



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 06:32 pm GMT

PDB ID : 5OF4
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)

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

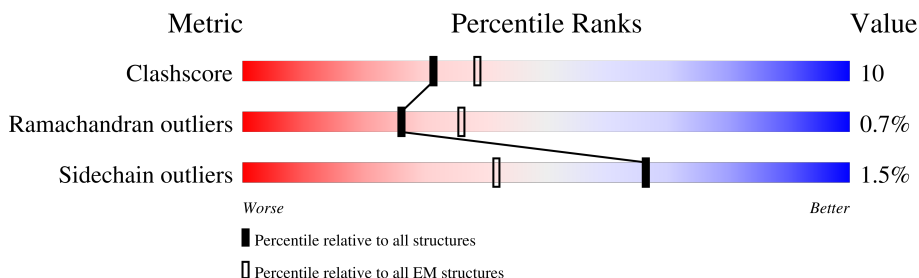
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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.



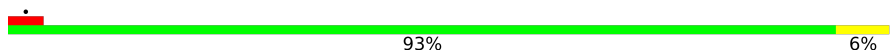
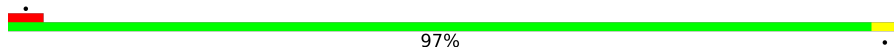
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	553	17% (red), 61% (green), 27% (yellow), 10% (grey)
2	B	760	13% (red), 63% (green), 29% (yellow), 5% (grey)
3	D	85	33% (red), 76% (green), 18% (yellow), 5% (grey)
4	E	395	5% (red), 33% (green), 13% (yellow), 53% (grey)
5	F	308	7% (red), 54% (green), 12% (yellow), 33% (grey)
6	G	71	25% (red), 65% (green), 25% (yellow), 7% (grey)
7	H	124	6% (red), 99% (green)
8	Z	270	25% (red), 97% (green)

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Mol	Chain	Length	Quality of chain
9	Y	232	 93% 6%
10	X	78	 97%

2 Entry composition [i](#)

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
			Total	C	N	O	S		
1	A	499	3887	2469	676	718	24	0	0

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

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

- 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
			Total	C	N	O	S		
3	D	81	643	412	118	112	1	0	0

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

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

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

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

- 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		

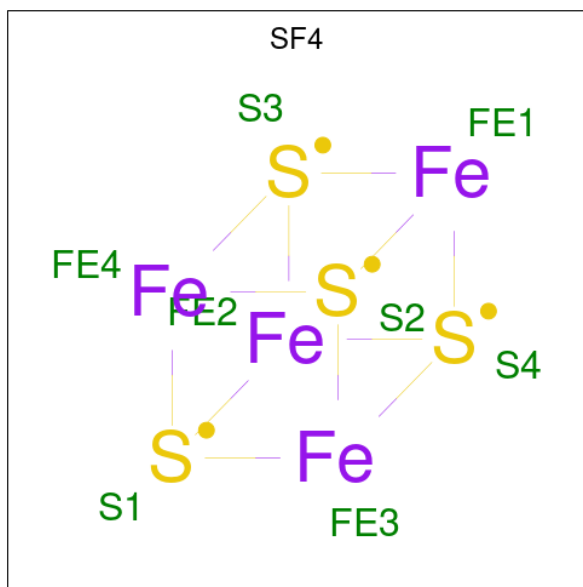
- Molecule 9 is a protein called Unassigned secondary structure elements (p52 region).

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 (three-letter code: SF4) (formula: Fe₄S₄).

