



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 06:03 AM UTC

PDB ID : 5OF4 / pdb_00005of4
EMDB ID : EMD-3802
Title : The cryo-EM structure of human TFIIH
Authors : Greber, B.J.; Nguyen, T.H.D.; Fang, J.; Afonine, P.V.; Adams, P.D.; Nogales, E.
Deposited on : 2017-07-10
Resolution : 4.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

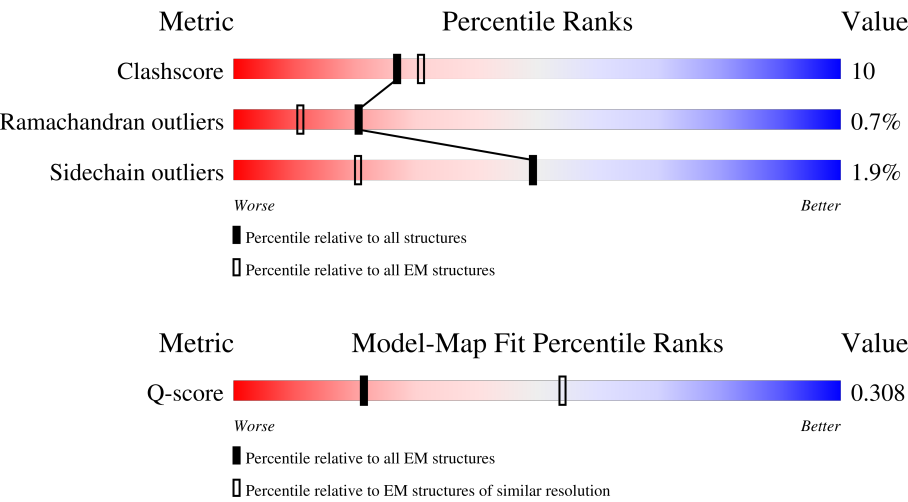
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
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 4.40 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	3132 (3.91 - 4.90)

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

Mol	Chain	Length	Quality of chain
1	A	553	17% 59% 28% 10%
2	B	760	13% 64% 28% 5%
3	D	85	33% 73% 22% 5%
4	E	395	5% 32% 13% 53%

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Mol	Chain	Length	Quality of chain
5	F	308	
6	G	71	
7	H	124	
8	Z	270	
9	Y	232	
10	X	78	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17200 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 TFIID basal transcription factor complex helicase XPB subunit,XPB,TFIID basal transcription factor complex helicase XPB subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	499	Total	C	N	O	S	0	0
			3887	2469	676	718	24		

- Molecule 2 is a protein called TFIID basal transcription factor complex helicase XPD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	724	Total	C	N	O	S	0	0
			5671	3626	992	1025	28		

- Molecule 3 is a protein called General transcription factor IID subunit 4,p52,General transcription factor IID subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	81	Total	C	N	O	S	0	0
			643	412	118	112	1		

- Molecule 4 is a protein called General transcription factor IID subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	184	Total	C	N	O	S	0	0
			1451	918	251	272	10		

- Molecule 5 is a protein called General transcription factor IID subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	205	Total	C	N	O	S	0	0
			1498	954	257	276	11		

- Molecule 6 is a protein called General transcription factor IID subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	66	Total	C	N	O	S	0	0
			522	336	83	100	3		

- Molecule 7 is a protein called MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	124	Total	C	N	O		0	0
			620	372	124	124			

- Molecule 8 is a protein called Unassigned secondary structure elements..

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	270	Total	C	N	O		0	0
			1350	810	270	270			

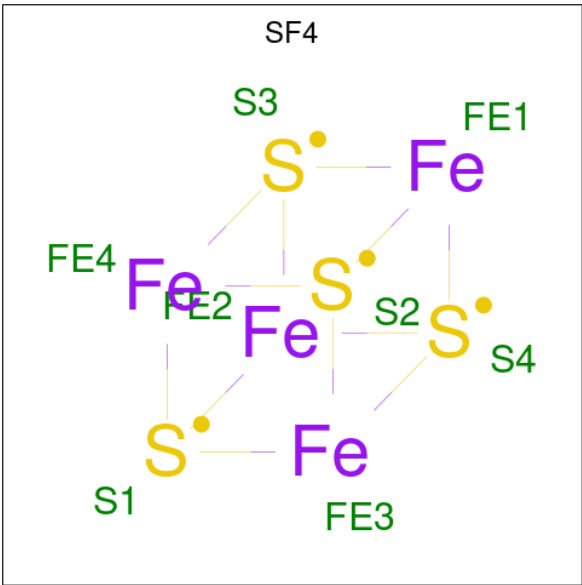
- Molecule 9 is a protein called Unassigned secondary structure elements (p52 region).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Y	232	Total	C	N	O		0	0
			1160	696	232	232			

- Molecule 10 is a protein called Unassigned secondary structure elements (XPB NTE region).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	78	Total	C	N	O		0	0
			390	234	78	78			

- Molecule 11 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

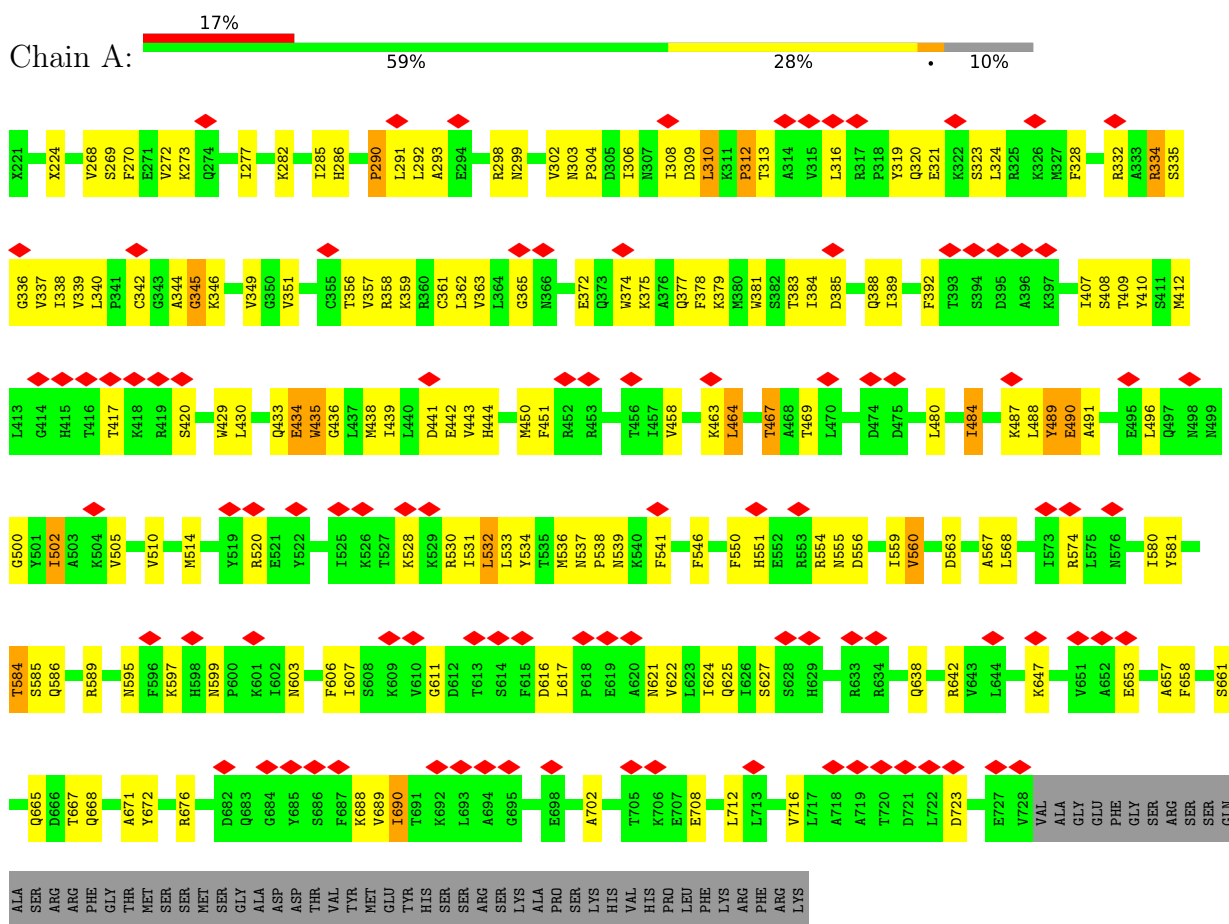


Mol	Chain	Residues	Atoms			AltConf
11	B	1	Total	Fe	S	0
			8	4	4	

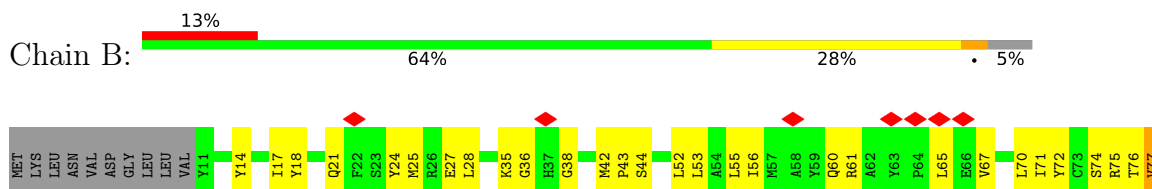
3 Residue-property plots

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.

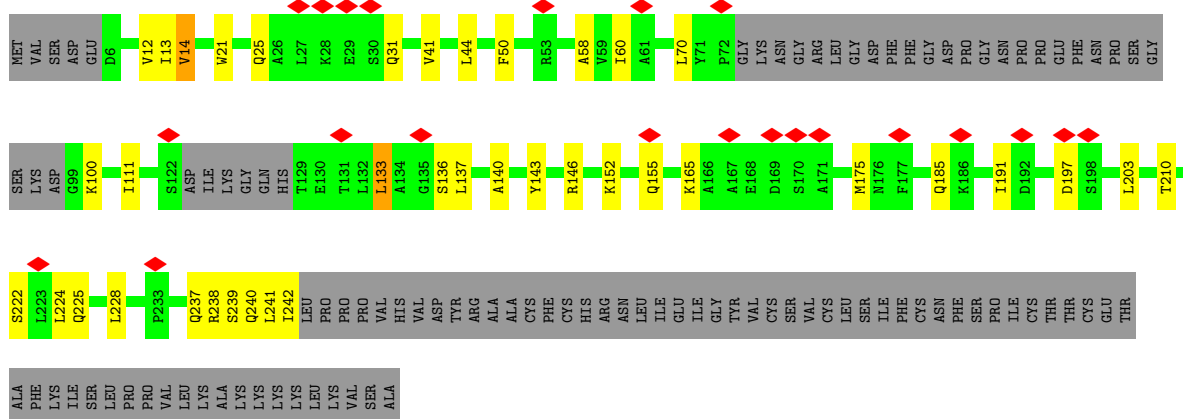
- Molecule 1: TFIIH basal transcription factor complex helicase XPB subunit,XPB,TFIIH basal transcription factor complex helicase XPB subunit



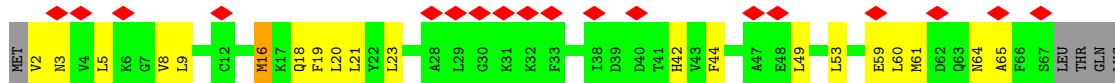
- Molecule 2: TFIIH basal transcription factor complex helicase XPD subunit



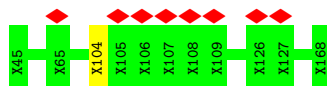
- Molecule 5: General transcription factor IIH subunit 3



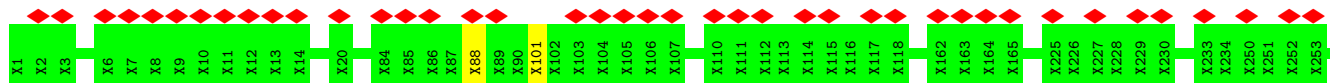
- Molecule 6: General transcription factor IIH subunit 5

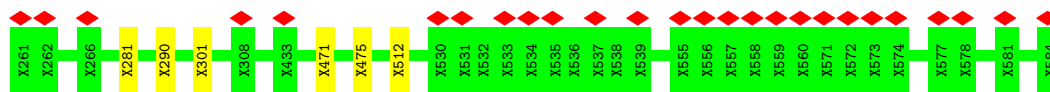


- Molecule 7: MAT1

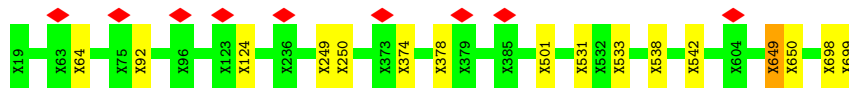


- Molecule 8: Unassigned secondary structure elements.

