



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:42 AM UTC

PDB ID : 8BEE / pdb\_00008bee  
EMDB ID : EMD-15999  
Title : Cryo-EM structure of the Arabidopsis thaliana I+III2 supercomplex (CI peripheral core)  
Authors : Klusch, N.; Kuehlbrandt, W.  
Deposited on : 2022-10-21  
Resolution : 2.04 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](mailto: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>.

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

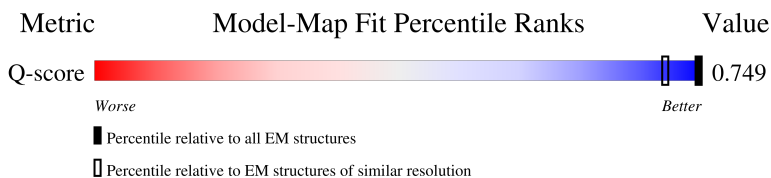
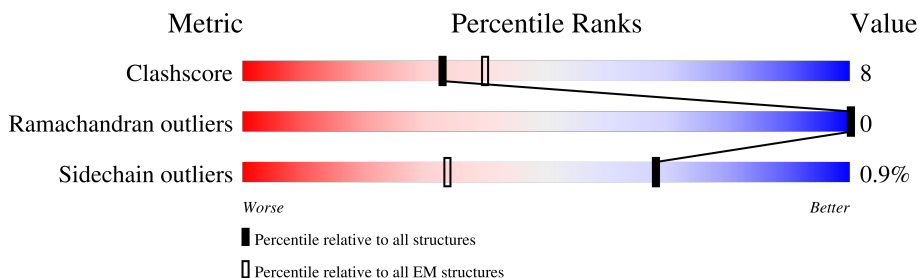
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.04 Å.

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





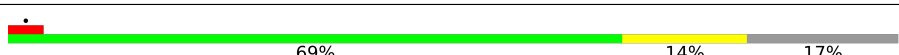
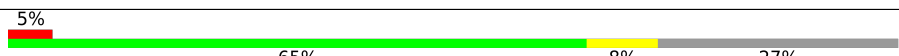

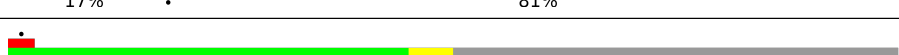
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1810 ( 1.55 - 2.54 )

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  $\geq 3$ , 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	56% (green), 15% (yellow), 28% (grey)
2	C	190	79% (green), 15% (yellow), 5% (orange), 1% (red)
3	D	394	80% (green), 18% (yellow), 2% (orange), 1% (red)
4	I	222	56% (green), 15% (yellow), 29% (grey)

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Mol	Chain	Length	Quality of chain
5	P	402	
6	U	126	
7	V	169	
8	W	133	
9	Z	143	
10	q	159	

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
11	SF4	I	500	-	-	X	-

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 13780 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	181	1545	997	266	276	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] iron-sulfur protein 8-A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	I	157	1282	813	215	244	10	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	P	316	2453	1580	414	444	15	0	0

- Molecule 6 is a protein called Acyl carrier protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	U	87	677	427	110	139	1	0	0

- Molecule 7 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		
7	V	140	1123	712	187	219	5	0	0

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	W	97	773	490	142	138	3	0	0

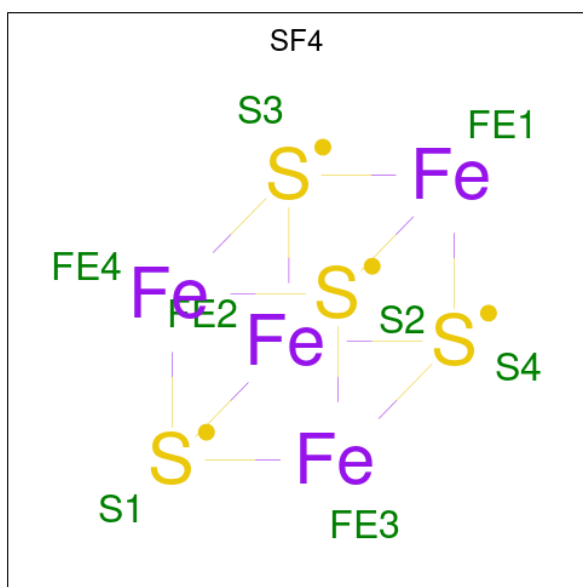
- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A.

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

- Molecule 10 is a protein called Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

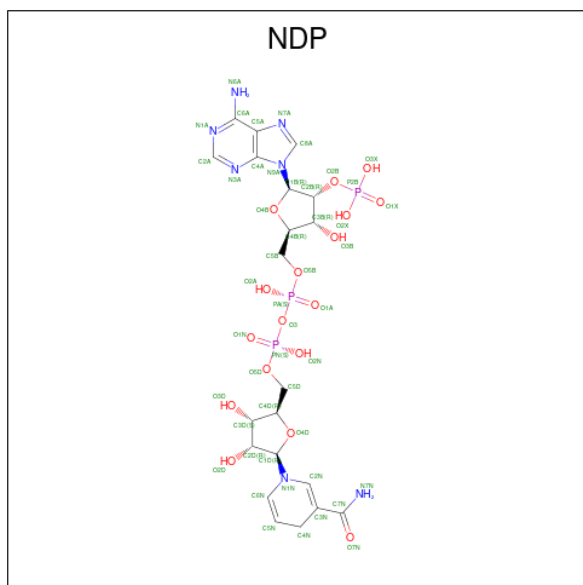
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	q	80	669	427	120	120	2	1	0

- Molecule 11 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
11	B	1	Total Fe S 8 4 4	0
11	I	1	Total Fe S 8 4 4	0
11	I	1	Total Fe S 8 4 4	0

- Molecule 12 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ) (labeled as "Ligand of Interest" by depositor).





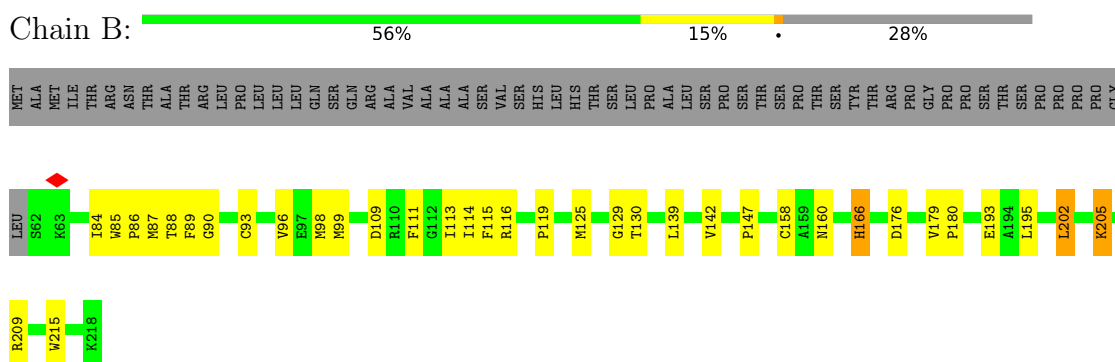
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
14	Z	6	Total 6	O 6	0
14	q	33	Total 33	O 33	0

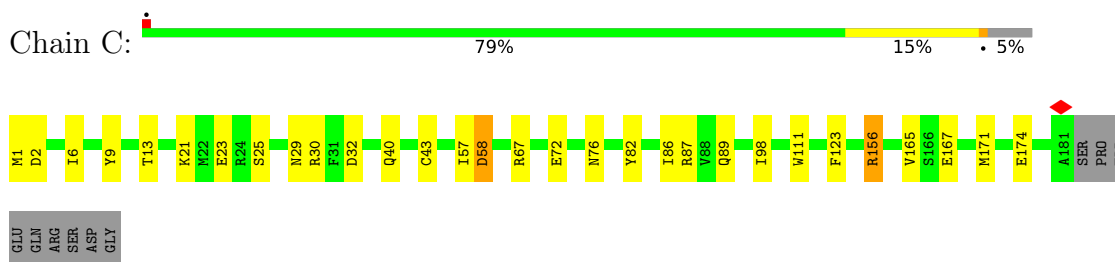
### 3 Residue-property plots [i](#)

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.

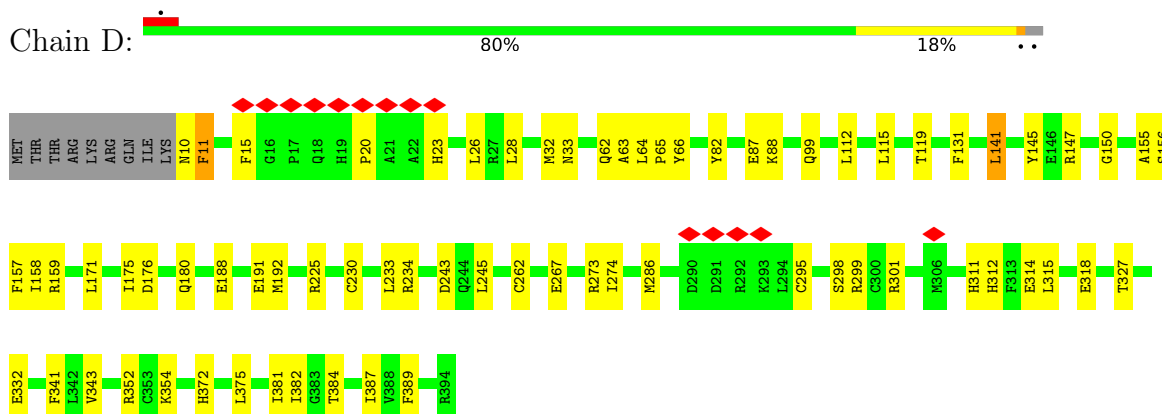
- Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



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



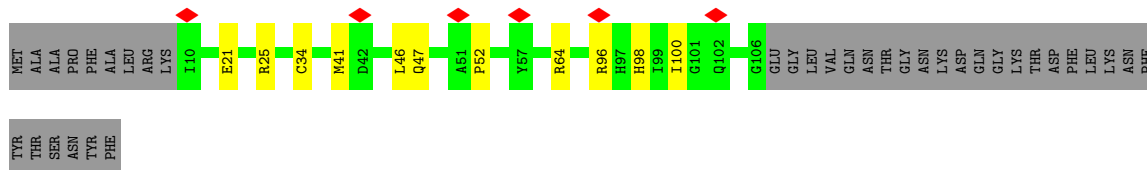
- Molecule 3: NADH dehydrogenase subunit 7