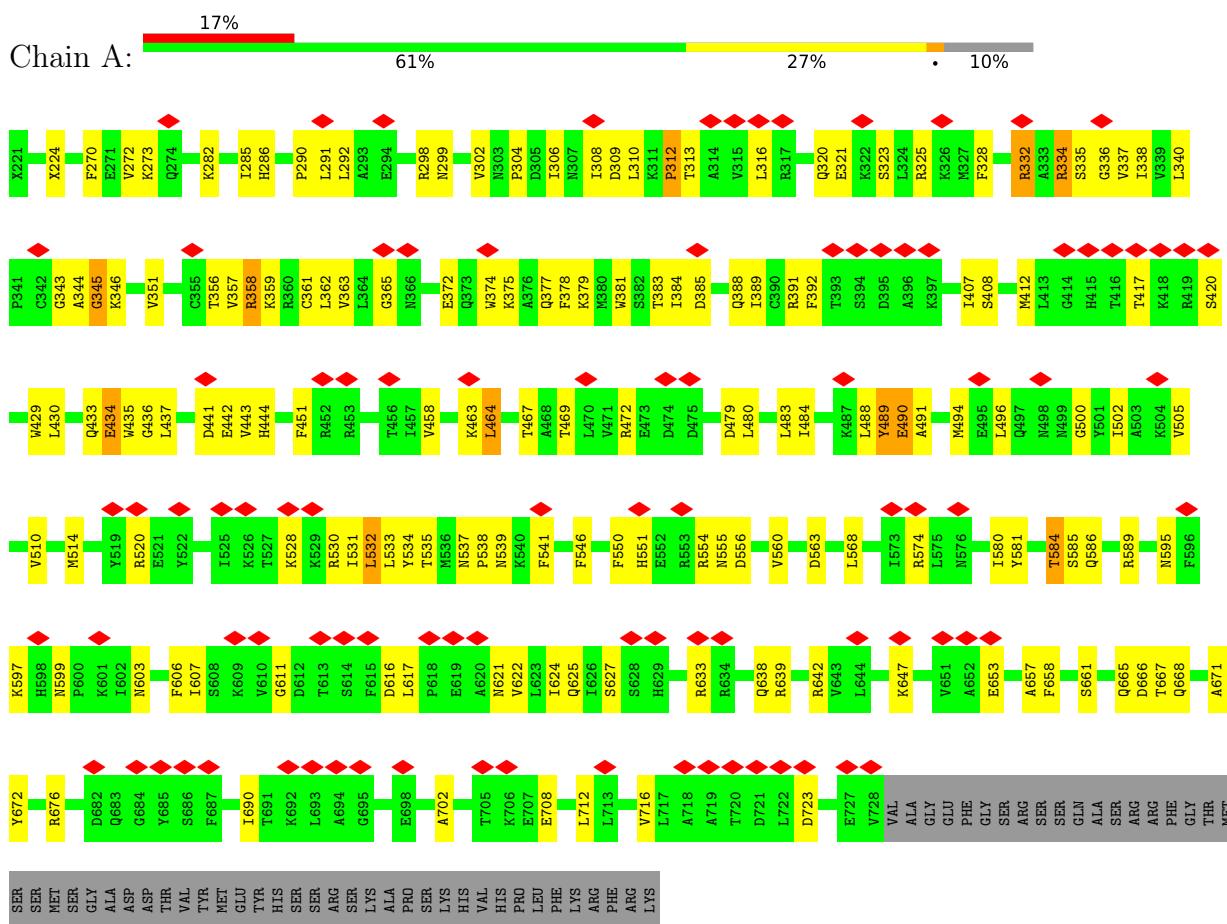


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
11	B	1	8	4	4	0

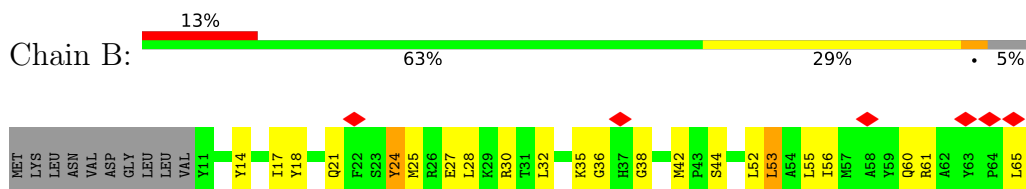
3 Residue-property plots

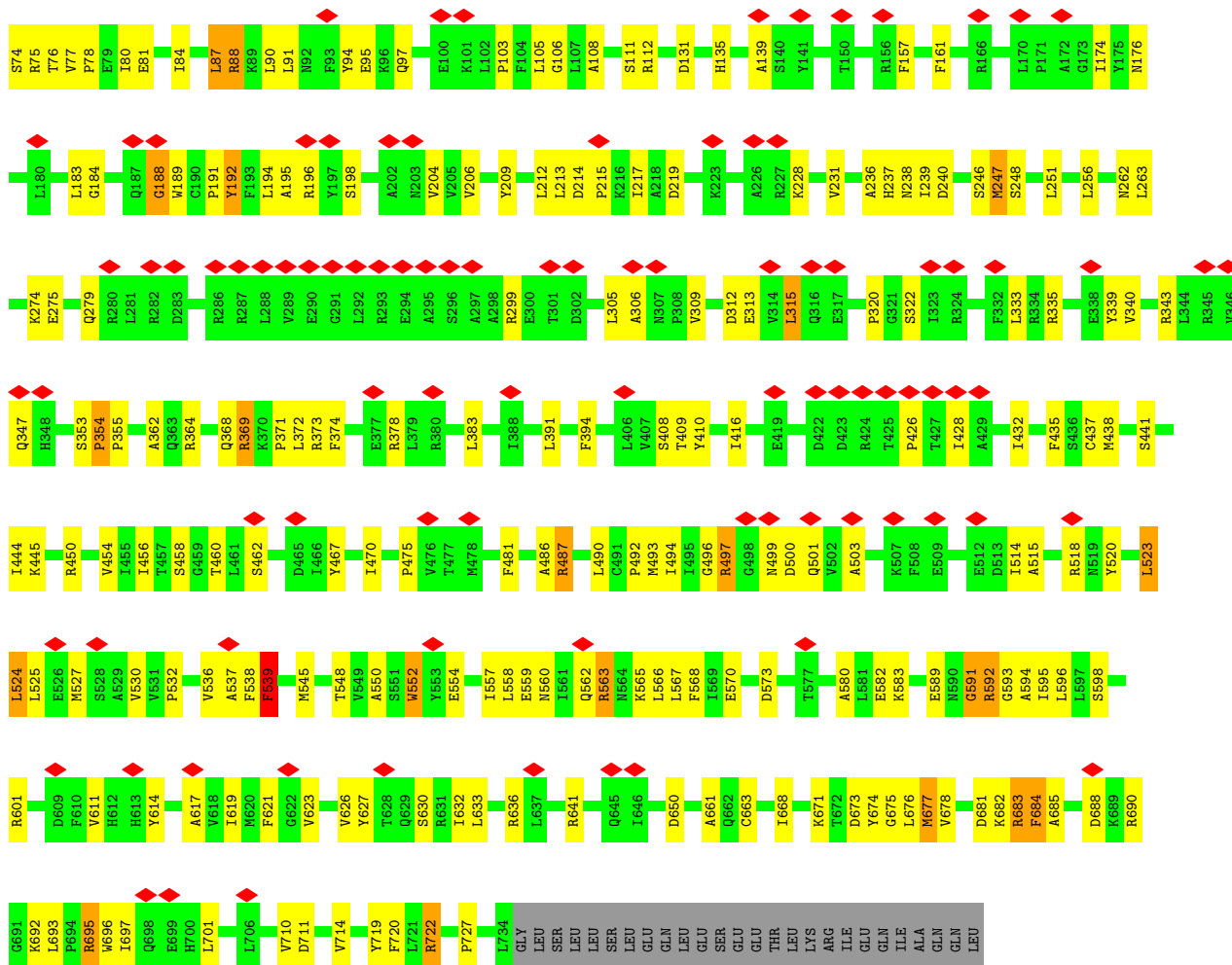
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

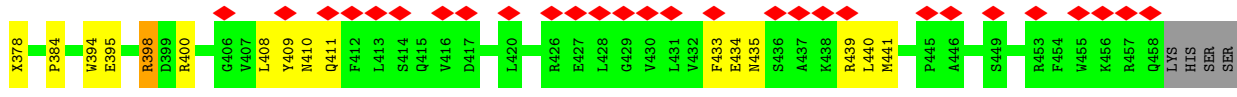
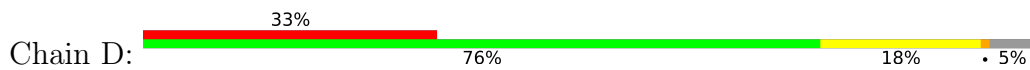


- Molecule 2: TFIIH basal transcription factor complex helicase XPD subunit

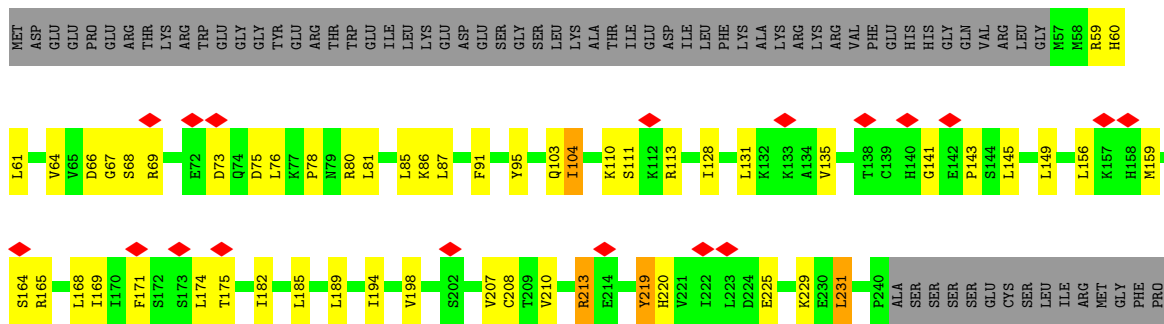
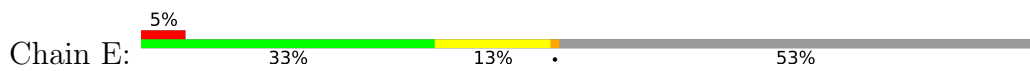




• Molecule 3: General transcription factor IIH subunit 4,p52,General transcription factor IIH subunit 4



• Molecule 4: General transcription factor IIH subunit 2



GLN	HIS	THR	ILE	ALA	SER	LEU	SER	ASP	GLN	ASP	ALA	LYS	PRO	SER	PHE	GLN	MET	ALA	HIS	LEU	ASP	GLY	ASN	THR	GLU	PRO	GLY	THR	LEU	LEU	GLY	TYR	GLN	PHE	CYS	PRO	GLN	CYS	ARG	LYS	TYR	CYS	GLU	LEU	PRO	VAL	GLY	VAL	ASP	GLY	THR	LEU	VAL	ALA
PRO	HIS	LEU	ALA	ARG	SER	TYR	HIS	LEU	GLN	PHE	LEU	HIS	PRO	ASP	ALA	PHE	GLN	GLU	ILE	PRO	LEU	GLU	TYR	ASN	GLY	GLU	ARG	PHE	CYS	TYR	GLY	CYS	GLN	TYR	VAL	VAL	CYS	ALA	VAL	VAL	CYS	GLN	ASN	VAL	PHE	VAL	ASP	GLY	THR	LEU	VAL	VAL		
HIS	ASP	SER	LEU	HIS	CYS	PRO	GLY	CYS	ILE	HIS	LYS	ILE	PRO	ALA	PHE	ALA	GLN	SER	ILE	PRO	LEU	GLU	ASN	GLY	VAL																													

• Molecule 5: General transcription factor IIH subunit 3



MET	VAL	SER	ASP	GLU	D6	L10	L11	V12	I13	V14	W21	Q25	A26	K28	E29	S30	Q31	V41	L44	F50	R53	L57	A58	Y59	I60	A61	L70	Y71	P72	GLY	LYS	ASN	GLY	ARG	VAL	LEU	VAL	GLY	ASP	PHE	LEU	ASP	GLY	PRO	ASN	GLY	PRO	PRO	PRO	PHE	ASN
PRO	SER	GLY	SER	LYS	ASP	G99	I111	S122	ASP	ILE	LYS	GLY	HIS	T129	E130	T131	L132	L133	A134	G135	S136	L137	A138	K139	A140	L141	C142	Y143	R146	E150	V151	K152	Q155	L162	K165	A166	A167	E168	D169	S170	A171	F177	K186	I191	D192	D197	S198				
L203	T210	S222	L223	L224	Q225	L228	P233	S239	Q240	L241	I242	LEU	PRO	PRO	PRO	VAL	HIS	VAL	ASP	TYR	ARG	ALA	ALA	ALA	PHE	CYS	HIS	ARG	ASN	ILE	ILE	GLY	TYR	VAL	CYS	SER	VAL	LEU	SER	ILE	LEU	THR	THR	THR							
CYS	GLU	THR	ALA	PHE	LYS	ILE	SER	PRO	PRO	VAL	LEU	LYS	LYS	LYS	LYS	LEU	VAL	VAL	SER	SER	ALA																														

• Molecule 6: General transcription factor IIH subunit 5



MET	V2	N3	V4	L5	K6	G7	L9	G12	M16	K17	F19	L20	L21	Y22	L23	A28	L29	G30	K31	K32	F33	I38	D39	D40	T41	H42	V43	F44	A47	E48	L49	L53	E59	L60	M61	D62	O63	N64	F66	S67	LEU	THR	GLN	LYS
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• Molecule 7: MAT1



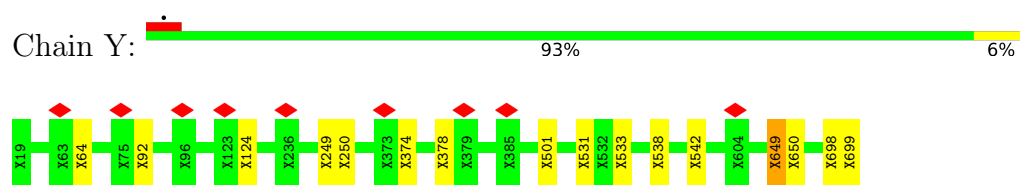
X45	X65	X104	X105	X106	X107	X108	X109	X126	X127	X168
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• Molecule 8: Unassigned secondary structure elements.

