



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:02 PM UTC

PDB ID : 8BZ1 / pdb_00008bz1
EMDB ID : EMD-16335
Title : RNA polymerase II core pre-initiation complex with the proximal +1 nucleosome (cPIC-Nuc10W)
Authors : Abril-Garrido, J.; Dienemann, C.; Grabbe, F.; Velychko, T.; Lidschreiber, M.; Wang, H.; Cramer, P.
Deposited on : 2022-12-14
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

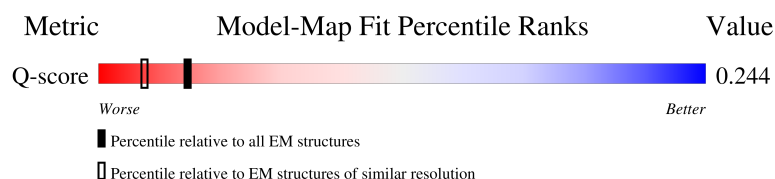
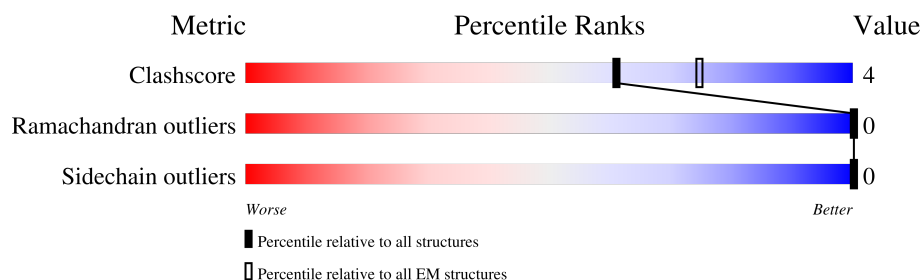
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	1970	
2	B	1174	
3	C	275	
4	D	142	

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Mol	Chain	Length	Quality of chain
5	E	210	
6	F	127	
7	G	172	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	316	
14	N	210	
15	O	339	
16	Q	517	
17	R	249	
18	T	210	
19	U	376	
20	V	109	
21	a	136	
21	e	136	
22	b	103	
22	f	103	
23	c	130	
23	g	130	
24	d	126	
24	h	126	

2 Entry composition [i](#)

There are 26 unique types of molecules in this entry. The entry contains 103616 atoms, of which 50237 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 DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1423	Total	C	H	N	O	S	0	0
			22693	7092	11419	2016	2094	72		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	1136	Total	C	H	N	O	S	0	0
			18198	5739	9122	1597	1676	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	257	Total	C	H	N	O	S	0	0
			4071	1294	2012	351	408	6		

- Molecule 4 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	128	Total	C	H	N	O	S	0	0
			2084	656	1034	178	212	4		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	209	Total	C	H	N	O	S	0	0
			3459	1089	1738	300	324	8		

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	89	Total	C	H	N	O	S	0	0
			1351	435	666	118	127	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	171	Total	C	H	N	O	S	0	0
			2710	875	1359	219	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	148	Total	C	H	N	O	S	0	0
			2334	750	1148	194	237	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	114	Total	C	H	N	O	S	0	0
			1796	571	868	166	180	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	64	Total	C	H	N	O	S	0	0
			1034	328	527	86	87	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	115	Total	C	H	N	O	S	0	0
			1862	593	942	152	173	2		

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	44	Total	C	H	N	O	S	0	0
			756	231	383	72	64	6		

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	252	Total	C	H	N	O	S	0	0
			3945	1224	1992	346	366	17		

- Molecule 14 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	198	Total	C	H	N	O	P	0	0
			6271	1921	2220	746	1187	197		

- Molecule 15 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	179	Total	C	H	N	O	S	0	0
			2937	923	1515	251	241	7		

- Molecule 16 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	Q	138	Total	C	H	N	O	S	0	0
			2242	719	1104	208	208	3		

- Molecule 17 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	R	222	Total	C	H	N	O	S	0	0
			3609	1127	1821	320	338	3		

- Molecule 18 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	T	198	Total	C	H	N	O	P	0	0
			6280	1924	2219	755	1185	197		

- Molecule 19 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	U	113	Total	C	H	N	O	S	0	0
			1820	585	890	152	189	4		

- Molecule 20 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	V	99	Total	C	H	N	O	S	0	0
			1624	510	818	142	151	3		

- Molecule 21 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	a	97	Total	C	H	N	O	S	0	0
			1643	506	841	155	138	3		
21	e	98	Total	C	H	N	O	S	0	0
			1665	512	854	157	139	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	103	ALA	GLY	engineered mutation	UNP P84233
e	103	ALA	GLY	engineered mutation	UNP P84233

- Molecule 22 is a protein called Histone H4.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	b	82	Total	C	H	N	O	S	0	0
			1350	412	697	127	113	1		
22	f	82	Total	C	H	N	O	S	0	0
			1350	412	697	127	113	1		

- Molecule 23 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	c	109	Total	C	H	N	O		0	0
			1752	531	909	167	145			
23	g	106	Total	C	H	N	O		0	0
			1696	516	878	160	142			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	100	ARG	GLY	engineered mutation	UNP P06897
g	100	ARG	GLY	engineered mutation	UNP P06897

- Molecule 24 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	d	97	Total	C	H	N	O	S	0	0
			1561	480	795	142	142	2		
24	h	95	Total	C	H	N	O	S	0	0
			1513	468	769	134	140	2		

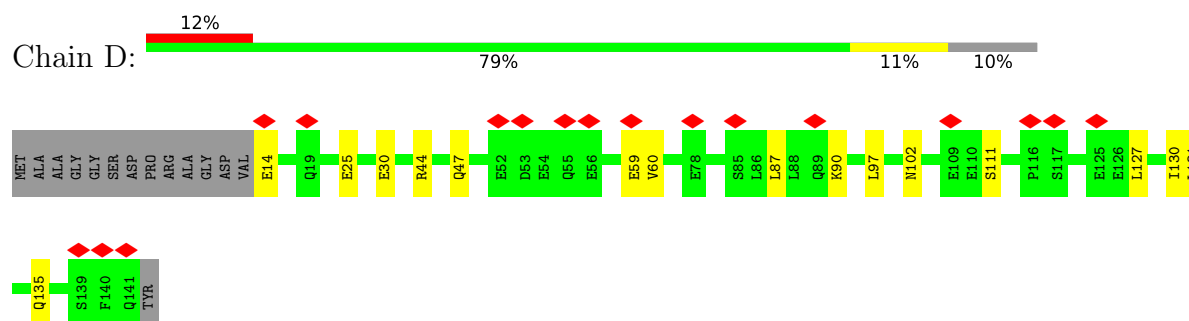
- Molecule 25 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
25	A	2	Total 2	Zn 2	0
25	B	1	Total 1	Zn 1	0
25	C	1	Total 1	Zn 1	0
25	I	2	Total 2	Zn 2	0
25	J	1	Total 1	Zn 1	0
25	L	1	Total 1	Zn 1	0
25	M	1	Total 1	Zn 1	0

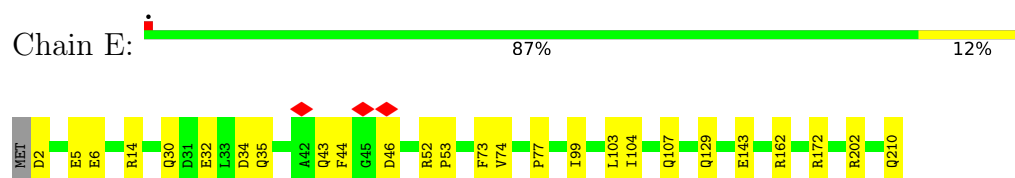
- Molecule 26 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
26	A	1	Total 1	Mg 1	0

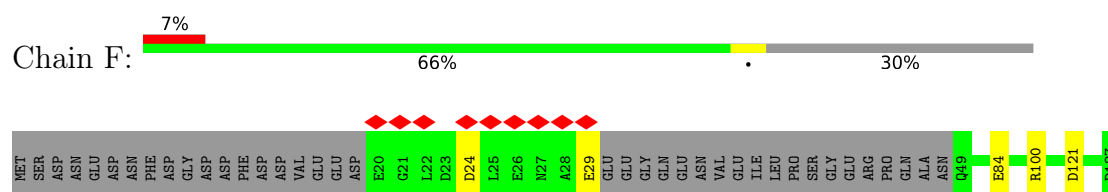
- Molecule 4: RNA polymerase II subunit D



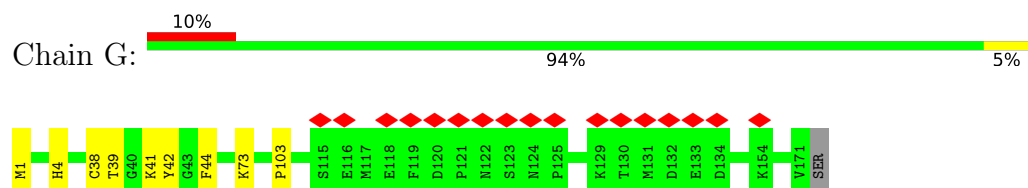
- Molecule 5: DNA-directed RNA polymerase II subunit E



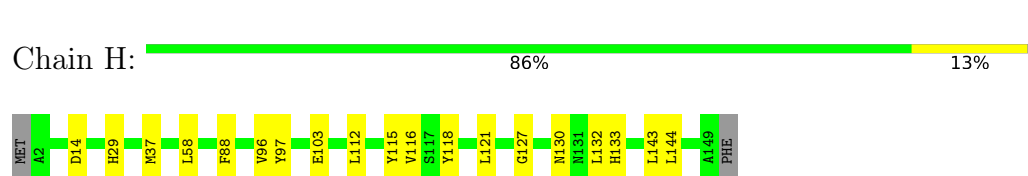
- Molecule 6: DNA-directed RNA polymerase II subunit F



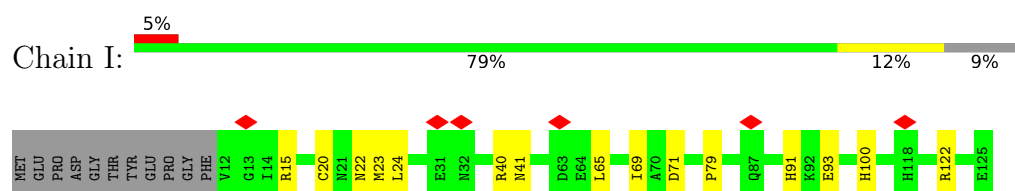
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

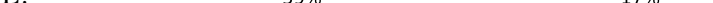


- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

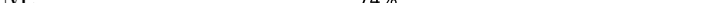
M1
I2
I3
R6
C7
F8
T9
I13
V14
L40
K41
R42
C45
R46
R47
M48
L49
P64
LEU
GLU
LYS

- Chain K: 89% 9%

M1	S9	V63	H69	K70	I71	Y81	A86	F87	T88	N89	A90	I91	R104	F105	G115	I1E	GLU
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- Chain L:  59% 17% 24%

MET	ASP	THR	GLN	LYS	ASP	VAL	GLN	PRO	PRO	LYS	GLN	GLN	M15	I16	Y17	R31	D32	C36	R37	Y41	R42	I43	M44	A57	R58
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- Chain M:  74% 5% 20%

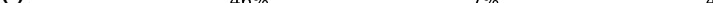
MET	ALA	SER	THR	SER	ARG	LEU	ASP	LEU	LEU	PRO	ARG	VAL	T14	C15	H18	D26	C37	D43	I46	D47	T54	PHE	SER	ASN	ASP	ASP	LYS	ALA	ALA	THR	LYS	ASP	PRO	SER	ARG	VAL	GLY	ASP	SER	SER	GLN	ASN	ASN	PRO	LEU	LEU	LEU	SER	SER	THR	MET	ILE	GLY
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GLY	THR	GLY	ALA	ALA	SER	PER	ASP	GLU	PHE	GLY	ASN	SER	LYS	TYR	GLN	ASN	ARG	ARG	T106	R127	I128	P131	I134	R154	P174	V183	D213	A264	D303	D311	K312	L313	P314	Q315	V316
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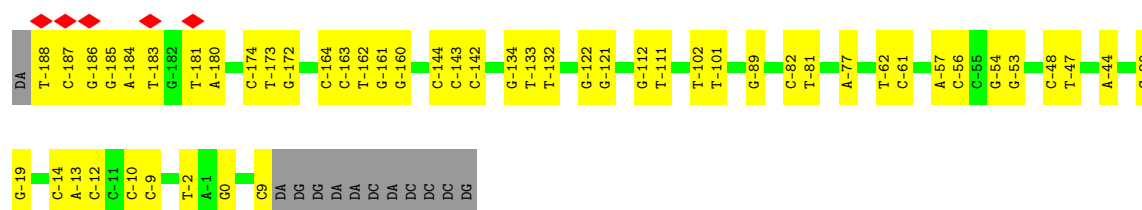
- Chain N:  66% 29% 6%

