



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:59 PM UTC

PDB ID : 8I02 / pdb_00008i02
EMDB ID : EMD-35092
Title : Cryo-EM structure of the SIN3S complex from *S. pombe*
Authors : Wang, C.; Guo, Z.; Zhan, X.
Deposited on : 2023-01-10
Resolution : 2.90 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

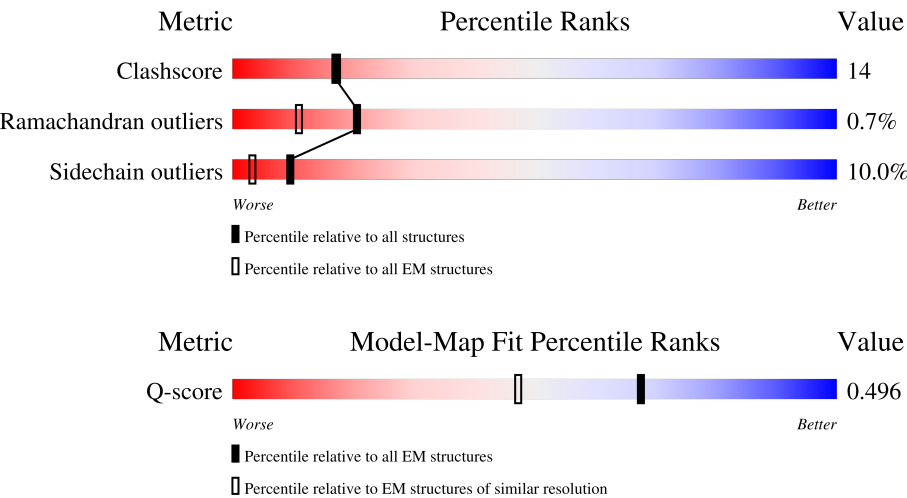
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	F	404	
2	A	1075	
3	B	405	
4	C	431	

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Mol	Chain	Length	Quality of chain
5	D	337	29%16%51%
5	E	337	25%20%53%
6	G	607	32%14%53%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19876 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 Cph1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	235	Total	C	N	O	S	0	0
			1702	1076	303	313	10		

- Molecule 2 is a protein called Paired amphipathic helix protein pst2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	864	Total	C	N	O	S	0	0
			7173	4628	1206	1315	24		

- Molecule 3 is a protein called Histone deacetylase clr6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	369	Total	C	N	O	S	0	0
			2957	1879	503	556	19		

- Molecule 4 is a protein called RbAp48-related WD40 repeat-containing protein prw1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	380	Total	C	N	O	S	0	0
			3046	1923	523	584	16		

- Molecule 5 is a protein called Chromatin modification-related protein eaf3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	165	Total	C	N	O	S	0	0
			1378	890	229	253	6		
5	E	160	Total	C	N	O	S	0	0
			1337	863	221	246	7		

- Molecule 6 is a protein called Uncharacterized protein C2F7.07c.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	284	Total	C	N	O	S	0	0
			2275	1443	392	419	21		

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

Mol	Chain	Residues	Atoms		AltConf
7	F	2	Total	Zn	0
			2	2	
7	B	1	Total	Zn	0
			1	1	
7	G	3	Total	Zn	0
			3	3	

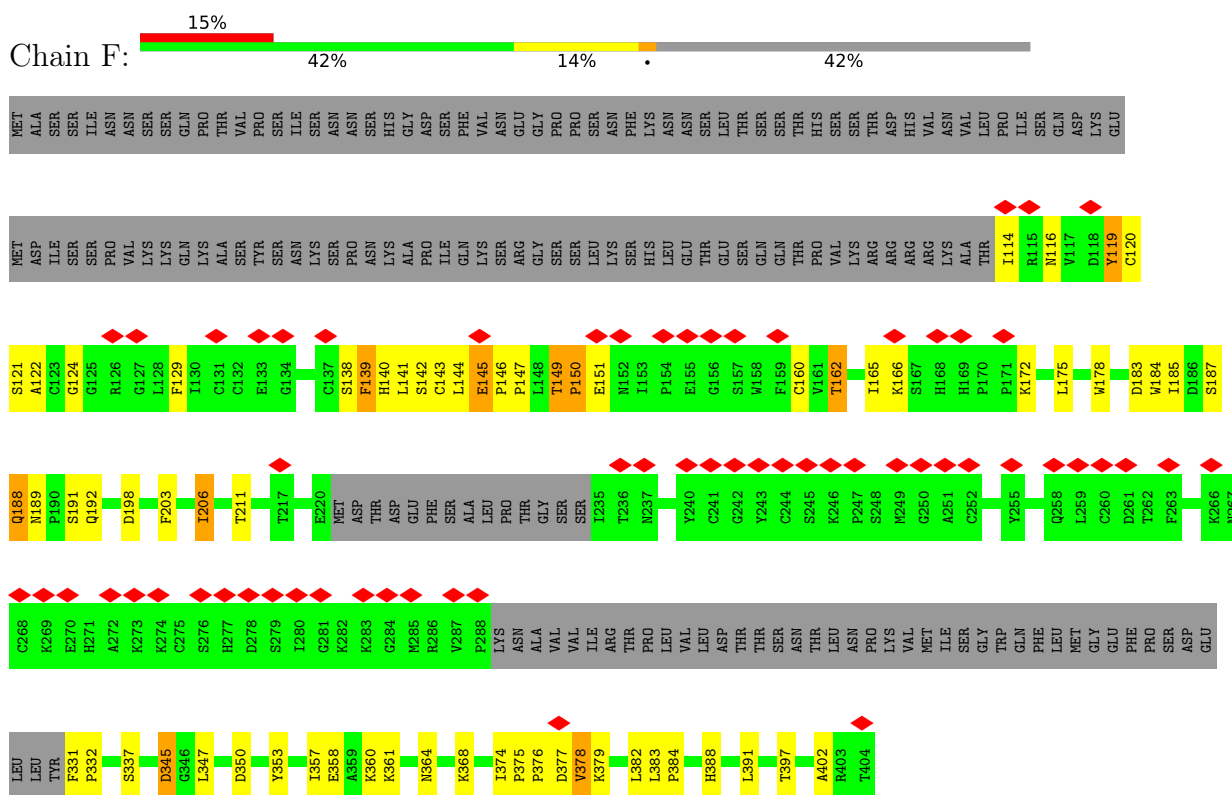
- Molecule 8 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
8	B	2	Total	K	0
			2	2	

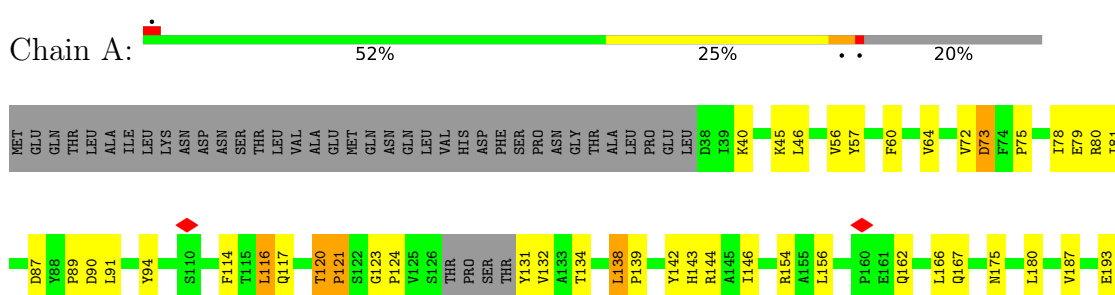
3 Residue-property plots

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

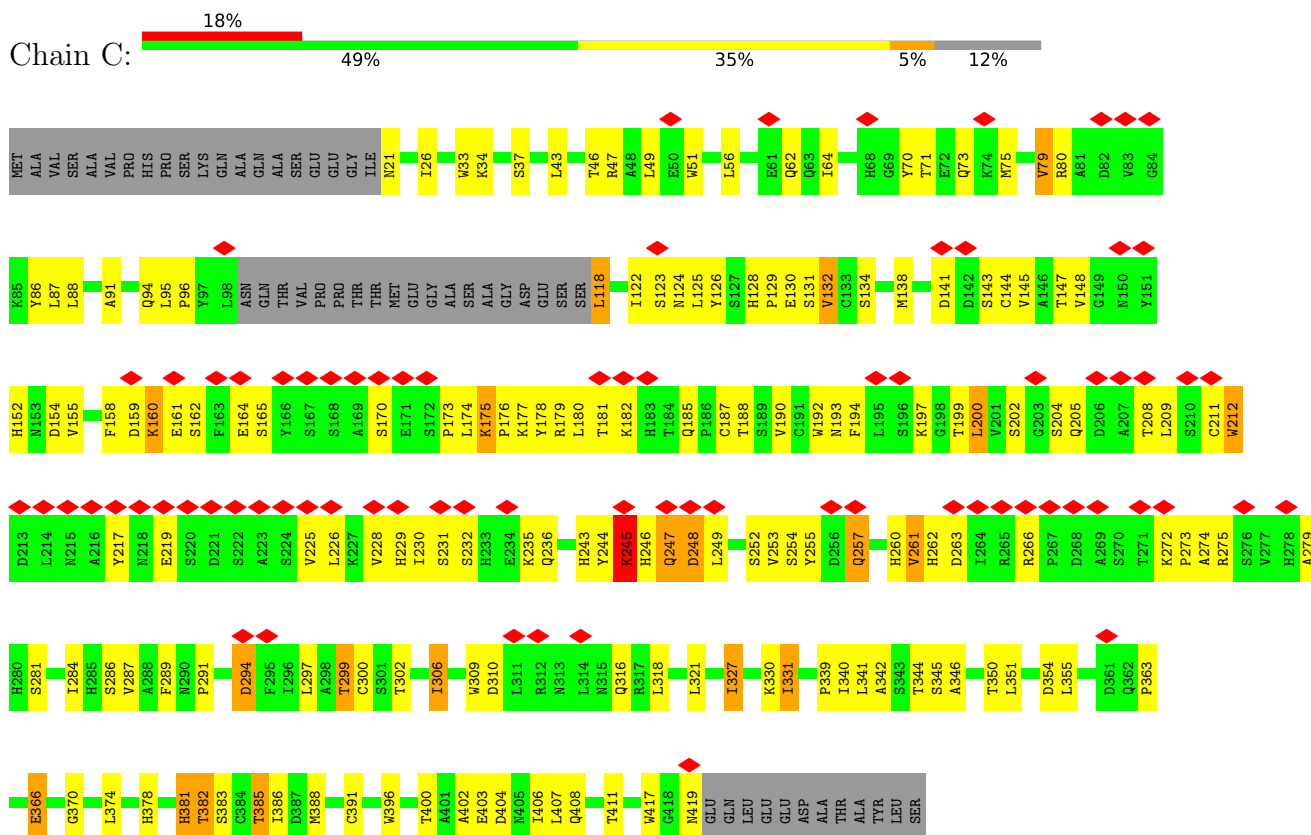
• Molecule 1: Cph1



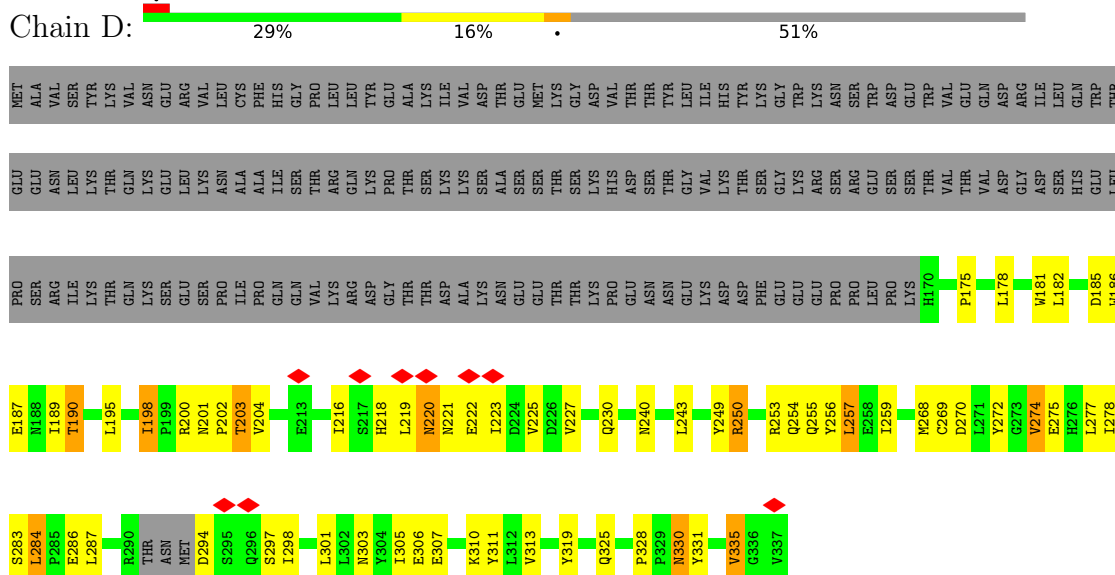
• Molecule 2: Paired amphipathic helix protein pst2



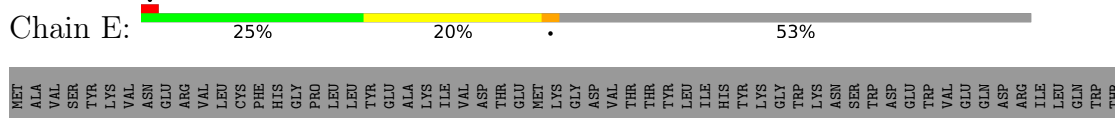
Chain C:



Chain D:



Chain E:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	777199	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	7.429	Depositor
Minimum map value	-4.765	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.102	Depositor
Recommended contour level	0.5	Depositor
Map size ($\text{\AA}$)	391.32, 391.32, 391.32	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.087, 1.087, 1.087	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: ZN, K

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	F	0.26	0/1744	0.47	0/2376
2	A	0.75	26/7348 (0.4%)	0.81	41/9919 (0.4%)
3	B	0.44	0/3036	0.53	0/4119
4	C	0.22	0/3131	0.48	1/4266 (0.0%)
5	D	0.30	0/1408	0.49	0/1907
5	E	0.27	0/1366	0.51	1/1851 (0.1%)
6	G	0.34	0/2334	0.57	0/3173
All	All	0.52	26/20367 (0.1%)	0.64	43/27611 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
2	A	0	7
5	D	0	1
5	E	0	1
6	G	0	2
All	All	0	12