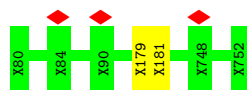




- Molecule 9: Unassigned secondary structure elements (p52 region)



- Molecule 10: Unassigned secondary structure elements (XPB NTE region)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	122900	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Correction in RELION based on values determined in CTFFIND4.	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	37879	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.129	Depositor
Minimum map value	-0.075	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	337.92, 337.92, 337.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.26	21/3779 (0.6%)	1.19	11/5102 (0.2%)
2	B	1.35	30/5790 (0.5%)	1.29	28/7853 (0.4%)
3	D	1.05	2/631 (0.3%)	1.00	3/855 (0.4%)
4	E	1.39	8/1478 (0.5%)	1.33	7/2001 (0.3%)
5	F	1.31	10/1518 (0.7%)	1.26	5/2061 (0.2%)
6	G	0.87	0/528	0.99	1/713 (0.1%)
All	All	1.30	71/13724 (0.5%)	1.24	55/18585 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
2	B	0	9
3	D	0	1
6	G	0	1
7	H	0	1
8	Z	0	2
9	Y	0	3
All	All	0	23

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	489	TYR	C-O	-15.42	1.05	1.24
2	B	539	PHE	N-CA	-10.27	1.31	1.45
1	A	270	PHE	C-O	9.09	1.34	1.24
1	A	464	LEU	C-O	-8.52	1.13	1.24
2	B	109	LEU	CA-C	-8.44	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	591	GLY	C-O	8.38	1.35	1.23
2	B	629	GLN	CA-C	8.05	1.63	1.52
1	A	490	GLU	C-O	7.72	1.33	1.23
1	A	310	LEU	C-O	-7.65	1.16	1.24
5	F	237	GLN	C-O	7.55	1.32	1.23
2	B	417	ILE	N-CA	-7.05	1.38	1.46
4	E	207	VAL	C-O	-6.95	1.15	1.24
2	B	496	GLY	C-O	-6.86	1.14	1.23
2	B	732	ASP	C-O	6.86	1.32	1.24
1	A	690	ILE	C-O	-6.84	1.16	1.24
4	E	168	LEU	C-O	-6.77	1.15	1.24
1	A	334	ARG	CZ-NH1	6.61	1.42	1.32
2	B	494	ILE	CB-CG1	6.61	1.66	1.53
4	E	168	LEU	CA-C	-6.43	1.44	1.52
1	A	345	GLY	C-O	-6.42	1.15	1.23
4	E	220	HIS	N-CA	6.42	1.53	1.46
1	A	489	TYR	CA-C	6.37	1.60	1.52
2	B	43	PRO	C-O	-6.27	1.15	1.24
2	B	109	LEU	N-CA	6.26	1.54	1.46
2	B	214	ASP	C-O	-6.18	1.17	1.24
2	B	522	ASN	C-O	6.11	1.31	1.24
1	A	409	THR	C-O	6.09	1.31	1.23
2	B	524	LEU	CB-CG	6.02	1.65	1.53
2	B	490	LEU	CA-C	-6.01	1.45	1.52
1	A	324	LEU	CA-C	5.99	1.60	1.52
5	F	224	LEU	CA-C	5.92	1.60	1.52
2	B	112	ARG	C-O	-5.89	1.17	1.23
2	B	535	ILE	CA-C	5.71	1.59	1.52
2	B	674	TYR	CA-C	-5.68	1.45	1.52
5	F	143	TYR	C-O	-5.66	1.17	1.24
1	A	293	ALA	C-O	5.66	1.30	1.23
3	D	392	ARG	CA-C	-5.63	1.45	1.52
4	E	61	LEU	CA-C	-5.62	1.45	1.52
5	F	185	GLN	CA-C	-5.62	1.45	1.52
4	E	91	PHE	CG-CD1	5.61	1.50	1.38
2	B	436	SER	C-O	5.61	1.31	1.23
2	B	620	MET	C-O	-5.60	1.17	1.24
5	F	13	ILE	CB-CG1	5.57	1.64	1.53
2	B	531	VAL	N-CA	-5.52	1.39	1.46
1	A	290	PRO	N-CA	-5.51	1.40	1.47
1	A	269	SER	C-O	-5.51	1.17	1.24
4	E	169	ILE	N-CA	-5.45	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	220	HIS	CA-C	-5.43	1.46	1.52
1	A	467	THR	C-O	-5.43	1.17	1.23
2	B	217	ILE	C-O	-5.41	1.17	1.24
2	B	687	GLY	N-CA	5.41	1.52	1.45
1	A	438	MET	C-O	-5.37	1.17	1.24
1	A	339	VAL	C-O	-5.37	1.18	1.24
5	F	240	GLN	N-CA	5.37	1.53	1.46
2	B	727	PRO	C-O	5.31	1.30	1.24
2	B	679	PHE	CA-C	-5.29	1.46	1.53
2	B	626	VAL	C-O	5.29	1.30	1.24
2	B	723	GLN	CA-C	-5.22	1.45	1.52
3	D	394	TRP	CE3-CZ3	5.22	1.54	1.38
5	F	14	VAL	CA-C	-5.21	1.46	1.52
1	A	268	VAL	C-O	-5.19	1.18	1.24
5	F	146	ARG	CD-NE	5.19	1.53	1.46
1	A	319	TYR	C-O	5.15	1.30	1.24
1	A	439	ILE	CA-CB	-5.14	1.47	1.53
2	B	77	VAL	CA-C	5.12	1.58	1.52
5	F	240	GLN	CA-C	5.10	1.59	1.52
5	F	100	LYS	CA-C	5.06	1.59	1.52
2	B	569	ILE	CA-C	-5.05	1.46	1.52
2	B	548	THR	C-O	-5.05	1.18	1.24
2	B	499	ASN	C-O	-5.04	1.17	1.24
1	A	560	VAL	C-O	-5.01	1.18	1.24

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	207	VAL	CG1-CB-CG2	8.03	128.47	110.80
1	A	490	GLU	N-CA-C	-7.38	97.66	109.76
2	B	533	ASP	N-CA-C	7.36	121.84	112.86
2	B	184	GLY	O-C-N	6.66	128.58	122.19
4	E	220	HIS	CB-CA-C	-6.45	98.63	110.62
2	B	628	THR	N-CA-C	6.44	121.00	113.20
2	B	493	MET	CA-C-O	6.37	128.16	120.27
5	F	146	ARG	CB-CG-CD	6.33	125.86	111.30
2	B	687	GLY	N-CA-C	-6.28	104.73	112.77
6	G	16	MET	CB-CG-SD	6.11	131.02	112.70
1	A	316	LEU	CA-C-N	6.09	136.65	121.80
1	A	316	LEU	C-N-CA	6.09	136.65	121.80
2	B	109	LEU	CB-CA-C	-6.08	103.00	112.12
2	B	310	LEU	CA-C-N	-5.90	113.90	120.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	310	LEU	C-N-CA	-5.90	113.90	120.45
1	A	273	LYS	CB-CG-CD	5.89	124.85	111.30
2	B	425	THR	CA-C-N	5.85	127.15	119.84
2	B	425	THR	C-N-CA	5.85	127.15	119.84
1	A	320	GLN	CB-CA-C	5.80	120.42	110.79
4	E	211	LEU	CD1-CG-CD2	-5.79	98.06	110.80
2	B	112	ARG	CG-CD-NE	5.67	124.47	112.00
2	B	497	ARG	NE-CZ-NH2	5.65	124.29	119.20
1	A	489	TYR	O-C-N	-5.61	116.63	123.30
2	B	533	ASP	CB-CA-C	-5.48	102.42	111.36
1	A	303	ASN	CA-C-N	-5.42	115.01	120.21
1	A	303	ASN	C-N-CA	-5.42	115.01	120.21
4	E	193	LYS	CG-CD-CE	5.37	123.65	111.30
2	B	591	GLY	O-C-N	5.35	129.65	122.70
2	B	699	GLU	CB-CG-CD	5.33	121.67	112.60
2	B	247	MET	CB-CG-SD	-5.33	96.71	112.70
1	A	435	TRP	N-CA-C	-5.32	106.37	112.92
2	B	77	VAL	CA-C-N	-5.26	113.11	118.85
2	B	77	VAL	C-N-CA	-5.26	113.11	118.85
4	E	86	LYS	CA-CB-CG	5.23	124.56	114.10
3	D	402	ARG	CA-C-N	5.22	128.26	120.90
3	D	402	ARG	C-N-CA	5.22	128.26	120.90
4	E	205	VAL	CB-CA-C	5.21	118.35	111.21
5	F	238	ARG	CA-C-N	5.20	131.48	121.54
5	F	238	ARG	C-N-CA	5.20	131.48	121.54
5	F	146	ARG	NE-CZ-NH2	5.20	123.88	119.20
2	B	677	MET	N-CA-C	5.20	116.65	107.61
3	D	394	TRP	CA-CB-CG	5.18	123.45	113.60
2	B	626	VAL	CG1-CB-CG2	5.15	122.13	110.80
2	B	595	ILE	N-CA-C	5.14	116.04	109.30
2	B	663	CYS	N-CA-C	5.12	116.67	111.14
1	A	270	PHE	CA-C-N	-5.11	113.38	122.07
1	A	270	PHE	C-N-CA	-5.11	113.38	122.07
2	B	503	ALA	N-CA-C	-5.11	96.79	107.37
4	E	222	ILE	N-CA-C	5.11	115.63	108.17
2	B	677	MET	CB-CG-SD	-5.11	97.37	112.70
2	B	612	HIS	N-CA-C	5.10	118.97	112.34
2	B	703	ASP	N-CA-C	-5.09	105.38	111.03
2	B	299	ARG	N-CA-C	5.04	121.54	110.80
5	F	146	ARG	NE-CZ-NH1	-5.04	116.46	121.50
2	B	85	GLU	CB-CG-CD	5.00	121.11	112.60

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	272	VAL	Peptide
1	A	312	PRO	Peptide
1	A	328	PHE	Peptide
1	A	412	MET	Peptide
1	A	434	GLU	Peptide
1	A	500	GLY	Peptide
2	B	111	SER	Peptide
2	B	188	GLY	Peptide
2	B	313	GLU	Peptide
2	B	486	ALA	Peptide
2	B	490	LEU	Peptide
2	B	532	PRO	Peptide
2	B	557	ILE	Peptide
2	B	627	TYR	Peptide
2	B	727	PRO	Peptide
3	D	378	UNK	Peptide
6	G	59	GLU	Peptide
7	H	104	UNK	Peptide
9	Y	249	UNK	Peptide
9	Y	649	UNK	Peptide
9	Y	92	UNK	Peptide
8	Z	281	UNK	Peptide
8	Z	88	UNK	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	A	3887	0	3750	98	0
2	B	5671	0	5575	144	0
3	D	643	0	622	15	0
4	E	1451	0	1492	33	0
5	F	1498	0	1414	19	0
6	G	522	0	528	14	0
7	H	620	0	131	0	0
8	Z	1350	0	315	5	0
9	Y	1160	0	279	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	X	390	0	96	1	0
11	B	8	0	0	0	0
All	All	17200	0	14202	312	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 10.

