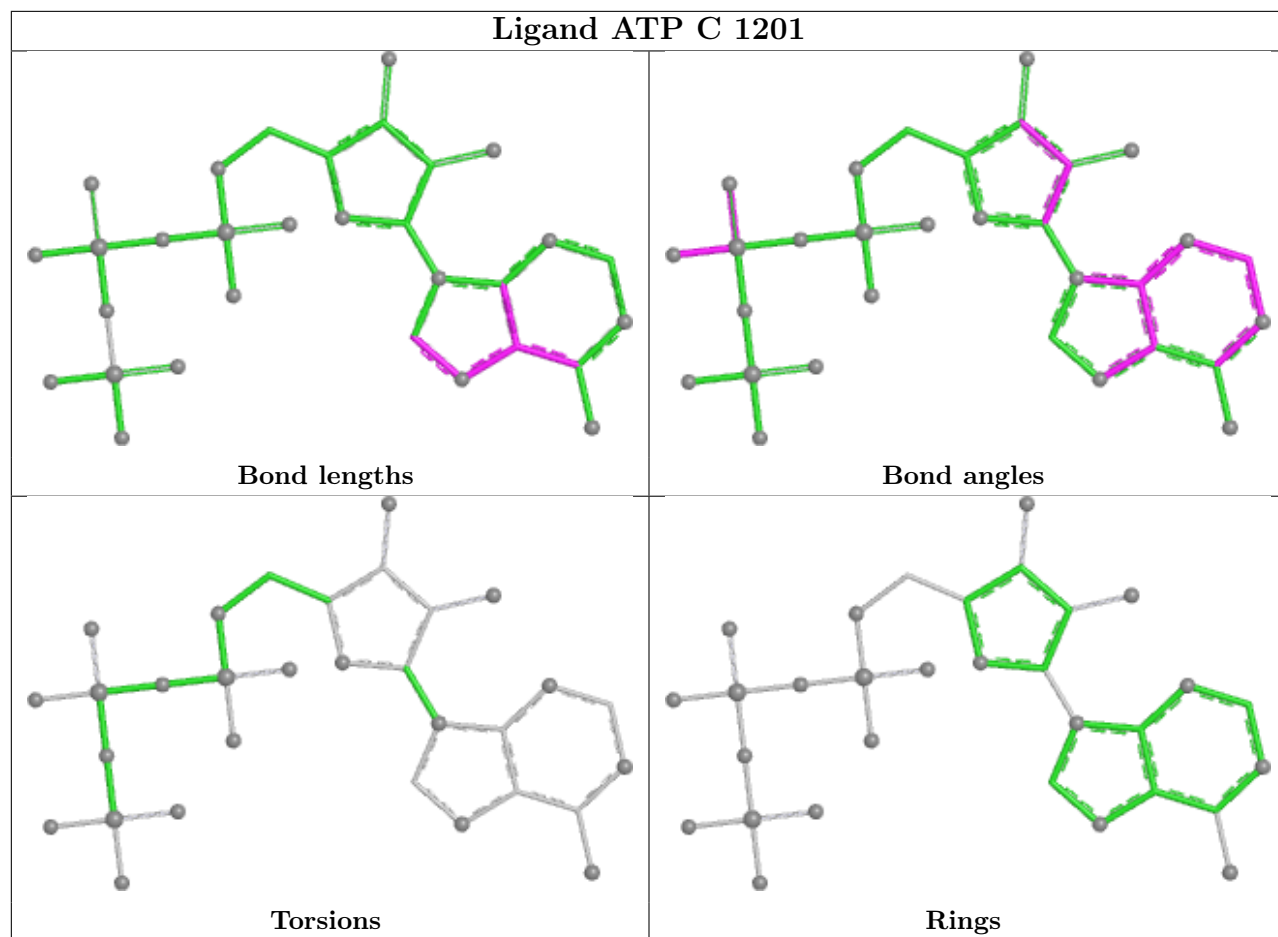
There are no ring outliers.