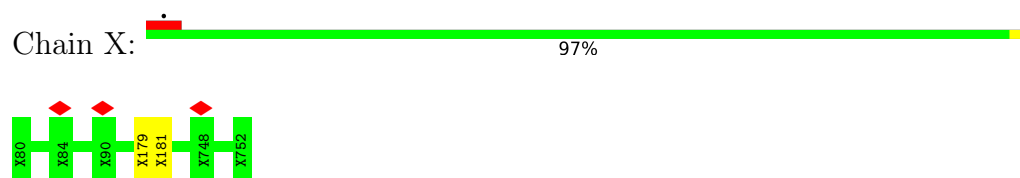


X1	X2	X3	X6	X7	X8	X9	X10	X11	X12	X13	X14	X20	X84	X85	X86	X87	X88	X89	X90	X101	X102	X103	X104	X105	X106	X107	X110	X111	X112	X113	X114	X115	X116	X117	X118	X162	X163	X164	X165	X225	X226	X227	X228	X229	X230	X233	X234	X250	X251	X252	X253
X261	X262	X266	X281	X301	X308	X433	X471	X475	X512	X530	X531	X532	X533	X534	X535	X536	X537	X538	X539	X555	X556	X557	X558	X559	X560	X571	X572	X573	X574	X577	X578	X581	X584																		

- 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 (\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 (\AA)	1.32, 1.32, 1.32	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	1.00	7/3779 (0.2%)	1.07	17/5102 (0.3%)
2	B	1.08	11/5790 (0.2%)	1.22	44/7853 (0.6%)
3	D	0.92	1/631 (0.2%)	0.96	2/855 (0.2%)
4	E	1.13	3/1478 (0.2%)	1.24	10/2001 (0.5%)
5	F	1.02	1/1518 (0.1%)	1.11	12/2061 (0.6%)
6	G	0.72	0/528	0.86	2/713 (0.3%)
All	All	1.04	23/13724 (0.2%)	1.15	87/18585 (0.5%)

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 (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	489	TYR	C-O	-9.39	1.05	1.23
3	D	394	TRP	CE3-CZ3	9.33	1.54	1.38
4	E	91	PHE	CG-CD1	7.93	1.50	1.38
2	B	591	GLY	C-O	7.24	1.35	1.23
2	B	539	PHE	N-CA	-7.20	1.31	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	334	ARG	CZ-NH1	6.89	1.42	1.33
2	B	720	PHE	CG-CD1	6.83	1.49	1.38
2	B	614	TYR	CE1-CZ	-6.81	1.29	1.38
2	B	539	PHE	CG-CD1	6.34	1.48	1.38
1	A	270	PHE	C-O	5.82	1.34	1.23
4	E	207	VAL	CB-CG1	5.76	1.65	1.52
2	B	719	TYR	CG-CD1	5.63	1.46	1.39
2	B	496	GLY	C-O	-5.62	1.14	1.23
2	B	552	TRP	CZ3-CH2	-5.61	1.31	1.40
1	A	345	GLY	C-O	-5.25	1.15	1.23
1	A	334	ARG	CZ-NH2	5.24	1.39	1.33
1	A	464	LEU	C-O	-5.23	1.13	1.23
2	B	552	TRP	CB-CG	5.19	1.59	1.50
4	E	208	CYS	CB-SG	5.16	1.91	1.82
5	F	143	TYR	CG-CD2	-5.12	1.32	1.39
1	A	490	GLU	C-O	5.09	1.33	1.23
2	B	467	TYR	CG-CD2	5.05	1.45	1.39
2	B	570	GLU	CD-OE1	5.04	1.31	1.25

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	207	VAL	CG1-CB-CG2	10.98	128.47	110.90
2	B	196	ARG	NE-CZ-NH1	10.96	125.78	120.30
1	A	639	ARG	NE-CZ-NH2	-9.64	115.48	120.30
2	B	684	PHE	CB-CG-CD1	9.34	127.34	120.80
1	A	332	ARG	NE-CZ-NH1	8.44	124.52	120.30
2	B	695	ARG	NE-CZ-NH1	8.02	124.31	120.30
2	B	497	ARG	NE-CZ-NH2	7.97	124.29	120.30
2	B	364	ARG	NE-CZ-NH1	7.95	124.27	120.30
3	D	398	ARG	NE-CZ-NH1	7.83	124.22	120.30
5	F	146	ARG	NE-CZ-NH1	-7.67	116.46	120.30
2	B	481	PHE	CB-CG-CD1	-7.36	115.65	120.80
2	B	518	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	A	666	ASP	CB-CG-OD1	7.33	124.89	118.30
4	E	59	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	A	391	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	A	334	ARG	NE-CZ-NH1	-7.21	116.69	120.30
5	F	146	ARG	NE-CZ-NH2	7.16	123.88	120.30
1	A	437	LEU	CB-CG-CD1	-7.13	98.88	111.00
2	B	626	VAL	CG1-CB-CG2	7.02	122.13	110.90
2	B	711	ASP	CB-CG-OD2	7.02	124.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	224	LEU	CB-CG-CD2	6.95	122.82	111.00
2	B	589	GLU	OE1-CD-OE2	-6.85	115.08	123.30
2	B	573	ASP	CB-CG-OD2	6.82	124.44	118.30
2	B	383	LEU	CB-CG-CD2	6.79	122.54	111.00
1	A	437	LEU	CB-CG-CD2	6.75	122.47	111.00
5	F	10	LEU	CB-CG-CD1	6.67	122.34	111.00
2	B	487	ARG	NE-CZ-NH2	-6.66	116.97	120.30
2	B	719	TYR	CB-CG-CD2	-6.50	117.10	121.00
2	B	53	LEU	CB-CG-CD2	6.47	121.99	111.00
2	B	219	ASP	CB-CG-OD1	-6.45	112.50	118.30
2	B	196	ARG	NE-CZ-NH2	-6.44	117.08	120.30
2	B	536	VAL	CG1-CB-CG2	6.43	121.19	110.90
2	B	494	ILE	CG1-CB-CG2	6.34	125.34	111.40
1	A	494	MET	CG-SD-CE	6.22	110.16	100.20
2	B	524	LEU	CB-CG-CD1	6.22	121.57	111.00
6	G	16	MET	CB-CG-SD	6.21	131.02	112.40
2	B	32	LEU	CB-CG-CD2	-6.13	100.58	111.00
2	B	112	ARG	CG-CD-NE	6.03	124.47	111.80
1	A	494	MET	CA-CB-CG	6.03	123.55	113.30
1	A	316	LEU	C-N-CA	5.98	136.65	121.70
1	A	358	ARG	NE-CZ-NH2	-5.97	117.31	120.30
5	F	143	TYR	CB-CG-CD2	-5.96	117.43	121.00
6	G	61	MET	CG-SD-CE	5.94	109.70	100.20
2	B	247	MET	CG-SD-CE	5.93	109.68	100.20
5	F	162	LEU	CB-CG-CD1	5.90	121.03	111.00
4	E	220	HIS	CB-CA-C	-5.89	98.63	110.40
2	B	391	LEU	CB-CG-CD1	5.88	121.00	111.00
2	B	601	ARG	NE-CZ-NH2	5.86	123.23	120.30
2	B	695	ARG	NE-CZ-NH2	-5.82	117.39	120.30
5	F	139	LYS	CD-CE-NZ	5.78	124.99	111.70
2	B	373	ARG	NE-CZ-NH1	5.74	123.17	120.30
4	E	207	VAL	CA-CB-CG2	-5.72	102.31	110.90
5	F	141	LEU	CB-CG-CD1	-5.66	101.38	111.00
5	F	137	LEU	CB-CG-CD1	5.65	120.60	111.00
4	E	231	LEU	CA-CB-CG	-5.64	102.32	115.30
2	B	369	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	483	LEU	CB-CG-CD2	5.54	120.42	111.00
5	F	146	ARG	CB-CG-CD	5.49	125.86	111.60
4	E	189	LEU	CB-CG-CD1	5.42	120.20	111.00
2	B	683	ARG	NE-CZ-NH1	5.40	123.00	120.30
4	E	213	ARG	NE-CZ-NH2	-5.39	117.61	120.30
5	F	150	GLU	OE1-CD-OE2	-5.34	116.90	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	450	ARG	NE-CZ-NH2	-5.31	117.64	120.30
2	B	503	ALA	N-CA-C	-5.26	96.79	111.00
2	B	247	MET	CB-CG-SD	-5.23	96.71	112.40
1	A	391	ARG	NE-CZ-NH2	-5.19	117.70	120.30
2	B	194	LEU	CB-CG-CD1	5.19	119.83	111.00
1	A	479	ASP	CB-CG-OD1	5.19	122.97	118.30
2	B	315	LEU	CA-CB-CG	5.17	127.20	115.30
2	B	30	ARG	NE-CZ-NH1	5.17	122.88	120.30
3	D	394	TRP	CA-CB-CG	5.13	123.45	113.70
2	B	596	LEU	CB-CG-CD1	-5.13	102.28	111.00
2	B	611	VAL	CG1-CB-CG2	-5.12	102.71	110.90
2	B	24	TYR	CB-CG-CD2	-5.12	117.93	121.00
2	B	90	LEU	CB-CG-CD2	-5.10	102.32	111.00
1	A	273	LYS	CB-CG-CD	5.10	124.85	111.60
2	B	450	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	B	192	TYR	CZ-CE2-CD2	-5.07	115.23	119.80
4	E	86	LYS	CA-CB-CG	5.07	124.56	113.40
4	E	219	TYR	CG-CD2-CE2	-5.07	117.25	121.30
1	A	325	ARG	NE-CZ-NH1	5.05	122.83	120.30
2	B	373	ARG	NE-CZ-NH2	-5.04	117.78	120.30
5	F	53	ARG	NE-CZ-NH1	5.04	122.82	120.30
4	E	213	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	320	GLN	CB-CA-C	5.01	120.42	110.40
2	B	88	ARG	NE-CZ-NH1	5.01	122.81	120.30
2	B	677	MET	CB-CG-SD	-5.01	97.37	112.40