All (312) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:GLY:HA2	2:B:204:VAL:O	1.71	0.91
1:A:671:ALA:HB2	6:G:65:ALA:HB1	1.56	0.88
1:A:224:UNK:O	1:A:292:LEU:HA	1.74	0.87
1:A:429:TRP:O	1:A:433:GLN:HB2	1.75	0.85
3:D:408:LEU:HB3	6:G:5:LEU:HD12	1.59	0.84
3:D:433:PHE:O	3:D:441:MET:HA	1.78	0.81
9:Y:698:UNK:O	9:Y:699:UNK:O	1.96	0.81
1:A:336:GLY:O	1:A:464:LEU:HA	1.82	0.79
2:B:539:PHE:HB2	2:B:598:SER:O	1.83	0.78
2:B:438:MET:HG2	2:B:636:ARG:HA	1.67	0.77
4:E:60:HIS:HD2	4:E:103:GLN:HE21	1.33	0.76
2:B:697:ILE:HA	2:B:701:LEU:HB3	1.69	0.75
1:A:444:HIS:HD2	1:A:467:THR:HG23	1.52	0.74
4:E:198:VAL:O	4:E:219:TYR:HA	1.88	0.74
5:F:14:VAL:HG13	5:F:60:ILE:HD11	1.68	0.74
2:B:248:SER:HA	2:B:435:PHE:O	1.88	0.74
5:F:242:ILE:CB	8:Z:301:UNK:CB	2.66	0.73
1:A:374:TRP:O	1:A:378:PHE:HB2	1.90	0.72
1:A:337:VAL:HG21	1:A:484:ILE:HD13	1.73	0.71
2:B:184:GLY:HA2	2:B:189:TRP:HA	1.72	0.70
1:A:298:ARG:HB2	1:A:359:LYS:HZ3	1.57	0.69
2:B:231:VAL:O	2:B:454:VAL:HA	1.91	0.69
2:B:492:PRO:HA	2:B:677:MET:O	1.92	0.69
9:Y:698:UNK:O	9:Y:699:UNK:C	2.41	0.69
2:B:335:ARG:O	2:B:339:TYR:HB2	1.92	0.69
2:B:565:LYS:HB3	2:B:594:ALA:H	1.57	0.69
2:B:236:ALA:HB1	2:B:239:ILE:HD11	1.73	0.68
2:B:72:TYR:O	2:B:206:VAL:HA	1.92	0.68
2:B:61:ARG:NH2	2:B:103:PRO:O	2.26	0.68
3:D:395:GLU:OE2	9:Y:501:UNK:HA	1.94	0.68
1:A:356:THR:HB	2:B:501:GLN:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:ALA:HA	2:B:206:VAL:O	1.94	0.67
1:A:510:VAL:HG22	1:A:690:ILE:HB	1.77	0.65
3:D:409:TYR:O	3:D:440:LEU:HA	1.95	0.65
4:E:87:LEU:HD22	4:E:229:LYS:HD3	1.78	0.64
1:A:338:ILE:HG23	1:A:489:TYR:HB3	1.78	0.64
1:A:581:TYR:H	1:A:589:ARG:HH12	1.46	0.64
2:B:88:ARG:NH1	2:B:174:ILE:O	2.31	0.64
2:B:191:PRO:O	2:B:195:ALA:HB2	1.98	0.63
4:E:159:MET:O	4:E:165:ARG:NH2	2.31	0.63
2:B:17:ILE:HD13	2:B:21:GLN:HB2	1.81	0.62
2:B:262:ASN:HD21	2:B:394:PHE:HA	1.63	0.62
2:B:70:LEU:HB3	2:B:204:VAL:HG22	1.81	0.62
2:B:558:LEU:HD21	2:B:567:LEU:HD11	1.82	0.62
1:A:334:ARG:NH1	1:A:335:SER:O	2.33	0.61
1:A:434:GLU:HB2	1:A:436:GLY:H	1.66	0.61
2:B:444:ILE:HG21	2:B:470:ILE:HG23	1.82	0.61
3:D:411:GLN:O	6:G:2:VAL:HG21	2.00	0.61
2:B:566:LEU:O	2:B:594:ALA:HA	2.00	0.61
4:E:60:HIS:CD2	4:E:103:GLN:HE21	2.18	0.61
1:A:417:THR:HG23	1:A:420:SER:HB3	1.83	0.61
1:A:429:TRP:O	1:A:433:GLN:CB	2.48	0.60
2:B:231:VAL:HB	2:B:454:VAL:HG12	1.84	0.60
2:B:617:ALA:HB1	2:B:676:LEU:HD23	1.83	0.60
4:E:156:LEU:HG	4:E:165:ARG:HD3	1.83	0.60
1:A:310:LEU:HD23	2:B:515:ALA:HB2	1.83	0.59
1:A:374:TRP:NE1	1:A:441:ASP:OD2	2.34	0.59
2:B:56:ILE:HG21	2:B:70:LEU:HD22	1.84	0.59
2:B:72:TYR:HB3	2:B:206:VAL:HG22	1.85	0.59
4:E:68:SER:HB3	4:E:143:PRO:HD3	1.84	0.59
2:B:240:ASP:OD2	2:B:636:ARG:NH2	2.36	0.59
1:A:556:ASP:HB3	1:A:621:ASN:HD22	1.68	0.58
1:A:410:TYR:HB3	1:A:450:MET:HE2	1.85	0.58
1:A:377:GLN:O	1:A:381:TRP:HB2	2.03	0.58
2:B:81:GLU:HA	2:B:84:ILE:HD12	1.85	0.58
1:A:469:THR:OG1	1:A:638:GLN:NE2	2.37	0.58
2:B:460:THR:HG23	2:B:661:ALA:HB3	1.86	0.58
4:E:156:LEU:HD21	4:E:165:ARG:HB3	1.84	0.58
4:E:182:ILE:HG13	4:E:185:LEU:HD12	1.86	0.58
1:A:560:VAL:HG22	1:A:624:ILE:HB	1.86	0.58
2:B:692:LYS:HG2	2:B:701:LEU:HD13	1.85	0.57
5:F:41:VAL:HA	5:F:44:LEU:HD12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:619:ILE:HG23	2:B:678:VAL:HG23	1.86	0.57
2:B:75:ARG:HH12	2:B:238:ASN:H	1.51	0.57
5:F:137:LEU:HD12	5:F:140:ALA:HB3	1.85	0.57
5:F:152:LYS:HB2	5:F:155:GLN:HA	1.86	0.57
1:A:514:MET:HG2	1:A:665:GLN:HE21	1.69	0.57
9:Y:533:UNK:O	9:Y:538:UNK:HA	2.05	0.57
2:B:559:GLU:O	2:B:563:ARG:N	2.38	0.57
1:A:365:GLY:HA2	1:A:441:ASP:HB2	1.86	0.56
2:B:493:MET:HB3	2:B:678:VAL:HG12	1.86	0.56
1:A:442:GLU:OE1	1:A:444:HIS:NE2	2.34	0.56
2:B:71:ILE:HB	2:B:231:VAL:HG22	1.87	0.56
3:D:408:LEU:HD11	3:D:440:LEU:HB3	1.87	0.56
1:A:308:ILE:HB	1:A:388:GLN:HE22	1.71	0.56
2:B:353:SER:O	2:B:416:ILE:HB	2.05	0.56
5:F:175:MET:HE3	8:Z:290:UNK:CB	2.36	0.56
1:A:668:GLN:OE1	6:G:64:ASN:O	2.24	0.56
2:B:623:VAL:HG21	2:B:683:ARG:HD2	1.88	0.56
1:A:385:ASP:HA	1:A:389:ILE:HD11	1.88	0.56
1:A:312:PRO:HD3	1:A:383:THR:HG23	1.89	0.55
1:A:555:ASN:O	1:A:603:ASN:ND2	2.39	0.55
5:F:70:LEU:HD13	5:F:111:ILE:HA	1.88	0.55
5:F:225:GLN:HA	5:F:228:LEU:HD12	1.88	0.55
1:A:356:THR:OG1	2:B:501:GLN:NE2	2.40	0.55
1:A:625:GLN:O	1:A:661:SER:HA	2.07	0.55
2:B:183:LEU:O	2:B:188:GLY:N	2.39	0.55
1:A:299:ASN:HB3	1:A:332:ARG:HB3	1.88	0.55
1:A:622:VAL:HG22	1:A:658:PHE:HB2	1.89	0.54
4:E:61:LEU:O	4:E:104:ILE:HA	2.07	0.54
2:B:497:ARG:HD3	2:B:710:VAL:HG23	1.90	0.54
1:A:363:VAL:HB	1:A:407:ILE:HG12	1.89	0.54
2:B:552:TRP:HB3	2:B:558:LEU:HD23	1.90	0.54
2:B:42:MET:HE3	2:B:44:SER:HA	1.90	0.54
2:B:309:VAL:HG11	2:B:409:THR:HB	1.90	0.54
2:B:630:SER:HB3	2:B:633:LEU:HD13	1.90	0.54
2:B:335:ARG:O	2:B:339:TYR:CB	2.56	0.54
4:E:76:LEU:HD22	4:E:225:GLU:HG2	1.90	0.53
1:A:310:LEU:CD2	2:B:515:ALA:HB2	2.38	0.53
1:A:586:GLN:HA	1:A:589:ARG:HD2	1.90	0.53
1:A:285:ILE:HG23	1:A:290:PRO:HG2	1.90	0.53
2:B:315:LEU:HB2	2:B:374:PHE:HZ	1.73	0.53
2:B:525:LEU:HD22	2:B:560:ASN:HD21	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:TYR:O	1:A:589:ARG:NH1	2.41	0.53
2:B:369:ARG:H	2:B:372:LEU:HD12	1.74	0.53
1:A:344:ALA:HB2	1:A:502:ILE:HD11	1.89	0.53
6:G:19:PHE:HE1	6:G:60:LEU:HD22	1.74	0.52
2:B:650:ASP:OD1	2:B:690:ARG:NH2	2.41	0.52
1:A:282:LYS:HG2	1:A:292:LEU:HD11	1.90	0.52
3:D:434:GLU:HA	3:D:441:MET:HG2	1.91	0.52
1:A:505:VAL:HG22	1:A:657:ALA:HB3	1.90	0.52
2:B:70:LEU:O	2:B:204:VAL:HA	2.09	0.52
2:B:562:GLN:HE22	8:Z:512:UNK:CB	2.23	0.52
4:E:210:VAL:HA	4:E:213:ARG:HG2	1.92	0.52
5:F:50:PHE:CE1	9:Y:124:UNK:HA	2.45	0.52
2:B:263:LEU:HD13	2:B:333:LEU:HD23	1.92	0.51
2:B:362:ALA:O	2:B:368:GLN:NE2	2.42	0.51
2:B:67:VAL:HB	2:B:228:LYS:HD2	1.92	0.51
2:B:632:ILE:HG23	2:B:633:LEU:HD12	1.93	0.51
2:B:237:HIS:CD2	2:B:460:THR:HB	2.45	0.51
5:F:191:ILE:HD12	5:F:210:THR:HG21	1.92	0.51
2:B:21:GLN:O	2:B:25:MET:HB2	2.11	0.51
2:B:76:THR:HB	2:B:78:PRO:HD2	1.93	0.51
2:B:722:ARG:NH2	4:E:75:ASP:OD2	2.44	0.51
1:A:530:ARG:HA	1:A:533:LEU:HD12	1.93	0.51
1:A:361:CYS:SG	1:A:362:LEU:N	2.84	0.50
2:B:251:LEU:O	2:B:432:ILE:HA	2.10	0.50
2:B:372:LEU:HB3	2:B:408:SER:HB2	1.93	0.50
2:B:673:ASP:OD1	2:B:674:TYR:N	2.44	0.50
6:G:8:VAL:O	6:G:44:PHE:HA	2.12	0.50
1:A:298:ARG:HH12	1:A:435:TRP:HE3	1.59	0.50
1:A:528:LYS:HG2	1:A:531:ILE:HD12	1.94	0.50
2:B:275:GLU:O	2:B:279:GLN:N	2.36	0.50
2:B:497:ARG:HH11	2:B:710:VAL:H	1.59	0.50
9:Y:374:UNK:O	9:Y:378:UNK:CB	2.59	0.50
1:A:302:VAL:HG22	1:A:304:PRO:HD2	1.93	0.50
2:B:191:PRO:O	2:B:195:ALA:CB	2.59	0.50
2:B:520:TYR:HA	2:B:523:LEU:HD23	1.92	0.50
5:F:225:GLN:HE22	9:Y:64:UNK:C	2.24	0.50
4:E:85:LEU:HD21	4:E:135:VAL:HG22	1.94	0.50
6:G:20:LEU:HD23	6:G:23:LEU:HD12	1.93	0.50
2:B:28:LEU:HD13	2:B:55:LEU:HB2	1.94	0.49
2:B:343:ARG:O	2:B:347:GLN:HB2	2.12	0.49
3:D:398:ARG:NH2	9:Y:250:UNK:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:MET:N	2:B:458:SER:O	2.40	0.49
1:A:533:LEU:HA	1:A:716:VAL:HG11	1.95	0.49
2:B:668:ILE:HD11	2:B:675:GLY:HA3	1.93	0.49
1:A:340:LEU:HD23	1:A:491:ALA:HB2	1.95	0.49
2:B:91:LEU:O	2:B:95:GLU:HB2	2.12	0.49
1:A:337:VAL:H	1:A:488:LEU:HD13	1.77	0.49