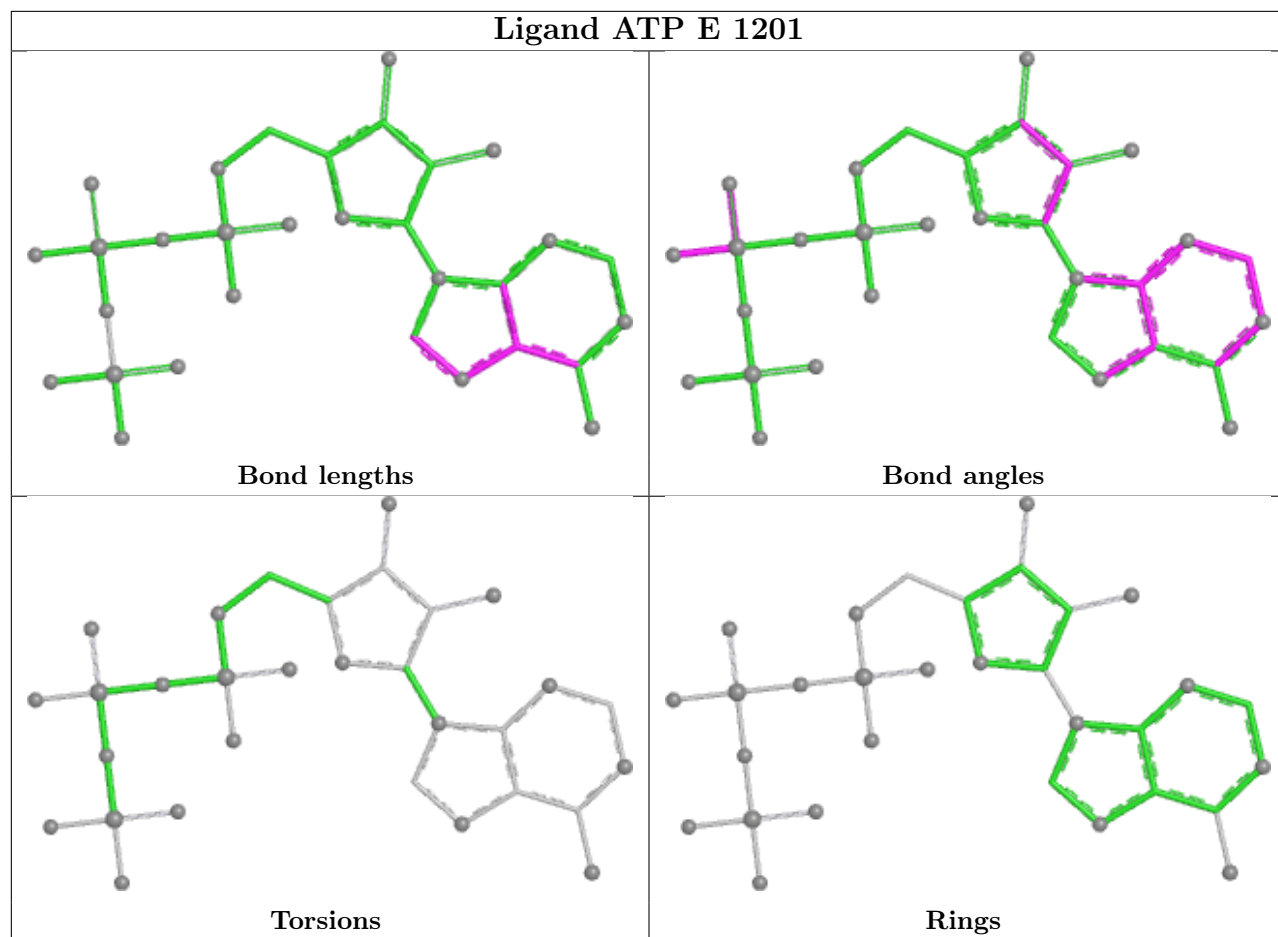
4 monomers are involved in 7 short contacts:

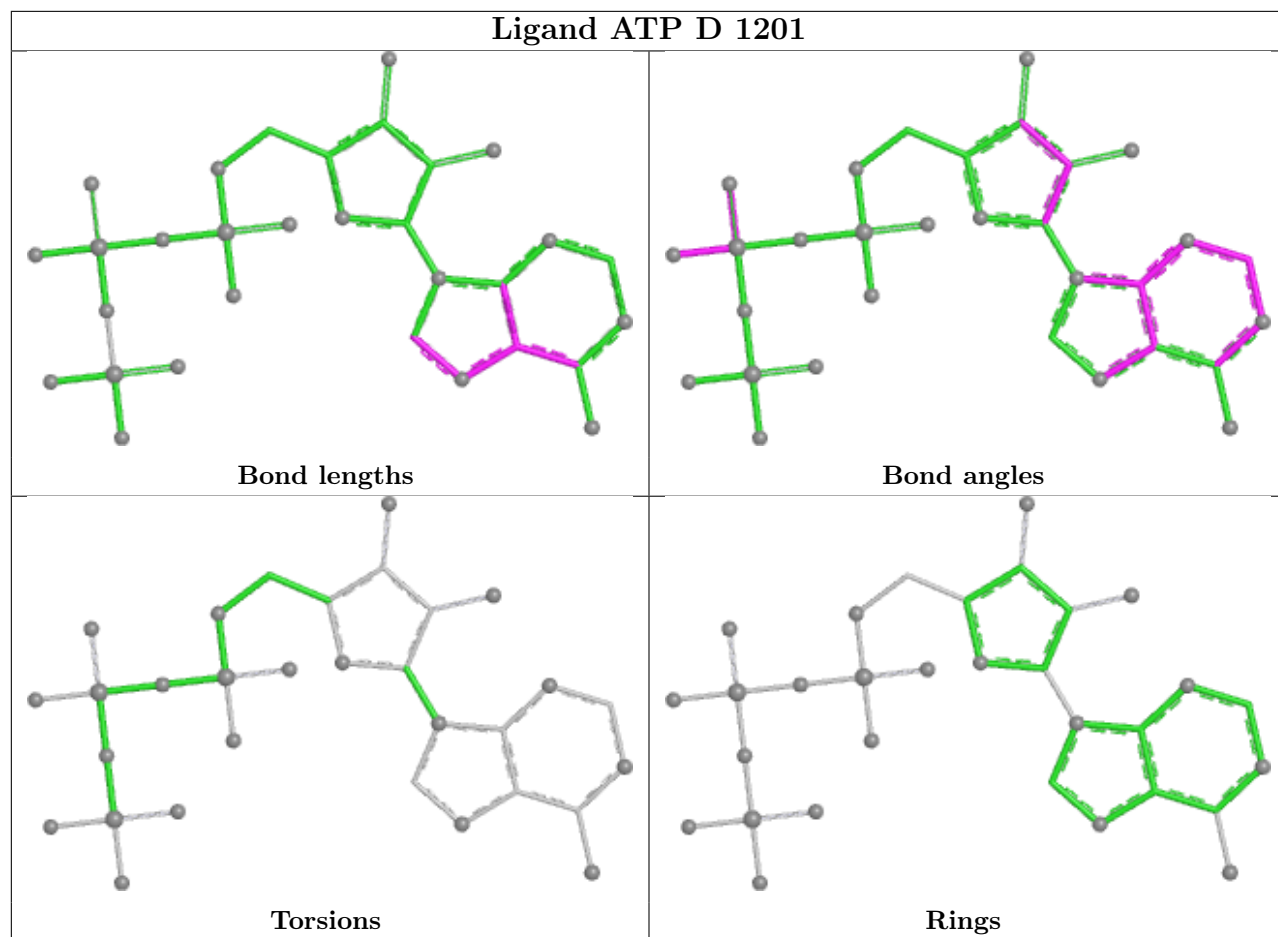
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1201	ATP	2	0
4	E	1201	ATP	1	0
4	D	1201	ATP	2	0
4	B	1201	ATP	2	0