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	337	CYS	C-O	-17.91	1.01	1.24
2	A	372	PRO	N-CA	17.80	1.70	1.47
2	A	359	PHE	C-O	-13.05	1.09	1.24
2	A	370	SER	C-O	-12.32	1.08	1.23
2	A	352	SER	C-O	-12.02	1.09	1.24
2	A	364	LEU	C-O	-11.07	1.10	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	338	GLY	C-O	-10.92	1.09	1.24
2	A	377	GLU	C-O	-10.19	1.09	1.24
2	A	339	PRO	C-O	-10.13	1.09	1.24
2	A	379	SER	C-O	-10.11	1.12	1.24
2	A	372	PRO	C-O	-9.99	1.10	1.24
2	A	360	ALA	C-O	-9.49	1.11	1.24
2	A	363	ILE	C-O	-9.27	1.13	1.24
2	A	340	SER	C-O	-8.22	1.15	1.23
2	A	351	ILE	C-O	-7.21	1.16	1.24
2	A	356	ARG	C-O	-6.90	1.14	1.23
2	A	352	SER	CA-CB	-6.70	1.44	1.53
2	A	339	PRO	N-CD	-6.43	1.38	1.47
2	A	365	ASN	C-O	-6.08	1.17	1.24
2	A	370	SER	CA-CB	-6.05	1.42	1.53
2	A	378	GLU	C-O	-5.83	1.16	1.24
2	A	355	GLY	C-O	-5.81	1.16	1.23
2	A	354	SER	C-O	-5.58	1.16	1.24
2	A	365	ASN	CG-OD1	-5.44	1.13	1.23
2	A	377	GLU	CD-OE1	-5.29	1.15	1.25
2	A	373	THR	C-O	-5.25	1.16	1.23

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	371	HIS	CA-C-N	14.22	137.62	119.84
2	A	371	HIS	C-N-CA	14.22	137.62	119.84
2	A	378	GLU	N-CA-C	12.56	127.03	112.72
2	A	369	VAL	O-C-N	-10.40	110.83	122.69
2	A	365	ASN	CB-CA-C	-10.01	95.25	110.26
2	A	378	GLU	N-CA-CB	-8.76	97.65	110.70
2	A	358	ASP	CA-C-N	8.74	131.81	120.44
2	A	358	ASP	C-N-CA	8.74	131.81	120.44
2	A	372	PRO	CA-N-CD	-8.57	100.00	112.00
2	A	370	SER	CA-C-O	-8.52	111.50	121.46
2	A	358	ASP	O-C-N	7.67	130.38	122.09
2	A	375	ALA	CA-C-N	7.53	135.93	121.54
2	A	375	ALA	C-N-CA	7.53	135.93	121.54
2	A	339	PRO	N-CA-CB	-7.38	96.51	103.52
2	A	351	ILE	CA-C-O	-6.51	114.19	121.36
2	A	365	ASN	CA-C-N	6.48	132.74	122.11
2	A	365	ASN	C-N-CA	6.48	132.74	122.11
2	A	352	SER	N-CA-C	6.43	119.00	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	361	TRP	N-CA-C	-6.37	105.34	113.23
2	A	371	HIS	CA-CB-CG	6.29	120.09	113.80
2	A	340	SER	CA-C-O	-6.29	114.74	121.78
2	A	372	PRO	CA-C-N	6.18	134.67	121.45
2	A	372	PRO	C-N-CA	6.18	134.67	121.45
2	A	375	ALA	N-CA-C	-6.07	105.18	112.59
4	C	245	LYS	N-CA-C	-6.04	105.87	113.18
2	A	378	GLU	O-C-N	-6.02	114.95	122.35
2	A	359	PHE	CA-C-O	-5.88	114.64	120.82
2	A	359	PHE	CA-CB-CG	5.85	119.65	113.80
2	A	350	ASN	CA-C-O	-5.80	112.63	119.48
2	A	356	ARG	NE-CZ-NH2	5.80	124.42	119.20
2	A	373	THR	CA-CB-CG2	5.63	120.08	110.50
2	A	362	GLY	CA-C-N	5.60	132.06	121.97
2	A	362	GLY	C-N-CA	5.60	132.06	121.97
2	A	381	PHE	CB-CA-C	-5.53	101.93	110.78
2	A	349	ARG	CB-CG-CD	-5.49	98.67	111.30
2	A	381	PHE	CA-CB-CG	5.46	119.25	113.80
5	E	275	GLU	N-CA-C	-5.44	108.41	114.62
2	A	358	ASP	CA-C-O	-5.21	115.34	120.70
2	A	351	ILE	CA-C-N	-5.17	115.82	123.05
2	A	351	ILE	C-N-CA	-5.17	115.82	123.05
2	A	361	TRP	CA-CB-CG	5.10	123.29	113.60
2	A	365	ASN	CA-CB-CG	5.07	117.67	112.60
2	A	339	PRO	N-CA-C	5.03	120.47	113.98

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	331	CYS	Peptide
2	A	332	SER	Peptide
2	A	336	GLU	Mainchain
2	A	369	VAL	Mainchain
2	A	373	THR	Mainchain
2	A	790	LYS	Peptide
2	A	972	LYS	Peptide
5	D	284	LEU	Peptide
5	E	198	ILE	Peptide
1	F	145	GLU	Peptide
6	G	294	ILE	Peptide
6	G	438	ASN	Peptide

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	F	1702	0	1525	56	0
2	A	7173	0	7114	195	0
3	B	2957	0	2811	78	0
4	C	3046	0	2908	111	0
5	D	1378	0	1368	46	0
5	E	1337	0	1325	54	0
6	G	2275	0	2198	57	0
7	B	1	0	0	0	0
7	F	2	0	0	0	0
7	G	3	0	0	0	0
8	B	2	0	0	0	0
All	All	19876	0	19249	539	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 14.