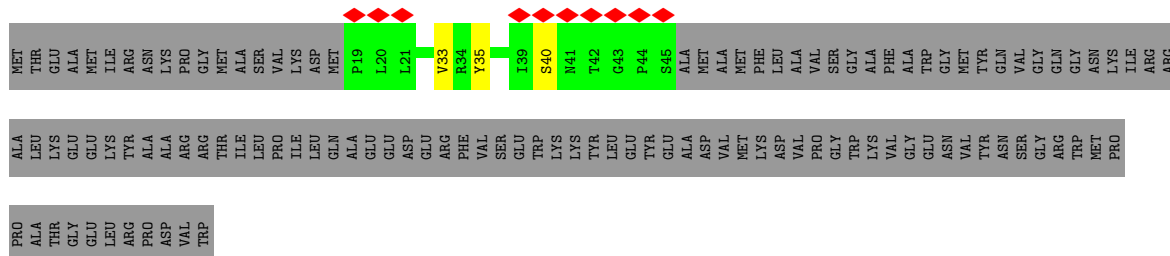




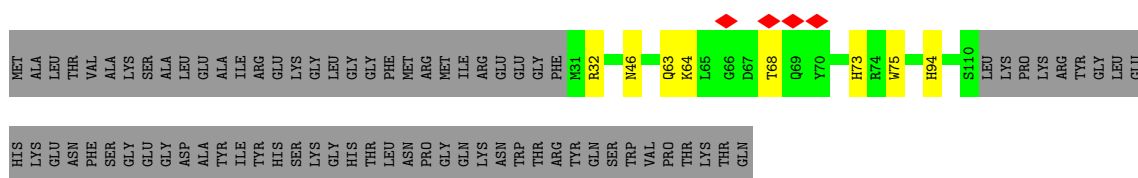
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A



- Molecule 10: Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	213993	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	215000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	17.742	Depositor
Minimum map value	-8.300	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.420	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	127.779, 133.509, 126.633	wwPDB
Map dimensions	221, 233, 223	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.573, 0.573, 0.573	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: SF4, NDP, 8Q1

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	0.90	6/1279 (0.5%)	0.83	0/1734
2	C	0.68	0/1590	0.75	3/2152 (0.1%)
3	D	0.75	12/3147 (0.4%)	0.73	1/4256 (0.0%)
4	I	0.57	3/1310 (0.2%)	0.57	2/1771 (0.1%)
5	P	0.62	2/2509 (0.1%)	0.79	3/3401 (0.1%)
6	U	0.19	0/687	0.41	0/929
7	V	0.70	2/1146 (0.2%)	0.79	0/1555
8	W	0.51	0/788	0.74	2/1069 (0.2%)
9	Z	0.13	0/206	0.35	0/281
10	q	0.25	0/690	0.37	0/936
All	All	0.66	25/13352 (0.2%)	0.71	11/18084 (0.1%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	V	107	ASP	C-O	-9.01	1.19	1.23
7	V	129	HIS	C-O	-7.68	1.14	1.24
4	I	134	PRO	C-O	-7.20	1.14	1.24
1	B	147	PRO	C-O	-6.84	1.16	1.23
3	D	147	ARG	C-O	-6.81	1.16	1.24
1	B	166	HIS	C-O	-6.54	1.15	1.24
3	D	63	ALA	C-O	-6.52	1.15	1.24
3	D	65	PRO	C-O	-6.39	1.15	1.24
1	B	180	PRO	C-O	-6.28	1.16	1.23
3	D	66	TYR	C-O	-6.26	1.16	1.24
3	D	141	LEU	C-O	-6.25	1.16	1.24
4	I	161	LYS	C-O	-5.98	1.16	1.24
3	D	159	ARG	C-O	-5.92	1.18	1.24
3	D	155	ALA	C-O	-5.80	1.17	1.24
4	I	167	PHE	C-O	-5.77	1.17	1.24
3	D	158	ILE	C-O	-5.74	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	202	LEU	C-O	-5.68	1.17	1.24
3	D	99	GLN	C-O	-5.63	1.17	1.24
1	B	119	PRO	C-O	-5.59	1.16	1.24
1	B	205	LYS	C-O	-5.50	1.17	1.24
3	D	87	GLU	C-O	-5.24	1.18	1.24
5	P	98	PRO	C-O	-5.22	1.17	1.23
3	D	157	PHE	C-O	-5.11	1.17	1.24
3	D	62	GLN	C-O	-5.08	1.17	1.24
5	P	287	VAL	C-O	-5.05	1.18	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	124	ASP	CA-CB-CG	8.46	121.06	112.60
3	D	11	PHE	CA-CB-CG	7.53	121.33	113.80
8	W	98	HIS	N-CA-CB	-6.57	101.49	110.56
5	P	289	THR	CB-CA-C	6.47	121.16	109.83
2	C	29	ASN	N-CA-CB	5.81	118.52	109.97
5	P	296	ILE	N-CA-C	-5.80	104.71	110.62
2	C	58	ASP	N-CA-C	5.37	116.30	108.14
4	I	190	HIS	CA-CB-CG	5.34	119.14	113.80
2	C	156	ARG	CG-CD-NE	-5.34	100.25	112.00
8	W	98	HIS	CA-CB-CG	-5.20	108.60	113.80
4	I	167	PHE	O-C-N	5.12	127.55	122.12