2:B:256:LEU:HD13	2:B:340:VAL:HG22	1.94	0.49
1:A:538:PRO:HG3	1:A:712:LEU:HD23	1.95	0.49
2:B:84:ILE:HD13	2:B:176:ASN:HA	1.95	0.49
3:D:435:ASN:O	3:D:439:ARG:HA	2.13	0.49
4:E:128:ILE:HA	4:E:131:LEU:HD12	1.94	0.49
1:A:357:VAL:HG11	1:A:359:LYS:HE2	1.95	0.48
5:F:165:LYS:HD2	5:F:203:LEU:HD11	1.95	0.48
4:E:145:LEU:HD11	4:E:169:ILE:HD13	1.96	0.48
1:A:563:ASP:HA	1:A:627:SER:HB2	1.95	0.48
1:A:580:ILE:HG13	1:A:607:ILE:HA	1.94	0.48
6:G:49:LEU:O	6:G:53:LEU:N	2.45	0.48
4:E:95:TYR:CE2	4:E:104:ILE:HG12	2.49	0.48
1:A:306:ILE:HG23	1:A:358:ARG:HG3	1.95	0.48
5:F:222:SER:HA	5:F:225:GLN:HE21	1.78	0.48
2:B:21:GLN:O	2:B:25:MET:CB	2.61	0.48
5:F:25:GLN:O	5:F:31:GLN:NE2	2.46	0.48
2:B:591:GLY:O	2:B:592:ARG:HB2	2.13	0.47
2:B:592:ARG:HA	4:E:175:THR:HG23	1.95	0.47
2:B:320:PRO:HG2	2:B:371:PRO:HG3	1.96	0.47
1:A:442:GLU:OE2	1:A:642:ARG:NH2	2.48	0.47
2:B:36:GLY:HA3	2:B:475:PRO:HG3	1.95	0.47
2:B:38:GLY:H	2:B:475:PRO:HD2	1.79	0.47
1:A:321:GLU:HB3	2:B:499:ASN:HD21	1.79	0.47
2:B:462:SER:HB2	2:B:693:LEU:HD23	1.95	0.47
1:A:595:ASN:HA	1:A:599:ASN:HD22	1.80	0.47
2:B:322:SER:OG	2:B:378:ARG:NH2	2.47	0.47
5:F:21:TRP:HE1	5:F:197:ASP:HB2	1.79	0.47
1:A:531:ILE:HA	1:A:534:TYR:CE1	2.50	0.47
3:D:435:ASN:HB3	3:D:440:LEU:H	1.78	0.47
1:A:688:LYS:NZ	1:A:689:VAL:O	2.33	0.46
2:B:560:ASN:O	2:B:563:ARG:HB3	2.15	0.46
6:G:9:LEU:HD11	6:G:42:HIS:HB3	1.97	0.46
1:A:351:VAL:HG22	1:A:378:PHE:HD1	1.80	0.46
2:B:106:GLY:HA3	2:B:174:ILE:HD12	1.96	0.46
1:A:536:MET:HE2	1:A:712:LEU:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:CYS:HA	1:A:346:LYS:HZ1	1.80	0.46
2:B:539:PHE:CZ	2:B:548:THR:HG21	2.50	0.46
2:B:44:SER:H	2:B:696:TRP:HZ2	1.63	0.46
2:B:527:MET:HG2	2:B:619:ILE:HD11	1.98	0.46
2:B:695:ARG:HD3	2:B:696:TRP:HD1	1.81	0.46
2:B:497:ARG:HE	2:B:500:ASP:HB2	1.80	0.46
3:D:410:ASN:HD21	6:G:3:ASN:HB2	1.80	0.46
1:A:451:PHE:CE2	1:A:480:LEU:HD13	2.51	0.46
2:B:538:PHE:CD2	2:B:663:CYS:HB3	2.50	0.46
2:B:681:ASP:OD1	2:B:682:LYS:N	2.49	0.46
10:X:179:UNK:O	10:X:181:UNK:N	2.49	0.46
2:B:157:PHE:CD2	2:B:189:TRP:HB2	2.51	0.46
2:B:537:ALA:HB1	2:B:621:PHE:HE2	1.81	0.46
1:A:537:ASN:HD21	1:A:539:ASN:HD22	1.64	0.45
1:A:443:VAL:HG22	1:A:467:THR:HG21	1.98	0.45
1:A:310:LEU:HD11	2:B:514:ILE:HD11	1.99	0.45
1:A:372:GLU:HA	1:A:375:LYS:HG2	1.98	0.45
1:A:430:LEU:HD21	1:A:458:VAL:HA	1.98	0.45
2:B:215:PRO:HG2	2:B:247:MET:HB2	1.98	0.45
2:B:309:VAL:HB	2:B:312:ASP:HB2	1.97	0.45
2:B:488:VAL:HG13	2:B:700:HIS:HD1	1.81	0.45
1:A:574:ARG:NH2	1:A:708:GLU:OE2	2.50	0.45
2:B:214:ASP:HA	2:B:246:SER:HB2	1.97	0.45
1:A:323:SER:HB2	1:A:338:ILE:HG21	1.98	0.45
2:B:161:PHE:HB2	2:B:189:TRP:HE1	1.81	0.45
4:E:76:LEU:HD12	4:E:80:ARG:HG2	1.98	0.45
2:B:35:LYS:HE2	2:B:65:LEU:HD11	1.99	0.45
2:B:657:MET:HE1	2:B:684:PHE:HE1	1.82	0.45
2:B:692:LYS:HE3	2:B:696:TRP:HB3	1.99	0.45
1:A:392:PHE:HB2	1:A:408:SER:HA	1.98	0.45
1:A:463:LYS:HD3	1:A:484:ILE:HG22	1.99	0.44
2:B:582:GLU:OE2	8:Z:101:UNK:CB	2.66	0.44
3:D:435:ASN:O	3:D:439:ARG:N	2.51	0.44
6:G:61:MET:O	6:G:64:ASN:HB3	2.17	0.44
1:A:379:LYS:HA	1:A:385:ASP:HB3	1.99	0.44
2:B:693:LEU:HD12	2:B:696:TRP:CE2	2.52	0.44
1:A:595:ASN:OD1	1:A:599:ASN:ND2	2.49	0.44
2:B:539:PHE:HD1	2:B:539:PHE:HA	1.74	0.44
3:D:400:ARG:O	6:G:16:MET:HE3	2.18	0.44
2:B:236:ALA:HB3	2:B:456:ILE:HG13	1.99	0.44
1:A:520:ARG:HB2	6:G:18:GLN:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:LEU:HD21	1:A:606:PHE:HB3	2.00	0.43
2:B:74:SER:O	2:B:209:TYR:N	2.50	0.43
1:A:532:LEU:HD11	1:A:723:ASP:HB2	2.00	0.43
4:E:66:ASP:OD1	4:E:67:GLY:N	2.51	0.43
5:F:60:ILE:HD13	5:F:136:SER:HB2	2.00	0.43
2:B:550:ALA:O	2:B:554:GLU:HB3	2.18	0.43
2:B:568:PHE:HB3	2:B:580:ALA:HB1	2.01	0.43
4:E:168:LEU:HD12	4:E:168:LEU:HA	1.84	0.43
2:B:343:ARG:HA	2:B:343:ARG:HD3	1.87	0.43
1:A:356:THR:HB	2:B:501:GLN:CG	2.49	0.43
1:A:546:PHE:O	1:A:550:PHE:HB2	2.18	0.43
2:B:18:TYR:CE1	2:B:671:LYS:HB2	2.54	0.43
2:B:71:ILE:O	2:B:231:VAL:HA	2.19	0.43
2:B:135:HIS:CE1	2:B:139:ALA:HB3	2.54	0.43
5:F:133:LEU:HB2	5:F:165:LYS:HE2	2.01	0.43
1:A:597:LYS:NZ	1:A:617:LEU:O	2.51	0.43
1:A:536:MET:HE3	1:A:567:ALA:HA	2.00	0.43
2:B:524:LEU:HD11	2:B:595:ILE:HD12	2.01	0.43
4:E:111:SER:HA	4:E:141:GLY:HA3	1.99	0.43
2:B:657:MET:HE1	2:B:684:PHE:CE1	2.54	0.43
2:B:677:MET:HE2	2:B:677:MET:HB3	1.71	0.43
4:E:110:LYS:O	4:E:113:ARG:HB2	2.18	0.43
2:B:315:LEU:HB2	2:B:374:PHE:CZ	2.54	0.42
3:D:435:ASN:O	3:D:439:ARG:CA	2.67	0.42
1:A:496:LEU:HB3	1:A:502:ILE:HD12	2.01	0.42
2:B:131:ASP:OD2	2:B:192:TYR:OH	2.26	0.42
2:B:539:PHE:HD2	2:B:545:MET:HG3	1.85	0.42
4:E:81:LEU:O	4:E:85:LEU:HB2	2.20	0.42
2:B:563:ARG:HH22	4:E:69:ARG:HD2	1.84	0.42
1:A:541:PHE:HE2	1:A:702:ALA:HB3	1.84	0.42
2:B:441:SER:HB2	2:B:445:LYS:HE3	2.01	0.42
2:B:530:VAL:HG21	2:B:714:VAL:HG13	2.02	0.42
1:A:356:THR:HB	2:B:501:GLN:CB	2.44	0.42
2:B:523:LEU:O	2:B:527:MET:HB2	2.19	0.42
1:A:625:GLN:NE2	1:A:627:SER:O	2.53	0.42
1:A:665:GLN:O	1:A:667:THR:OG1	2.36	0.42
2:B:52:LEU:HD23	2:B:52:LEU:HA	1.92	0.42
2:B:217:ILE:HG23	2:B:306:ALA:H	1.85	0.42
9:Y:531:UNK:O	9:Y:542:UNK:N	2.53	0.42
4:E:73:ASP:O	4:E:80:ARG:HG3	2.20	0.42
4:E:95:TYR:HE2	4:E:104:ILE:HG12	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:18:GLN:HG3	6:G:21:LEU:HD12	2.01	0.42
1:A:309:ASP:HA	1:A:384:ILE:HG12	2.01	0.42
2:B:212:LEU:HG	2:B:213:LEU:HD12	2.01	0.42
4:E:149:LEU:HD12	4:E:182:ILE:HD11	2.01	0.42
3:D:409:TYR:HD2	3:D:441:MET:HE3	1.85	0.41
2:B:538:PHE:CE2	2:B:663:CYS:HB3	2.55	0.41
4:E:64:VAL:HB	4:E:169:ILE:HA	2.02	0.41
4:E:231:LEU:HD23	4:E:231:LEU:HA	1.83	0.41
8:Z:471:UNK:O	8:Z:475:UNK:CB	2.68	0.41
2:B:217:ILE:HG12	2:B:305:LEU:HA	2.01	0.41
4:E:169:ILE:HG22	4:E:171:PHE:HB2	2.02	0.41
9:Y:649:UNK:O	9:Y:650:UNK:CB	2.68	0.41
1:A:667:THR:HG22	1:A:668:GLN:H	1.85	0.41
2:B:684:PHE:O	2:B:688:ASP:HB2	2.20	0.41
1:A:514:MET:H	1:A:665:GLN:NE2	2.18	0.41
1:A:556:ASP:OD2	1:A:647:LYS:NZ	2.40	0.41
2:B:53:LEU:HD13	2:B:87:LEU:HB3	2.02	0.41
2:B:105:LEU:HD21	2:B:198:SER:HB2	2.03	0.41
2:B:568:PHE:CZ	2:B:583:LYS:HB3	2.55	0.41
2:B:558:LEU:HD13	2:B:562:GLN:HG3	2.02	0.41
5:F:203:LEU:HD23	5:F:203:LEU:HA	1.79	0.41
1:A:611:GLY:O	1:A:616:ASP:N	2.43	0.41
1:A:672:TYR:HE2	1:A:676:ARG:HH11	1.69	0.41
2:B:24:TYR:HA	2:B:27:GLU:HB2	2.03	0.41
2:B:567:LEU:HD23	2:B:595:ILE:HG23	2.03	0.41
1:A:286:HIS:ND1	1:A:291:LEU:HD13	2.36	0.40
1:A:551:HIS:HA	1:A:554:ARG:HB2	2.03	0.40
1:A:584:THR:HG22	1:A:585:SER:H	1.86	0.40
1:A:653:GLU:HG2	4:E:78:PRO:HG3	2.03	0.40
2:B:354:PRO:HG2	2:B:355:PRO:HD3	2.03	0.40
2:B:77:VAL:HA	2:B:80:ILE:HD12	2.03	0.40
2:B:94:TYR:HA	2:B:97:GLN:HB2	2.02	0.40
2:B:56:ILE:HG22	2:B:60:GLN:HE21	1.86	0.40
4:E:71:MET:HE3	4:E:172:SER:HB3	2.03	0.40
5:F:12:VAL:HA	5:F:58:ALA:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	461/553 (83%)	402 (87%)	57 (12%)	2 (0%)	30	66
2	B	722/760 (95%)	614 (85%)	101 (14%)	7 (1%)	12	47
3	D	75/85 (88%)	71 (95%)	3 (4%)	1 (1%)	9	41
4	E	182/395 (46%)	171 (94%)	11 (6%)	0	100	100
5	F	199/308 (65%)	182 (92%)	15 (8%)	2 (1%)	12	47
6	G	64/71 (90%)	56 (88%)	8 (12%)	0	100	100
All	All	1703/2172 (78%)	1496 (88%)	195 (12%)	12 (1%)	20	55

