



Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 02:17 am GMT

PDB ID : 6RFL
EMDB ID : EMD-4868
Title : Structure of the complete Vaccinia DNA-dependent RNA polymerase complex
Authors : Grimm, C.; Hillen, S.H.; Bedenk, K.; Bartuli, J.; Neyer, S.; Zhang, Q.; Huettenhofer, A.; Erlacher, M.; Dienemann, C.; Schlosser, A.; Urlaub, H.; Boettcher, B.; Szalay, A.A.; Cramer, P.; Fischer, U.
Deposited on : 2019-04-15
Resolution : 2.76 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:

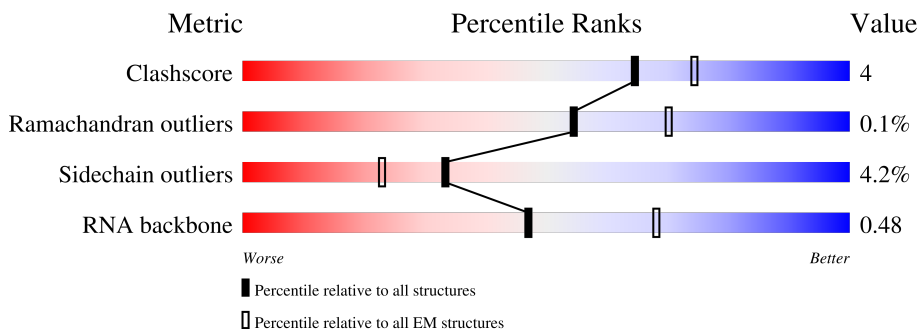
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 2.76 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
RNA backbone	4643	859

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	B	1164	
2	E	185	
3	F	164	
4	G	161	
5	I	795	
6	J	63	
7	L	287	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	O	844	<p>11% 85% 12% ..</p>
9	Q	129	<p>5% 79% 15% . .</p>
9	R	129	<p>5% 88% 10% .</p>
10	K	710	<p>11% . 87%</p>
11	U	72	<p>64% 22% . 12%</p>
12	A	1286	<p>. 83% 15% ..</p>
13	Y	631	<p>6% 81% 14% 5%</p>
14	C	305	<p>. 86% 14%</p>
15	S	259	<p>11% 54% 8% . 38%</p>

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 51788 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 DNA-dependent RNA polymerase subunit rpo132.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	1129	9091	5794	1554	1695	48	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	184	1495	966	248	276	5	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase 19 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	F	103	849	545	148	153	3	0	0

- Molecule 4 is a protein called DNA-dependent RNA polymerase subunit rpo18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	153	1192	753	198	235	6	0	0

- Molecule 5 is a protein called Putative H4L RNA polymerase-associated transcription factor RAP94.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I	773	6446	4210	1025	1190	21	0	0

- Molecule 6 is a protein called DNA-dependent RNA polymerase subunit rpo7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	J	61	490	310	88	88	4	0	0

- Molecule 7 is a protein called Small subunit of mRNA capping enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	L	284	Total	C	N	O	S	0	0
			2320	1492	385	430	13		

- Molecule 8 is a protein called Large subunit of mRNA capping enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	O	826	Total	C	N	O	S	0	0
			6693	4317	1099	1259	18		

- Molecule 9 is a protein called Virion core protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	R	129	Total	C	N	O	S	1	0
			1056	689	165	197	5		
9	Q	124	Total	C	N	O	S	0	0
			1013	660	158	190	5		

- Molecule 10 is a protein called Transcription factor VETF 82kDa large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K	91	Total	C	N	O	S	0	0
			749	476	131	133	9		

- Molecule 11 is a RNA chain called chr17.trna16-GlnTTG.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	U	63	Total	C	N	O	P	6	0
			1465	654	251	491	69		

- Molecule 12 is a protein called DNA-dependent RNA polymerase subunit rpo147.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	A	1272	Total	C	N	O	S	0	0
			10223	6578	1683	1917	45		

- Molecule 13 is a protein called Nucleoside triphosphate phosphohydrolase-I.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	Y	600	Total	C	N	O	S	0	0
			4845	3105	826	889	25		

- Molecule 14 is a protein called DNA-directed RNA polymerase 35 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	C	304	2484	1608	399	464	13	0	0

- Molecule 15 is a protein called DNA-directed RNA polymerase 30 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
15	S	161	1311	820	211	273	3	4	0	0

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
16	B	1	Total	Zn	0
			1	1	
16	I	1	Total	Zn	0
			1	1	
16	A	2	Total	Zn	0
			2	2	

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		AltConf
18	B	28	Total	O	0
			28	28	
18	E	2	Total	O	0
			2	2	
18	F	1	Total	O	0
			1	1	
18	G	2	Total	O	0
			2	2	
18	I	3	Total	O	0
			3	3	
18	J	3	Total	O	0
			3	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
18	K	1	Total 1	O 1	0
18	A	16	Total 16	O 16	0
18	Y	2	Total 2	O 2	0
18	C	3	Total 3	O 3	0

A184
ASP


- Molecule 3: DNA-directed RNA polymerase 19 kDa subunit

Chain F:  57% 6% 37%

MET	ALA	ASP	THR	ASP	ASP	ILE	ASP	ASP	TYR	GLU	SER	ASP	ASP	LEU	THR	THR	TYR	GLU	ASP	ASP	GLU	GLU	GLU	GLU	GLU	GLY	GLU	SER	SER	LEU	GLU	THR	SER	ASP	ILE	ASP	ASP	PRO	LYS	SER	SER	SER	TYR	LYS	LYS	ILE	VAL	GLU	SER	SER	ALA	SER	SER	THR	HIS	ILE	GLU	ASP	ALA	HIS	SER	SER	ASN	LEU	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----


HIS	I62	K70	R75	R76	I77	N112	H115	V116	I117	P127	K132	L136	Y164
-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------

- Molecule 4: DNA-dependent RNA polymerase subunit rpo18

Chain G:  83% 12% 5%

MET	S2	N7	V12	T20	E52	E55	L58	N64	I84	V85	R86	I91	N96	V97	T98	I99	C106	S109	H110	D111	F117	SER	ASP	SER	SER	LYS	TYR	C123	A130	V137	T138	E149	V159	ASP	SER
-----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	-----	-----

- Molecule 5: Putative H4L RNA polymerase-associated transcription factor RAP94

Chain I:  5% 85% 11% ..

