



Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 05:46 pm GMT

PDB ID : 7AQR
EMDB ID : EMD-11873
Title : Cryo-EM structure of Arabidopsis thaliana Complex-I (peripheral arm)
Authors : Klusch, N.; Kuehlbrandt, W.; Yildiz, O.
Deposited on : 2020-10-22
Resolution : 2.91 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.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

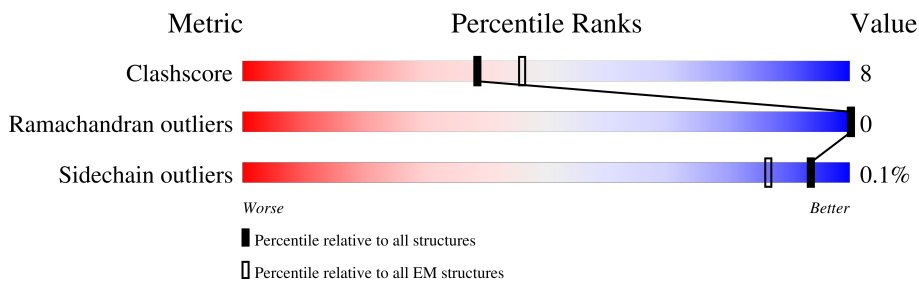
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.91 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	218	
2	C	190	
3	D	394	
4	E	255	
5	F	486	
6	G	748	
7	I	222	
8	P	402	

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Mol	Chain	Length	Quality of chain
9	Q	154	
10	R	110	
11	S	97	
12	U	126	
13	V	169	
14	W	133	
15	Z	143	
16	q	159	
17	r	131	

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
18	SF4	F	501	-	-	X	-

2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 25751 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 NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	157	1244	797	218	215	14	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	185	1581	1021	271	283	6	0	0

- Molecule 3 is a protein called NADH dehydrogenase subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	385	3077	1954	542	557	24	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	363	SER	LEU	variant	UNP A0A2P2CLH2

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	192	1500	954	248	287	11	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	434	3368	2125	600	618	25	0	0

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	688	5252	3291	921	1001	39	0	0

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8-A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I	165	1349	849	229	261	10	0	0

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	P	332	2560	1643	439	463	15	0	0

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	Q	119	939	600	163	175	1	0	0

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	R	62	482	304	84	89	5	0	0

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	S	93	727	459	129	133	6	0	0

- Molecule 12 is a protein called Acyl carrier protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	U	83	650	411	103	135	1	0	0

- Molecule 13 is a protein called Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	V	140	1123	712	187	219	5	0	0

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	W	112	904	578	161	162	3	0	0

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	Z	27	199	126	38	35	0	0

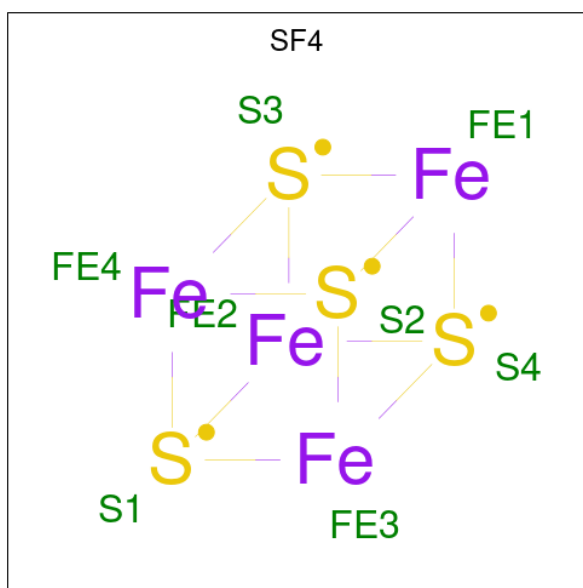
- Molecule 16 is a protein called Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	q	65	536	342	95	99	0	0

- Molecule 17 is a protein called Furry.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	r	10	89	56	18	15	0	0

- Molecule 18 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



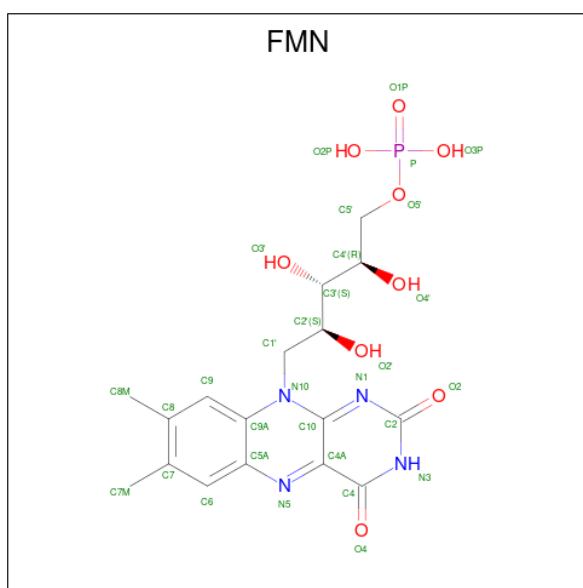
Mol	Chain	Residues	Atoms			AltConf
18	B	1	Total	Fe	S	0
			8	4	4	
18	F	1	Total	Fe	S	0
			8	4	4	
18	G	1	Total	Fe	S	0
			16	8	8	
18	G	1	Total	Fe	S	0
			16	8	8	
18	I	1	Total	Fe	S	0
			16	8	8	
18	I	1	Total	Fe	S	0
			16	8	8	

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
19	E	1	Total	Fe	S	0
			4	2	2	
19	G	1	Total	Fe	S	0
			4	2	2	

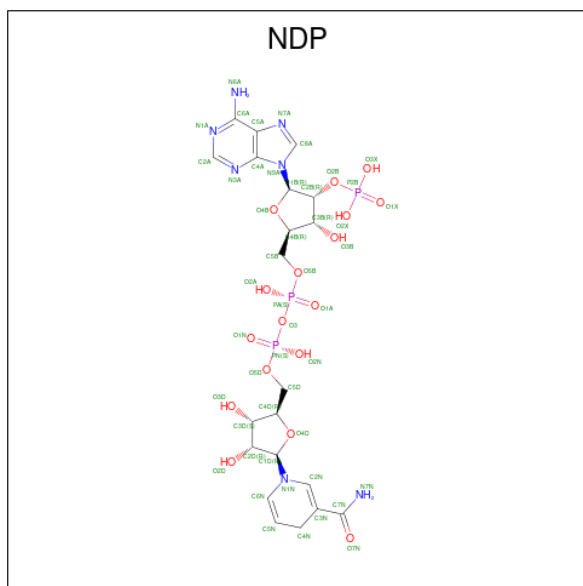
- Molecule 20 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



Mol	Chain	Residues	Atoms				AltConf	
20	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 21 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE

PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

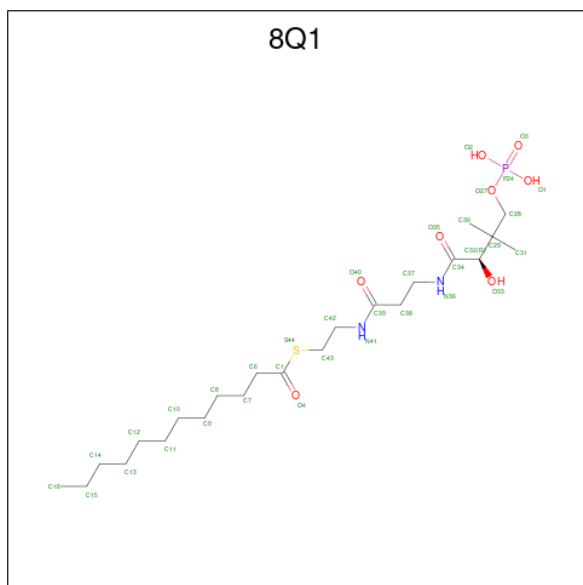


Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
21	P	1	48	21	7	17	3	0

- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
22	R	1	1	1	0

- Molecule 23 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$).

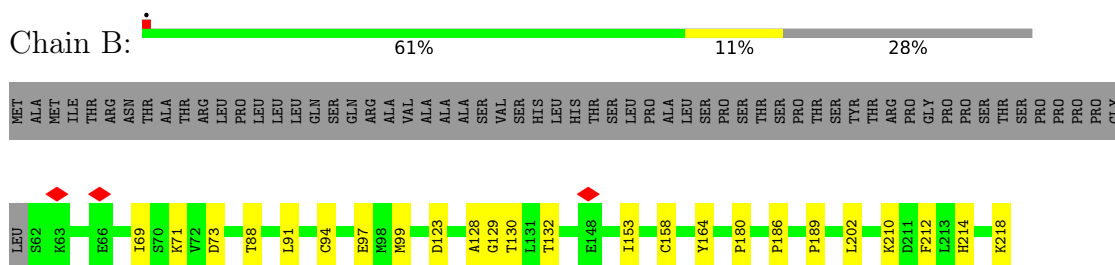


Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
23	W	1	35	23	2	8	1	1	0

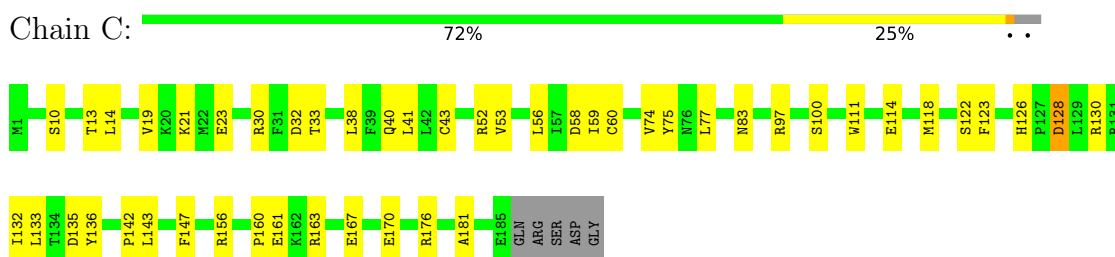
3 Residue-property plots [i](#)

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

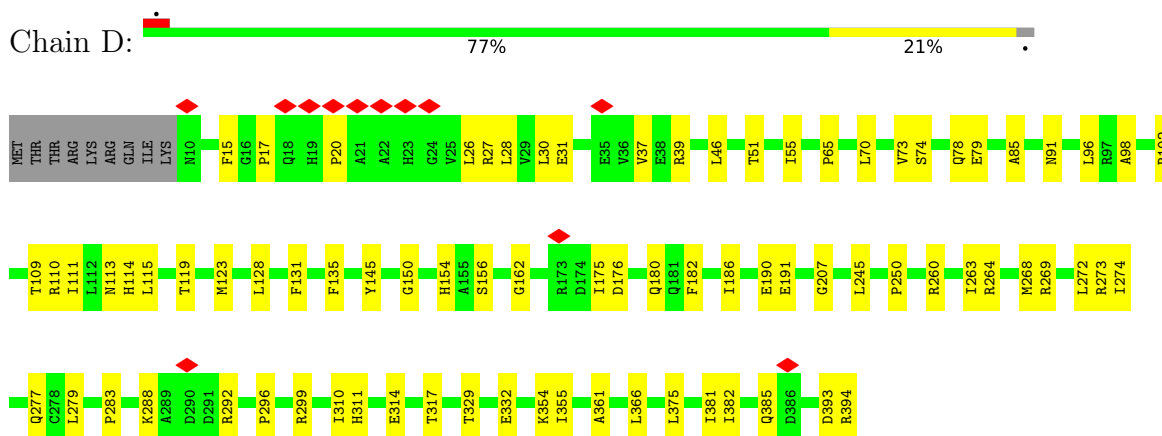
- Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



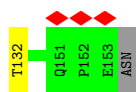
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3



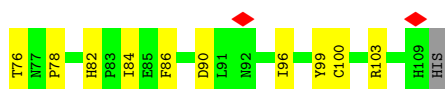
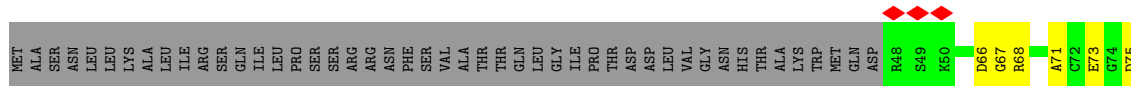
- Molecule 3: NADH dehydrogenase subunit 7



- Molecule 4: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



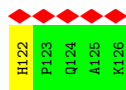
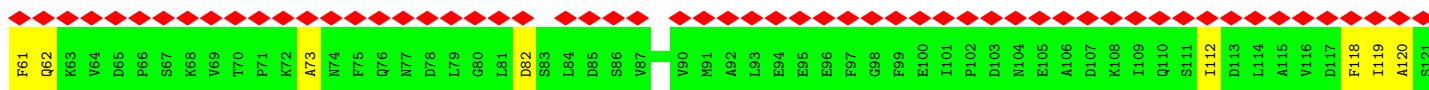
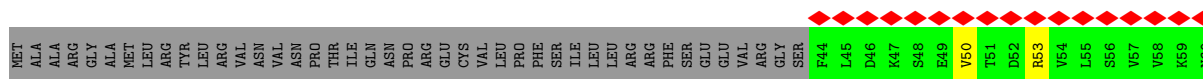
- Molecule 10: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