All (539) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:372:PRO:N	2:A:372:PRO:CA	1.70	1.41
2:A:354:SER:OG	3:B:67:ASP:OD2	1.55	1.25
2:A:348:GLU:OE1	5:D:328:PRO:HB3	1.37	1.21
2:A:341:TYR:CE2	3:B:185:TYR:CZ	2.59	0.91
2:A:80:ARG:NH1	2:A:234:ASN:O	2.05	0.89
2:A:306:SER:OG	2:A:310:ARG:NH1	2.06	0.89
2:A:369:VAL:HG11	2:A:371:HIS:NE2	1.89	0.86
4:C:185:GLN:HB2	4:C:205:GLN:HB3	1.59	0.84
2:A:348:GLU:OE1	5:D:328:PRO:CB	2.25	0.83
5:D:243:LEU:HD23	5:D:268:MET:HB3	1.63	0.80
2:A:791:ILE:HG12	2:A:793:ARG:H	1.46	0.80
5:E:223:ILE:HG23	6:G:479:ARG:HB3	1.63	0.79
2:A:746:TYR:HB3	2:A:903:GLU:HG2	1.66	0.78
2:A:341:TYR:CE2	3:B:185:TYR:OH	2.35	0.78
2:A:385:ARG:NH2	2:A:385:ARG:O	2.17	0.77
5:E:243:LEU:HD23	5:E:268:MET:HB3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:341:TYR:CZ	3:B:185:TYR:CZ	2.74	0.76
2:A:582:CYS:SG	2:A:583:ASN:ND2	2.59	0.76
2:A:747:SER:H	2:A:903:GLU:HG2	1.50	0.76
5:D:219:LEU:HB3	5:D:225:VAL:HG22	1.68	0.75
2:A:365:ASN:ND2	2:A:368:TRP:O	2.19	0.75
2:A:794:ASP:OD1	2:A:797:ASN:ND2	2.19	0.75
2:A:142:TYR:OH	6:G:573:ASN:ND2	2.20	0.75
5:D:204:VAL:HG13	5:D:277:LEU:HD22	1.70	0.74
2:A:357:ASP:OD1	2:A:357:ASP:N	2.19	0.74
4:C:187:CYS:HA	4:C:204:SER:HA	1.70	0.73
3:B:373:ALA:O	6:G:585:ARG:NH1	2.22	0.73
2:A:1018:TYR:OH	2:A:1020:ASP:OD1	2.07	0.72
2:A:1034:CYS:SG	2:A:1035:GLN:N	2.61	0.72
4:C:261:VAL:HG13	4:C:275:ARG:HB2	1.71	0.72
5:D:240:ASN:ND2	5:D:269:CYS:SG	2.63	0.71
5:D:243:LEU:HD21	5:D:272:TYR:CG	2.25	0.71
2:A:256:GLU:HA	2:A:259:ASP:HB2	1.71	0.71
1:F:149:THR:HG22	1:F:151:GLU:HG2	1.73	0.71
2:A:259:ASP:O	2:A:263:ASN:ND2	2.24	0.71
6:G:394:ARG:HB3	6:G:447:ASN:HD22	1.57	0.70
2:A:369:VAL:HG11	2:A:371:HIS:CD2	2.27	0.70
4:C:62:GLN:OE1	4:C:73:GLN:NE2	2.25	0.69
2:A:1035:GLN:OE1	2:A:1038:ARG:NH2	2.25	0.69
4:C:245:LYS:O	4:C:245:LYS:HG3	1.91	0.69
2:A:306:SER:HG	2:A:310:ARG:NH1	1.91	0.69
2:A:1043:ARG:HG3	4:C:339:PRO:HB3	1.75	0.69
3:B:140:LYS:NZ	3:B:182:GLU:OE2	2.26	0.69
2:A:214:LYS:NZ	3:B:235:GLU:OE2	2.21	0.69
6:G:291:ASP:HB3	6:G:292:PRO:HD2	1.75	0.68
6:G:263:ASN:N	6:G:263:ASN:OD1	2.25	0.68
3:B:284:PHE:O	3:B:287:SER:OG	2.12	0.68
2:A:1002:CYS:HB2	2:A:1009:LEU:HD21	1.75	0.68
4:C:154:ASP:HB3	4:C:181:THR:HG23	1.76	0.67
4:C:247:GLN:O	4:C:249:LEU:HG	1.93	0.67
1:F:382:LEU:HB3	1:F:384:PRO:HD2	1.75	0.67
5:D:216:ILE:HG13	5:D:219:LEU:HD12	1.77	0.67
4:C:350:THR:HB	4:C:378:HIS:HB3	1.77	0.67
6:G:337:VAL:O	6:G:340:GLN:HG3	1.95	0.67
3:B:261:ASP:OD1	3:B:261:ASP:N	2.28	0.66
2:A:796:TRP:HD1	2:A:799:LEU:HD12	1.60	0.66
2:A:364:LEU:HD11	3:B:158:LEU:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:420:ILE:HG22	2:A:477:LEU:HD21	1.78	0.66
4:C:187:CYS:SG	4:C:202:SER:OG	2.53	0.65
2:A:892:ARG:HH22	2:A:971:GLU:HB2	1.60	0.65
1:F:147:PRO:HG2	5:E:260:ARG:HG2	1.77	0.65
2:A:341:TYR:OH	3:B:181:GLU:OE1	2.13	0.65
2:A:1030:ASP:HA	2:A:1033:ASP:HB3	1.78	0.65
5:D:274:VAL:HG21	5:D:319:TYR:HB3	1.78	0.65
4:C:79:VAL:HG23	4:C:87:LEU:HB3	1.78	0.64
5:E:184:ASP:O	5:E:188:ASN:ND2	2.30	0.64
4:C:187:CYS:SG	4:C:188:THR:N	2.71	0.64
5:D:328:PRO:HG2	5:D:331:TYR:HB2	1.78	0.64
4:C:193:ASN:OD1	4:C:194:PHE:N	2.31	0.64
4:C:185:GLN:O	4:C:204:SER:OG	2.17	0.63
2:A:341:TYR:CZ	3:B:185:TYR:CE2	2.87	0.63
2:A:1039:LYS:NZ	4:C:354:ASP:OD2	2.26	0.63
5:E:226:ASP:O	5:E:230:GLN:NE2	2.31	0.63
5:D:284:LEU:HD12	5:D:287:LEU:HB2	1.81	0.63
2:A:1035:GLN:NE2	4:C:417:TRP:O	2.31	0.63
2:A:574:TYR:O	2:A:578:THR:OG1	2.12	0.63
3:B:306:ALA:O	3:B:310:THR:OG1	2.16	0.63
5:E:187:GLU:OE2	5:E:192:ASN:ND2	2.32	0.63
2:A:964:PRO:HB3	4:C:33:TRP:HB2	1.80	0.63
2:A:80:ARG:NH2	2:A:134:THR:O	2.32	0.62
4:C:128:HIS:ND1	4:C:130:GLU:O	2.27	0.62
6:G:364:ARG:HD3	6:G:468:GLU:HA	1.82	0.62
1:F:178:TRP:HE1	5:E:231:ALA:HA	1.65	0.62
2:A:782:PRO:HA	2:A:792:TRP:HE1	1.64	0.62
1:F:120:CYS:HB3	1:F:124:GLY:H	1.65	0.62
4:C:327:ILE:C	4:C:345:SER:HG	2.07	0.62
2:A:358:ASP:OD2	2:A:358:ASP:N	2.33	0.62
3:B:169:TYR:OH	3:B:171:ASP:OD2	2.12	0.62
4:C:88:LEU:HG	4:C:128:HIS:HB2	1.80	0.61
4:C:243:HIS:HB3	4:C:246:HIS:HA	1.81	0.61
5:D:203:THR:OG1	5:D:204:VAL:N	2.31	0.61
2:A:154:ARG:NH1	6:G:606:SER:HB3	2.16	0.61
2:A:243:ARG:O	2:A:310:ARG:NH2	2.33	0.61
1:F:375:PRO:HB2	1:F:378:VAL:HB	1.83	0.61
5:D:230:GLN:HB3	6:G:335:VAL:HG21	1.81	0.61
2:A:1002:CYS:HB3	2:A:1005:SER:O	2.01	0.61
3:B:272:ASN:O	3:B:272:ASN:ND2	2.33	0.61
2:A:378:GLU:HG2	3:B:201:TYR:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:330:TYR:HB3	3:B:333:TYR:CD2	2.36	0.60
2:A:610:PHE:O	2:A:614:LEU:HB2	2.00	0.60
2:A:400:ARG:NH1	3:B:332:GLN:O	2.34	0.60
5:E:185:ASP:OD1	5:E:324:TYR:OH	2.17	0.60
2:A:120:THR:OG1	2:A:121:PRO:HD3	2.01	0.60
2:A:877:ASN:O	2:A:877:ASN:ND2	2.32	0.60
2:A:373:THR:HB	3:B:204:GLY:HA3	1.83	0.60
2:A:910:TRP:HE1	2:A:912:ASN:ND2	1.99	0.60
5:E:173:SER:O	5:E:173:SER:OG	2.20	0.60
2:A:332:SER:O	2:A:333:ASP:HB2	2.01	0.60
1:F:360:LYS:O	1:F:364:ASN:ND2	2.34	0.60
5:E:196:ILE:O	5:E:255:GLN:NE2	2.34	0.60
2:A:381:PHE:HD1	2:A:381:PHE:N	2.00	0.60
2:A:810:GLU:O	2:A:814:VAL:HG23	2.02	0.60
3:B:58:ARG:NH1	3:B:71:GLU:OE2	2.27	0.60
2:A:744:PHE:HB2	2:A:894:GLU:HG2	1.83	0.60
4:C:148:VAL:HG11	4:C:187:CYS:HB3	1.83	0.59
4:C:310:ASP:HB2	4:C:318:LEU:HD11	1.82	0.59
2:A:1015:GLU:HB3	4:C:47:ARG:HD2	1.83	0.59
3:B:79:ASP:OD1	3:B:79:ASP:N	2.36	0.59
1:F:376:PRO:HB3	1:F:397:THR:HG21	1.84	0.59
2:A:801:ASP:OD1	2:A:801:ASP:N	2.22	0.59
3:B:64:CYS:HB2	3:B:183:PHE:CE1	2.38	0.59
4:C:217:TYR:OH	4:C:219:GLU:OE1	2.15	0.59
5:D:330:ASN:OD1	5:D:330:ASN:N	2.30	0.59
2:A:143:HIS:ND1	3:B:247:GLN:OE1	2.33	0.59
4:C:381:HIS:HD2	4:C:385:THR:HG22	1.67	0.59
5:D:186:TRP:O	5:D:190:THR:OG1	2.20	0.59
2:A:1046:TRP:O	2:A:1050:LEU:HB2	2.02	0.59
2:A:378:GLU:CG	3:B:201:TYR:O	2.50	0.59
5:E:274:VAL:HG13	5:E:277:LEU:HB3	1.85	0.59
3:B:85:GLN:HA	3:B:88:GLN:HE21	1.68	0.58
2:A:903:GLU:H	2:A:925:ALA:HB3	1.68	0.58
1:F:402:ALA:HB2	6:G:595:VAL:HG23	1.85	0.58
2:A:888:ASP:OD2	2:A:888:ASP:N	2.35	0.58
2:A:905:LEU:HD23	2:A:922:MET:HB2	1.85	0.58
2:A:132:VAL:HG13	3:B:353:ARG:HH12	1.67	0.58
2:A:503:ARG:HD2	2:A:791:ILE:HB	1.85	0.58
5:E:237:ILE:HG22	5:E:241:LYS:HE3	1.86	0.58
3:B:139:ALA:O	3:B:151:ASN:ND2	2.33	0.57
6:G:411:ARG:NH1	6:G:436:CYS:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:381:PHE:N	2:A:381:PHE:CD1	2.73	0.57
5:D:198:ILE:O	5:D:200:ARG:HG2	2.05	0.57
5:D:216:ILE:HA	5:D:219:LEU:HG	1.87	0.57
5:D:310:LYS:HA	5:D:313:VAL:HG12	1.87	0.57
6:G:416:ALA:HB2	6:G:422:ILE:HB	1.86	0.57
2:A:369:VAL:CG1	2:A:371:HIS:CD2	2.88	0.57
4:C:208:THR:HG22	4:C:231:SER:HA	1.86	0.57
4:C:244:TYR:HD2	4:C:291:PRO:HA	1.70	0.57
4:C:246:HIS:O	4:C:248:ASP:N	2.37	0.57
1:F:185:ILE:HG13	5:E:238:TYR:HE1	1.69	0.57
4:C:257:GLN:NE2	4:C:281:SER:O	2.38	0.57
2:A:437:LEU:HD13	2:A:441:LEU:HG	1.87	0.57
3:B:348:GLU:CD	3:B:348:GLU:H	2.13	0.57
5:E:198:ILE:HG12	5:E:259:ILE:HG13	1.87	0.56
4:C:245:LYS:C	4:C:247:GLN:H	2.09	0.56
5:E:172:ILE:HD13	5:E:174:VAL:HG23	1.87	0.56
5:E:205:ARG:NH2	5:E:267:GLU:OE2	2.38	0.56
5:E:316:LYS:HB2	5:E:320:PHE:HD2	1.71	0.56
2:A:991:ALA:HB2	2:A:1021:ALA:HA	1.86	0.56
4:C:159:ASP:OD1	4:C:160:LYS:N	2.34	0.56
2:A:516:SER:OG	3:B:345:ASN:OD1	2.24	0.56
2:A:221:PRO:HG2	3:B:244:HIS:CD2	2.40	0.56
3:B:249:PHE:HD1	3:B:251:PRO:HG3	1.71	0.56
2:A:909:CYS:SG	2:A:910:TRP:N	2.78	0.56
3:B:119:GLN:HG3	3:B:159:GLU:CD	2.31	0.56
4:C:306:ILE:HG13	4:C:321:LEU:HB2	1.88	0.56
6:G:422:ILE:HG13	6:G:433:HIS:CD2	2.41	0.56
2:A:154:ARG:HH12	6:G:606:SER:HB3	1.71	0.56
2:A:73:ASP:OD1	2:A:73:ASP:N	2.29	0.55
5:D:198:ILE:HG21	5:D:259:ILE:HD13	1.88	0.55
3:B:92:ASN:ND2	3:B:144:ALA:O	2.29	0.55
4:C:80:ARG:HG3	4:C:86:TYR:CZ	2.40	0.55
4:C:134:SER:HB2	4:C:190:VAL:HG22	1.87	0.55
1:F:145:GLU:HB3	5:E:245:ASN:HB3	1.88	0.55
2:A:590:LYS:HA	2:A:593:HIS:HB3	1.88	0.55
2:A:783:ASN:HB3	2:A:786:SER:OG	2.06	0.55
5:D:250:ARG:NH1	5:D:335:VAL:O	2.39	0.55
1:F:364:ASN:O	1:F:368:LYS:HG2	2.07	0.55
5:D:189:ILE:HD11	5:D:249:TYR:CD2	2.42	0.55
2:A:429:GLU:HA	2:A:432:ARG:HD3	1.88	0.55
2:A:995:SER:O	2:A:995:SER:OG	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:232:SER:HB2	4:C:273:PRO:HD3	1.88	0.55
2:A:281:LEU:HD23	2:A:294:LEU:HD11	1.89	0.55
1:F:183:ASP:O	1:F:187:SER:OG	2.24	0.55
4:C:386:ILE:HD11	4:C:403:GLU:HG3	1.88	0.55
5:E:219:LEU:HD11	5:E:228:PHE:HD2	1.71	0.55
2:A:420:ILE:HG12	2:A:441:LEU:HD23	1.89	0.54
5:D:175:PRO:HD2	5:D:178:LEU:HD12	1.90	0.54
1:F:358:GLU:OE2	2:A:284:TYR:OH	2.21	0.54
4:C:235:LYS:HG2	4:C:236:GLN:H	1.71	0.54
5:D:195:LEU:O	5:D:325:GLN:N	2.35	0.54
2:A:369:VAL:CG1	2:A:371:HIS:NE2	2.66	0.54
4:C:88:LEU:HD21	4:C:132:VAL:HG11	1.90	0.54
2:A:796:TRP:CD1	2:A:799:LEU:HD12	2.43	0.54
2:A:615:ASP:OD2	2:A:619:ARG:NH2	2.41	0.54
5:D:275:GLU:N	5:D:275:GLU:OE2	2.41	0.54
1:F:361:LYS:HA	1:F:364:ASN:HD21	1.73	0.53
1:F:138:SER:OG	1:F:138:SER:O	2.27	0.53
5:D:253:ARG:O	5:D:256:TYR:HB3	2.08	0.53
2:A:1039:LYS:HE3	4:C:340:ILE:HD11	1.91	0.53
2:A:364:LEU:HD22	3:B:183:PHE:HD1	1.72	0.53
2:A:448:ILE:O	2:A:452:THR:HG22	2.08	0.53
1:F:116:ASN:HD21	1:F:138:SER:HB3	1.74	0.53
2:A:240:SER:HB2	2:A:241:GLN:HE21	1.74	0.53
5:D:311:TYR:OH	5:D:319:TYR:OH	2.26	0.53
2:A:567:ILE:HG23	2:A:717:HIS:CD2	2.44	0.53
2:A:601:LEU:O	2:A:741:LYS:HD2	2.08	0.53
2:A:549:PHE:O	2:A:553:SER:HB3	2.10	0.52
3:B:68:GLU:HG3	3:B:91:PHE:HZ	1.73	0.52
4:C:96:PRO:HD3	4:C:118:LEU:HD13	1.89	0.52
5:D:201:ASN:HB3	5:D:202:PRO:HD3	1.92	0.52
4:C:123:SER:OG	4:C:124:ASN:N	2.43	0.52
6:G:285:PHE:HZ	6:G:349:ASN:HD21	1.56	0.52
6:G:354:HIS:CD2	6:G:355:LEU:H	2.27	0.52
6:G:554:ARG:HG3	6:G:555:ASP:N	2.24	0.52
2:A:968:ARG:NH2	4:C:370:GLY:O	2.43	0.52
2:A:875:GLU:O	2:A:878:SER:OG	2.25	0.52
2:A:791:ILE:HG23	2:A:792:TRP:H	1.75	0.51
3:B:60:ASP:OD1	3:B:60:ASP:N	2.40	0.51
2:A:1033:ASP:O	2:A:1037:LYS:HB2	2.11	0.51
3:B:201:TYR:OH	3:B:268:LEU:O	2.27	0.51
6:G:381:LYS:N	6:G:448:LEU:O	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:714:TYR:CD2	2:A:715:PRO:HD2	2.45	0.51
2:A:592:GLU:OE2	2:A:596:LYS:NZ	2.29	0.51
5:D:204:VAL:HG23	5:D:272:TYR:O	2.10	0.51
6:G:339:MET:SD	6:G:339:MET:N	2.83	0.51
4:C:138:MET:HB3	4:C:192:TRP:CG	2.45	0.51
2:A:599:LEU:O	2:A:603:PHE:HB2	2.11	0.51
2:A:746:TYR:HD1	2:A:903:GLU:HB3	1.76	0.51
6:G:291:ASP:CB	6:G:292:PRO:HD2	2.41	0.51
4:C:248:ASP:N	4:C:248:ASP:OD1	2.43	0.51
5:D:175:PRO:O	5:D:178:LEU:N	2.42	0.51
2:A:167:GLN:NE2	6:G:567:ALA:O	2.28	0.51
2:A:471:ARG:HG3	2:A:472:MET:SD	2.51	0.51
6:G:422:ILE:HG13	6:G:433:HIS:HD2	1.75	0.51
2:A:414:ILE:HD13	2:A:485:GLU:HG2	1.91	0.50
1:F:384:PRO:O	6:G:581:ARG:NH2	2.45	0.50
2:A:75:PRO:O	2:A:79:GLU:HG2	2.11	0.50
4:C:209:LEU:HD21	4:C:252:SER:HB3	1.94	0.50
1:F:184:TRP:NE1	1:F:188:GLN:HE22	2.09	0.50
4:C:263:ASP:HB3	4:C:266:ARG:HD2	1.94	0.50
5:D:227:VAL:HA	5:D:230:GLN:HE21	1.77	0.50
4:C:141:ASP:OD2	4:C:143:SER:OG	2.28	0.50
4:C:351:LEU:HD22	4:C:374:LEU:HD11	1.93	0.50
4:C:299:THR:OG1	4:C:300:CYS:N	2.45	0.49
4:C:339:PRO:HB2	4:C:355:LEU:HB2	1.94	0.49
1:F:122:ALA:HB1	1:F:191:SER:HA	1.94	0.49
1:F:144:LEU:O	5:E:253:ARG:NH2	2.45	0.49
2:A:576:VAL:O	2:A:580:ILE:HG13	2.12	0.49
4:C:260:HIS:HA	4:C:275:ARG:O	2.12	0.49
1:F:191:SER:O	5:E:246:MET:HA	2.12	0.49
1:F:383:LEU:N	1:F:384:PRO:HD2	2.28	0.49
4:C:383:SER:OG	4:C:404:ASP:OD2	2.31	0.49
2:A:571:ASP:OD2	2:A:714:TYR:OH	2.30	0.49
3:B:275:MET:O	3:B:279:SER:OG	2.14	0.49
5:E:198:ILE:HD12	5:E:272:TYR:OH	2.12	0.49
1:F:116:ASN:ND2	1:F:138:SER:HB3	2.27	0.49
3:B:85:GLN:HB3	3:B:86:PRO:HD3	1.95	0.49
5:E:186:TRP:O	5:E:190:THR:OG1	2.26	0.49
6:G:515:PHE:O	6:G:516:LYS:HB2	2.12	0.49
2:A:803:PRO:HB2	2:A:811:ASN:HD22	1.78	0.49
4:C:199:THR:OG1	4:C:211:CYS:SG	2.70	0.49
4:C:254:SER:OG	4:C:255:TYR:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:46:LEU:HD23	2:A:57:TYR:HE2	1.78	0.48
2:A:413:THR:OG1	2:A:452:THR:HG21	2.12	0.48
6:G:339:MET:HA	6:G:342:CYS:HB3	1.95	0.48
1:F:185:ILE:HG13	5:E:238:TYR:CE1	2.47	0.48
4:C:70:TYR:HB2	4:C:94:GLN:HG3	1.95	0.48
4:C:180:LEU:HD23	4:C:212:TRP:CD2	2.48	0.48
5:D:223:ILE:O	5:D:227:VAL:HG23	2.12	0.48
4:C:34:LYS:HG2	6:G:519:PHE:HD2	1.78	0.48
5:D:221:ASN:O	5:D:225:VAL:HG23	2.13	0.48
5:E:198:ILE:CG1	5:E:259:ILE:HG13	2.43	0.48
1:F:353:TYR:CZ	1:F:357:ILE:HD11	2.49	0.48
2:A:341:TYR:OH	3:B:185:TYR:CE2	2.67	0.48