MET	D2	K16	L20	D21	A22	N23	I24	S25	P26	K27	S34	K37	I42	S48	T49	I50	T51	E52	I55	R56	L57	N65	I66	D67	A68	D69	D70	Q71	K83	F84	E85	S97	F98	N99	D100	T104	D105	Y109	D113	R124	Q125	K126	K127	V136
-----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------

ARG	GLY	ASP	V140	K145	ASN	SER	ASP	LEU	VAL	SER	SER	PHE	ASN	ALA	GLU	LEU	GLU	P159	P173	R183	L220	K233	Y234	V235	M253	L256	S280	Y281	H282	L283	H284	S285	R293	F301	R317	D318	V319	R320	V321	C326	E327	E334	K337	V338
-----	-----	-----	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

G359	L375	D376	D379	N383	T384	V385	I386	V387	D626	S388	T389	E398	D418	N419	I420	T425	F439	Q448	E449	K452	E457	L462	E473	SER	GLN	VAL	SER	SER	F479	E480	L481	F482	V497	T522	S558	L564	E593	S594	R595	G596	E597	F746	V749	L599
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

P600	L604	V614	H621	T622	C623	V624	E625	D626	K627	I628	D651	E652	D653	I654	D662	T663	T666	K676	I679	E680	R681	K682	K683	L691	K698	R710	D713	P714	M715	P716	D723	H726	V727	K730	N735	R738	V747	F748	V749	N753
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

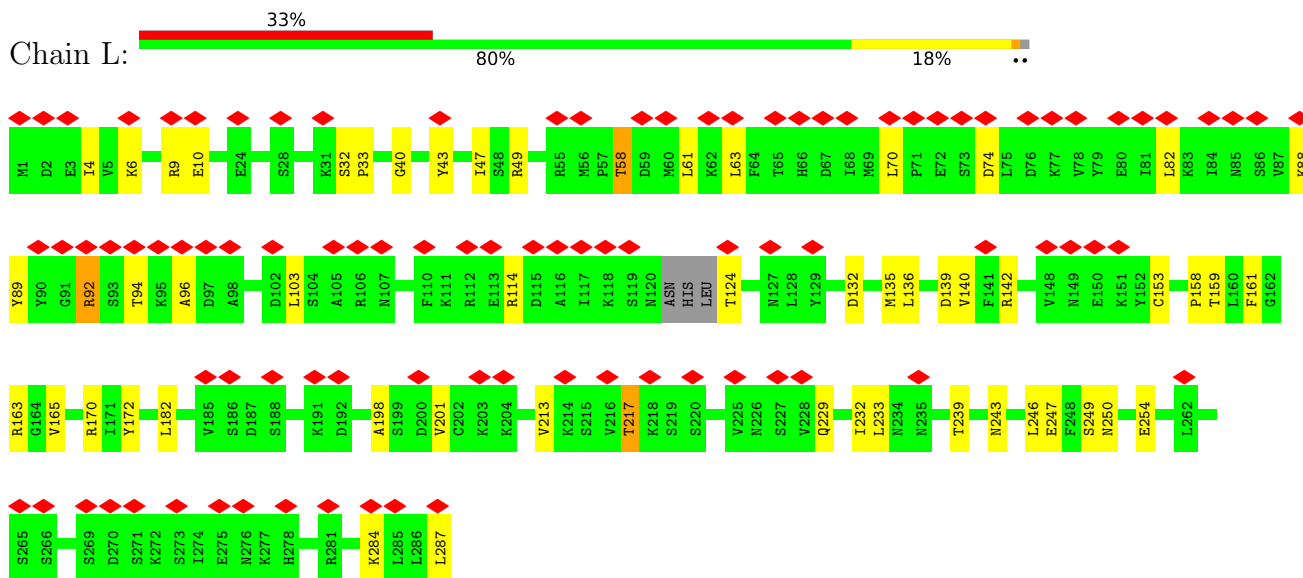
R757	L760	F793	N794	N795
------	------	------	------	------

- Molecule 6: DNA-dependent RNA polymerase subunit rpo7

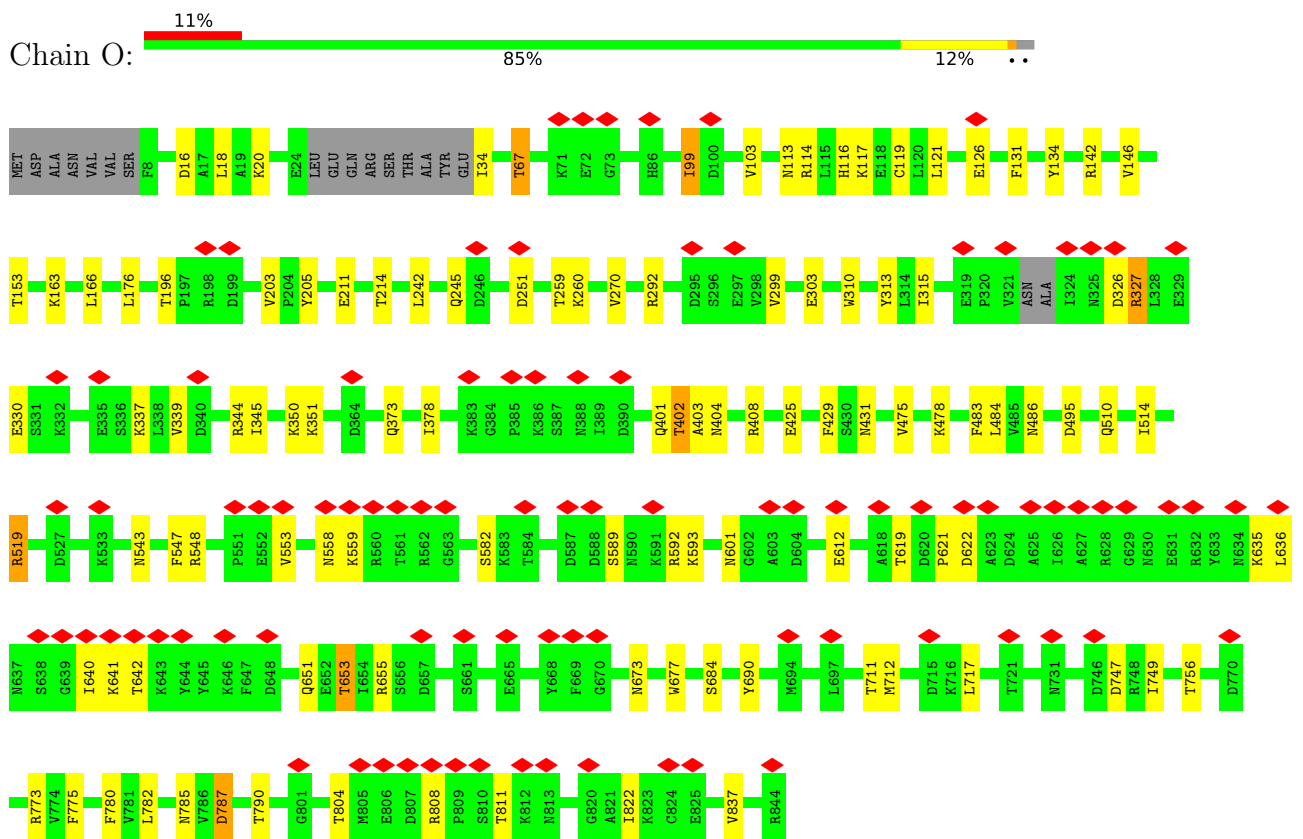
Chain J:  75% 22% .

