



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 11:53 PM EDT

PDB ID : 7KRO / pdb_00007kro
EMDB ID : EMD-23008
Title : Structure of SARS-CoV-2 backtracked complex complex bound to nsp13 helicase - nsp13(2)-BTC
Authors : Chen, J.; Malone, B.; Campbell, E.A.; Darst, S.A.
Deposited on : 2020-11-20
Resolution : 3.60 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.dev133
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) : 2.50

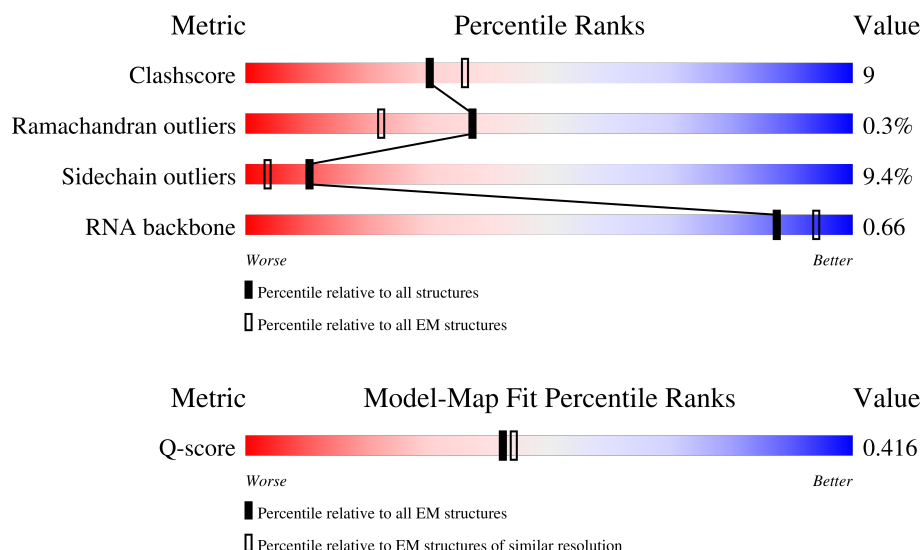
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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.



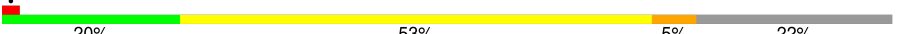
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	932	
2	B	199	
2	D	199	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	88	
4	E	605	
4	F	605	
5	P	40	
6	T	55	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	1N7	A	1005	X	-	-	-
11	AF3	E	706	-	-	X	-
11	AF3	F	1005	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 21988 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 RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	927	Total	C	N	O	S	0	0
			7470	4770	1253	1393	54		

- Molecule 2 is a protein called Non-structural protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	186	Total	C	N	O	S	0	0
			1424	894	243	276	11		
2	D	185	Total	C	N	O	S	0	0
			1427	895	243	278	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P0DTD1
D	0	MET	-	initiating methionine	UNP P0DTD1

- Molecule 3 is a protein called Non-structural protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	75	Total	C	N	O	S	0	0
			576	362	94	113	7		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	expression tag	UNP P0DTD1
C	-3	PRO	-	expression tag	UNP P0DTD1
C	-2	VAL	-	expression tag	UNP P0DTD1
C	-1	ASP	-	expression tag	UNP P0DTD1
C	0	MET	-	expression tag	UNP P0DTD1

- Molecule 4 is a protein called Helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	590	Total	C	N	O	S	0	0
			4602	2926	781	861	34		
4	F	590	Total	C	N	O	S	0	0
			4602	2926	781	861	34		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	expression tag	UNP P0DTD1
E	-2	PRO	-	expression tag	UNP P0DTD1
E	-1	HIS	-	expression tag	UNP P0DTD1
E	0	MET	-	expression tag	UNP P0DTD1
F	-3	GLY	-	expression tag	UNP P0DTD1
F	-2	PRO	-	expression tag	UNP P0DTD1
F	-1	HIS	-	expression tag	UNP P0DTD1
F	0	MET	-	expression tag	UNP P0DTD1

- Molecule 5 is a RNA chain called RNA (37-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	37	Total	C	N	O	P	0	0
			776	348	132	259	37		

- Molecule 6 is a RNA chain called RNA (43-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	43	Total	C	N	O	P	0	0
			914	409	161	301	43		

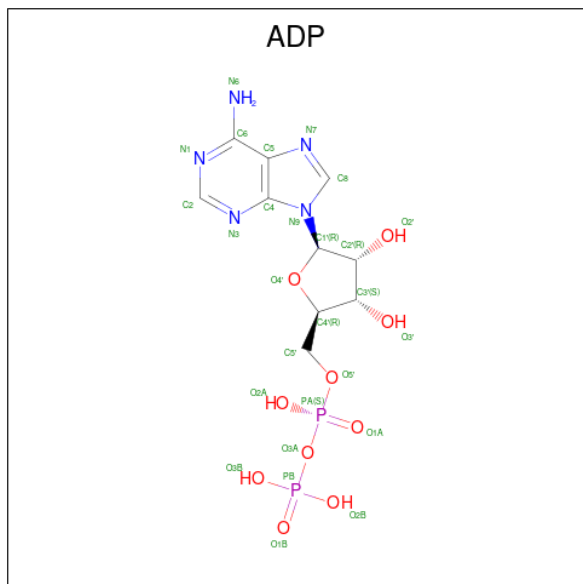
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	A	2	Total	Zn	0
			2	2	
7	E	3	Total	Zn	0
			3	3	
7	F	3	Total	Zn	0
			3	3	

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

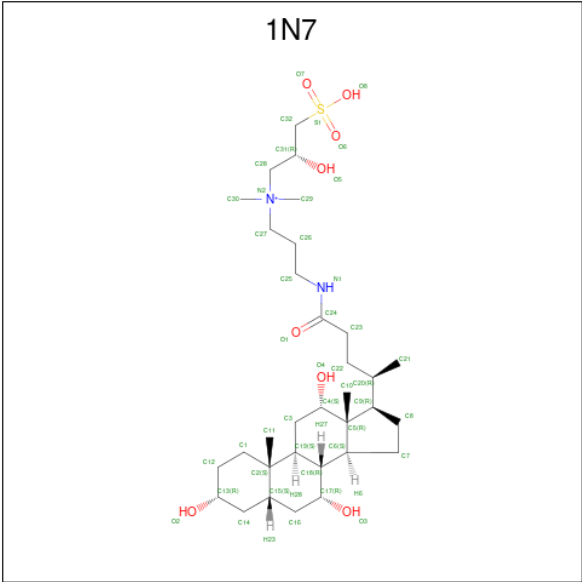
Mol	Chain	Residues	Atoms	AltConf
8	A	1	Total Mg 1 1	0
8	E	1	Total Mg 1 1	0
8	F	1	Total Mg 1 1	0

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



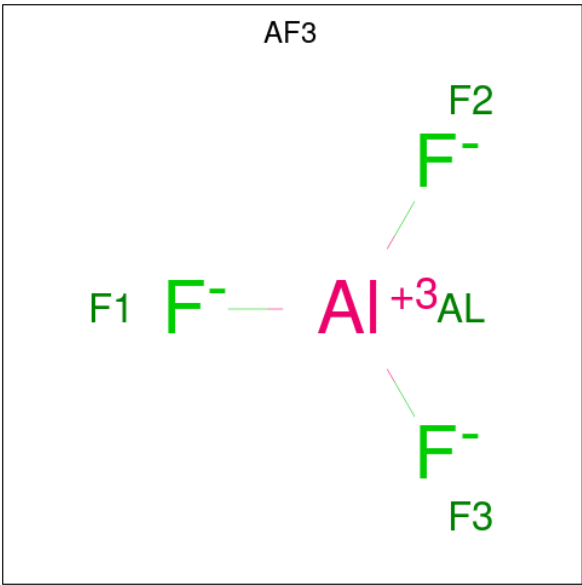
Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total 27	C 10	N 5	O 10	P 2	0
9	E	1	Total 27	C 10	N 5	O 10	P 2	0
9	F	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 10 is CHAPSO (CCD ID: 1N7) (formula: $\text{C}_{32}\text{H}_{59}\text{N}_2\text{O}_8\text{S}$).



Mol	Chain	Residues	Atoms				AltConf
10	A	1	Total	C	N	O	0
			35	29	2	4	
10	A	1	Total	C	O		0
			26	23	3		
10	E	1	Total	C	N	O	0
			36	30	2	4	

- Molecule 11 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF₃).



Mol	Chain	Residues	Atoms			AltConf
11	E	1	Total	Al	F	0
			4	1	3	

Continued on next page...

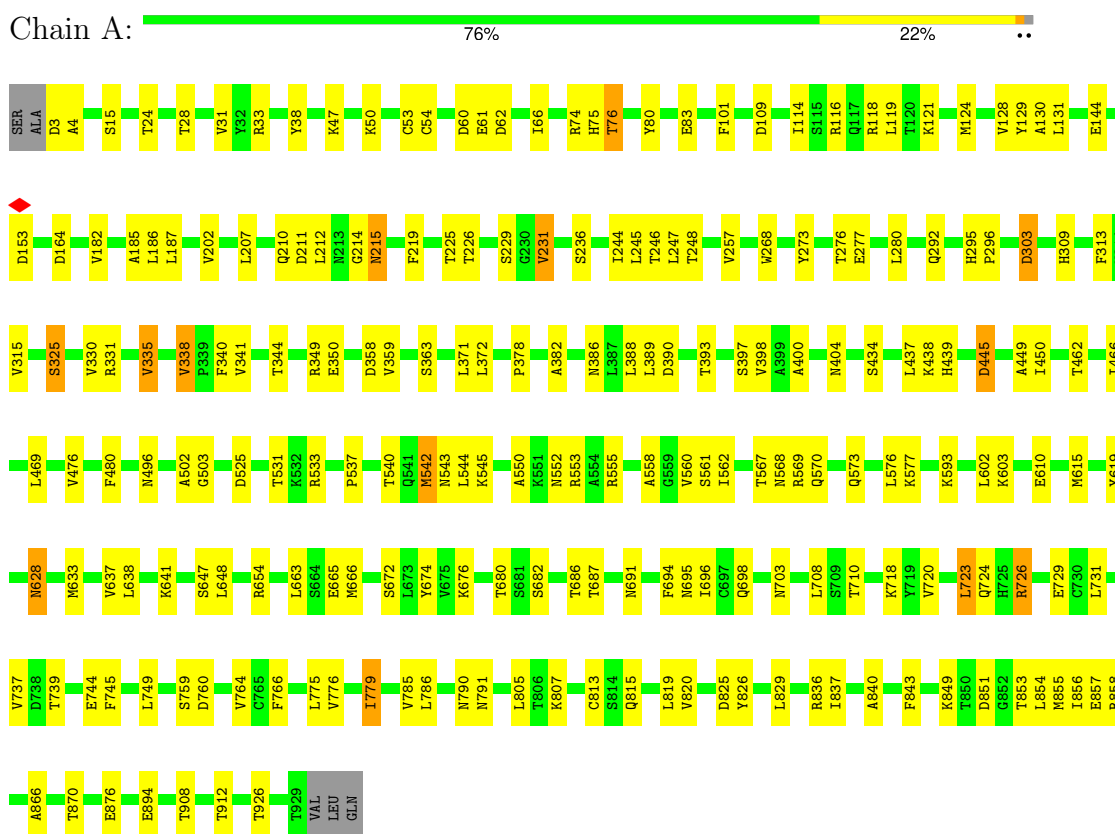
Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
			Total	Al	F	
11	F	1	4	1	3	0