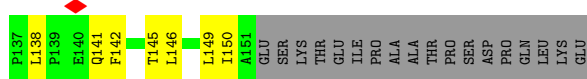
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 12: Acyl carrier protein 2, mitochondrial



- Molecule 13: Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5, mitochondrial



- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	459177	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 ($e^-/\text{\AA}^2$)	43	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	0.083	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	502.2, 502.2, 502.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, FES, ZN, SF4, 8Q1, FMN

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	B	0.26	0/1279	0.48	0/1734
2	C	0.26	0/1629	0.52	1/2207 (0.0%)
3	D	0.26	0/3147	0.51	0/4256
4	E	0.25	0/1535	0.48	0/2084
5	F	0.26	0/3441	0.49	0/4641
6	G	0.26	0/5347	0.49	0/7242
7	I	0.26	0/1378	0.50	0/1862
8	P	0.26	0/2617	0.49	0/3544
9	Q	0.26	0/966	0.46	0/1305
10	R	0.26	0/493	0.43	0/668
11	S	0.26	0/739	0.51	0/996
12	U	0.24	0/660	0.42	0/892
13	V	0.25	0/1146	0.48	0/1555
14	W	0.25	0/923	0.46	0/1249
15	Z	0.25	0/206	0.53	0/281
16	q	0.24	0/553	0.47	0/750
17	r	0.23	0/89	0.60	0/118
All	All	0.26	0/26148	0.49	1/35384 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	128	ASP	CB-CG-OD2	5.80	123.53	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	B	1244	0	1231	18	0
2	C	1581	0	1529	38	0
3	D	3077	0	3043	58	0
4	E	1500	0	1472	37	0
5	F	3368	0	3352	53	0
6	G	5252	0	5241	94	0
7	I	1349	0	1293	16	0
8	P	2560	0	2605	50	0
9	Q	939	0	928	8	0
10	R	482	0	478	9	0
11	S	727	0	759	12	0
12	U	650	0	635	8	0
13	V	1123	0	1112	21	0
14	W	904	0	901	19	0
15	Z	199	0	198	3	0
16	q	536	0	495	0	0
17	r	89	0	95	0	0
18	B	8	0	0	0	0
18	F	8	0	0	2	0
18	G	16	0	0	0	0
18	I	16	0	0	0	0
19	E	4	0	0	1	0
19	G	4	0	0	0	0
20	F	31	0	19	3	0
21	P	48	0	26	0	0
22	R	1	0	0	0	0
23	W	35	0	0	1	0
All	All	25751	0	25412	391	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 8.