MET	V2	F3	Q4	C10	R18	Y19	K20	L21	V31	L32	C39	C40	R41	Q47	N53	I62	ASN
-----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

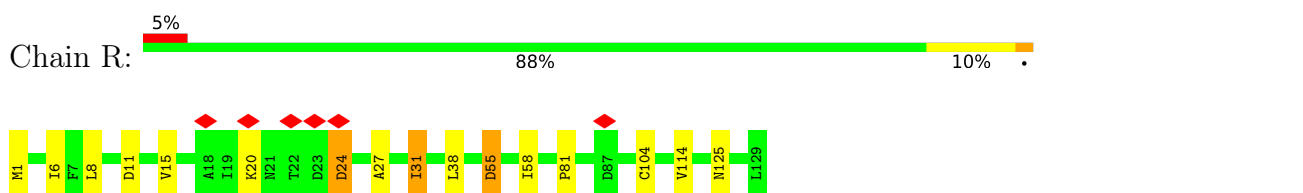
- Molecule 7: Small subunit of mRNA capping enzyme

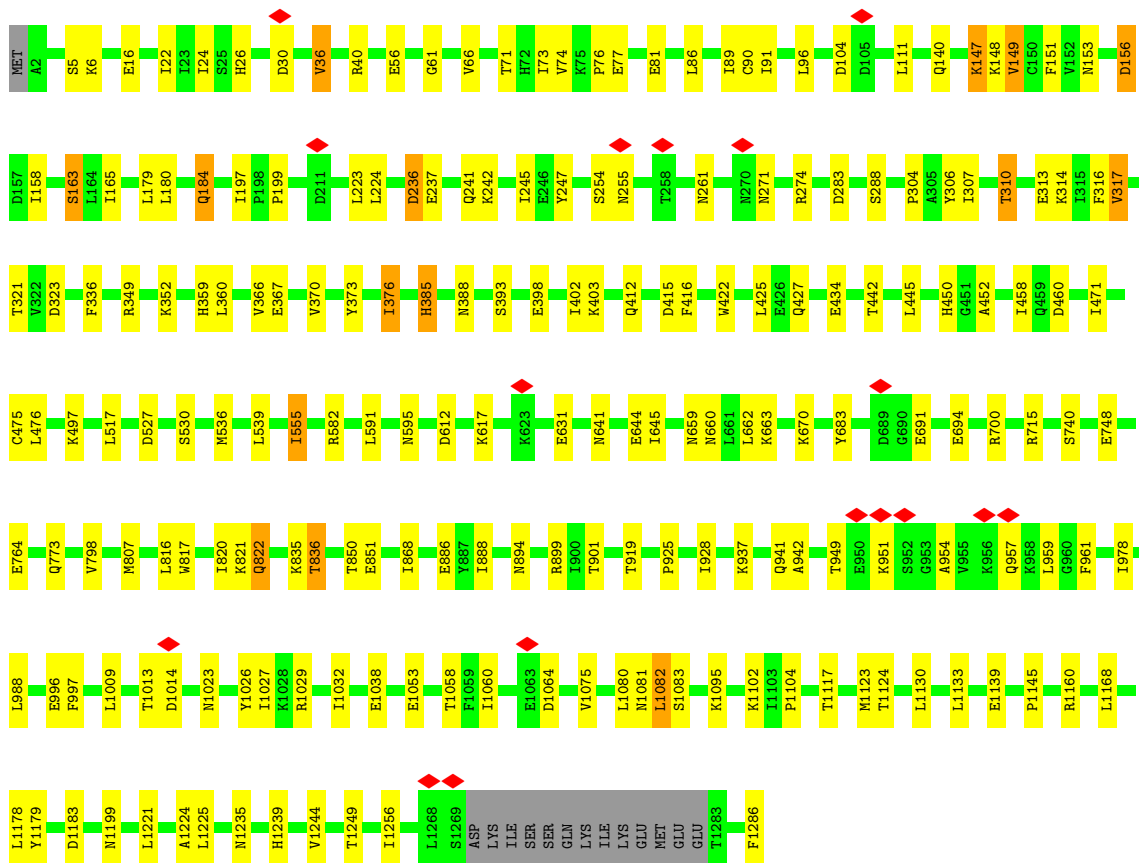


• Molecule 8: Large subunit of mRNA capping enzyme

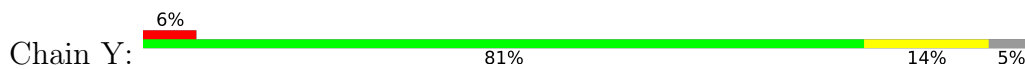


• Molecule 9: Virion core protein

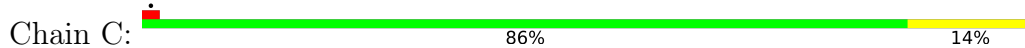


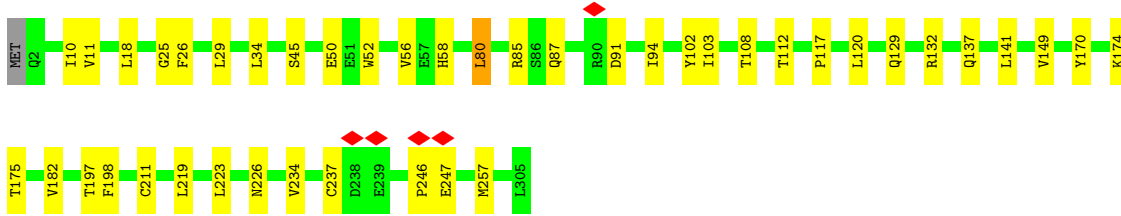


• Molecule 13: Nucleoside triphosphate phosphohydrolase-I

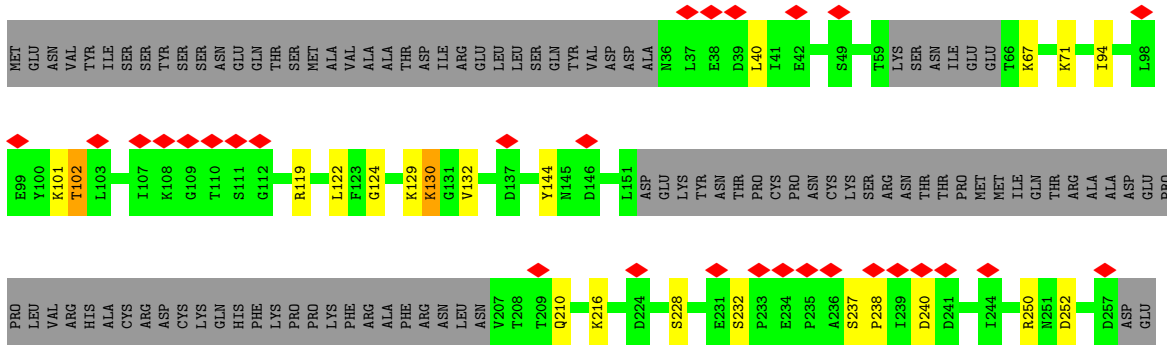


• Molecule 14: DNA-directed RNA polymerase 35 kDa subunit





• Molecule 15: DNA-directed RNA polymerase 30 kDa polypeptide



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	618338	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.562	Depositor
Minimum map value	-0.348	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	536.004, 536.004, 536.004	wwPDB
Map dimensions	504, 504, 504	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0635, 1.0635, 1.0635	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: MG, SEP, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	B	0.32	0/9281	0.52	0/12537
2	E	0.30	0/1522	0.56	0/2069
3	F	0.31	0/863	0.47	0/1158
4	G	0.32	0/1209	0.51	0/1639
5	I	0.30	0/6590	0.50	1/8918 (0.0%)
6	J	0.33	0/494	0.53	0/663
7	L	0.27	0/2365	0.47	0/3189
8	O	0.27	0/6832	0.48	0/9238
9	Q	0.29	0/1035	0.48	0/1402
9	R	0.30	0/1081	0.50	0/1463
10	K	0.28	0/767	0.49	0/1030
11	U	0.37	0/1635	1.04	10/2545 (0.4%)
12	A	0.32	0/10429	0.51	1/14098 (0.0%)
13	Y	0.28	0/4936	0.48	0/6638
14	C	0.32	0/2540	0.52	1/3440 (0.0%)
15	S	0.27	0/1302	0.51	0/1749
All	All	0.30	0/52881	0.53	13/71776 (0.0%)

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	B	0	1
2	E	0	1
5	I	0	1
7	L	1	0
12	A	0	3
All	All	1	6

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	I	220	LEU	CA-CB-CG	6.49	130.23	115.30
11	U	36[A]	G	C4-N9-C1'	6.34	134.74	126.50
11	U	36[B]	G	C4-N9-C1'	6.34	134.74	126.50
11	U	36[A]	G	N3-C4-C5	-5.98	125.61	128.60
11	U	36[B]	G	N3-C4-C5	-5.98	125.61	128.60
12	A	1082	LEU	CA-CB-CG	5.90	128.88	115.30
11	U	36[A]	G	N3-C4-N9	5.89	129.53	126.00
11	U	36[B]	G	N3-C4-N9	5.89	129.53	126.00
14	C	80	LEU	CA-CB-CG	5.87	128.81	115.30
11	U	26	U	N3-C2-O2	-5.46	118.38	122.20
11	U	36[A]	G	C8-N9-C1'	-5.30	120.11	127.00
11	U	36[B]	G	C8-N9-C1'	-5.30	120.11	127.00
11	U	26	U	N1-C2-O2	5.28	126.49	122.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	L	12	THR	CB