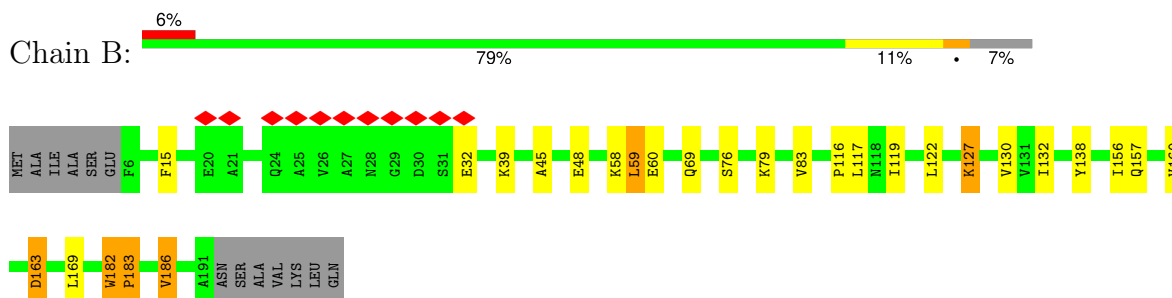
3 Residue-property plots

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

• Molecule 1: RNA-directed RNA polymerase

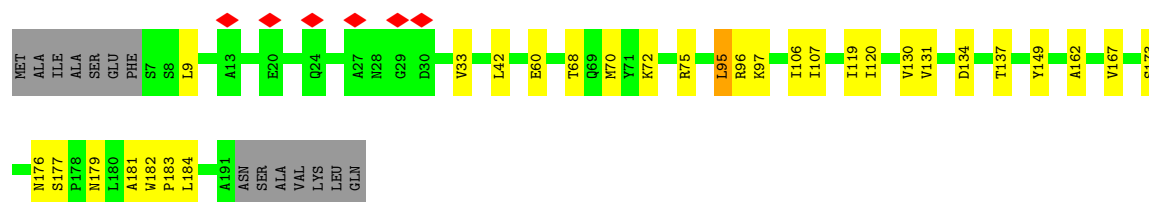


• Molecule 2: Non-structural protein 8



- Molecule 2: Non-structural protein 8

Chain D:  78% 15% 7%



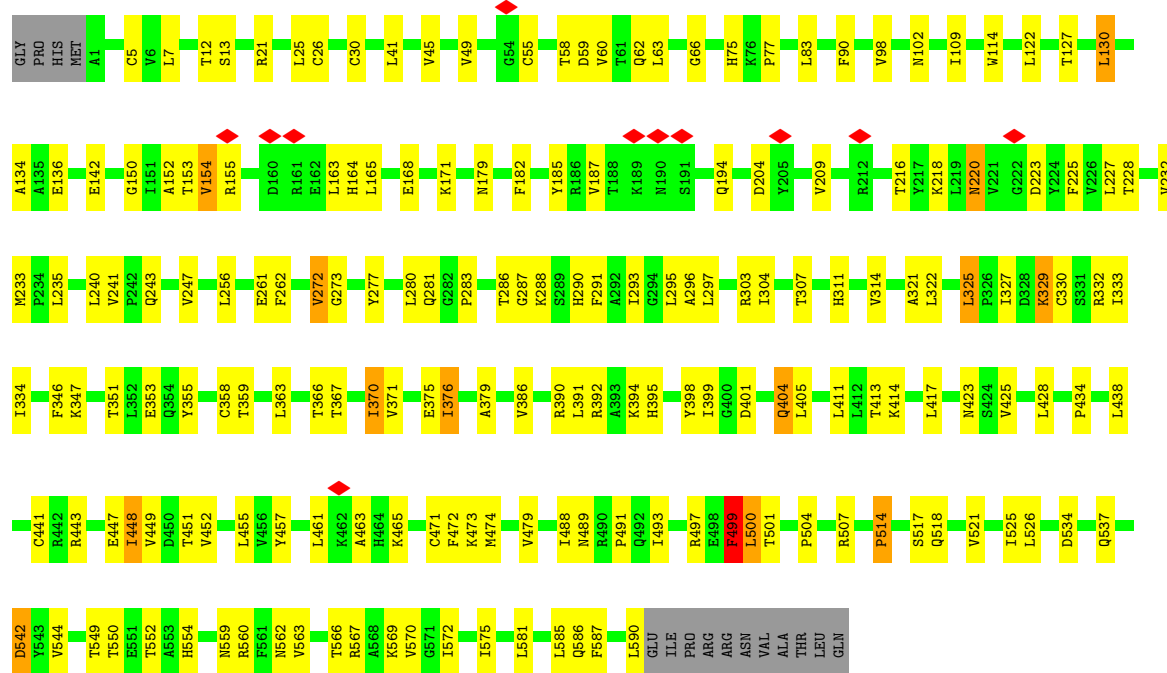
- Molecule 3: Non-structural protein 7

Chain C:  70% 15% 15%



- Molecule 4: Helicase

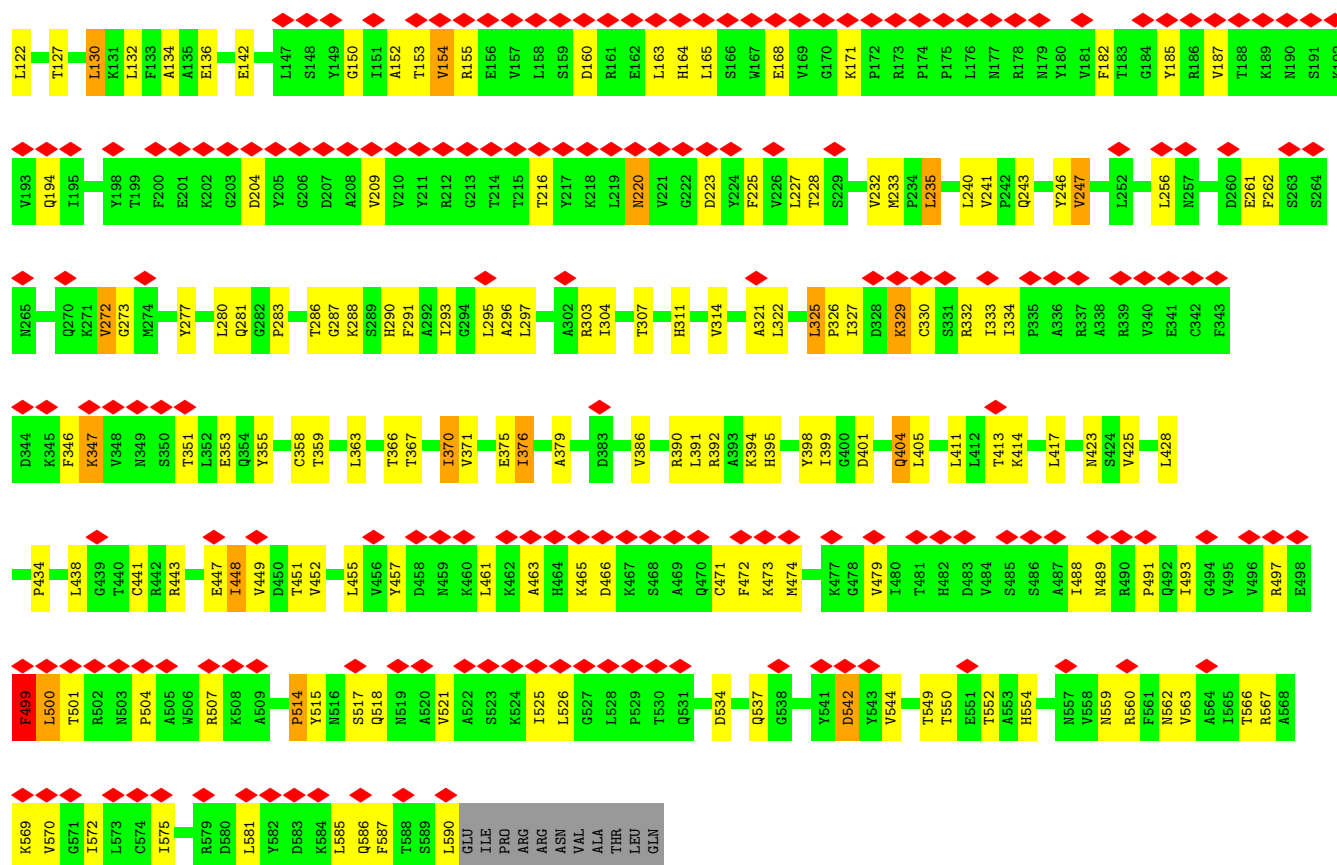
Chain E:  67% 28% 5%



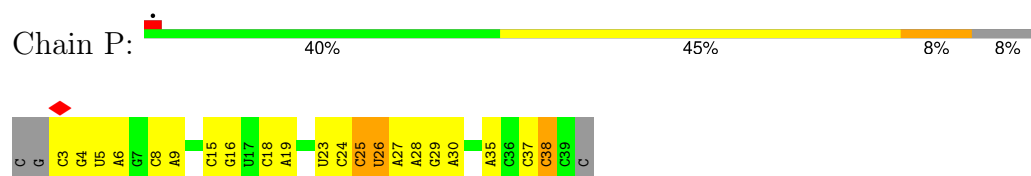
- Molecule 4: Helicase

Chain F:  31% 66% 29%

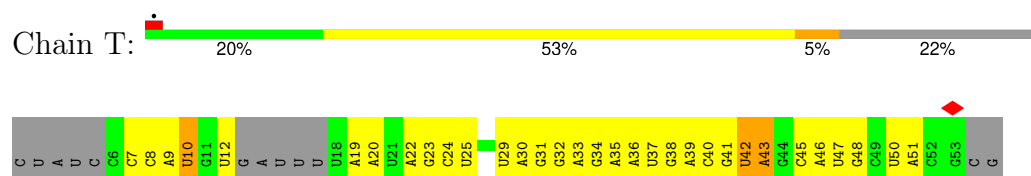




• Molecule 5: RNA (37-MER)



• Molecule 6: RNA (43-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	235147	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 ($e^-/\text{\AA}^2$)	66	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.563	Depositor
Minimum map value	-2.801	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.091	Depositor
Recommended contour level	0.4	Depositor
Map size ($\text{\AA}$)	340.80002, 340.80002, 340.80002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.065, 1.065, 1.065	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AF3, MG, ADP, ZN, 1N7

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	0.44	1/7659 (0.0%)	0.48	1/10394 (0.0%)
2	B	0.29	0/1443	0.40	0/1955
2	D	0.27	0/1446	0.43	0/1958
3	C	0.39	0/579	0.39	0/779
4	E	0.20	0/4706	0.40	0/6402
4	F	0.20	0/4706	0.40	0/6402
5	P	0.23	0/864	0.31	0/1341
6	T	0.25	0/1020	0.27	0/1584
All	All	0.32	1/22423 (0.0%)	0.42	1/30815 (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
2	B	0	1
2	D	0	1
4	E	0	2
4	F	0	2
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130	ALA	CA-C	-6.13	1.44	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	856	ILE	N-CA-C	-6.99	105.97	112.96

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	182	TRP	Peptide
2	D	181	ALA	Peptide
4	E	499	PHE	Peptide
4	E	514	PRO	Peptide
4	F	499	PHE	Peptide
4	F	514	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	7470	0	7206	109	0
2	B	1424	0	1437	15	0
2	D	1427	0	1445	14	0
3	C	576	0	608	8	0
4	E	4602	0	4576	97	0
4	F	4602	0	4576	105	0
5	P	776	0	399	23	0
6	T	914	0	463	35	0
7	A	2	0	0	0	0
7	E	3	0	0	0	0
7	F	3	0	0	0	0
8	A	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
9	A	27	0	12	1	0
9	E	27	0	12	2	0
9	F	27	0	12	2	0
10	A	61	0	86	2	0
10	E	36	0	52	3	0
11	E	4	0	0	2	0
11	F	4	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	21988	0	20884	385	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 9.