DG	DG	DG	DG	DG	DG	DG	DT	DT	DT	DT	DT	G-9	T1	C21	G22	T27	C35	T36	C37	C45	G46	A47	C53	C54	C59	C60	C68	T69	C70	A71	A72	T73	G79	T80	A81	G82	T100	A101	A102	A103	G109	T110	T119	C120	C121	C122	C123
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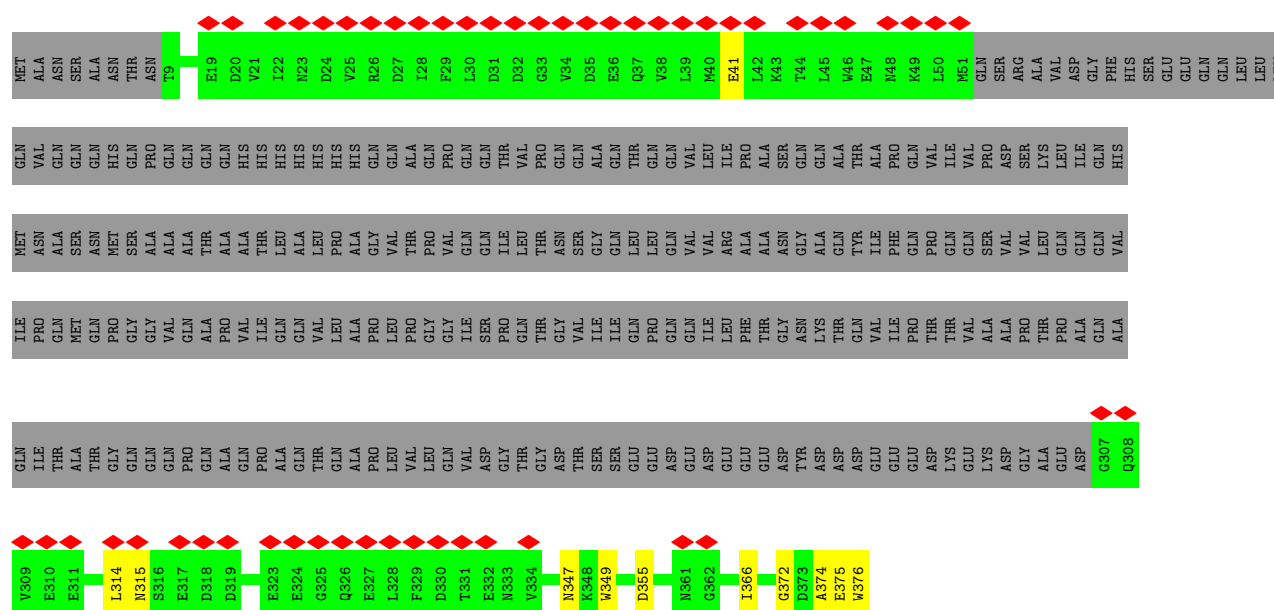
T131	A132	A140	G141	G142	G143	C152	C153	T154	A155	C161	A162	G163	G164	C165	T169	G170	T171	C172	A179	T180	A181	C182	A183	T184	C185	C186	G187	A188	DT
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- Chain 0:  46% 7% 47%

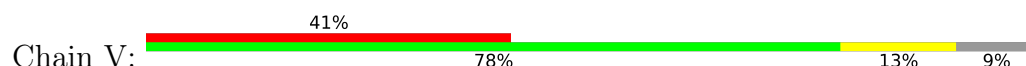
[illegible][illegible]



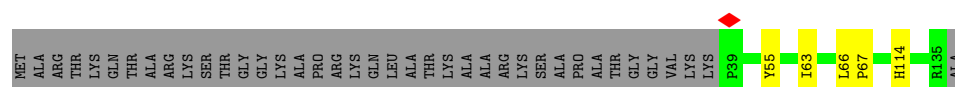
• Molecule 19: Transcription initiation factor IIA subunit 1



• Molecule 20: Transcription initiation factor IIA subunit 2



• Molecule 21: Histone H3.2





MET	PRO	GLU	PRO	PRO	ALA	LYS	SER	ALA	PRO	ALA	PRO	LYS	LYS	GLY	SER	LYS	LYS	ALA	VAL	THR	LYS	THR	GLN	LYS	LYS	ASP	GLY	LYS	LYS	ARG	ARG	K32
																																E36
																																M60
																																V99
																																K126

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	214161	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.45	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1300	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	37.902	Depositor
Minimum map value	-16.786	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.5	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.21	0/11479	0.57	3/15496 (0.0%)
2	B	0.21	0/9257	0.55	0/12493
3	C	0.16	0/2102	0.52	0/2857
4	D	0.11	0/1064	0.42	0/1428
5	E	0.13	0/1752	0.47	0/2366
6	F	0.15	0/694	0.47	0/936
7	G	0.12	0/1382	0.42	0/1874
8	H	0.13	0/1207	0.47	0/1628
9	I	0.14	0/949	0.49	0/1284
10	J	0.17	0/516	0.51	0/696
11	K	0.15	0/939	0.40	0/1271
12	L	0.18	0/378	0.68	0/500
13	M	0.15	0/1983	0.47	0/2679
14	N	0.23	0/4543	0.60	0/7009
15	O	0.12	0/1448	0.50	0/1948
16	Q	0.12	0/1167	0.44	0/1576
17	R	0.12	0/1817	0.43	0/2445
18	T	0.24	0/4557	0.59	3/7033 (0.0%)
19	U	0.14	0/945	0.45	0/1274
20	V	0.15	0/816	0.46	0/1105
21	a	0.15	0/814	0.54	0/1092
21	e	0.15	0/823	0.51	0/1104
22	b	0.15	0/660	0.52	0/883
22	f	0.16	0/660	0.53	0/883
23	c	0.14	0/853	0.50	0/1149
23	g	0.14	0/828	0.50	0/1117
24	d	0.18	0/777	0.53	0/1041
24	h	0.18	0/755	0.51	0/1013
All	All	0.19	0/55165	0.54	6/76180 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	T	-14	DC	O3'-P-O5'	5.89	112.83	104.00
18	T	-13	DA	C1'-O4'-C4'	-5.75	101.07	109.70
18	T	-12	DC	C1'-O4'-C4'	-5.54	101.40	109.70
1	A	1120	GLY	CA-C-N	5.31	125.52	120.43
1	A	1120	GLY	C-N-CA	5.31	125.52	120.43
1	A	862	ARG	NE-CZ-NH2	5.25	123.93	119.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11274	11419	11407	110	0
2	B	9076	9122	9116	95	0
3	C	2059	2012	2008	27	0
4	D	1050	1034	1033	11	0
5	E	1721	1738	1737	18	0
6	F	685	666	688	13	0
7	G	1351	1359	1358	7	0
8	H	1186	1148	1147	10	0
9	I	928	868	859	11	0
10	J	507	527	523	12	0
11	K	920	942	942	8	0
12	L	373	383	379	9	0
13	M	1953	1992	1990	12	0
14	N	4051	2220	2222	43	0
15	O	1422	1515	1514	16	0
16	Q	1138	1104	1103	14	0
17	R	1788	1821	1819	12	0
18	T	4061	2219	2221	33	0
19	U	930	890	888	10	0
20	V	806	818	818	12	0
21	a	802	841	841	4	0
21	e	811	854	853	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	b	653	697	696	8	0
22	f	653	697	696	5	0
23	c	843	909	908	6	0
23	g	818	878	877	7	0
24	d	766	795	797	2	0
24	h	744	769	771	3	0
25	A	2	0	0	0	0
25	B	1	0	0	0	0
25	C	1	0	0	0	0
25	I	2	0	0	0	0
25	J	1	0	0	0	0
25	L	1	0	0	0	0
25	M	1	0	0	0	0
26	A	1	0	0	0	0
All	All	53379	50237	50211	429	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 4.