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	26	0
2	C	1545	0	1501	29	0
3	D	3077	0	3043	50	0
4	I	1282	0	1236	28	0
5	P	2453	0	2493	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	U	677	0	665	20	0
7	V	1123	0	1112	20	0
8	W	773	0	782	12	0
9	Z	199	0	198	2	0
10	q	669	0	630	7	0
11	B	8	0	0	1	0
11	I	16	0	0	2	0
12	P	48	0	26	0	0
13	W	35	0	0	0	0
14	B	88	0	0	5	0
14	C	105	0	0	3	0
14	D	222	0	0	18	0
14	I	94	0	0	11	0
14	P	44	0	0	7	0
14	V	31	0	0	4	0
14	W	8	0	0	1	0
14	Z	6	0	0	0	0
14	q	33	0	0	0	0
All	All	13780	0	12917	219	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 (219) 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)
3:D:372:HIS:HE1	14:D:516:HOH:O	1.15	1.30
2:C:57:ILE:HA	14:D:477:HOH:O	1.31	1.25
1:B:202:LEU:HA	14:B:669:HOH:O	1.39	1.21
4:I:159:MET:HA	14:I:687:HOH:O	1.44	1.18
3:D:145:TYR:HD1	14:D:469:HOH:O	1.47	0.98
2:C:165:VAL:HB	8:W:96:ARG:CZ	1.95	0.95
5:P:194:SER:OG	5:P:342:ASP:OD1	1.90	0.89
2:C:57:ILE:HD13	14:D:477:HOH:O	1.72	0.88
3:D:10:ASN:OD1	3:D:33:ASN:OD1	1.92	0.88
4:I:84:LEU:HA	14:I:685:HOH:O	1.74	0.85
3:D:372:HIS:CE1	14:D:516:HOH:O	2.02	0.83
5:P:254:GLN:HG2	5:P:287:VAL:HG22	1.60	0.82
7:V:63:GLN:HE21	7:V:141:GLN:HG2	1.44	0.80
5:P:194:SER:CB	5:P:342:ASP:OD1	2.30	0.79
3:D:145:TYR:CD1	14:D:469:HOH:O	2.28	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:HIS:NE2	2:C:171:MET:HE1	2.00	0.77
2:C:165:VAL:HB	8:W:96:ARG:NH1	1.99	0.76
5:P:319:ALA:O	14:P:601:HOH:O	2.03	0.76
2:C:72:GLU:OE1	2:C:89:GLN:NE2	2.19	0.75
3:D:191:GLU:OE2	4:I:82:LEU:HD23	1.89	0.73
6:U:70:THR:HG23	6:U:72:LYS:H	1.54	0.73
4:I:157:ILE:HB	14:I:647:HOH:O	1.90	0.71
3:D:10:ASN:CG	3:D:33:ASN:OD1	2.33	0.71
4:I:84:LEU:HD12	14:I:685:HOH:O	1.89	0.70
1:B:205:LYS:HB3	14:B:669:HOH:O	1.91	0.68
1:B:88:THR:HG23	1:B:115:PHE:CD1	2.28	0.68
1:B:209:ARG:NH1	5:P:104:ASP:OD2	2.27	0.68
3:D:299:ARG:NH2	4:I:175:ASP:OD1	2.28	0.67
6:U:115:ALA:O	6:U:119:ILE:HD12	1.94	0.67
2:C:43:CYS:SG	14:V:230:HOH:O	2.52	0.67
7:V:63:GLN:NE2	7:V:141:GLN:HG2	2.10	0.66
3:D:156:SER:HB2	14:I:660:HOH:O	1.94	0.66
2:C:30:ARG:HB2	14:C:232:HOH:O	1.95	0.66
6:U:50:VAL:HG12	6:U:116:VAL:HG23	1.77	0.66
2:C:165:VAL:HG23	2:C:167:GLU:OE1	1.96	0.66
3:D:262:CYS:SG	14:D:611:HOH:O	2.54	0.65
6:U:61:PHE:HZ	6:U:88:GLU:HB3	1.62	0.65
1:B:160:ASN:ND2	14:B:603:HOH:O	2.29	0.64
6:U:81:LEU:HD22	6:U:85:ASP:HB3	1.79	0.64
4:I:162:CYS:HB3	14:I:687:HOH:O	1.97	0.63
8:W:21:GLU:OE1	8:W:25:ARG:NH2	2.30	0.63
8:W:47:GLN:OE1	8:W:47:GLN:N	2.21	0.63
4:I:195:TYR:HB2	14:I:647:HOH:O	1.99	0.63
5:P:135:MET:HE1	5:P:171:ALA:HA	1.82	0.62
3:D:28:LEU:HD11	3:D:382:ILE:HD11	1.82	0.62
3:D:286:MET:HA	3:D:286:MET:HE2	1.81	0.61
3:D:23:HIS:CD2	3:D:26:LEU:HD22	2.36	0.60
3:D:234:ARG:NH2	14:D:409:HOH:O	2.33	0.60
5:P:181:ILE:HD13	5:P:215:THR:HB	1.84	0.60
10:q:46:ASN:OD1	10:q:75[A]:TRP:NE1	2.31	0.60
8:W:96:ARG:HD3	14:W:302:HOH:O	2.01	0.59
5:P:314:ILE:O	5:P:318:MET:HG3	2.02	0.59
4:I:99:GLU:OE2	14:I:601:HOH:O	2.17	0.59
7:V:83:CYS:HB2	7:V:89:LEU:HD21	1.85	0.58
1:B:87:MET:HE1	1:B:142:VAL:HG11	1.85	0.58
3:D:23:HIS:NE2	3:D:387:ILE:HB	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:141:LEU:HD12	14:D:610:HOH:O	2.04	0.57
5:P:126:ARG:NH1	5:P:158:ASP:OD2	2.33	0.57
10:q:64:LYS:HB2	10:q:73:HIS:HB3	1.87	0.56
2:C:40:GLN:NE2	14:C:202:HOH:O	2.25	0.56
5:P:140:VAL:HG11	5:P:269:LEU:HD21	1.87	0.56
7:V:91:GLU:OE2	14:V:201:HOH:O	2.18	0.56
3:D:298:SER:OG	3:D:301:ARG:HG2	2.06	0.56
3:D:191:GLU:CD	4:I:82:LEU:HD23	2.31	0.55
7:V:49:GLU:O	7:V:55:LYS:NZ	2.39	0.55
1:B:88:THR:HB	1:B:98:MET:CE	2.37	0.55
4:I:141:GLU:HG3	4:I:154:ARG:HD2	1.88	0.55
7:V:140:GLU:CG	7:V:144:LYS:HE3	2.37	0.55
5:P:107:ARG:HD2	14:P:633:HOH:O	2.07	0.55
2:C:165:VAL:CB	8:W:96:ARG:CZ	2.77	0.55
6:U:70:THR:HG22	6:U:73:ALA:HB2	1.89	0.55
5:P:205:GLU:O	5:P:209:ASN:ND2	2.39	0.54
3:D:245:LEU:HD13	3:D:274:ILE:HG23	1.89	0.54
3:D:119:THR:HB	3:D:131:PHE:HA	1.91	0.53
5:P:233:TRP:CH2	5:P:290:THR:HG23	2.43	0.53
4:I:84:LEU:CA	14:I:685:HOH:O	2.45	0.53
3:D:315:LEU:HD12	14:D:582:HOH:O	2.08	0.53
1:B:88:THR:HG23	1:B:115:PHE:HD1	1.72	0.53
2:C:86:ILE:HD12	2:C:87:ARG:H	1.74	0.53
3:D:188:GLU:O	3:D:191:GLU:HG3	2.08	0.53
3:D:230:CYS:SG	14:D:585:HOH:O	2.59	0.53
2:C:25:SER:CB	7:V:122:ASN:HB3	2.39	0.53
3:D:315:LEU:CD1	14:D:582:HOH:O	2.57	0.53
4:I:78:ARG:NH2	9:Z:40:SER:OG	2.43	0.52
1:B:89:PHE:CD1	1:B:139:LEU:HD23	2.44	0.52
4:I:59:ASP:OD2	4:I:61:ASN:ND2	2.42	0.52
5:P:107:ARG:O	5:P:110:LYS:HG3	2.10	0.52
5:P:215:THR:HA	14:P:602:HOH:O	2.09	0.52
5:P:135:MET:HE3	5:P:141:VAL:HG21	1.90	0.52
5:P:204:GLU:HG2	5:P:216:ILE:HD12	1.92	0.52
7:V:72:GLU:N	7:V:72:GLU:OE1	2.44	0.51
5:P:292:GLU:HA	5:P:295:GLU:OE1	2.10	0.51
3:D:23:HIS:HB2	3:D:26:LEU:HB2	1.93	0.51
5:P:157:GLU:H	5:P:157:GLU:CD	2.19	0.51
6:U:61:PHE:CZ	6:U:88:GLU:HB3	2.45	0.51
5:P:194:SER:CA	5:P:342:ASP:OD1	2.59	0.51
3:D:314:GLU:OE1	3:D:318:GLU:HB3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:115:LEU:HD12	14:D:610:HOH:O	2.11	0.50
4:I:82:LEU:HD12	4:I:85:LYS:HD3	1.92	0.50
1:B:130:THR:HA	1:B:158:CYS:HB3	1.94	0.50
7:V:134:ARG:NH1	14:V:203:HOH:O	2.30	0.50
3:D:176:ASP:O	3:D:180:GLN:HG2	2.11	0.50
4:I:111:HIS:CE1	11:I:500:SF4:S4	3.05	0.50
4:I:195:TYR:CB	14:I:647:HOH:O	2.59	0.50
2:C:171:MET:HG2	2:C:174:GLU:HA	1.94	0.49
3:D:312:HIS:ND1	14:D:411:HOH:O	2.34	0.49
4:I:123:CYS:O	4:I:151:ARG:NH1	2.44	0.49
5:P:186:LEU:HA	5:P:218:ARG:HB3	1.94	0.49
3:D:273:ARG:HD2	9:Z:35:TYR:CZ	2.47	0.49
3:D:243:ASP:OD1	14:D:401:HOH:O	2.20	0.49
5:P:173:GLU:HA	5:P:173:GLU:OE2	2.13	0.48
5:P:273:GLY:O	5:P:276:MET:HG3	2.13	0.48
3:D:341:PHE:HB3	3:D:354:LYS:HB3	1.96	0.48
5:P:161:HIS:HA	5:P:203:ALA:HB2	1.95	0.48
3:D:381:ILE:O	3:D:384:THR:HG22	2.13	0.48
6:U:91:MET:HE2	8:W:34:CYS:HB3	1.95	0.48
5:P:194:SER:OG	5:P:342:ASP:CG	2.55	0.48
10:q:32:ARG:HA	10:q:32:ARG:HD2	1.68	0.48
6:U:55:LEU:HD12	6:U:112:ILE:HD13	1.96	0.47
5:P:196:MET:HB3	5:P:342:ASP:OD2	2.14	0.47
3:D:245:LEU:HB3	14:D:421:HOH:O	2.14	0.47
5:P:252:LYS:HB2	5:P:352:LEU:HD11	1.96	0.47
7:V:28:ASN:OD1	7:V:28:ASN:N	2.48	0.47
3:D:11:PHE:CE1	3:D:32:MET:HB2	2.49	0.47
6:U:111:SER:OG	6:U:113:ASP:OD2	2.31	0.47
5:P:301:ILE:HG13	5:P:303:GLU:HB2	1.96	0.47
2:C:25:SER:HB3	7:V:122:ASN:HB3	1.96	0.46
2:C:43:CYS:SG	14:V:222:HOH:O	2.49	0.46
8:W:46:LEU:HD11	8:W:100:ILE:HD11	1.96	0.46
1:B:111:PHE:HB2	1:B:113:ILE:HD12	1.98	0.46
2:C:67:ARG:O	14:C:201:HOH:O	2.20	0.46
7:V:56:ALA:HB2	7:V:149:LEU:HD11	1.98	0.46
1:B:88:THR:HB	1:B:98:MET:HE3	1.96	0.46
1:B:129:GLY:HA2	11:B:500:SF4:S3	2.56	0.46
3:D:233:LEU:HB2	3:D:332:GLU:HB2	1.97	0.46
4:I:99:GLU:OE2	10:q:75[B]:TRP:NE1	2.49	0.46
5:P:69:ILE:HD12	5:P:91:MET:HE1	1.98	0.46
3:D:15:PHE:HE2	3:D:375:LEU:HD11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:192:MET:HG3	14:D:573:HOH:O	2.15	0.45
6:U:91:MET:HE2	8:W:34:CYS:SG	2.56	0.45
5:P:76:ALA:HB3	5:P:97:VAL:HG13	1.98	0.45
5:P:104:ASP:HB3	14:P:630:HOH:O	2.16	0.45
6:U:126:LYS:HB2	6:U:126:LYS:HE2	1.69	0.45
3:D:26:LEU:HD21	3:D:382:ILE:HD13	1.98	0.45
3:D:301:ARG:HA	3:D:301:ARG:HD2	1.76	0.45
3:D:225:ARG:NH2	3:D:267:GLU:OE2	2.45	0.45
5:P:194:SER:HA	5:P:342:ASP:OD1	2.16	0.45
2:C:9:TYR:CZ	2:C:13:THR:HG21	2.51	0.45
4:I:86:TYR:HA	4:I:89:ASP:OD2	2.17	0.44
5:P:135:MET:HE1	5:P:171:ALA:CA	2.45	0.44
4:I:111:HIS:NE2	11:I:500:SF4:S4	2.91	0.44
2:C:2:ASP:O	2:C:6:ILE:HG13	2.18	0.44
1:B:90:GLY:HA3	3:D:20:PRO:HD3	1.99	0.44
1:B:96:VAL:HA	1:B:99:MET:HE3	2.00	0.44
1:B:109:ASP:OD2	1:B:114:ILE:HD11	2.18	0.44
3:D:112:LEU:HA	14:D:610:HOH:O	2.18	0.43
5:P:229:ILE:C	5:P:232:PRO:HD2	2.43	0.43
5:P:301:ILE:O	5:P:302:ARG:C	2.61	0.43
6:U:51:THR:OG1	6:U:116:VAL:HG21	2.19	0.43
6:U:109:ILE:HD13	6:U:115:ALA:HA	2.01	0.43
6:U:74:ASN:OD1	6:U:76:GLN:N	2.51	0.43
1:B:176:ASP:HB2	14:B:632:HOH:O	2.17	0.43
2:C:23:GLU:HA	7:V:120:ILE:O	2.18	0.43
1:B:179:VAL:C	5:P:111:LEU:HD11	2.43	0.43
7:V:81:LEU:HA	7:V:81:LEU:HD23	1.80	0.43
2:C:25:SER:HB2	7:V:122:ASN:HB3	2.00	0.43
5:P:291:HIS:O	5:P:295:GLU:HG3	2.19	0.43
5:P:298:TYR:CZ	5:P:305:PRO:HA	2.54	0.43
2:C:156:ARG:NE	2:C:167:GLU:OE2	2.52	0.42
3:D:150:GLY:HA3	4:I:106:ARG:O	2.19	0.42
7:V:140:GLU:HG3	7:V:144:LYS:HE3	2.00	0.42
5:P:373:TYR:HD1	5:P:373:TYR:HA	1.71	0.42
5:P:361:GLN:HG2	14:P:638:HOH:O	2.20	0.42
2:C:1:MET:HA	7:V:138:LEU:HD11	2.02	0.42
3:D:23:HIS:CD2	3:D:389:PHE:HE2	2.38	0.42
4:I:210:GLU:OE2	10:q:94:HIS:HB3	2.20	0.42
5:P:204:GLU:OE2	5:P:216:ILE:HG21	2.19	0.42
5:P:315:ALA:HB1	5:P:344:ILE:HD13	2.01	0.42
7:V:72:GLU:CD	7:V:72:GLU:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:q:63:GLN:HA	10:q:73:HIS:O	2.19	0.42
6:U:94:GLU:CG	6:U:101:ILE:HG22	2.49	0.42
8:W:41:MET:HE2	8:W:52:PRO:HG3	2.01	0.42
5:P:103:GLU:HG3	14:P:640:HOH:O	2.19	0.42
5:P:165:GLU:O	5:P:169:LEU:HG	2.19	0.42
6:U:98:GLY:O	6:U:126:LYS:NZ	2.48	0.42
3:D:64:LEU:HD23	3:D:82:TYR:HD2	1.85	0.42
6:U:105:GLU:HG2	6:U:118:PHE:CE1	2.55	0.42
1:B:193:GLU:HB3	4:I:183:PHE:CE2	2.55	0.42
4:I:82:LEU:CD1	4:I:85:LYS:HD3	2.50	0.42
6:U:57:VAL:CG2	6:U:96:GLU:HG3	2.49	0.42
7:V:80:ARG:HE	7:V:80:ARG:HB3	1.74	0.42
2:C:165:VAL:CG1	8:W:96:ARG:NE	2.84	0.41
7:V:100:ILE:O	7:V:104:ILE:HG12	2.19	0.41
4:I:61:ASN:OD1	4:I:62:THR:N	2.53	0.41
1:B:88:THR:HB	1:B:98:MET:HE1	2.01	0.41
3:D:343:VAL:HB	3:D:352:ARG:HB3	2.03	0.41
1:B:195:LEU:HB2	14:B:685:HOH:O	2.21	0.41
1:B:215:TRP:CZ2	5:P:332:PRO:HG2	2.56	0.41
1:B:85:TRP:HB3	1:B:116:ARG:HG2	2.03	0.41
2:C:21:LYS:HB2	2:C:32:ASP:HB2	2.02	0.41
2:C:98:ILE:O	2:C:123:PHE:HA	2.21	0.41
5:P:98:PRO:HA	5:P:121:MET:O	2.20	0.41
6:U:82:ASP:CG	8:W:64:ARG:HH22	2.28	0.41
10:q:68:THR:HB	10:q:73:HIS:CE1	2.56	0.41
5:P:302:ARG:NH1	5:P:302:ARG:HG3	2.36	0.41
4:I:194:LEU:HB2	14:I:627:HOH:O	2.21	0.40
2:C:58:ASP:HB2	2:C:111:TRP:NE1	2.35	0.40
2:C:76:ASN:ND2	2:C:87:ARG:HG3	2.36	0.40
3:D:88:LYS:HD3	3:D:327:THR:HG21	2.03	0.40
5:P:100:ARG:HD2	14:P:639:HOH:O	2.19	0.40
1:B:84:ILE:O	1:B:86:PRO:HD3	2.21	0.40
5:P:157:GLU:CD	5:P:157:GLU:N	2.79	0.40
5:P:293:LEU:HD12	5:P:293:LEU:HA	1.87	0.40
5:P:152:ARG:HH21	5:P:332:PRO:HG3	1.86	0.40
1:B:125:MET:SD	1:B:139:LEU:HD21	2.62	0.40
2:C:1:MET:HB3	2:C:82:TYR:HB3	2.04	0.40
3:D:171:LEU:O	3:D:175:ILE:HG13	2.21	0.40
3:D:295:CYS:O	3:D:311:HIS:CE1	2.75	0.40
4:I:189:THR:OG1	4:I:192:GLU:HG3	2.21	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%)	149 (96%)	6 (4%)	0	100	100
2	C	179/190 (94%)	176 (98%)	3 (2%)	0	100	100
3	D	383/394 (97%)	366 (96%)	17 (4%)	0	100	100
4	I	153/222 (69%)	151 (99%)	2 (1%)	0	100	100
5	P	314/402 (78%)	301 (96%)	13 (4%)	0	100	100
6	U	85/126 (68%)	77 (91%)	8 (9%)	0	100	100
7	V	138/169 (82%)	135 (98%)	3 (2%)	0	100	100
8	W	95/133 (71%)	87 (92%)	8 (8%)	0	100	100
9	Z	25/143 (18%)	25 (100%)	0	0	100	100
10	q	79/159 (50%)	75 (95%)	4 (5%)	0	100	100
All	All	1606/2156 (74%)	1542 (96%)	64 (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%)	131 (99%)	1 (1%)	73	77
2	C	171/179 (96%)	171 (100%)	0	100	100
3	D	331/340 (97%)	331 (100%)	0	100	100
4	I	140/195 (72%)	137 (98%)	3 (2%)	47	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	P	263/334 (79%)	258 (98%)	5 (2%)	50	50
6	U	78/113 (69%)	77 (99%)	1 (1%)	61	63
7	V	123/148 (83%)	122 (99%)	1 (1%)	73	77
8	W	84/114 (74%)	84 (100%)	0	100	100
9	Z	21/115 (18%)	20 (95%)	1 (5%)	23	16
10	q	69/133 (52%)	69 (100%)	0	100	100
All	All	1412/1855 (76%)	1400 (99%)	12 (1%)	68	77