3:B:119:GLN:HG3	3:B:159:GLU:OE2	2.14	0.48
4:C:21:ASN:N	4:C:21:ASN:OD1	2.45	0.48
6:G:558:LEU:HB3	6:G:559:PRO:HD3	1.96	0.48
4:C:193:ASN:HB2	4:C:199:THR:HG22	1.96	0.48
3:B:69:TYR:HB2	3:B:91:PHE:CE1	2.48	0.48
4:C:159:ASP:HB2	4:C:177:LYS:HE3	1.94	0.48
4:C:176:PRO:HG2	4:C:179:ARG:CZ	2.43	0.48
4:C:200:LEU:O	4:C:212:TRP:HD1	1.97	0.48
2:A:886:TYR:HE2	2:A:889:PHE:HD1	1.61	0.48
2:A:714:TYR:CD1	2:A:810:GLU:HG2	2.49	0.48
2:A:859:HIS:O	2:A:859:HIS:ND1	2.45	0.48
4:C:26:ILE:HG22	4:C:382:THR:HG22	1.95	0.48
2:A:981:SER:O	2:A:985:THR:HG22	2.14	0.47
3:B:198:PHE:CB	3:B:224:PRO:HB3	2.44	0.47
3:B:138:HIS:CD2	3:B:202:PHE:HE1	2.32	0.47
4:C:345:SER:OG	4:C:346:ALA:N	2.46	0.47
5:E:243:LEU:HD21	5:E:272:TYR:CE2	2.50	0.47
3:B:37:ASN:O	3:B:40:VAL:HG12	2.15	0.47
3:B:207:HIS:ND1	3:B:209:LYS:HB2	2.29	0.47
4:C:75:MET:HE3	4:C:91:ALA:HB3	1.96	0.47
5:D:221:ASN:OD1	5:D:222:GLU:N	2.48	0.47
5:E:215:LYS:HD2	5:E:228:PHE:HE2	1.79	0.47
1:F:144:LEU:HB3	1:F:146:PRO:HD2	1.97	0.47
2:A:46:LEU:HD23	2:A:57:TYR:CE2	2.49	0.47
2:A:79:GLU:OE2	2:A:131:TYR:OH	2.22	0.47
2:A:549:PHE:HB3	2:A:552:ARG:HG3	1.95	0.47
6:G:276:LEU:HD23	6:G:304:TRP:HZ2	1.79	0.47
1:F:121:SER:HB3	1:F:139:PHE:CD2	2.50	0.47
2:A:230:PHE:CZ	6:G:419:SER:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:263:LEU:HD11	3:B:308:VAL:HG21	1.97	0.47
5:D:255:GLN:O	5:D:259:ILE:HD12	2.14	0.47
5:E:314:LEU:HG	5:E:315:HIS:CD2	2.50	0.47
6:G:458:ASP:OD1	6:G:458:ASP:N	2.47	0.47
3:B:268:LEU:HD12	3:B:300:TYR:CE2	2.49	0.47
4:C:244:TYR:CD2	4:C:291:PRO:HA	2.49	0.47
4:C:182:LYS:HG3	4:C:226:LEU:HD21	1.96	0.47
3:B:211:THR:O	3:B:211:THR:OG1	2.22	0.46
5:D:268:MET:C	5:D:270:ASP:H	2.24	0.46
2:A:457:TYR:CE2	2:A:480:VAL:HG23	2.50	0.46
2:A:849:LYS:HE3	2:A:849:LYS:HB2	1.69	0.46
3:B:72:PHE:HE2	3:B:84:PHE:HB3	1.79	0.46
5:E:211:PHE:O	5:E:214:SER:HB3	2.15	0.46
2:A:798:ASP:OD1	2:A:798:ASP:N	2.49	0.46
2:A:975:THR:HG22	2:A:976:VAL:H	1.80	0.46
5:D:257:LEU:HG	6:G:293:PRO:HB2	1.98	0.46
1:F:149:THR:O	1:F:151:GLU:N	2.48	0.46
2:A:243:ARG:C	2:A:310:ARG:HE	2.24	0.46
4:C:145:VAL:HB	4:C:158:PHE:HB2	1.98	0.46
5:E:288:ILE:HG21	5:E:298:ILE:HG23	1.97	0.46
6:G:291:ASP:OD1	6:G:291:ASP:N	2.49	0.46
6:G:356:PRO:HG2	6:G:359:ILE:HG13	1.97	0.46
2:A:997:LEU:HD21	2:A:1010:TYR:HE1	1.81	0.46
4:C:86:TYR:CG	4:C:131:SER:HA	2.51	0.46
2:A:587:GLY:C	2:A:589:LYS:H	2.24	0.46
4:C:246:HIS:O	4:C:249:LEU:N	2.41	0.46
2:A:591:VAL:O	2:A:595:PHE:HD2	1.99	0.46
3:B:64:CYS:HB2	3:B:183:PHE:HE1	1.80	0.46
3:B:74:TRP:HE3	3:B:75:ARG:HG2	1.80	0.46
5:E:283:SER:O	5:E:283:SER:OG	2.33	0.46
6:G:354:HIS:HD2	6:G:355:LEU:O	1.98	0.46
4:C:330:LYS:HB3	4:C:388:MET:HE3	1.98	0.46
6:G:357:HIS:O	6:G:361:SER:HB3	2.16	0.46
3:B:235:GLU:HG3	3:B:239:LYS:HE3	1.98	0.45
3:B:349:ASN:OD1	3:B:350:HIS:N	2.49	0.45
4:C:174:LEU:HD12	4:C:175:LYS:H	1.80	0.45
2:A:216:PRO:HG2	2:A:219:SER:HB3	1.98	0.45
2:A:423:ARG:HA	2:A:426:GLU:CD	2.42	0.45
5:E:204:VAL:HG21	5:E:239:PHE:CE1	2.51	0.45
4:C:130:GLU:HB3	4:C:152:HIS:CE1	2.51	0.45
4:C:138:MET:HB3	4:C:192:TRP:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:457:SER:O	6:G:461:THR:HG23	2.16	0.45
4:C:88:LEU:HB2	4:C:126:TYR:HB2	1.97	0.45
5:E:204:VAL:HG22	5:E:272:TYR:O	2.15	0.45
2:A:973:GLU:OE2	2:A:982:ARG:NH2	2.49	0.45
4:C:96:PRO:HD3	4:C:118:LEU:CD1	2.46	0.45
3:B:104:TYR:O	3:B:108:SER:OG	2.34	0.45
4:C:274:ALA:HB1	4:C:275:ARG:NH1	2.32	0.45
4:C:286:SER:HB3	4:C:331:ILE:HG23	1.99	0.45
4:C:381:HIS:HE1	4:C:408:GLN:HG3	1.81	0.45
6:G:452:LYS:HD2	6:G:459:HIS:CE1	2.52	0.45
1:F:374:ILE:HD11	1:F:388:HIS:CE1	2.52	0.45
1:F:129:PHE:HB3	1:F:139:PHE:O	2.17	0.45
1:F:149:THR:HG22	1:F:151:GLU:CG	2.44	0.45
2:A:132:VAL:HG13	3:B:353:ARG:NH1	2.32	0.45
6:G:364:ARG:HH11	6:G:468:GLU:HA	1.82	0.45
6:G:378:ASP:OD1	6:G:378:ASP:N	2.49	0.45
1:F:119:TYR:CD2	1:F:124:GLY:HA2	2.52	0.44
2:A:860:HIS:C	2:A:862:VAL:H	2.25	0.44
3:B:179:GLY:O	3:B:183:PHE:HD2	2.00	0.44
4:C:129:PRO:HB3	4:C:173:PRO:HB2	1.98	0.44
4:C:212:TRP:HE3	4:C:225:VAL:HG13	1.82	0.44
6:G:369:GLY:N	6:G:373:GLU:O	2.47	0.44
2:A:242:SER:O	2:A:242:SER:OG	2.33	0.44
2:A:369:VAL:CG1	2:A:371:HIS:CE1	3.00	0.44
2:A:782:PRO:HB3	2:A:792:TRP:CZ2	2.51	0.44
4:C:87:LEU:HD11	4:C:125:LEU:HD23	1.98	0.44
1:F:139:PHE:HE2	1:F:189:ASN:HD21	1.65	0.44
2:A:396:LEU:O	2:A:400:ARG:HG3	2.17	0.44
3:B:332:GLN:HE21	3:B:332:GLN:HB3	1.53	0.44
1:F:147:PRO:HG3	5:E:256:TYR:CE1	2.53	0.44
2:A:187:VAL:HG21	2:A:201:PHE:CZ	2.52	0.44
5:E:183:VAL:O	5:E:186:TRP:HB3	2.16	0.44
2:A:446:LYS:HB3	2:A:446:LYS:HE2	1.74	0.44
2:A:962:ARG:O	2:A:963:CYS:HB2	2.18	0.44
3:B:322:ASP:OD1	3:B:324:ASN:N	2.36	0.44
4:C:177:LYS:HD3	4:C:178:TYR:CE2	2.52	0.44
5:E:189:ILE:HG23	5:E:251:PHE:HB3	2.00	0.44
2:A:214:LYS:HE3	2:A:214:LYS:HB2	1.76	0.44
2:A:563:TYR:HB3	2:A:569:LEU:HD13	1.99	0.44
2:A:747:SER:OG	2:A:903:GLU:HG3	2.17	0.44
3:B:68:GLU:HG3	3:B:91:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:402:ALA:HB3	4:C:406:ILE:HB	1.99	0.44
5:E:219:LEU:HD13	5:E:224:ASP:HB3	1.99	0.44
2:A:306:SER:HG	2:A:310:ARG:HH11	1.63	0.44
2:A:713:LYS:HB2	2:A:713:LYS:HE2	1.54	0.44
2:A:116:LEU:HD23	2:A:117:GLN:O	2.18	0.44
2:A:477:LEU:HD12	2:A:477:LEU:HA	1.85	0.44
5:D:218:HIS:O	5:D:220:ASN:ND2	2.50	0.44
6:G:484:LYS:HB3	6:G:484:LYS:HE2	1.77	0.44
1:F:175:LEU:HG	6:G:476:GLY:HA2	2.00	0.44
2:A:87:ASP:C	2:A:89:PRO:HD3	2.43	0.44
2:A:121:PRO:HG2	2:A:207:SER:HB3	1.99	0.44
2:A:709:LYS:HE3	2:A:709:LYS:HB3	1.85	0.44
4:C:124:ASN:N	4:C:124:ASN:OD1	2.50	0.44
5:D:306:GLU:O	5:D:310:LYS:HG2	2.17	0.44
1:F:350:ASP:OD1	6:G:479:ARG:HG2	2.17	0.43
3:B:53:PRO:HB3	3:B:113:GLY:HA2	2.00	0.43
6:G:463:ARG:O	6:G:463:ARG:HD3	2.18	0.43
3:B:160:LEU:HD12	3:B:255:ILE:HD11	2.00	0.43
6:G:546:SER:O	6:G:546:SER:OG	2.36	0.43
1:F:172:LYS:HE3	1:F:172:LYS:HA	2.01	0.43
2:A:395:LYS:O	2:A:399:GLU:HG3	2.19	0.43
3:B:20:HIS:NE2	3:B:22:GLY:O	2.52	0.43
5:E:211:PHE:HA	5:E:214:SER:HB3	2.00	0.43
6:G:354:HIS:HD2	6:G:355:LEU:H	1.64	0.43
2:A:383:VAL:HG12	2:A:384:GLN:H	1.82	0.43
2:A:460:GLU:HG3	2:A:461:HIS:CD2	2.53	0.43
4:C:279:ALA:HB2	4:C:309:TRP:HZ2	1.83	0.43
5:D:301:LEU:O	5:D:305:ILE:HG12	2.18	0.43
2:A:134:THR:HG22	2:A:213:SER:HB3	2.00	0.43
2:A:448:ILE:HA	2:A:451:LYS:HD3	2.01	0.43
2:A:718:PRO:HG2	2:A:721:LEU:HD13	2.00	0.43
2:A:1036:ASN:O	2:A:1040:GLN:HG3	2.18	0.43
3:B:74:TRP:CE3	3:B:75:ARG:HG2	2.53	0.43
2:A:366:ASP:OD1	3:B:141:LYS:NZ	2.52	0.43
5:E:316:LYS:HB2	5:E:316:LYS:HE3	1.75	0.43
2:A:357:ASP:HB2	2:A:358:ASP:H	1.57	0.43
2:A:997:LEU:HD11	2:A:1010:TYR:HD1	1.82	0.43
2:A:997:LEU:HA	2:A:1014:THR:HB	2.01	0.43
1:F:375:PRO:HA	1:F:376:PRO:HD3	1.89	0.43
2:A:506:GLU:CD	3:B:335:GLY:HA2	2.44	0.43
4:C:396:TRP:O	4:C:411:THR:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:348:GLU:C	2:A:350:ASN:H	2.27	0.43
2:A:744:PHE:CB	2:A:894:GLU:HG2	2.49	0.43
4:C:235:LYS:HB3	4:C:235:LYS:HE3	1.78	0.43
4:C:302:THR:HB	4:C:327:ILE:HG23	2.01	0.43
5:E:175:PRO:HD3	5:E:310:LYS:HE3	2.00	0.43
5:E:196:ILE:O	5:E:198:ILE:HG23	2.19	0.42
1:F:203:PHE:HB2	1:F:206:ILE:HG12	2.01	0.42
1:F:149:THR:C	1:F:151:GLU:H	2.27	0.42
4:C:155:VAL:HG13	4:C:180:LEU:HB2	2.00	0.42
4:C:230:ILE:HG21	4:C:262:HIS:CE1	2.54	0.42
5:D:294:ASP:HA	5:D:298:ILE:HD13	2.01	0.42
5:E:303:ASN:O	5:E:306:GLU:HG3	2.19	0.42
6:G:434:PRO:HB3	6:G:441:LEU:HB2	2.02	0.42
6:G:437:LEU:H	6:G:437:LEU:HG	1.63	0.42
2:A:348:GLU:O	2:A:350:ASN:N	2.52	0.42
5:D:274:VAL:HA	5:D:277:LEU:HB3	2.00	0.42
1:F:360:LYS:HE3	1:F:360:LYS:HB3	1.87	0.42
3:B:176:HIS:HB3	3:B:203:PRO:HG2	2.02	0.42
3:B:231:ASP:OD2	3:B:273:LEU:HA	2.20	0.42
4:C:161:GLU:O	4:C:165:SER:OG	2.22	0.42
4:C:253:VAL:HG11	4:C:284:ILE:HG21	2.01	0.42
6:G:266:CYS:HB2	6:G:286:HIS:ND1	2.34	0.42
2:A:46:LEU:HD12	2:A:91:LEU:HD13	2.02	0.42
2:A:156:LEU:HD23	2:A:162:GLN:HB2	2.01	0.42
2:A:260:PHE:O	2:A:264:VAL:HG23	2.19	0.42
2:A:308:LEU:HD23	2:A:308:LEU:HA	1.70	0.42
2:A:503:ARG:CD	2:A:791:ILE:HB	2.50	0.42
4:C:287:VAL:HG13	4:C:297:LEU:HD11	2.02	0.42
5:E:204:VAL:HG23	5:E:269:CYS:O	2.20	0.42
6:G:302:ASP:HB3	6:G:304:TRP:CE2	2.54	0.42
3:B:162:LYS:HE3	3:B:162:LYS:HB2	1.81	0.42
3:B:176:HIS:H	3:B:203:PRO:HG2	1.85	0.42
3:B:351:ASN:N	3:B:351:ASN:OD1	2.52	0.42
4:C:284:ILE:HD12	4:C:284:ILE:H	1.84	0.42
4:C:388:MET:HB3	4:C:400:THR:HG22	2.01	0.42
5:E:248:LEU:HD12	5:E:253:ARG:NH1	2.35	0.42
6:G:515:PHE:C	6:G:517:LEU:H	2.28	0.42
2:A:554:ARG:O	2:A:920:LYS:NZ	2.40	0.42
4:C:138:MET:HE3	4:C:144:CYS:HB2	2.02	0.42
5:D:303:ASN:O	5:D:307:GLU:HG3	2.20	0.42
1:F:162:THR:HA	1:F:165:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:353:TYR:O	1:F:357:ILE:HG13	2.19	0.41
4:C:71:THR:HG22	4:C:95:LEU:O	2.20	0.41
4:C:294:ASP:OD1	4:C:294:ASP:N	2.28	0.41
4:C:302:THR:O	4:C:302:THR:OG1	2.39	0.41
2:A:458:THR:O	2:A:461:HIS:N	2.35	0.41
2:A:758:LEU:O	2:A:762:ARG:HG2	2.20	0.41
4:C:243:HIS:HD2	4:C:289:PHE:CD1	2.38	0.41
5:E:316:LYS:HE3	5:E:320:PHE:CD2	2.55	0.41
6:G:550:PHE:O	6:G:554:ARG:HG2	2.20	0.41
1:F:129:PHE:HE1	1:F:140:HIS:NE2	2.17	0.41
1:F:162:THR:OG1	1:F:166:LYS:NZ	2.53	0.41
1:F:331:PHE:HA	1:F:332:PRO:HD3	1.93	0.41
2:A:121:PRO:HG2	2:A:207:SER:CB	2.51	0.41
2:A:428:PRO:HB2	2:A:430:GLU:OE1	2.20	0.41
4:C:132:VAL:HG12	4:C:147:THR:HB	2.02	0.41
4:C:341:LEU:HD23	4:C:342:ALA:N	2.35	0.41
2:A:142:TYR:O	2:A:146:ILE:HG13	2.20	0.41
2:A:1003:LEU:HD22	2:A:1003:LEU:H	1.86	0.41
4:C:381:HIS:HB3	4:C:383:SER:O	2.20	0.41
5:E:318:GLU:OE2	5:E:318:GLU:N	2.47	0.41
6:G:291:ASP:O	6:G:292:PRO:C	2.63	0.41
1:F:203:PHE:CE2	5:E:183:VAL:HG11	2.56	0.41
2:A:138:LEU:N	2:A:139:PRO:HD2	2.36	0.41
4:C:197:LYS:HD3	4:C:197:LYS:C	2.45	0.41
5:E:322:LYS:HD3	5:E:322:LYS:HA	1.81	0.41
1:F:140:HIS:CE1	5:E:250:ARG:HH21	2.38	0.41
1:F:345:ASP:OD1	1:F:345:ASP:N	2.46	0.41
2:A:791:ILE:HG23	2:A:792:TRP:N	2.35	0.41
6:G:304:TRP:HA	6:G:304:TRP:CE3	2.56	0.41
6:G:364:ARG:HD2	6:G:364:ARG:HA	1.89	0.41
2:A:144:ARG:NE	2:A:221:PRO:O	2.54	0.41
2:A:305:ASN:HB3	2:A:308:LEU:HB2	2.03	0.41
2:A:372:PRO:HA	3:B:203:PRO:O	2.21	0.41
2:A:378:GLU:HG3	3:B:201:TYR:O	2.19	0.41
2:A:923:LYS:C	2:A:924:ARG:HD2	2.46	0.41
4:C:316:GLN:OE1	4:C:316:GLN:N	2.54	0.41
4:C:344:THR:HG21	4:C:385:THR:OG1	2.20	0.41
4:C:363:PRO:HD2	4:C:366:GLU:OE2	2.21	0.41
5:D:181:TRP:CZ3	5:D:278:ILE:HD11	2.56	0.41
5:D:182:LEU:HD11	5:D:282:VAL:HG21	2.03	0.41
5:D:298:ILE:HD12	5:D:298:ILE:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:169:LYS:HE2	5:E:169:LYS:HB3	1.78	0.41
5:E:223:ILE:H	5:E:223:ILE:HG13	1.68	0.41
5:E:306:GLU:OE2	5:E:310:LYS:NZ	2.53	0.41
2:A:45:LYS:HD2	2:A:94:TYR:CE2	2.56	0.41
2:A:535:LEU:HD21	2:A:747:SER:HB3	2.03	0.41
2:A:783:ASN:ND2	3:B:324:ASN:HB3	2.36	0.41
3:B:15:ASP:OD1	3:B:15:ASP:N	2.53	0.41
5:D:254:GLN:HB2	5:D:335:VAL:HG13	2.03	0.41
5:E:239:PHE:CZ	5:E:243:LEU:HD22	2.56	0.41
1:F:140:HIS:HB2	1:F:143:CYS:HB2	2.02	0.40
2:A:60:PHE:O	2:A:64:VAL:HG23	2.20	0.40
2:A:123:GLY:HA2	2:A:124:PRO:HD3	1.83	0.40
2:A:879:SER:HB2	2:A:886:TYR:CE1	2.57	0.40
4:C:80:ARG:HG3	4:C:86:TYR:CE1	2.56	0.40
1:F:185:ILE:HD13	1:F:185:ILE:HA	1.94	0.40
2:A:291:ARG:O	2:A:295:VAL:HG23	2.21	0.40
2:A:420:ILE:HG21	2:A:441:LEU:HD23	2.03	0.40
2:A:1024:LEU:HB2	2:A:1025:ARG:CZ	2.52	0.40
3:B:114:SER:OG	3:B:152:ASP:HB2	2.21	0.40
1:F:139:PHE:CE1	1:F:160:CYS:HB3	2.56	0.40
2:A:381:PHE:HD1	2:A:381:PHE:H	1.69	0.40
2:A:708:ILE:C	2:A:710:ALA:H	2.29	0.40
3:B:198:PHE:HB2	3:B:224:PRO:HB3	2.02	0.40
1:F:379:LYS:HE2	1:F:383:LEU:H	1.86	0.40
2:A:746:TYR:CD1	2:A:903:GLU:HB3	2.56	0.40
3:B:275:MET:HG3	3:B:308:VAL:HG22	2.03	0.40
4:C:177:LYS:HD3	4:C:178:TYR:CD2	2.57	0.40
5:E:241:LYS:HE2	5:E:241:LYS:HB3	1.72	0.40
1:F:141:LEU:HD21	1:F:150:PRO:HD3	2.03	0.40
1:F:378:VAL:HG22	1:F:379:LYS:H	1.86	0.40
6:G:483:ASN:ND2	6:G:487:ILE:HG23	2.36	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	F	229/404 (57%)	200 (87%)	28 (12%)	1 (0%)	30	59
2	A	850/1075 (79%)	750 (88%)	91 (11%)	9 (1%)	11	36
3	B	367/405 (91%)	333 (91%)	34 (9%)	0	100	100
4	C	376/431 (87%)	324 (86%)	51 (14%)	1 (0%)	36	65
5	D	161/337 (48%)	142 (88%)	19 (12%)	0	100	100
5	E	156/337 (46%)	139 (89%)	17 (11%)	0	100	100
6	G	276/607 (46%)	226 (82%)	45 (16%)	5 (2%)	6	25
All	All	2415/3596 (67%)	2114 (88%)	285 (12%)	16 (1%)	20	48