All (391) 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)
6:G:658:ARG:NH1	6:G:662:GLU:HG3	1.66	1.11
6:G:658:ARG:HH12	6:G:662:GLU:CG	1.72	1.02
6:G:658:ARG:NH1	6:G:662:GLU:CG	2.25	1.00
6:G:658:ARG:HH12	6:G:662:GLU:HG2	1.34	0.93
6:G:176:GLY:O	6:G:182:GLN:NE2	2.10	0.84
2:C:60:CYS:HB3	3:D:354:LYS:HD2	1.63	0.80
2:C:170:GLU:HG2	8:P:64:SER:HB3	1.63	0.79
2:C:21:LYS:HB3	2:C:32:ASP:HB3	1.65	0.77
4:E:180:MET:HG2	4:E:199:GLU:HA	1.66	0.77
2:C:23:GLU:OE1	2:C:30:ARG:NH2	2.17	0.76
4:E:128:LEU:HB2	4:E:182:THR:HB	1.66	0.76
4:E:132:THR:O	5:F:392:ARG:NH2	2.21	0.74
4:E:136:MET:HB3	5:F:392:ARG:NH1	2.05	0.72
14:W:34:CYS:HB3	14:W:56:ARG:HH21	1.54	0.72
11:S:13:GLU:OE1	11:S:15:ARG:NH1	2.23	0.71
6:G:409:TRP:HB2	6:G:414:ALA:HB1	1.71	0.70
8:P:249:GLY:HA2	8:P:290:THR:HB	1.74	0.69
4:E:136:MET:HB3	5:F:392:ARG:HH12	1.58	0.69
5:F:350:ILE:HG23	5:F:354:ILE:HG13	1.75	0.69
2:C:33:THR:HG21	2:C:41:LEU:HD22	1.76	0.68
2:C:135:ASP:OD1	2:C:136:TYR:N	2.26	0.68
13:V:63:GLN:OE1	13:V:141:GLN:NE2	2.20	0.68
6:G:658:ARG:HH11	6:G:662:GLU:HG3	1.57	0.68
8:P:58:LYS:HB3	8:P:66:VAL:HB	1.74	0.68
6:G:556:TYR:HB2	6:G:559:GLN:HG3	1.75	0.68
5:F:181:ILE:HD11	5:F:192:LEU:HD23	1.77	0.67
2:C:132:ILE:HG23	2:C:133:LEU:HG	1.76	0.67
6:G:658:ARG:NE	6:G:668:LEU:HB2	2.09	0.67
5:F:240:GLU:OE1	5:F:247:ARG:NH2	2.27	0.67
3:D:74:SER:O	3:D:78:GLN:NE2	2.27	0.66
5:F:334:TRP:NE1	5:F:356:GLU:OE2	2.27	0.66
12:U:73:ALA:H	12:U:112:ILE:HG22	1.60	0.66
5:F:385:ASP:OD1	5:F:472:ARG:NH2	2.28	0.66
6:G:299:VAL:O	6:G:632:ASN:ND2	2.29	0.65
3:D:109:THR:OG1	3:D:145:TYR:OH	2.14	0.65
8:P:218:ARG:NH2	8:P:281:GLU:OE2	2.30	0.65
4:E:132:THR:HG22	4:E:133:THR:H	1.61	0.64
2:C:161:GLU:HG3	2:C:163:ARG:HG2	1.79	0.64
6:G:429:THR:OG1	6:G:548:ASN:O	2.16	0.64
11:S:74:LEU:HD22	11:S:82:ILE:HG12	1.79	0.64
3:D:26:LEU:HD21	3:D:382:ILE:HD13	1.80	0.63
6:G:317:PRO:HG3	6:G:328:ILE:HG12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:603:GLN:HE21	6:G:656:ILE:HD12	1.64	0.62
1:B:88:THR:HG23	3:D:20:PRO:HD2	1.80	0.62
4:E:128:LEU:HB3	4:E:169:MET:HB3	1.81	0.62
3:D:190:GLU:OE1	15:Z:37:ARG:NH1	2.31	0.62
2:C:19:VAL:HA	2:C:33:THR:HG22	1.81	0.62
14:W:21:GLU:OE1	14:W:24:ARG:NH2	2.29	0.62
11:S:19:CYS:O	11:S:29:ARG:NH1	2.33	0.61
3:D:110:ARG:NH2	3:D:332:GLU:O	2.28	0.61
8:P:298:TYR:HA	8:P:301:ILE:HG22	1.82	0.61
2:C:114:GLU:OE1	3:D:394:ARG:NH2	2.33	0.61
6:G:338:GLY:O	6:G:606:HIS:NE2	2.32	0.61
4:E:136:MET:HA	4:E:140:SER:H	1.66	0.61
6:G:292:THR:HG22	6:G:293:ILE:H	1.66	0.60
6:G:345:SER:HB2	6:G:648:GLY:HA3	1.83	0.60
3:D:96:LEU:HD23	3:D:283:PRO:HG3	1.84	0.60
10:R:82:HIS:CD2	10:R:100:CYS:SG	2.93	0.60
5:F:293:ASN:HD21	5:F:361:ASP:HB3	1.67	0.60
5:F:402:CYS:HA	6:G:242:ARG:HG3	1.83	0.60
6:G:108:HIS:HD2	6:G:223:ARG:HH21	1.49	0.60
13:V:146:LEU:O	13:V:150:ILE:HG12	2.01	0.60
3:D:299:ARG:NH2	7:I:175:ASP:OD1	2.34	0.60
5:F:343:GLY:H	5:F:347:VAL:HG21	1.65	0.60
6:G:629:THR:HG22	6:G:639:GLN:HG2	1.84	0.60
7:I:189:THR:HB	7:I:192:GLU:HG3	1.84	0.59
4:E:78:ASP:O	4:E:82:GLN:HG3	2.02	0.59
10:R:96:ILE:HG12	10:R:103:ARG:HG2	1.84	0.59
2:C:128:ASP:OD1	2:C:130:ARG:NH1	2.34	0.59
8:P:289:THR:HG22	8:P:292:GLU:HG3	1.85	0.59
3:D:110:ARG:HG3	3:D:114:HIS:CE1	2.38	0.59
9:Q:129:LYS:HE3	9:Q:130:PRO:HD2	1.84	0.58
6:G:171:PRO:O	6:G:283:ARG:NH2	2.36	0.58
3:D:207:GLY:O	3:D:260:ARG:NH2	2.36	0.58
5:F:257:GLY:HA3	5:F:263:THR:HG22	1.85	0.58
11:S:11:MET:HE1	11:S:14:LEU:HB2	1.85	0.58
3:D:114:HIS:HD2	3:D:264:ARG:HG3	1.66	0.57
14:W:44:TYR:OH	14:W:94:LYS:O	2.19	0.57
1:B:97:GLU:HG3	1:B:189:PRO:HB2	1.86	0.57
6:G:607:GLY:HA2	6:G:611:VAL:HG21	1.86	0.57
3:D:162:GLY:HA3	3:D:288:LYS:HA	1.87	0.56
2:C:53:VAL:HG11	2:C:77:LEU:HB3	1.86	0.56
12:U:50:VAL:HG21	12:U:120:ALA:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:331:ARG:O	5:F:336:ASN:ND2	2.38	0.56
5:F:351:PRO:HD2	5:F:354:ILE:HD11	1.87	0.56
2:C:52:ARG:HD2	13:V:92:GLU:HG2	1.85	0.56
3:D:175:ILE:HG22	3:D:279:LEU:HD11	1.87	0.56
7:I:130:GLU:HB2	7:I:140:ILE:HD12	1.87	0.56
4:E:78:ASP:OD1	4:E:79:LEU:N	2.39	0.56
5:F:64:ILE:HG23	5:F:276:THR:HG21	1.87	0.56
10:R:75:ASP:OD1	10:R:76:THR:N	2.40	0.55
14:W:41:MET:O	14:W:47:GLN:NE2	2.39	0.55
10:R:66:ASP:OD2	10:R:67:GLY:N	2.39	0.55
14:W:55:LEU:O	14:W:59:ILE:HD12	2.06	0.55
3:D:114:HIS:CD2	3:D:264:ARG:HG3	2.41	0.55
4:E:174:CYS:HA	5:F:146:GLY:HA2	1.89	0.55
4:E:201:VAL:HA	4:E:205:LYS:HD2	1.89	0.55
8:P:151:THR:HG22	8:P:153:ASN:H	1.71	0.55
5:F:339:ALA:HB1	5:F:349:LEU:HD11	1.88	0.55
14:W:15:ASN:HD21	14:W:73:LYS:HG2	1.70	0.55
4:E:42:LYS:HE2	4:E:44:ASP:HB2	1.87	0.55
3:D:292:ARG:NH1	3:D:296:PRO:O	2.39	0.54
8:P:157:GLU:OE2	8:P:161:HIS:ND1	2.40	0.54
11:S:53:CYS:SG	11:S:54:SER:N	2.78	0.54
4:E:49:PHE:O	4:E:83:GLN:NE2	2.40	0.54
5:F:89:LYS:HG3	5:F:212:SER:HB3	1.89	0.54
8:P:223:ILE:HD12	8:P:230:LEU:HD23	1.89	0.54
4:E:172:MET:HB2	5:F:185:TYR:HE1	1.72	0.54
3:D:317:THR:HG23	7:I:128:LEU:HD12	1.91	0.53
6:G:689:HIS:ND1	11:S:53:CYS:SG	2.81	0.53
8:P:253:PHE:CE2	8:P:255:PRO:HG3	2.43	0.53
3:D:190:GLU:OE2	3:D:269:ARG:NH2	2.40	0.53
5:F:348:PRO:HG3	5:F:456:TRP:HB3	1.90	0.53
8:P:289:THR:HG23	8:P:291:HIS:H	1.73	0.53
4:E:188:ASN:HB3	4:E:192:GLY:HA3	1.90	0.53
8:P:186:LEU:HA	8:P:218:ARG:HG2	1.90	0.53
13:V:58:GLU:HG2	13:V:62:ARG:NH1	2.23	0.53
3:D:273:ARG:HG2	3:D:277:GLN:HE21	1.74	0.53
7:I:181:PRO:HG3	7:I:210:GLU:HG2	1.91	0.53
12:U:53:ARG:HD2	12:U:119:ILE:HG21	1.90	0.53
5:F:76:LEU:O	5:F:80:MET:HG2	2.09	0.52
6:G:292:THR:HG22	6:G:293:ILE:N	2.24	0.52
14:W:98:HIS:NE2	14:W:102:GLN:OE1	2.43	0.52
4:E:38:SER:OG	4:E:41:ASN:OD1	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:LYS:O	1:B:214:HIS:ND1	2.43	0.52
6:G:444:GLY:HA3	6:G:520:LEU:HD21	1.92	0.52
7:I:152:THR:O	7:I:197:LYS:NZ	2.42	0.52
10:R:71:ALA:HB1	10:R:84:ILE:HD11	1.90	0.52
6:G:591:VAL:HG11	6:G:610:ALA:HA	1.91	0.52
5:F:293:ASN:ND2	5:F:361:ASP:HB3	2.25	0.52
3:D:245:LEU:HD13	3:D:274:ILE:HG23	1.92	0.52
8:P:282:LEU:HD12	8:P:360:PHE:CZ	2.45	0.52
8:P:131:ILE:HG22	8:P:170:VAL:HG11	1.93	0.51
13:V:98:THR:O	13:V:102:LYS:HG3	2.10	0.51
3:D:111:ILE:HG12	3:D:268:MET:HG3	1.93	0.51
1:B:69:ILE:HG23	1:B:212:PHE:HD2	1.76	0.51
4:E:32:LEU:HD23	4:E:34:TYR:CZ	2.45	0.51
4:E:113:PHE:HB2	5:F:243:GLN:HE21	1.75	0.51
6:G:385:GLY:HA2	6:G:411:GLU:HG3	1.93	0.51
8:P:161:HIS:NE2	8:P:165:GLU:OE2	2.43	0.51
13:V:118:GLU:N	13:V:118:GLU:OE2	2.44	0.51
6:G:64:ARG:NH1	9:Q:132:THR:O	2.43	0.51
3:D:182:PHE:HD2	3:D:272:LEU:HD13	1.76	0.51
6:G:500:HIS:ND1	6:G:501:PRO:HD2	2.26	0.51
14:W:120:LYS:HD3	14:W:124:LEU:HD23	1.93	0.51
1:B:153:ILE:HD11	1:B:202:LEU:HD22	1.93	0.51
4:E:32:LEU:O	4:E:119:ARG:NH1	2.36	0.51
4:E:135:CYS:HB2	4:E:140:SER:HB3	1.92	0.51
3:D:311:HIS:ND1	6:G:186:MET:SD	2.81	0.50
5:F:161:LEU:HD13	5:F:268:VAL:HG13	1.93	0.50
5:F:267:ASN:N	20:F:500:FMN:O1P	2.41	0.50
2:C:118:MET:HB3	2:C:143:LEU:HB2	1.93	0.50
8:P:76:ALA:HB3	8:P:97:VAL:HG13	1.94	0.50
3:D:119:THR:HB	3:D:131:PHE:HA	1.94	0.50
6:G:395:VAL:HG21	6:G:654:TRP:HB2	1.92	0.50
8:P:238:LYS:HE2	8:P:301:ILE:HD11	1.92	0.50
5:F:341:ILE:HB	5:F:378:ILE:HB	1.93	0.50
7:I:105:PRO:HB2	7:I:218:GLU:OE1	2.12	0.50
9:Q:111:GLU:HG2	9:Q:115:LYS:HE2	1.94	0.50
5:F:121:LYS:NZ	20:F:500:FMN:O3P	2.41	0.49
1:B:189:PRO:HD3	3:D:154:HIS:CD2	2.47	0.49
2:C:52:ARG:NH2	13:V:95:ASP:OD2	2.42	0.49
2:C:58:ASP:HB2	3:D:354:LYS:HE2	1.95	0.49
6:G:500:HIS:HB3	6:G:503:CYS:SG	2.52	0.49
7:I:206:ARG:NH1	7:I:207:TRP:CZ2	2.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:U:118:PHE:O	12:U:122:HIS:ND1	2.44	0.49
5:F:185:TYR:HB3	5:F:188:GLU:HB2	1.94	0.49
2:C:161:GLU:OE1	8:P:373:TYR:OH	2.23	0.49
6:G:96:GLU:OE2	6:G:104:ARG:NH2	2.46	0.49
8:P:255:PRO:HB2	8:P:370:LEU:HD22	1.94	0.49
8:P:114:ASP:O	8:P:115:LEU:HD12	2.13	0.49
6:G:91:VAL:HG13	6:G:144:ILE:HG12	1.93	0.49
5:F:151:ARG:HH11	5:F:155:ARG:HH11	1.59	0.49
5:F:313:GLU:OE1	5:F:326:HIS:NE2	2.44	0.49
5:F:408:CYS:HB2	18:F:501:SF4:S3	2.53	0.49
2:C:111:TRP:HH2	3:D:361:ALA:HB2	1.78	0.48
3:D:28:LEU:HD23	3:D:30:LEU:HD21	1.95	0.48
3:D:31:GLU:OE2	3:D:39:ARG:NH2	2.45	0.48
4:E:169:MET:HE1	19:E:500:FES:S2	2.33	0.48
3:D:17:PRO:HG2	3:D:26:LEU:HB3	1.94	0.48
6:G:336:TYR:HA	6:G:339:LEU:HD12	1.96	0.48
13:V:67:VAL:HG22	13:V:80:ARG:HH12	1.77	0.48
4:E:177:ASN:O	4:E:180:MET:HG3	2.12	0.48
6:G:659:ALA:O	6:G:663:VAL:HG23	2.13	0.48
8:P:147:ARG:HD2	8:P:149:TYR:CE2	2.49	0.48
3:D:51:THR:O	3:D:55:ILE:HG12	2.13	0.48
8:P:359:LYS:HD2	8:P:361:GLN:HE22	1.79	0.48
2:C:40:GLN:NE2	13:V:106:TRP:CD2	2.81	0.48
2:C:40:GLN:NE2	13:V:106:TRP:CG	2.82	0.48
8:P:337:GLN:HG2	8:P:338:ILE:N	2.29	0.48
5:F:428:LYS:H	5:F:431:GLU:HG3	1.78	0.48
8:P:184:SER:OG	8:P:185:CYS:N	2.47	0.48
6:G:172:ILE:HG23	7:I:124:ILE:HD12	1.96	0.48
9:Q:49:HIS:HB3	9:Q:98:TYR:HE1	1.77	0.47
2:C:43:CYS:SG	13:V:102:LYS:NZ	2.68	0.47
3:D:27:ARG:HG3	3:D:46:LEU:HD11	1.95	0.47
8:P:201:ALA:O	8:P:204:GLU:HB2	2.14	0.47
5:F:361:ASP:HB2	5:F:364:ALA:HB3	1.97	0.47
6:G:173:CYS:O	6:G:283:ARG:NH1	2.40	0.47
12:U:82:ASP:HB3	14:W:64:ARG:HH22	1.79	0.47
2:C:60:CYS:SG	2:C:74:VAL:HB	2.55	0.47
5:F:63:ARG:NH1	5:F:312:GLU:O	2.48	0.47
5:F:306:ASN:HB2	5:F:328:GLY:HA3	1.96	0.47
10:R:68:ARG:NH2	10:R:90:ASP:OD2	2.41	0.47
1:B:123:ASP:OD1	1:B:123:ASP:N	2.46	0.47
3:D:30:LEU:HD22	3:D:37:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:164:GLY:HA2	5:F:275:PRO:HD3	1.96	0.47
5:F:237:GLU:HG3	5:F:245:LYS:O	2.15	0.47
5:F:91:LEU:HD11	5:F:279:ARG:HG3	1.97	0.47
6:G:324:ASN:OD1	6:G:325:GLU:N	2.48	0.47
8:P:152:ARG:HH21	8:P:327:ASN:N	2.13	0.46
8:P:80:LEU:HD23	8:P:144:LEU:HD22	1.97	0.46
9:Q:41:LYS:HE2	14:W:68:HIS:CE1	2.50	0.46
1:B:130:THR:HA	1:B:158:CYS:HB3	1.97	0.46
8:P:182:GLN:HG3	8:P:207:VAL:HG21	1.96	0.46
13:V:51:GLU:HG2	13:V:109:TRP:CE3	2.50	0.46
13:V:145:THR:O	13:V:149:LEU:HG	2.15	0.46
6:G:407:ASN:HB3	6:G:409:TRP:HZ3	1.79	0.46
8:P:60:THR:HG22	9:Q:82:LEU:HD21	1.97	0.46
1:B:91:LEU:HB2	1:B:129:GLY:HA3	1.97	0.46
2:C:38:LEU:HD21	2:C:75:TYR:CZ	2.50	0.46
13:V:58:GLU:O	13:V:62:ARG:HG3	2.15	0.46
2:C:83:ASN:OD1	13:V:133:HIS:ND1	2.30	0.46
8:P:328:LYS:HG3	8:P:329:VAL:H	1.81	0.46
13:V:71:GLU:OE1	13:V:76:MET:HB3	2.16	0.46
15:Z:20:LEU:H	15:Z:20:LEU:HD23	1.81	0.46
2:C:126:HIS:O	14:W:11:GLY:HA2	2.17	0.45
6:G:110:ARG:NH2	6:G:321:GLU:OE2	2.49	0.45
6:G:724:MET:SD	6:G:730:ARG:HA	2.56	0.45
6:G:738:CYS:O	6:G:742:LEU:HB2	2.16	0.45
6:G:658:ARG:CD	6:G:668:LEU:HB2	2.47	0.45
8:P:110:LYS:HE3	8:P:110:LYS:HB3	1.77	0.45
8:P:231:ASN:OD1	8:P:381:TYR:OH	2.25	0.45
3:D:28:LEU:HD21	3:D:366:LEU:HD21	1.97	0.45
3:D:250:PRO:HG2	3:D:263:ILE:HG23	1.99	0.45
6:G:364:ALA:O	6:G:368:VAL:HG22	2.16	0.45
6:G:512:PRO:HB2	6:G:542:VAL:HG12	1.99	0.45
4:E:179:PRO:O	4:E:201:VAL:HG12	2.17	0.45
5:F:234:ALA:HB2	5:F:246:PRO:HG3	1.98	0.45
6:G:287:LEU:HB3	6:G:306:ASP:HB3	1.99	0.45
5:F:69:TYR:HB2	5:F:71:LEU:HD13	1.98	0.45
6:G:266:ASP:OD1	6:G:333:ARG:NH2	2.48	0.45
8:P:142:ILE:HD11	8:P:269:LEU:HD11	1.99	0.45
4:E:133:THR:HG21	5:F:393:LEU:HD22	1.97	0.45
14:W:34:CYS:HB3	14:W:56:ARG:NH2	2.25	0.45
2:C:97:ARG:HG2	2:C:122:SER:HB3	1.99	0.45
6:G:169:ASP:HA	10:R:99:TYR:OH	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:W:22:ALA:O	14:W:26:VAL:HG23	2.16	0.45
3:D:70:LEU:HD11	3:D:355:ILE:HD13	1.99	0.44
5:F:85:TRP:CD2	5:F:204:LEU:HD13	2.52	0.44
1:B:71:LYS:HD3	1:B:71:LYS:HA	1.69	0.44
2:C:142:PRO:HA	2:C:147:PHE:CD2	2.52	0.44
6:G:411:GLU:OE2	6:G:586:ALA:HA	2.17	0.44
6:G:662:GLU:OE1	14:W:124:LEU:HB2	2.17	0.44
4:E:47:TRP:HE1	4:E:84:ASN:HD22	1.66	0.44
6:G:423:TYR:OH	6:G:700:PRO:HA	2.18	0.44
6:G:653:ASP:O	6:G:657:VAL:HG23	2.18	0.44
14:W:121:THR:HG22	14:W:123:PHE:H	1.81	0.44
2:C:38:LEU:HD21	2:C:75:TYR:CE1	2.52	0.44
5:F:102:GLU:HA	5:F:105:LYS:HE2	1.99	0.44
5:F:443:GLU:OE1	5:F:456:TRP:NE1	2.50	0.44
1:B:73:ASP:OD1	1:B:210:LYS:HA	2.17	0.44
6:G:304:ARG:NH2	6:G:306:ASP:OD2	2.42	0.44
2:C:128:ASP:O	2:C:128:ASP:OD2	2.35	0.44
7:I:124:ILE:HG22	7:I:151:ARG:HH12	1.84	0.43
1:B:99:MET:HB3	3:D:135:PHE:HE2	1.83	0.43
3:D:15:PHE:CE2	3:D:375:LEU:HD11	2.53	0.43
8:P:105:SER:OG	8:P:106:PRO:HD3	2.18	0.43
8:P:230:LEU:HD12	8:P:378:LEU:HD11	2.00	0.43
5:F:298:LEU:HD23	5:F:312:GLU:HB2	1.99	0.43
5:F:446:THR:HB	18:F:501:SF4:S3	2.58	0.43
6:G:83:VAL:HG21	6:G:98:ALA:HB2	2.00	0.43
8:P:56:ALA:H	8:P:68:GLY:H	1.65	0.43
12:U:61:PHE:O	12:U:62:GLN:HG2	2.18	0.43
2:C:118:MET:SD	2:C:142:PRO:HG2	2.57	0.43
3:D:98:ALA:O	3:D:102:ARG:HG3	2.18	0.43
6:G:652:ASP:O	6:G:656:ILE:HG13	2.18	0.43
10:R:73:GLU:HG2	10:R:78:PRO:HA	2.00	0.43
6:G:603:GLN:NE2	6:G:656:ILE:HD12	2.31	0.43
11:S:10:SER:HB2	11:S:94:ALA:HB3	2.00	0.43
3:D:115:LEU:HD23	3:D:115:LEU:HA	1.91	0.43
5:F:319:LEU:HD21	5:F:340:ILE:HD13	2.01	0.43
14:W:31:ARG:O	14:W:35:ARG:HG3	2.19	0.43
3:D:182:PHE:CE2	3:D:186:ILE:HD11	2.54	0.43
4:E:109:GLU:HG2	6:G:239:ILE:O	2.19	0.43
6:G:310:PRO:HA	6:G:645:PRO:HD2	2.01	0.43
8:P:98:PRO:HB2	8:P:123:PHE:CD1	2.54	0.43
13:V:24:ASP:OD2	13:V:24:ASP:N	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:181:ALA:HB3	9:Q:70:LYS:HE3	2.01	0.43
3:D:182:PHE:O	3:D:186:ILE:HG13	2.19	0.43
3:D:310:ILE:HG23	6:G:182:GLN:HB2	2.01	0.43
6:G:422:ARG:HA	6:G:425:TYR:CE2	2.54	0.43
3:D:150:GLY:HA3	7:I:108:ARG:HG3	2.00	0.42
4:E:169:MET:HE1	4:E:197:TYR:HE1	1.84	0.42
4:E:202:THR:HG22	4:E:204:GLU:H	1.82	0.42
6:G:198:MET:HG3	10:R:86:PHE:CE1	2.54	0.42
6:G:118:ARG:O	6:G:158:VAL:HG21	2.19	0.42
6:G:413:THR:H	6:G:559:GLN:NE2	2.17	0.42
7:I:160:THR:HG21	7:I:190:HIS:CE1	2.54	0.42
6:G:410:CYS:SG	6:G:411:GLU:N	2.92	0.42
3:D:176:ASP:O	3:D:180:GLN:HG2	2.19	0.42
5:F:368:VAL:HG12	5:F:368:VAL:O	2.19	0.42
6:G:300:GLY:HA3	6:G:632:ASN:HD21	1.83	0.42
8:P:245:LEU:HD12	8:P:309:LYS:HD3	2.01	0.42
11:S:64:TYR:HB2	11:S:68:VAL:HB	2.01	0.42
12:U:119:ILE:HA	12:U:122:HIS:ND1	2.35	0.42
2:C:13:THR:HG23	13:V:53:TYR:HA	2.02	0.42
6:G:377:PRO:O	6:G:405:SER:HB2	2.20	0.42
6:G:409:TRP:HD1	6:G:410:CYS:O	2.02	0.42
1:B:180:PRO:HB2	8:P:107:ARG:HG2	2.01	0.42
3:D:314:GLU:HG3	6:G:186:MET:HG3	2.02	0.42
5:F:208:ASN:OD1	5:F:213:GLY:N	2.43	0.42
5:F:366:LYS:HA	5:F:370:SER:O	2.20	0.42
6:G:293:ILE:HD13	6:G:638:GLN:HB2	2.02	0.42
2:C:10:SER:O	2:C:14:LEU:HB2	2.20	0.42
2:C:56:LEU:HD21	2:C:59:ILE:HD11	2.02	0.42
7:I:140:ILE:HG12	7:I:155:TYR:CD2	2.55	0.42
2:C:156:ARG:NH1	2:C:167:GLU:OE2	2.44	0.42
4:E:65:PRO:HG2	4:E:68:TYR:HB2	2.01	0.42
6:G:445:THR:HG23	6:G:447:PRO:HD3	2.01	0.42
6:G:483:LYS:HG2	6:G:485:LEU:HD23	2.02	0.42
11:S:31:PHE:O	11:S:35:ASN:HB2	2.19	0.42
3:D:79:GLU:OE1	3:D:156:SER:HA	2.20	0.41
6:G:523:ARG:NH2	6:G:711:SER:OG	2.53	0.41
11:S:30:THR:O	11:S:34:LYS:HG2	2.20	0.41
13:V:138:LEU:HD13	13:V:142:PHE:CD2	2.55	0.41
14:W:31:ARG:NH2	14:W:35:ARG:HH22	2.18	0.41
6:G:684:ALA:HB3	6:G:687:LEU:HD12	2.01	0.41
6:G:472:VAL:HG22	6:G:485:LEU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:543:VAL:HG13	6:G:543:VAL:O	2.21	0.41
8:P:321:PRO:HA	8:P:324:PHE:CZ	2.55	0.41
3:D:39:ARG:HG2	3:D:39:ARG:HH11	1.85	0.41
5:F:341:ILE:O	5:F:377:VAL:HA	2.20	0.41
13:V:57:VAL:HA	13:V:60:PHE:CE1	2.55	0.41
1:B:218:LYS:HB3	8:P:100:ARG:HH12	1.85	0.41
3:D:123:MET:HG3	3:D:128:LEU:HD23	2.01	0.41
6:G:146:THR:O	6:G:155:ARG:NH2	2.52	0.41
6:G:518:ALA:HB2	6:G:554:LEU:HA	2.01	0.41
8:P:337:GLN:OE1	8:P:337:GLN:N	2.53	0.41
8:P:360:PHE:CD2	8:P:367:PRO:HG3	2.55	0.41
4:E:135:CYS:CB	4:E:140:SER:HB3	2.50	0.41
4:E:136:MET:HB3	5:F:392:ARG:CZ	2.50	0.41
6:G:280:PHE:HB3	7:I:150:ARG:HG3	2.02	0.41
6:G:376:LYS:HB2	6:G:379:GLU:HG2	2.01	0.41
6:G:520:LEU:HD12	6:G:529:ILE:HG21	2.03	0.41
4:E:95:ALA:O	4:E:99:VAL:HG23	2.21	0.41
6:G:325:GLU:HB2	6:G:457:ARG:HH22	1.85	0.41
6:G:440:PHE:HB2	6:G:469:VAL:HG22	2.03	0.41
8:P:201:ALA:O	8:P:205:GLU:OE1	2.38	0.41
14:W:23:ARG:NH2	23:W:200:8Q1:O3	2.52	0.41
2:C:176:ARG:NH2	7:I:138:ILE:O	2.52	0.41
6:G:584:MET:HG3	6:G:603:GLN:OE1	2.21	0.41
12:U:50:VAL:HA	12:U:53:ARG:NE	2.36	0.41
14:W:37:ILE:O	14:W:41:MET:HG2	2.21	0.41
1:B:164:TYR:OH	3:D:65:PRO:HG2	2.21	0.41
1:B:186:PRO:HD3	7:I:186:ALA:HA	2.03	0.41
3:D:73:VAL:HG12	3:D:113:ASN:HA	2.02	0.41
3:D:85:ALA:HA	3:D:329:THR:HG21	2.03	0.41
3:D:393:ASP:OD1	3:D:393:ASP:N	2.54	0.41
4:E:129:VAL:HG23	4:E:130:CYS:N	2.35	0.41
4:E:178:ALA:HB3	4:E:179:PRO:HD3	2.03	0.41
6:G:170:CYS:N	6:G:171:PRO:HD2	2.36	0.41
6:G:554:LEU:H	6:G:633:THR:HG22	1.85	0.41
6:G:581:VAL:HB	6:G:600:VAL:HG22	2.03	0.41
6:G:693:ARG:HA	6:G:693:ARG:HD3	1.82	0.41
8:P:292:GLU:O	8:P:296:ILE:HG13	2.20	0.41
2:C:160:PRO:HG2	8:P:86:GLN:HG2	2.03	0.41
4:E:206:VAL:HA	4:E:209:ILE:HG12	2.03	0.41
8:P:254:GLN:NE2	8:P:284:GLY:O	2.54	0.41
8:P:337:GLN:HG2	8:P:338:ILE:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:381:ILE:O	3:D:385:GLN:HG3	2.22	0.40
6:G:304:ARG:CZ	6:G:316:ILE:HD11	2.51	0.40
6:G:503:CYS:O	6:G:507:LYS:HG2	2.21	0.40
6:G:521:PHE:HE1	6:G:530:LEU:HD21	1.86	0.40
6:G:590:ASN:OD1	6:G:590:ASN:N	2.54	0.40
8:P:159:ALA:HA	8:P:163:ILE:HD12	2.03	0.40
8:P:246:ILE:HD11	8:P:347:LEU:HD22	2.03	0.40
2:C:100:SER:HB2	2:C:123:PHE:HB3	2.02	0.40
3:D:91:ASN:HD21	13:V:125:PRO:HB2	1.86	0.40
6:G:391:GLU:O	6:G:395:VAL:HG23	2.22	0.40
11:S:4:ARG:NH2	11:S:35:ASN:OD1	2.46	0.40
3:D:191:GLU:OE1	15:Z:37:ARG:NH2	2.53	0.40
5:F:138:VAL:HG11	5:F:161:LEU:HD11	2.03	0.40
20:F:500:FMN:H1'1	20:F:500:FMN:H9	1.81	0.40
6:G:93:GLN:O	6:G:97:VAL:HG23	2.22	0.40
1:B:132:THR:OG1	3:D:46:LEU:O	2.27	0.40
4:E:169:MET:HE2	4:E:171:CYS:HA	2.03	0.40
9:Q:79:VAL:O	9:Q:79:VAL:HG12	2.21	0.40
11:S:77:LEU:HD23	11:S:81:GLN:HB3	2.03	0.40
1:B:94:CYS:HB3	1:B:128:ALA:HB1	2.02	0.40
6:G:300:GLY:HA3	6:G:632:ASN:ND2	2.37	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	B	155/218 (71%)	151 (97%)	4 (3%)	0	100	100
2	C	183/190 (96%)	180 (98%)	3 (2%)	0	100	100
3	D	383/394 (97%)	369 (96%)	14 (4%)	0	100	100
4	E	190/255 (74%)	182 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	432/486 (89%)	421 (98%)	11 (2%)	0	100	100
6	G	686/748 (92%)	668 (97%)	18 (3%)	0	100	100
7	I	163/222 (73%)	161 (99%)	2 (1%)	0	100	100
8	P	330/402 (82%)	317 (96%)	13 (4%)	0	100	100
9	Q	117/154 (76%)	112 (96%)	5 (4%)	0	100	100
10	R	60/110 (54%)	58 (97%)	2 (3%)	0	100	100
11	S	91/97 (94%)	83 (91%)	8 (9%)	0	100	100
12	U	81/126 (64%)	75 (93%)	6 (7%)	0	100	100
13	V	138/169 (82%)	135 (98%)	3 (2%)	0	100	100
14	W	108/133 (81%)	102 (94%)	6 (6%)	0	100	100
15	Z	25/143 (18%)	24 (96%)	1 (4%)	0	100	100
16	q	63/159 (40%)	57 (90%)	6 (10%)	0	100	100
17	r	8/131 (6%)	7 (88%)	1 (12%)	0	100	100
All	All	3213/4137 (78%)	3102 (96%)	111 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	132/184 (72%)	132 (100%)	0	100	100
2	C	175/179 (98%)	175 (100%)	0	100	100
3	D	331/340 (97%)	331 (100%)	0	100	100
4	E	166/220 (76%)	165 (99%)	1 (1%)	86	95
5	F	353/396 (89%)	353 (100%)	0	100	100
6	G	571/625 (91%)	571 (100%)	0	100	100
7	I	147/195 (75%)	147 (100%)	0	100	100
8	P	273/334 (82%)	273 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	Q	100/128 (78%)	100 (100%)	0	100	100
10	R	55/97 (57%)	55 (100%)	0	100	100
11	S	82/85 (96%)	82 (100%)	0	100	100
12	U	75/113 (66%)	75 (100%)	0	100	100
13	V	123/148 (83%)	123 (100%)	0	100	100
14	W	98/114 (86%)	98 (100%)	0	100	100
15	Z	21/115 (18%)	20 (95%)	1 (5%)	25	57
16	q	54/133 (41%)	54 (100%)	0	100	100
17	r	10/118 (8%)	10 (100%)	0	100	100
All	All	2766/3524 (78%)	2764 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	135	CYS
15	Z	38	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
6	G	320	ASN
6	G	638	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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
18	SF4	I	500	7	0,12,12	-	-	-		
21	NDP	P	500	-	45,52,52	2.27	4 (8%)	53,80,80	1.74	10 (18%)
19	FES	E	500	4	0,4,4	-	-	-		
18	SF4	F	501	5	0,12,12	-	-	-		
18	SF4	I	501	7	0,12,12	-	-	-		
23	8Q1	W	200	-	31,34,34	1.70	6 (19%)	40,43,43	1.58	4 (10%)
20	FMN	F	500	-	33,33,33	1.08	2 (6%)	48,50,50	1.22	8 (16%)
18	SF4	G	803	6	0,12,12	-	-	-		
19	FES	G	801	6	0,4,4	-	-	-		
18	SF4	G	802	6	0,12,12	-	-	-		
18	SF4	B	500	1	0,12,12	-	-	-		