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	93	CYS
4	I	100	LYS
4	I	124	ILE
4	I	220	LEU
5	P	111	LEU
5	P	147	ARG
5	P	151	THR
5	P	289	THR
5	P	308	VAL
6	U	70	THR
7	V	39	LYS
9	Z	33	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	201	GLN
3	D	23	HIS
3	D	78	GLN
3	D	281	GLN
3	D	372	HIS
5	P	94	GLN
5	P	327	ASN
7	V	45	GLN
8	W	54	GLN
8	W	66	ASN
9	Z	41	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	NDP	P	500	-	51,52,52	0.58	0	71,80,80	0.70	0
11	SF4	B	500	1	0,12,12	-	-	-		
11	SF4	I	501	4	0,12,12	-	-	-		
11	SF4	I	500	4	0,12,12	-	-	-		
13	8Q1	W	200	-	32,34,34	0.33	0	39,43,43	0.46	0

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
11	SF4	B	500	1	-	-	0/6/5/5
12	NDP	P	500	-	-	6/34/77/77	0/5/5/5
11	SF4	I	501	4	-	-	0/6/5/5
13	8Q1	W	200	-	-	11/41/41/41	-
11	SF4	I	500	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

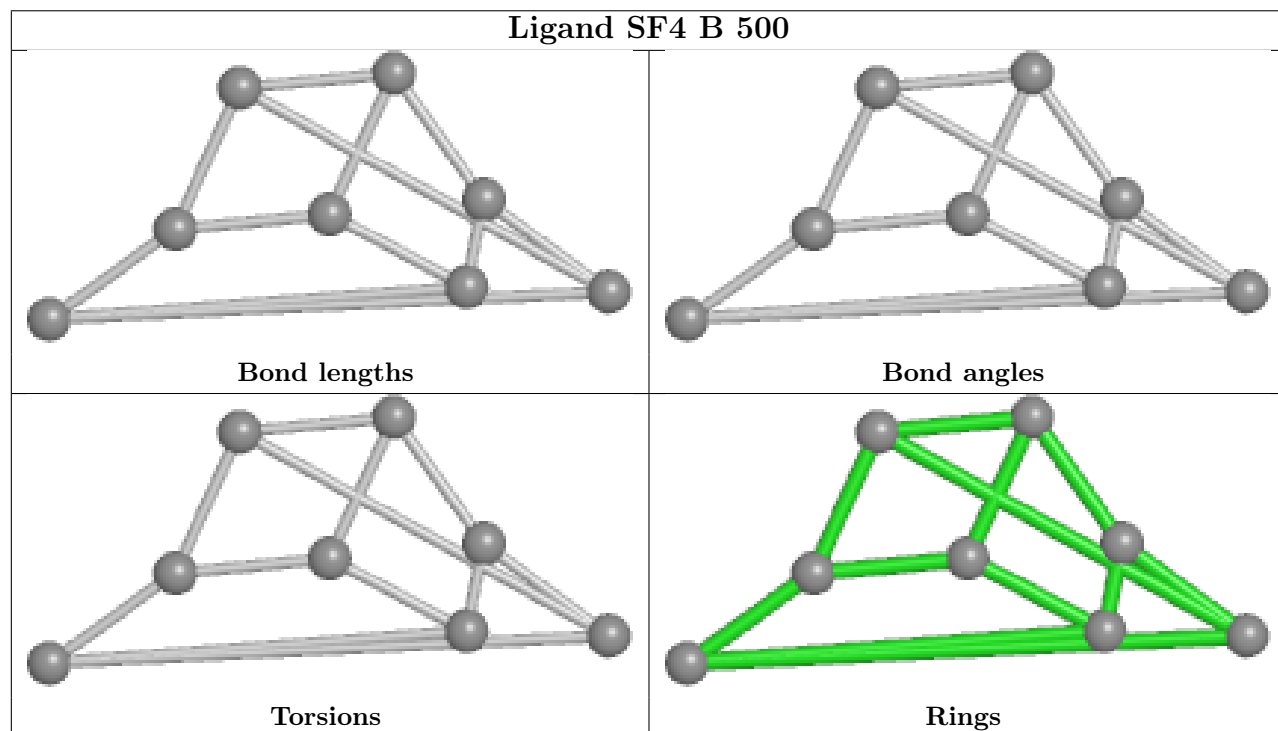
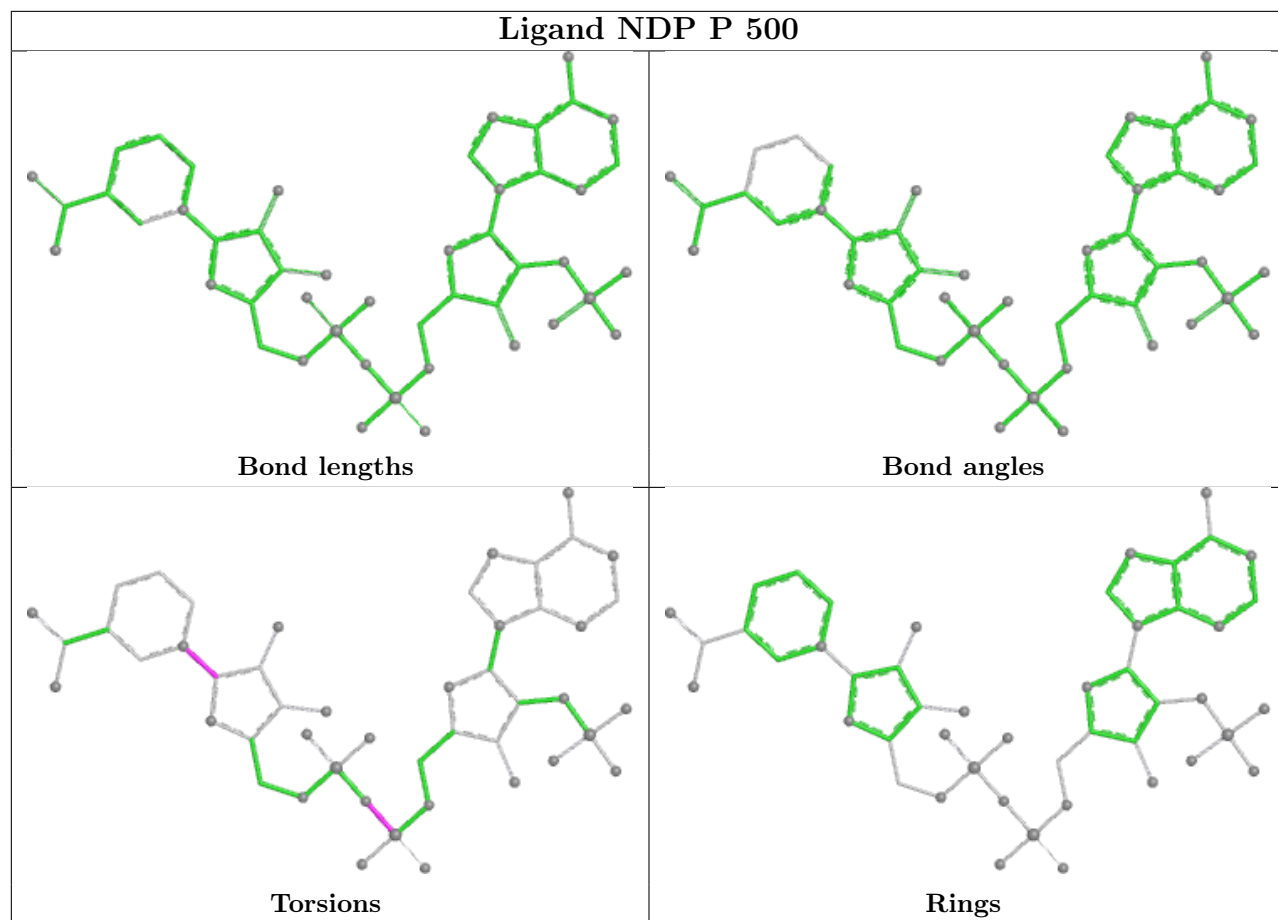
Mol	Chain	Res	Type	Atoms
13	W	200	8Q1	O27-C28-C29-C30
13	W	200	8Q1	O27-C28-C29-C31
13	W	200	8Q1	O27-C28-C29-C32
13	W	200	8Q1	C29-C28-O27-P24
13	W	200	8Q1	C28-C29-C32-C34
13	W	200	8Q1	C28-C29-C32-O33
13	W	200	8Q1	C30-C29-C32-O33
13	W	200	8Q1	C31-C29-C32-C34
13	W	200	8Q1	C31-C29-C32-O33
13	W	200	8Q1	C28-O27-P24-O1
12	P	500	NDP	C2D-C1D-N1N-C6N
12	P	500	NDP	C2D-C1D-N1N-C2N
12	P	500	NDP	PN-O3-PA-O1A
13	W	200	8Q1	C30-C29-C32-C34
12	P	500	NDP	O4D-C1D-N1N-C6N
12	P	500	NDP	O4D-C1D-N1N-C2N
12	P	500	NDP	PN-O3-PA-O2A