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	247	GLN
6	G	291	ASP
2	A	332	SER
2	A	337	CYS
2	A	372	PRO
2	A	792	TRP
2	A	333	ASP
2	A	376	SER
2	A	901	PRO
1	F	150	PRO
2	A	175	ASN
6	G	290	ILE
6	G	462	PRO
6	G	350	PRO
6	G	439	PRO
2	A	121	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	161/365 (44%)	144 (89%)	17 (11%)	6	22
2	A	806/994 (81%)	725 (90%)	81 (10%)	7	24
3	B	320/351 (91%)	297 (93%)	23 (7%)	13	39
4	C	342/382 (90%)	305 (89%)	37 (11%)	6	21
5	D	153/312 (49%)	138 (90%)	15 (10%)	7	25
5	E	149/312 (48%)	128 (86%)	21 (14%)	3	11
6	G	261/553 (47%)	236 (90%)	25 (10%)	8	26
All	All	2192/3269 (67%)	1973 (90%)	219 (10%)	9	24

All (219) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	114	ILE
1	F	119	TYR
1	F	139	PHE
1	F	142	SER
1	F	149	THR
1	F	162	THR
1	F	188	GLN
1	F	192	GLN
1	F	198	ASP
1	F	206	ILE
1	F	211	THR
1	F	337	SER
1	F	345	ASP
1	F	347	LEU
1	F	377	ASP
1	F	378	VAL
1	F	391	LEU
2	A	40	LYS
2	A	56	VAL
2	A	72	VAL
2	A	73	ASP
2	A	78	ILE
2	A	81	ILE
2	A	90	ASP
2	A	114	PHE
2	A	116	LEU
2	A	120	THR
2	A	138	LEU
2	A	166	LEU

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Mol	Chain	Res	Type
2	A	180	LEU
2	A	193	GLU
2	A	207	SER
2	A	258	SER
2	A	271	VAL
2	A	272	GLU
2	A	290	ASP
2	A	302	LEU
2	A	311	SER
2	A	319	SER
2	A	329	SER
2	A	339	PRO
2	A	350	ASN
2	A	354	SER
2	A	357	ASP
2	A	358	ASP
2	A	372	PRO
2	A	374	TRP
2	A	381	PHE
2	A	382	ILE
2	A	385	ARG
2	A	386	LYS
2	A	420	ILE
2	A	436	THR
2	A	439	GLU
2	A	446	LYS
2	A	447	SER
2	A	472	MET
2	A	493	SER
2	A	504	SER
2	A	519	VAL
2	A	562	VAL
2	A	603	PHE
2	A	611	SER
2	A	614	LEU
2	A	716	SER
2	A	722	LEU
2	A	738	ASP
2	A	742	GLU
2	A	764	TYR
2	A	772	GLN
2	A	774	SER

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Mol	Chain	Res	Type
2	A	781	ILE
2	A	787	GLN
2	A	792	TRP
2	A	794	ASP
2	A	801	ASP
2	A	807	THR
2	A	812	THR
2	A	823	ILE
2	A	846	THR
2	A	862	VAL
2	A	877	ASN
2	A	879	SER
2	A	886	TYR
2	A	887	ASP
2	A	888	ASP
2	A	893	LEU
2	A	894	GLU
2	A	895	ILE
2	A	903	GLU
2	A	909	CYS
2	A	975	THR
2	A	981	SER
2	A	989	ARG
2	A	992	GLU
2	A	1004	ASP
2	A	1032	LEU
2	A	1050	LEU
3	B	14	GLU
3	B	37	ASN
3	B	44	LEU
3	B	45	TYR
3	B	60	ASP
3	B	79	ASP
3	B	99	VAL
3	B	101	ASP
3	B	108	SER
3	B	138	HIS
3	B	153	ILE
3	B	173	ASP
3	B	180	VAL
3	B	191	MET
3	B	194	SER

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Mol	Chain	Res	Type
3	B	201	TYR
3	B	211	THR
3	B	243	SER
3	B	260	THR
3	B	261	ASP
3	B	322	ASP
3	B	344	SER
3	B	351	ASN
4	C	37	SER
4	C	43	LEU
4	C	46	THR
4	C	49	LEU
4	C	51	TRP
4	C	56	LEU
4	C	64	ILE
4	C	79	VAL
4	C	118	LEU
4	C	122	ILE
4	C	132	VAL
4	C	160	LYS
4	C	162	SER
4	C	164	GLU
4	C	170	SER
4	C	175	LYS
4	C	200	LEU
4	C	212	TRP
4	C	228	VAL
4	C	229	HIS
4	C	245	LYS
4	C	248	ASP
4	C	257	GLN
4	C	261	VAL
4	C	272	LYS
4	C	294	ASP
4	C	299	THR
4	C	306	ILE
4	C	327	ILE
4	C	331	ILE
4	C	366	GLU
4	C	381	HIS
4	C	382	THR
4	C	385	THR