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
18	SF4	I	500	7	-	-	0/6/5/5
21	NDP	P	500	-	-	9/30/77/77	0/5/5/5
18	SF4	B	500	1	-	-	0/6/5/5
19	FES	E	500	4	-	-	0/1/1/1
18	SF4	I	501	7	-	-	0/6/5/5
23	8Q1	W	200	-	-	25/41/41/41	-
20	FMN	F	500	-	-	7/18/18/18	0/3/3/3
18	SF4	G	803	6	-	-	0/6/5/5
19	FES	G	801	6	-	-	0/1/1/1
18	SF4	G	802	6	-	-	0/6/5/5
18	SF4	F	501	5	-	-	0/6/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	P	500	NDP	P2B-O2B	12.74	1.83	1.59
23	W	200	8Q1	C34-N36	5.52	1.45	1.33
23	W	200	8Q1	C39-N41	5.36	1.45	1.33
21	P	500	NDP	PN-O5D	3.96	1.75	1.59
20	F	500	FMN	C4A-N5	3.81	1.38	1.30
21	P	500	NDP	O2B-C2B	-3.00	1.33	1.44
23	W	200	8Q1	C1-S44	2.43	1.82	1.76
20	F	500	FMN	C10-N1	2.41	1.38	1.33
21	P	500	NDP	C2A-N1A	2.22	1.38	1.33
23	W	200	8Q1	O40-C39	-2.21	1.18	1.23
23	W	200	8Q1	O35-C34	-2.19	1.19	1.23
23	W	200	8Q1	C6-C1	2.08	1.53	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	P	500	NDP	PN-O3-PA	-7.10	108.48	132.83
23	W	200	8Q1	C6-C1-S44	5.75	120.15	113.46
23	W	200	8Q1	O4-C1-C6	-3.79	119.51	123.99
21	P	500	NDP	O2B-P2B-O1X	-3.32	96.59	109.39
20	F	500	FMN	C4-N3-C2	-3.18	119.77	125.64
21	P	500	NDP	PA-O5B-C5B	-3.06	103.74	121.68
21	P	500	NDP	PN-O5D-C5D	-2.92	104.53	121.68
23	W	200	8Q1	C43-S44-C1	2.82	110.66	101.87
20	F	500	FMN	C4A-C4-N3	2.73	120.11	113.19
20	F	500	FMN	O4-C4-C4A	-2.59	119.74	126.60
21	P	500	NDP	O4B-C4B-C3B	2.56	110.19	105.11
21	P	500	NDP	O3X-P2B-O2X	2.53	117.32	107.64
20	F	500	FMN	C4A-C10-N10	2.53	120.17	116.48
23	W	200	8Q1	C38-C39-N41	2.47	120.58	116.42
21	P	500	NDP	C2A-N1A-C6A	-2.38	114.67	118.75
21	P	500	NDP	O2N-PN-O1N	2.34	123.83	112.24
21	P	500	NDP	O5D-PN-O1N	-2.29	100.10	109.07
20	F	500	FMN	C4A-C10-N1	-2.22	119.57	124.73
20	F	500	FMN	C10-C4A-N5	-2.19	120.22	124.86
21	P	500	NDP	C5B-C4B-C3B	-2.14	107.17	115.18
20	F	500	FMN	C9A-C5A-N5	-2.08	120.17	122.43
20	F	500	FMN	C5A-C9A-N10	2.07	120.09	117.95