All (385) 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)
2:B:69:GLN:HG3	4:F:68:MET:HE3	1.66	0.78
1:A:83:GLU:HG3	1:A:219:PHE:HB2	1.69	0.74
4:F:489:ASN:HB2	4:F:549:THR:HG23	1.74	0.69
1:A:215:ASN:OD1	1:A:215:ASN:N	2.24	0.69
4:E:489:ASN:HB2	4:E:549:THR:HG23	1.74	0.68
4:E:405:LEU:HD22	4:E:563:VAL:HG11	1.77	0.67
4:F:405:LEU:HD22	4:F:563:VAL:HG11	1.77	0.66
3:C:74:GLU:HB2	2:D:96:ARG:HH12	1.60	0.66
4:E:394:LYS:O	4:E:395:HIS:ND1	2.29	0.66
1:A:628:ASN:HB3	1:A:663:LEU:HD21	1.78	0.66
4:F:394:LYS:O	4:F:395:HIS:ND1	2.29	0.66
1:A:813:CYS:SG	5:P:35:A:O2'	2.55	0.64
1:A:445:ASP:OD1	1:A:445:ASP:N	2.26	0.64
4:E:280:LEU:HB3	4:E:399:ILE:HG22	1.80	0.63
4:E:379:ALA:O	4:E:423:ASN:ND2	2.32	0.62
4:F:283:PRO:HG2	4:F:286:THR:HG21	1.80	0.62
4:F:379:ALA:O	4:F:423:ASN:ND2	2.32	0.62
1:A:80:TYR:HE1	1:A:101:PHE:HB3	1.64	0.61
4:E:283:PRO:HG2	4:E:286:THR:HG21	1.81	0.61
4:F:280:LEU:HB3	4:F:399:ILE:HG22	1.80	0.61
1:A:851:ASP:OD1	2:D:75:ARG:NH2	2.33	0.61
1:A:303:ASP:N	1:A:303:ASP:OD1	2.31	0.61
1:A:849:LYS:HG2	1:A:855:MET:HE3	1.82	0.61
4:F:499:PHE:O	4:F:501:THR:N	2.25	0.61
1:A:378:PRO:HG3	1:A:666:MET:HG3	1.81	0.61
1:A:449:ALA:HB2	1:A:544:LEU:HD11	1.82	0.61
1:A:568:ASN:OD1	1:A:654:ARG:NH2	2.34	0.60
4:E:473:LYS:HG3	4:E:587:PHE:HB2	1.84	0.60
4:F:283:PRO:O	4:F:288:LYS:NZ	2.34	0.60
4:F:542:ASP:HA	4:F:569:LYS:HB3	1.84	0.60
4:E:303:ARG:NH2	4:E:351:THR:O	2.35	0.60
5:P:26:U:H2'	5:P:27:A:H8	1.66	0.60
1:A:50:LYS:NZ	1:A:53:CYS:SG	2.66	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:303:ARG:NH2	4:F:351:THR:O	2.35	0.59
4:E:283:PRO:O	4:E:288:LYS:NZ	2.34	0.59
4:E:142:GLU:HG2	4:E:411:LEU:HD23	1.85	0.59
1:A:555:ARG:NE	5:P:37:C:O2	2.36	0.58
2:D:182:TRP:O	2:D:184:LEU:N	2.35	0.58
4:F:49:VAL:HG12	4:F:58:THR:HG22	1.85	0.58
4:F:473:LYS:HG3	4:F:587:PHE:HB2	1.84	0.58
4:F:296:ALA:HB1	4:F:355:TYR:HE2	1.68	0.58
4:E:296:ALA:HB1	4:E:355:TYR:HE2	1.68	0.58
4:E:542:ASP:HA	4:E:569:LYS:HB3	1.84	0.58
4:F:142:GLU:HG2	4:F:411:LEU:HD23	1.85	0.58
2:B:58:LYS:HG2	4:F:79:ILE:HG21	1.85	0.58
4:E:401:ASP:OD2	4:E:457:TYR:OH	2.21	0.58
4:E:150:GLY:HA2	4:E:171:LYS:HE3	1.86	0.58
2:B:156:ILE:HG21	2:B:169:LEU:HD21	1.85	0.57
4:E:49:VAL:HG12	4:E:58:THR:HG22	1.85	0.57
2:B:130:VAL:HB	2:B:186:VAL:HG13	1.86	0.57
4:F:518:GLN:OE1	4:F:549:THR:OG1	2.22	0.57
4:E:499:PHE:O	4:E:501:THR:N	2.26	0.57
4:E:66:GLY:HA3	4:E:77:PRO:HG3	1.87	0.57
4:E:413:THR:HG23	4:E:414:LYS:HG3	1.86	0.57
1:A:15:SER:OG	1:A:118:ARG:NH2	2.37	0.57
1:A:116:ARG:NH2	9:A:1004:ADP:O3B	2.38	0.57
4:F:401:ASP:OD2	4:F:457:TYR:OH	2.21	0.57
4:F:66:GLY:HA3	4:F:77:PRO:HG3	1.87	0.57
4:F:150:GLY:HA2	4:F:171:LYS:HE3	1.86	0.57
1:A:615:MET:HB2	1:A:766:PHE:HE2	1.70	0.56
5:P:26:U:H2'	5:P:27:A:C8	2.40	0.56
4:E:7:LEU:HD11	4:E:102:ASN:HB3	1.88	0.56
4:F:413:THR:HG23	4:F:414:LYS:HG3	1.86	0.56
1:A:647:SER:OG	1:A:648:LEU:N	2.39	0.55
4:E:367:THR:HA	4:E:392:ARG:HG3	1.89	0.55
4:F:7:LEU:HD11	4:F:102:ASN:HB3	1.88	0.55
4:E:375:GLU:OE1	4:E:537:GLN:NE2	2.39	0.55
4:F:375:GLU:OE1	4:F:537:GLN:NE2	2.39	0.55
4:F:367:THR:HA	4:F:392:ARG:HG3	1.89	0.55
6:T:38:G:H2'	6:T:39:A:H8	1.69	0.55
1:A:760:ASP:OD1	1:A:760:ASP:N	2.40	0.55
4:E:443:ARG:NH1	9:E:704:ADP:O3A	2.40	0.55
4:E:518:GLN:OE1	4:E:549:THR:OG1	2.22	0.55
4:F:443:ARG:NH1	9:F:1003:ADP:O3A	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ASP:N	1:A:109:ASP:OD1	2.40	0.54
4:E:443:ARG:HH22	4:E:567:ARG:HH21	1.56	0.54
4:E:293:ILE:HG23	4:E:325:LEU:HD13	1.91	0.53
1:A:211:ASP:N	1:A:211:ASP:OD1	2.40	0.53
4:E:534:ASP:OD1	4:E:560:ARG:NH1	2.41	0.53
1:A:358:ASP:OD1	1:A:533:ARG:NH2	2.41	0.53
1:A:619:TYR:OH	1:A:695:ASN:OD1	2.16	0.53
4:F:443:ARG:HH22	4:F:567:ARG:HH21	1.56	0.53
6:T:40:C:H2'	6:T:41:G:H8	1.74	0.53
1:A:476:VAL:HG12	1:A:637:VAL:HG11	1.91	0.52
1:A:480:PHE:O	1:A:641:LYS:NZ	2.34	0.52
4:F:293:ILE:HG23	4:F:325:LEU:HD13	1.90	0.52
4:F:534:ASP:OD1	4:F:560:ARG:NH1	2.41	0.52
4:F:549:THR:HG22	4:F:550:THR:HG23	1.91	0.52
4:E:179:ASN:HB3	6:T:10:U:H5	1.74	0.52
5:P:25:C:H2'	5:P:26:U:H6	1.74	0.52
4:E:497:ARG:HA	4:E:500:LEU:HD22	1.92	0.52
1:A:840:ALA:O	1:A:858:ARG:NH2	2.42	0.52
4:F:243:GLN:HB2	4:F:277:TYR:HE1	1.74	0.52
4:E:552:THR:HG23	4:E:554:HIS:H	1.74	0.51
1:A:502:ALA:HB1	1:A:562:ILE:HB	1.92	0.51
1:A:819:LEU:HD11	1:A:826:TYR:HB3	1.93	0.51
2:B:15:PHE:HA	2:B:45:ALA:HB1	1.93	0.51
4:E:243:GLN:HB2	4:E:277:TYR:HE1	1.75	0.51
1:A:390:ASP:OD2	1:A:674:TYR:OH	2.25	0.51
2:B:163:ASP:OD1	2:B:163:ASP:N	2.31	0.51
4:E:549:THR:HG22	4:E:550:THR:HG23	1.91	0.51
1:A:358:ASP:OD2	1:A:533:ARG:NH1	2.41	0.51
1:A:378:PRO:HD2	1:A:537:PRO:HB2	1.93	0.51
4:F:497:ARG:HD3	4:F:525:ILE:HG22	1.93	0.51
4:F:497:ARG:HA	4:F:500:LEU:HD22	1.92	0.51
4:F:552:THR:HG23	4:F:554:HIS:H	1.74	0.51
1:A:569:ARG:O	1:A:573:GLN:HB2	2.10	0.51
1:A:325:SER:O	1:A:325:SER:OG	2.24	0.50
4:E:497:ARG:HD3	4:E:525:ILE:HG22	1.93	0.50
6:T:38:G:H2'	6:T:39:A:C8	2.46	0.50
4:F:370:ILE:HA	4:F:395:HIS:O	2.12	0.50
4:F:441:CYS:HB2	4:F:463:ALA:HB2	1.94	0.50
4:F:376:ILE:HD13	4:F:398:TYR:HB3	1.93	0.50
2:D:173:SER:O	2:D:177:SER:N	2.45	0.50
4:E:262:PHE:HE2	4:E:297:LEU:HD12	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:272:VAL:HG11	4:E:295:LEU:HD21	1.94	0.50
4:F:363:LEU:HD22	4:F:391:LEU:HD11	1.94	0.50
4:F:542:ASP:OD1	4:F:542:ASP:N	2.44	0.50
4:E:370:ILE:HA	4:E:395:HIS:O	2.12	0.50
4:F:262:PHE:HE2	4:F:297:LEU:HD12	1.77	0.50
4:E:542:ASP:OD1	4:E:542:ASP:N	2.44	0.49
4:F:152:ALA:HB1	4:F:165:LEU:HD22	1.94	0.49
4:F:273:GLY:O	4:F:395:HIS:NE2	2.44	0.49
6:T:50:U:H2'	6:T:51:A:H8	1.77	0.49
4:E:45:VAL:HG11	10:E:707:1N7:H21	1.95	0.49
4:E:441:CYS:HB2	4:E:463:ALA:HB2	1.94	0.49
4:F:272:VAL:HG11	4:F:295:LEU:HD21	1.94	0.49
1:A:720:VAL:HG11	1:A:775:LEU:HD13	1.94	0.49
5:P:25:C:H2'	5:P:26:U:C6	2.47	0.49
6:T:34:G:H2'	6:T:35:A:H8	1.78	0.49
6:T:35:A:H2'	6:T:36:A:H8	1.77	0.49
6:T:19:A:H2'	6:T:20:A:C8	2.47	0.49
4:E:479:VAL:HG23	4:E:491:PRO:HG3	1.95	0.49
4:F:21:ARG:HG3	4:F:136:GLU:HG2	1.94	0.48
6:T:31:G:H2'	6:T:32:G:H8	1.78	0.48
4:E:152:ALA:HB1	4:E:165:LEU:HD22	1.94	0.48
4:E:363:LEU:HD22	4:E:391:LEU:HD11	1.94	0.48
1:A:545:LYS:HE2	1:A:555:ARG:HD3	1.96	0.48
4:E:376:ILE:HD13	4:E:398:TYR:HB3	1.93	0.48
1:A:615:MET:HB2	1:A:766:PHE:CE2	2.48	0.48
4:E:5:CYS:SG	4:E:26:CYS:N	2.74	0.48
4:F:479:VAL:HG23	4:F:491:PRO:HG3	1.95	0.48
1:A:335:VAL:HG23	1:A:338:VAL:HG12	1.96	0.48
2:D:95:LEU:HD23	2:D:107:ILE:HD11	1.94	0.48
4:F:5:CYS:SG	4:F:26:CYS:N	2.74	0.48
6:T:50:U:H2'	6:T:51:A:C8	2.49	0.47
4:E:21:ARG:NE	4:E:136:GLU:OE2	2.47	0.47
4:E:218:LYS:HB2	4:F:246:TYR:C	2.39	0.47
4:E:21:ARG:HG3	4:E:136:GLU:HG2	1.94	0.47
4:E:12:THR:OG1	4:E:13:SER:N	2.47	0.47
4:E:473:LYS:HD3	4:E:585:LEU:HG	1.96	0.47
4:F:12:THR:OG1	4:F:13:SER:N	2.47	0.47
4:F:473:LYS:HD3	4:F:585:LEU:HG	1.96	0.47
5:P:3:C:H2'	5:P:4:G:H8	1.79	0.47
4:E:90:PHE:HZ	10:E:707:1N7:H7	1.78	0.47
4:F:220:ASN:OD1	4:F:220:ASN:N	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:GLY:HA3	1:A:561:SER:HA	1.97	0.47
3:C:20:LEU:HD11	3:C:66:VAL:HG13	1.97	0.47
4:E:220:ASN:N	4:E:220:ASN:OD1	2.48	0.47
4:F:504:PRO:HB3	4:F:507:ARG:HH12	1.80	0.47
5:P:18:C:H2'	5:P:19:A:H8	1.79	0.47
1:A:437:LEU:HD23	1:A:437:LEU:HA	1.79	0.47
4:E:504:PRO:HB3	4:E:507:ARG:HH12	1.80	0.47
4:F:326:PRO:HB2	4:F:329:LYS:HZ1	1.79	0.47
1:A:273:TYR:HB3	2:B:116:PRO:HG3	1.97	0.47
4:F:21:ARG:NE	4:F:136:GLU:OE2	2.47	0.47
4:E:321:ALA:O	4:E:325:LEU:N	2.48	0.46
4:F:321:ALA:O	4:F:325:LEU:N	2.48	0.46
4:E:304:ILE:HG12	4:E:370:ILE:HG23	1.97	0.46
4:F:25:LEU:HD13	4:F:30:CYS:HA	1.97	0.46
6:T:24:C:H2'	6:T:25:U:H6	1.80	0.46
1:A:182:VAL:O	1:A:185:ALA:HB3	2.14	0.46
1:A:691:ASN:HB3	1:A:759:SER:O	2.15	0.46
4:F:304:ILE:HG12	4:F:370:ILE:HG23	1.97	0.46
4:F:404:GLN:OE1	11:F:1005:AF3:F2	2.24	0.46
6:T:42:U:H2'	6:T:43:A:H8	1.81	0.46
1:A:434:SER:OG	1:A:876:GLU:OE1	2.26	0.46
4:E:330:CYS:HA	4:E:355:TYR:O	2.16	0.46
4:E:488:ILE:HD11	4:E:517:SER:HB3	1.97	0.46
4:F:474:MET:HB2	4:F:575:ILE:HG22	1.98	0.46
6:T:45:C:H2'	6:T:46:A:H8	1.81	0.46
1:A:121:LYS:NZ	1:A:144:GLU:OE2	2.42	0.46
1:A:593:LYS:HE3	1:A:815:GLN:HE22	1.79	0.46
4:F:488:ILE:HD11	4:F:517:SER:HB3	1.97	0.46
6:T:29:U:H2'	6:T:30:A:H8	1.80	0.46
1:A:388:LEU:HD13	1:A:400:ALA:HB2	1.98	0.46
1:A:843:PHE:HE2	3:C:11:VAL:HG21	1.80	0.46
4:E:109:ILE:HD12	4:E:130:LEU:HD12	1.96	0.46
4:E:204:ASP:OD1	4:E:204:ASP:N	2.49	0.46
4:F:330:CYS:HA	4:F:355:TYR:O	2.16	0.46
6:T:40:C:H2'	6:T:41:G:C8	2.51	0.46
1:A:38:TYR:OH	1:A:729:GLU:OE2	2.26	0.46
1:A:292:GLN:HB3	1:A:309:HIS:HE1	1.80	0.46
1:A:628:ASN:OD1	1:A:628:ASN:N	2.49	0.46
1:A:726:ARG:NH1	1:A:744:GLU:OE1	2.49	0.46
1:A:837:ILE:HG13	1:A:866:ALA:HB2	1.98	0.46
4:E:287:GLY:HA2	9:E:704:ADP:H5'1	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:83:LEU:HD22	4:F:90:PHE:HB3	1.98	0.46
5:P:15:C:H2'	5:P:16:G:H8	1.80	0.46
1:A:128:VAL:HG22	1:A:244:ILE:HG13	1.98	0.45
1:A:749:LEU:HD23	1:A:749:LEU:HA	1.78	0.45
4:E:25:LEU:HD13	4:E:30:CYS:HA	1.97	0.45
4:E:404:GLN:OE1	11:E:706:AF3:F2	2.24	0.45
5:P:3:C:H2'	5:P:4:G:C8	2.51	0.45
5:P:24:C:H2'	5:P:25:C:C6	2.51	0.45
5:P:8:C:H2'	5:P:9:A:H8	1.82	0.45
6:T:31:G:H2'	6:T:32:G:C8	2.51	0.45
4:F:109:ILE:HD12	4:F:130:LEU:HD12	1.96	0.45
1:A:226:THR:O	1:A:229:SER:OG	2.33	0.45
1:A:825:ASP:OD1	1:A:825:ASP:N	2.50	0.45
4:F:240:LEU:HD21	4:F:425:VAL:HG22	1.99	0.45
4:F:287:GLY:HA2	9:F:1003:ADP:H5'1	1.99	0.45
6:T:32:G:H2'	6:T:33:A:H8	1.81	0.45
4:E:83:LEU:HD22	4:E:90:PHE:HB3	1.98	0.45
1:A:116:ARG:HB3	1:A:119:LEU:HD21	1.98	0.45
1:A:462:THR:OG1	1:A:791:ASN:OD1	2.25	0.45
3:C:56:LEU:HD23	2:D:106:ILE:HD11	1.99	0.45
4:E:273:GLY:O	4:E:395:HIS:NE2	2.44	0.45
5:P:5:U:H2'	5:P:6:A:H8	1.81	0.45
4:F:63:LEU:HD23	4:F:63:LEU:HA	1.83	0.45
5:P:24:C:H2'	5:P:25:C:H6	1.82	0.45
4:E:474:MET:HB2	4:E:575:ILE:HG22	1.98	0.45
1:A:525:ASP:OD1	1:A:570:GLN:NE2	2.50	0.44
3:C:58:VAL:HG22	2:D:119:ILE:HG12	1.99	0.44
1:A:186:LEU:HD11	1:A:245:LEU:HD11	1.99	0.44
1:A:382:ALA:HB3	2:B:117:LEU:HD11	2.00	0.44
1:A:619:TYR:HD1	1:A:786:LEU:HD21	1.82	0.44
4:E:155:ARG:HD2	4:E:164:HIS:CE1	2.53	0.44
4:E:449:VAL:HG11	4:E:463:ALA:HB3	1.98	0.44
4:F:155:ARG:HD2	4:F:164:HIS:CE1	2.53	0.44
4:F:515:TYR:OH	4:F:550:THR:OG1	2.27	0.44
5:P:29:G:H2'	5:P:30:A:H8	1.83	0.44
1:A:3:ASP:OD1	1:A:4:ALA:N	2.48	0.44
1:A:207:LEU:HD23	1:A:207:LEU:HA	1.82	0.44
1:A:854:LEU:HD22	2:D:72:LYS:HB2	2.00	0.44
4:E:240:LEU:HD21	4:E:425:VAL:HG22	1.99	0.44
1:A:33:ARG:HG3	1:A:50:LYS:HD3	1.98	0.44
1:A:236:SER:O	1:A:236:SER:OG	2.34	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:THR:HG23	1:A:296:PRO:HG2	2.00	0.44
4:F:204:ASP:OD1	4:F:204:ASP:N	2.49	0.44
4:F:466:ASP:OD1	4:F:466:ASP:N	2.50	0.44
1:A:202:VAL:HG13	1:A:231:VAL:HG13	1.99	0.44
1:A:779:ILE:HD13	1:A:779:ILE:HA	1.83	0.44
1:A:836:ARG:NH2	1:A:840:ALA:HB2	2.32	0.44
4:E:21:ARG:HD2	4:E:21:ARG:HA	1.79	0.44
4:E:109:ILE:HD13	4:E:134:ALA:HB2	1.98	0.44
4:F:386:VAL:HG13	4:F:390:ARG:HE	1.83	0.44
4:F:449:VAL:HG11	4:F:463:ALA:HB3	1.98	0.44
6:T:35:A:H2'	6:T:36:A:C8	2.53	0.44
1:A:553:ARG:HD2	5:P:38:C:H4'	1.99	0.44
4:F:154:VAL:HB	4:F:163:LEU:HD11	2.00	0.44
6:T:47:U:H2'	6:T:48:G:H8	1.82	0.44
1:A:60:ASP:HB3	1:A:66:ILE:HD13	2.00	0.44
1:A:330:VAL:HG11	2:B:117:LEU:HD13	1.99	0.44
4:E:287:GLY:O	4:E:291:PHE:N	2.47	0.44
6:T:32:G:H2'	6:T:33:A:C8	2.53	0.44
6:T:47:U:H2'	6:T:48:G:C8	2.52	0.44
4:E:386:VAL:HG13	4:E:390:ARG:HE	1.83	0.43
4:F:109:ILE:HD13	4:F:134:ALA:HB2	1.98	0.43
10:A:1006:1N7:H14	10:A:1006:1N7:H29	1.86	0.43
2:D:162:ALA:HB2	2:D:183:PRO:HG2	2.00	0.43
4:E:544:VAL:O	4:E:572:ILE:HA	2.19	0.43
4:E:329:LYS:HZ3	4:E:329:LYS:N	2.16	0.43
1:A:552:ASN:OD1	1:A:552:ASN:N	2.37	0.43
4:F:332:ARG:NH1	4:F:333:ILE:O	2.52	0.43
1:A:389:LEU:HB3	2:B:130:VAL:HG22	2.01	0.43
5:P:27:A:H2'	5:P:28:A:C8	2.53	0.43
6:T:29:U:H2'	6:T:30:A:C8	2.54	0.43
4:E:448:ILE:HD11	4:E:566:THR:HA	2.00	0.43
5:P:5:U:H2'	5:P:6:A:C8	2.54	0.43
5:P:18:C:H2'	5:P:19:A:C8	2.54	0.43
1:A:331:ARG:HD2	1:A:344:THR:HG21	2.01	0.43
1:A:665:GLU:HG2	1:A:676:LYS:HE2	1.99	0.43
1:A:386:ASN:HB3	2:B:127:LYS:HB3	2.00	0.43
2:B:59:LEU:HD11	4:F:80:SER:H	1.84	0.43
1:A:603:LYS:HD3	1:A:603:LYS:HA	1.91	0.43
4:E:281:GLN:HB3	4:E:434:PRO:HB3	2.00	0.43
4:E:472:PHE:HD1	4:E:590:LEU:HD21	1.84	0.43
10:E:707:1N7:H14	10:E:707:1N7:H29	1.77	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:CYS:SG	1:A:74:ARG:NH2	2.92	0.43
4:E:218:LYS:HG3	4:F:247:VAL:HG13	2.00	0.43
4:F:448:ILE:HD11	4:F:566:THR:HA	2.00	0.43
2:D:95:LEU:HD12	2:D:95:LEU:HA	1.84	0.42
4:E:154:VAL:HB	4:E:163:LEU:HD11	2.00	0.42
4:F:297:LEU:HD23	4:F:297:LEU:HA	1.82	0.42
6:T:33:A:H2'	6:T:34:G:C8	2.54	0.42
1:A:187:LEU:HD23	1:A:187:LEU:HA	1.83	0.42
6:T:34:G:H2'	6:T:35:A:C8	2.54	0.42
6:T:45:C:H2'	6:T:46:A:C8	2.54	0.42
4:F:281:GLN:HB3	4:F:434:PRO:HB3	2.00	0.42
5:P:27:A:H2'	5:P:28:A:H8	1.84	0.42
1:A:75:HIS:CG	1:A:76:THR:H	2.37	0.42
1:A:540:THR:HG22	1:A:560:VAL:HA	2.02	0.42
1:A:723:LEU:HD21	1:A:745:PHE:HD1	1.83	0.42
10:A:1005:1N7:H14	10:A:1005:1N7:H29	1.73	0.42
4:E:182:PHE:HB3	4:E:225:PHE:HB3	2.01	0.42
4:E:185:TYR:O	4:E:223:ASP:HA	2.19	0.42
4:E:332:ARG:NH1	4:E:333:ILE:O	2.52	0.42
4:E:375:GLU:OE2	11:E:706:AF3:F3	2.27	0.42
4:F:130:LEU:HD13	4:F:130:LEU:HA	1.86	0.42
3:C:4:SER:O	3:C:4:SER:OG	2.34	0.42
4:F:182:PHE:HB3	4:F:225:PHE:HB3	2.02	0.42
4:F:233:MET:HE2	4:F:233:MET:HB3	1.89	0.42
4:F:347:LYS:H	4:F:347:LYS:HG2	1.66	0.42
4:F:544:VAL:O	4:F:572:ILE:HA	2.18	0.42
1:A:210:GLN:HE21	1:A:214:GLY:HA2	1.85	0.42
2:D:70:MET:HE3	2:D:70:MET:HB2	1.92	0.42
4:F:472:PHE:HD1	4:F:590:LEU:HD21	1.84	0.42
6:T:30:A:H2'	6:T:31:G:H8	1.84	0.42
4:F:307:THR:HA	4:F:358:CYS:O	2.19	0.42
1:A:124:MET:HG3	1:A:210:GLN:HG2	2.02	0.42
1:A:439:HIS:CD2	1:A:550:ALA:HB2	2.54	0.42
4:E:307:THR:HA	4:E:358:CYS:O	2.19	0.42
4:E:376:ILE:H	4:E:376:ILE:HG12	1.44	0.42
4:F:114:TRP:HH2	4:F:134:ALA:HB1	1.84	0.42
4:F:185:TYR:O	4:F:223:ASP:HA	2.19	0.42
6:T:37:U:H2'	6:T:38:G:C8	2.55	0.42
1:A:638:LEU:HD12	1:A:638:LEU:HA	1.85	0.42
1:A:654:ARG:HD2	1:A:654:ARG:HA	1.79	0.42
4:E:322:LEU:HD13	4:E:346:PHE:HE1	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:41:LEU:HD13	4:F:58:THR:HB	2.02	0.42
4:F:375:GLU:OE2	11:F:1005:AF3:F3	2.27	0.42
1:A:476:VAL:HG22	1:A:696:ILE:HG22	2.02	0.42
2:B:132:ILE:HG21	2:B:138:TYR:HB2	2.02	0.41
4:F:423:ASN:OD1	4:F:423:ASN:N	2.53	0.41
1:A:371:LEU:HD12	1:A:371:LEU:HA	1.83	0.41
1:A:633:MET:HE3	1:A:633:MET:HB3	1.78	0.41
1:A:708:LEU:HD11	1:A:731:LEU:HD12	2.01	0.41
4:E:114:TRP:HH2	4:E:134:ALA:HB1	1.84	0.41
4:E:451:THR:HG22	4:E:586:GLN:H	1.85	0.41
4:F:293:ILE:HD13	4:F:293:ILE:HA	1.82	0.41
4:F:322:LEU:HD13	4:F:346:PHE:HE1	1.85	0.41
4:E:559:ASN:OD1	4:E:559:ASN:N	2.52	0.41
4:F:451:THR:HG22	4:F:586:GLN:H	1.85	0.41
6:T:19:A:H2'	6:T:20:A:H8	1.82	0.41
6:T:36:A:H2'	6:T:37:U:C6	2.55	0.41
1:A:398:VAL:HG21	1:A:666:MET:HE1	2.02	0.41
1:A:404:ASN:N	1:A:404:ASN:OD1	2.50	0.41
6:T:22:A:H2'	6:T:23:G:C8	2.56	0.41
1:A:469:LEU:HD12	1:A:469:LEU:HA	1.76	0.41
4:E:55:CYS:HB2	4:E:75:HIS:CE1	2.55	0.41
4:F:471:CYS:HA	4:F:572:ILE:O	2.21	0.41
1:A:335:VAL:HG12	1:A:363:SER:HB2	2.02	0.41
4:E:63:LEU:HD23	4:E:63:LEU:HA	1.83	0.41
4:F:55:CYS:HB2	4:F:75:HIS:CE1	2.55	0.41
1:A:542:MET:HE2	1:A:558:ALA:HB2	2.02	0.41
1:A:545:LYS:HE2	1:A:545:LYS:HB3	1.92	0.41
4:F:455:LEU:HD23	4:F:455:LEU:HA	1.86	0.41
6:T:30:A:H2'	6:T:31:G:C8	2.55	0.41
4:E:471:CYS:HB3	4:E:587:PHE:CD2	2.56	0.41
6:T:33:A:H2'	6:T:34:G:H8	1.85	0.41
1:A:791:ASN:HD22	1:A:791:ASN:HA	1.70	0.41
2:B:132:ILE:O	2:B:183:PRO:HA	2.21	0.41
4:E:233:MET:HE2	4:E:233:MET:HB3	1.89	0.41
4:F:165:LEU:HD12	4:F:209:VAL:HG21	2.03	0.41
5:P:23:U:H2'	5:P:24:C:C6	2.56	0.41
6:T:24:C:H2'	6:T:25:U:C6	2.54	0.41
3:C:28:LEU:HD12	3:C:28:LEU:HA	1.80	0.41
3:C:7:LYS:O	3:C:10:SER:OG	2.37	0.40
2:D:120:ILE:HD11	2:D:149:TYR:HE1	1.86	0.40
2:D:134:ASP:O	2:D:137:THR:OG1	2.38	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:455:LEU:HD23	4:E:455:LEU:HA	1.86	0.40
5:P:15:C:H2'	5:P:16:G:C8	2.56	0.40
1:A:908:THR:HG21	2:D:60:GLU:HG3	2.04	0.40
4:E:41:LEU:HD13	4:E:58:THR:HB	2.02	0.40
4:E:218:LYS:HA	4:F:247:VAL:HG22	2.03	0.40
4:E:423:ASN:OD1	4:E:423:ASN:N	2.53	0.40
4:E:451:THR:CG2	4:E:586:GLN:H	2.34	0.40
4:F:287:GLY:O	4:F:291:PHE:N	2.47	0.40
4:F:559:ASN:OD1	4:F:559:ASN:N	2.52	0.40
5:P:29:G:H2'	5:P:30:A:C8	2.56	0.40
1:A:47:LYS:HD2	1:A:129:TYR:HE2	1.86	0.40
1:A:225:THR:OG1	1:A:226:THR:N	2.54	0.40
1:A:829:LEU:HD23	1:A:829:LEU:HA	1.87	0.40
2:B:58:LYS:HG2	4:F:79:ILE:HD13	2.03	0.40
4:F:132:LEU:HD22	4:F:235:LEU:HD13	2.03	0.40
4:F:451:THR:CG2	4:F:586:GLN:H	2.34	0.40
1:A:186:LEU:HD23	1:A:186:LEU:HA	1.90	0.40
1:A:577:LYS:NZ	6:T:22:A:OP1	2.37	0.40
1:A:718:LYS:HE3	1:A:718:LYS:HB3	1.94	0.40
4:E:165:LEU:HD12	4:E:209:VAL:HG21	2.03	0.40
4:F:160:ASP:N	4:F:160:ASP:OD1	2.55	0.40
6:T:36:A:H2'	6:T:37:U:H6	1.87	0.40
1:A:694:PHE:HE1	1:A:698:GLN:HE21	1.69	0.40
4:F:471:CYS:HB3	4:F:587:PHE:CD2	2.56	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	925/932 (99%)	867 (94%)	58 (6%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	184/199 (92%)	176 (96%)	6 (3%)	2 (1%)	11	43
2	D	183/199 (92%)	175 (96%)	8 (4%)	0	100	100
3	C	73/88 (83%)	72 (99%)	1 (1%)	0	100	100
4	E	588/605 (97%)	533 (91%)	52 (9%)	3 (0%)	24	57
4	F	588/605 (97%)	534 (91%)	51 (9%)	3 (0%)	24	57
All	All	2541/2628 (97%)	2357 (93%)	176 (7%)	8 (0%)	37	65