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Mol	Chain	Res	Type
4	C	391	CYS
4	C	407	LEU
4	C	419	ASN
5	D	185	ASP
5	D	187	GLU
5	D	190	THR
5	D	198	ILE
5	D	203	THR
5	D	220	ASN
5	D	250	ARG
5	D	257	LEU
5	D	274	VAL
5	D	282	VAL
5	D	283	SER
5	D	286	GLU
5	D	297	SER
5	D	330	ASN
5	D	335	VAL
5	E	169	LYS
5	E	170	HIS
5	E	172	ILE
5	E	176	ASP
5	E	185	ASP
5	E	188	ASN
5	E	193	GLN
5	E	195	LEU
5	E	198	ILE
5	E	204	VAL
5	E	216	ILE
5	E	222	GLU
5	E	236	VAL
5	E	246	MET
5	E	249	TYR
5	E	267	GLU
5	E	278	ILE
5	E	282	VAL
5	E	291	THR
5	E	300	CYS
5	E	305	ILE
6	G	263	ASN
6	G	279	GLU
6	G	305	TYR

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Mol	Chain	Res	Type
6	G	341	LEU
6	G	342	CYS
6	G	344	TYR
6	G	348	HIS
6	G	354	HIS
6	G	397	LEU
6	G	398	LEU
6	G	418	VAL
6	G	426	ASP
6	G	428	CYS
6	G	435	ASP
6	G	458	ASP
6	G	460	VAL
6	G	472	VAL
6	G	486	ASN
6	G	488	VAL
6	G	490	ASP
6	G	542	ILE
6	G	550	PHE
6	G	565	ASP
6	G	574	ASP
6	G	585	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	116	ASN
1	F	152	ASN
1	F	168	HIS
1	F	173	HIS
1	F	188	GLN
1	F	364	ASN
1	F	390	ASN
2	A	52	HIS
2	A	175	ASN
2	A	234	ASN
2	A	241	GLN
2	A	263	ASN
2	A	286	GLN
2	A	305	ASN
2	A	406	HIS
2	A	425	ASN

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Mol	Chain	Res	Type
2	A	461	HIS
2	A	544	GLN
2	A	583	ASN
2	A	597	ASN
2	A	616	GLN
2	A	717	HIS
2	A	757	ASN
2	A	777	GLN
2	A	912	ASN
2	A	926	ASN
2	A	1040	GLN
3	B	37	ASN
3	B	88	GLN
3	B	165	GLN
3	B	332	GLN
4	C	21	ASN
4	C	68	HIS
4	C	150	ASN
4	C	218	ASN
4	C	236	GLN
4	C	262	HIS
4	C	278	HIS
4	C	315	ASN
4	C	362	GLN
4	C	381	HIS
4	C	419	ASN
5	D	230	GLN
5	E	192	ASN
5	E	230	GLN
5	E	261	GLN
5	E	315	HIS
6	G	349	ASN
6	G	354	HIS
6	G	357	HIS
6	G	429	ASN
6	G	447	ASN
6	G	456	HIS
6	G	459	HIS
6	G	486	ASN
6	G	526	ASN
6	G	529	ASN
6	G	573	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](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

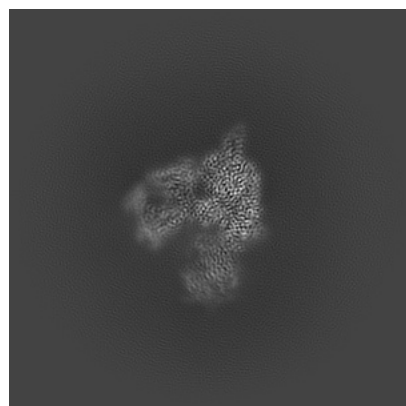
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35092. These allow visual inspection of the internal detail of the map and identification of artifacts.

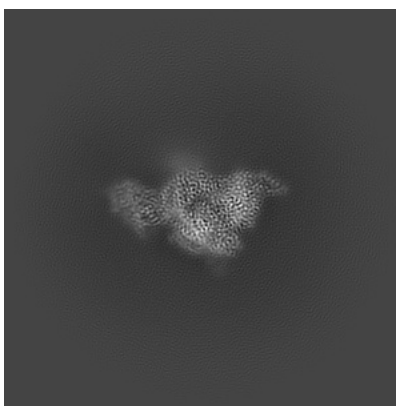
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

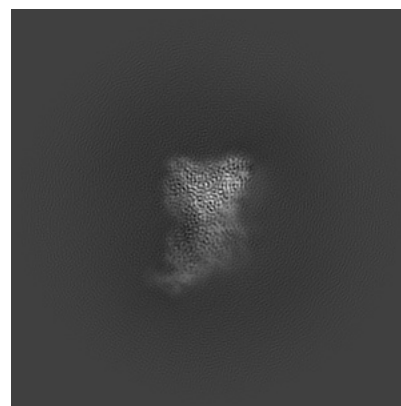
6.1.1 Primary map



X

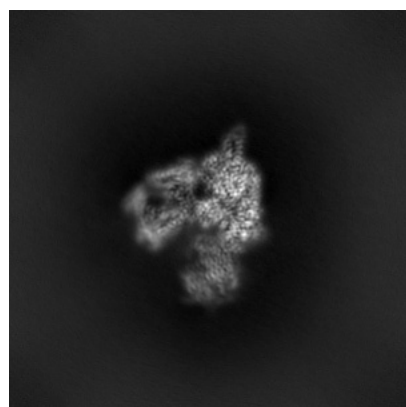


Y

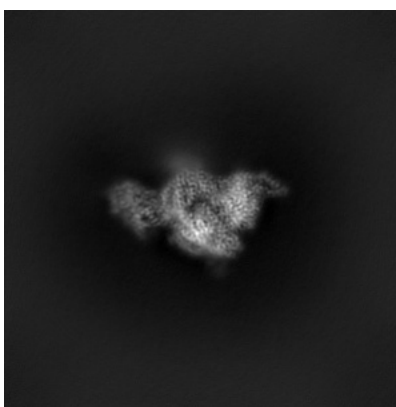


Z

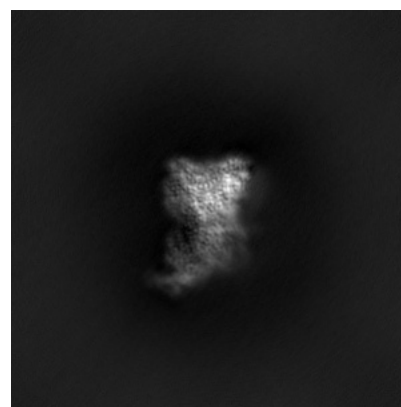
6.1.2 Raw map



X



Y

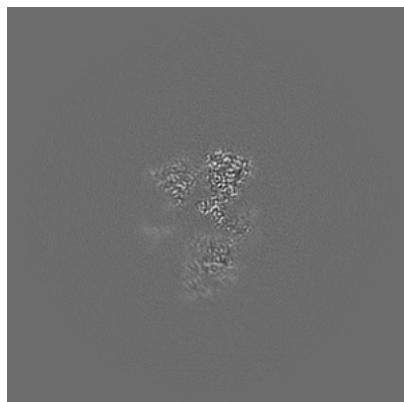


Z

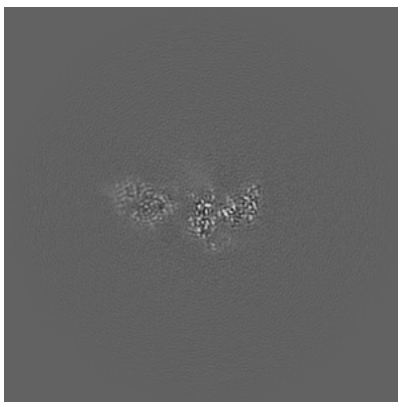
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

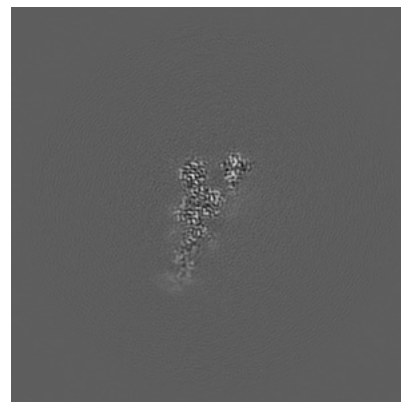
6.2.1 Primary map



X Index: 180

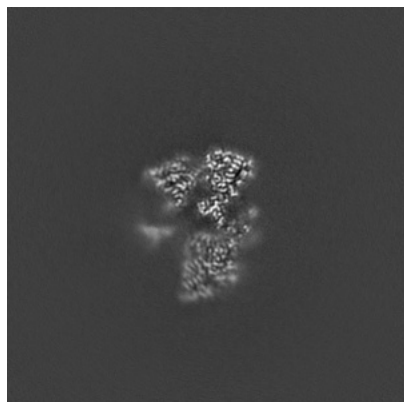


Y Index: 180

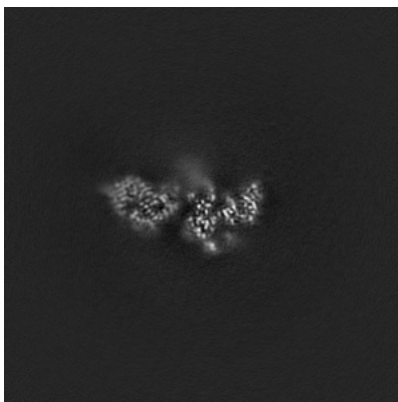


Z Index: 180

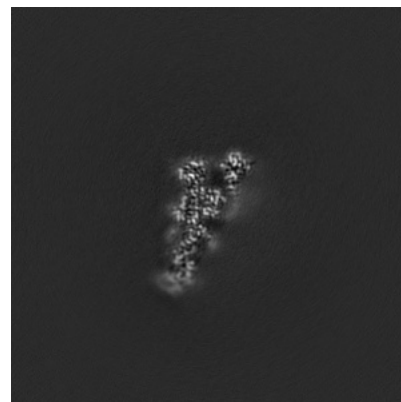
6.2.2 Raw map



X Index: 180



Y Index: 180

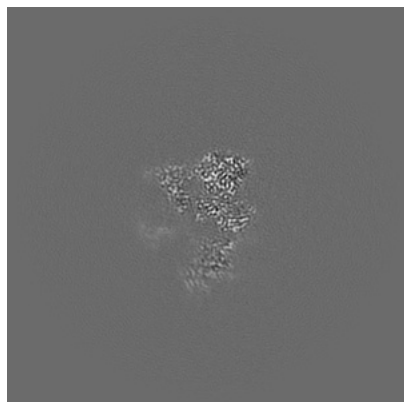


Z Index: 180

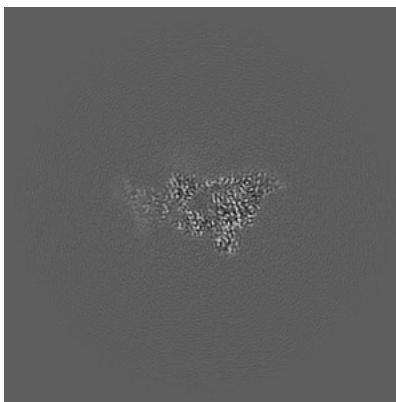
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

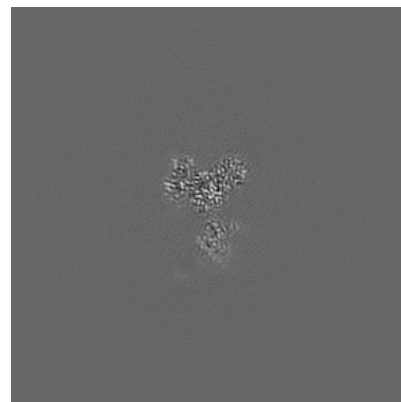
6.3.1 Primary map



X Index: 175

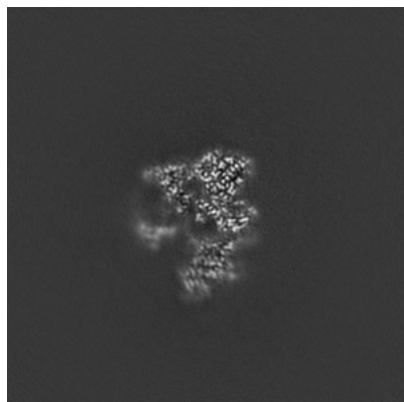


Y Index: 200

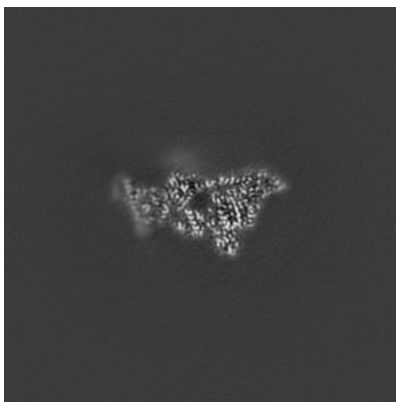


Z Index: 203

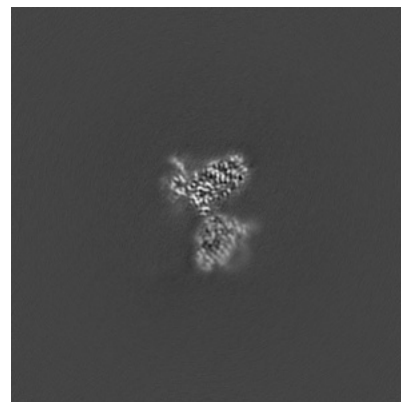
6.3.2 Raw map



X Index: 175



Y Index: 200

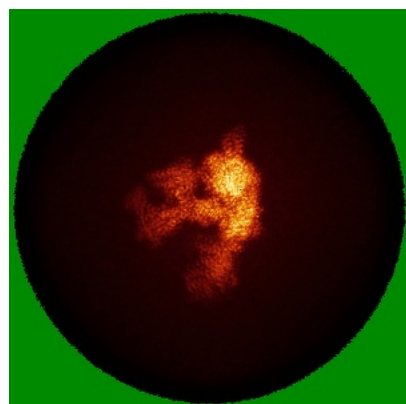


Z Index: 209

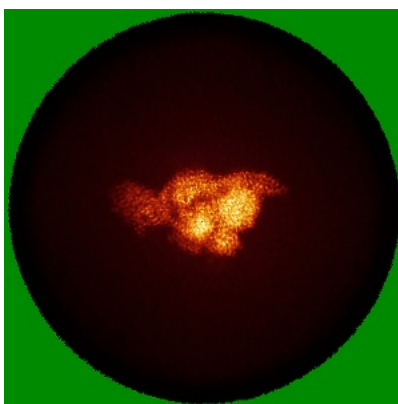
The images above show the largest variance slices of the map in three orthogonal directions.