There are no chirality outliers.

All (41) torsion outliers are listed below:

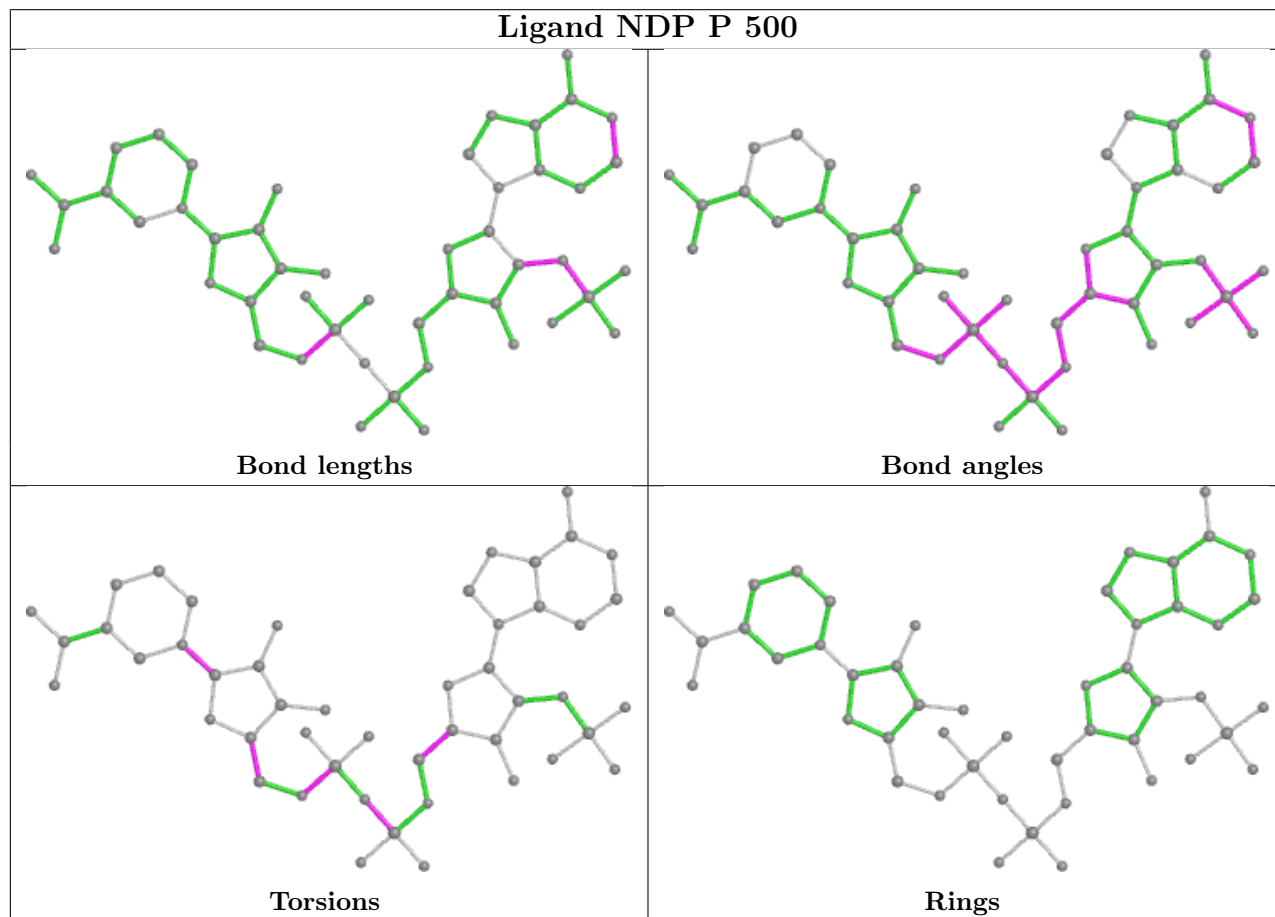
Mol	Chain	Res	Type	Atoms
20	F	500	FMN	N10-C1'-C2'-O2'
20	F	500	FMN	N10-C1'-C2'-C3'
20	F	500	FMN	C1'-C2'-C3'-O3'
20	F	500	FMN	C1'-C2'-C3'-C4'
21	P	500	NDP	C5D-O5D-PN-O3
21	P	500	NDP	C5D-O5D-PN-O1N
21	P	500	NDP	O4D-C4D-C5D-O5D
23	W	200	8Q1	O4-C1-S44-C43
23	W	200	8Q1	C6-C1-S44-C43
23	W	200	8Q1	O27-C28-C29-C30
23	W	200	8Q1	O27-C28-C29-C31
23	W	200	8Q1	O27-C28-C29-C32
23	W	200	8Q1	C28-C29-C32-C34
23	W	200	8Q1	C31-C29-C32-C34
23	W	200	8Q1	C29-C32-C34-O35
23	W	200	8Q1	O33-C32-C34-N36
23	W	200	8Q1	N41-C42-C43-S44
23	W	200	8Q1	C28-O27-P24-O3
23	W	200	8Q1	C28-O27-P24-O2
23	W	200	8Q1	C28-O27-P24-O1
21	P	500	NDP	C3D-C4D-C5D-O5D
20	F	500	FMN	O2'-C2'-C3'-C4'
20	F	500	FMN	O2'-C2'-C3'-O3'
23	W	200	8Q1	O33-C32-C34-O35
23	W	200	8Q1	C30-C29-C32-O33
23	W	200	8Q1	C31-C29-C32-O33
21	P	500	NDP	PN-O3-PA-O1A
23	W	200	8Q1	C29-C32-C34-N36
23	W	200	8Q1	O4-C1-C6-C7
23	W	200	8Q1	S44-C1-C6-C7
21	P	500	NDP	O4D-C1D-N1N-C6N
23	W	200	8Q1	C28-C29-C32-O33
20	F	500	FMN	C5'-O5'-P-O1P
21	P	500	NDP	PN-O3-PA-O2A
23	W	200	8Q1	C7-C8-C9-C10
23	W	200	8Q1	C11-C10-C9-C8
21	P	500	NDP	O4B-C4B-C5B-O5B
23	W	200	8Q1	C12-C13-C14-C15
23	W	200	8Q1	C30-C29-C32-C34
23	W	200	8Q1	C29-C28-O27-P24
21	P	500	NDP	C2D-C1D-N1N-C6N

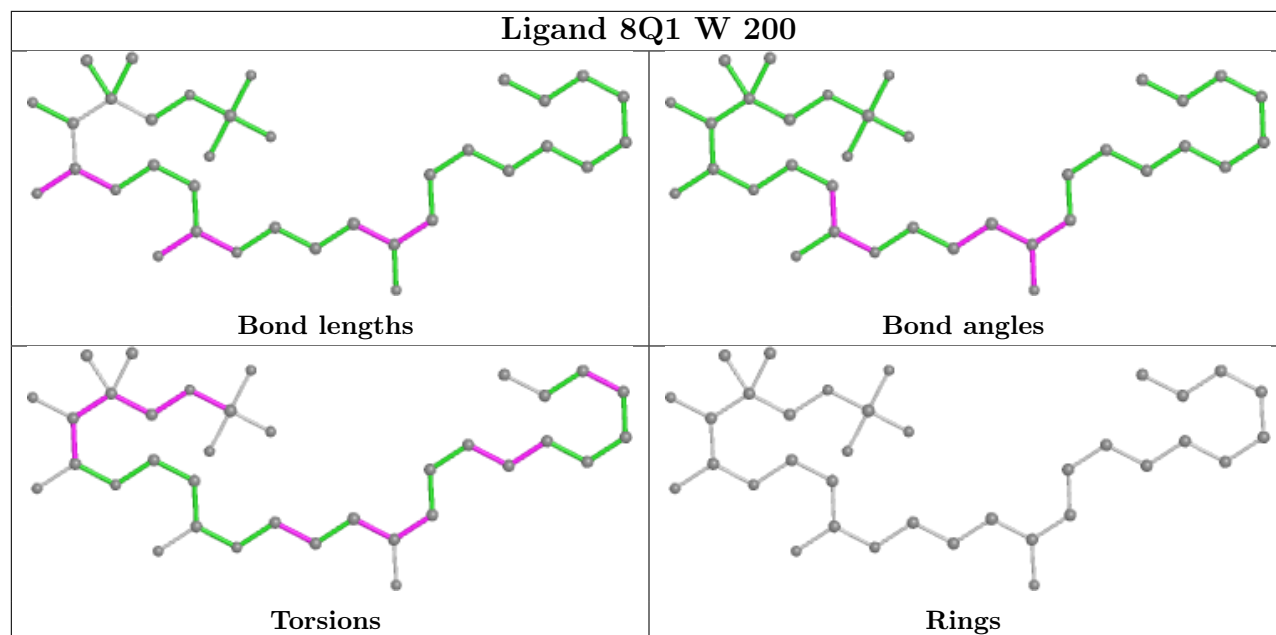
There are no ring outliers.