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	A	147	LYS	Peptide
12	A	458	ILE	Peptide
12	A	582	ARG	Peptide
1	B	1097	ILE	Peptide
2	E	116	LEU	Peptide
5	I	481	LEU	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	B	9091	0	9146	100	0
2	E	1495	0	1548	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	849	0	874	8	0
4	G	1192	0	1181	9	0
5	I	6446	0	6502	53	0
6	J	490	0	530	6	0
7	L	2320	0	2363	28	0
8	O	6693	0	6766	48	0
9	Q	1013	0	998	11	0
9	R	1056	0	1056	11	0
10	K	749	0	727	6	0
11	U	1465	0	738	5	0
12	A	10223	0	10337	107	0
13	Y	4845	0	4911	50	0
14	C	2484	0	2470	24	0
15	S	1311	0	1268	15	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	I	1	0	0	0	0
17	A	1	0	0	0	0
18	A	16	0	0	1	0
18	B	28	0	0	0	0
18	C	3	0	0	0	0
18	E	2	0	0	0	0
18	F	1	0	0	0	0
18	G	2	0	0	0	0
18	I	3	0	0	0	0
18	J	3	0	0	0	0
18	K	1	0	0	0	0
18	Y	2	0	0	0	0
All	All	51788	0	51415	433	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 (433) 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)
7:L:43:TYR:O	7:L:47:ILE:HB	1.75	0.85
14:C:25:GLY:O	14:C:29:LEU:HB2	1.85	0.75
12:A:817:TRP:O	12:A:821:LYS:HB3	1.89	0.72
13:Y:268:GLU:HG2	13:Y:272:GLN:HE22	1.57	0.69
5:I:233:LYS:HB2	11:U:41:C:H5'	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:149:VAL:HG21	12:A:242:LYS:HB2	1.77	0.64
6:J:2:VAL:HA	6:J:18:ARG:HD3	1.80	0.64
7:L:159:THR:HG22	7:L:161:PHE:H	1.63	0.63
1:B:178:PRO:HB3	1:B:192:PHE:HB3	1.79	0.63
5:I:109:TYR:O	5:I:113:ASP:HB2	2.00	0.62
12:A:36:VAL:HG21	12:A:224:LEU:HB3	1.82	0.62
2:E:172:GLY:HA3	12:A:820:ILE:HB	1.82	0.61
1:B:1141:ASP:HB2	12:A:6:LYS:HB3	1.82	0.61
13:Y:386:GLU:HG2	13:Y:444:SER:H	1.66	0.61
1:B:542:PRO:HA	1:B:545:ILE:HD13	1.83	0.60
1:B:431:HIS:HB3	1:B:701:LEU:HD21	1.82	0.60
12:A:271:ASN:HB2	12:A:274:ARG:HG2	1.84	0.60
1:B:242:ARG:O	5:I:738:ARG:NH2	2.33	0.60
12:A:81:GLU:HG3	12:A:1225:LEU:HD21	1.84	0.60
8:O:621:PRO:HB3	8:O:653:THR:HG22	1.84	0.60
1:B:540:LEU:HD23	1:B:545:ILE:HD12	1.83	0.59
10:K:443:PHE:HB2	10:K:447:GLN:HE21	1.67	0.59
5:I:735:ASN:ND2	5:I:747:VAL:O	2.36	0.59
13:Y:416:LYS:HA	13:Y:419:ARG:HD2	1.83	0.59
12:A:61:GLY:HA3	12:A:199:PRO:HB3	1.83	0.59
14:C:117:PRO:HD2	14:C:120:LEU:HD22	1.85	0.59
9:Q:46:GLN:HG3	9:Q:107:ILE:HD12	1.85	0.58
1:B:102:ILE:HG13	1:B:397:VAL:HG11	1.85	0.58
7:L:6:LYS:O	7:L:10:GLU:HB2	2.03	0.58
13:Y:278:GLU:HG2	13:Y:283:ILE:HD11	1.84	0.58
1:B:1071:THR:HG21	12:A:1244:VAL:HG22	1.84	0.58
12:A:184:GLN:NE2	12:A:1224:ALA:O	2.37	0.58
12:A:76:PRO:HB3	12:A:245:ILE:HG12	1.84	0.57
12:A:1160:ARG:NH1	12:A:1183:ASP:OD1	2.37	0.57
1:B:761:LYS:HD2	1:B:899:GLU:HG3	1.86	0.57
9:R:55:ASP:OD1	9:R:55:ASP:N	2.38	0.57
13:Y:406:ILE:O	13:Y:408:ASN:ND2	2.37	0.57
7:L:153:CYS:HB3	7:L:198:ALA:HB3	1.86	0.56
7:L:88:LYS:HE3	7:L:94:THR:HB	1.87	0.56
12:A:996:GLU:O	12:A:1095:LYS:NZ	2.38	0.56
12:A:450:HIS:HD2	12:A:452:ALA:H	1.53	0.56
12:A:349:ARG:HB2	12:A:352:LYS:HB2	1.87	0.56
8:O:34:ILE:N	8:O:126:GLU:O	2.38	0.56
2:E:1:MET:SD	2:E:46:THR:OG1	2.64	0.56
1:B:430:PRO:O	1:B:436:GLN:NE2	2.38	0.56
1:B:680:ASN:HD21	1:B:957:SER:HA	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:881:ASP:OD2	1:B:1017:ARG:NH2	2.39	0.56
5:I:457:GLU:HB3	5:I:462:LEU:HD13	1.88	0.56
5:I:713:ASP:HB2	5:I:726:HIS:HE1	1.71	0.56
8:O:582:SER:O	8:O:592:ARG:NH1	2.40	0.55
1:B:255:ASP:O	1:B:574:HIS:ND1	2.39	0.55
1:B:709:ILE:HG23	1:B:870:LEU:HB2	1.88	0.55