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	THR
2	B	428	ILE
2	B	592	ARG
2	B	14	TYR
2	B	685	ALA
5	F	239	SER
5	F	241	LEU
2	B	299	ARG
2	B	354	PRO
2	B	426	PRO
3	D	384	PRO
1	A	345	GLY

5.3.2 Protein sidechains

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	400/454 (88%)	391 (98%)	9 (2%)	44	63
2	B	586/664 (88%)	576 (98%)	10 (2%)	53	67
3	D	64/73 (88%)	63 (98%)	1 (2%)	55	69
4	E	169/352 (48%)	163 (96%)	6 (4%)	31	52
5	F	144/272 (53%)	143 (99%)	1 (1%)	76	79
6	G	59/64 (92%)	59 (100%)	0	100	100
All	All	1422/1879 (76%)	1395 (98%)	27 (2%)	49	66

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	ILE
1	A	349	VAL
1	A	484	ILE
1	A	487	LYS
1	A	490	GLU
1	A	502	ILE
1	A	532	LEU
1	A	559	ILE
1	A	584	THR
2	B	87	LEU
2	B	383	LEU
2	B	410	TYR
2	B	437	CYS
2	B	446	PRO
2	B	523	LEU
2	B	539	PHE
2	B	558	LEU
2	B	571	THR
2	B	722	ARG
3	D	387	ILE
4	E	104	ILE
4	E	107	ILE
4	E	164	SER
4	E	174	LEU
4	E	194	ILE
4	E	207	VAL
5	F	133	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	320	GLN
1	A	373	GLN
1	A	388	GLN
1	A	539	ASN
1	A	564	ASN
1	A	595	ASN
1	A	599	ASN
1	A	621	ASN
1	A	638	GLN
1	A	665	GLN
2	B	21	GLN
2	B	262	ASN
2	B	384	HIS
2	B	501	GLN
2	B	519	ASN
2	B	522	ASN
2	B	562	GLN
2	B	590	ASN
2	B	726	GLN
3	D	448	HIS
4	E	60	HIS
4	E	147	ASN
4	E	154	GLN
4	E	220	HIS
4	E	235	HIS
5	F	31	GLN
5	F	205	GLN
5	F	225	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
11	SF4	B	1000	2	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	SF4	B	1000	2	-	-	0/6/5/5

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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	Y	18
8	Z	15
10	X	6
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	181:UNK	C	201:UNK	N	103.83
1	Z	165:UNK	C	171:UNK	N	91.40
1	Z	20:UNK	C	82:UNK	N	60.92
1	Y	320:UNK	C	373:UNK	N	57.49
1	Z	487:UNK	C	501:UNK	N	56.59
1	Y	75:UNK	C	92:UNK	N	50.69
1	Y	147:UNK	C	236:UNK	N	50.24
1	Y	385:UNK	C	498:UNK	N	49.12
1	Y	543:UNK	C	601:UNK	N	43.70
1	Z	294:UNK	C	301:UNK	N	37.51
1	Y	250:UNK	C	261:UNK	N	36.80
1	Y	272:UNK	C	303:UNK	N	34.35
1	Y	28:UNK	C	36:UNK	N	31.44
1	Z	90:UNK	C	101:UNK	N	30.33
1	Z	118:UNK	C	159:UNK	N	29.75
1	Y	612:UNK	C	641:UNK	N	29.36
1	Z	234:UNK	C	250:UNK	N	27.04
1	Z	313:UNK	C	401:UNK	N	26.49
1	Z	520:UNK	C	530:UNK	N	26.25
1	Z	269:UNK	C	281:UNK	N	24.88
1	A	256:UNK	C	266:GLN	N	24.41
1	Y	512:UNK	C	520:UNK	N	22.77
1	Y	50:UNK	C	61:UNK	N	21.77
1	Z	560:UNK	C	571:UNK	N	21.75
1	Y	524:UNK	C	530:UNK	N	21.02
1	X	92:UNK	C	134:UNK	N	19.25
1	Y	671:UNK	C	687:UNK	N	18.46
1	Z	421:UNK	C	430:UNK	N	15.09
1	X	144:UNK	C	147:UNK	N	11.32
1	Z	455:UNK	C	465:UNK	N	11.20
1	X	187:UNK	C	737:UNK	N	10.67
1	Y	23:UNK	C	25:UNK	N	10.29

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Y	654:UNK	C	662:UNK	N	10.05
1	Z	539:UNK	C	551:UNK	N	10.03
1	X	158:UNK	C	160:UNK	N	8.14
1	X	172:UNK	C	174:UNK	N	6.07
1	Y	119:UNK	C	121:UNK	N	5.02
1	Y	105:UNK	C	107:UNK	N	4.84
1	Y	534:UNK	C	537:UNK	N	4.11
1	X	179:UNK	C	181:UNK	N	3.54

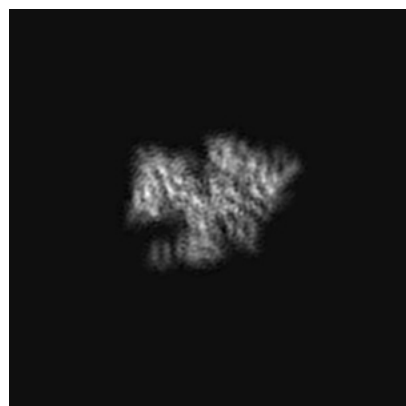
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3802. These allow visual inspection of the internal detail of the map and identification of artifacts.

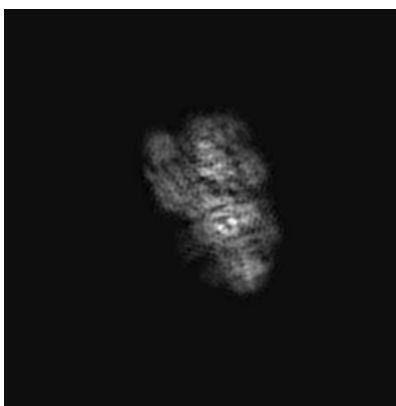
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

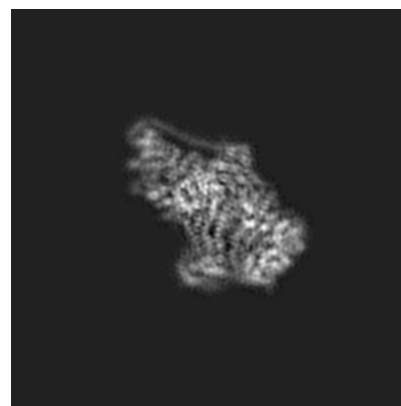
6.1.1 Primary map



X

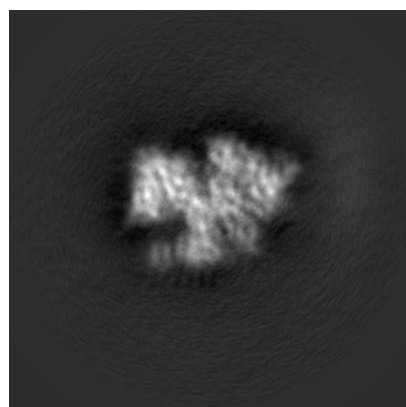


Y

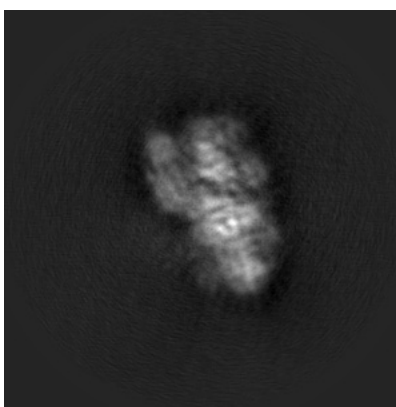


Z

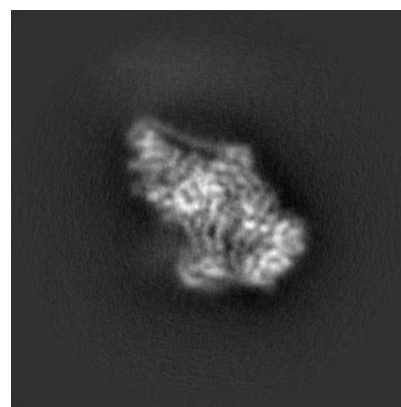
6.1.2 Raw map



X



Y

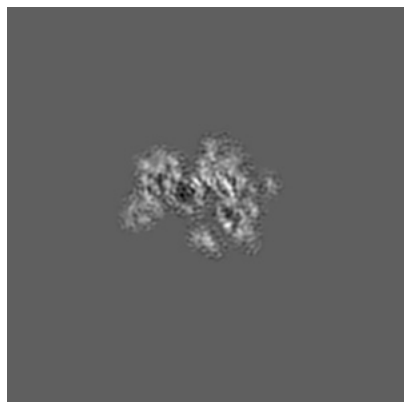


Z

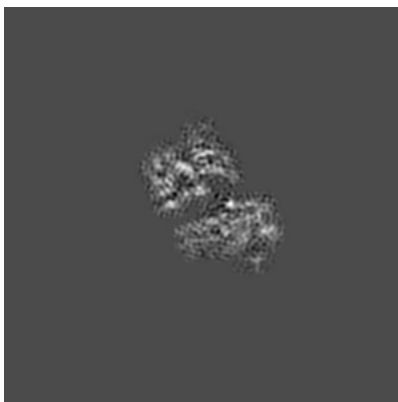
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

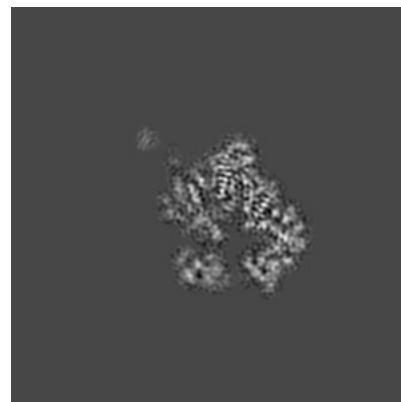
6.2.1 Primary map



X Index: 128

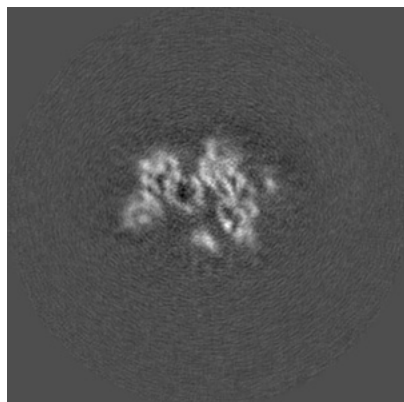


Y Index: 128

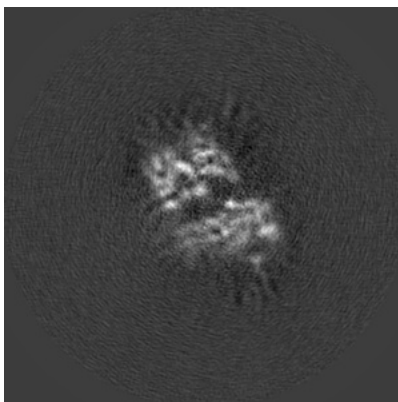


Z Index: 128

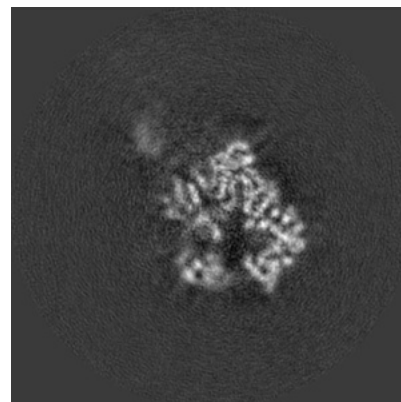
6.2.2 Raw map



X Index: 128



Y Index: 128

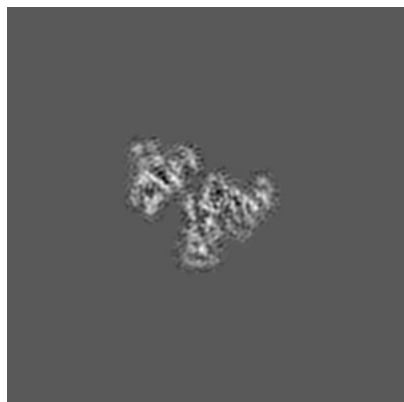


Z Index: 128

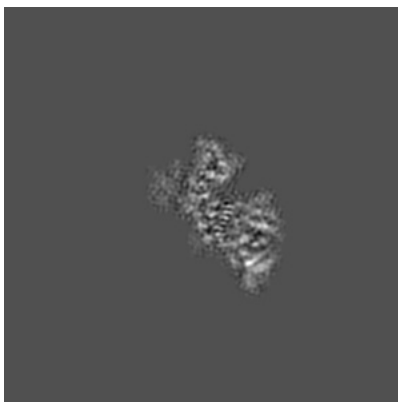
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