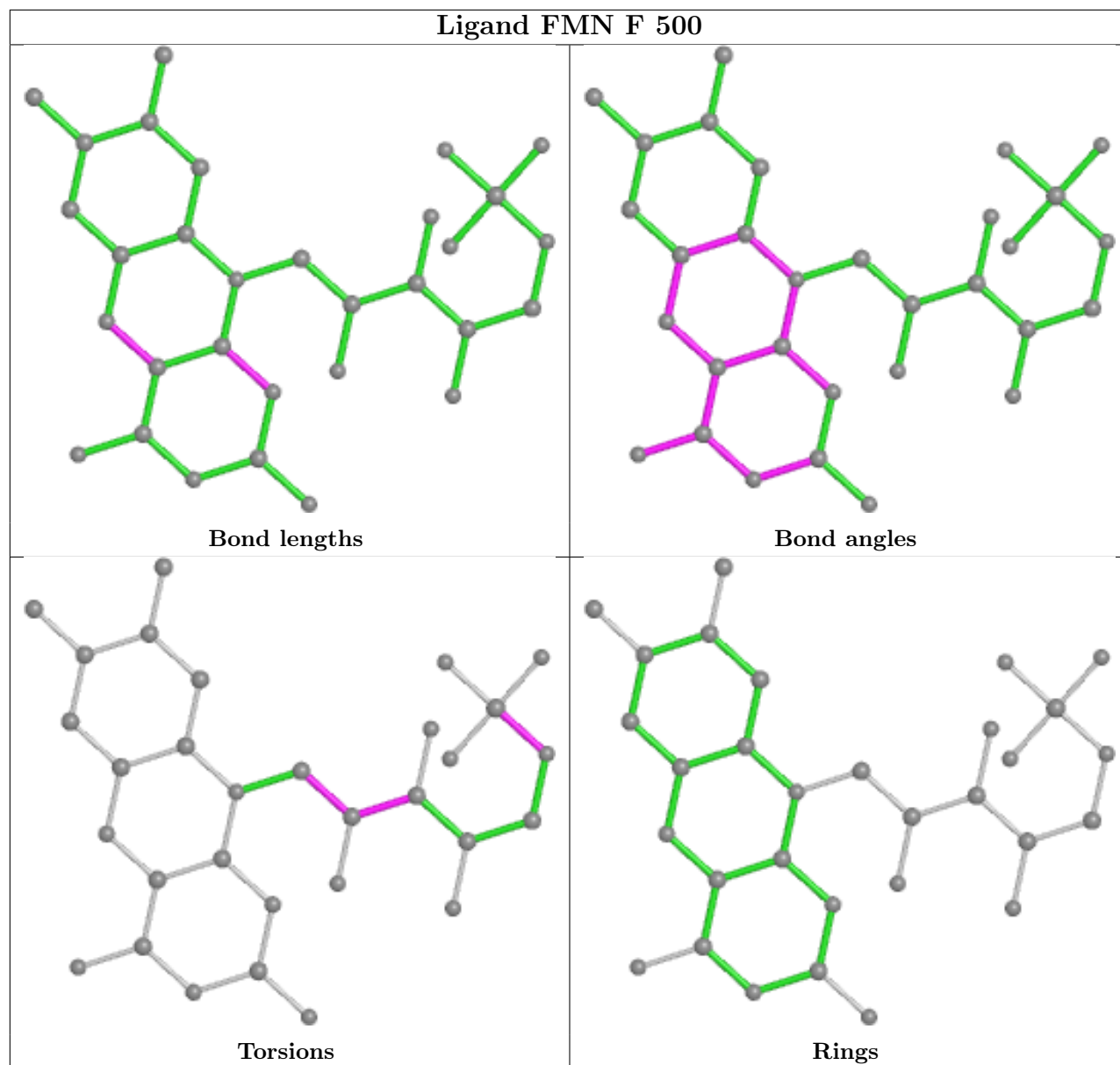
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	E	500	FES	1	0
18	F	501	SF4	2	0
23	W	200	8Q1	1	0
20	F	500	FMN	3	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

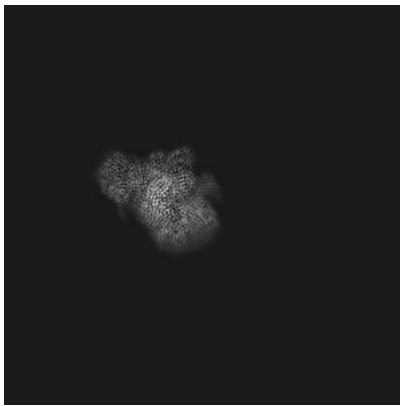
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11873. These allow visual inspection of the internal detail of the map and identification of artifacts.

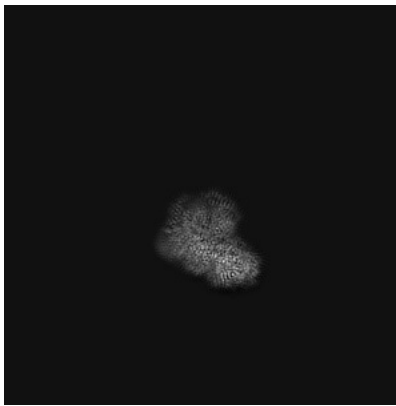
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

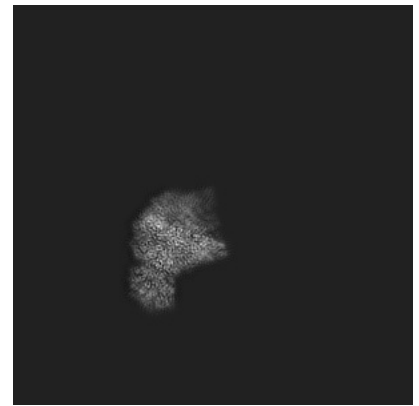
6.1.1 Primary map



X

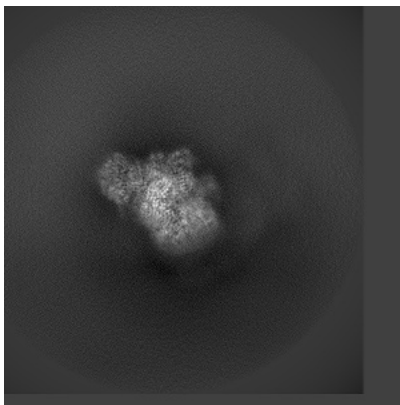


Y

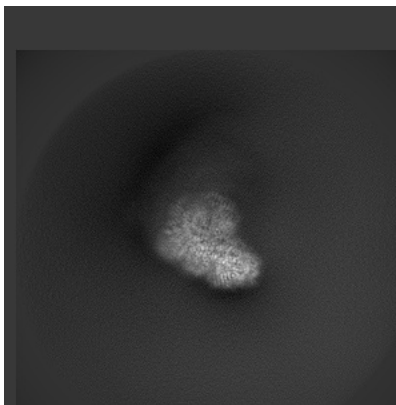


Z

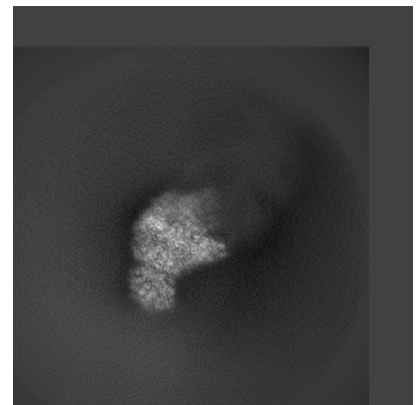
6.1.2 Raw map



X



Y



Z

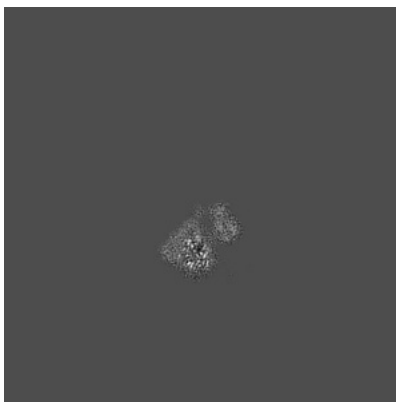
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

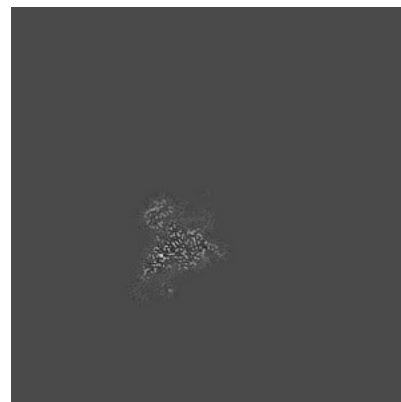
6.2.1 Primary map



X Index: 300



Y Index: 300

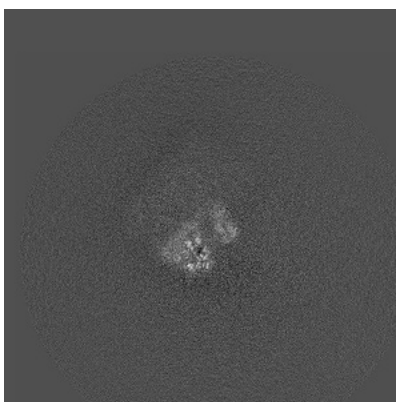


Z Index: 300

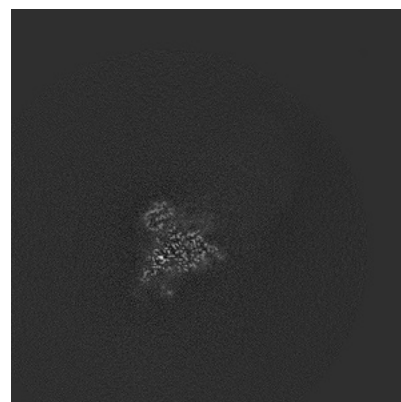
6.2.2 Raw map



X Index: 300



Y Index: 300

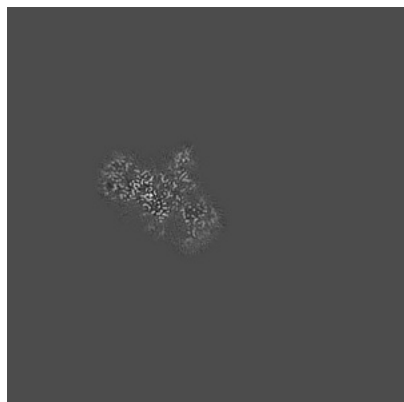


Z Index: 300

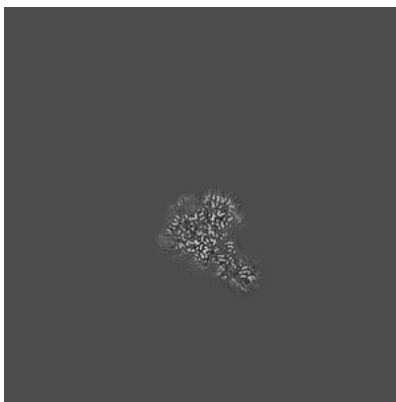
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 222

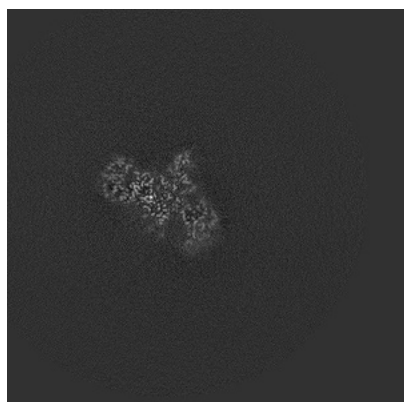


Y Index: 240

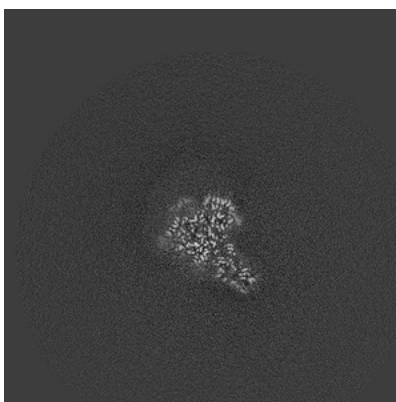


Z Index: 328

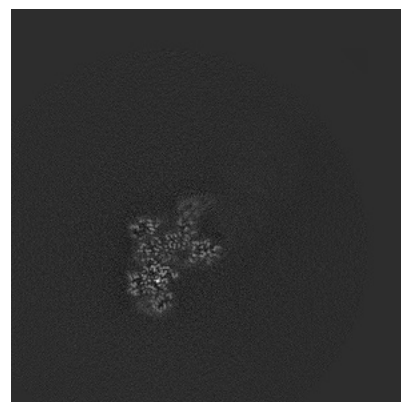
6.3.2 Raw map



X Index: 222



Y Index: 240

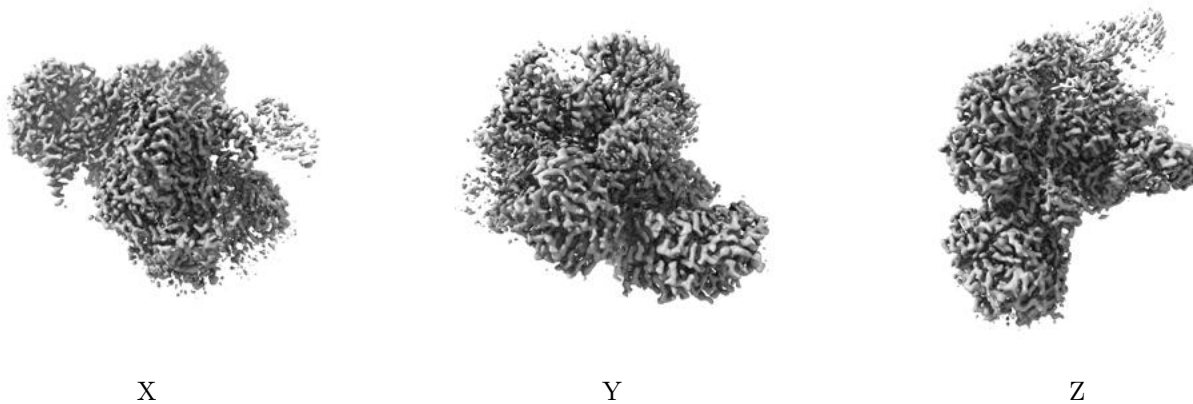


Z Index: 334

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

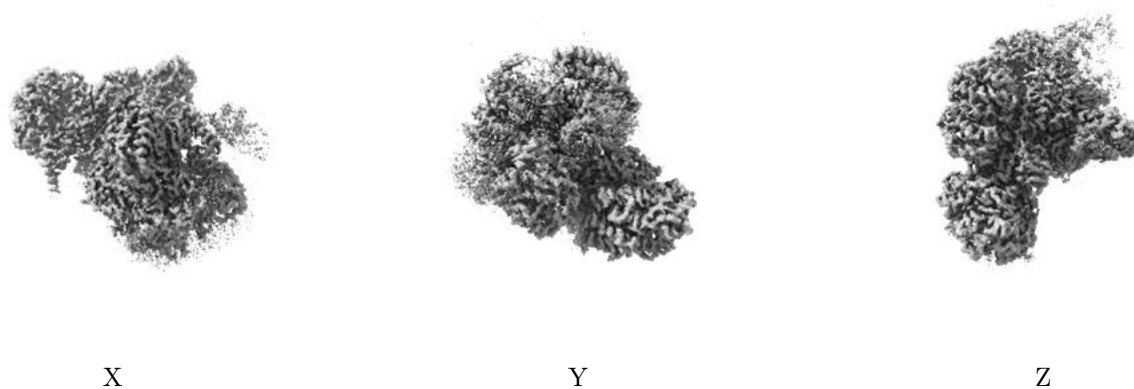
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