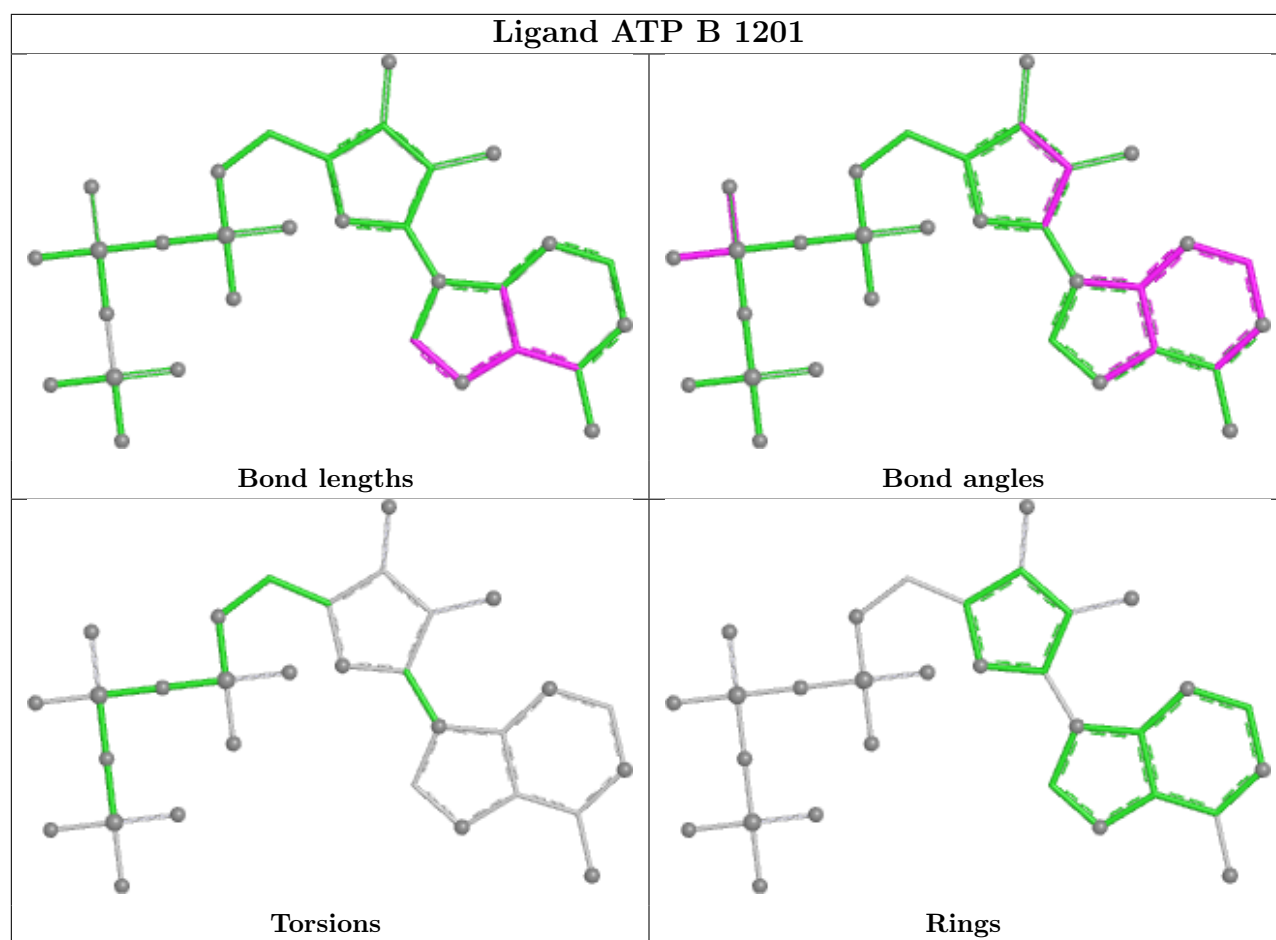
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