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	500	LEU
4	F	500	LEU
2	B	182	TRP
2	B	183	PRO
4	E	514	PRO
4	F	514	PRO
4	E	499	PHE
4	F	499	PHE

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	819/823 (100%)	745 (91%)	74 (9%)	9	33
2	B	153/168 (91%)	138 (90%)	15 (10%)	7	31
2	D	155/168 (92%)	144 (93%)	11 (7%)	13	40
3	C	70/81 (86%)	67 (96%)	3 (4%)	26	52
4	E	513/526 (98%)	460 (90%)	53 (10%)	7	30
4	F	513/526 (98%)	460 (90%)	53 (10%)	7	30
All	All	2223/2292 (97%)	2014 (91%)	209 (9%)	10	32

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	THR
1	A	28	THR
1	A	31	VAL
1	A	61	GLU
1	A	62	ASP
1	A	76	THR
1	A	114	ILE
1	A	131	LEU
1	A	153	ASP
1	A	164	ASP
1	A	212	LEU
1	A	215	ASN
1	A	231	VAL
1	A	246	THR
1	A	247	LEU
1	A	248	THR
1	A	257	VAL
1	A	268	TRP
1	A	277	GLU
1	A	280	LEU
1	A	295	HIS
1	A	303	ASP
1	A	313	PHE
1	A	315	VAL
1	A	325	SER
1	A	335	VAL
1	A	338	VAL
1	A	340	PHE
1	A	341	VAL
1	A	349	ARG
1	A	350	GLU
1	A	359	VAL
1	A	372	LEU
1	A	393	THR
1	A	397	SER
1	A	438	LYS
1	A	445	ASP
1	A	450	ILE
1	A	466	ILE
1	A	496	ASN
1	A	531	THR
1	A	542	MET
1	A	543	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	567	THR
1	A	576	LEU
1	A	602	LEU
1	A	610	GLU
1	A	628	ASN
1	A	672	SER
1	A	680	THR
1	A	682	SER
1	A	686	THR
1	A	687	THR
1	A	703	ASN
1	A	710	THR
1	A	723	LEU
1	A	724	GLN
1	A	726	ARG
1	A	737	VAL
1	A	739	THR
1	A	764	VAL
1	A	776	VAL
1	A	779	ILE
1	A	785	VAL
1	A	790	ASN
1	A	805	LEU
1	A	807	LYS
1	A	820	VAL
1	A	853	THR
1	A	857	GLU
1	A	870	THR
1	A	894	GLU
1	A	912	THR
1	A	926	THR
2	B	32	GLU
2	B	39	LYS
2	B	48	GLU
2	B	59	LEU
2	B	60	GLU
2	B	76	SER
2	B	79	LYS
2	B	83	VAL
2	B	119	ILE
2	B	122	LEU
2	B	127	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	157	GLN
2	B	160	VAL
2	B	163	ASP
2	B	186	VAL
3	C	33	VAL
3	C	61	SER
3	C	71	LEU
2	D	9	LEU
2	D	33	VAL
2	D	42	LEU
2	D	68	THR
2	D	95	LEU
2	D	97	LYS
2	D	130	VAL
2	D	131	VAL
2	D	167	VAL
2	D	176	ASN
2	D	179	ASN
4	E	59	ASP
4	E	60	VAL
4	E	62	GLN
4	E	98	VAL
4	E	122	LEU
4	E	127	THR
4	E	130	LEU
4	E	153	THR
4	E	154	VAL
4	E	168	GLU
4	E	187	VAL
4	E	194	GLN
4	E	216	THR
4	E	220	ASN
4	E	227	LEU
4	E	228	THR
4	E	232	VAL
4	E	235	LEU
4	E	241	VAL
4	E	247	VAL
4	E	256	LEU
4	E	261	GLU
4	E	272	VAL
4	E	290	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	E	311	HIS
4	E	314	VAL
4	E	325	LEU
4	E	327	ILE
4	E	329	LYS
4	E	334	ILE
4	E	347	LYS
4	E	353	GLU
4	E	359	THR
4	E	366	THR
4	E	370	ILE
4	E	371	VAL
4	E	376	ILE
4	E	404	GLN
4	E	417	LEU
4	E	428	LEU
4	E	438	LEU
4	E	447	GLU
4	E	448	ILE
4	E	452	VAL
4	E	461	LEU
4	E	465	LYS
4	E	493	ILE
4	E	521	VAL
4	E	526	LEU
4	E	542	ASP
4	E	562	ASN
4	E	570	VAL
4	E	581	LEU
4	F	59	ASP
4	F	60	VAL
4	F	62	GLN
4	F	98	VAL
4	F	122	LEU
4	F	127	THR
4	F	130	LEU
4	F	153	THR
4	F	154	VAL
4	F	168	GLU
4	F	187	VAL
4	F	194	GLN
4	F	216	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	F	220	ASN
4	F	227	LEU
4	F	228	THR
4	F	232	VAL
4	F	235	LEU
4	F	241	VAL
4	F	247	VAL
4	F	256	LEU
4	F	261	GLU
4	F	272	VAL
4	F	290	HIS
4	F	311	HIS
4	F	314	VAL
4	F	325	LEU
4	F	327	ILE
4	F	329	LYS
4	F	334	ILE
4	F	347	LYS
4	F	353	GLU
4	F	359	THR
4	F	366	THR
4	F	370	ILE
4	F	371	VAL
4	F	376	ILE
4	F	404	GLN
4	F	417	LEU
4	F	428	LEU
4	F	438	LEU
4	F	447	GLU
4	F	448	ILE
4	F	452	VAL
4	F	461	LEU
4	F	465	LYS
4	F	493	ILE
4	F	521	VAL
4	F	526	LEU
4	F	542	ASP
4	F	562	ASN
4	F	570	VAL
4	F	581	LEU

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	5	GLN
1	A	75	HIS
1	A	81	GLN
1	A	168	ASN
1	A	198	ASN
1	A	295	HIS
1	A	362	HIS
1	A	414	ASN
2	B	100	ASN
2	B	179	ASN
3	C	18	GLN
2	D	140	ASN
2	D	157	GLN
4	E	9	ASN
4	E	86	ASN
4	E	311	HIS
4	E	381	ASN
4	E	404	GLN
4	E	503	ASN
4	E	531	GLN
4	F	9	ASN
4	F	86	ASN
4	F	381	ASN
4	F	404	GLN
4	F	531	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	P	36/40 (90%)	2 (5%)	1 (2%)
6	T	41/55 (74%)	7 (17%)	0
All	All	77/95 (81%)	9 (11%)	1 (1%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	P	26	U
5	P	38	C
6	T	7	C
6	T	8	C
6	T	9	A
6	T	10	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	T	12	U
6	T	42	U
6	T	43	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	P	25	C

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 19 ligands modelled in this entry, 11 are monoatomic - leaving 8 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
9	ADP	A	1004	8	28,29,29	1.35	4 (14%)	43,45,45	1.81	8 (18%)
9	ADP	F	1003	11,8	28,29,29	1.40	4 (14%)	43,45,45	1.81	8 (18%)
10	1N7	A	1005	-	38,38,46	2.82	21 (55%)	58,58,72	3.13	26 (44%)
9	ADP	E	704	11,8	28,29,29	1.40	4 (14%)	43,45,45	1.81	8 (18%)
10	1N7	A	1006	-	29,29,46	2.69	16 (55%)	47,47,72	2.35	20 (42%)
10	1N7	E	707	-	39,39,46	2.57	21 (53%)	61,61,72	2.54	27 (44%)
11	AF3	F	1005	9	0,3,3	-	-	-	-	-
11	AF3	E	706	9	0,3,3	-	-	-	-	-