All (429) 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:494:LYS:O	6:F:29:GLU:CA	1.78	1.30
2:B:494:LYS:O	6:F:29:GLU:HA	1.26	1.23
2:B:495:LEU:O	6:F:29:GLU:O	1.67	1.12
1:A:1125:LYS:NZ	6:F:24:ASP:HA	1.84	0.91
2:B:494:LYS:O	6:F:29:GLU:N	2.13	0.81
2:B:494:LYS:O	6:F:29:GLU:C	2.28	0.76
5:E:77:PRO:O	5:E:107:GLN:NE2	2.18	0.74
1:A:1125:LYS:HZ2	6:F:24:ASP:HA	1.51	0.73
1:A:74:CYS:SG	1:A:84:HIS:CE1	2.79	0.73
1:A:1036:ASN:OD1	5:E:202:ARG:NH2	2.23	0.71
2:B:495:LEU:O	6:F:29:GLU:C	2.35	0.70
1:A:1411:LEU:O	1:A:1421:ARG:NH1	2.24	0.69
1:A:1125:LYS:HZ1	6:F:24:ASP:HA	1.53	0.69
2:B:495:LEU:C	6:F:29:GLU:O	2.34	0.69
4:D:25:GLU:OE1	7:G:41:LYS:NZ	2.25	0.68
2:B:953:ASP:OD1	3:C:36:ARG:NH1	2.25	0.68
15:O:267:PRO:HG2	15:O:337:LYS:HB3	1.74	0.68
1:A:428:ASP:OD2	1:A:430:ARG:NH2	2.27	0.67
5:E:46:ASP:O	5:E:52:ARG:NH2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1059:ILE:O	2:B:1080:ARG:NH1	2.26	0.66
1:A:1218:ARG:NH1	1:A:1252:ALA:O	2.29	0.66
2:B:294:ASP:OD2	2:B:379:ARG:NH2	2.25	0.65
1:A:1208:SER:HA	1:A:1266:GLU:HG3	1.77	0.65
3:C:150:ILE:HG22	3:C:151:VAL:H	1.62	0.65
15:O:174:LEU:HD12	15:O:178:LEU:HD11	1.78	0.65
18:T:-44:DA:OP1	21:e:38:LYS:NZ	2.26	0.65
3:C:37:VAL:HG13	3:C:41:GLU:HB2	1.79	0.64
2:B:777:ASN:O	10:J:47:ARG:NH2	2.30	0.64
2:B:910:THR:HG22	12:L:43:ILE:HA	1.79	0.63
13:M:154:ARG:NH2	18:T:-10:DC:OP1	2.31	0.62
14:N:46:DG:H2''	14:N:47:DA:C8	2.36	0.61
1:A:410:ASN:HD22	1:A:430:ARG:HB3	1.64	0.61
2:B:721:ARG:NH2	2:B:940:GLY:O	2.34	0.61
8:H:58:LEU:HD11	8:H:143:LEU:HD11	1.83	0.61
5:E:2:ASP:N	5:E:5:GLU:OE2	2.33	0.61
14:N:79:DG:H2''	14:N:80:DT:C6	2.36	0.61
2:B:905:ASP:OD1	2:B:924:ARG:NH2	2.33	0.60
2:B:388:TYR:CZ	2:B:505:LEU:HD21	2.36	0.60
1:A:460:ARG:HB2	1:A:501:MET:HE3	1.84	0.60
2:B:677:MET:H	2:B:682:LEU:HG	1.66	0.60
1:A:1439:LEU:HD13	2:B:1162:LEU:HD21	1.84	0.59
2:B:433:LEU:O	13:M:127:ARG:NH1	2.35	0.59
16:Q:159:GLU:OE2	16:Q:180:ARG:NH1	2.32	0.59
2:B:495:LEU:C	6:F:29:GLU:C	2.71	0.59
13:M:174:PRO:HD2	13:M:213:ASP:HB3	1.84	0.59
15:O:297:LYS:HB3	15:O:298:PRO:HD3	1.84	0.59
1:A:233:CYS:SG	1:A:244:ARG:NH2	2.76	0.59
1:A:465:HIS:ND1	1:A:467:MET:HE2	2.17	0.58
14:N:123:DC:H5''	22:f:48:SER:HA	1.84	0.58
2:B:1062:ARG:NH2	2:B:1081:ASP:O	2.32	0.58
18:T:-133:DT:H2''	18:T:-132:DT:C6	2.39	0.58
2:B:939:HIS:NE2	2:B:983:GLU:OE1	2.32	0.57
3:C:180:ALA:O	10:J:42:ARG:NH1	2.38	0.57
1:A:479:TRP:HB2	1:A:483:ARG:NH1	2.19	0.57
1:A:539:GLN:OE1	2:B:968:ASN:ND2	2.37	0.57
1:A:1218:ARG:NH2	1:A:1250:ASP:OD1	2.37	0.57
5:E:35:GLN:NE2	5:E:43:GLN:OE1	2.33	0.57
17:R:179:ASP:OD1	17:R:179:ASP:N	2.37	0.57
3:C:44:ILE:HG21	3:C:178:PRO:HB3	1.86	0.57
18:T:-48:DC:H2''	18:T:-47:DT:C6	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ARG:NH2	1:A:414:PRO:O	2.38	0.57
5:E:172:ARG:NH2	5:E:210:GLN:OE1	2.38	0.57
12:L:41:TYR:CE2	12:L:43:ILE:HB	2.40	0.56
1:A:525:ILE:HA	1:A:535:MET:HE3	1.86	0.56
2:B:60:GLU:OE2	17:R:140:ARG:NH2	2.37	0.56
3:C:260:GLN:HB2	11:K:91:ILE:HG21	1.88	0.56
13:M:264:ALA:HB2	13:M:313:LEU:HD21	1.86	0.56
2:B:934:LYS:HG2	2:B:944:THR:HG22	1.87	0.56
14:N:161:DC:H2''	14:N:162:DA:C5	2.40	0.56
9:I:69:ILE:HG22	9:I:71:ASP:H	1.71	0.56
21:a:63:ILE:HD11	22:b:38:LEU:HD11	1.88	0.56
1:A:542:LEU:HD23	1:A:774:ALA:HA	1.89	0.55
4:D:60:VAL:HG13	7:G:103:PRO:HB3	1.87	0.55
16:Q:48:GLU:OE2	16:Q:101:ARG:NH1	2.35	0.55
14:N:45:DC:H2''	14:N:46:DG:C8	2.41	0.55
2:B:755:GLN:HE22	10:J:48:MET:HE2	1.71	0.55
7:G:4:HIS:CE1	7:G:73:LYS:HD2	2.41	0.55
1:A:510:GLU:OE1	2:B:1101:GLN:NE2	2.39	0.55
2:B:926:VAL:HG21	3:C:62:GLU:HG3	1.89	0.55
19:U:355:ASP:OD1	20:V:6:TYR:OH	2.25	0.55
6:F:100:ARG:NH1	6:F:121:ASP:O	2.40	0.55
1:A:433:PRO:HA	1:A:438:LEU:HD11	1.90	0.54
15:O:199:ALA:HB2	15:O:214:PHE:CE2	2.43	0.54
2:B:198:GLU:OE2	2:B:391:LYS:NZ	2.29	0.54
2:B:157:ARG:NH1	2:B:177:CYS:O	2.40	0.54
2:B:399:LEU:HB3	2:B:453:TRP:CZ3	2.42	0.54
1:A:346:LYS:HA	1:A:351:ARG:HD3	1.89	0.54
1:A:811:ILE:HD12	9:I:79:PRO:HB3	1.89	0.54
12:L:32:ASP:OD2	12:L:37:ARG:NH1	2.34	0.54
14:N:72:DA:OP1	23:c:33:ARG:NH2	2.40	0.54
17:R:206:THR:HG21	17:R:213:LEU:HD13	1.90	0.54
1:A:1210:TRP:CE2	1:A:1282:ASP:HB3	2.42	0.54
4:D:44:ARG:NH2	4:D:47:GLN:OE1	2.40	0.54
22:b:60:LYS:NZ	22:b:64:GLU:OE2	2.34	0.54
2:B:59:VAL:HG21	2:B:91:ILE:HD11	1.90	0.53
16:Q:26:TYR:HA	17:R:97:THR:HG22	1.89	0.53
1:A:1434:GLU:HG2	1:A:1437:ASP:HB2	1.90	0.53
19:U:41:GLU:HG3	20:V:27:GLN:HE22	1.73	0.53
1:A:430:ARG:HH12	13:M:26:ASP:CG	2.16	0.53
1:A:491:PRO:HD3	1:A:535:MET:HB3	1.90	0.53
18:T:-10:DC:H2''	18:T:-9:DC:C6	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:387:HIS:NE2	2:B:671:GLU:OE2	2.42	0.53
15:O:192:TYR:HB2	15:O:200:VAL:HG22	1.91	0.53
3:C:56:SER:HB2	3:C:158:GLU:H	1.73	0.52
16:Q:119:THR:HB	16:Q:122:THR:HB	1.91	0.52
11:K:9:SER:HA	11:K:69:HIS:CD2	2.43	0.52
1:A:364:ARG:HB3	2:B:1060:HIS:NE2	2.24	0.52
1:A:79:THR:HG21	13:M:43:ASP:HB2	1.92	0.52
1:A:1005:HIS:HD2	1:A:1006:PRO:HD2	1.75	0.52
18:T:-122:DG:H2''	18:T:-121:DG:C8	2.44	0.52
1:A:556:GLU:OE2	1:A:583:ARG:NH2	2.43	0.52
2:B:453:TRP:NE1	2:B:466:VAL:HB	2.24	0.52
14:N:68:DC:H2''	14:N:69:DT:C5	2.45	0.52
2:B:343:LEU:O	2:B:361:LYS:NZ	2.42	0.52
5:E:46:ASP:HB3	5:E:52:ARG:HB3	1.91	0.51
2:B:812:ARG:NH2	2:B:900:GLU:OE2	2.39	0.51
16:Q:44:GLN:HE22	16:Q:46:ARG:HG3	1.74	0.51
2:B:794:VAL:HG13	2:B:965:ILE:HG23	1.91	0.51
14:N:81:DA:H2''	14:N:82:DG:C8	2.45	0.51
1:A:1228:MET:HE3	1:A:1228:MET:HA	1.91	0.51
22:f:53:GLU:OE2	22:f:56:ARG:NH2	2.43	0.51
1:A:118:LEU:HD12	1:A:148:CYS:HB3	1.93	0.51
1:A:1430:CYS:HB3	1:A:1435:THR:HG23	1.92	0.51
8:H:130:ASN:HA	8:H:133:HIS:CD2	2.46	0.51
9:I:41:ASN:HA	16:Q:177:MET:HE2	1.93	0.51
14:N:59:DC:H2''	14:N:60:DC:C2	2.46	0.51
23:c:55:VAL:HG21	24:d:99:VAL:HG21	1.92	0.51
1:A:34:MET:HA	2:B:1138:ARG:HB3	1.92	0.51
12:L:17:TYR:HB3	12:L:44:MET:HB3	1.93	0.51
18:T:-112:DG:H2''	18:T:-111:DT:C5	2.46	0.51
3:C:7:PRO:O	11:K:104:ARG:NH2	2.33	0.50
1:A:192:ARG:HE	14:N:27:DT:H5''	1.76	0.50
1:A:1208:SER:HB2	1:A:1261:ILE:HB	1.93	0.50
11:K:81:TYR:OH	11:K:89:ASN:OD1	2.29	0.50
15:O:204:ILE:HD12	15:O:207:PRO:HG2	1.92	0.50
20:V:16:GLN:NE2	20:V:20:ASP:OD2	2.44	0.50
20:V:66:ARG:HB2	20:V:73:THR:HB	1.94	0.50
18:T:-188:DT:H2''	18:T:-187:DC:H5'	1.94	0.50
1:A:1262:MET:SD	1:A:1264:SER:OG	2.70	0.50
1:A:1228:MET:HE2	1:A:1257:LEU:HD12	1.94	0.50
18:T:-57:DA:H2''	18:T:-56:DC:C6	2.46	0.49
18:T:-54:DG:H2''	18:T:-53:DG:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:347:ASN:ND2	19:U:376:TRP:O	2.44	0.49
23:c:101:VAL:HG11	22:f:99:TYR:CE2	2.48	0.49
1:A:1450:PRO:HB2	1:A:1452:LYS:HG2	1.94	0.49
13:M:18:HIS:CE1	13:M:37:CYS:HB2	2.47	0.49
23:g:55:VAL:HG21	24:h:99:VAL:HG21	1.95	0.49
18:T:-143:DC:H2"	18:T:-142:DC:C5	2.48	0.49
1:A:1138:SER:OG	1:A:1338:THR:O	2.25	0.49
4:D:59:GLU:OE1	4:D:59:GLU:N	2.44	0.49
1:A:930:LEU:HB3	1:A:939:VAL:HG22	1.95	0.49
2:B:387:HIS:CD2	2:B:504:THR:HG21	2.49	0.48
8:H:112:LEU:HB2	8:H:132:LEU:HD12	1.93	0.48
1:A:395:THR:HG22	1:A:396:PRO:HD2	1.96	0.48
2:B:1119:CYS:HB2	2:B:1137:CYS:SG	2.53	0.48
2:B:305:LEU:HD13	9:I:23:MET:HG3	1.95	0.48
15:O:206:GLU:HB3	15:O:207:PRO:HD3	1.96	0.48
10:J:6:ARG:HD3	10:J:13:ILE:HD13	1.96	0.48
1:A:1242:ASP:HA	1:A:1262:MET:HE3	1.94	0.48
1:A:467:MET:HE3	1:A:534:VAL:HG21	1.95	0.48
2:B:64:PRO:HG3	2:B:87:LYS:HD3	1.95	0.48
8:H:118:TYR:HB2	8:H:121:LEU:HB2	1.96	0.48
14:N:21:DC:N4	14:N:22:DG:O6	2.47	0.48
1:A:863:ARG:HB3	1:A:1414:ILE:HG21	1.96	0.47
23:g:25:GLN:N	23:g:57:GLU:OE1	2.41	0.47
1:A:901:VAL:HA	1:A:980:PRO:HA	1.96	0.47
22:b:99:TYR:CE2	23:g:101:VAL:HG11	2.49	0.47