4:G:99:ILE:HB	4:G:106:CYS:HB2	1.89	0.55
8:O:344:ARG:NH1	12:A:1286:PHE:O	2.40	0.55
1:B:1105:ARG:HD3	12:A:16:GLU:HB3	1.89	0.55
4:G:7:ASN:O	5:I:293:ARG:NH2	2.39	0.55
5:I:104:THR:OG1	5:I:105:ASP:N	2.39	0.55
7:L:239:THR:O	7:L:243:ASN:ND2	2.40	0.55
12:A:336:PHE:HB2	12:A:367:GLU:HB2	1.89	0.55
14:C:103:ILE:HG13	14:C:112:THR:HG23	1.88	0.55
11:U:35[A]:U:H3	13:Y:163:SER:HG	1.54	0.55
14:C:85:ARG:HG2	14:C:94:ILE:HG12	1.89	0.55
14:C:85:ARG:NH2	14:C:91:ASP:O	2.40	0.55
12:A:236:ASP:N	12:A:236:ASP:OD1	2.39	0.55
7:L:40:GLY:HA3	7:L:246:LEU:HD11	1.89	0.54
8:O:303:GLU:HG3	8:O:315:ILE:HD11	1.88	0.54
1:B:951:PRO:HD2	5:I:604:LEU:H	1.72	0.54
12:A:691:GLU:HG2	12:A:951:LYS:HE2	1.90	0.54
12:A:156:ASP:OD1	12:A:156:ASP:N	2.39	0.54
5:I:481:LEU:HD13	9:R:58:ILE:HD11	1.89	0.54
1:B:319:MET:HB3	1:B:322:THR:HB	1.90	0.54
12:A:140:GLN:OE1	12:A:153:ASN:ND2	2.41	0.54
9:Q:14:ARG:NH1	9:Q:95:GLU:OE1	2.41	0.54
14:C:34:LEU:HD12	14:C:182:VAL:HG12	1.90	0.54
2:E:149:VAL:HG13	2:E:159:LEU:HD23	1.90	0.53
12:A:223:LEU:HD13	12:A:247:TYR:HA	1.88	0.53
1:B:45:ARG:NH2	1:B:48:GLU:OE1	2.40	0.53
8:O:519:ARG:NH1	8:O:547:PHE:O	2.40	0.53
5:I:449:GLU:HA	5:I:452:LYS:HE2	1.89	0.53
8:O:116:HIS:HB3	8:O:119:CYS:H	1.74	0.53
1:B:853:ARG:NH1	14:C:50:GLU:OE1	2.41	0.53
1:B:1132:ASN:ND2	1:B:1136:VAL:O	2.39	0.53
5:I:183:ARG:NH2	12:A:163:SER:OG	2.42	0.53
13:Y:268:GLU:O	13:Y:272:GLN:NE2	2.42	0.53
12:A:86:LEU:HD21	12:A:165:ILE:HG23	1.91	0.53
13:Y:292:MET:HA	13:Y:295:THR:HG22	1.89	0.53
7:L:89:TYR:O	7:L:142:ARG:NH1	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:20:LYS:HE3	6:J:31:VAL:HG22	1.90	0.52
8:O:775:PHE:HB3	8:O:780:PHE:HB2	1.91	0.52
13:Y:412:SER:HB2	13:Y:443:SER:HB3	1.91	0.52
5:I:50:ILE:HD12	5:I:55:ILE:HD11	1.92	0.52
12:A:445:LEU:HD13	12:A:555:ILE:HD12	1.91	0.52
12:A:475:CYS:SG	12:A:476:LEU:N	2.83	0.52
1:B:922:SER:HB2	12:A:670:LYS:HD3	1.90	0.52
12:A:1029:ARG:NH2	15:S:144:TYR:OH	2.43	0.52
3:F:76:ARG:O	3:F:132:LYS:NZ	2.43	0.52
12:A:104:ASP:N	12:A:104:ASP:OD1	2.42	0.52
3:F:76:ARG:NH2	12:A:919:THR:O	2.43	0.52
5:I:280:SER:HB3	5:I:283:LEU:HB2	1.92	0.52
8:O:408:ARG:NH1	8:O:425:GLU:OE1	2.40	0.52
12:A:527:ASP:O	15:S:210:GLN:NE2	2.41	0.52
1:B:127:LEU:HD12	5:I:419:ASN:HB3	1.92	0.51
15:S:40:LEU:HD11	15:S:124:GLY:HA3	1.92	0.51
8:O:251:ASP:N	8:O:251:ASP:OD1	2.43	0.51
7:L:247:GLU:HG3	13:Y:349:ASP:HA	1.93	0.51
1:B:181:ARG:HB3	1:B:189:THR:HG22	1.92	0.51
1:B:319:MET:HG3	1:B:327:LYS:HG2	1.93	0.51
9:Q:75:PHE:HB3	9:Q:123:PHE:HB2	1.91	0.51
1:B:767:ARG:O	6:J:4:GLN:NE2	2.40	0.51
5:I:715:MET:O	5:I:757:ARG:NH2	2.44	0.51
7:L:246:LEU:HA	7:L:249:SER:HB2	1.93	0.51
8:O:260:LYS:NZ	8:O:303:GLU:OE2	2.41	0.51
8:O:402:THR:HG23	8:O:429:PHE:HB2	1.92	0.51
12:A:153:ASN:ND2	12:A:156:ASP:OD1	2.43	0.51
7:L:9:ARG:NH2	7:L:284:LYS:O	2.42	0.51
10:K:401:ARG:NH1	10:K:406:GLU:OE1	2.43	0.51
1:B:610:ARG:NH2	1:B:622:GLU:OE1	2.43	0.51
1:B:766:GLN:O	14:C:58:HIS:NE2	2.43	0.51
12:A:71:THR:HG23	12:A:237:GLU:HG2	1.93	0.51
12:A:937:LYS:HG2	12:A:1178:LEU:HD11	1.92	0.51
1:B:370:ALA:HA	1:B:407:LEU:HD21	1.93	0.51
1:B:1083:ASP:OD1	1:B:1083:ASP:N	2.38	0.51
8:O:166:LEU:HD22	8:O:176:LEU:HA	1.93	0.51
9:R:6:ILE:HG21	9:R:38:LEU:HD21	1.93	0.51
12:A:748:GLU:HB3	12:A:942:ALA:HB1	1.93	0.50
1:B:675:SER:HA	1:B:728:LEU:HD11	1.94	0.50
1:B:852:SER:HB3	1:B:871:THR:HB	1.93	0.50