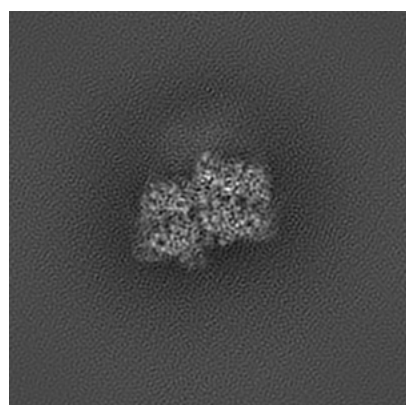
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9872. These allow visual inspection of the internal detail of the map and identification of artifacts.

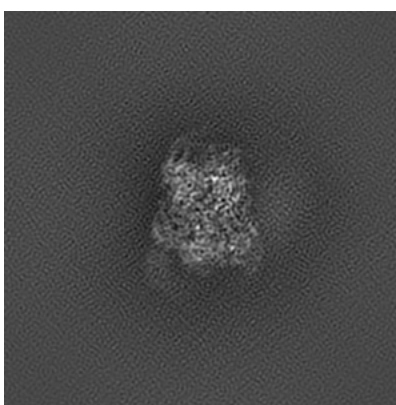
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

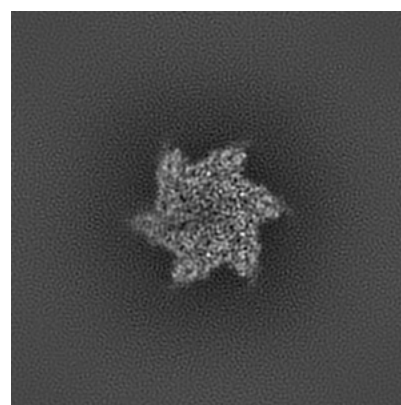
6.1.1 Primary map



X



Y

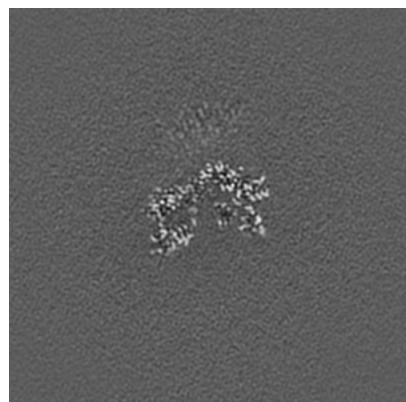


Z

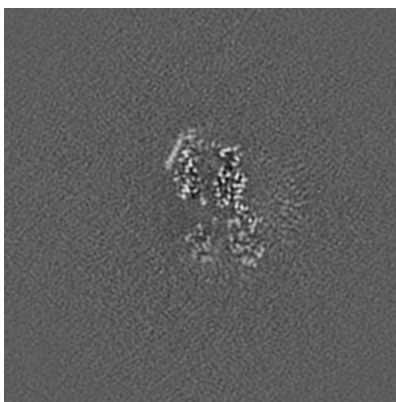
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

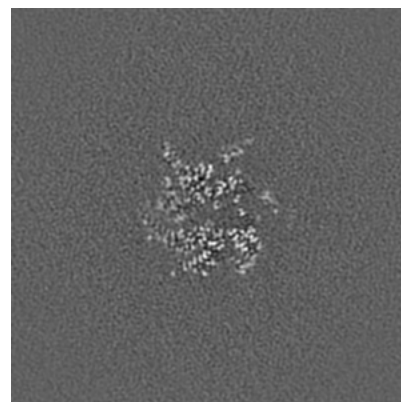
6.2.1 Primary map



X Index: 170



Y Index: 170

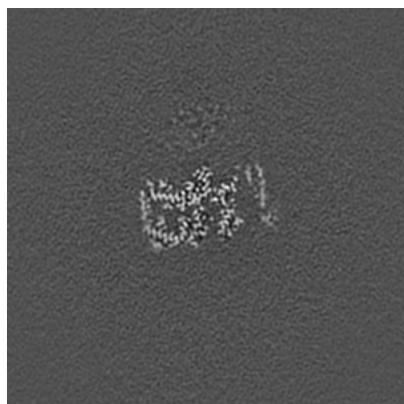


Z Index: 170

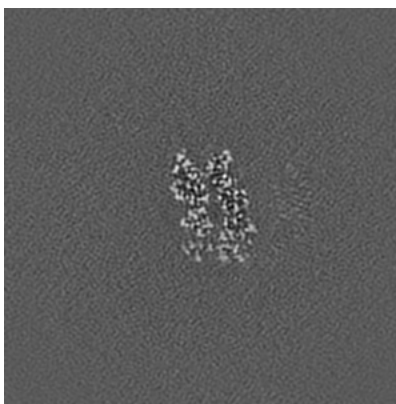
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