24:d:38:TYR:HA	24:d:41:TYR:HD2	1.80	0.47
1:A:1163:HIS:CD2	1:A:1302:GLU:HA	2.49	0.47
5:E:14:ARG:NH1	5:E:32:GLU:OE2	2.43	0.47
14:N:53:DC:H2"	14:N:54:DC:C6	2.49	0.47
2:B:93:LEU:HD21	2:B:154:ILE:HD11	1.95	0.47
20:V:15:LEU:HD21	20:V:36:VAL:HG12	1.97	0.47
2:B:117:ASN:HA	2:B:189:GLY:HA3	1.96	0.47
4:D:14:GLU:N	4:D:14:GLU:OE1	2.48	0.47
1:A:689:ILE:O	1:A:693:ILE:HG12	2.14	0.47
3:C:60:HIS:NE2	3:C:63:PHE:HB2	2.30	0.47
14:N:169:DT:H2"	14:N:170:DG:C8	2.50	0.47
1:A:454:ASP:HA	1:A:512:ARG:HH12	1.79	0.47
1:A:1005:HIS:CD2	1:A:1006:PRO:HD2	2.50	0.47
2:B:136:GLY:O	2:B:137:GLU:HG3	2.14	0.47
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.97	0.47
9:I:40:ARG:CZ	16:Q:173:HIS:HB2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:140:DA:H2''	14:N:141:DG:C8	2.49	0.47
13:M:128:ILE:HG23	13:M:183:VAL:HG11	1.96	0.47
14:N:73:DT:H5''	23:c:17:THR:HA	1.96	0.47
1:A:420:ILE:HB	1:A:445:LYS:HB2	1.97	0.47
1:A:497:ASP:O	2:B:942:LYS:HE2	2.15	0.47
1:A:1380:ARG:NH2	5:E:143:GLU:OE2	2.39	0.47
2:B:593:GLN:NE2	2:B:595:ASP:OD2	2.44	0.47
5:E:2:ASP:N	5:E:6:GLU:OE2	2.48	0.47
18:T:-144:DC:H2''	18:T:-143:DC:C6	2.50	0.47
1:A:531:ASN:OD1	1:A:1394:ASN:ND2	2.47	0.46
1:A:909:LEU:HD13	1:A:966:LEU:HB3	1.97	0.46
2:B:42:GLN:H	2:B:42:GLN:CD	2.23	0.46
15:O:239:ARG:NH1	19:U:315:ASN:OD1	2.47	0.46
18:T:-82:DC:H2''	18:T:-81:DT:C6	2.49	0.46
22:b:32:LYS:HE3	22:b:52:TYR:CE2	2.50	0.46
1:A:253:LEU:HD21	1:A:317:MET:HE1	1.96	0.46
1:A:1217:ASP:OD2	1:A:1219:LYS:NZ	2.44	0.46
4:D:90:LYS:HE3	4:D:130:ILE:HG12	1.98	0.46
14:N:183:DA:H2''	14:N:184:DT:C6	2.50	0.46
14:N:184:DT:H2''	14:N:185:DC:C6	2.51	0.46
19:U:375:GLU:O	20:V:62:LEU:N	2.46	0.46
23:g:63:ILE:HD13	23:g:94:LEU:HD13	1.97	0.46
1:A:871:VAL:HB	1:A:1088:GLY:HA3	1.97	0.46
14:N:80:DT:H2''	14:N:81:DA:N7	2.31	0.46
1:A:244:ARG:HB2	1:A:247:TRP:CD2	2.51	0.46
3:C:60:HIS:HD2	3:C:62:GLU:HG2	1.81	0.46
14:N:170:DG:H2''	14:N:171:DT:C5	2.50	0.46
15:O:169:VAL:HG13	15:O:222:THR:HG22	1.98	0.46
17:R:48:THR:N	17:R:51:ARG:O	2.44	0.46
18:T:-184:DA:H2''	18:T:-183:DT:H5'	1.97	0.46
1:A:575:PRO:HG3	1:A:594:LEU:HD11	1.97	0.46
3:C:70:LEU:HB3	10:J:6:ARG:HG2	1.97	0.46
15:O:188:ARG:O	20:V:64:THR:HG23	2.16	0.46
2:B:643:LEU:HD11	2:B:656:LEU:HD11	1.98	0.46
1:A:526:VAL:HA	1:A:533:PRO:HA	1.98	0.46
12:L:41:TYR:OH	12:L:43:ILE:HD12	2.16	0.46
14:N:181:DA:H2''	14:N:182:DC:C6	2.51	0.46
18:T:-160:DG:OP1	23:g:33:ARG:NH2	2.39	0.46
1:A:1147:SER:O	1:A:1154:ALA:HB2	2.16	0.46
2:B:194:LEU:HD21	2:B:448:LEU:HD23	1.98	0.46
2:B:975:ARG:HB3	2:B:977:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:119:DT:H2''	14:N:120:DC:C5	2.51	0.46
2:B:191:GLU:CD	2:B:743:ARG:HH12	2.23	0.45
2:B:715:ASP:N	2:B:715:ASP:OD1	2.49	0.45
4:D:30:GLU:OE2	7:G:4:HIS:ND1	2.47	0.45
14:N:120:DC:H2''	14:N:121:DC:C5	2.51	0.45
15:O:163:PRO:HA	15:O:262:CYS:HB3	1.98	0.45
1:A:239:GLU:HG3	1:A:241:ARG:HG2	1.98	0.45
1:A:937:ASP:OD1	1:A:937:ASP:N	2.50	0.45
1:A:1163:HIS:HB2	1:A:1301:ILE:O	2.17	0.45
2:B:623:ARG:NH1	2:B:697:GLU:OE2	2.29	0.45
6:F:84:GLU:N	6:F:84:GLU:OE1	2.49	0.45
10:J:40:LEU:HD22	10:J:45:CYS:HB3	1.99	0.45
14:N:36:DT:H2'	14:N:37:DC:C6	2.50	0.45
14:N:109:DG:H2''	14:N:110:DT:C6	2.51	0.45
13:M:131:PRO:HD2	13:M:134:ILE:HD12	1.99	0.45
14:N:131:DT:H2''	14:N:132:DA:C8	2.50	0.45
14:N:152:DC:H2''	14:N:153:DC:C5	2.51	0.45
18:T:-164:DC:H2''	18:T:-163:DC:C5	2.51	0.45
21:a:114:HIS:NE2	21:e:124:ASP:OD1	2.46	0.45
8:H:14:ASP:HB2	8:H:29:HIS:HB2	1.99	0.45
15:O:305:PHE:CZ	18:T:-2:DT:H1'	2.52	0.45
1:A:369:PRO:HB3	1:A:496:PHE:CE2	2.52	0.45
1:A:904:GLN:NE2	1:A:981:CYS:O	2.43	0.45
5:E:52:ARG:HD3	5:E:53:PRO:HD3	1.98	0.45
8:H:37:MET:SD	8:H:127:GLY:HA3	2.56	0.45
19:U:366:ILE:HD11	20:V:48:LEU:HG	1.99	0.45
3:C:99:VAL:HG21	3:C:127:VAL:HG21	1.99	0.45
5:E:73:PHE:CE2	5:E:99:ILE:HG13	2.52	0.45
10:J:14:VAL:HB	10:J:49:LEU:HD11	1.98	0.45
15:O:250:PHE:HB2	19:U:314:LEU:HD21	1.99	0.45
23:g:33:ARG:NH1	24:h:36:GLU:OE1	2.48	0.45
24:h:60:MET:HE3	24:h:60:MET:O	2.16	0.45
1:A:1287:CYS:HB3	2:B:247:ALA:HB1	1.98	0.45
2:B:601:VAL:HG22	2:B:616:THR:HG23	1.99	0.45
2:B:1109:GLU:OE1	2:B:1150:ARG:NH1	2.50	0.45
20:V:64:THR:HB	20:V:75:VAL:HB	1.98	0.45
21:e:80:LYS:HB3	21:e:83:LEU:HD11	1.99	0.44
1:A:67:ARG:NH2	13:M:46:ILE:O	2.50	0.44
9:I:20:CYS:SG	9:I:22:ASN:ND2	2.89	0.44
16:Q:173:HIS:O	16:Q:176:ILE:HG22	2.17	0.44
2:B:1035:ARG:NH2	2:B:1036:LYS:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:44:PHE:CB	5:E:52:ARG:HG3	2.48	0.44
16:Q:14:TYR:HB2	16:Q:135:PHE:CD2	2.52	0.44
17:R:228:ILE:HG23	17:R:230:LYS:O	2.17	0.44
1:A:395:THR:CG2	1:A:396:PRO:HD2	2.47	0.44
14:N:171:DT:H2''	14:N:172:DC:C5	2.51	0.44
15:O:239:ARG:HH21	15:O:239:ARG:HG3	1.83	0.44
1:A:194:SER:HB2	1:A:199:TYR:CE2	2.52	0.44
1:A:264:VAL:O	1:A:272:ASN:N	2.48	0.44
1:A:1143:LEU:HD13	1:A:1147:SER:HB2	1.99	0.44
2:B:109:MET:HE2	2:B:174:LEU:HD22	1.99	0.44
2:B:100:GLU:OE1	12:L:42:ARG:NH1	2.48	0.44
3:C:149:LEU:HD23	10:J:3:ILE:HG22	1.98	0.44
1:A:1211:LEU:HD11	1:A:1258:ARG:HB3	2.00	0.44
2:B:285:LEU:HD11	2:B:305:LEU:HD11	2.00	0.44
2:B:1112:ASP:OD1	2:B:1112:ASP:N	2.49	0.44
23:g:89:ARG:HB2	23:g:109:LEU:HD21	1.99	0.44
9:I:15:ARG:HB3	9:I:24:LEU:HD12	2.00	0.44
19:U:349:TRP:CG	20:V:62:LEU:HD13	2.52	0.44
2:B:385:ARG:O	2:B:391:LYS:HE3	2.18	0.43
14:N:185:DC:N4	18:T:-186:DG:O6	2.51	0.43
2:B:962:THR:O	10:J:9:THR:HG23	2.18	0.43
3:C:114:HIS:CD2	3:C:152:LYS:HE2	2.52	0.43
18:T:-133:DT:H2''	18:T:-132:DT:C5	2.53	0.43
19:U:372:GLY:HA3	20:V:58:PHE:CZ	2.53	0.43
1:A:1139:LEU:HD21	1:A:1343:LEU:HA	2.00	0.43
1:A:1139:LEU:HD13	1:A:1341:VAL:HA	2.00	0.43
3:C:9:VAL:HG11	11:K:105:PHE:CD2	2.53	0.43
4:D:102:ASN:HD22	7:G:1:MET:HE1	1.83	0.43
14:N:36:DT:H2'	14:N:37:DC:C5	2.53	0.43
14:N:121:DC:H2''	14:N:122:DC:C5	2.53	0.43
2:B:455:ASP:OD2	2:B:457:LYS:NZ	2.33	0.43
10:J:8:PHE:CD2	10:J:48:MET:HE1	2.53	0.43
16:Q:124:TYR:OH	17:R:22:LYS:HE2	2.18	0.43
18:T:-173:DT:H2''	18:T:-172:DG:C5	2.52	0.43
1:A:1147:SER:HB2	1:A:1154:ALA:HA	2.00	0.43
2:B:829:PHE:HE1	2:B:869:LYS:HD3	1.82	0.43
8:H:103:GLU:H	8:H:103:GLU:HG3	1.67	0.43
18:T:-77:DA:H5'	23:c:43:ARG:HG2	2.00	0.43
22:b:66:VAL:HA	22:b:94:GLN:HE22	1.84	0.43
2:B:789:ASN:O	2:B:968:ASN:HB2	2.19	0.43
2:B:812:ARG:CZ	2:B:897:ARG:HH12	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:72:PRO:HD3	10:J:13:ILE:HD11	2.01	0.43
3:C:150:ILE:HG22	3:C:151:VAL:N	2.30	0.43
14:N:35:DC:H2'	14:N:36:DT:C6	2.53	0.43
23:c:25:GLN:N	23:c:57:GLU:OE1	2.50	0.43
22:f:85:MET:HE1	22:f:103:GLY:HA3	2.01	0.43
1:A:653:VAL:HG11	1:A:669:TYR:OH	2.18	0.43
2:B:271:ILE:HD12	2:B:311:ILE:HD12	2.00	0.43
14:N:59:DC:H2''	14:N:60:DC:C6	2.53	0.43
14:N:103:DA:H3'	22:b:31:THR:HB	1.99	0.43
18:T:-186:DG:H2''	18:T:-185:DG:C8	2.54	0.43
1:A:279:LYS:HA	1:A:279:LYS:HE2	2.01	0.43
1:A:535:MET:O	1:A:669:TYR:OH	2.23	0.43
1:A:668:PHE:CZ	1:A:672:ILE:HD11	2.54	0.43
2:B:214:LYS:HE2	2:B:215:TYR:CE1	2.53	0.43
12:L:36:CYS:HB2	12:L:44:MET:HE1	2.00	0.43
18:T:-20:DC:H2'	18:T:-19:DG:O4'	2.19	0.43
1:A:334:ARG:NH2	1:A:335:PRO:O	2.52	0.43
2:B:187:ILE:HG21	2:B:449:ALA:HB2	2.00	0.43
2:B:388:TYR:CE1	2:B:505:LEU:HD21	2.54	0.43
4:D:87:LEU:HD22	4:D:97:LEU:HD22	2.01	0.43
3:C:263:LEU:HD22	11:K:87:PHE:HD2	1.84	0.43
5:E:30:GLN:HE21	5:E:34:ASP:CG	2.27	0.43
2:B:355:ASP:N	2:B:355:ASP:OD1	2.51	0.42
2:B:505:LEU:HD22	2:B:509:VAL:HB	2.02	0.42
3:C:114:HIS:NE2	3:C:152:LYS:HE2	2.34	0.42
8:H:96:VAL:HG22	8:H:116:VAL:HG22	2.00	0.42
9:I:65:LEU:O	9:I:122:ARG:NE	2.46	0.42
15:O:297:LYS:CB	15:O:298:PRO:HD3	2.49	0.42