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
9	ADP	A	1004	8	-	8/16/32/32	0/3/3/3
9	ADP	F	1003	11,8	-	1/16/32/32	0/3/3/3
9	ADP	E	704	11,8	-	1/16/32/32	0/3/3/3
10	1N7	A	1005	-	2/2/13/16	9/16/81/92	0/4/4/4
10	1N7	A	1006	-	-	6/6/71/92	0/4/4/4
10	1N7	E	707	-	-	6/17/82/92	0/4/4/4

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1005	1N7	C18-C17	5.92	1.64	1.53
10	E	707	1N7	C18-C17	5.44	1.63	1.53
10	A	1006	1N7	C18-C17	5.41	1.63	1.53
10	A	1006	1N7	C2-C19	4.85	1.64	1.56
10	A	1005	1N7	C23-C24	4.79	1.60	1.51
10	A	1005	1N7	C2-C19	4.71	1.64	1.56
10	A	1005	1N7	C24-N1	4.67	1.44	1.33
9	F	1003	ADP	C5-C4	4.59	1.47	1.39
9	E	704	ADP	C5-C4	4.55	1.47	1.39
10	E	707	1N7	C24-N1	4.55	1.44	1.33
10	E	707	1N7	C23-C24	4.53	1.60	1.51
9	A	1004	ADP	C5-C4	4.49	1.47	1.39
10	A	1005	1N7	C14-C13	4.42	1.59	1.52
10	A	1006	1N7	C3-C19	4.31	1.60	1.53
10	A	1005	1N7	C16-C17	4.22	1.60	1.52
10	A	1005	1N7	C20-C9	4.09	1.61	1.54
10	E	707	1N7	C14-C13	4.06	1.59	1.52
10	E	707	1N7	C2-C19	4.06	1.63	1.56
10	A	1005	1N7	C3-C19	4.04	1.60	1.53
10	A	1006	1N7	C14-C13	4.03	1.59	1.52
10	A	1005	1N7	C28-N2	4.01	1.58	1.46
10	E	707	1N7	C16-C17	3.91	1.60	1.52
10	A	1006	1N7	C20-C9	3.77	1.60	1.54
10	E	707	1N7	C20-C9	3.76	1.60	1.54
10	A	1006	1N7	C16-C17	3.76	1.59	1.52
10	E	707	1N7	C3-C19	3.67	1.59	1.53
10	A	1005	1N7	C5-C4	3.46	1.59	1.54
10	A	1005	1N7	C14-C15	3.36	1.59	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1006	1N7	C5-C4	3.25	1.59	1.54
10	A	1006	1N7	C14-C15	3.24	1.59	1.53
10	E	707	1N7	C28-N2	3.08	1.59	1.50
10	E	707	1N7	C14-C15	3.02	1.58	1.53
10	A	1005	1N7	C25-N1	3.00	1.52	1.46
10	E	707	1N7	C16-C15	2.93	1.58	1.53
10	A	1005	1N7	C18-C6	2.87	1.59	1.53
10	A	1005	1N7	C16-C15	2.87	1.58	1.53
10	A	1006	1N7	C1-C2	2.86	1.59	1.54
10	E	707	1N7	C25-N1	2.85	1.52	1.46
10	E	707	1N7	C5-C4	2.84	1.58	1.54
10	E	707	1N7	C29-N2	2.81	1.58	1.50
10	A	1006	1N7	C2-C15	2.79	1.59	1.55
10	A	1005	1N7	C5-C6	2.79	1.60	1.55
10	A	1006	1N7	C16-C15	2.78	1.58	1.53
10	A	1006	1N7	C18-C6	2.75	1.59	1.53
10	A	1006	1N7	C3-C4	2.70	1.57	1.53
10	A	1005	1N7	C1-C2	2.69	1.58	1.54
10	E	707	1N7	C1-C2	2.65	1.58	1.54
10	A	1005	1N7	C12-C13	2.63	1.57	1.51
9	A	1004	ADP	C5-C6	2.57	1.48	1.41
10	A	1006	1N7	C12-C13	2.55	1.57	1.51
9	E	704	ADP	C5-C6	2.55	1.48	1.41
10	A	1005	1N7	C18-C19	2.55	1.58	1.53
9	F	1003	ADP	C5-C6	2.55	1.48	1.41
10	A	1006	1N7	C18-C19	2.51	1.58	1.53
9	F	1003	ADP	C5-N7	-2.50	1.34	1.39
10	A	1005	1N7	C3-C4	2.50	1.57	1.53
9	E	704	ADP	C5-N7	-2.49	1.34	1.39
10	E	707	1N7	C18-C6	2.48	1.58	1.53
9	A	1004	ADP	C5-N7	-2.48	1.34	1.39
10	E	707	1N7	C12-C13	2.47	1.57	1.51
10	E	707	1N7	C2-C15	2.45	1.59	1.55
10	E	707	1N7	C18-C19	2.30	1.58	1.53
10	A	1005	1N7	C2-C15	2.25	1.58	1.55
10	E	707	1N7	C3-C4	2.23	1.56	1.53
9	F	1003	ADP	C8-N7	2.22	1.35	1.31
9	E	704	ADP	C8-N7	2.20	1.35	1.31
10	A	1006	1N7	C5-C6	2.19	1.59	1.55
9	A	1004	ADP	C8-N7	2.17	1.35	1.31
10	A	1005	1N7	C22-C23	2.09	1.59	1.52
10	E	707	1N7	C22-C23	2.03	1.59	1.52

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1005	1N7	C9-C5-C4	-12.48	106.44	117.67
10	E	707	1N7	C9-C5-C4	-6.87	111.49	117.67
10	E	707	1N7	C3-C4-C5	-6.46	104.69	111.26
10	A	1005	1N7	C6-C5-C4	6.39	113.26	107.42
10	A	1005	1N7	C9-C5-C6	6.22	106.35	100.11
10	A	1006	1N7	C9-C5-C4	-6.17	112.11	117.67
10	A	1005	1N7	C8-C9-C5	-6.09	97.63	103.54
10	E	707	1N7	C8-C9-C5	-5.94	97.78	103.54
9	A	1004	ADP	C5-C4-N3	-5.84	118.68	126.72
9	F	1003	ADP	C5-C4-N3	-5.81	118.72	126.72
9	E	704	ADP	C5-C4-N3	-5.80	118.72	126.72
10	A	1006	1N7	C8-C9-C5	-5.63	98.08	103.54
10	E	707	1N7	C6-C18-C17	5.30	118.89	111.85
10	A	1006	1N7	C11-C2-C1	-4.98	100.38	108.31
10	A	1005	1N7	C5-C9-C20	-4.97	113.47	119.48
10	A	1005	1N7	C23-C24-N1	4.94	125.34	116.34
9	E	704	ADP	N3-C4-N9	4.64	135.06	127.17
9	F	1003	ADP	N3-C4-N9	4.63	135.04	127.17
10	A	1005	1N7	C6-C18-C17	4.62	117.99	111.85
9	A	1004	ADP	N3-C4-N9	4.59	134.97	127.17
10	A	1005	1N7	C8-C9-C20	4.58	119.12	112.18
10	E	707	1N7	C23-C24-N1	4.30	124.19	116.34
10	E	707	1N7	C5-C9-C20	-4.30	114.27	119.48
10	E	707	1N7	C11-C2-C1	-4.26	101.53	108.31
10	A	1006	1N7	C6-C18-C17	4.08	117.26	111.85
10	A	1005	1N7	C7-C6-C18	-4.05	112.80	118.36
10	A	1005	1N7	C16-C17-C18	4.00	115.87	111.50
10	E	707	1N7	C7-C6-C5	-3.99	99.67	103.54
10	A	1005	1N7	C11-C2-C1	-3.83	102.21	108.31
10	A	1005	1N7	C2-C19-C18	3.77	116.04	111.84
10	A	1006	1N7	C3-C4-C5	-3.76	107.44	111.26
9	E	704	ADP	C2-N3-C4	3.71	120.89	111.83
9	F	1003	ADP	C2-N3-C4	3.70	120.86	111.83
9	A	1004	ADP	C2-N3-C4	3.66	120.77	111.83
10	E	707	1N7	C9-C5-C6	3.62	103.75	100.11
10	A	1006	1N7	C7-C6-C5	-3.47	100.17	103.54
10	A	1006	1N7	C19-C2-C15	3.43	113.27	108.51
10	A	1005	1N7	C16-C15-C2	-3.39	109.06	112.66
9	E	704	ADP	N3-C2-N1	-3.34	123.53	128.58
9	F	1003	ADP	N3-C2-N1	-3.29	123.60	128.58
9	A	1004	ADP	C4-C5-N7	-3.27	106.84	110.58
9	F	1003	ADP	C4-C5-N7	-3.27	106.84	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1005	1N7	C19-C2-C15	3.24	113.01	108.51
9	E	704	ADP	C4-C5-N7	-3.23	106.89	110.58
9	A	1004	ADP	N3-C2-N1	-3.18	123.76	128.58
10	E	707	1N7	C29-N2-C28	-3.14	100.73	108.98
10	A	1006	1N7	C2-C19-C18	3.11	115.31	111.84
10	A	1005	1N7	C3-C4-C5	-3.08	108.13	111.26
10	A	1005	1N7	O1-C24-C23	-3.06	116.47	122.02
10	A	1005	1N7	C23-C22-C20	3.06	120.17	114.46
10	E	707	1N7	C3-C19-C2	-3.02	110.64	113.70
10	A	1005	1N7	C10-C5-C4	2.99	112.05	109.06
10	A	1006	1N7	C6-C5-C4	2.97	110.13	107.42
10	E	707	1N7	C1-C2-C15	2.95	111.98	107.75
10	A	1006	1N7	C1-C2-C15	2.94	111.96	107.75
10	E	707	1N7	C27-C26-C25	2.90	116.63	110.95
10	A	1005	1N7	C1-C12-C13	2.87	114.29	110.48
10	A	1005	1N7	C15-C16-C17	2.87	117.81	114.40
10	E	707	1N7	C10-C5-C4	2.80	111.86	109.06
10	A	1006	1N7	C1-C12-C13	2.79	114.18	110.48
10	E	707	1N7	O1-C24-C23	-2.78	116.98	122.02
10	E	707	1N7	C1-C12-C13	2.76	114.14	110.48
10	A	1006	1N7	C5-C9-C20	-2.73	116.18	119.48
10	E	707	1N7	C7-C8-C9	2.71	110.44	105.14
10	E	707	1N7	C30-N2-C28	-2.69	101.91	108.98
10	A	1005	1N7	C19-C3-C4	2.64	117.74	114.29
10	A	1006	1N7	C10-C5-C4	2.60	111.66	109.06
10	A	1005	1N7	C3-C19-C2	-2.56	111.11	113.70
10	A	1005	1N7	C10-C5-C9	-2.51	107.27	111.20
10	E	707	1N7	C19-C2-C15	2.49	111.97	108.51
10	A	1005	1N7	O1-C24-N1	-2.46	118.19	123.03
9	E	704	ADP	C4-N9-C8	2.46	108.32	105.74
10	E	707	1N7	C11-C2-C19	-2.43	107.91	111.18
9	F	1003	ADP	C4-N9-C8	2.43	108.29	105.74
10	A	1005	1N7	C15-C14-C13	2.43	116.37	112.71
9	F	1003	ADP	C3'-C2'-C1'	2.42	106.03	101.46
10	A	1006	1N7	C19-C3-C4	2.42	117.46	114.29
9	E	704	ADP	C3'-C2'-C1'	2.42	106.03	101.46
9	A	1004	ADP	C5-N7-C8	2.40	107.22	103.45
10	A	1006	1N7	C7-C8-C9	2.39	109.82	105.14
9	F	1003	ADP	C5-N7-C8	2.37	107.17	103.45
9	E	704	ADP	C5-N7-C8	2.32	107.09	103.45
9	A	1004	ADP	C4-N9-C8	2.32	108.17	105.74
10	A	1006	1N7	C10-C5-C9	-2.28	107.63	111.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E	707	1N7	C8-C9-C20	2.25	115.59	112.18
10	A	1005	1N7	C25-N1-C24	2.24	127.00	122.82
10	E	707	1N7	C15-C14-C13	2.19	116.02	112.71
10	A	1006	1N7	C3-C19-C2	-2.16	111.51	113.70
10	E	707	1N7	O1-C24-N1	-2.14	118.84	123.03
10	E	707	1N7	C19-C18-C17	-2.13	109.17	111.86
10	A	1006	1N7	C8-C9-C20	2.13	115.40	112.18
10	E	707	1N7	C26-C27-N2	-2.12	108.18	115.97
10	E	707	1N7	C10-C5-C9	-2.10	107.91	111.20
10	E	707	1N7	C23-C22-C20	2.10	118.39	114.46
10	A	1006	1N7	C15-C14-C13	2.02	115.76	112.71
10	A	1006	1N7	O3-C17-C16	-2.02	104.84	109.86
9	A	1004	ADP	O2A-PA-O1A	2.01	121.78	112.44

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	A	1005	1N7	C6
10	A	1005	1N7	C18

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1004	ADP	PA-O3A-PB-O3B
9	A	1004	ADP	C5'-O5'-PA-O3A
10	A	1005	1N7	C21-C20-C9-C5
10	A	1005	1N7	C22-C20-C9-C5
10	A	1005	1N7	C22-C20-C9-C8
10	A	1005	1N7	C21-C20-C9-C8
10	E	707	1N7	C21-C20-C22-C23
10	A	1006	1N7	C22-C20-C9-C5
10	E	707	1N7	C9-C20-C22-C23
10	A	1006	1N7	C21-C20-C9-C5
10	E	707	1N7	C22-C20-C9-C5
10	E	707	1N7	C21-C20-C9-C5
10	A	1005	1N7	C20-C22-C23-C24
10	E	707	1N7	N1-C25-C26-C27
10	A	1005	1N7	C9-C20-C22-C23
10	A	1006	1N7	C21-C20-C9-C8
9	A	1004	ADP	C2'-C1'-N9-C8
10	A	1005	1N7	C22-C23-C24-O1
10	A	1005	1N7	C22-C23-C24-N1

Continued on next page...

Continued from previous page...