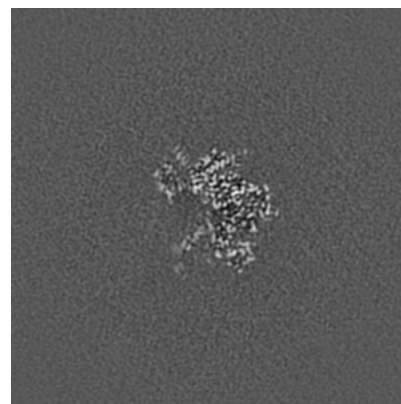
6.3.1 Primary map



X Index: 197



Y Index: 186

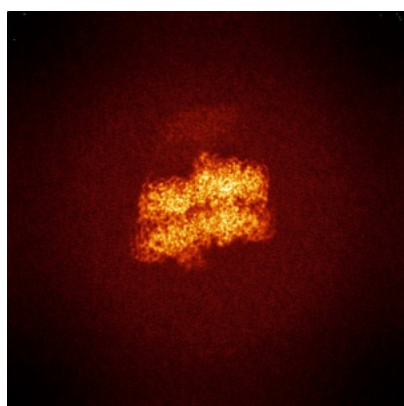


Z Index: 188

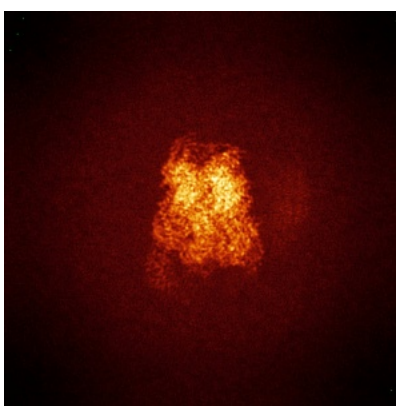
The images above show the largest variance slices of the map in three orthogonal directions.

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

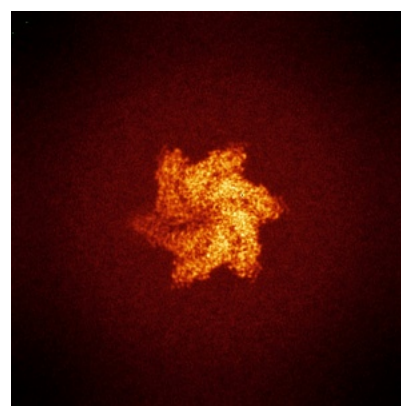
6.4.1 Primary map



X



Y

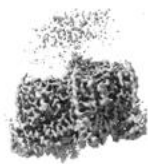


Z

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](#)

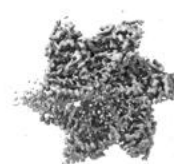
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

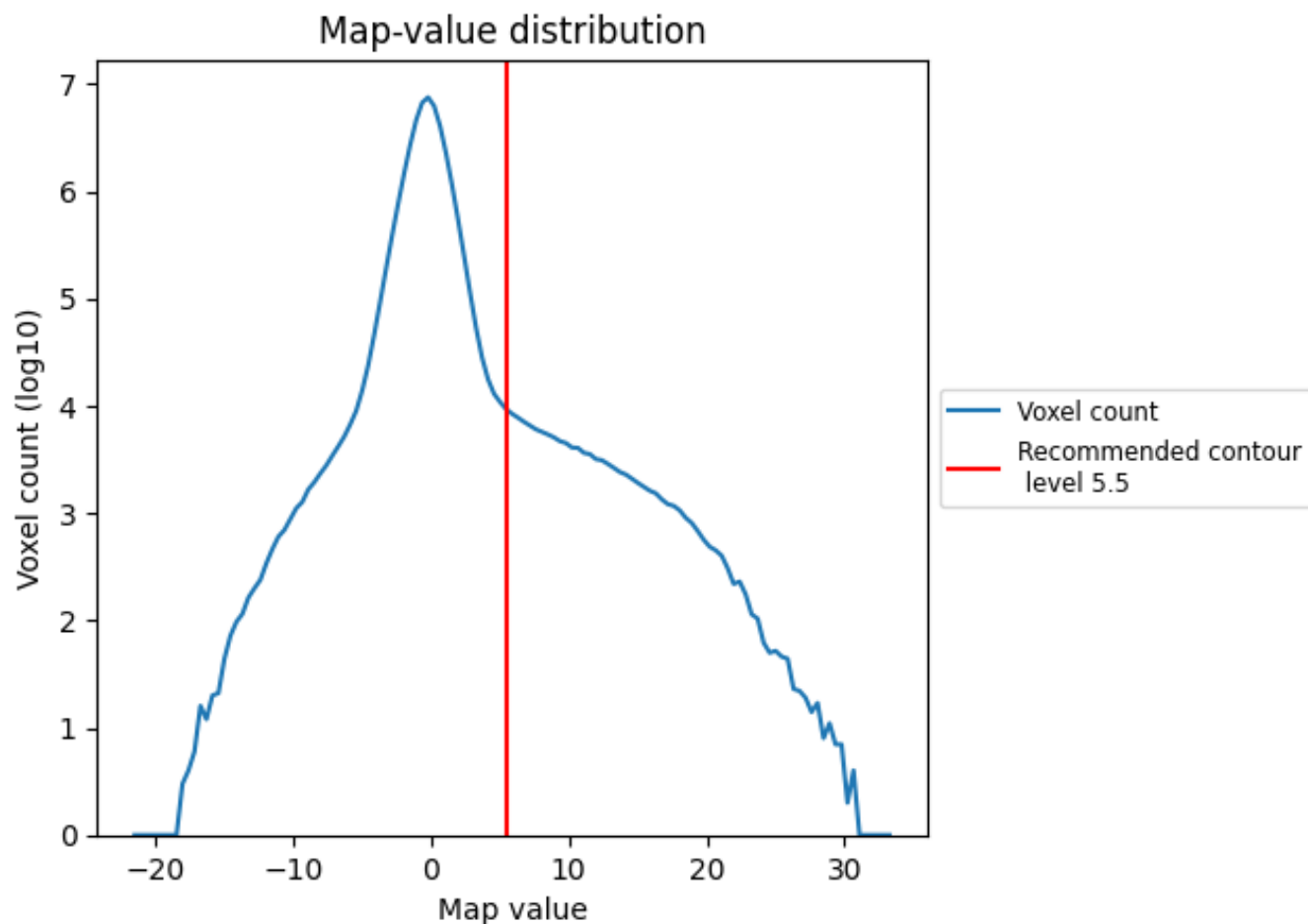
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