21:a:66:LEU:HB3	21:a:67:PRO:HD3	2.00	0.42
2:B:27:TRP:HZ2	2:B:1000:THR:HG21	1.84	0.42
2:B:907:VAL:HG22	2:B:921:ILE:HG12	2.01	0.42
14:N:1:DT:O2	18:T:0:DG:N2	2.52	0.42
14:N:69:DT:H2''	14:N:70:DC:C5	2.55	0.42
18:T:-134:DG:H2''	18:T:-133:DT:C5	2.54	0.42
1:A:194:SER:HB2	1:A:199:TYR:HE2	1.84	0.42
2:B:455:ASP:OD2	2:B:457:LYS:HG2	2.19	0.42
17:R:43:LEU:HD12	17:R:55:SER:O	2.20	0.42
2:B:1069:ILE:HG23	13:M:47:ASP:HB2	2.02	0.42
5:E:104:ILE:O	5:E:129:GLN:HA	2.20	0.42
17:R:58:LEU:HD11	17:R:62:LEU:HD23	2.01	0.42
18:T:-62:DT:H2''	18:T:-61:DC:C4	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:f:22:VAL:HG13	22:f:23:LEU:N	2.34	0.42
14:N:100:DT:H2''	14:N:101:DA:C8	2.55	0.42
1:A:481:THR:O	1:A:483:ARG:NH2	2.53	0.42
2:B:971:ALA:O	2:B:975:ARG:HD3	2.20	0.42
8:H:97:TYR:CZ	8:H:115:TYR:HB3	2.54	0.42
16:Q:111:LYS:O	16:Q:146:PHE:HA	2.20	0.42
1:A:548:PHE:CE1	1:A:555:LEU:HD11	2.54	0.42
1:A:988:TRP:HE1	1:A:992:LYS:HE3	1.84	0.42
5:E:74:VAL:HA	5:E:103:LEU:O	2.19	0.42
14:N:186:DC:H2''	14:N:187:DG:C8	2.55	0.42
18:T:-162:DT:H2''	18:T:-161:DG:C8	2.55	0.42
1:A:548:PHE:HE1	1:A:555:LEU:HD11	1.85	0.41
2:B:203:ASN:O	2:B:571:GLY:HA3	2.20	0.41
2:B:780:VAL:HG21	2:B:1048:TYR:CE1	2.55	0.41
2:B:815:LYS:HB2	2:B:918:PHE:CZ	2.55	0.41
5:E:2:ASP:O	5:E:6:GLU:HG2	2.20	0.41
14:N:163:DG:C5	14:N:164:DG:C6	3.08	0.41
9:I:91:HIS:HE1	9:I:93:GLU:HB3	1.85	0.41
1:A:544:ALA:HB2	1:A:680:LEU:HD13	2.01	0.41
1:A:1212:LEU:HD23	1:A:1259:ILE:HD12	2.01	0.41
2:B:529:MET:HE1	2:B:698:ILE:HD12	2.02	0.41
3:C:60:HIS:CE1	3:C:63:PHE:HB2	2.55	0.41
8:H:88:PHE:CG	8:H:144:LEU:HB3	2.55	0.41
16:Q:35:ASP:O	16:Q:108:ARG:NH1	2.46	0.41
18:T:-102:DT:H2''	18:T:-101:DT:C5	2.55	0.41
1:A:618:TYR:HB3	1:A:621:ILE:O	2.21	0.41
1:A:628:VAL:HA	1:A:638:GLY:HA3	2.03	0.41
2:B:786:THR:HG23	2:B:788:TYR:HD1	1.85	0.41
17:R:174:LYS:HB2	17:R:174:LYS:HE3	1.91	0.41
1:A:71:CYS:SG	1:A:74:CYS:HB2	2.60	0.41
9:I:91:HIS:CE1	9:I:93:GLU:HB3	2.55	0.41
11:K:81:TYR:CE2	11:K:86:ALA:HB2	2.55	0.41
16:Q:26:TYR:C	16:Q:27:ASN:HD22	2.29	0.41
17:R:23:VAL:HA	17:R:116:CYS:HB3	2.02	0.41
18:T:-181:DT:H2''	18:T:-180:DA:C8	2.56	0.41
1:A:774:ALA:O	1:A:775:LYS:HE2	2.21	0.41
2:B:1108:PHE:CE1	2:B:1113:PRO:HA	2.55	0.41
3:C:60:HIS:CD2	3:C:62:GLU:HG2	2.56	0.41
4:D:131:LEU:O	4:D:135:GLN:HG2	2.20	0.41
1:A:22:GLN:NE2	1:A:1446:GLY:O	2.53	0.41
2:B:759:VAL:HG12	2:B:999:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:-9:DG:N1	18:T:9:DC:O2	2.50	0.41
14:N:81:DA:H4'	14:N:82:DG:OP1	2.21	0.41
14:N:154:DT:H2''	14:N:155:DA:C8	2.56	0.41
3:C:70:LEU:O	10:J:6:ARG:NE	2.51	0.41
4:D:111:SER:OG	4:D:127:LEU:HD21	2.21	0.41
7:G:39:THR:HG23	7:G:42:TYR:H	1.86	0.41
14:N:164:DG:H2''	14:N:165:DC:C6	2.56	0.41
16:Q:18:VAL:O	17:R:35:SER:OG	2.28	0.41
18:T:-174:DC:H2''	18:T:-173:DT:C6	2.56	0.41
1:A:805:ARG:NH1	2:B:671:GLU:O	2.53	0.41
1:A:876:ASP:OD2	1:A:880:ARG:NH1	2.50	0.41
1:A:1216:LEU:HD11	1:A:1228:MET:HE1	2.03	0.41
1:A:1464:ALA:O	1:A:1469:GLY:HA3	2.21	0.41
2:B:110:PRO:HB3	2:B:156:LEU:HD21	2.02	0.41
2:B:737:ILE:HD12	2:B:737:ILE:HA	1.94	0.41
2:B:849:ASP:HB3	12:L:15:MET:HE1	2.02	0.41
13:M:15:CYS:HB3	13:M:18:HIS:O	2.20	0.41
18:T:-112:DG:H2''	18:T:-111:DT:C6	2.56	0.41
1:A:485:ASN:O	1:A:488:VAL:HG22	2.21	0.41
1:A:653:VAL:HG11	1:A:669:TYR:CZ	2.55	0.41
1:A:804:HIS:CE1	9:I:100:HIS:CD2	3.08	0.41
1:A:122:ASN:O	1:A:127:LYS:NZ	2.48	0.40
1:A:261:ARG:HD2	1:A:261:ARG:O	2.20	0.40
1:A:1030:SER:OG	5:E:162:ARG:NE	2.54	0.40
2:B:388:TYR:CE2	2:B:505:LEU:HD21	2.56	0.40
2:B:1066:PRO:HG2	2:B:1077:GLY:HA3	2.03	0.40
1:A:1304:ILE:HG23	1:A:1338:THR:HB	2.03	0.40
3:C:106:ARG:NH2	3:C:158:GLU:OE1	2.53	0.40
7:G:38:CYS:HB2	7:G:44:PHE:CD2	2.56	0.40
21:a:55:TYR:CZ	22:b:37:ARG:HG2	2.55	0.40
1:A:365:THR:HG22	1:A:482:PHE:CE2	2.56	0.40
1:A:892:GLY:C	1:A:894:ASP:H	2.28	0.40
11:K:63:VAL:HG12	11:K:71:ILE:HG22	2.04	0.40
18:T:-89:DG:H3'	22:b:80:LYS:HE2	2.03	0.40
1:A:775:LYS:HG3	2:B:974:SER:HB3	2.04	0.40
2:B:565:THR:HG21	2:B:580:PRO:HG3	2.03	0.40
2:B:924:ARG:HE	3:C:62:GLU:CD	2.29	0.40
15:O:288:PHE:CD1	15:O:289:PRO:HD2	2.56	0.40
19:U:374:ALA:HA	20:V:60:GLY:O	2.22	0.40
3:C:69:GLY:HA3	12:L:57:ALA:HB1	2.04	0.40
14:N:142:DG:H2''	14:N:143:DG:C8	2.57	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	1413/1970 (72%)	1381 (98%)	32 (2%)	0	100	100
2	B	1130/1174 (96%)	1102 (98%)	28 (2%)	0	100	100
3	C	253/275 (92%)	249 (98%)	4 (2%)	0	100	100
4	D	126/142 (89%)	126 (100%)	0	0	100	100
5	E	207/210 (99%)	206 (100%)	1 (0%)	0	100	100
6	F	85/127 (67%)	85 (100%)	0	0	100	100
7	G	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
8	H	146/150 (97%)	142 (97%)	4 (3%)	0	100	100
9	I	112/125 (90%)	107 (96%)	5 (4%)	0	100	100
10	J	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
11	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
12	L	42/58 (72%)	41 (98%)	1 (2%)	0	100	100
13	M	248/316 (78%)	243 (98%)	5 (2%)	0	100	100
15	O	177/339 (52%)	176 (99%)	1 (1%)	0	100	100
16	Q	134/517 (26%)	129 (96%)	5 (4%)	0	100	100
17	R	218/249 (88%)	216 (99%)	2 (1%)	0	100	100
19	U	109/376 (29%)	108 (99%)	1 (1%)	0	100	100
20	V	97/109 (89%)	95 (98%)	2 (2%)	0	100	100
21	a	95/136 (70%)	95 (100%)	0	0	100	100
21	e	96/136 (71%)	96 (100%)	0	0	100	100
22	b	80/103 (78%)	80 (100%)	0	0	100	100
22	f	80/103 (78%)	80 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	c	107/130 (82%)	107 (100%)	0	0	100	100
23	g	104/130 (80%)	103 (99%)	1 (1%)	0	100	100
24	d	95/126 (75%)	95 (100%)	0	0	100	100
24	h	93/126 (74%)	93 (100%)	0	0	100	100
All	All	5591/7483 (75%)	5490 (98%)	101 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	1254/1749 (72%)	1254 (100%)	0	100	100
2	B	994/1027 (97%)	994 (100%)	0	100	100
3	C	234/252 (93%)	234 (100%)	0	100	100
4	D	118/126 (94%)	118 (100%)	0	100	100
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	69/111 (62%)	69 (100%)	0	100	100
7	G	152/153 (99%)	152 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	103/112 (92%)	103 (100%)	0	100	100
10	J	53/56 (95%)	53 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	41/55 (74%)	41 (100%)	0	100	100
13	M	215/268 (80%)	215 (100%)	0	100	100
15	O	154/293 (53%)	154 (100%)	0	100	100
16	Q	121/448 (27%)	121 (100%)	0	100	100
17	R	196/218 (90%)	196 (100%)	0	100	100
19	U	105/324 (32%)	105 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	V	90/98 (92%)	90 (100%)	0	100	100
21	a	85/111 (77%)	85 (100%)	0	100	100
21	e	86/111 (78%)	86 (100%)	0	100	100
22	b	67/79 (85%)	67 (100%)	0	100	100
22	f	67/79 (85%)	67 (100%)	0	100	100
23	c	86/101 (85%)	86 (100%)	0	100	100
23	g	84/101 (83%)	84 (100%)	0	100	100
24	d	83/106 (78%)	83 (100%)	0	100	100
24	h	81/106 (76%)	81 (100%)	0	100	100
All	All	4962/6513 (76%)	4962 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	96	HIS
1	A	516	GLN
1	A	531	ASN
1	A	599	HIS
1	A	620	HIS
1	A	700	GLN
1	A	723	ASN
1	A	757	GLN
1	A	765	ASN
1	A	783	GLN
1	A	792	ASN
1	A	861	GLN
1	A	905	ASN
1	A	1394	ASN
2	B	117	ASN
2	B	145	GLN
2	B	197	GLN
2	B	312	GLN
2	B	486	ASN
2	B	755	GLN
2	B	1030	ASN
4	D	38	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	76	ASN
4	D	102	ASN
5	E	133	GLN
7	G	21	ASN
8	H	133	HIS
9	I	87	GLN
9	I	121	HIS
11	K	29	ASN
11	K	69	HIS
15	O	229	GLN
15	O	278	GLN
16	Q	10	ASN
16	Q	27	ASN
16	Q	53	ASN
16	Q	121	ASN
17	R	64	ASN
17	R	131	GLN
17	R	152	ASN
20	V	27	GLN
21	a	109	ASN
23	c	25	GLN
24	d	48	GLN
24	d	50	HIS
24	d	68	ASN
24	d	96	GLN
21	e	109	ASN
23	g	25	GLN
24	h	85	ASN
24	h	96	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