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

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Mol	Chain	Res	Type	Group
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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3887	0	3750	94	0
2	B	5671	0	5575	140	0
3	D	643	0	622	14	0
4	E	1451	0	1492	32	0
5	F	1498	0	1414	18	0
6	G	522	0	528	14	0
7	H	620	0	131	0	0
8	Z	1350	0	315	4	0
9	Y	1160	0	279	10	0
10	X	390	0	96	1	0
11	B	8	0	0	0	0
All	All	17200	0	14202	301	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 (301) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:298:ARG:HB2	1:A:359:LYS:HZ3	1.58	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:343:GLY:H	1:A:346:LYS:HZ2	1.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
2:B:565:LYS:HZ2	2:B:593:GLY:HA3	1.82	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
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
1:A:531:ILE:O	1:A:535:THR:OG1	2.25	0.43
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
2:B:524:LEU:HD11	2:B:595:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:111:SER:HA	4:E:141:GLY:HA3	1.99	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:400:ARG:HA	6:G:16:MET:HE1	2.03	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
5:F:12:VAL:HA	5:F:58:ALA:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	461/553 (83%)	402 (87%)	57 (12%)	2 (0%)	34	72
2	B	722/760 (95%)	614 (85%)	101 (14%)	7 (1%)	15	54
3	D	75/85 (88%)	71 (95%)	3 (4%)	1 (1%)	12	48
4	E	182/395 (46%)	171 (94%)	11 (6%)	0	100	100
5	F	199/308 (65%)	182 (92%)	15 (8%)	2 (1%)	15	54
6	G	64/71 (90%)	56 (88%)	8 (12%)	0	100	100
All	All	1703/2172 (78%)	1496 (88%)	195 (12%)	12 (1%)	26	62

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	400/454 (88%)	395 (99%)	5 (1%)	69	82
2	B	586/664 (88%)	576 (98%)	10 (2%)	60	78
3	D	64/73 (88%)	64 (100%)	0	100	100
4	E	169/352 (48%)	165 (98%)	4 (2%)	49	69
5	F	144/272 (53%)	142 (99%)	2 (1%)	67	81
6	G	59/64 (92%)	59 (100%)	0	100	100
All	All	1422/1879 (76%)	1401 (98%)	21 (2%)	66	80

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	472	ARG
1	A	490	GLU
1	A	532	LEU
1	A	584	THR
1	A	633	ARG
2	B	87	LEU
2	B	274	LYS

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Mol	Chain	Res	Type
2	B	410	TYR
2	B	437	CYS
2	B	487	ARG
2	B	523	LEU
2	B	539	PHE
2	B	563	ARG
2	B	641	ARG
2	B	722	ARG
4	E	104	ILE
4	E	164	SER
4	E	174	LEU
4	E	194	ILE
5	F	57	LEU
5	F	133	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	320	GLN
1	A	388	GLN
1	A	433	GLN
1	A	539	ASN
1	A	595	ASN
1	A	599	ASN
1	A	621	ASN
1	A	638	GLN
1	A	665	GLN
2	B	262	ASN
2	B	562	GLN
2	B	726	GLN
4	E	60	HIS
4	E	235	HIS
5	F	176	ASN
5	F	225	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [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 [i](#)

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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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
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

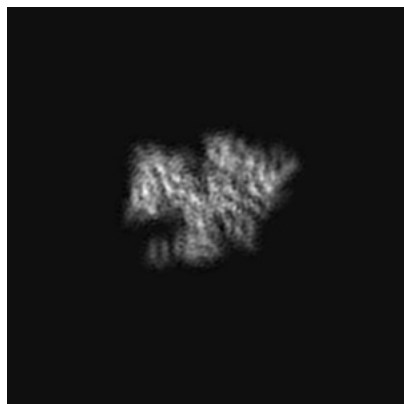
6 Map visualisation [i](#)

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.

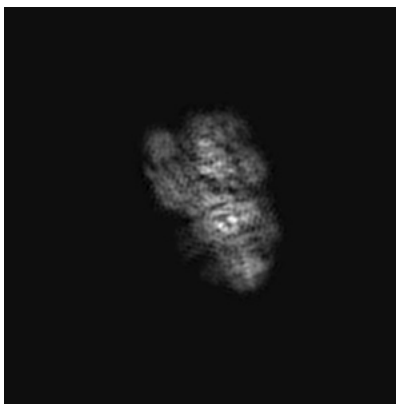
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

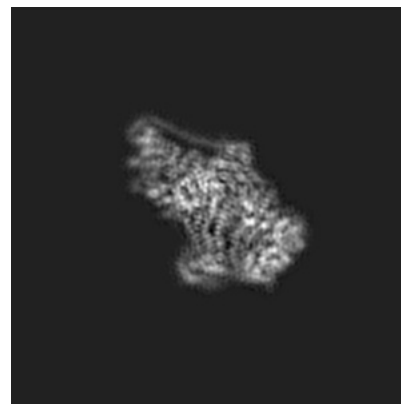
6.1.1 Primary map



X

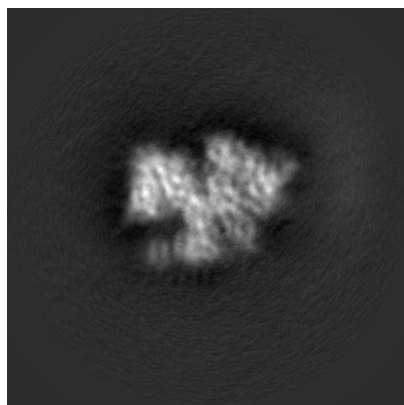


Y

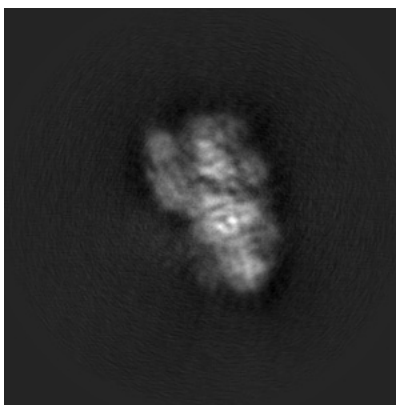


Z

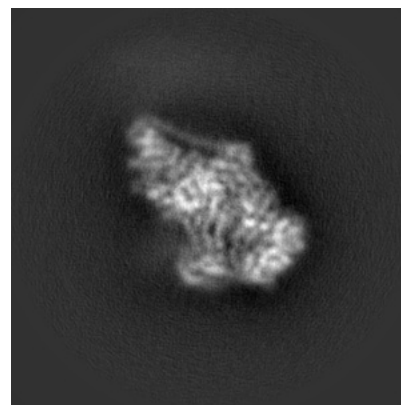
6.1.2 Raw map



X



Y

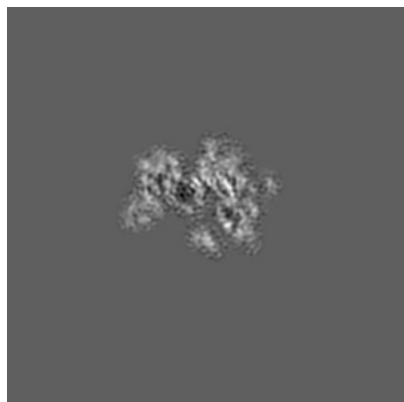


Z

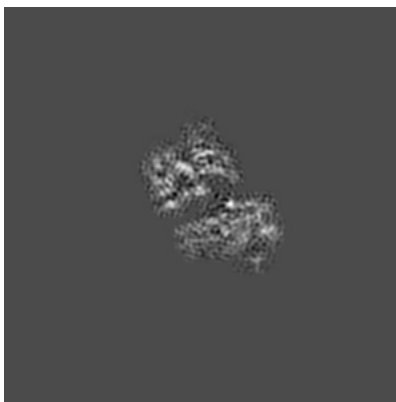
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