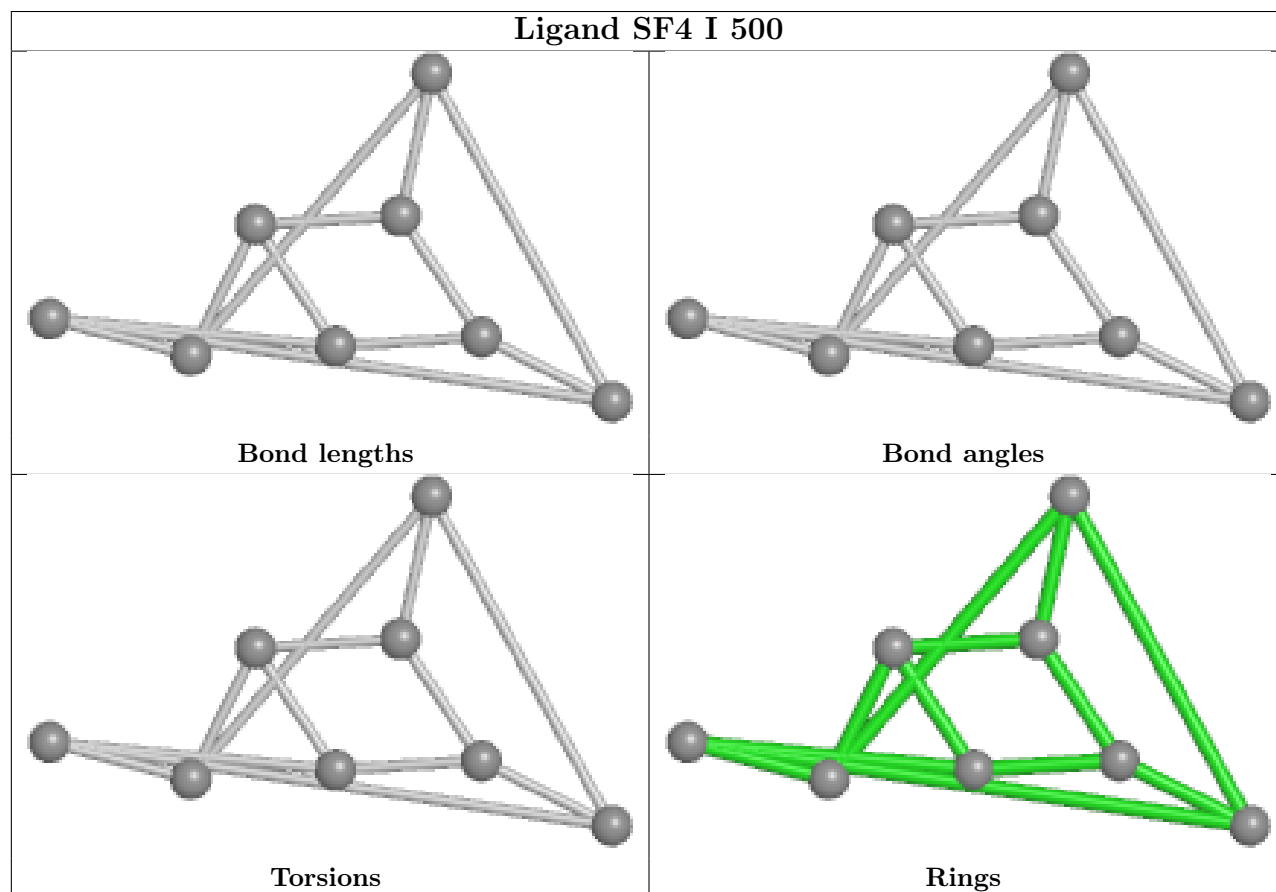
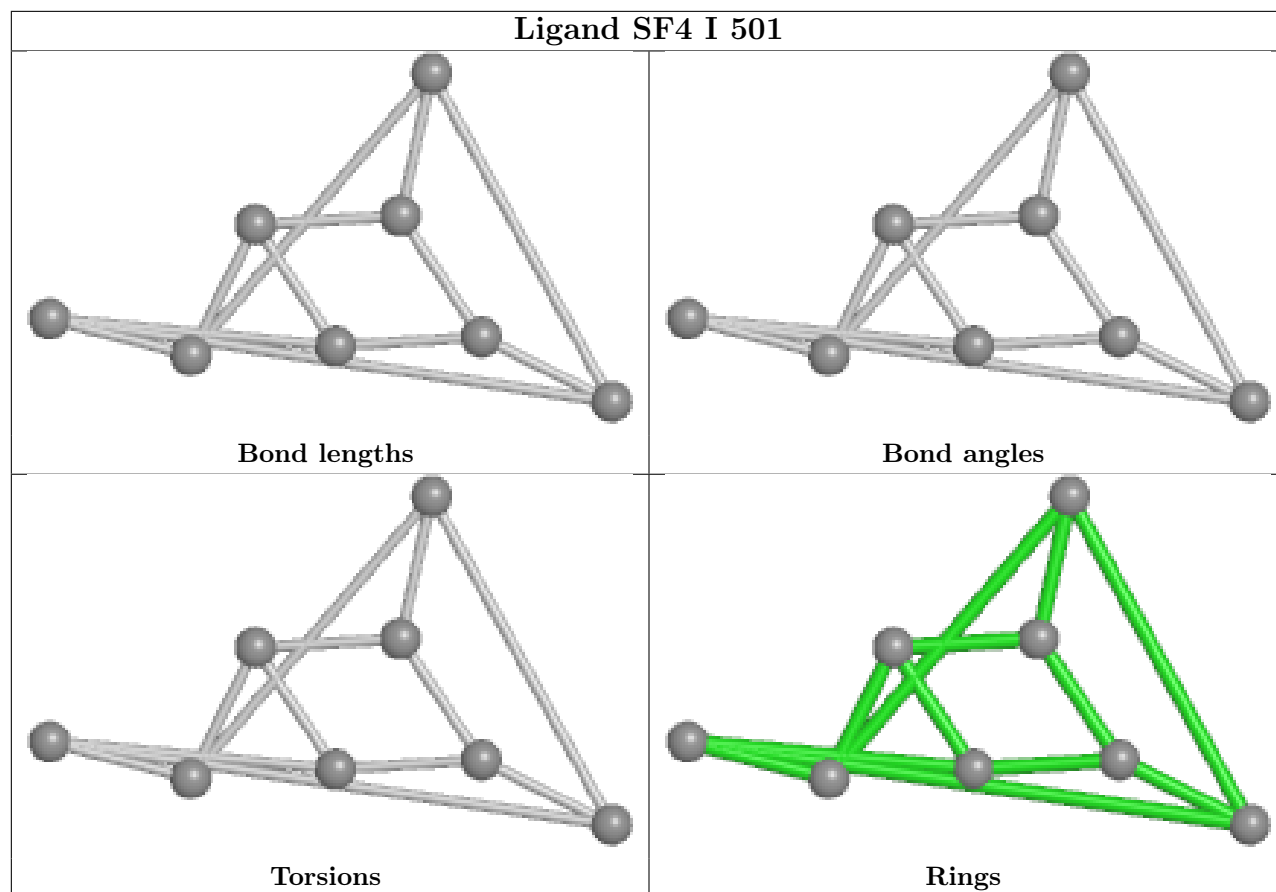
There are no ring outliers.

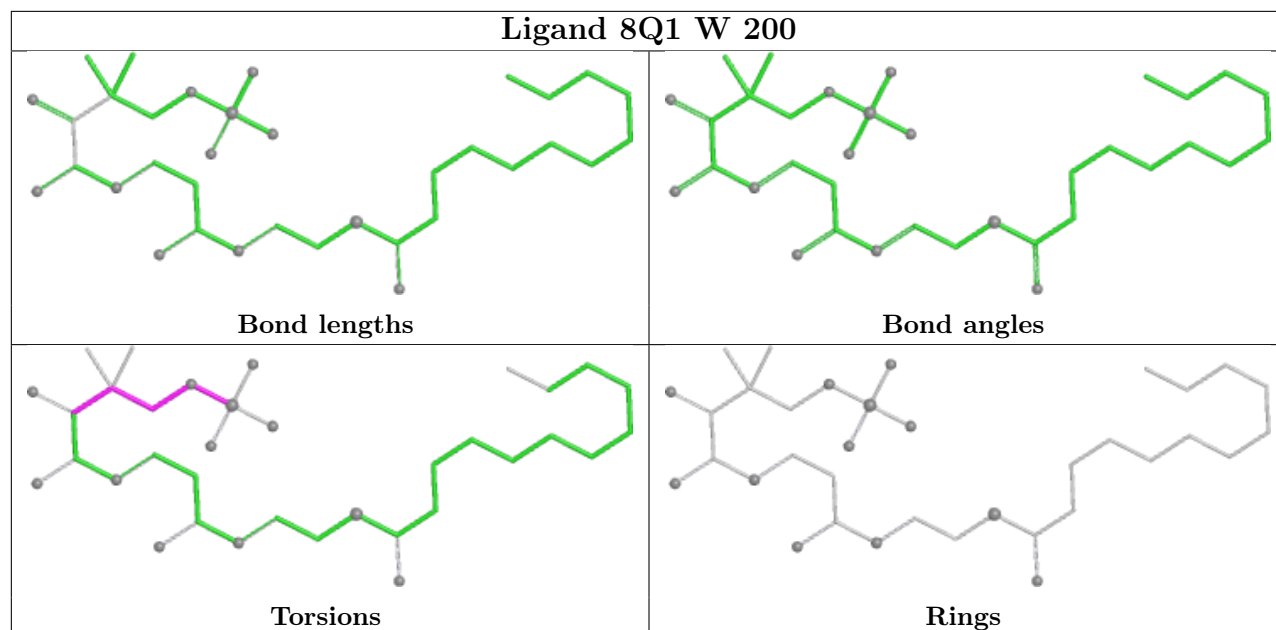
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	500	SF4	1	0
11	I	500	SF4	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.