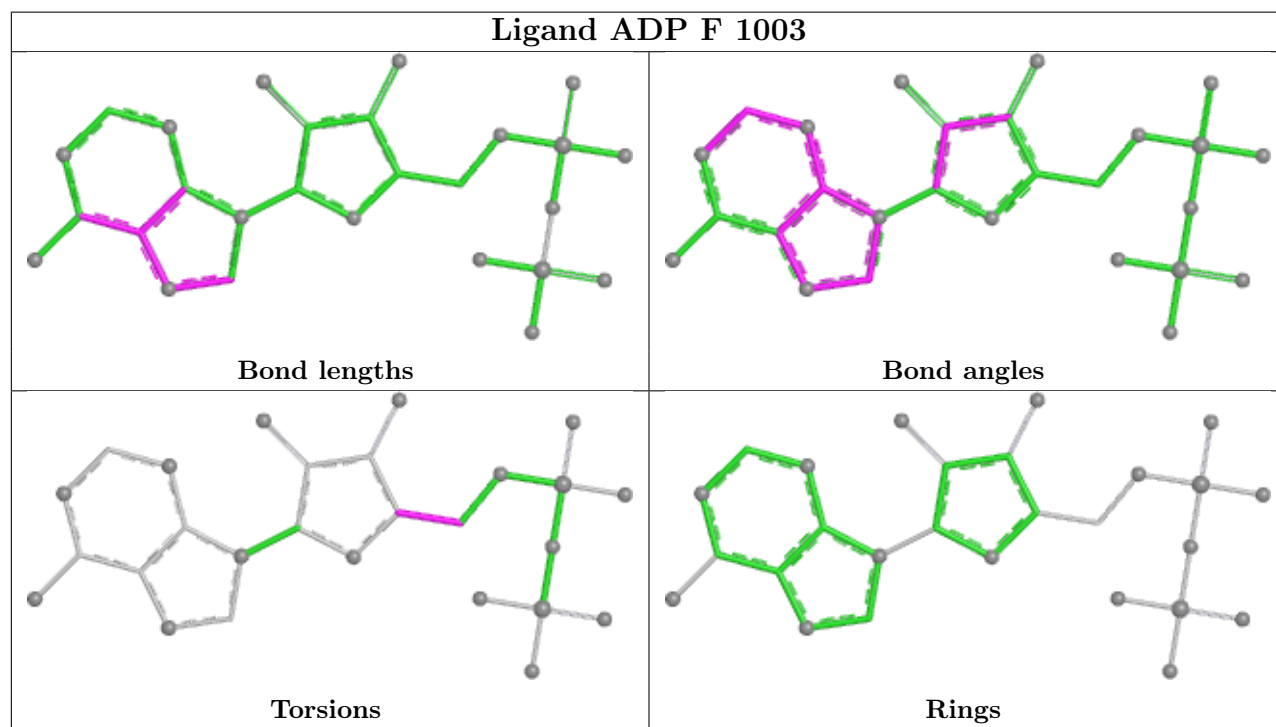
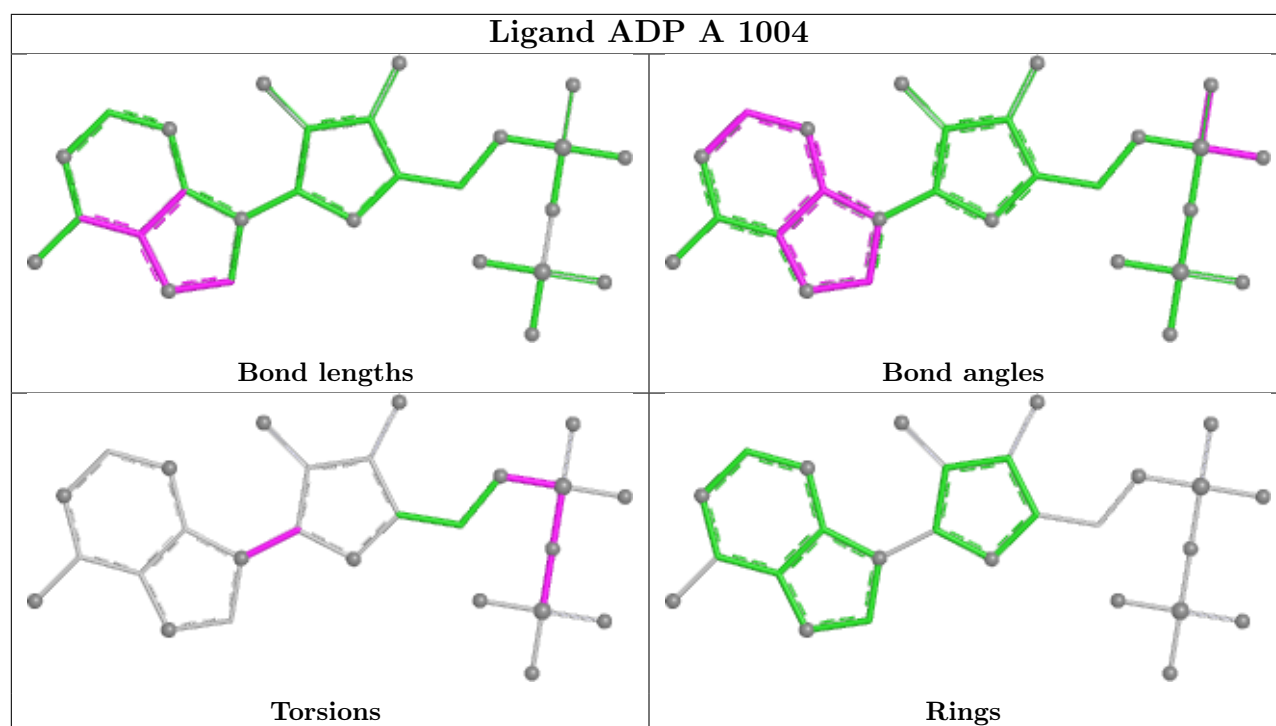
Mol	Chain	Res	Type	Atoms
10	A	1006	1N7	C22-C20-C9-C8
10	A	1005	1N7	C26-C27-N2-C28
10	A	1006	1N7	C9-C20-C22-C23
9	A	1004	ADP	C5'-O5'-PA-O1A
9	A	1004	ADP	C2'-C1'-N9-C4
9	E	704	ADP	O4'-C4'-C5'-O5'
9	F	1003	ADP	O4'-C4'-C5'-O5'
10	E	707	1N7	C22-C20-C9-C8
10	A	1006	1N7	C21-C20-C22-C23
9	A	1004	ADP	PB-O3A-PA-O1A
9	A	1004	ADP	O4'-C1'-N9-C8
9	A	1004	ADP	PB-O3A-PA-O2A

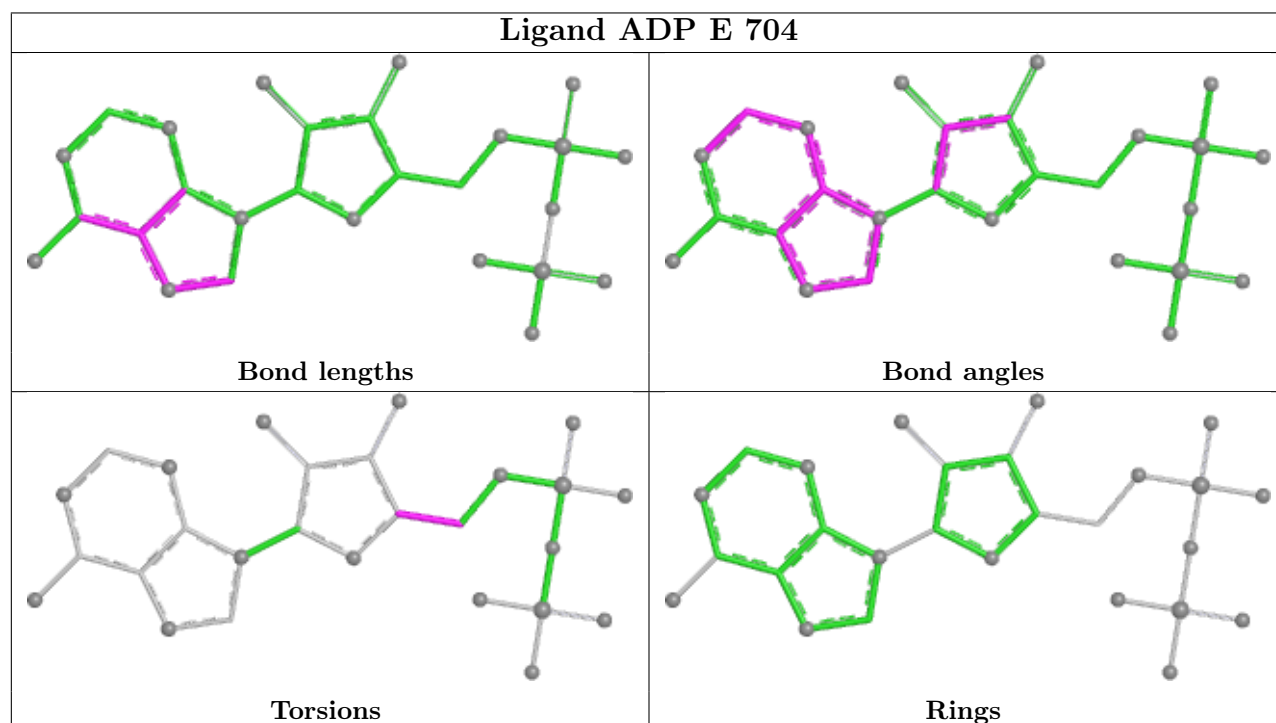
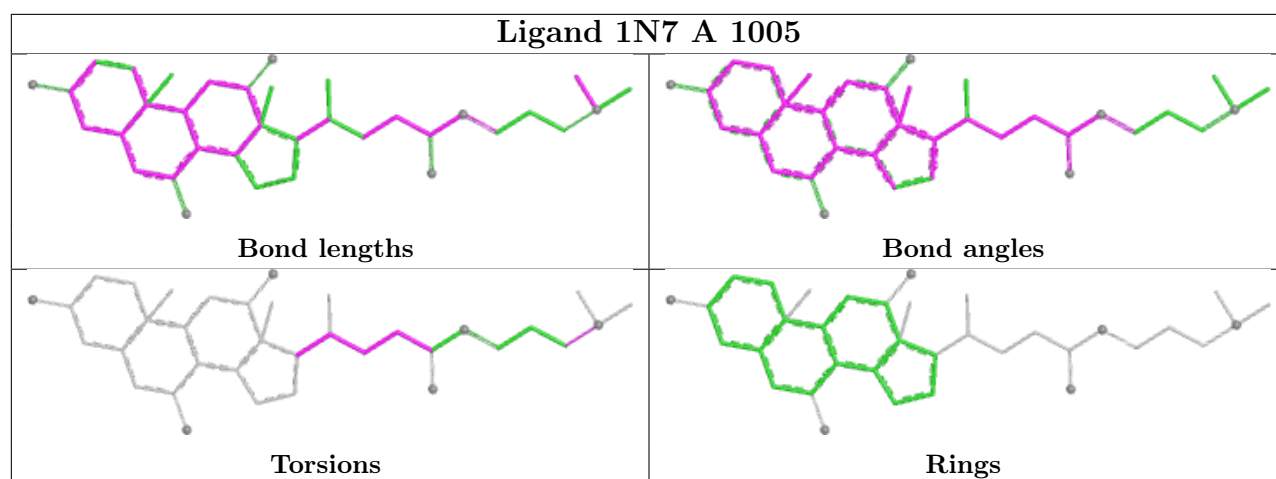
There are no ring outliers.

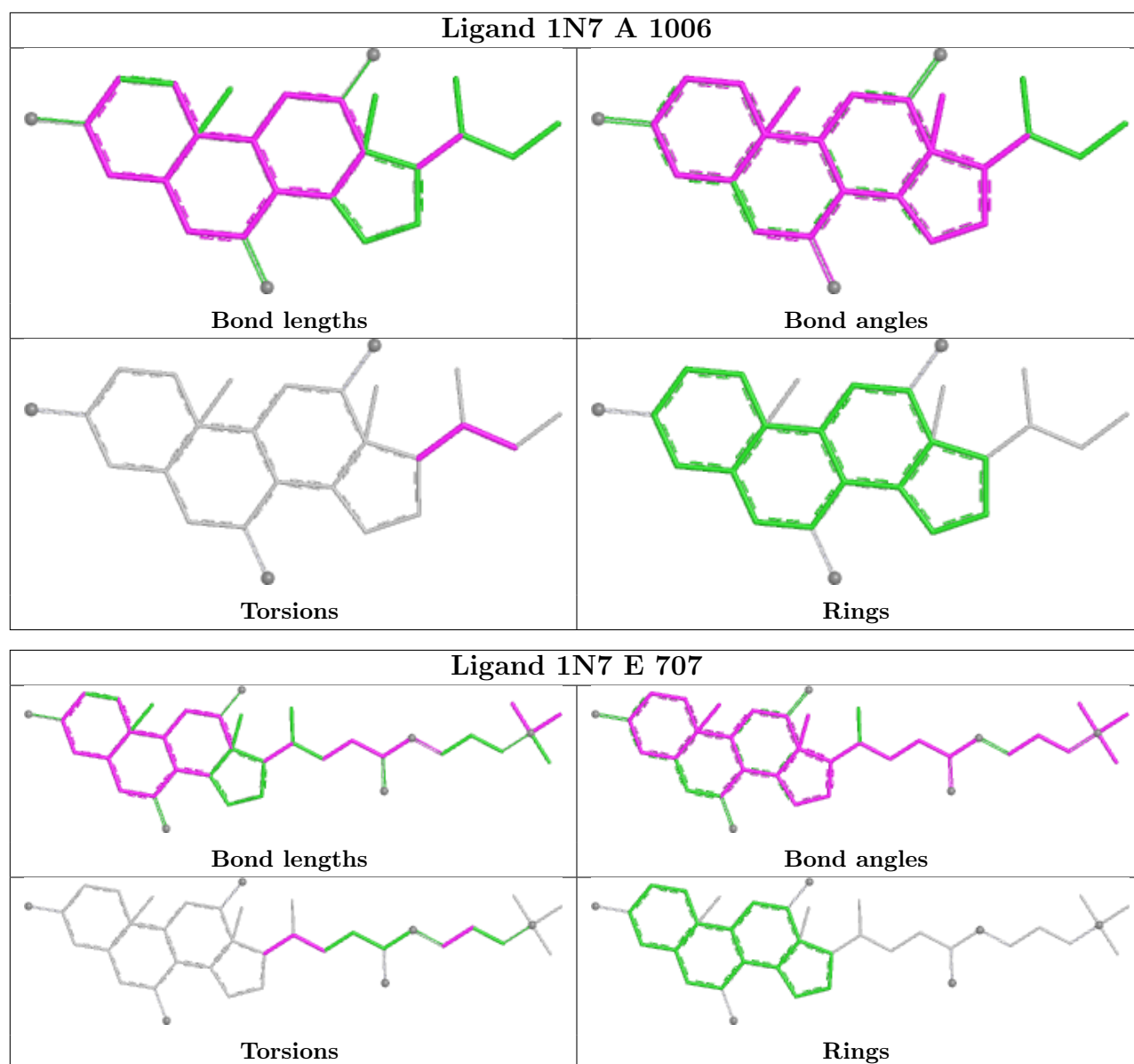
8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1004	ADP	1	0
9	F	1003	ADP	2	0
10	A	1005	1N7	1	0
9	E	704	ADP	2	0
10	A	1006	1N7	1	0
10	E	707	1N7	3	0
11	F	1005	AF3	2	0
11	E	706	AF3	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.

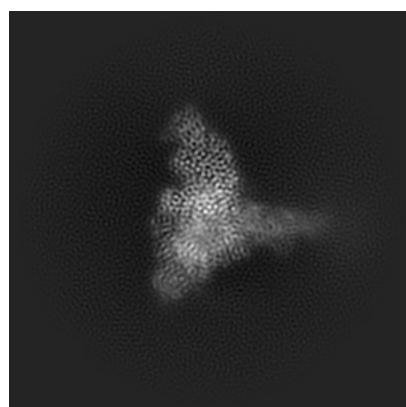
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23008. These allow visual inspection of the internal detail of the map and identification of artifacts.