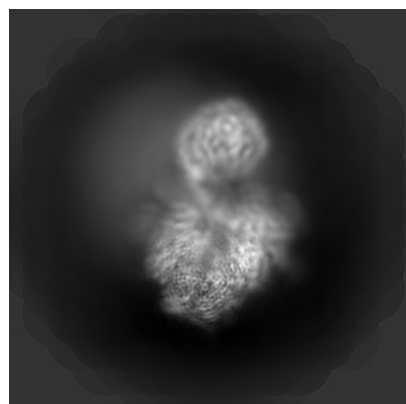
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16335. These allow visual inspection of the internal detail of the map and identification of artifacts.

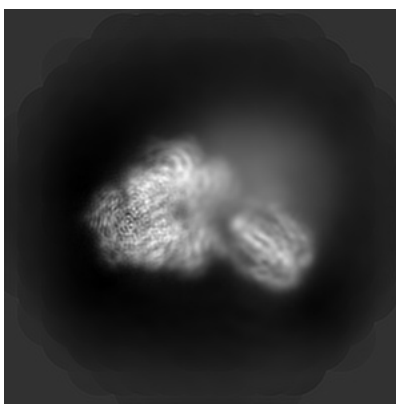
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

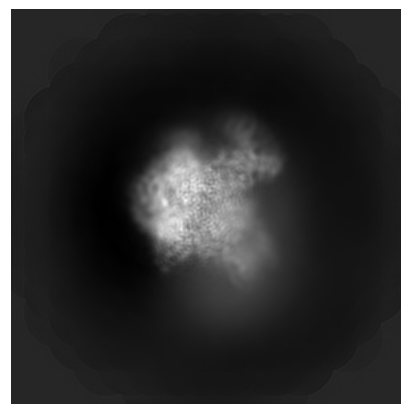
6.1.1 Primary map



X

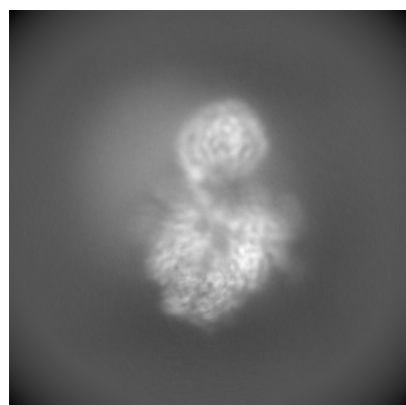


Y

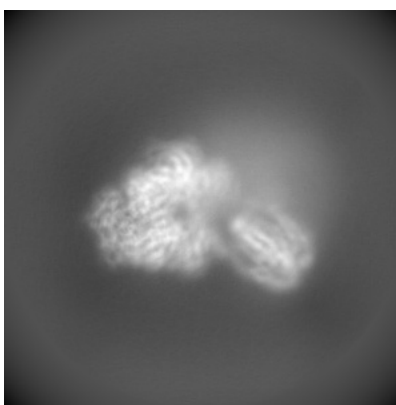


Z

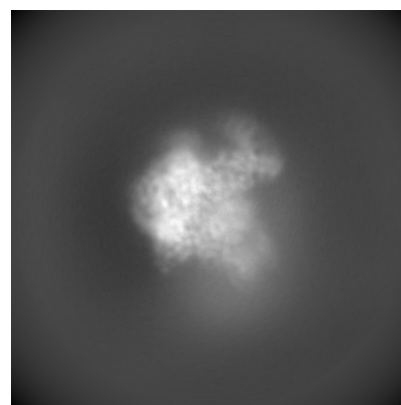
6.1.2 Raw map



X



Y

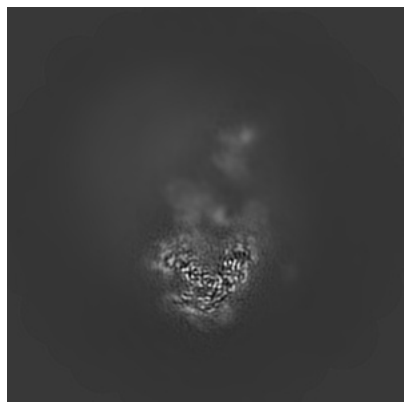


Z

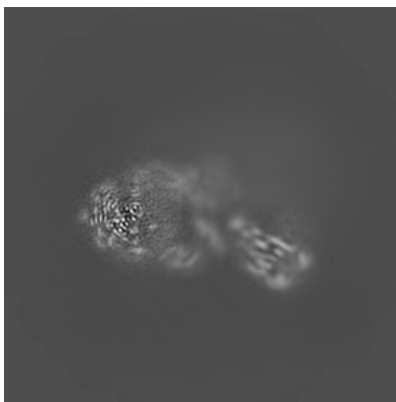
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

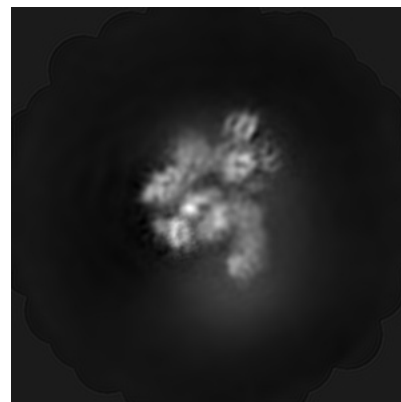
6.2.1 Primary map



X Index: 200

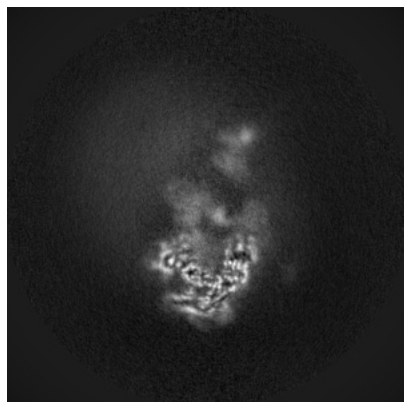


Y Index: 200

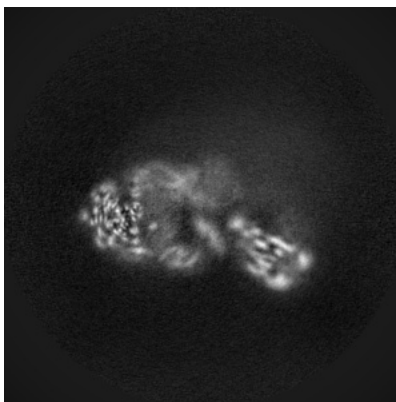


Z Index: 200

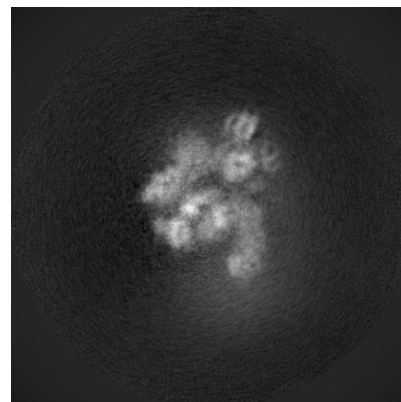
6.2.2 Raw map



X Index: 200



Y Index: 200

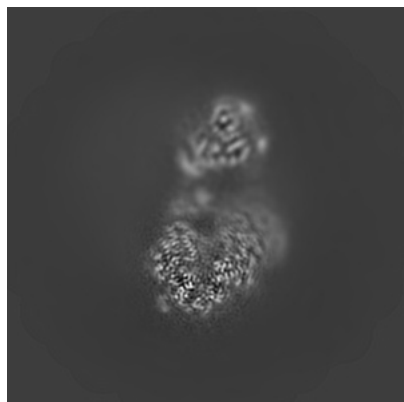


Z Index: 200

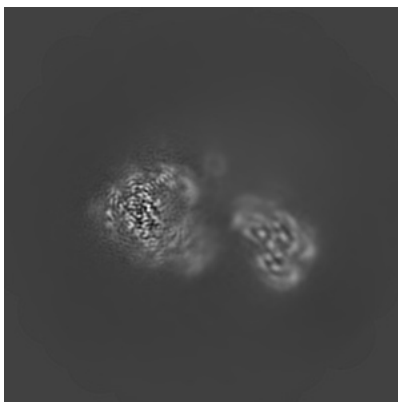
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

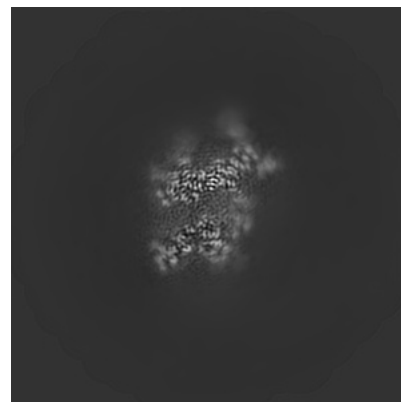
6.3.1 Primary map



X Index: 171

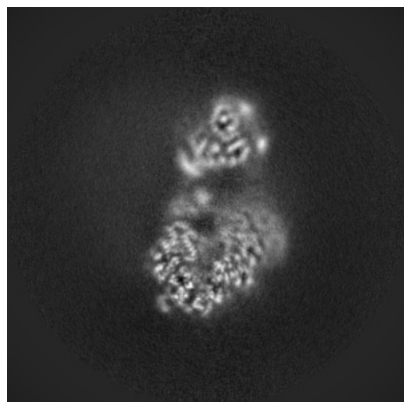


Y Index: 223

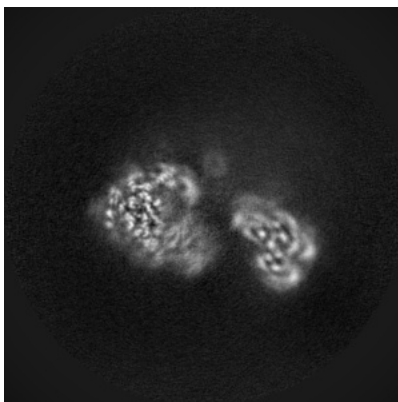


Z Index: 143

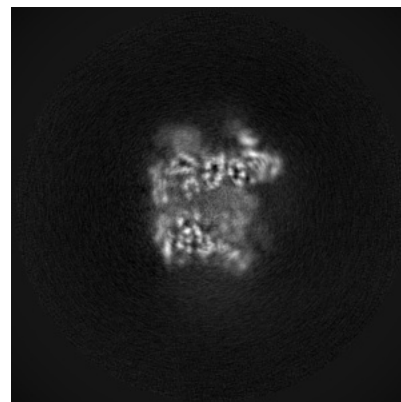
6.3.2 Raw map



X Index: 171



Y Index: 223

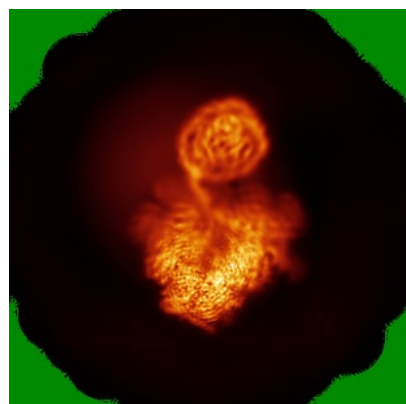


Z Index: 155

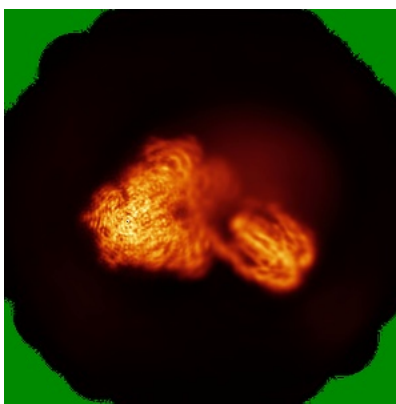
The images above show the largest variance slices of the map in three orthogonal directions.

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

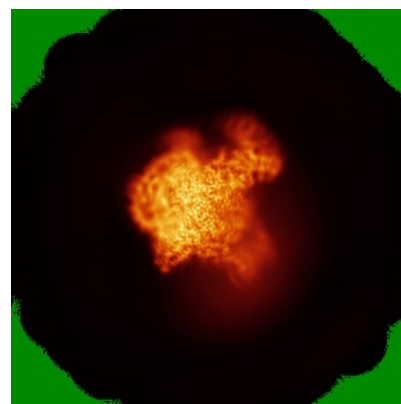
6.4.1 Primary map



X

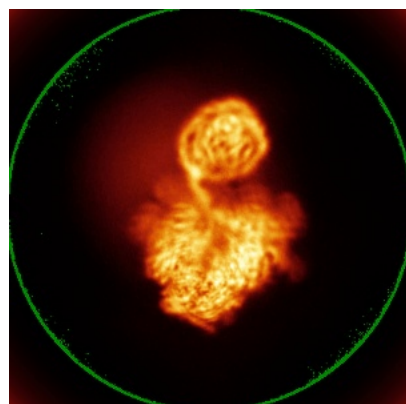


Y

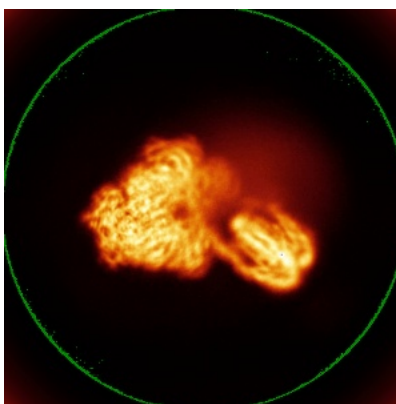


Z

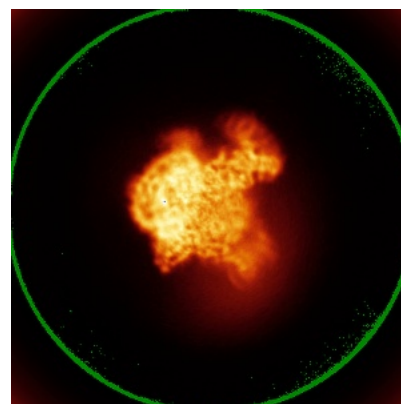
6.4.2 Raw map



X



Y

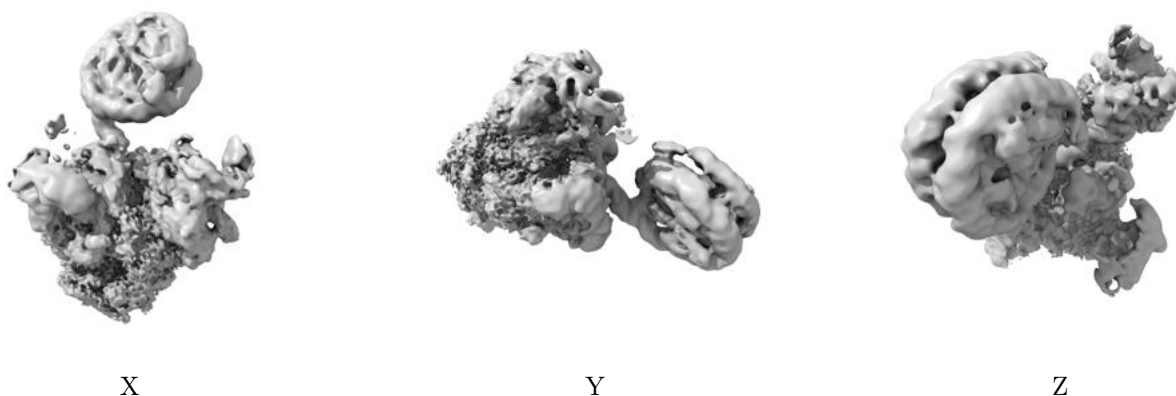


Z

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 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