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

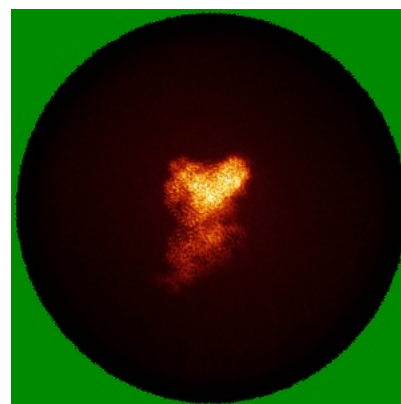
6.4.1 Primary map



X

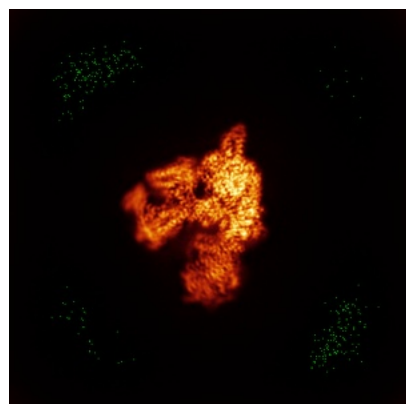


Y

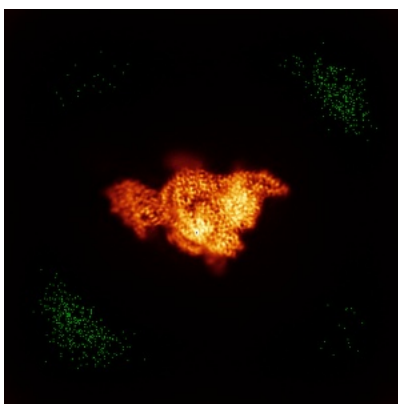


Z

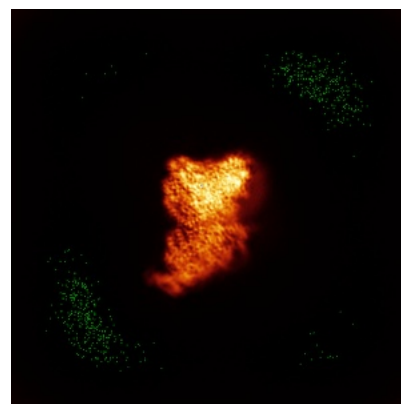
6.4.2 Raw map



X



Y

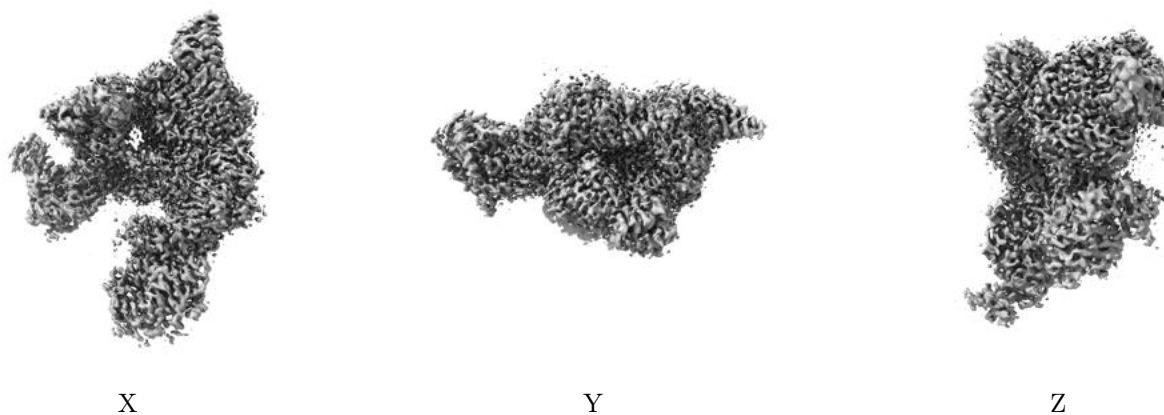


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

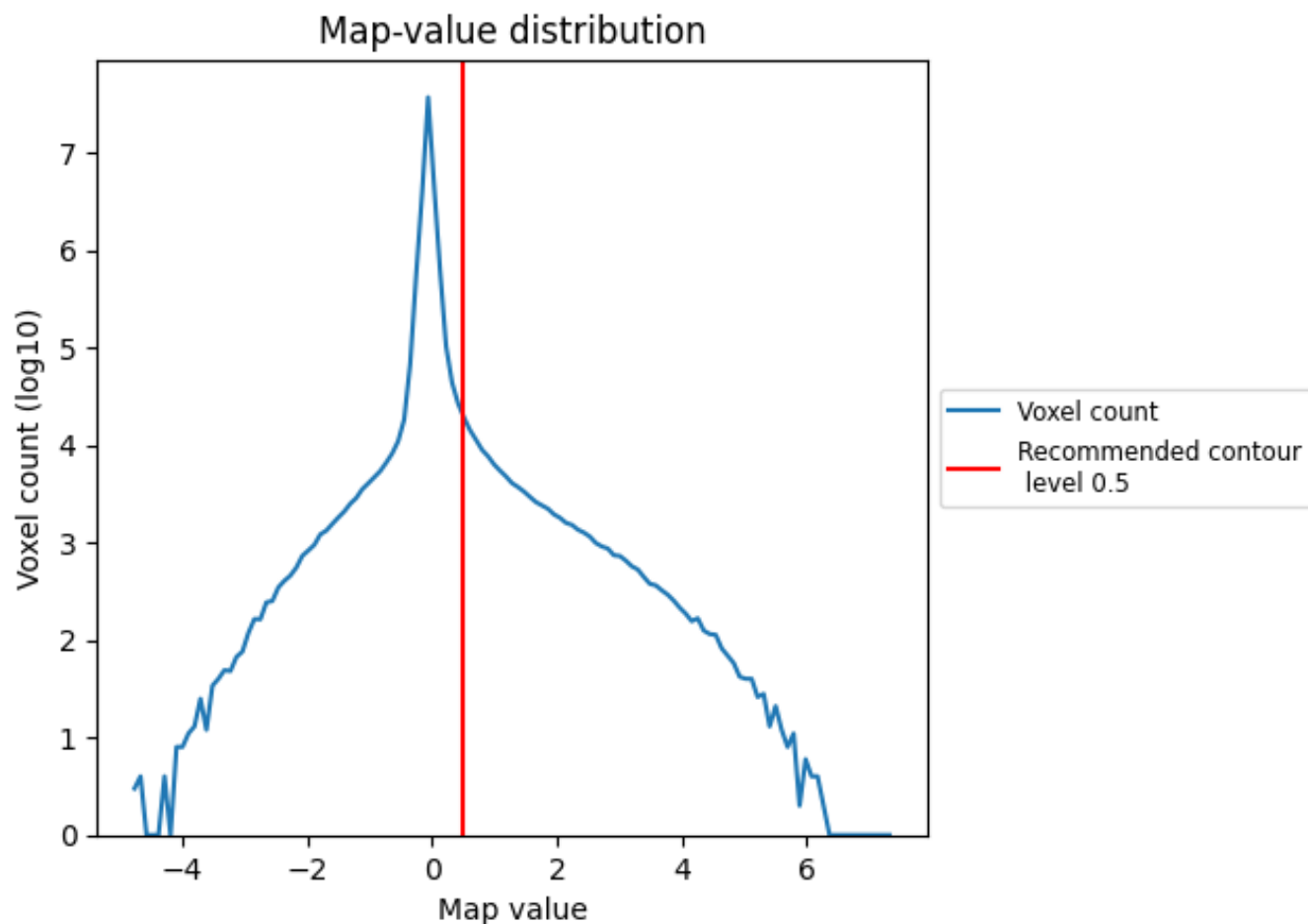
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

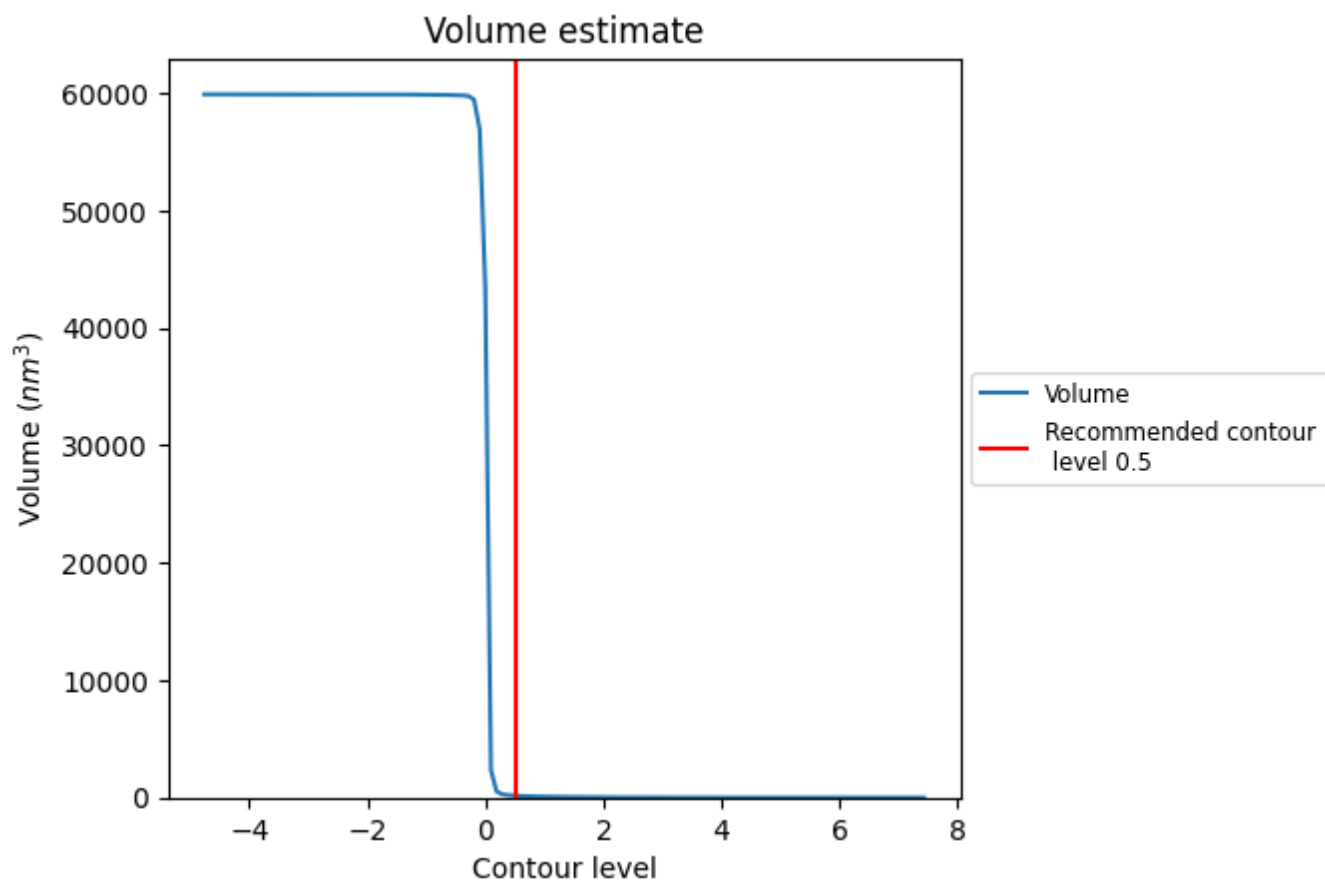
This section contains the results of statistical analysis of the map.

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.

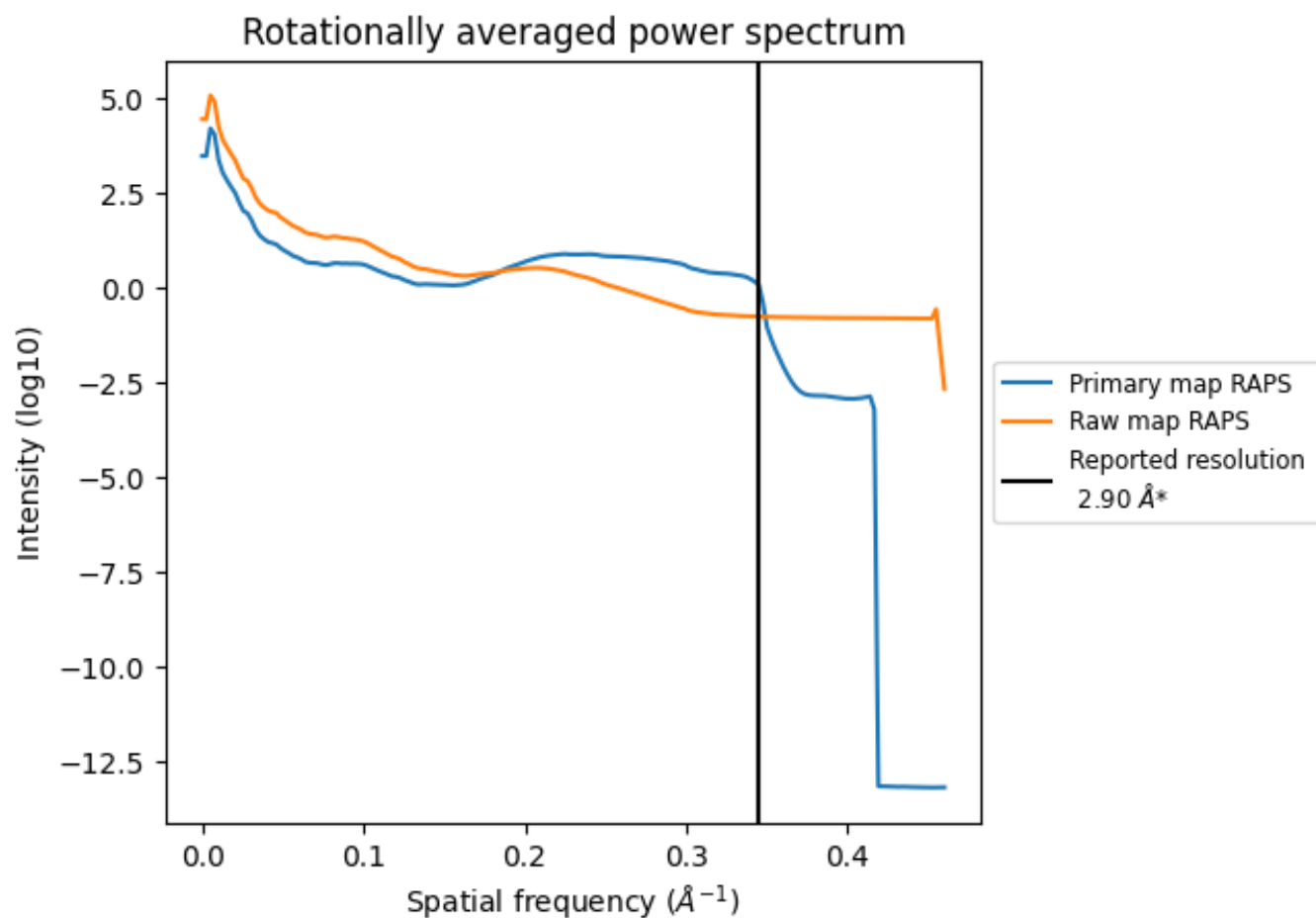
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 159 nm³; this corresponds to an approximate mass of 143 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