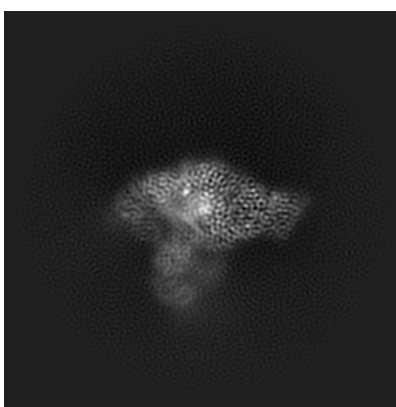
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

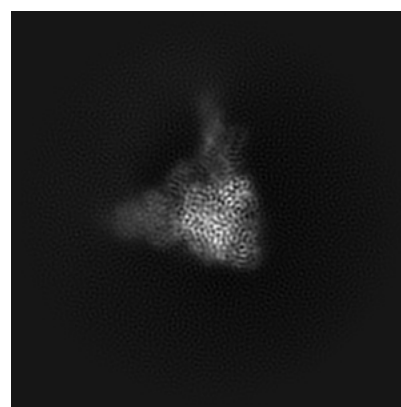
6.1.1 Primary map



X



Y

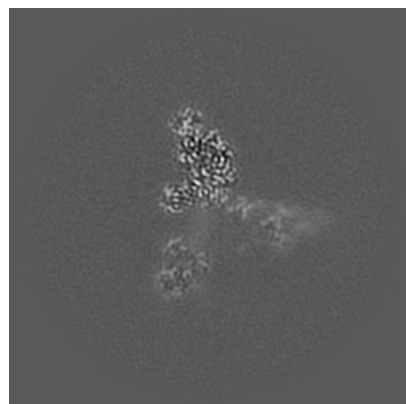


Z

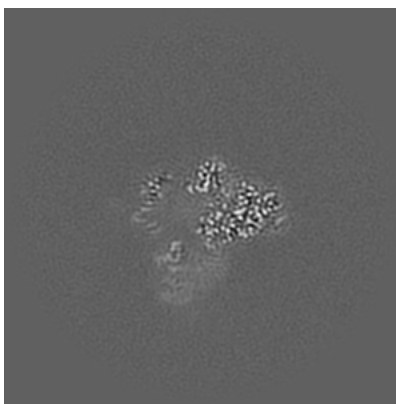
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

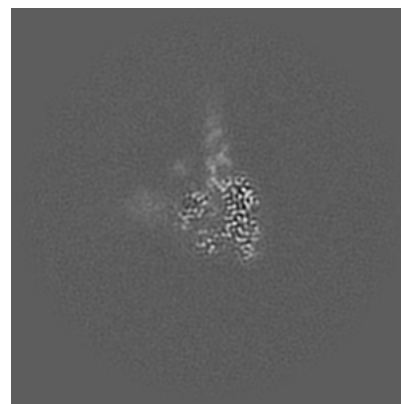
6.2.1 Primary map



X Index: 160



Y Index: 160

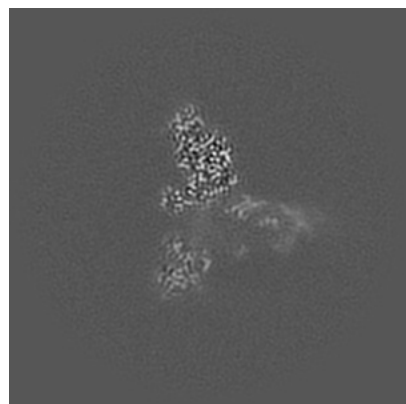


Z Index: 160

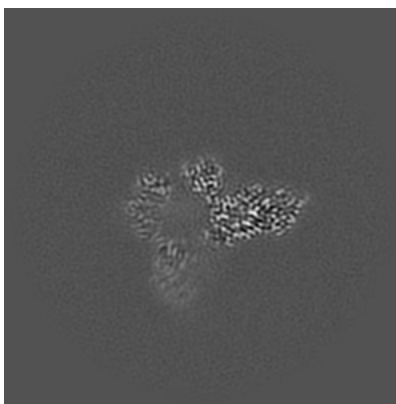
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

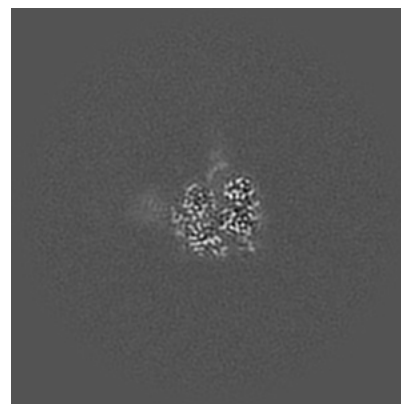
6.3.1 Primary map



X Index: 163



Y Index: 147

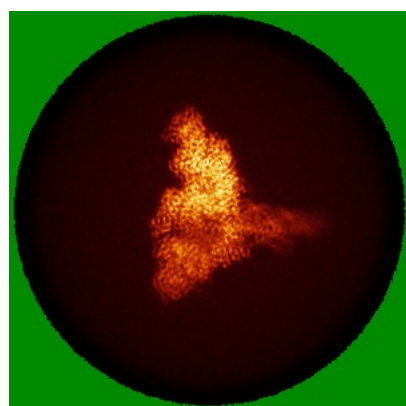


Z Index: 166

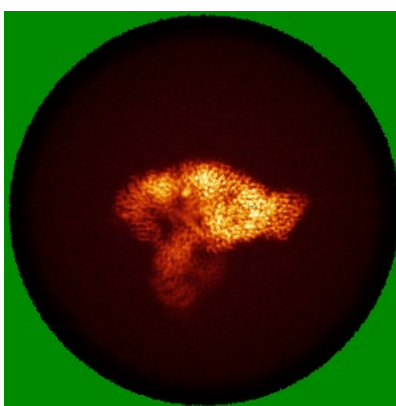
The images above show the largest variance slices of the map in three orthogonal directions.

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

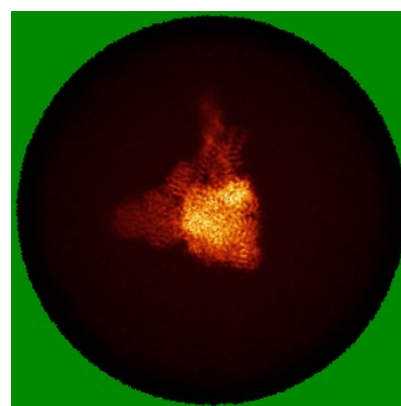
6.4.1 Primary map



X



Y

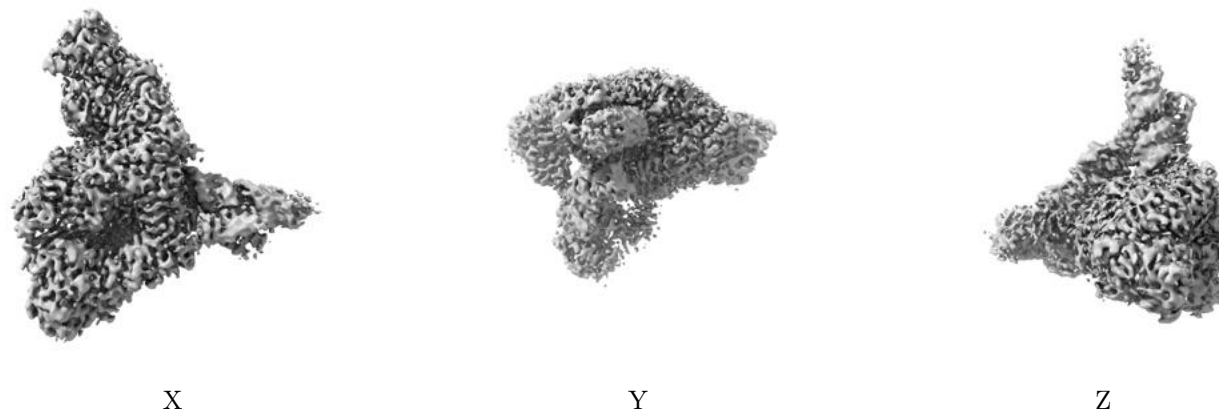


Z

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

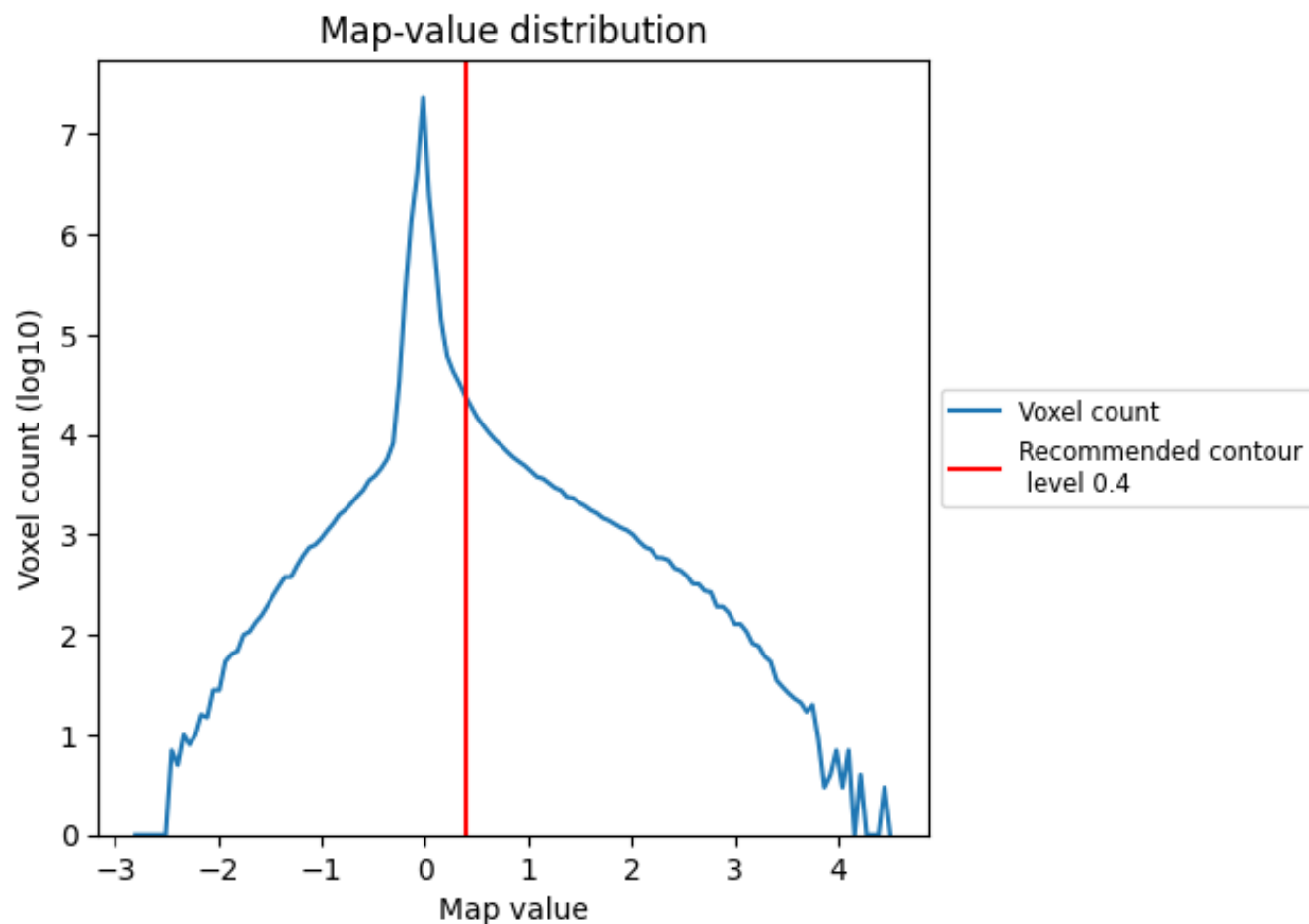
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

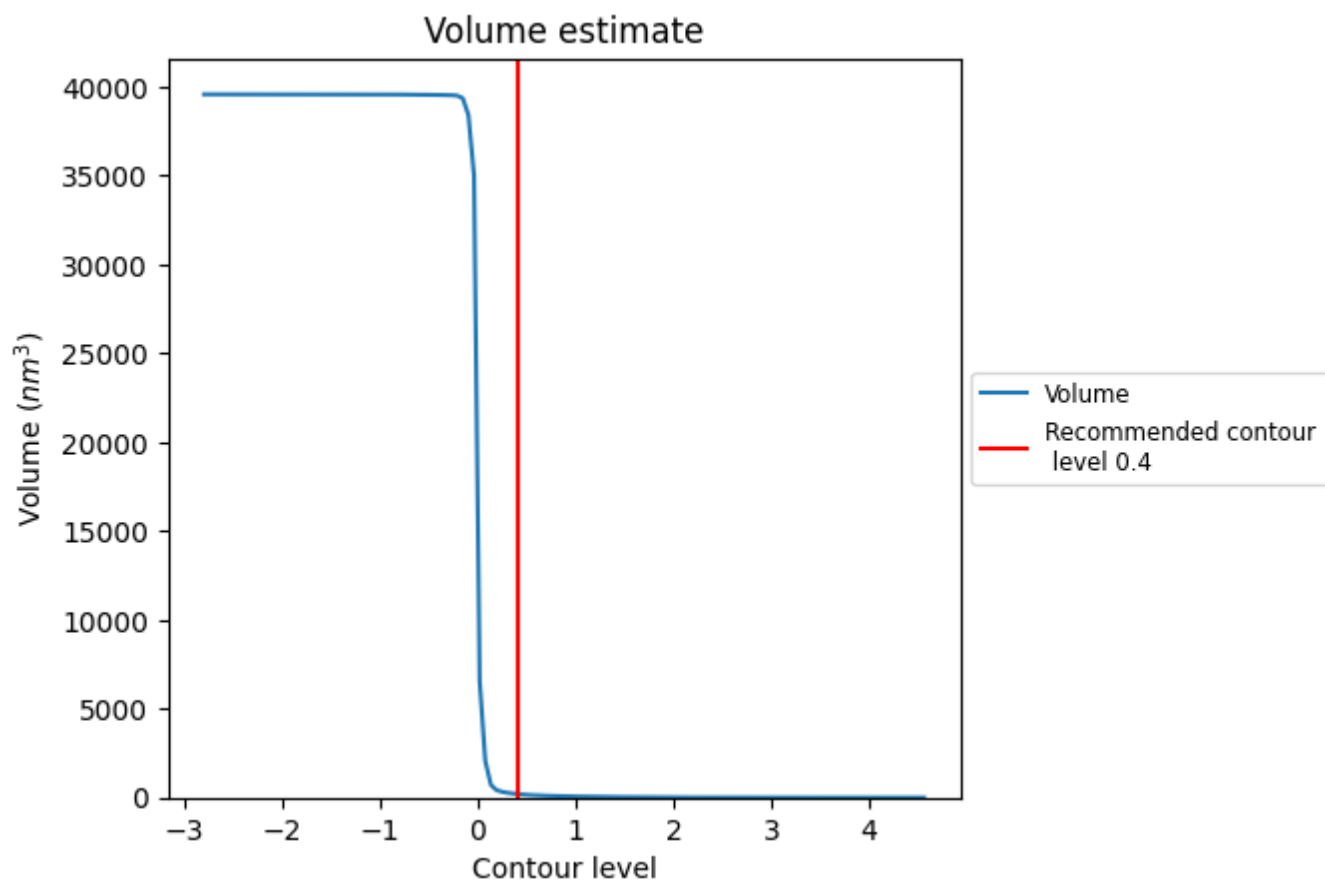
This section contains the results of statistical analysis of the map.

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.