8:O:404:ASN:HD21	8:O:478:LYS:HE3	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:476:ARG:HG2	13:Y:479:ARG:HH11	1.75	0.50
1:B:23:LYS:NZ	1:B:618:ASP:OD2	2.39	0.50
1:B:43:LEU:O	1:B:47:HIS:ND1	2.42	0.50
12:A:659:ASN:HB3	12:A:662:LEU:HB2	1.94	0.50
1:B:403:THR:HG21	5:I:420:ILE:HD11	1.94	0.50
2:E:5:ASN:HB2	2:E:100:LEU:HB3	1.93	0.50
5:I:627:LYS:NZ	5:I:628:ILE:O	2.45	0.50
14:C:56:VAL:HG21	14:C:141:LEU:HD13	1.94	0.50
1:B:255:ASP:H	1:B:336:ARG:HH12	1.59	0.50
8:O:655:ARG:NH1	8:O:684:SER:OG	2.44	0.50
8:O:782:LEU:HD21	8:O:785:ASN:HB2	1.94	0.50
12:A:237:GLU:O	12:A:241:GLN:HB2	2.11	0.50
12:A:304:PRO:HD2	12:A:307:ILE:HD12	1.94	0.50
4:G:84:ILE:HG22	10:K:383:ILE:HG23	1.94	0.50
3:F:112:ASN:HB3	3:F:115:HIS:HD2	1.77	0.50
5:I:497:VAL:HG22	5:I:564:LEU:HD21	1.93	0.50
3:F:127:PRO:HB2	12:A:1256:ILE:HG13	1.93	0.49
10:K:420:ASP:HB3	10:K:423:GLY:HA2	1.94	0.49
12:A:1023:ASN:HB3	12:A:1026:TYR:HD2	1.77	0.49
12:A:1130:LEU:HG	12:A:1133:LEU:HD12	1.93	0.49
4:G:91:ILE:HG12	4:G:97:VAL:HG13	1.93	0.49
1:B:140:ASN:OD1	1:B:140:ASN:N	2.45	0.49
1:B:491:LEU:HG	1:B:667:PHE:HB3	1.94	0.49
1:B:863:ASP:OD1	1:B:863:ASP:N	2.46	0.49
8:O:313:TYR:HB3	8:O:350:LYS:HG3	1.94	0.49
8:O:717:LEU:HD13	8:O:749:ILE:HD13	1.95	0.49
9:R:6:ILE:HD13	9:R:38:LEU:HD11	1.94	0.49
1:B:109:LYS:HD2	5:I:683:LYS:HD2	1.95	0.49
4:G:86:ARG:NH1	4:G:138:THR:OG1	2.41	0.49
8:O:403:ALA:HB2	8:O:483:PHE:HZ	1.78	0.49
8:O:711:THR:OG1	8:O:712:MET:N	2.46	0.49
1:B:18:LEU:HA	1:B:29:ARG:HG2	1.95	0.49
5:I:710:ARG:HG2	5:I:716:PRO:HB3	1.94	0.49
1:B:1058:ARG:NH2	12:A:764:GLU:OE1	2.45	0.49
1:B:372:ASP:OD1	15:S:250:ARG:NE	2.42	0.48
1:B:1062:ILE:HD11	12:A:1239:HIS:HE1	1.79	0.48
9:Q:4:VAL:HG11	9:Q:54:LYS:HE2	1.95	0.48
7:L:32:SER:HB2	7:L:229:GLN:HB3	1.95	0.48
12:A:954:ALA:HB2	12:A:1104:PRO:HD2	1.94	0.48
12:A:306:TYR:O	12:A:310:THR:OG1	2.31	0.48
1:B:244:SER:HB3	1:B:247:PHE:H	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:723:ASP:OD1	5:I:723:ASP:N	2.44	0.48
13:Y:483:HIS:HB3	13:Y:491:ARG:HG2	1.94	0.48
6:J:32:LEU:HD22	6:J:41:ARG:HG2	1.94	0.48
12:A:851:GLU:OE1	12:A:899:ARG:NE	2.45	0.48
8:O:260:LYS:HB2	8:O:378:ILE:HG12	1.95	0.48
12:A:835:LYS:HD3	15:S:216:LYS:HG2	1.94	0.48
12:A:1053:GLU:HB3	15:S:94:ILE:HD11	1.95	0.48
8:O:310:TRP:HB2	8:O:345:ILE:HG12	1.96	0.48
4:G:52:GLU:O	5:I:301:ARG:NH2	2.46	0.48
7:L:140:VAL:O	7:L:172:TYR:OH	2.31	0.48
12:A:836:THR:HB	12:A:888:ILE:HD11	1.95	0.48
1:B:744:ILE:HG22	1:B:913:VAL:HB	1.96	0.48
12:A:376:ILE:HD12	12:A:425:LEU:HD13	1.96	0.48
1:B:1097:ILE:HD11	1:B:1104:LEU:HD21	1.95	0.47
10:K:407:VAL:HG22	10:K:417:THR:HG22	1.94	0.47
11:U:35[A]:U:N3	13:Y:163:SER:OG	2.47	0.47
12:A:978:ILE:HG13	12:A:1145:PRO:HA	1.96	0.47
7:L:32:SER:HB2	7:L:229:GLN:HE21	1.80	0.47
13:Y:620:ILE:HB	13:Y:630:ILE:HB	1.96	0.47
1:B:706:ARG:NH2	14:C:45:SER:O	2.45	0.47
5:I:52:GLU:OE1	8:O:543:ASN:ND2	2.47	0.47
8:O:99:ILE:O	8:O:134:TYR:OH	2.28	0.47
12:A:978:ILE:HG12	12:A:1130:LEU:HD11	1.96	0.47
5:I:593:GLU:O	14:C:132:ARG:NH2	2.47	0.47
13:Y:504:ASN:OD1	13:Y:504:ASN:N	2.38	0.47
12:A:77:GLU:HG3	12:A:1221:LEU:HD22	1.97	0.47
1:B:242:ARG:NH2	1:B:284:ASP:OD2	2.46	0.47
1:B:514:ARG:HH12	5:I:753:ASN:HB2	1.79	0.47
12:A:1075:VAL:O	12:A:1081:ASN:ND2	2.46	0.47
13:Y:401:PHE:HB3	13:Y:408:ASN:HD22	1.80	0.47
1:B:491:LEU:HD13	1:B:590:PRO:HG2	1.97	0.47
7:L:74:ASP:N	7:L:74:ASP:OD1	2.47	0.47
12:A:868:ILE:HG21	12:A:886:GLU:HB2	1.97	0.47