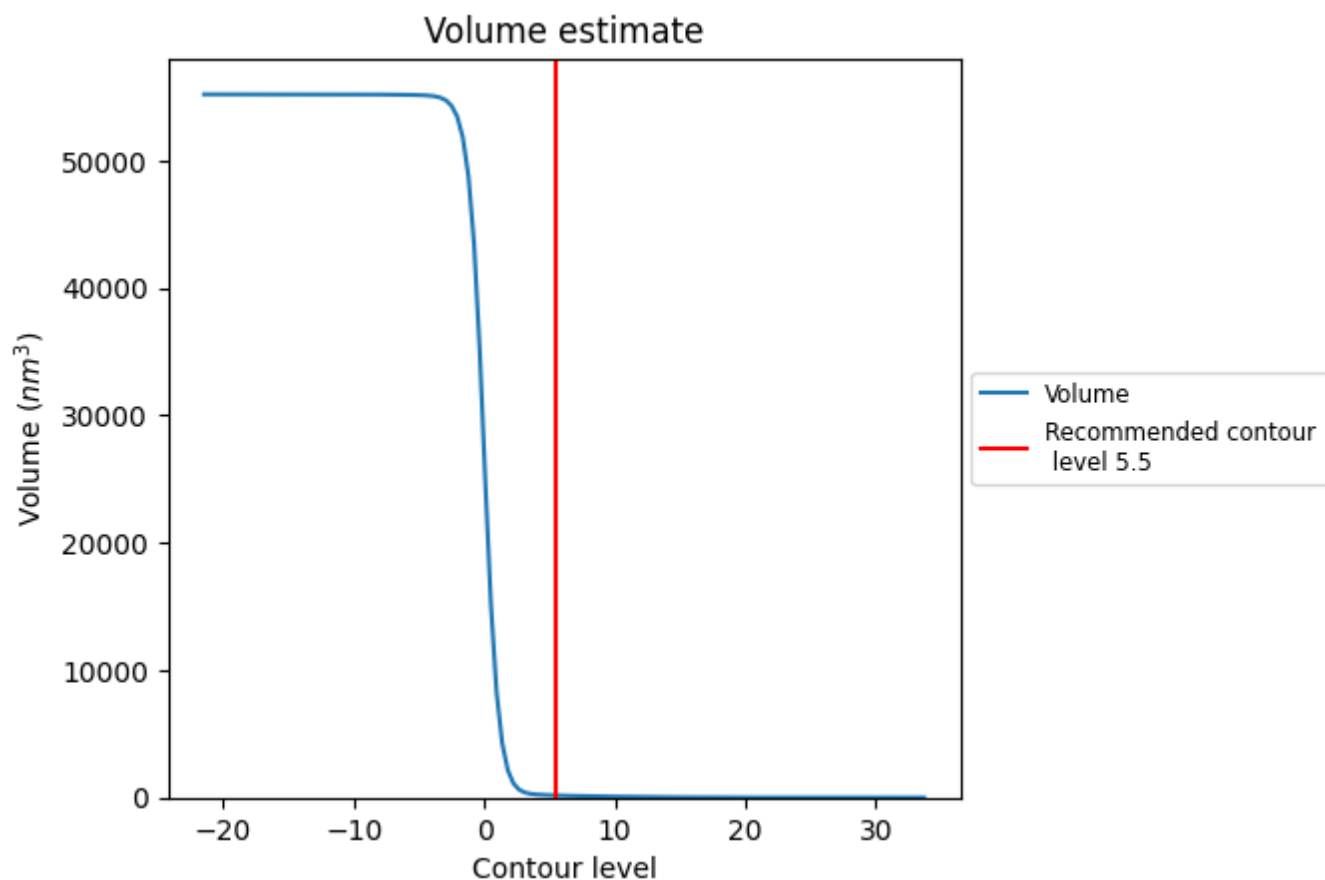
This section contains the results of statistical analysis of the map.