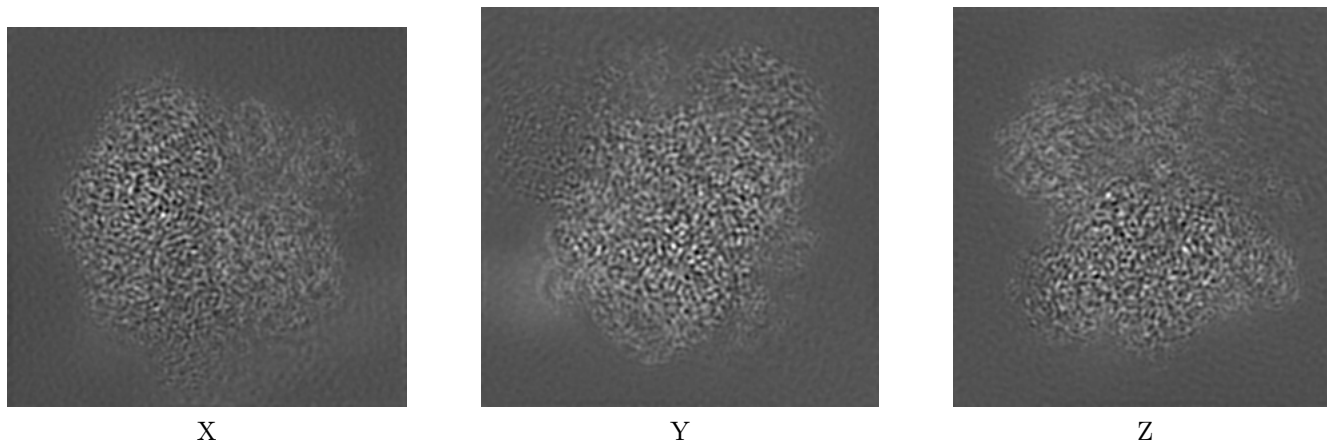
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15999. These allow visual inspection of the internal detail of the map and identification of artifacts.

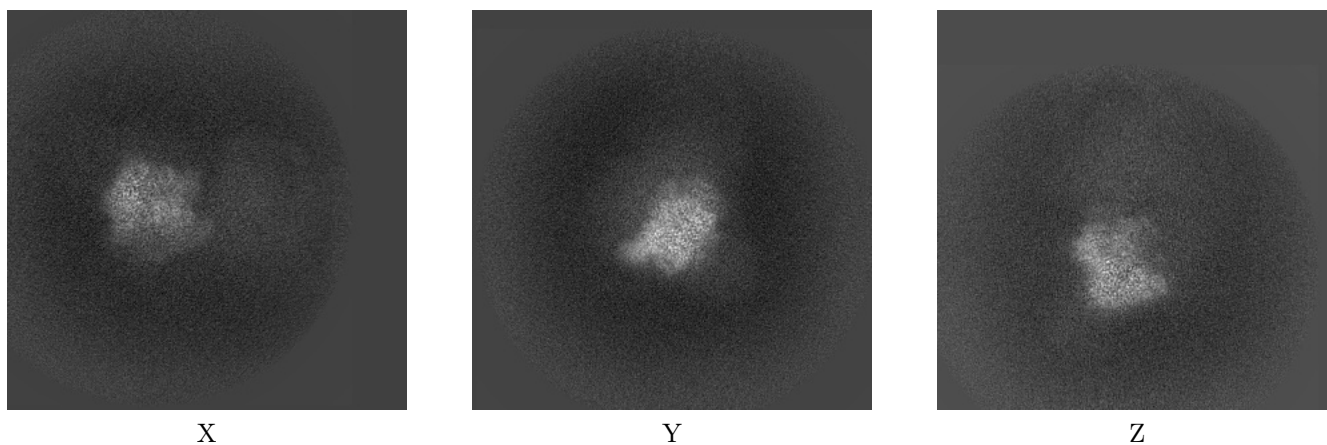
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



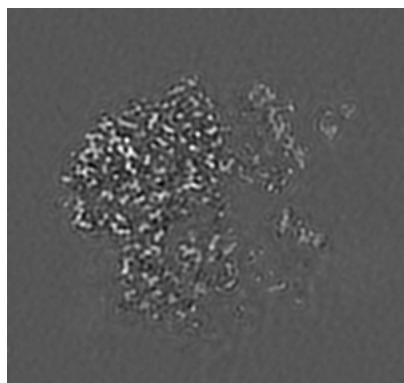
#### 6.1.2 Raw map



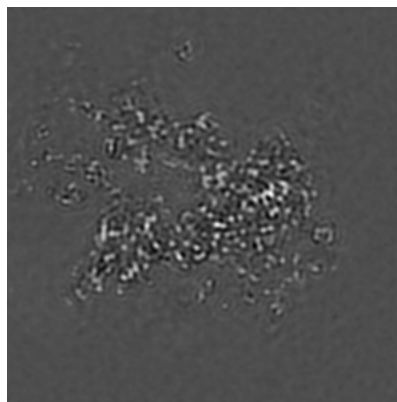
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

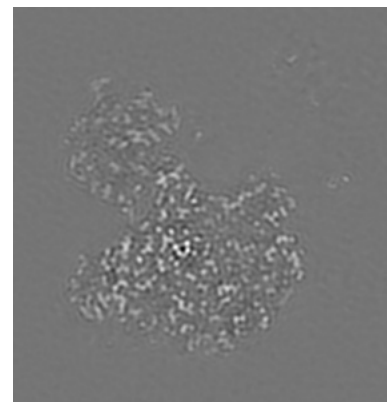
### 6.2.1 Primary map



X Index: 111

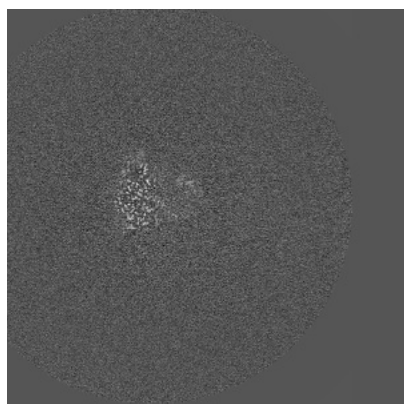


Y Index: 116

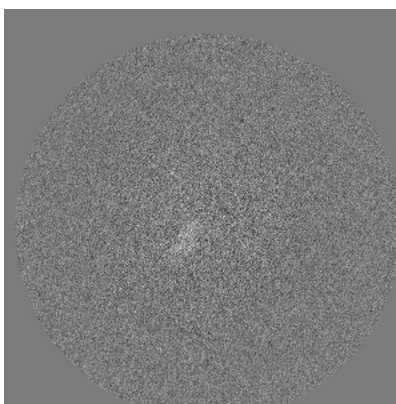


Z Index: 110

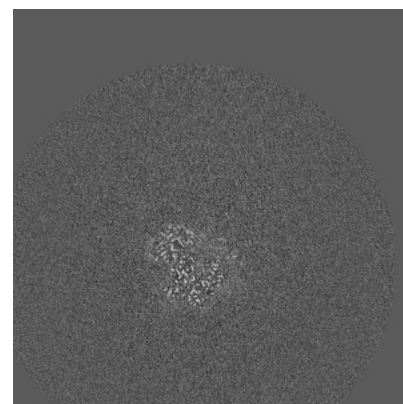
### 6.2.2 Raw map



X Index: 375



Y Index: 375

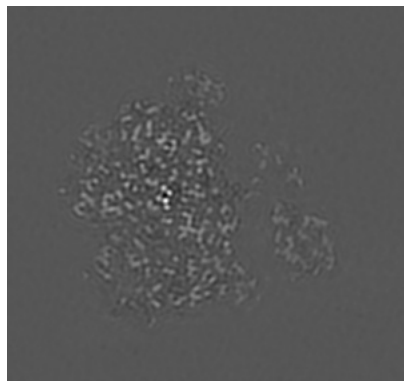


Z Index: 375

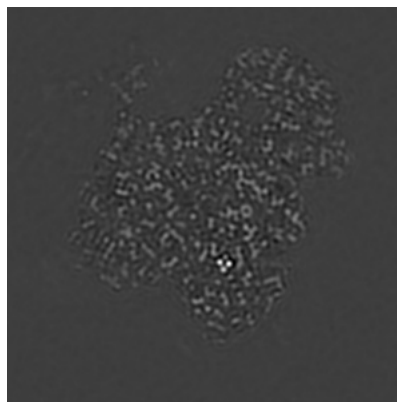
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