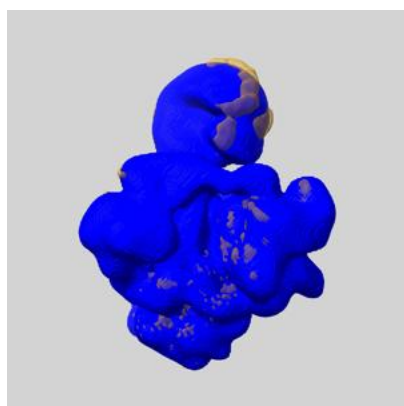
6.6 Mask visualisation [i](#)

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

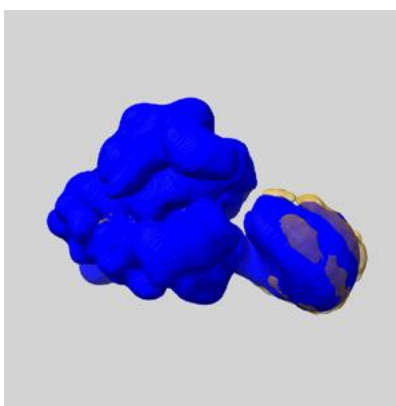
A mask typically either:

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

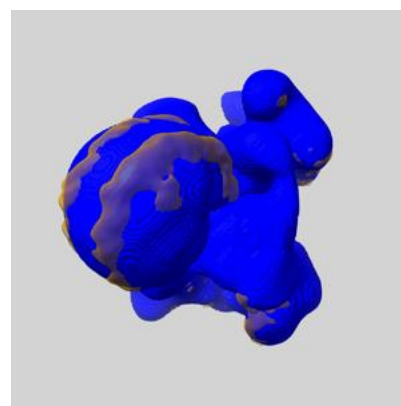
6.6.1 emd_16335_msk_1.map [i](#)



X



Y

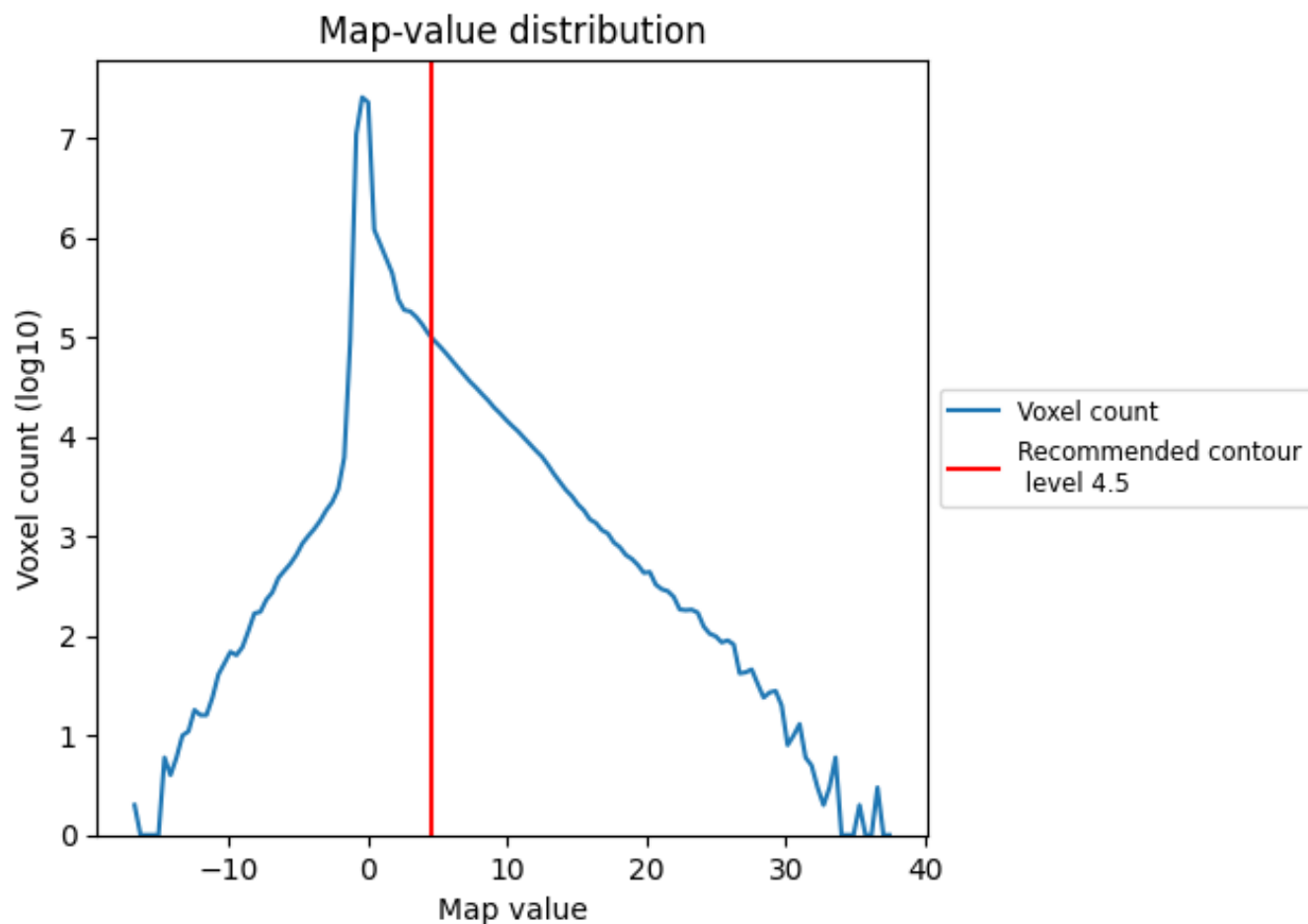


Z

7 Map analysis [i](#)

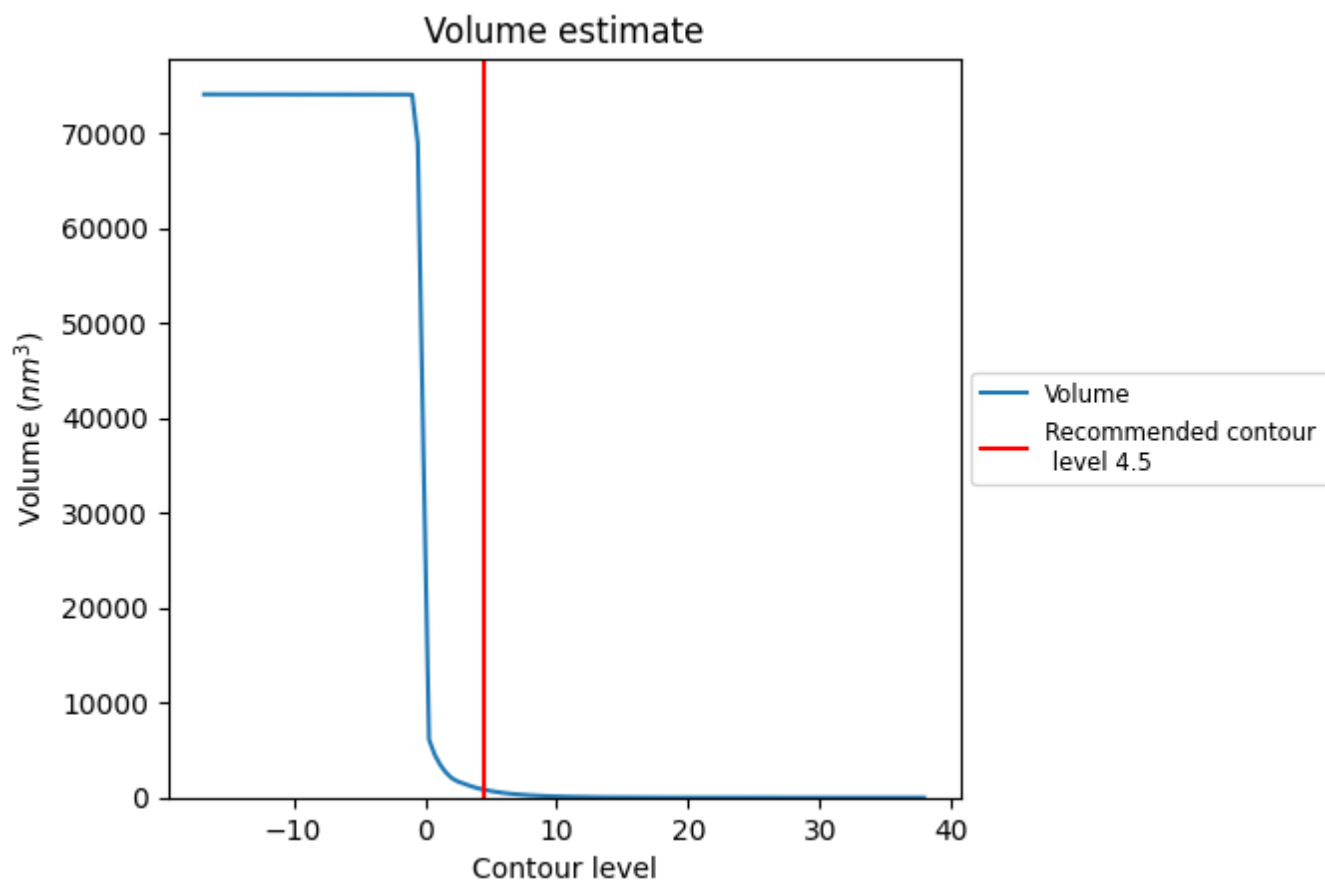
This section contains the results of statistical analysis of the map.

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.