1:B:65:ARG:NH2	1:B:105:GLU:OE2	2.48	0.46
5:I:16:LYS:O	5:I:20:LEU:HB2	2.15	0.46
9:R:24:ASP:OD1	9:R:24:ASP:N	2.48	0.46
12:A:694:GLU:OE1	12:A:715:ARG:NH1	2.47	0.46
13:Y:426:PHE:O	13:Y:431:ASN:ND2	2.48	0.46
1:B:96:ALA:HB3	1:B:128:ILE:HB	1.96	0.46
12:A:1060:ILE:O	15:S:130:LYS:NZ	2.38	0.46
1:B:569:THR:HG21	1:B:633:GLU:HG2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:398:GLU:O	13:Y:547:SER:OG	2.26	0.46
13:Y:278:GLU:OE1	13:Y:290:ARG:NE	2.46	0.46
8:O:67:THR:HG23	8:O:142:ARG:HB3	1.97	0.46
12:A:1038:GLU:OE1	15:S:119:ARG:NH1	2.45	0.46
5:I:594:SER:H	6:J:53:ASN:HD22	1.63	0.46
1:B:704:ASP:HB3	1:B:707:ASN:HB2	1.98	0.46
9:R:1:MET:HE1	9:R:27:ALA:HA	1.96	0.46
12:A:997:PHE:O	12:A:1102:LYS:NZ	2.48	0.46
5:I:125:GLN:HG3	5:I:127:LYS:H	1.80	0.46
5:I:418:ASP:OD1	5:I:425:THR:OG1	2.32	0.46
7:L:232:ILE:HG23	7:L:233:LEU:HG	1.97	0.46
8:O:113:ASN:HB3	8:O:121:LEU:HB3	1.98	0.46
13:Y:124:PHE:HA	13:Y:127:ILE:HG12	1.96	0.46
1:B:72:ASN:OD1	1:B:72:ASN:N	2.49	0.46
5:I:713:ASP:OD1	5:I:713:ASP:N	2.49	0.46
12:A:764:GLU:HG2	12:A:1235:ASN:HD22	1.81	0.46
8:O:495:ASP:OD1	8:O:495:ASP:N	2.49	0.45
8:O:558:ASN:HA	8:O:601:ASN:HD21	1.81	0.45
1:B:1148:SER:HB2	3:F:136:LEU:HD11	1.98	0.45
12:A:96:LEU:HD21	12:A:180:LEU:HD11	1.97	0.45
1:B:847:THR:O	1:B:1046:LYS:NZ	2.41	0.45
1:B:946:LYS:HE2	1:B:946:LYS:HB2	1.84	0.45
2:E:16:LYS:NZ	2:E:150:LYS:O	2.49	0.45
14:C:11:VAL:HG22	14:C:197:THR:HG23	1.99	0.45
9:Q:27:ALA:HB3	13:Y:485:LEU:HD23	1.98	0.45
1:B:600:MET:HA	1:B:603:VAL:HG22	1.98	0.45
1:B:754:GLN:NE2	12:A:460:ASP:OD1	2.43	0.45
1:B:765:ILE:HG23	1:B:877:PRO:HD2	1.98	0.45
7:L:132:ASP:HB3	7:L:135:MET:HG3	1.98	0.45
13:Y:457:ASP:OD2	13:Y:496:HIS:NE2	2.43	0.45
1:B:722:ILE:HD12	1:B:723:VAL:HG23	1.99	0.45
12:A:1027:ILE:HG23	12:A:1032:ILE:HG13	1.99	0.45
13:Y:538:TRP:O	13:Y:542:ASN:HB2	2.16	0.45
1:B:433:SER:OG	1:B:697:ALA:O	2.35	0.45
1:B:579:ARG:NE	1:B:633:GLU:OE1	2.48	0.45
7:L:124:THR:O	8:O:589:SER:OG	2.34	0.45
12:A:925:PRO:HB2	12:A:928:ILE:HG22	1.99	0.45
1:B:698:ILE:HD13	1:B:772:ILE:HG21	1.99	0.45
7:L:213:VAL:O	7:L:217:THR:OG1	2.32	0.45
8:O:114:ARG:HH21	8:O:117:LYS:HG3	1.82	0.45
8:O:146:VAL:HG22	8:O:163:LYS:HG2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:317:VAL:HG11	12:A:360:LEU:HB3	1.99	0.45
13:Y:85:VAL:HG12	13:Y:141:ASP:HB3	1.99	0.45
14:C:226:ASN:HB3	14:C:257:MET:HE1	1.99	0.45
12:A:434:GLU:OE2	12:A:1249:THR:OG1	2.30	0.45
1:B:54:ARG:NH1	1:B:375:GLU:OE1	2.40	0.44
1:B:1088:GLU:OE2	1:B:1116:THR:OG1	2.34	0.44
8:O:259:THR:HB	8:O:373:GLN:HG3	1.98	0.44
8:O:401:GLN:HE21	8:O:514:ILE:HD13	1.82	0.44
12:A:313:GLU:HG2	12:A:370:VAL:HA	1.98	0.44
13:Y:362:LYS:HB3	13:Y:362:LYS:HE3	1.79	0.44
4:G:55:GLU:HB2	5:I:301:ARG:HB3	2.00	0.44
8:O:211:GLU:HA	8:O:214:THR:HG22	1.99	0.44
12:A:314:LYS:HD3	12:A:427:GLN:HB2	1.99	0.44
1:B:16:LYS:HA	1:B:16:LYS:HD3	1.75	0.44
5:I:173:PRO:HG3	12:A:158:ILE:HD13	2.00	0.44
5:I:727:VAL:HG13	5:I:760:LEU:HD22	2.00	0.44
1:B:156:VAL:HG12	1:B:166:VAL:HG13	2.00	0.44
1:B:212:LEU:HD13	1:B:220:LEU:HD13	1.98	0.44
1:B:892:THR:OG1	12:A:416:PHE:O	2.32	0.44
2:E:36:THR:HG23	2:E:53:LYS:HE2	2.00	0.44
13:Y:220:GLU:OE2	13:Y:529:ARG:NH1	2.51	0.44
5:I:65:ASN:OD1	5:I:65:ASN:N	2.49	0.44
8:O:559:LYS:HA	8:O:756:THR:HG22	1.99	0.44
9:R:81:PRO:HG2	13:Y:20:PRO:HA	1.98	0.44
9:Q:3:LEU:HD21	9:Q:51:LEU:HD23	2.00	0.44