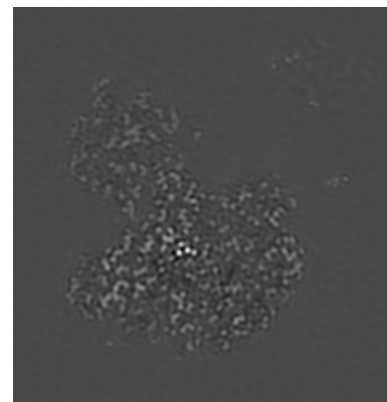
### 6.3.1 Primary map



X Index: 98

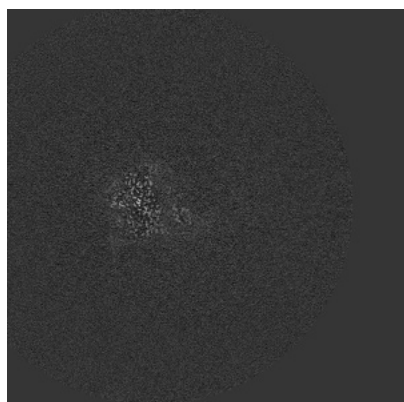


Y Index: 81

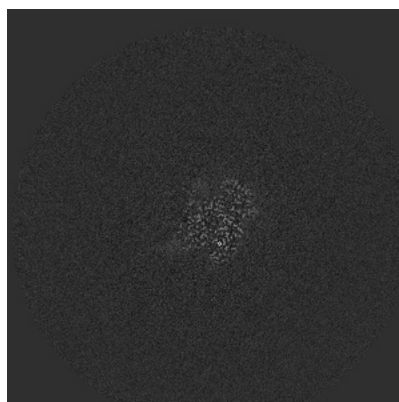


Z Index: 111

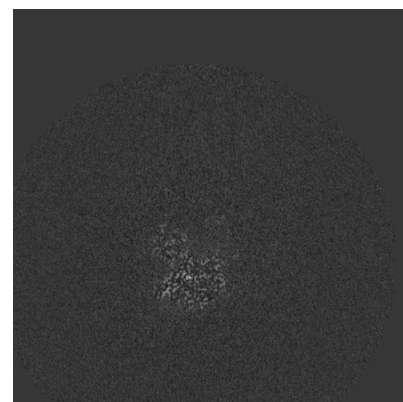
### 6.3.2 Raw map



X Index: 328



Y Index: 236

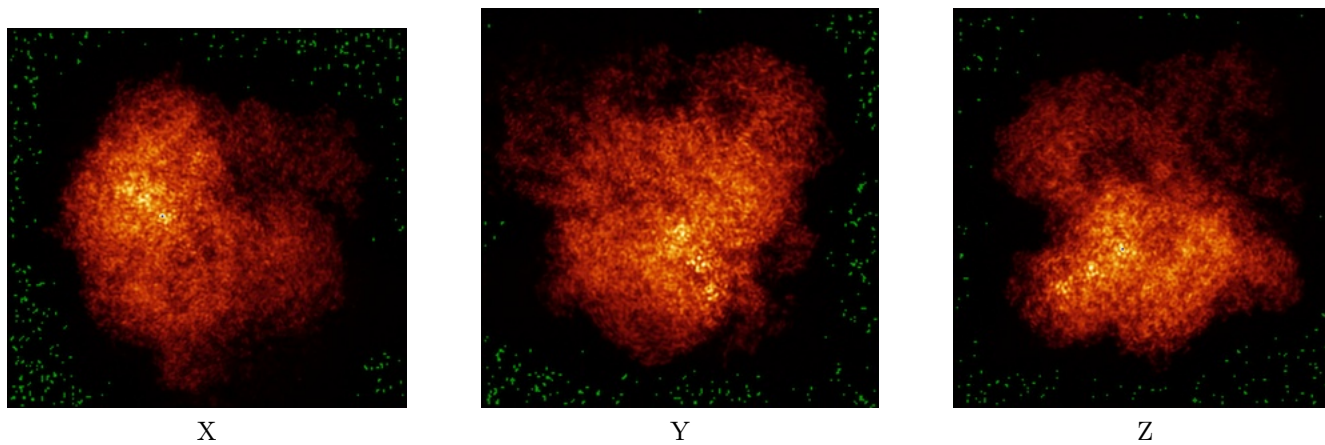


Z Index: 389

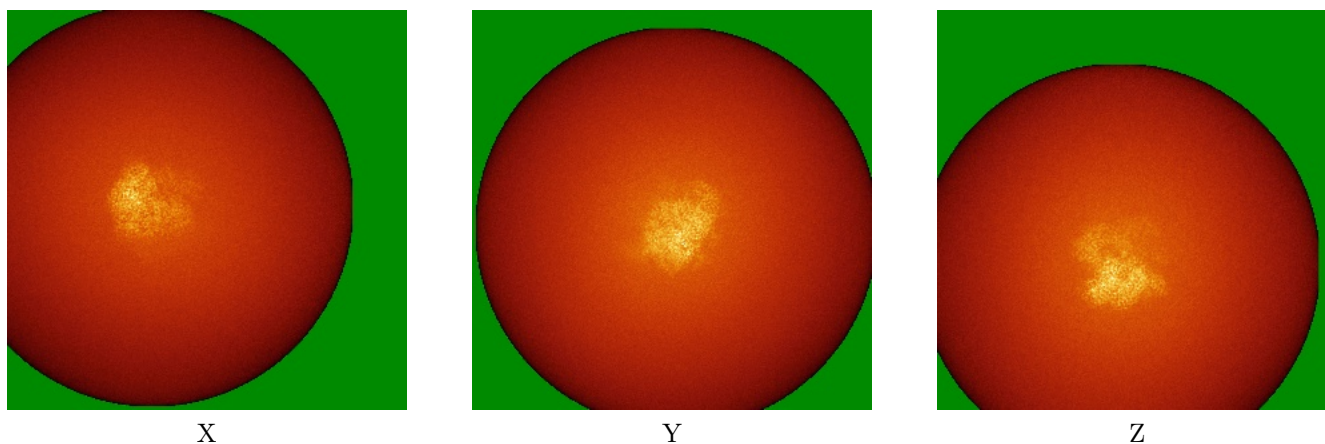
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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](#)

This section was not generated.

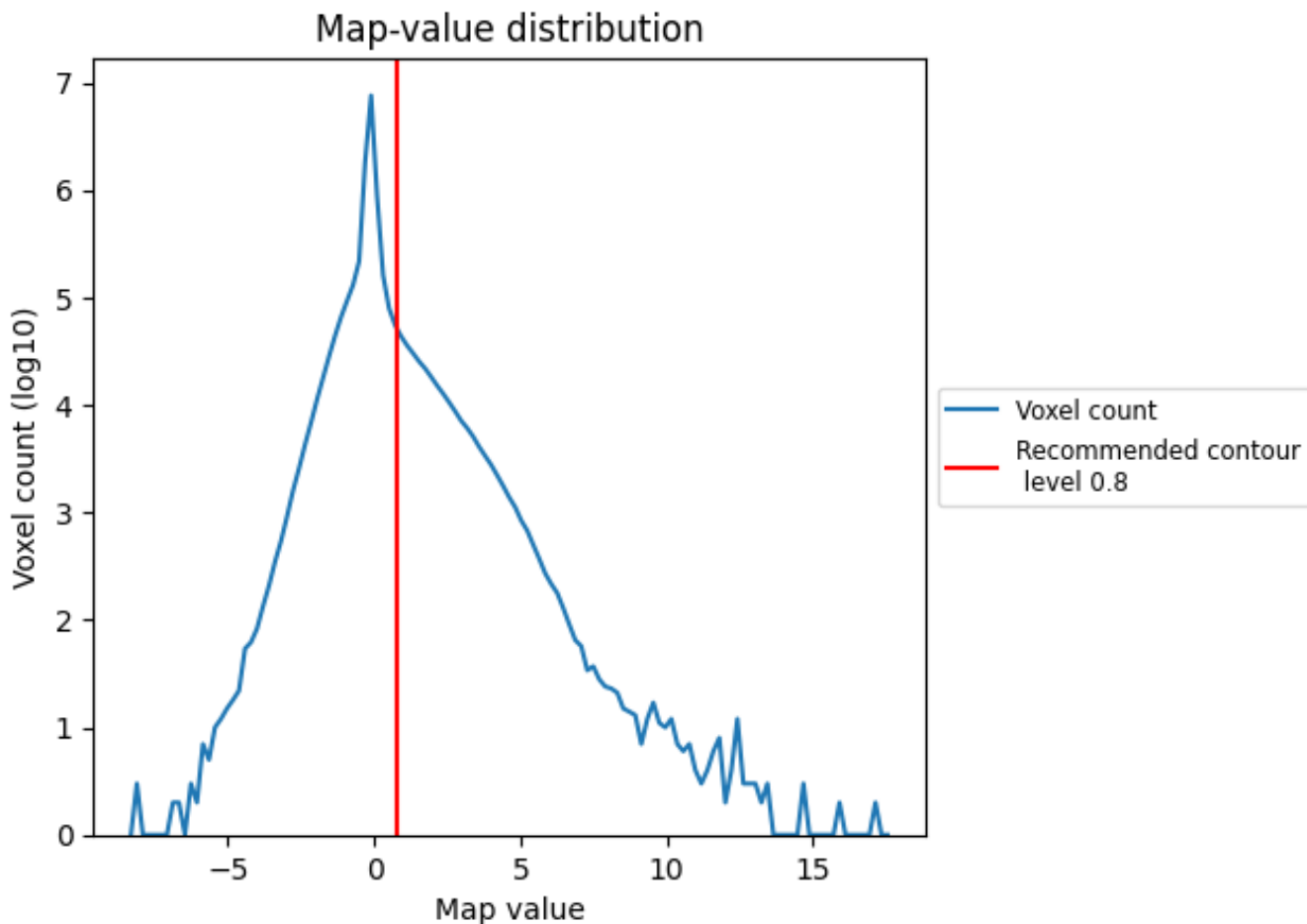
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

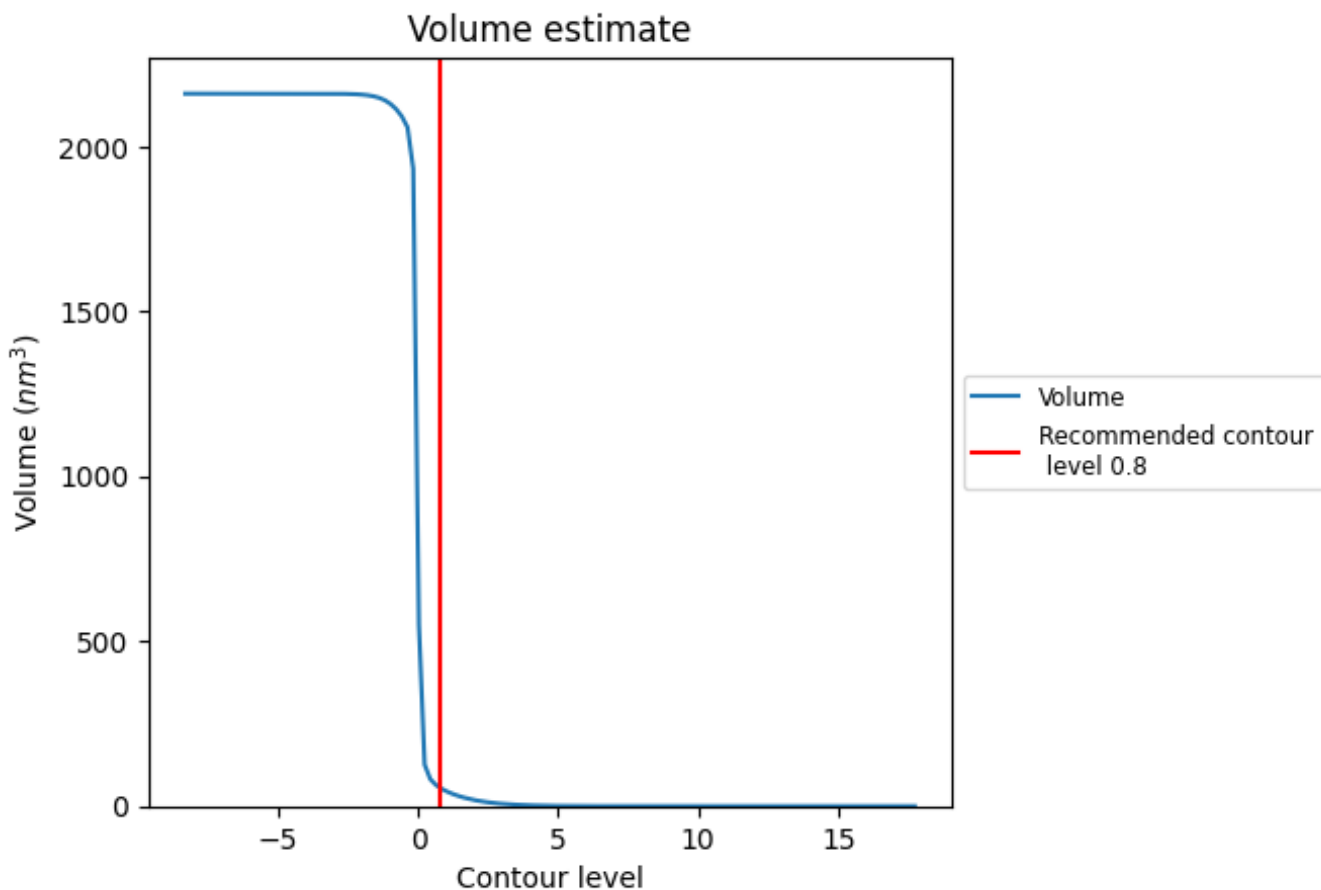
This section contains the results of statistical analysis of the map.

### 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 56  $\text{nm}^3$ ; this corresponds to an approximate mass of 50 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.