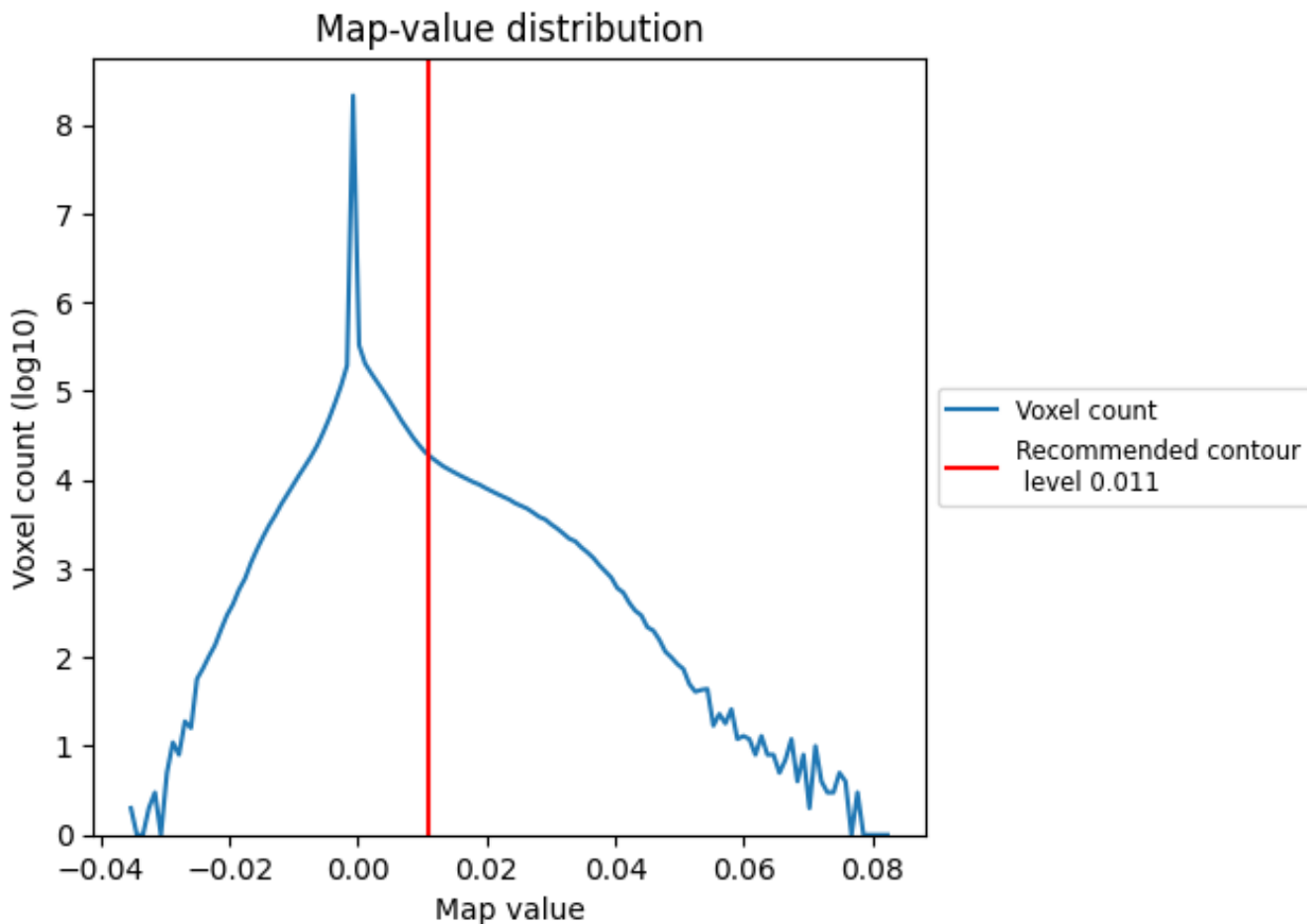
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

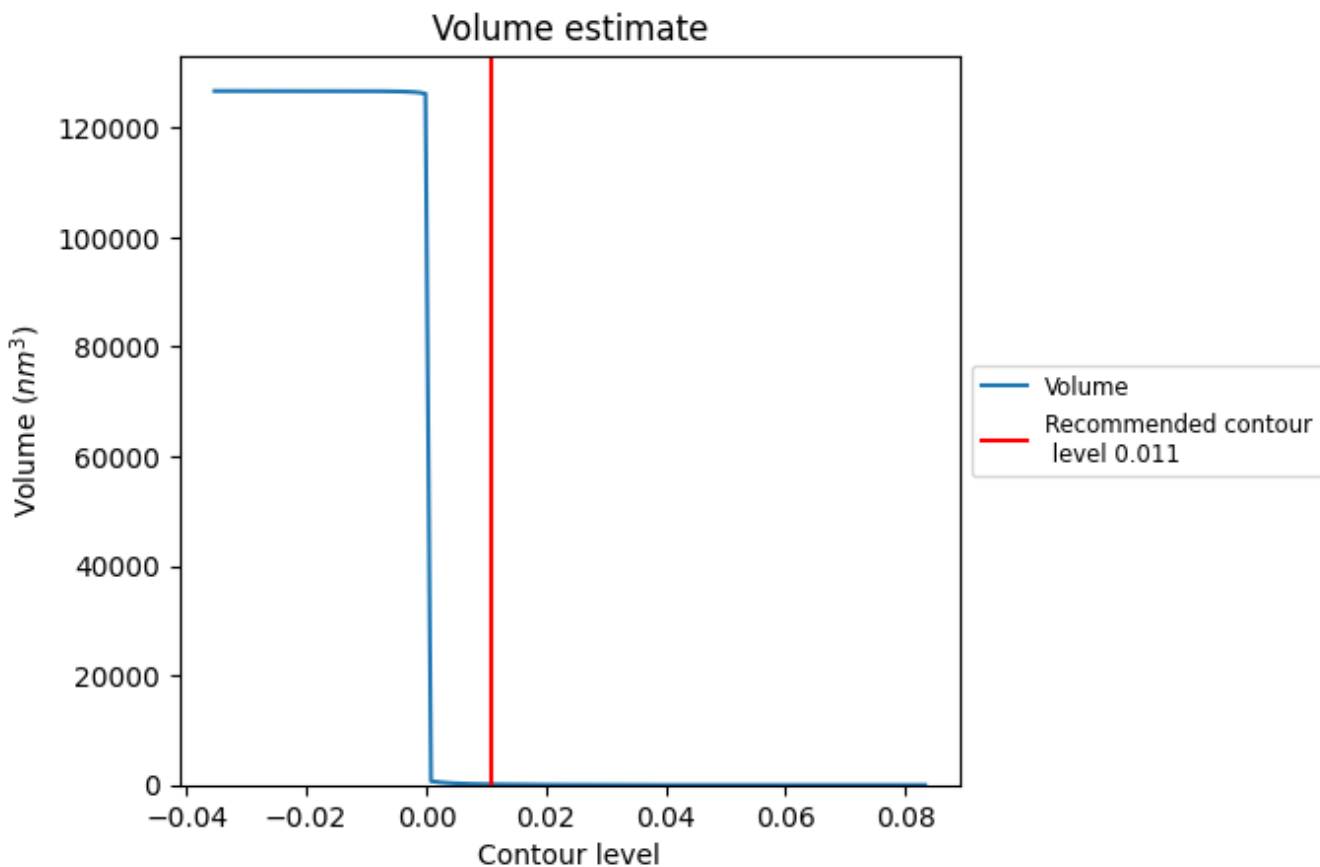
This section contains the results of statistical analysis of the map.

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.

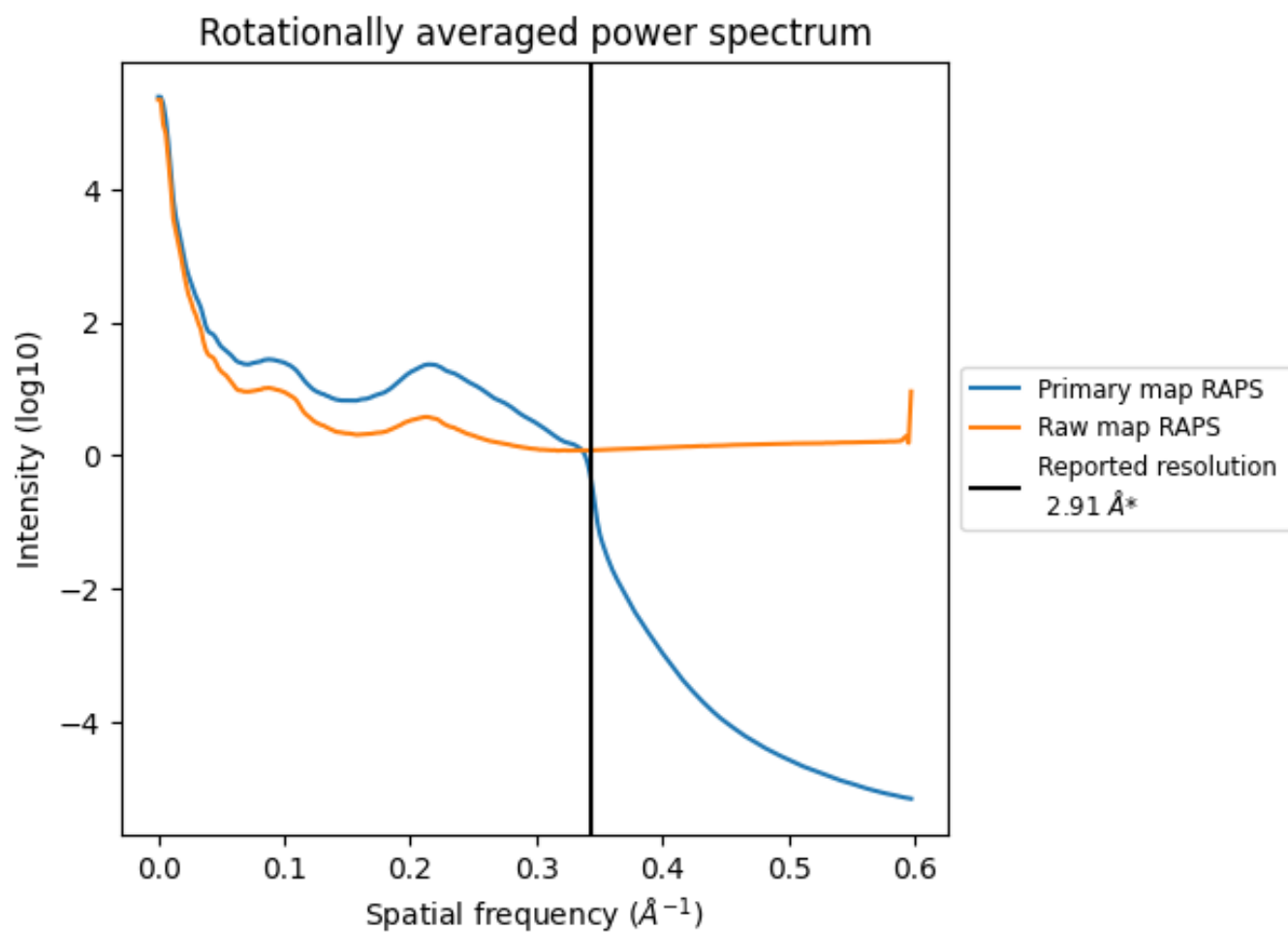
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 121 nm³; this corresponds to an approximate mass of 109 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