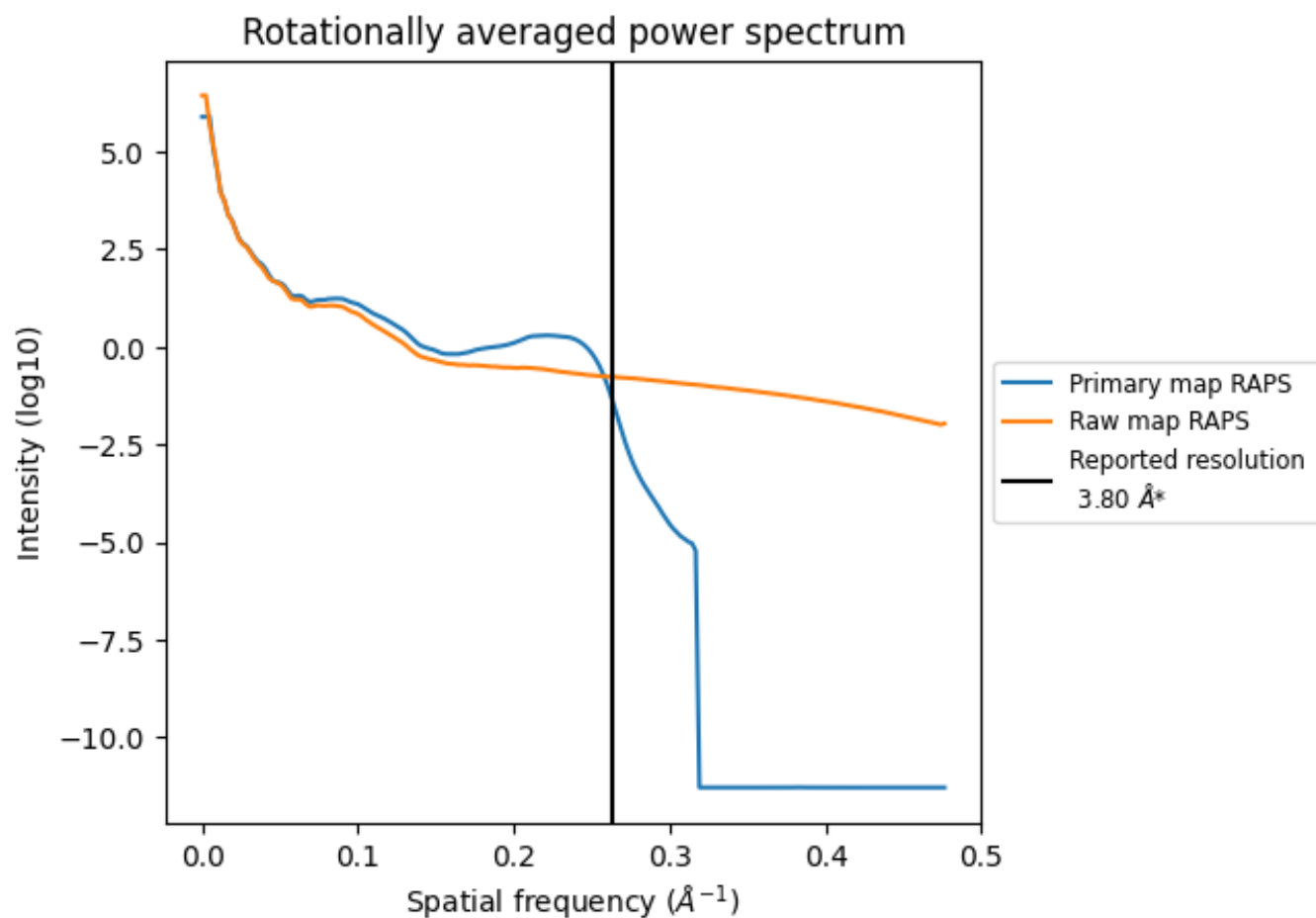
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 822 nm^3 ; this corresponds to an approximate mass of 742 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 ⓘ

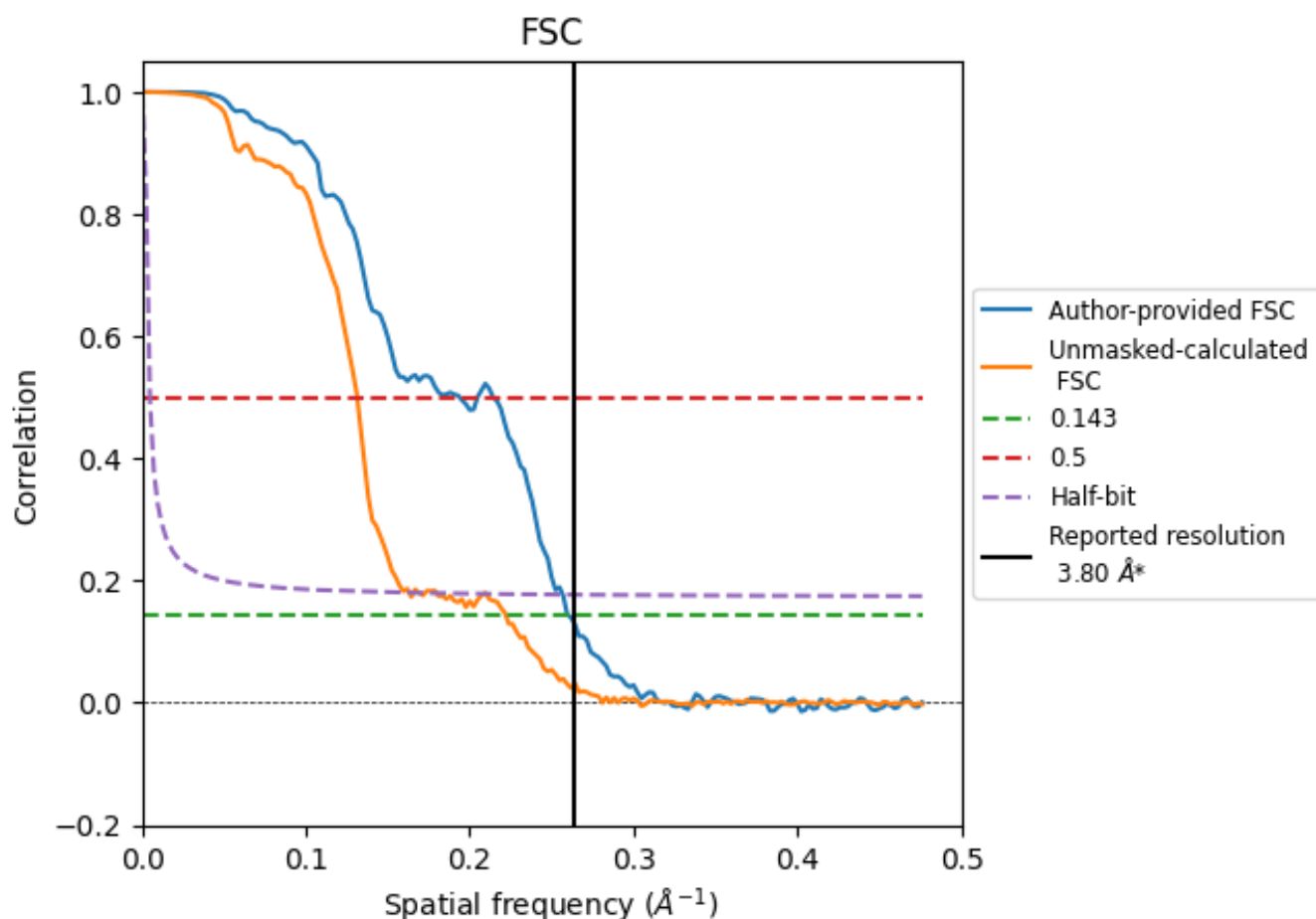


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.84	5.16	3.89
Unmasked-calculated*	4.50	7.62	6.13

*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 4.50 differs from the reported value 3.8 by more than 10 %

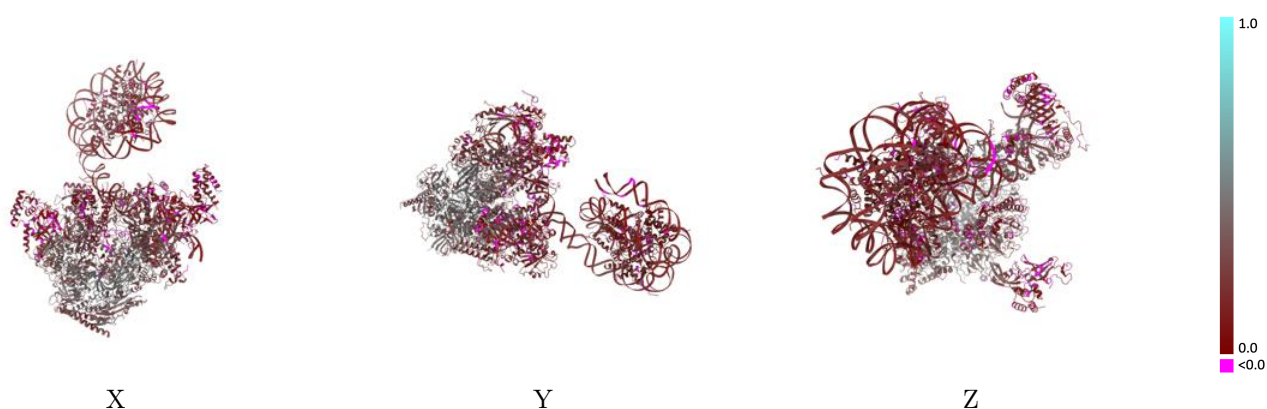
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16335 and PDB model 8BZ1. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

This section was not generated.

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

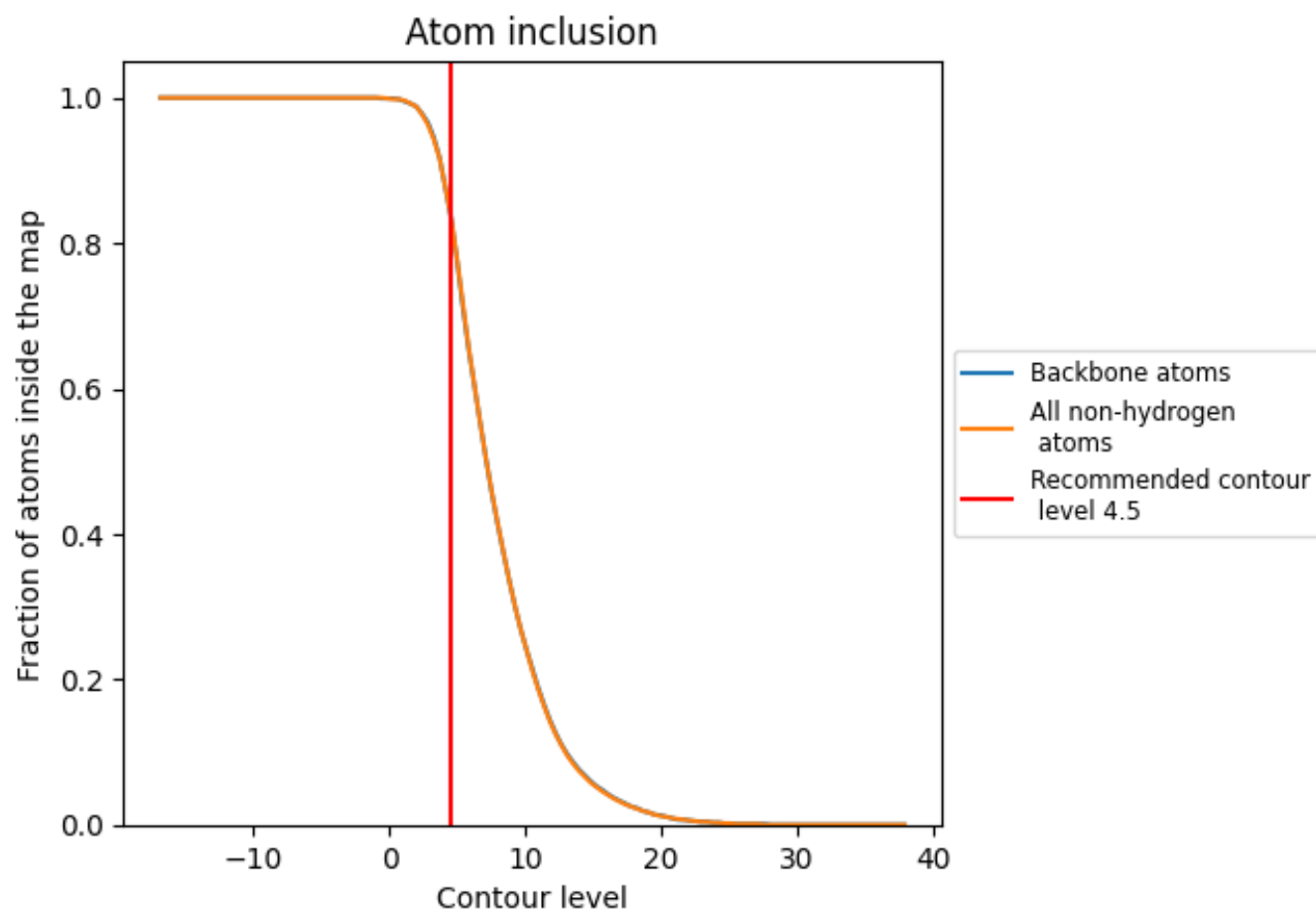


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 84% 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 (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8430	 0.2440
A	 0.8540	 0.2820
B	 0.9030	 0.3450
C	 0.8880	 0.3690
D	 0.7640	 0.1140
E	 0.8830	 0.2300
F	 0.8630	 0.3290
G	 0.8410	 0.1500
H	 0.8770	 0.3640
I	 0.8240	 0.2160
J	 0.9310	 0.3980
K	 0.8520	 0.3460
L	 0.9270	 0.3410
M	 0.8720	 0.2850
N	 0.8920	 0.1640
O	 0.8840	 0.1880
Q	 0.6970	 0.1260
R	 0.6630	 0.1410
T	 0.9050	 0.1720
U	 0.4360	 0.1070
V	 0.4570	 0.1070
a	 0.8330	 0.1350
b	 0.8170	 0.1500
c	 0.8440	 0.1670
d	 0.8940	 0.1750
e	 0.8690	 0.1440
f	 0.8310	 0.1550
g	 0.8320	 0.1560
h	 0.9090	 0.1690