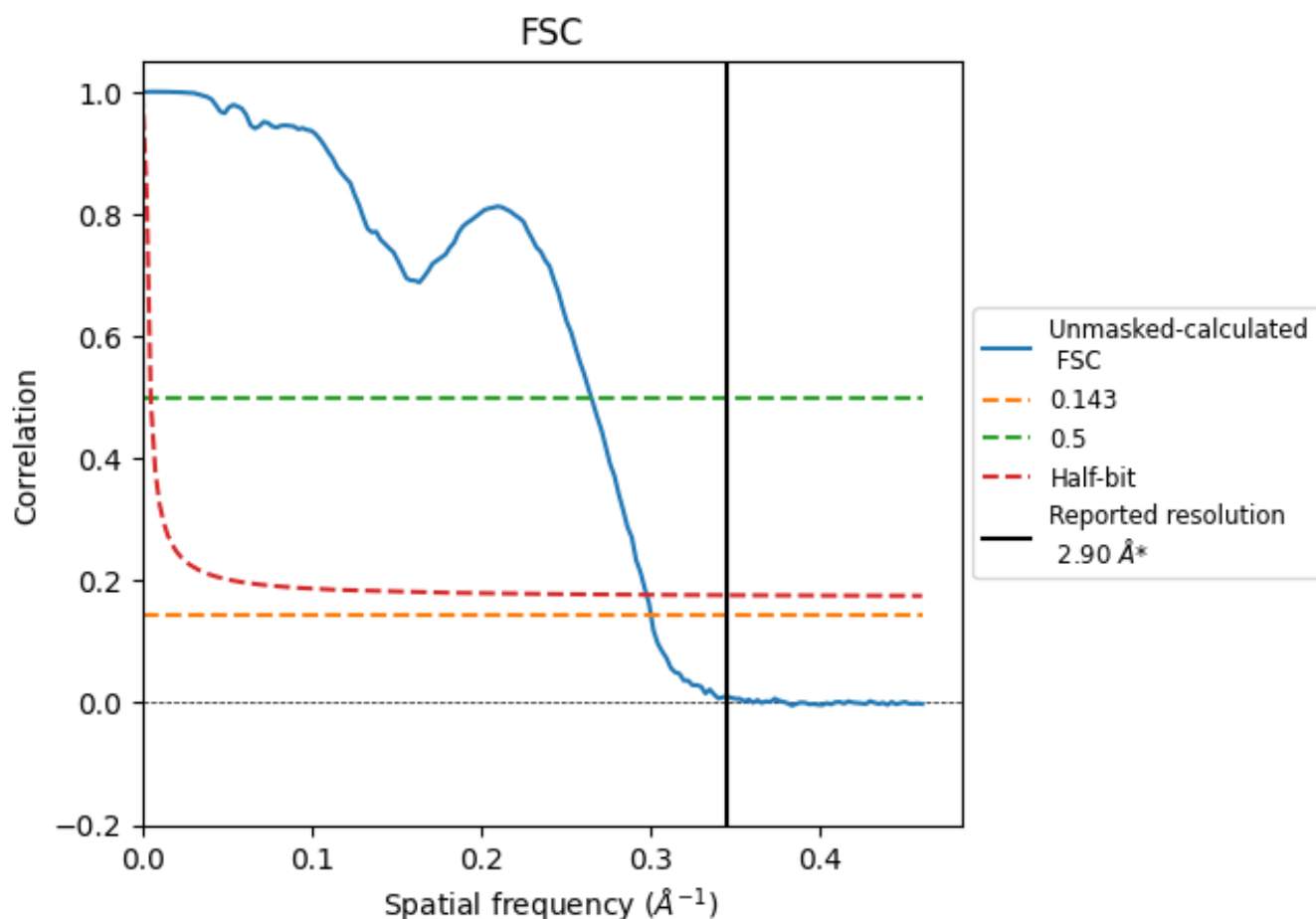


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

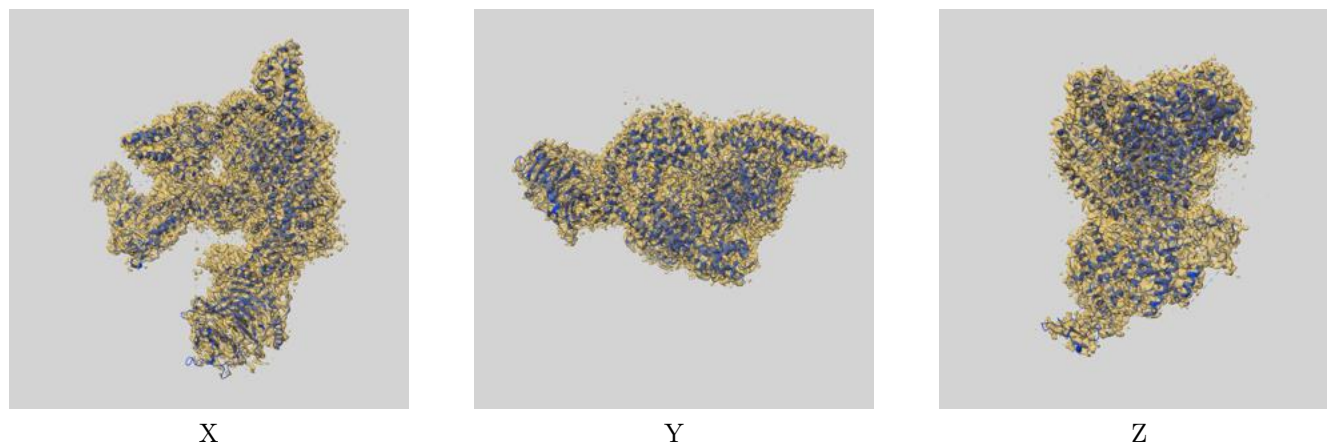
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.33	3.78	3.36

*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 3.33 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

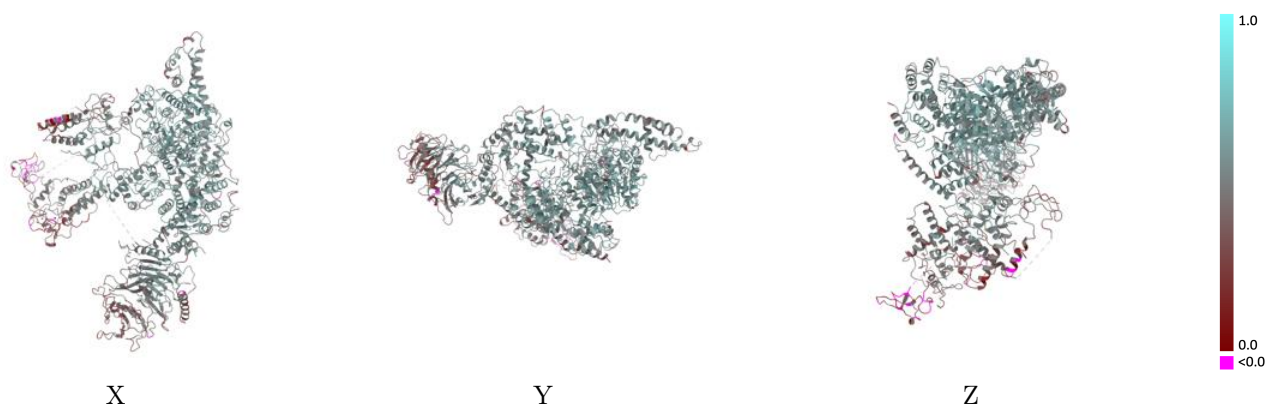
This section contains information regarding the fit between EMDB map EMD-35092 and PDB model 8I02. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



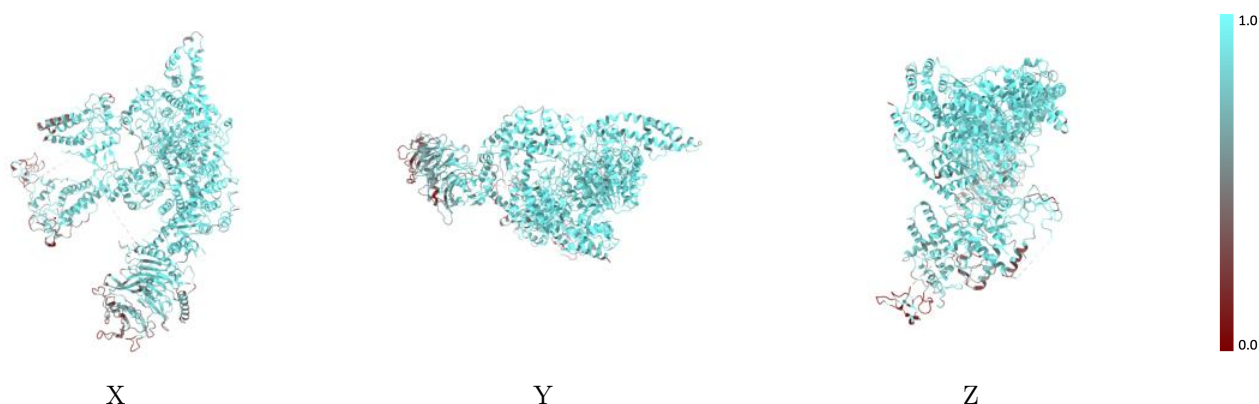
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



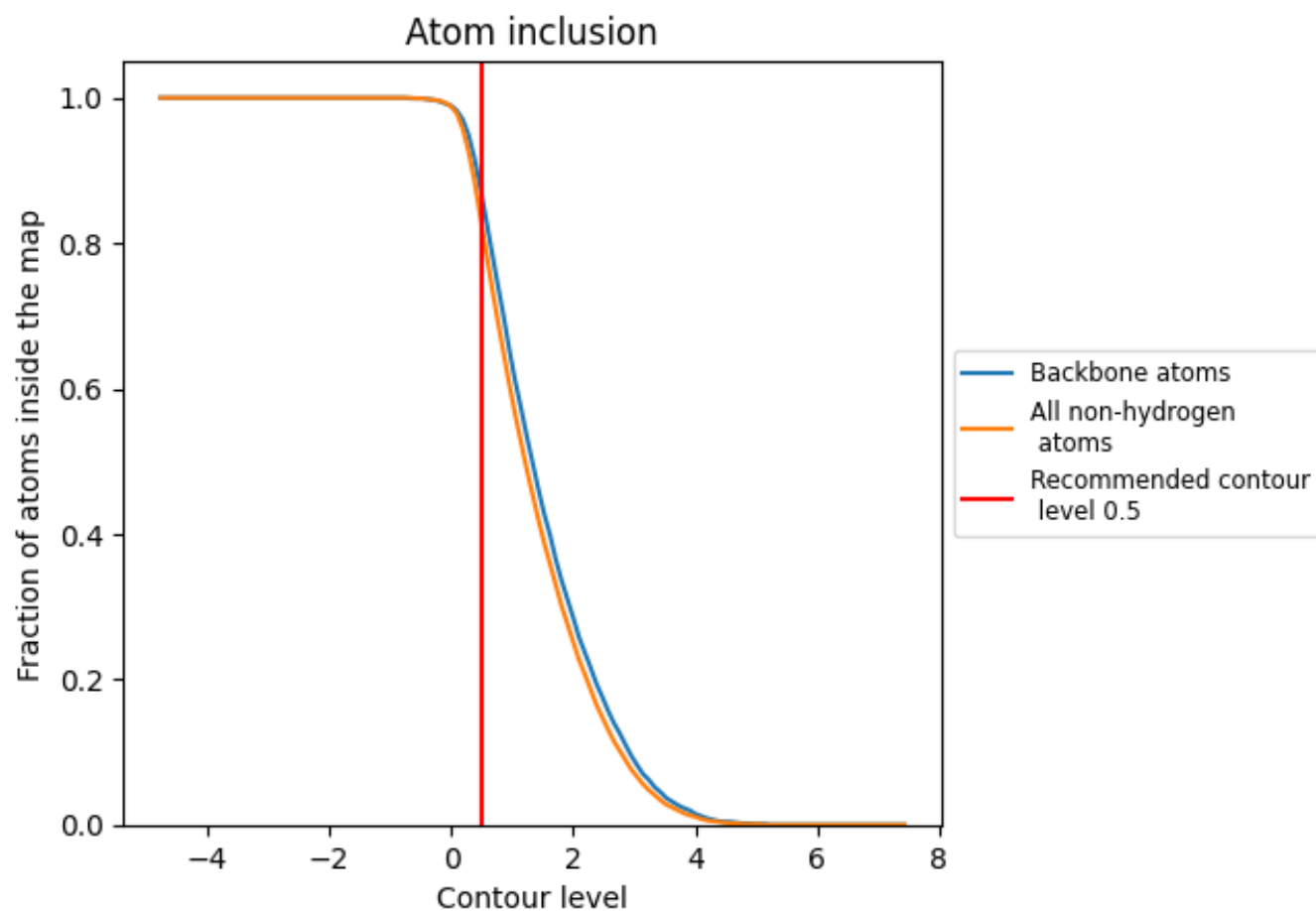
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8240	0.4960
A	0.8810	0.5270
B	0.9570	0.5920
C	0.6460	0.4370
D	0.8200	0.4760
E	0.7820	0.4300
F	0.6660	0.3580
G	0.8540	0.5040

1.0

0.0

<0.0