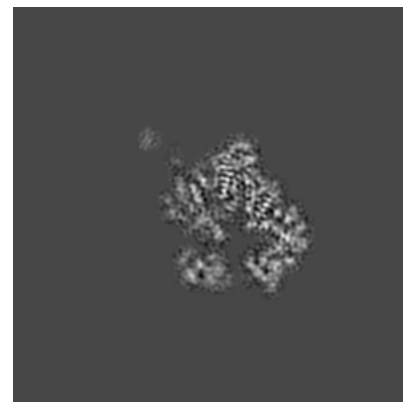
6.2.1 Primary map



X Index: 128

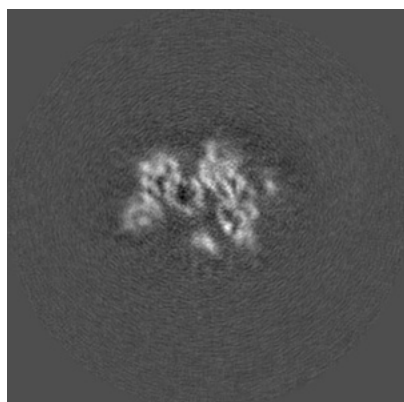


Y Index: 128

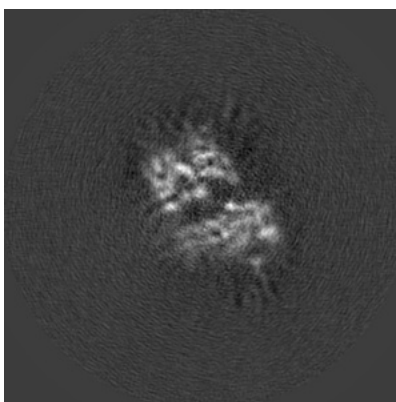


Z Index: 128

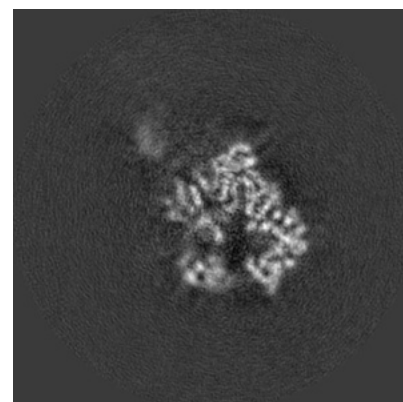
6.2.2 Raw map



X Index: 128



Y Index: 128

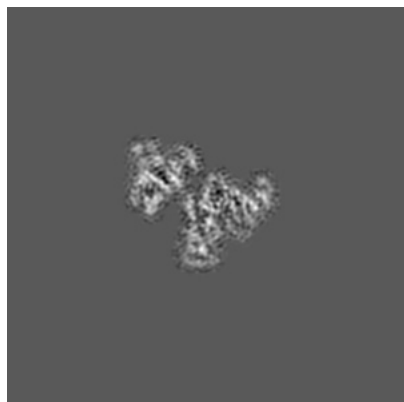


Z Index: 128

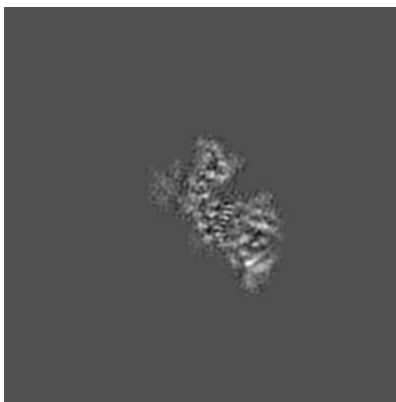
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

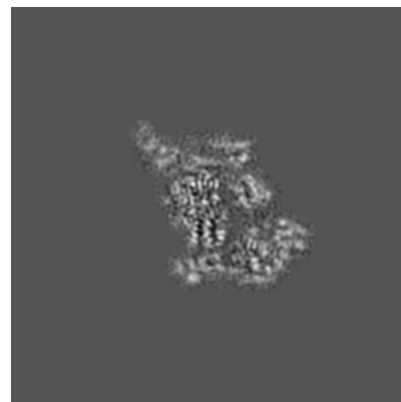
6.3.1 Primary map



X Index: 151

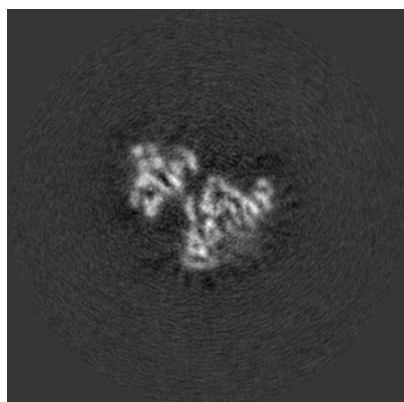


Y Index: 138

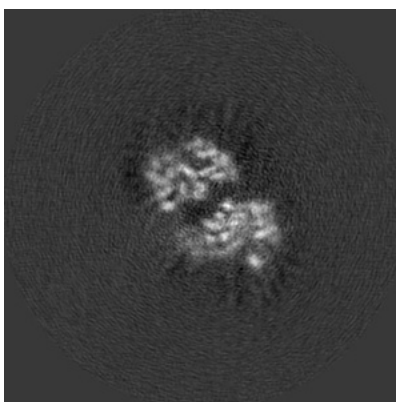


Z Index: 138

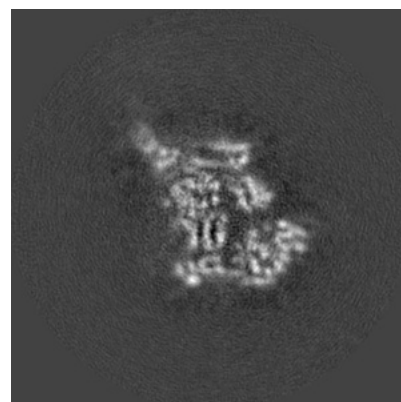
6.3.2 Raw map



X Index: 151



Y Index: 130



Z Index: 138

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

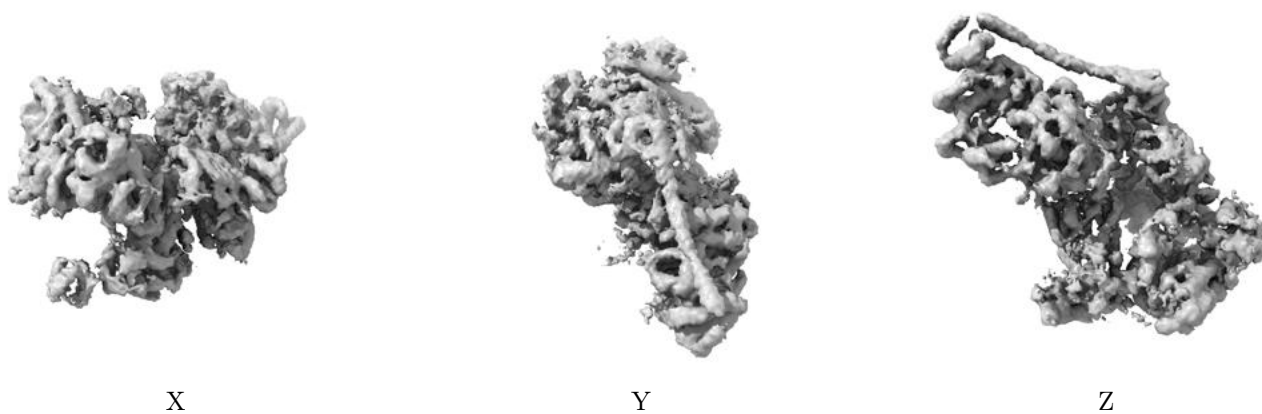
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

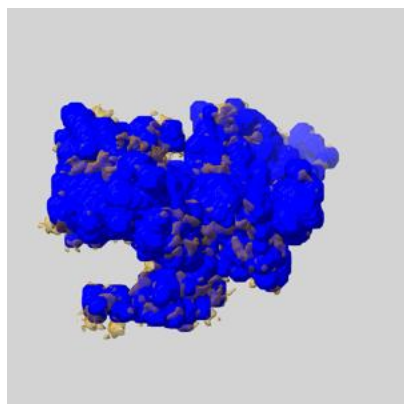
6.5 Mask visualisation [i](#)