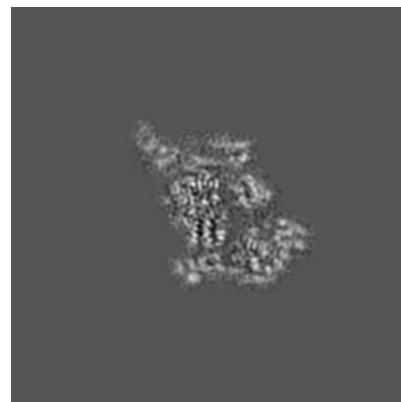
6.3.1 Primary map



X Index: 151

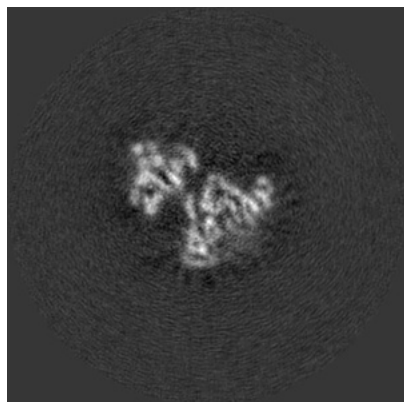


Y Index: 138

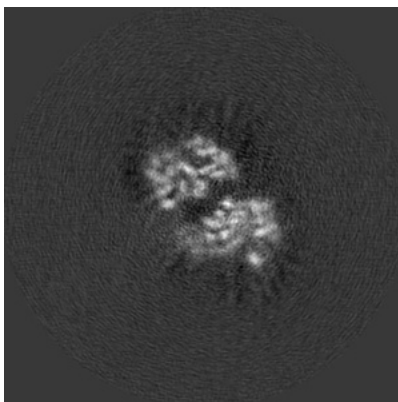


Z Index: 138

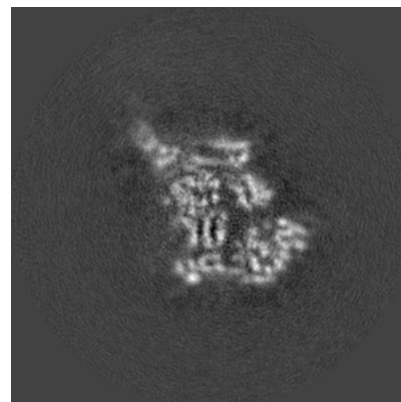
6.3.2 Raw map



X Index: 151



Y Index: 130

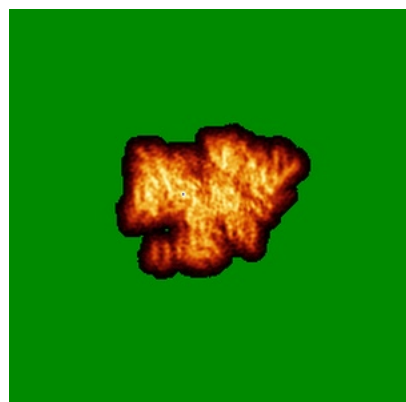


Z Index: 138

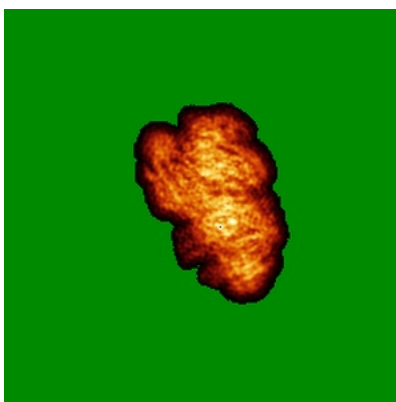
The images above show the largest variance slices of the map in three orthogonal directions.

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

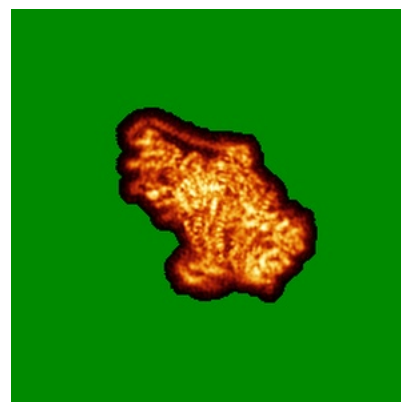
6.4.1 Primary map



X

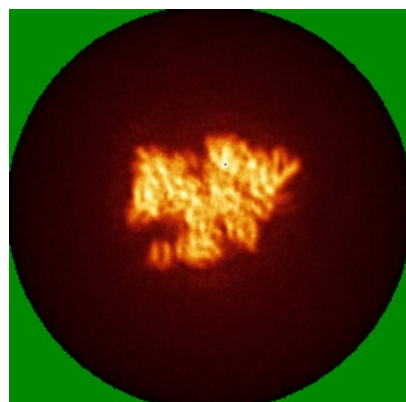


Y

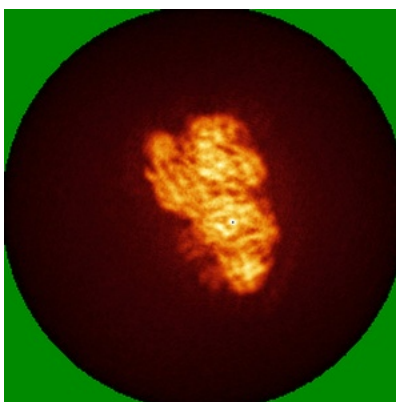


Z

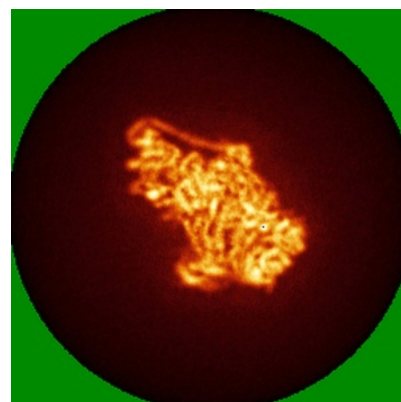
6.4.2 Raw map



X



Y

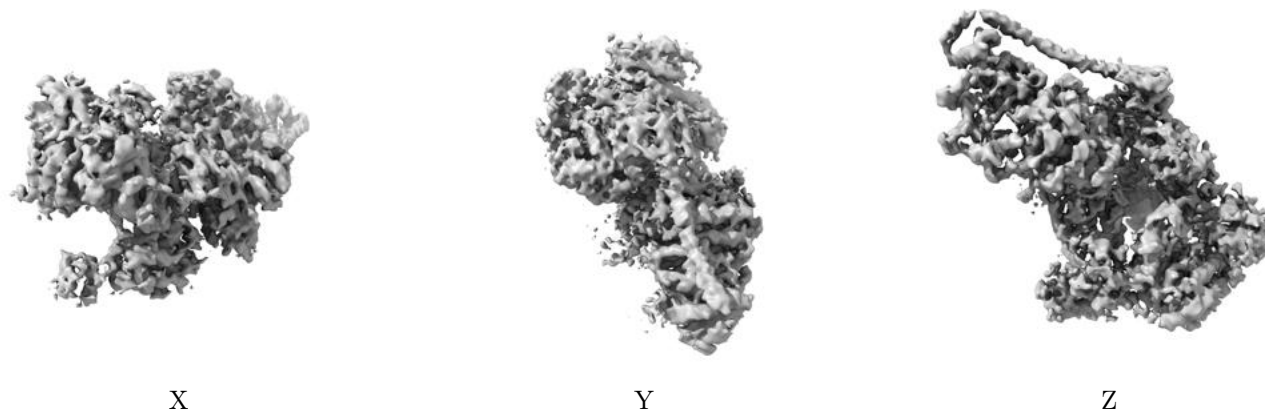


Z

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.

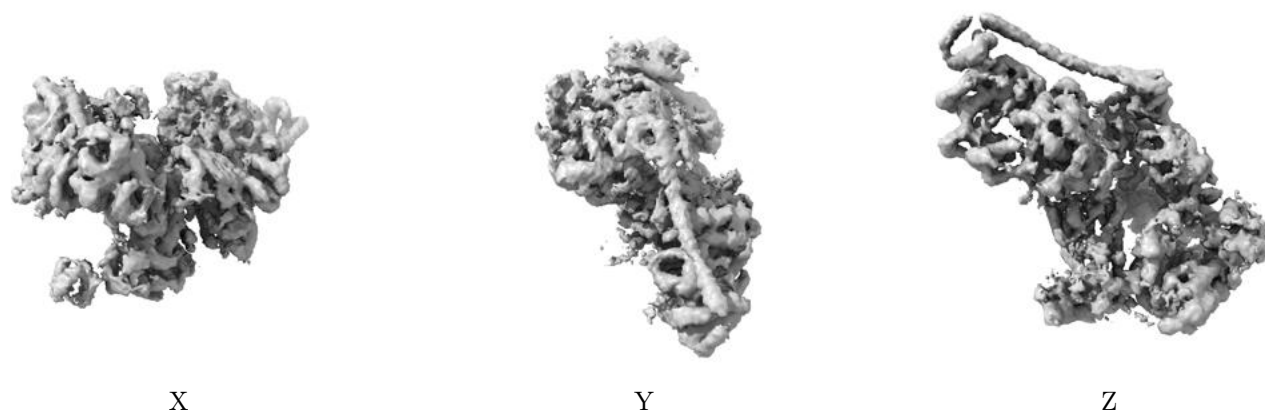
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

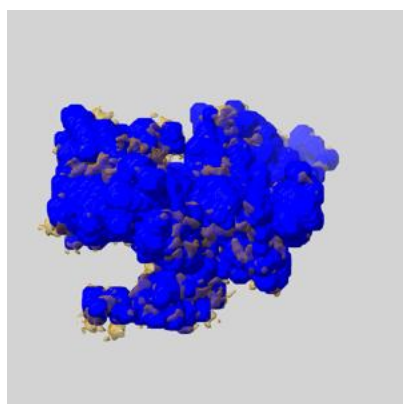
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

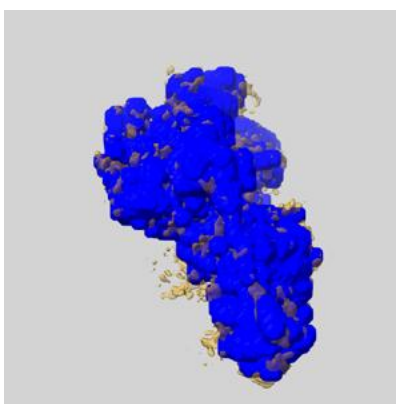
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

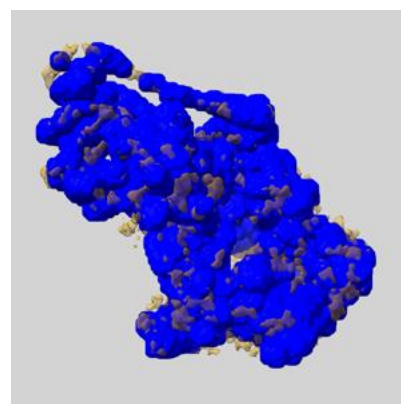
6.6.1 emd_3802_msk_1.map [i](#)