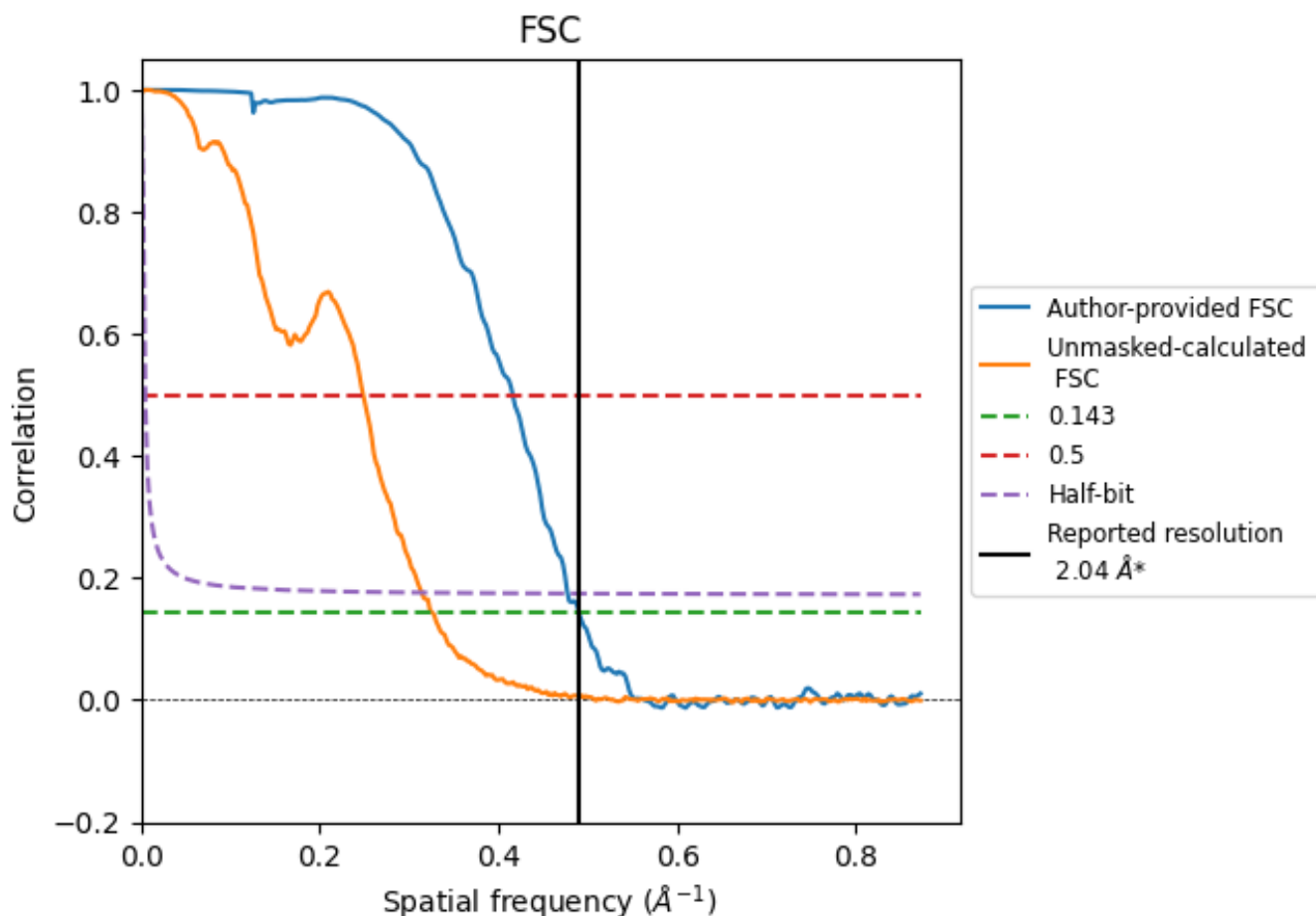
## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

## 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 0.490 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.04	-	-
Author-provided FSC curve	2.04	2.40	2.09
Unmasked-calculated*	3.07	4.02	3.18

\*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 3.07 differs from the reported value 2.04 by more than 10 %

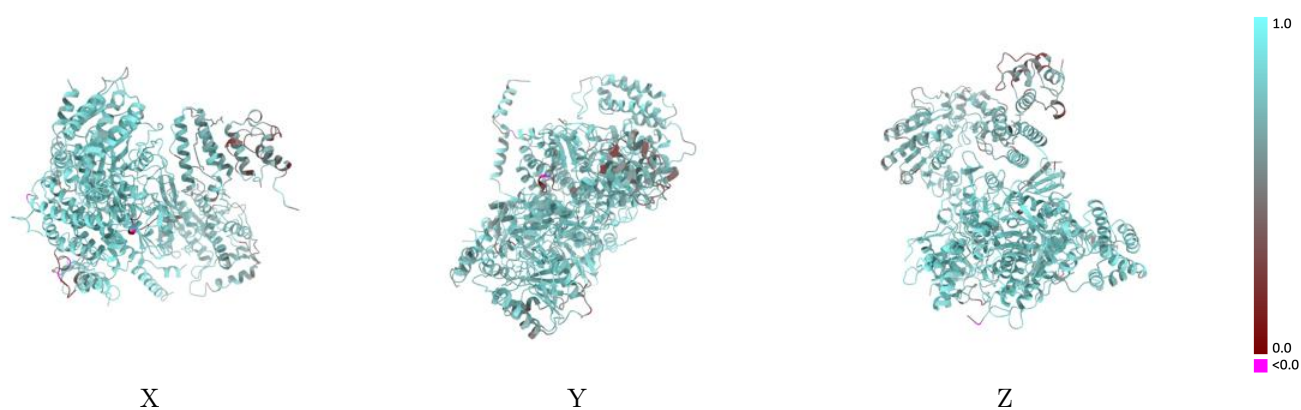
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15999 and PDB model 8BEE. Per-residue inclusion information can be found in section 3 on page 9.

### 9.1 Map-model overlay [i](#)

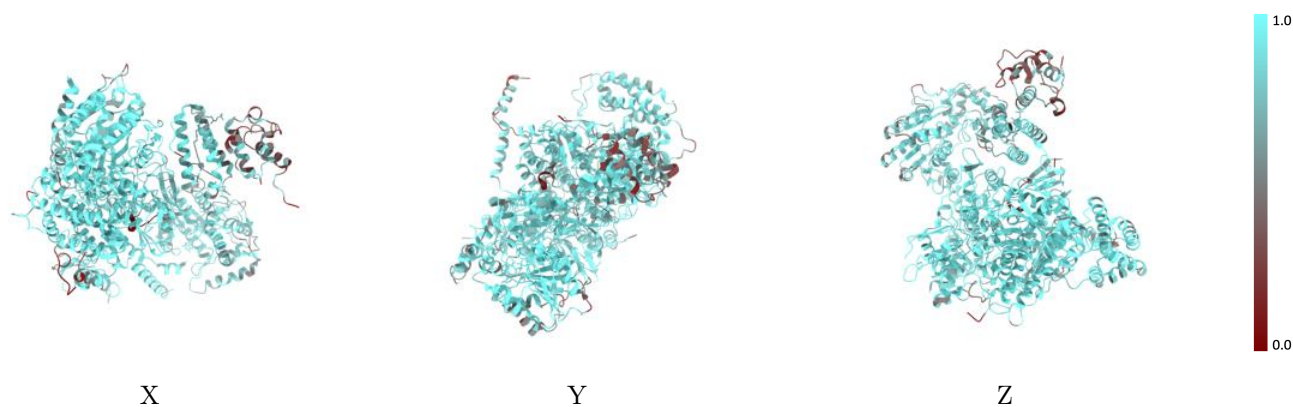
This section was not generated.

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



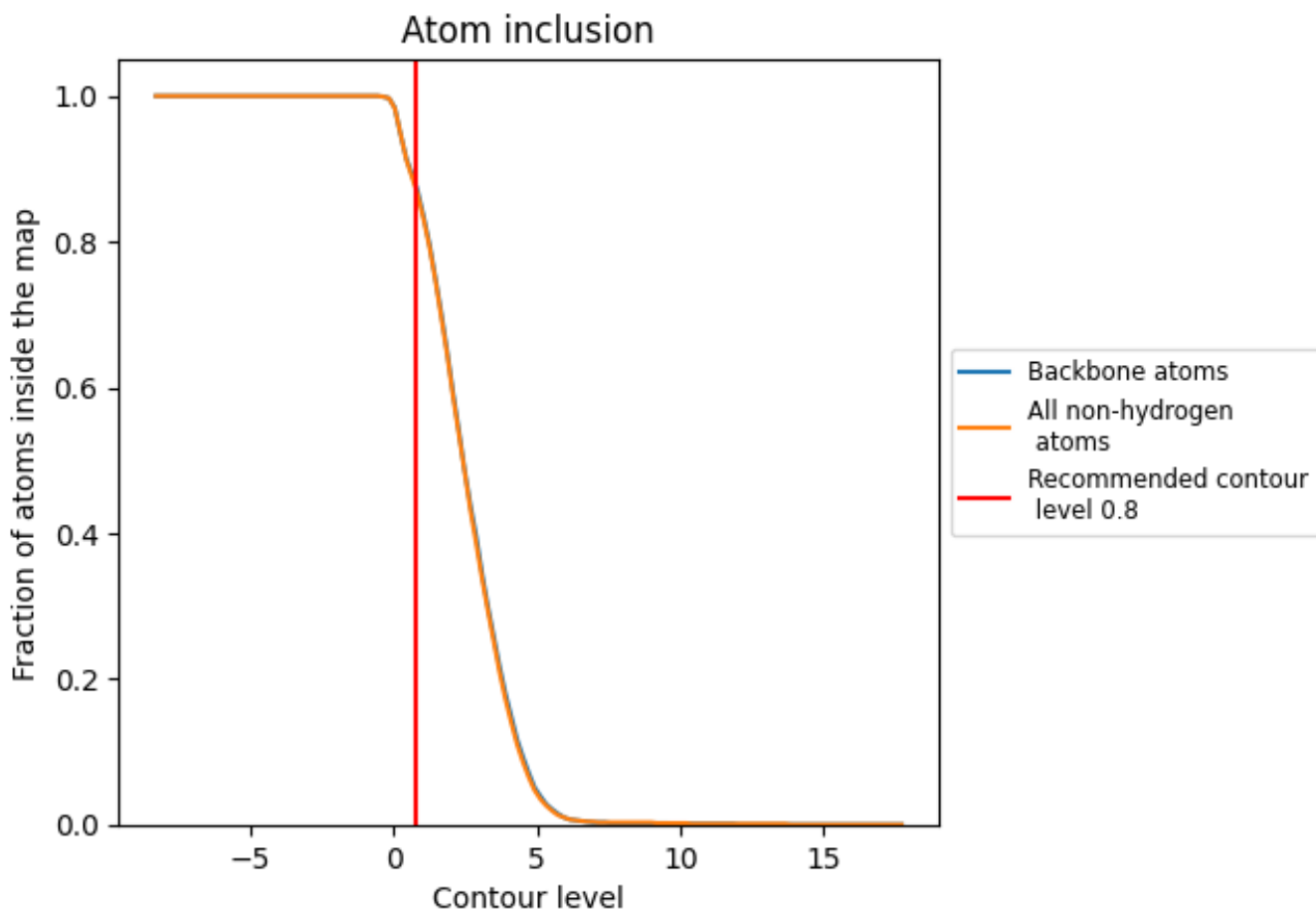
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 87% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8700	 0.7490
B	 0.9730	 0.8170
C	 0.9520	 0.8030
D	 0.9380	 0.8030
I	 0.9220	 0.7920
P	 0.8340	 0.6960
U	 0.4690	 0.5230
V	 0.8470	 0.7340
W	 0.8000	 0.6930
Z	 0.5830	 0.5610
q	 0.8940	 0.7410