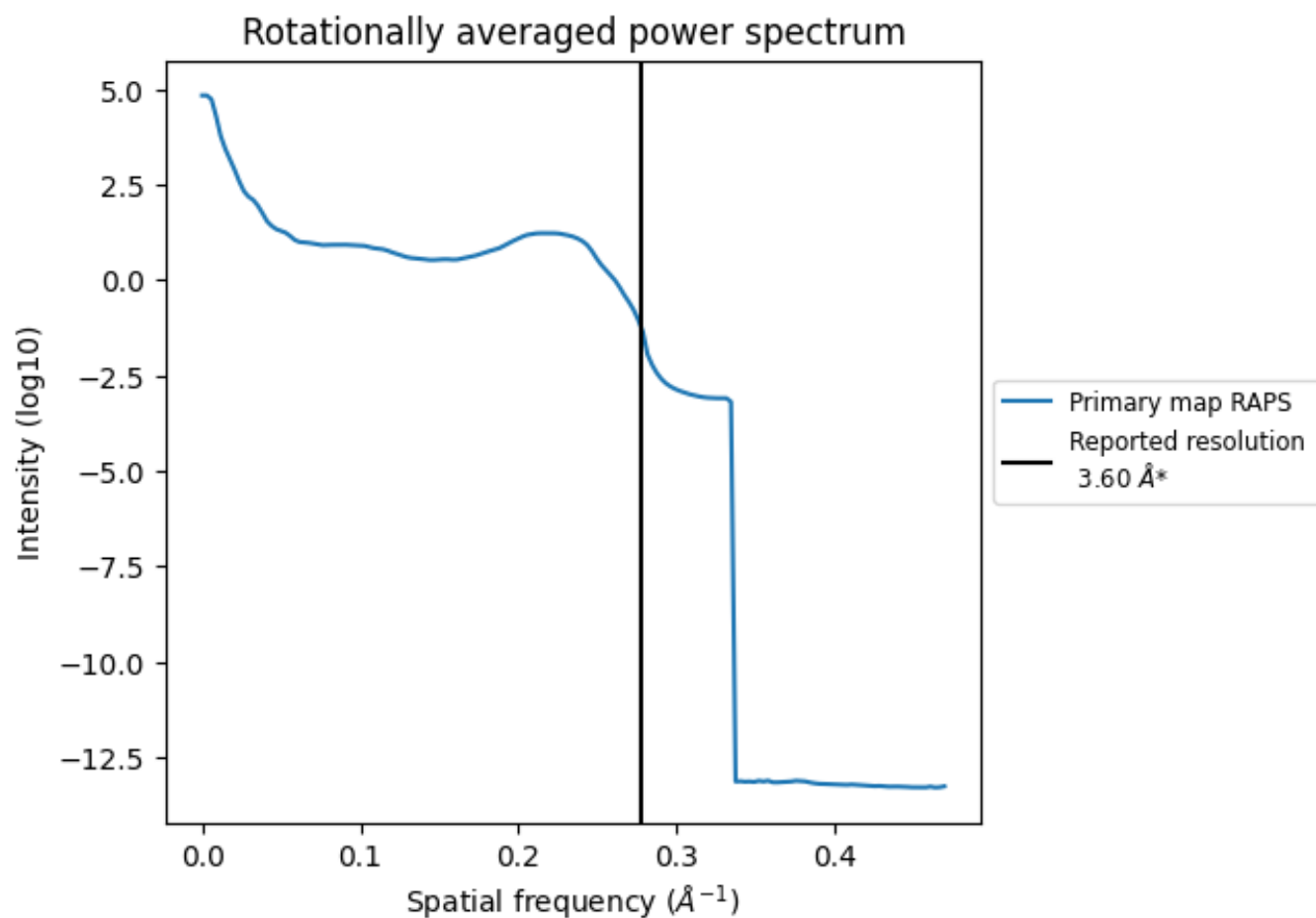
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 199 nm³; this corresponds to an approximate mass of 180 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 ⓘ

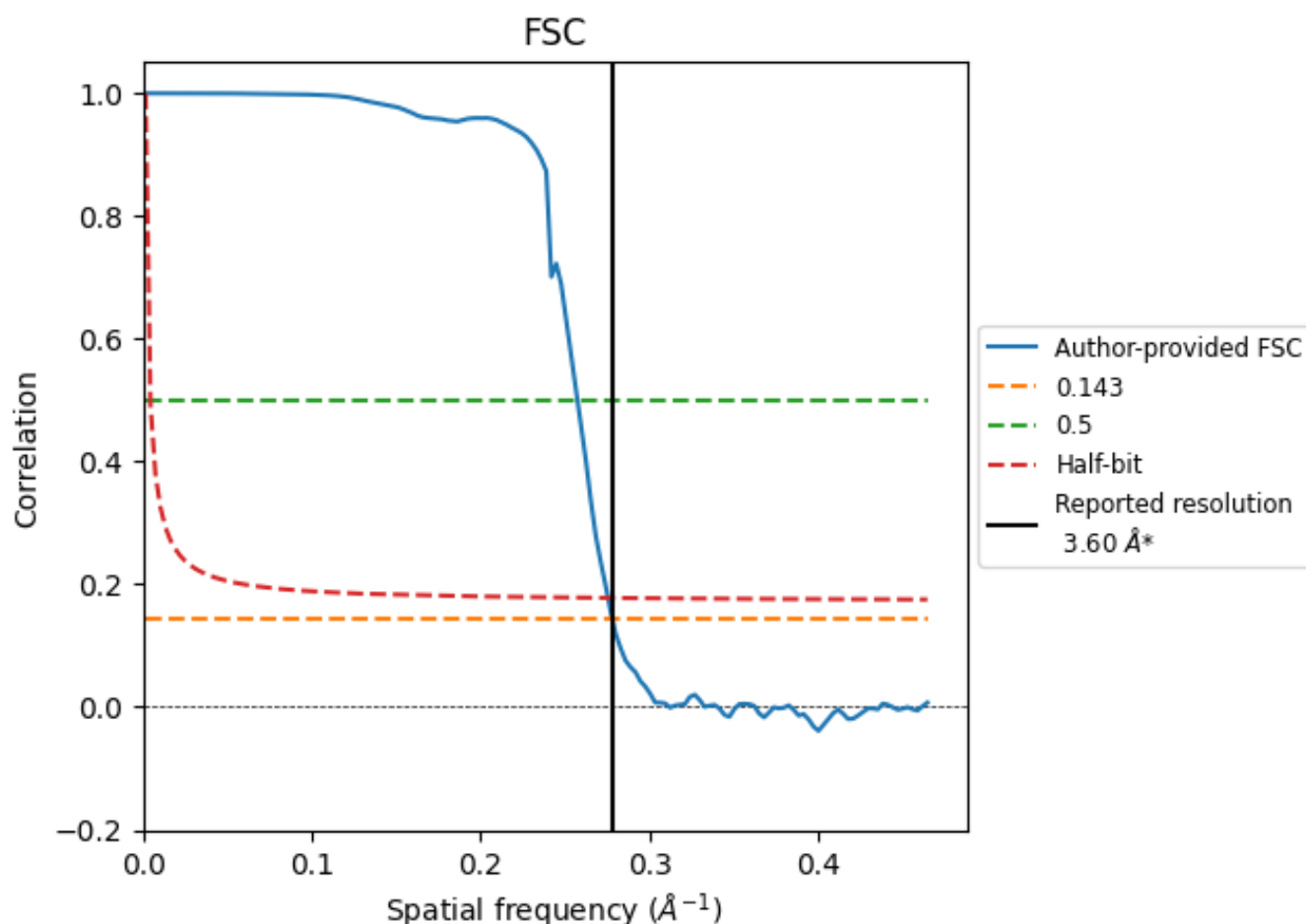


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

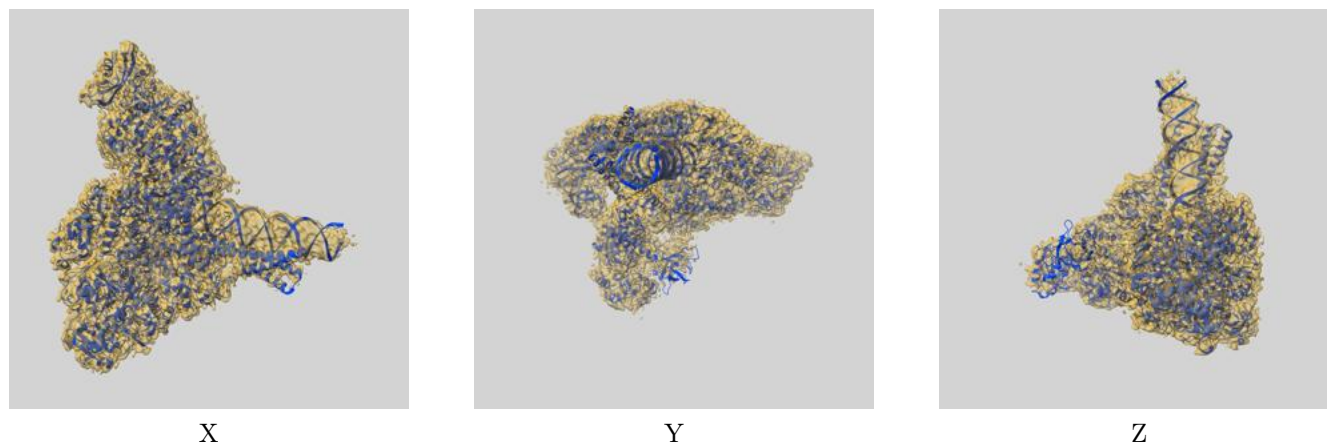
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.59	3.88	3.63
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

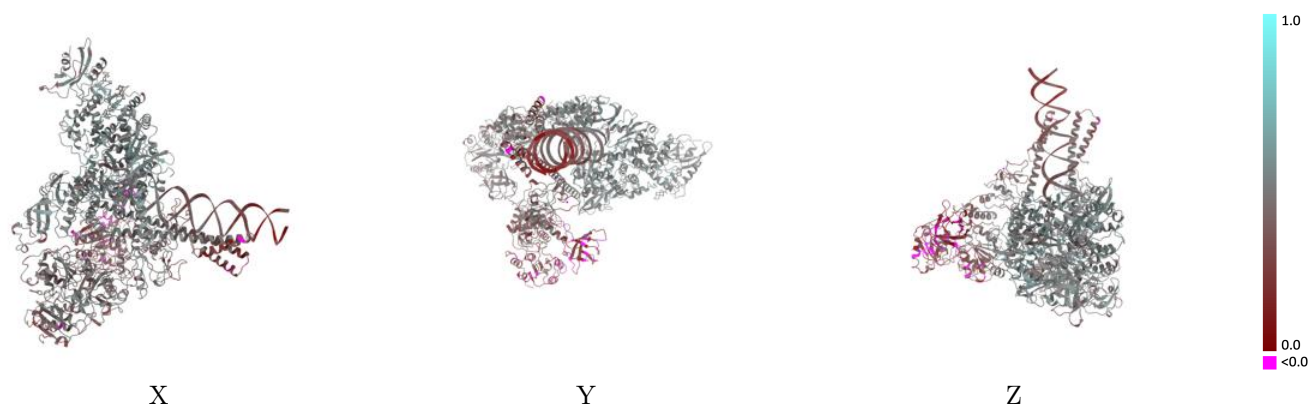
This section contains information regarding the fit between EMDB map EMD-23008 and PDB model 7KRO. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



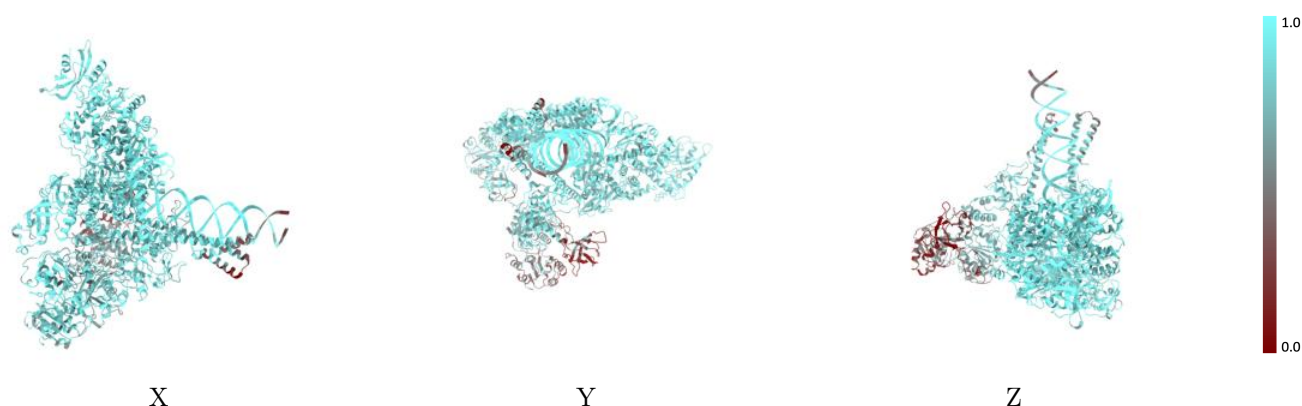
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



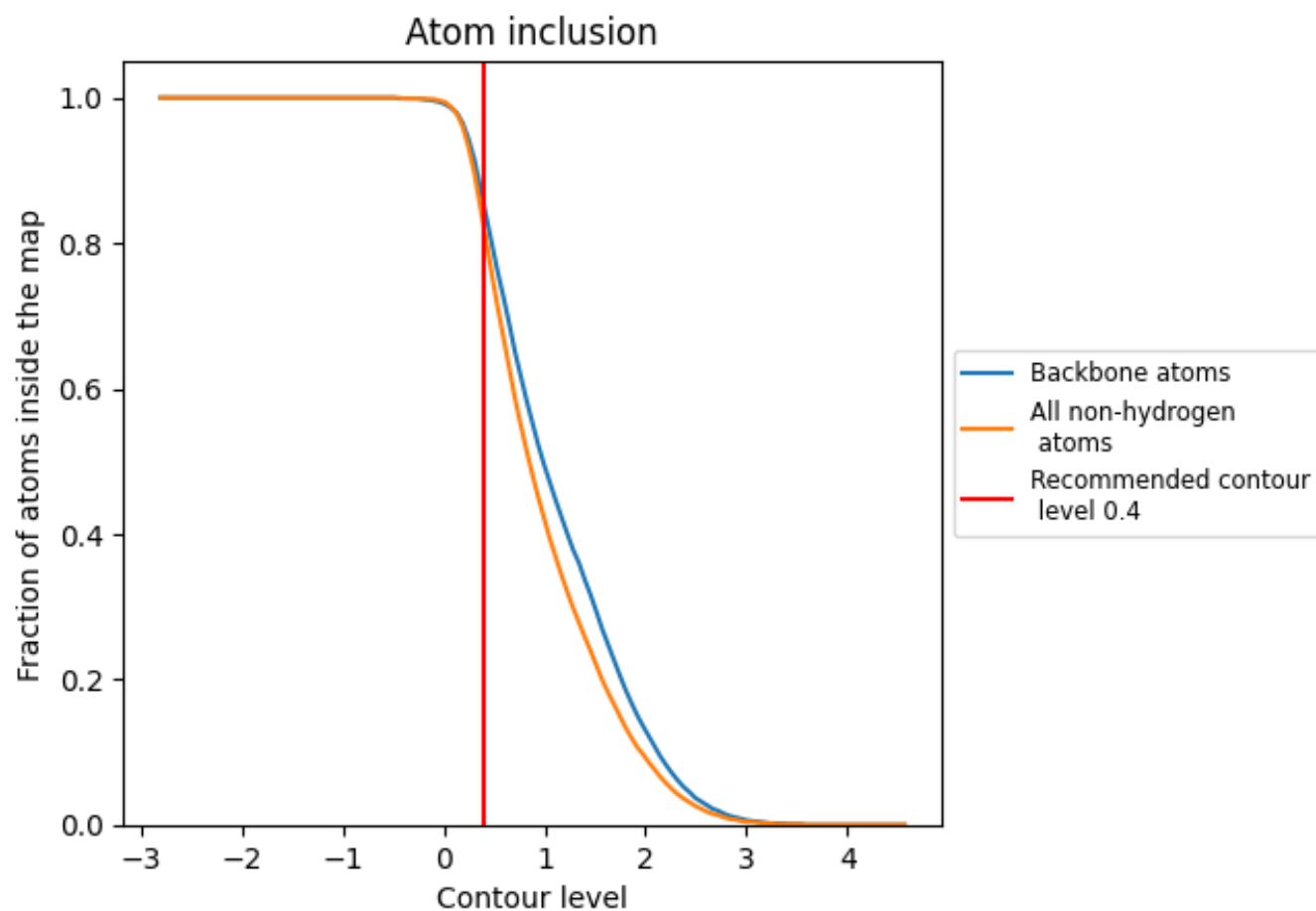
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 82% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8220	0.4160
A	0.9370	0.5130
B	0.8620	0.4400
C	0.9020	0.4950
D	0.8800	0.4520
E	0.8350	0.4330
F	0.5570	0.2410
P	0.8900	0.3350
T	0.8860	0.3490

1.0

0.0

<0.0