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

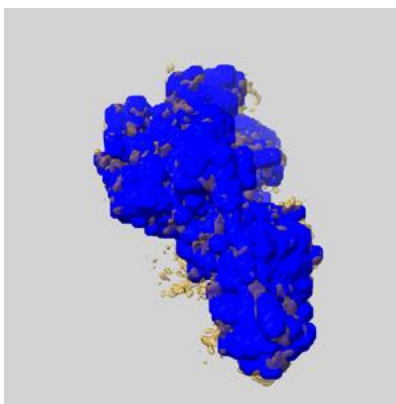
A mask typically either:

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

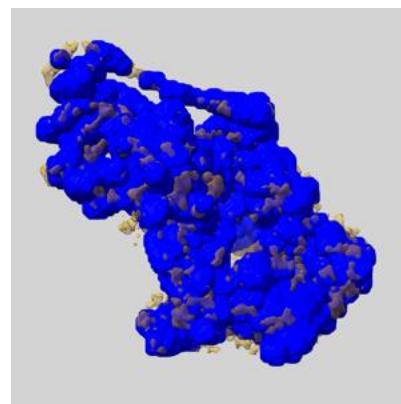
6.5.1 emd_3802_msk_1.map [i](#)



X



Y

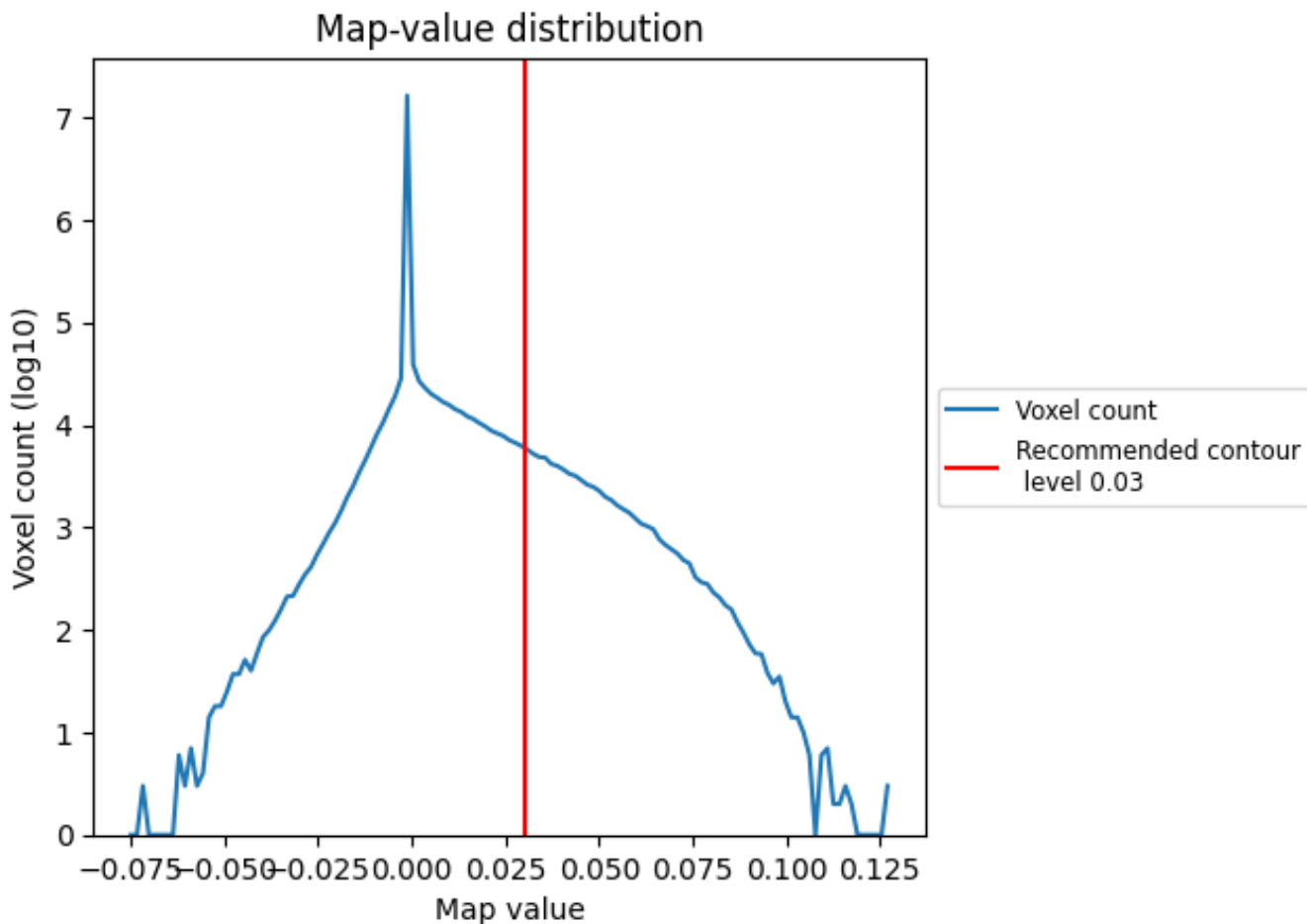


Z

7 Map analysis [i](#)

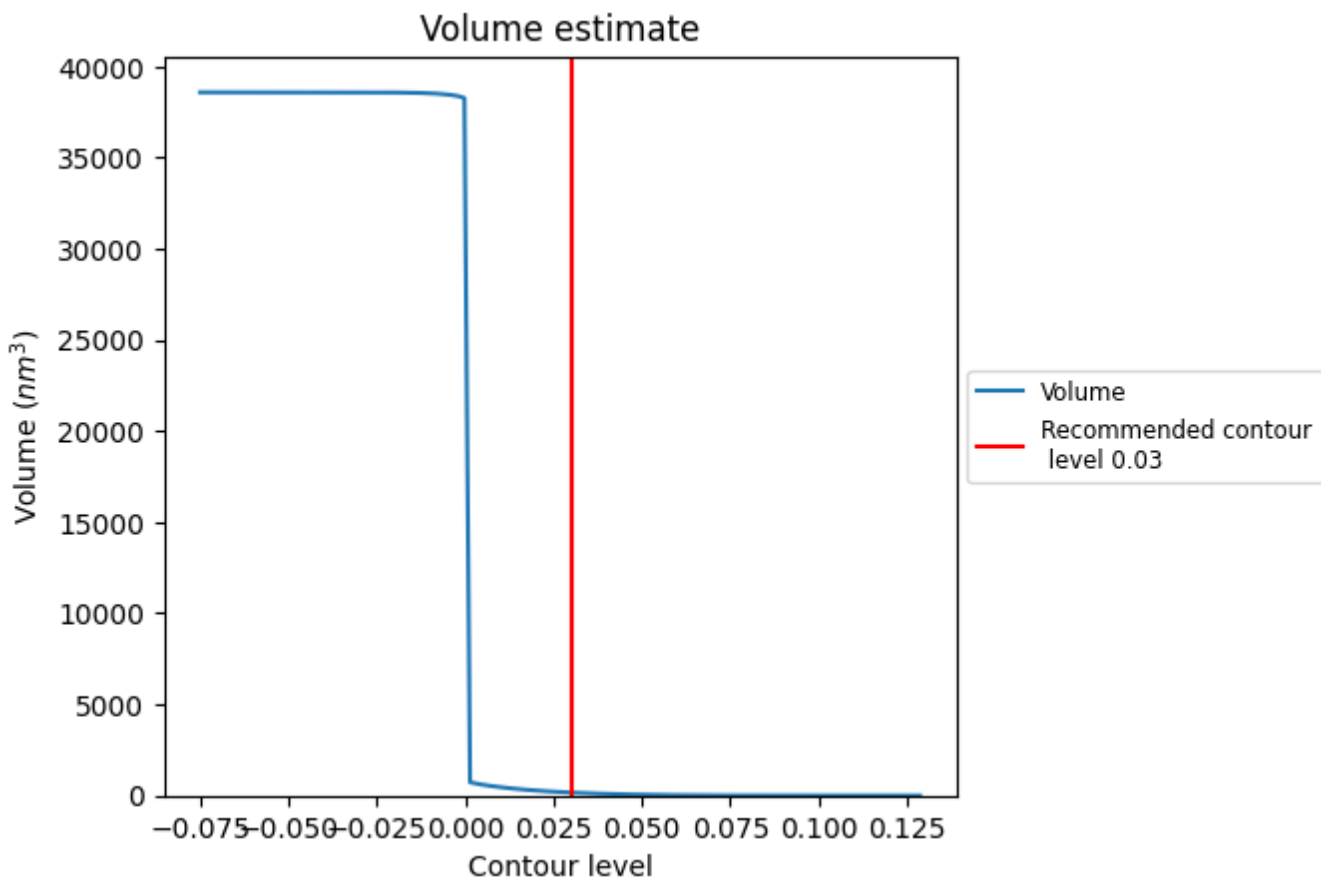
This section contains the results of statistical analysis of the map.