X



Y

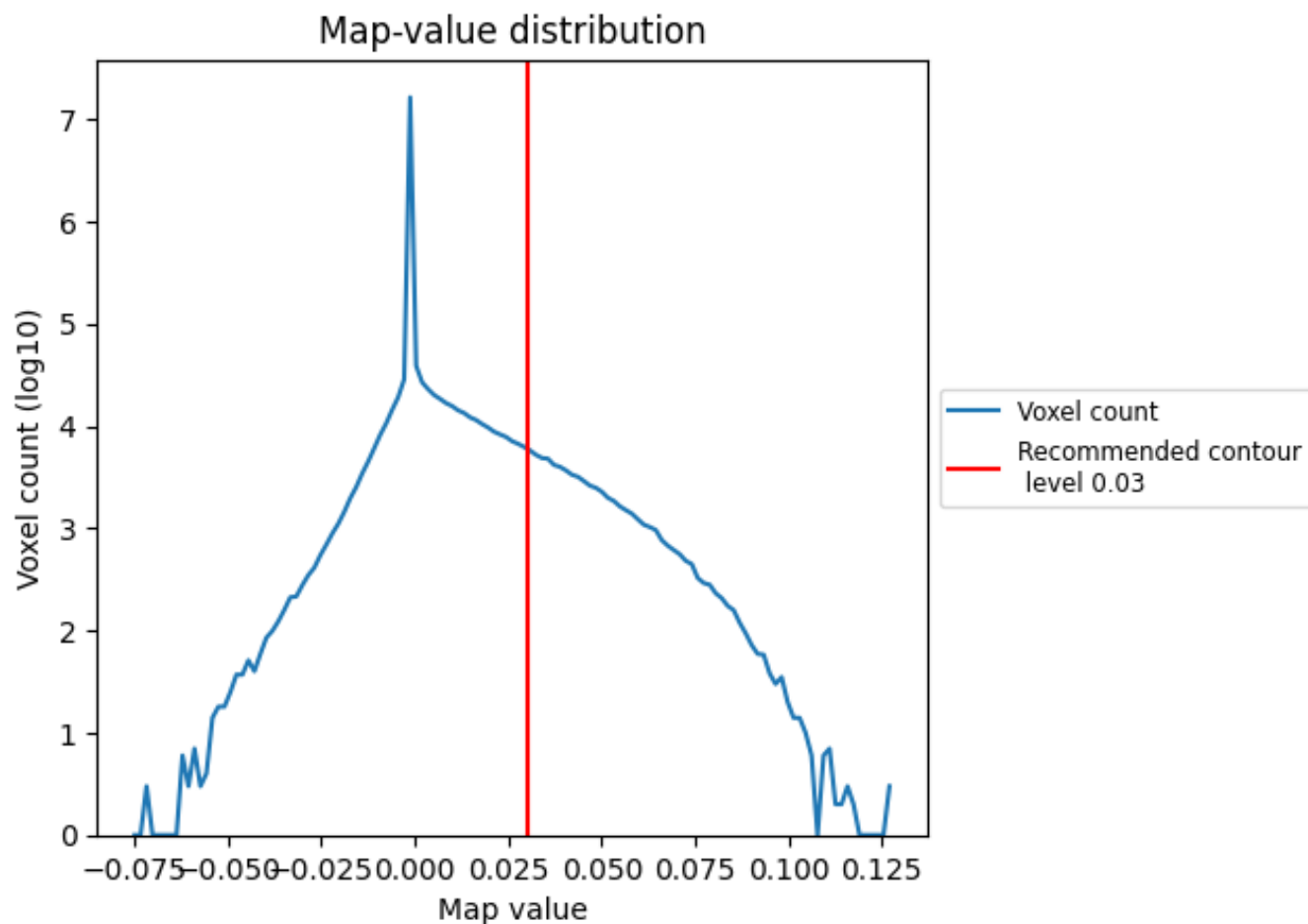


Z

7 Map analysis [i](#)

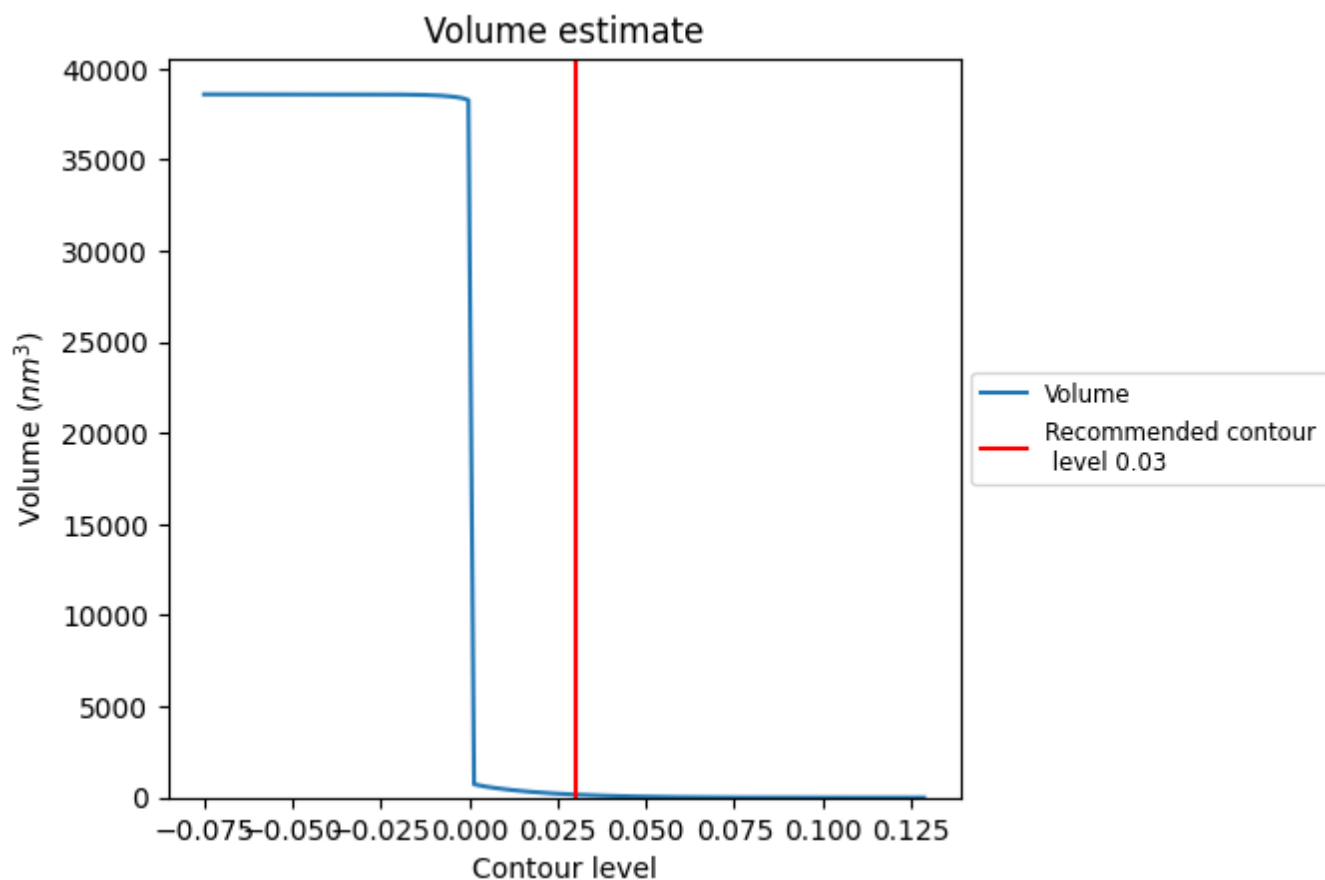
This section contains the results of statistical analysis of the map.

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.

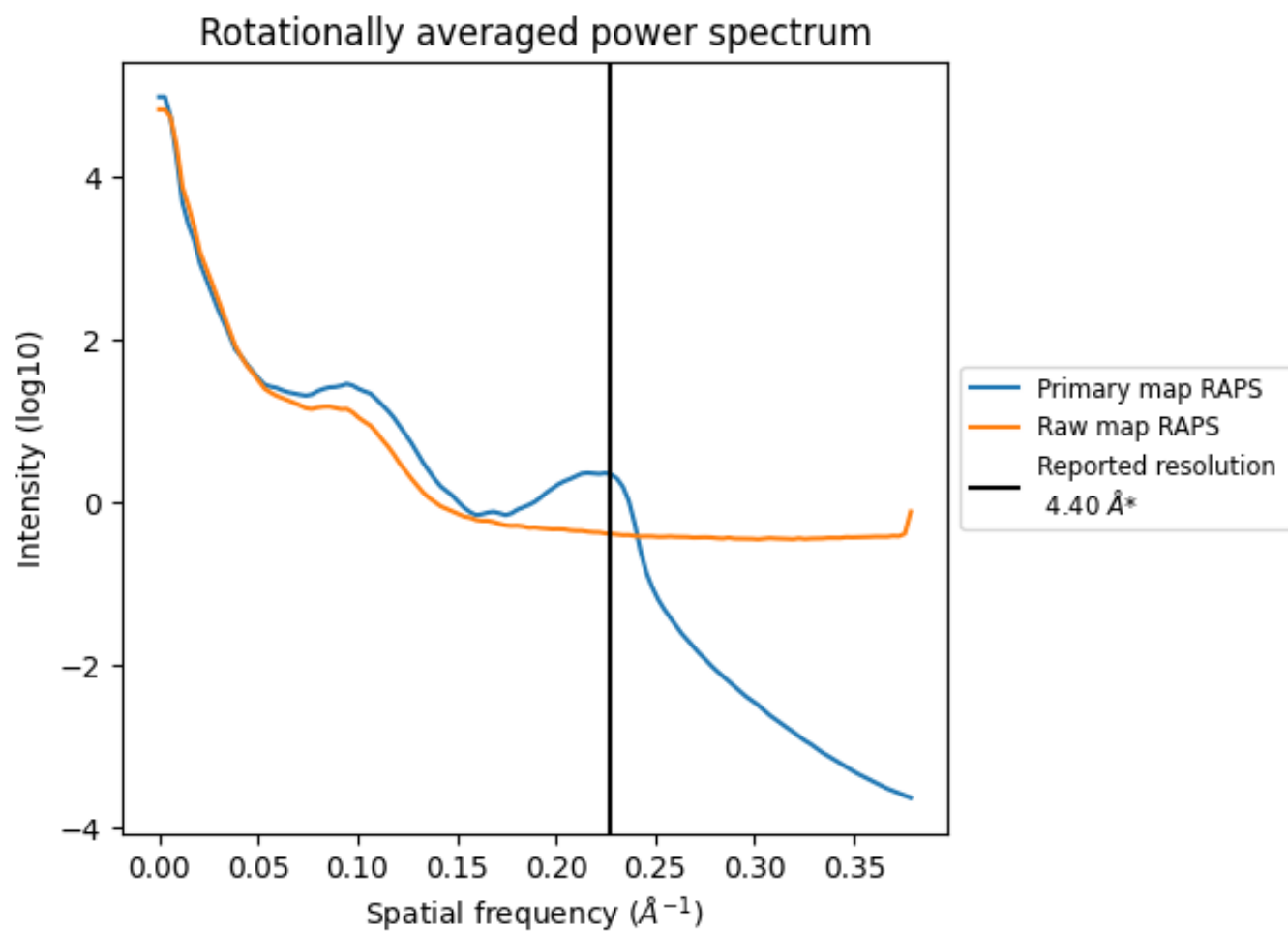
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 163 nm^3 ; this corresponds to an approximate mass of 147 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 ⓘ