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.

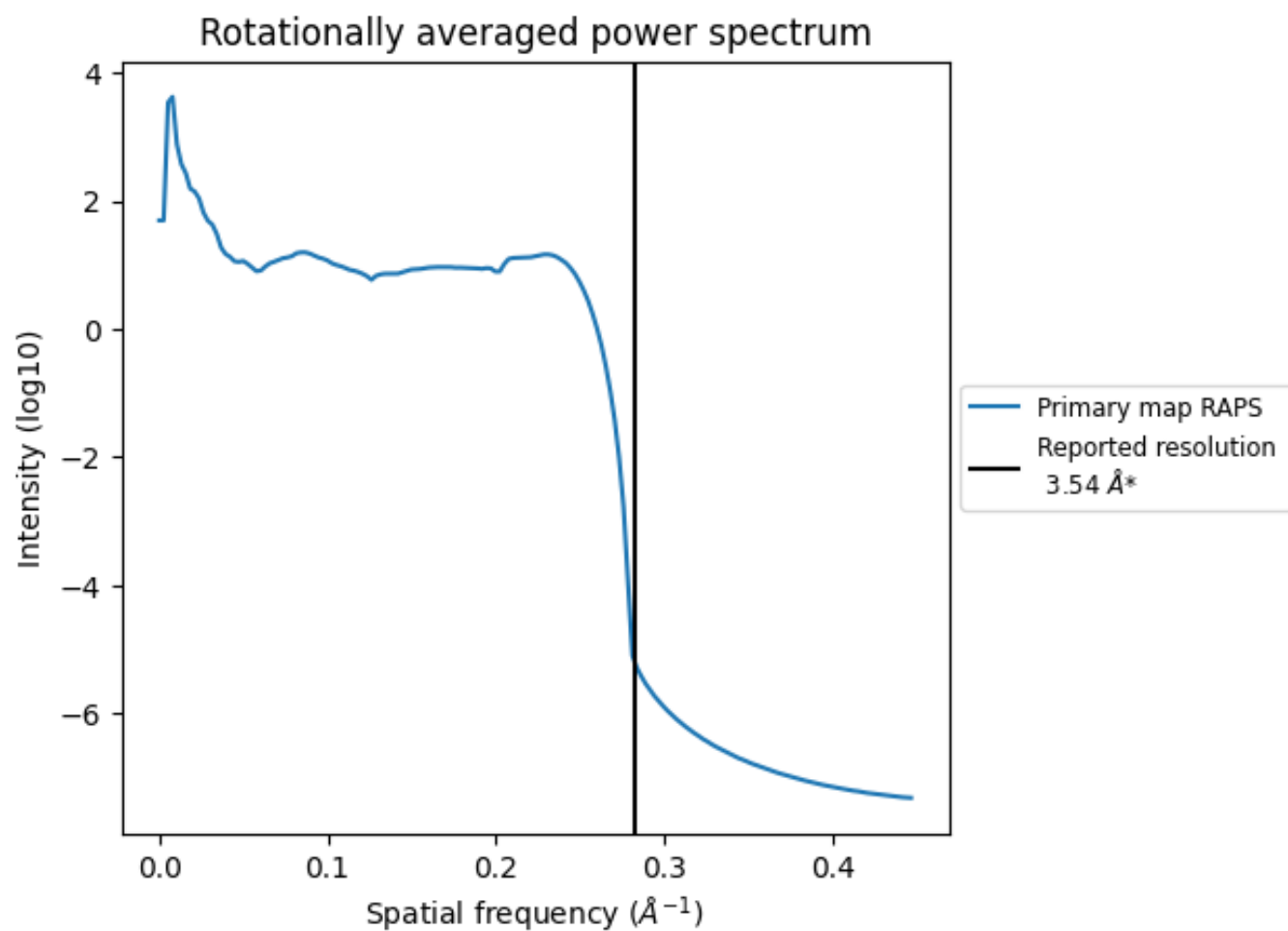
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 170 nm³; this corresponds to an approximate mass of 154 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 0.282 Å⁻¹