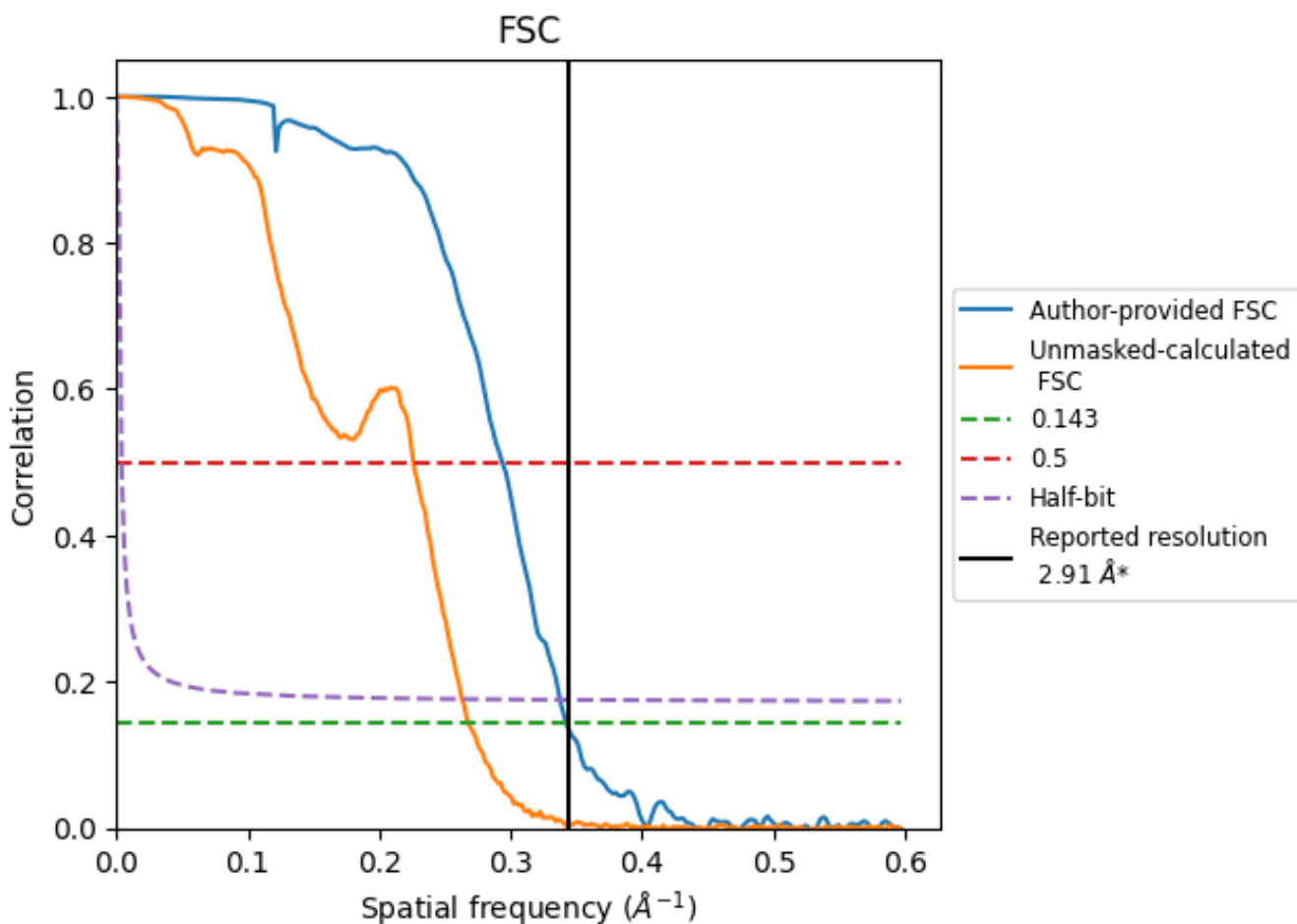


*Reported resolution corresponds to spatial frequency of 0.344 Å⁻¹

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 0.344 Å⁻¹

8.2 Resolution estimates [i](#)

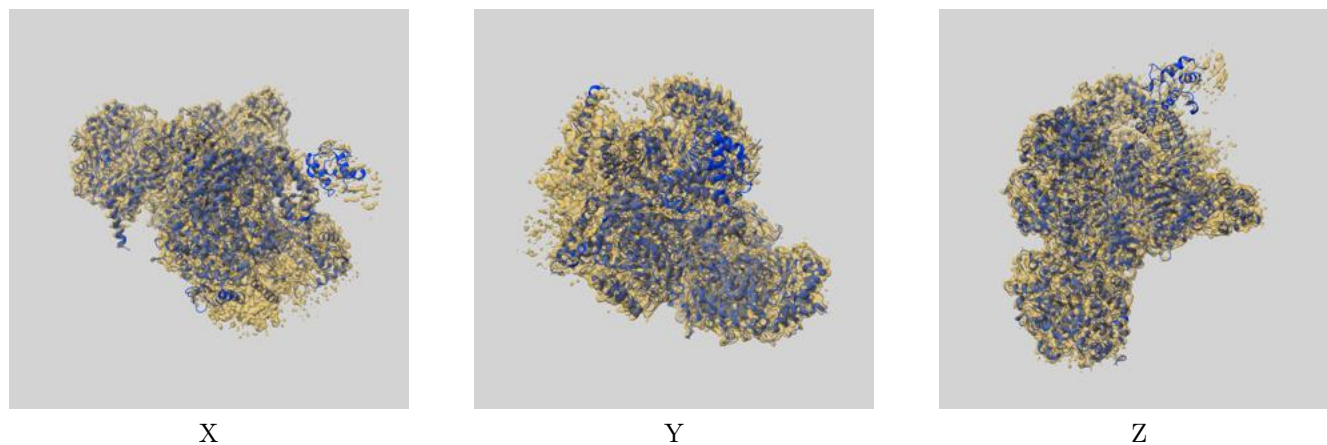
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.91	-	-
Author-provided FSC curve	2.92	3.40	2.96
Unmasked-calculated*	3.73	4.42	3.80

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.73 differs from the reported value 2.91 by more than 10 %

9 Map-model fit [i](#)

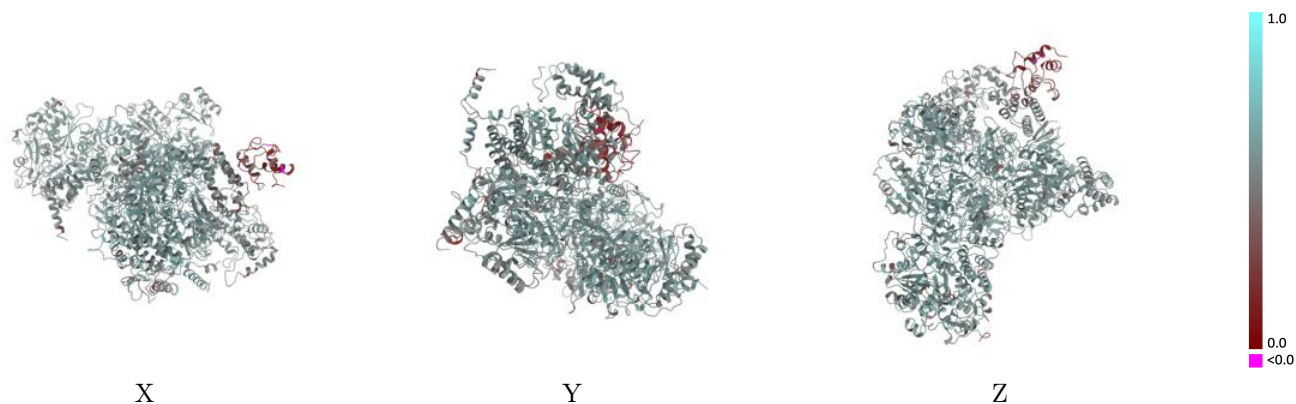
This section contains information regarding the fit between EMDB map EMD-11873 and PDB model 7AQR. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



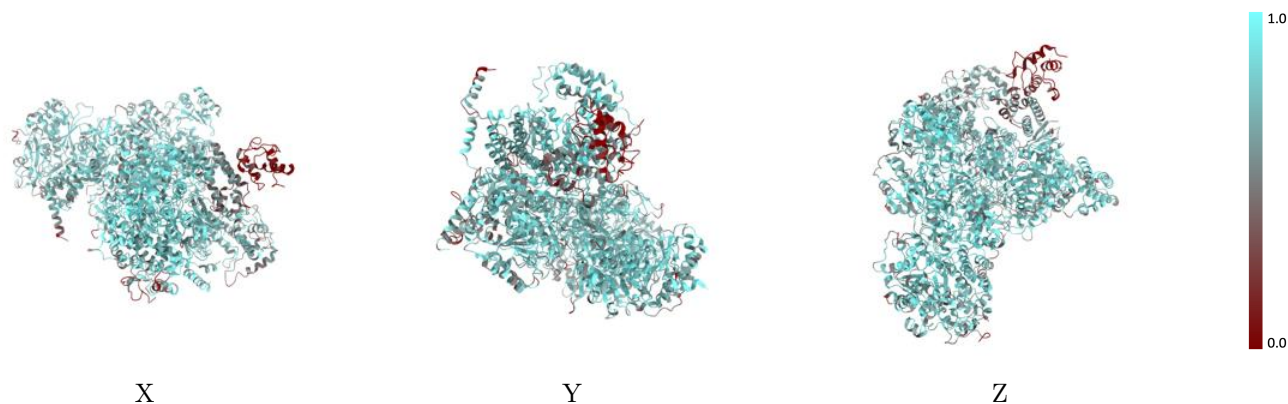
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



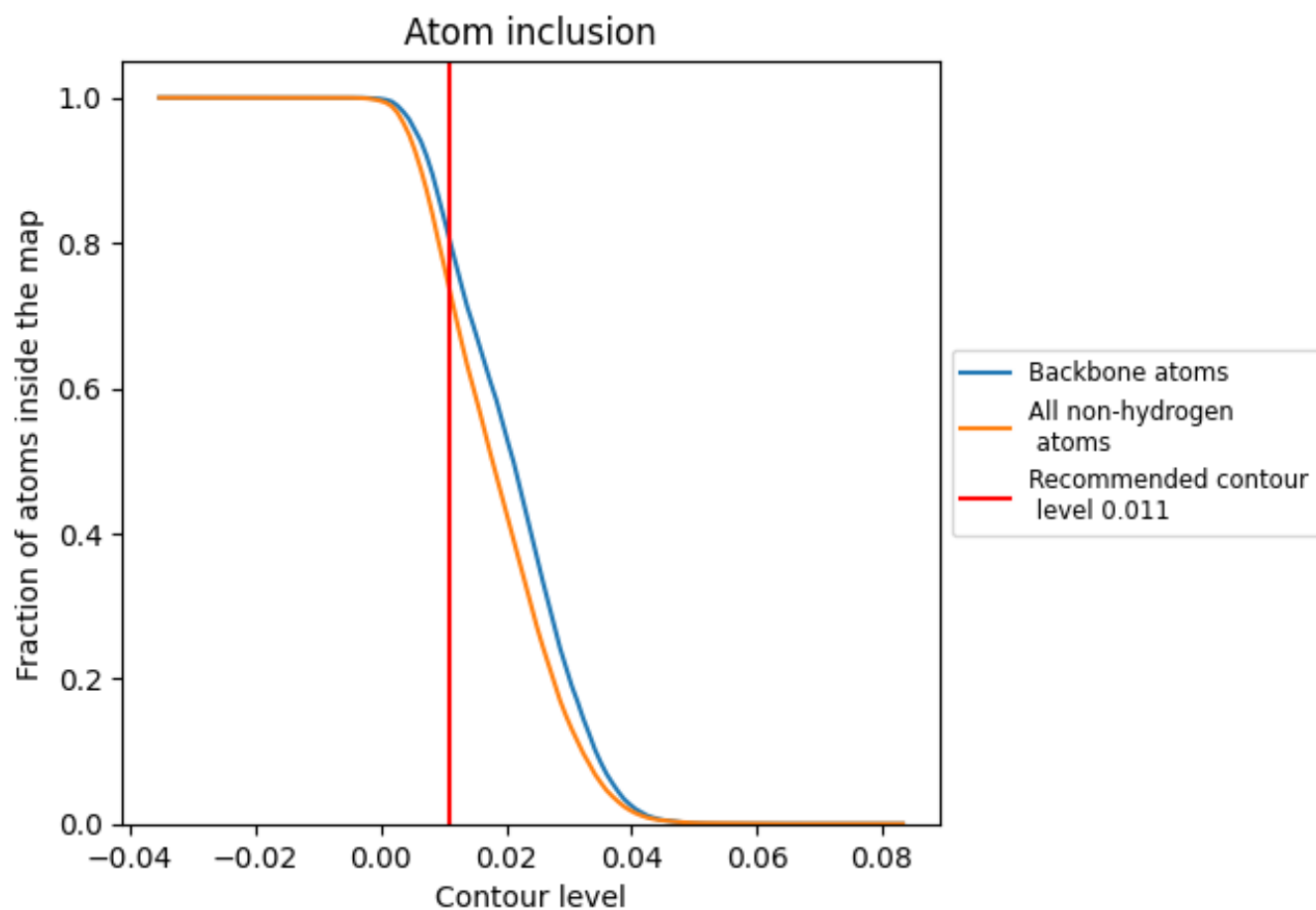
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.011).





































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 74% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7354	 0.5540
B	 0.8463	 0.5910
C	 0.8400	 0.5940
D	 0.8156	 0.5880
E	 0.7059	 0.5250
F	 0.7531	 0.5600
G	 0.7918	 0.5780
I	 0.8087	 0.5800
P	 0.6694	 0.5270
Q	 0.7538	 0.5890
R	 0.7642	 0.5830
S	 0.7637	 0.5580
U	 0.0864	 0.2510
V	 0.7468	 0.5380
W	 0.5120	 0.4900
Z	 0.5677	 0.5130
q	 0.4540	 0.4900
r	 0.3690	 0.4840