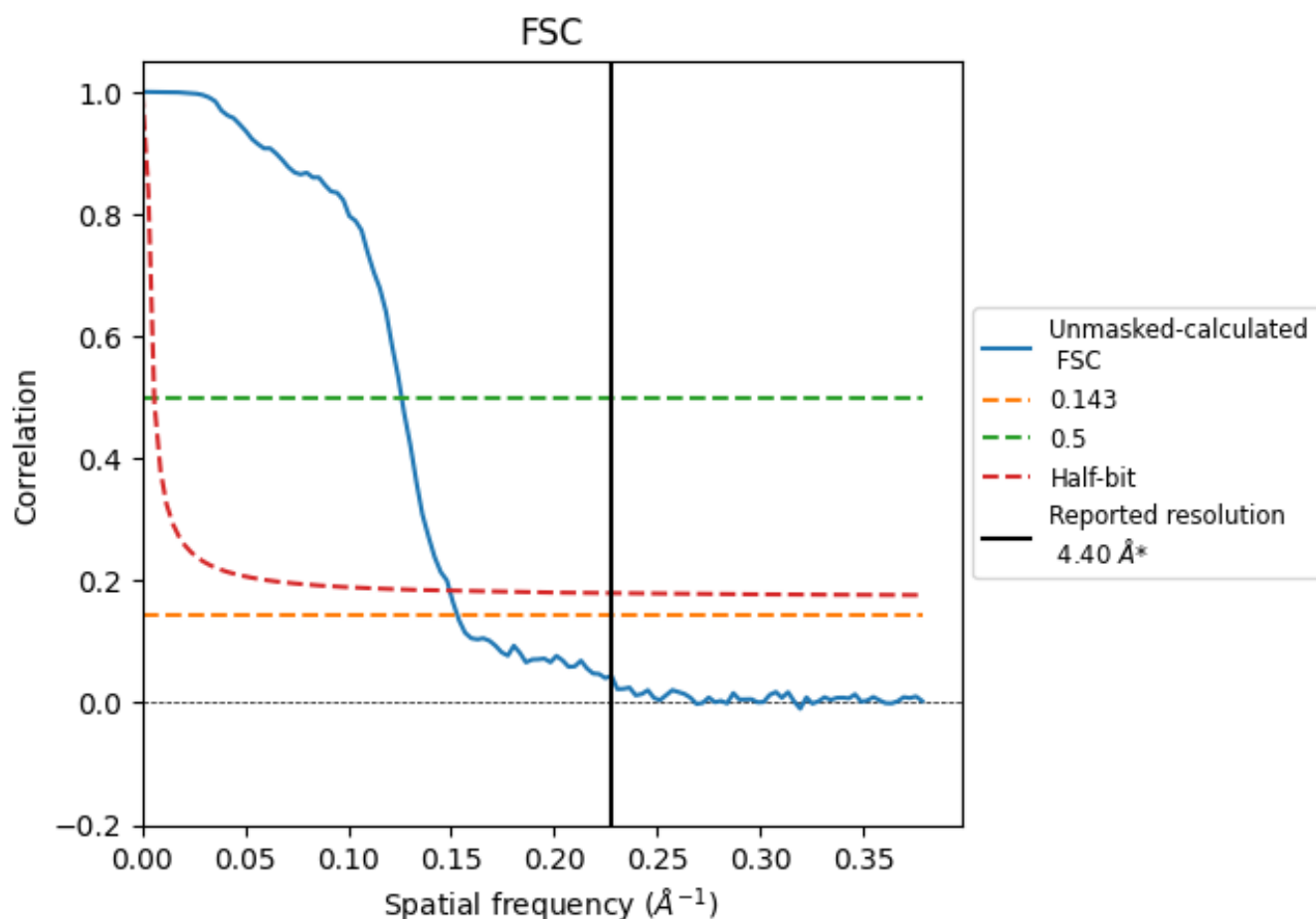


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

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 0.227 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

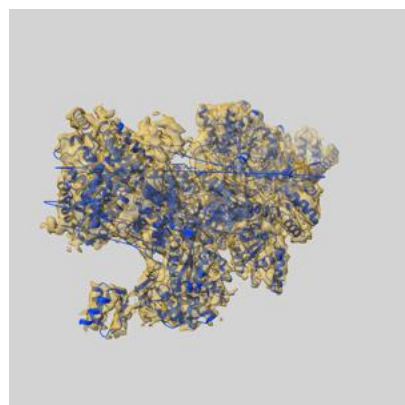
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.53	7.94	6.69

*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 6.53 differs from the reported value 4.4 by more than 10 %

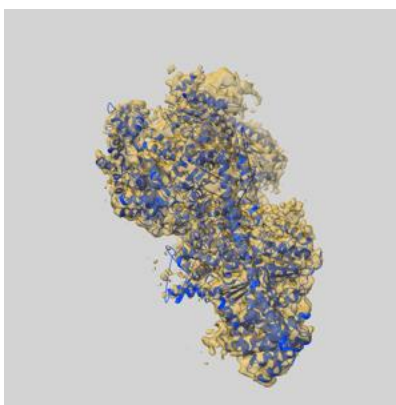
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3802 and PDB model 5OF4. Per-residue inclusion information can be found in section [3](#) on page [7](#).

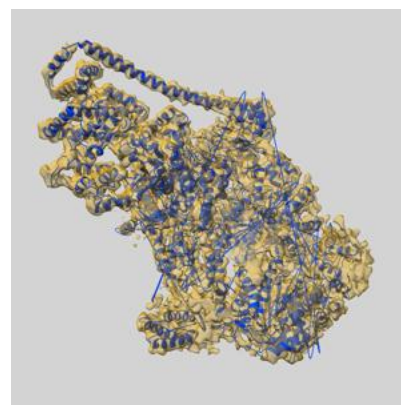
9.1 Map-model overlay [i](#)



X



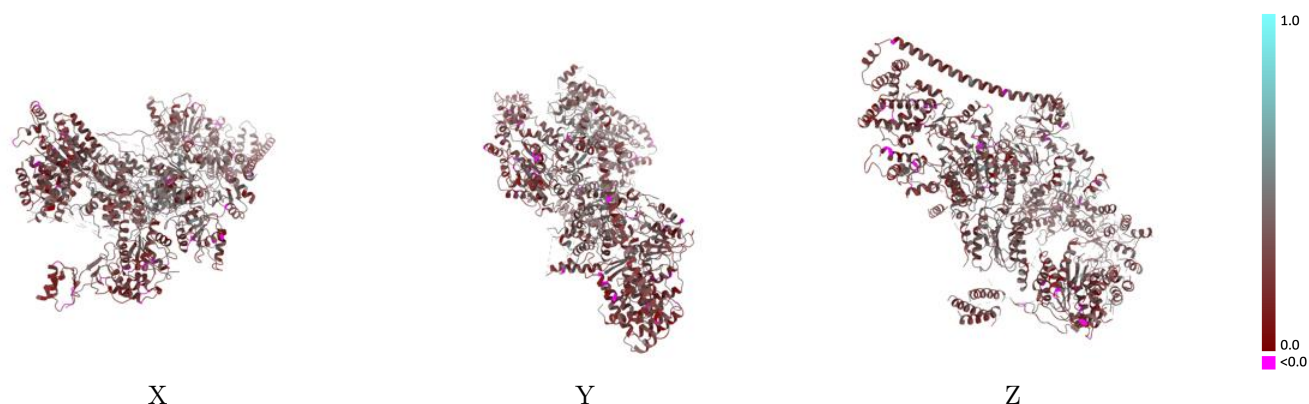
Y



Z

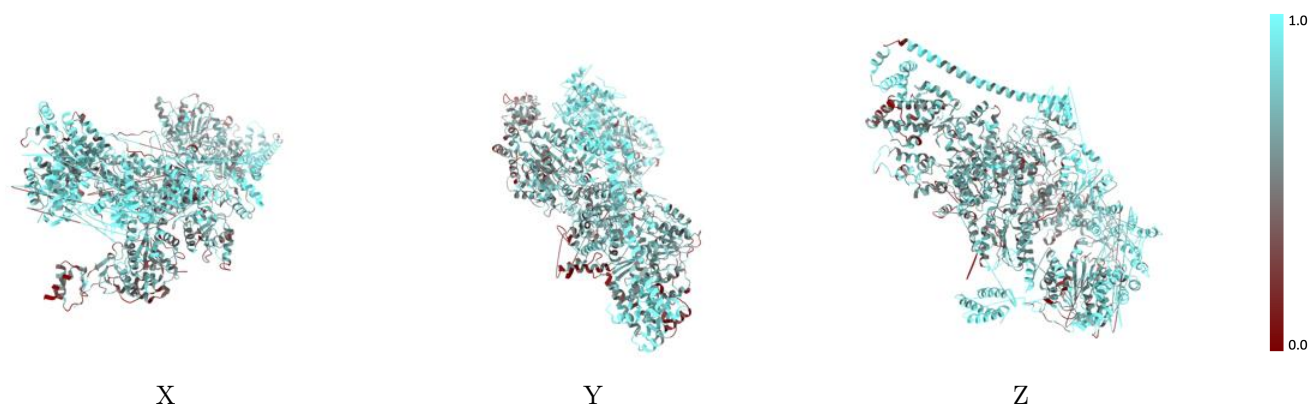
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



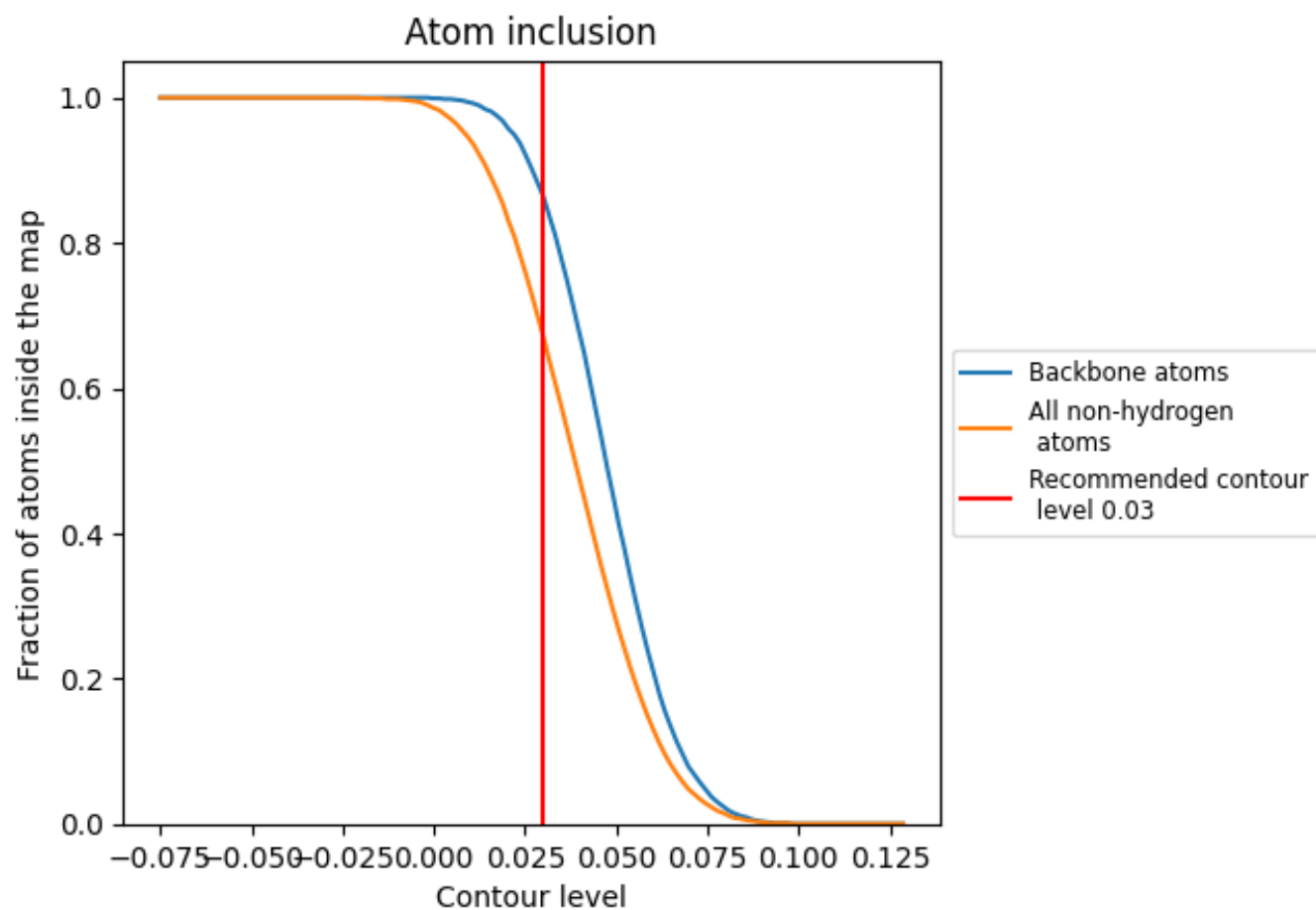
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 67% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6710	 0.3080
A	 0.6120	 0.2980
B	 0.6470	 0.3020
D	 0.5350	 0.2680
E	 0.6690	 0.3630
F	 0.6800	 0.2860
G	 0.5180	 0.2640
H	 0.8450	 0.2810
X	 0.9130	 0.3870
Y	 0.9010	 0.3510
Z	 0.7080	 0.3200