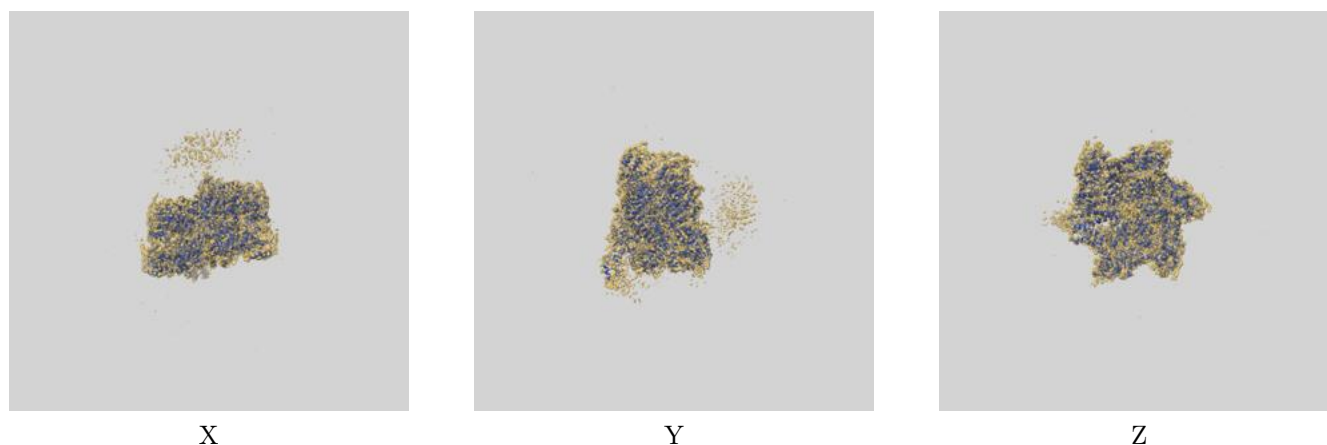
8 Fourier-Shell correlation ⓘ

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-9872 and PDB model 6JQ0. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 5.5 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](#)



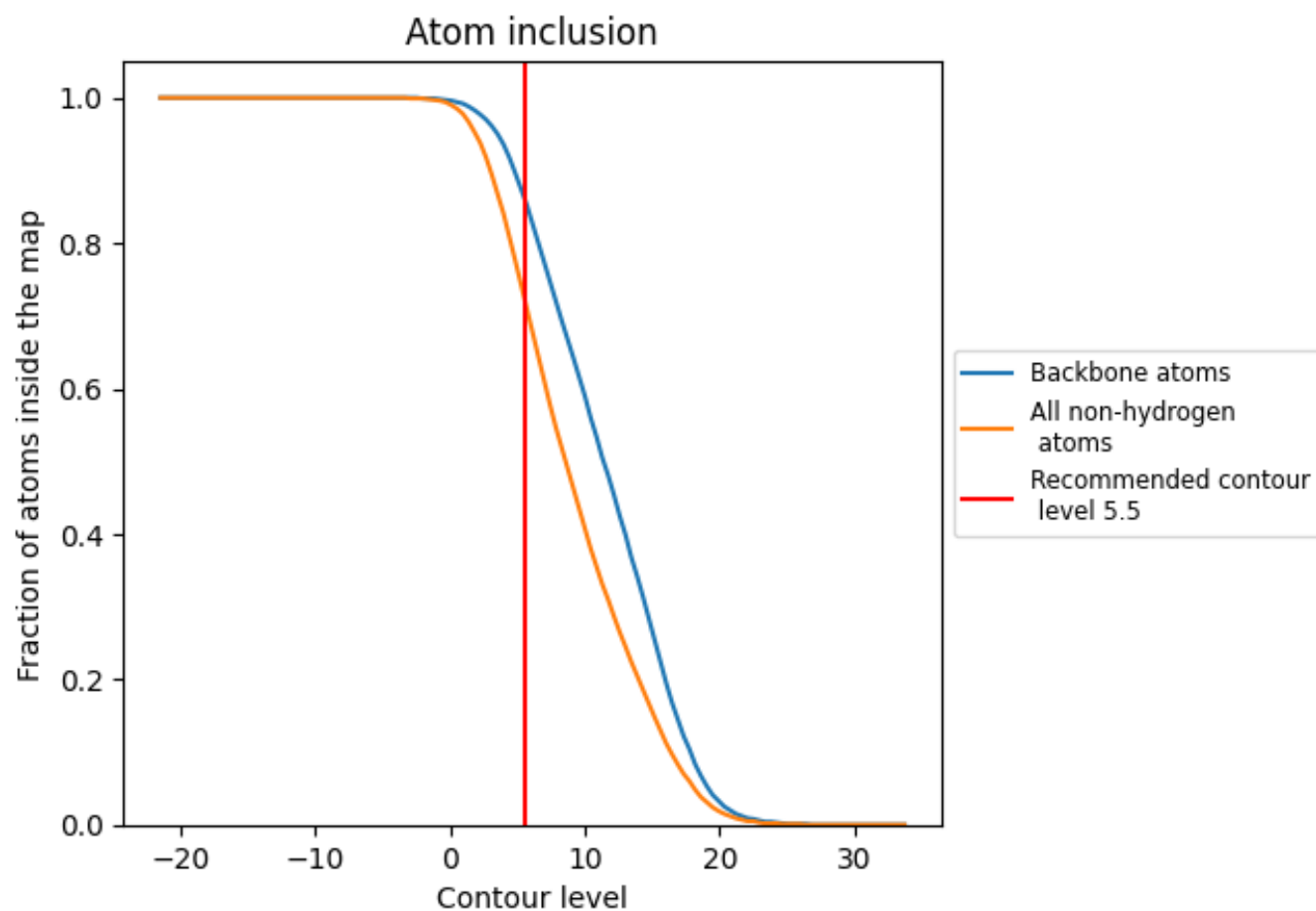
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 72% 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 (5.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7240	0.4630
A	0.5720	0.4220
B	0.7620	0.4710
C	0.8090	0.4910
D	0.8020	0.4900
E	0.7640	0.4720
F	0.6150	0.4220
G	0.7570	0.5510

1.0

0.0

<0.0