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.

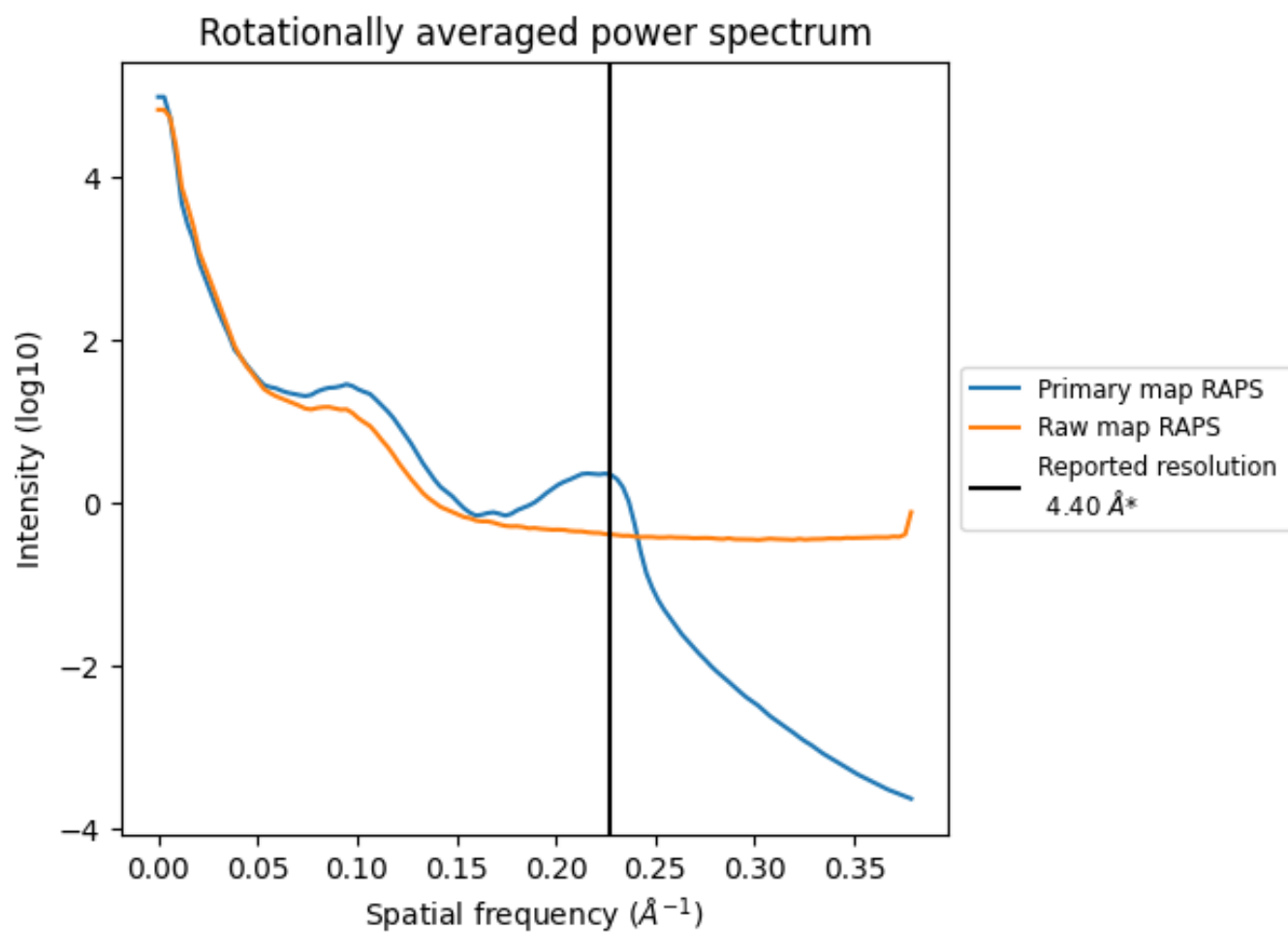
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 163 nm³; 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 i

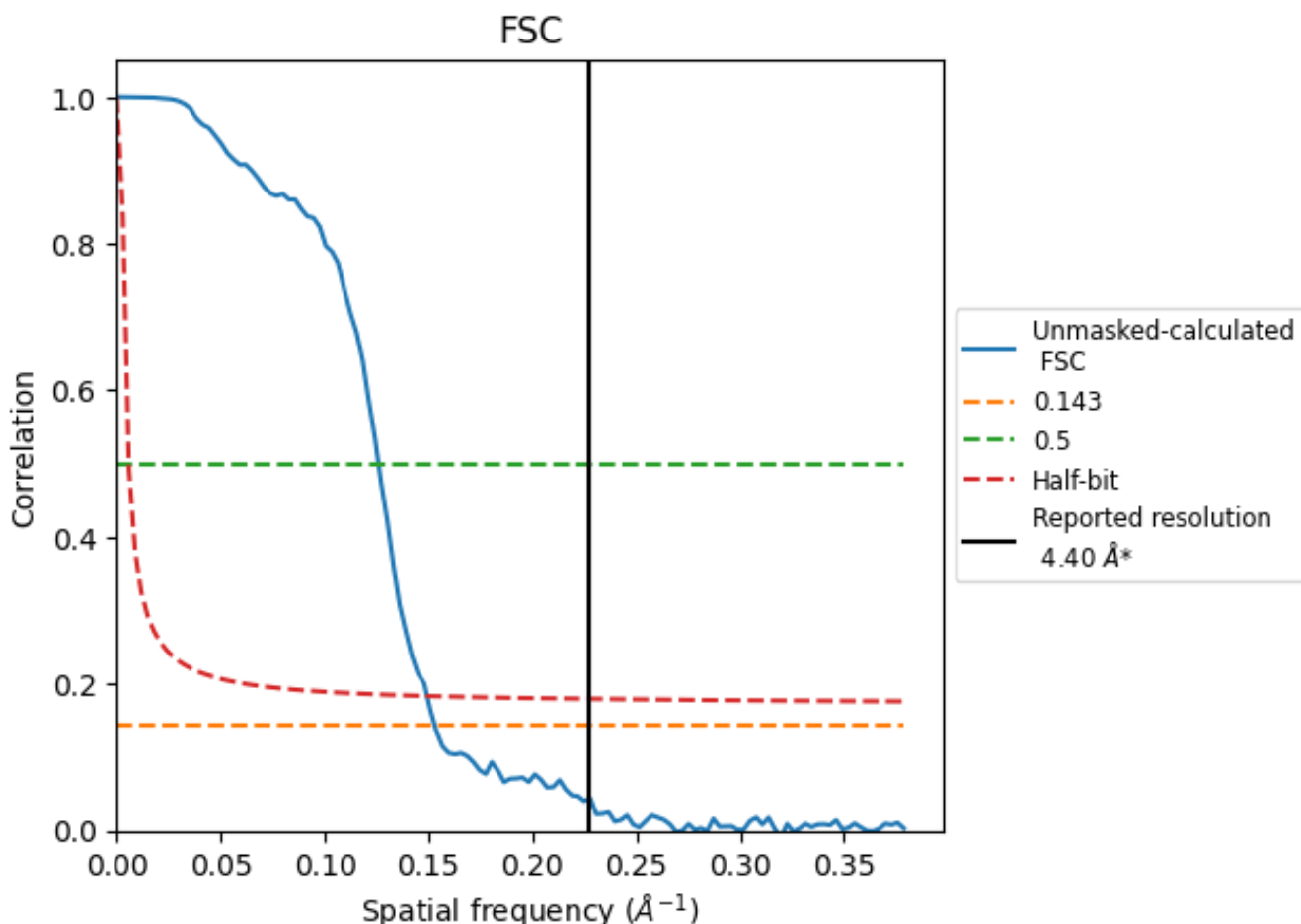


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

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 Å⁻¹

8.2 Resolution estimates [i](#)

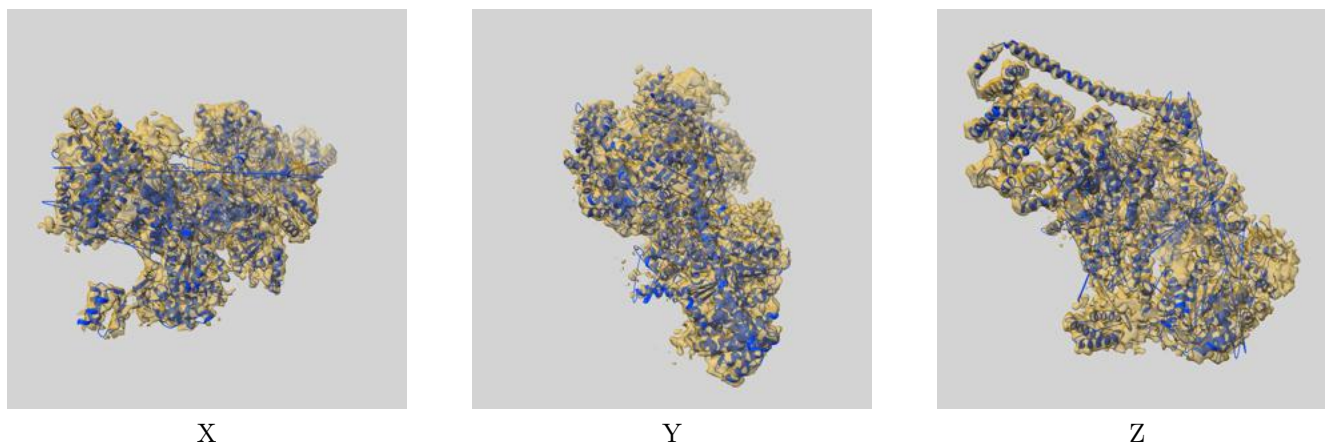
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.53	7.94	6.69

*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](#)

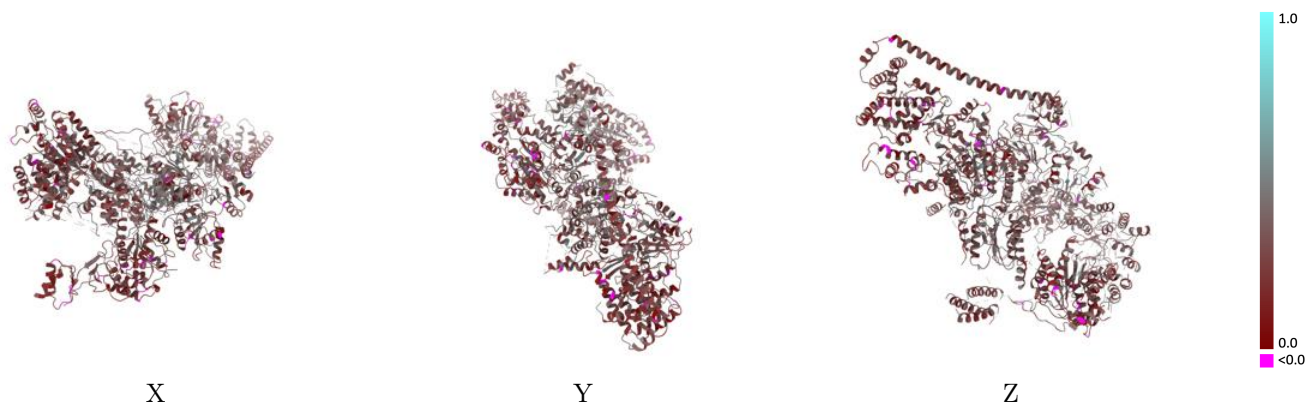
This section contains information regarding the fit between EMDB map EMD-3802 and PDB model 5OF4. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



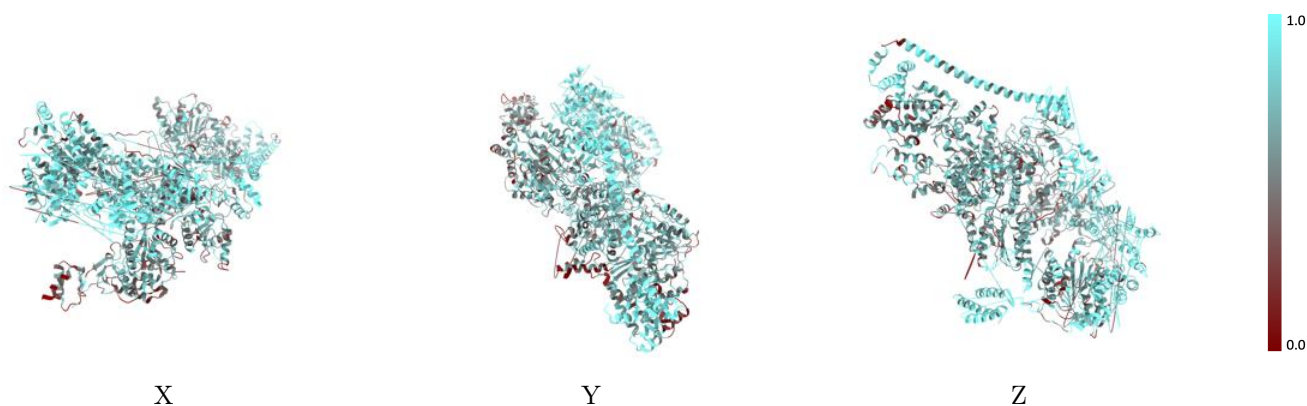
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



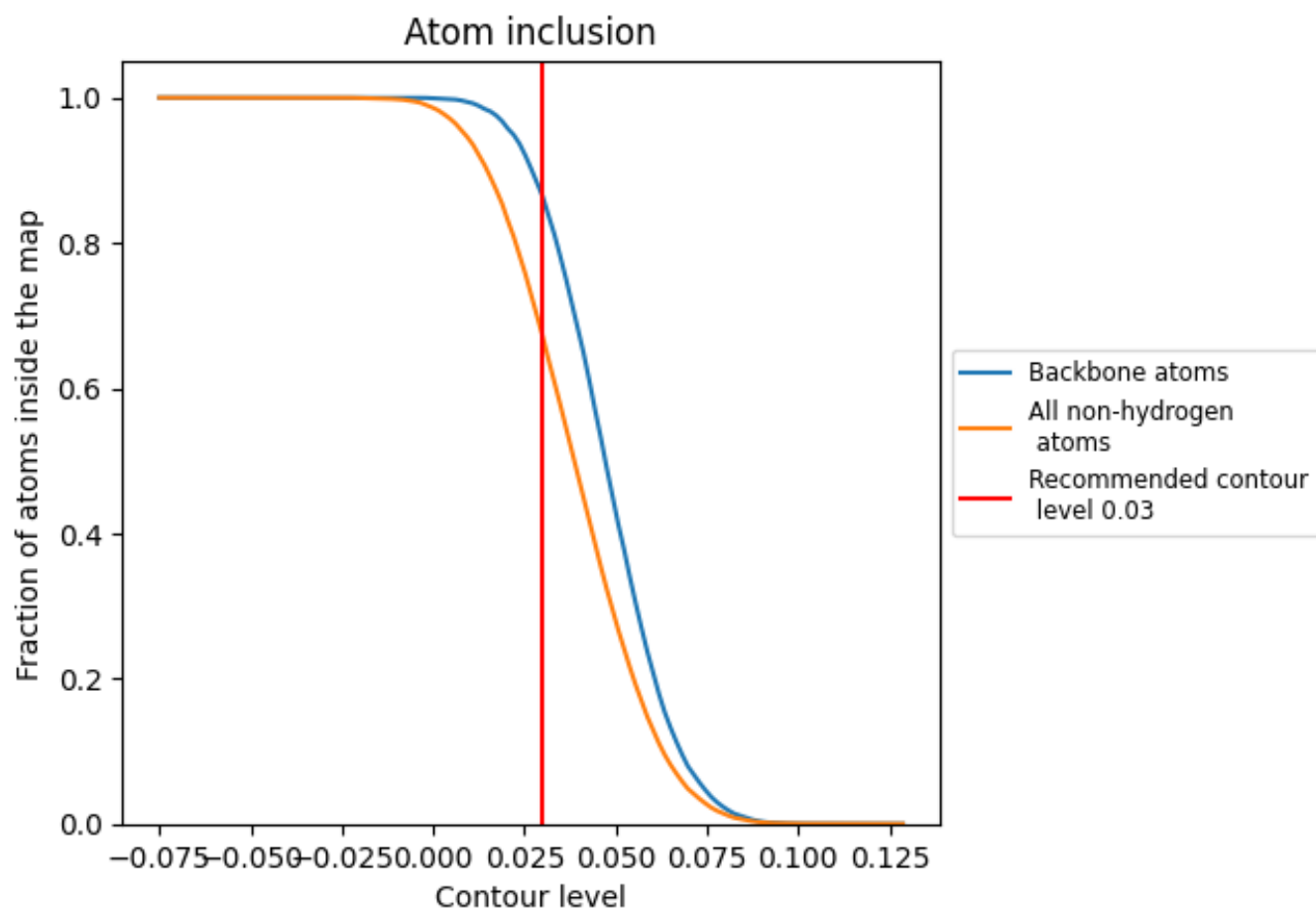
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.6714	 0.3080
A	 0.6120	 0.2980
B	 0.6469	 0.3020
D	 0.5353	 0.2680
E	 0.6690	 0.3630
F	 0.6802	 0.2860
G	 0.5183	 0.2640
H	 0.8452	 0.2810
X	 0.9128	 0.3870
Y	 0.9009	 0.3510
Z	 0.7081	 0.3200