13:Y:502:LEU:HD12	13:Y:506:MET:HB3	2.00	0.44
5:I:97:SER:OG	5:I:98:PHE:N	2.51	0.44
13:Y:600:ASP:OD1	13:Y:600:ASP:N	2.51	0.44
1:B:955:PRO:HG2	1:B:958:ASN:HA	1.99	0.44
5:I:22:ALA:HB3	5:I:27:LYS:HE3	2.00	0.44
5:I:334:GLU:HA	5:I:337:LYS:HE2	1.99	0.44
5:I:698:LYS:HA	5:I:793:PHE:HE2	1.83	0.44
12:A:254:SER:OG	12:A:255:ASN:N	2.51	0.44
12:A:316:PHE:O	12:A:321:THR:OG1	2.32	0.44
12:A:497:LYS:HA	12:A:497:LYS:HD3	1.81	0.44
13:Y:456:ASN:OD1	13:Y:490:ARG:NH2	2.51	0.44
12:A:22:ILE:HG12	12:A:40:ARG:HB3	2.00	0.43
12:A:988:LEU:HD13	12:A:1123:MET:HB2	2.00	0.43
2:E:66:GLU:HB2	2:E:85:THR:HA	1.99	0.43
5:I:124:ARG:HA	5:I:124:ARG:HD3	1.81	0.43
5:I:359:GLY:HA2	5:I:375:LEU:HD12	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:99:ILE:H	8:O:99:ILE:HG13	1.70	0.43
5:I:676:LYS:HD2	5:I:683:LYS:HD3	1.99	0.43
12:A:595:ASN:HD21	12:A:641:ASN:HD21	1.66	0.43
1:B:1039:ARG:NH2	12:A:56:GLU:O	2.41	0.43
2:E:111:PRO:HG2	2:E:113:PHE:HD2	1.84	0.43
10:K:401:ARG:HG3	10:K:406:GLU:HG2	2.01	0.43
13:Y:13:LEU:O	13:Y:40:ARG:NH2	2.41	0.43
5:I:281:TYR:HH	11:U:20[A]:U:P	2.41	0.43
12:A:74:VAL:HG21	12:A:151:PHE:HE1	1.83	0.43
12:A:388:ASN:HA	12:A:412:GLN:HG2	2.00	0.43
14:C:170:TYR:O	14:C:174:LYS:CB	2.66	0.43
4:G:109:SER:OG	4:G:111:ASP:OD1	2.35	0.43
8:O:292:ARG:NH2	8:O:337:LYS:O	2.45	0.43
12:A:147:LYS:HE3	12:A:147:LYS:HB3	1.84	0.43
7:L:33:PRO:HB2	7:L:163:ARG:HD3	2.01	0.43
7:L:70:LEU:HD21	7:L:287:LEU:HD21	2.00	0.43
12:A:323:ASP:N	12:A:323:ASP:OD1	2.52	0.43
13:Y:86:LYS:HD2	13:Y:145:ASN:HD22	1.84	0.43
13:Y:202:ARG:NH2	13:Y:228:GLY:O	2.41	0.43
7:L:103:LEU:HB2	7:L:158:PRO:HD3	2.01	0.43
8:O:787:ASP:OD1	8:O:787:ASP:N	2.52	0.43
9:R:8:LEU:HB2	9:R:15:VAL:HG22	2.00	0.43
9:R:11:ASP:OD1	9:R:11:ASP:N	2.51	0.43
13:Y:254:LYS:HD3	13:Y:478:ILE:HG21	2.01	0.43
13:Y:361:LEU:HD11	13:Y:403:VAL:HG11	2.01	0.43
14:C:52:TRP:HB3	14:C:141:LEU:HD21	2.01	0.43
15:S:240:ASP:OD1	15:S:240:ASP:N	2.52	0.43
4:G:117:PHE:HB3	4:G:123:CYS:HA	2.00	0.43
6:J:4:GLN:HB2	6:J:47:GLN:HE22	1.84	0.43
8:O:636:LEU:HD23	8:O:636:LEU:HA	1.90	0.43
12:A:612:ASP:HA	12:A:617:LYS:HD2	2.01	0.43
12:A:1064:ASP:OD1	12:A:1064:ASP:N	2.50	0.43
13:Y:278:GLU:HG3	13:Y:289:LEU:HB2	2.01	0.43
14:C:25:GLY:HA3	14:C:223:LEU:HD21	1.99	0.43
14:C:174:LYS:HE2	14:C:174:LYS:HB3	1.88	0.43
12:A:30:ASP:OD1	12:A:30:ASP:N	2.49	0.43
12:A:89:ILE:HG22	12:A:96:LEU:HD23	2.01	0.43
13:Y:266:LYS:HD3	13:Y:363:GLU:HB3	2.01	0.43
1:B:325:GLN:HE22	5:I:749:VAL:HA	1.82	0.42
1:B:686:ARG:NH2	1:B:888:SER:O	2.44	0.42
7:L:88:LYS:HB2	7:L:96:ALA:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R:104:CYS:SG	9:Q:116:SER:OG	2.71	0.42
12:A:941:GLN:NE2	18:A:1403:HOH:O	2.48	0.42
13:Y:33:ASP:OD1	13:Y:33:ASP:N	2.47	0.42
13:Y:202:ARG:HA	13:Y:203:PRO:HD3	1.92	0.42
14:C:26:PHE:HD2	14:C:219:LEU:HD22	1.83	0.42
1:B:223:SER:HB3	1:B:230:THR:HG23	2.00	0.42
7:L:246:LEU:O	7:L:250:ASN:ND2	2.52	0.42
12:A:24:ILE:HG13	12:A:197:ILE:HG13	2.01	0.42
12:A:822:GLN:O	12:A:822:GLN:NE2	2.50	0.42
13:Y:385:PHE:HE1	13:Y:473:ILE:HD12	1.84	0.42
14:C:10:ILE:HB	14:C:198:PHE:HB2	2.01	0.42
5:I:83:LYS:HG2	13:Y:579:THR:HG22	2.01	0.42
7:L:139:ASP:OD1	7:L:139:ASP:N	2.52	0.42
12:A:807:MET:SD	12:A:894:ASN:ND2	2.92	0.42
9:Q:21:ASN:OD1	9:Q:21:ASN:N	2.39	0.42
13:Y:283:ILE:HG13	13:Y:286:PHE:HA	2.00	0.42
15:S:101:LYS:HD3	15:S:101:LYS:HA	1.84	0.42
2:E:63:VAL:HG22	2:E:82:ILE:HB	2.01	0.42
13:Y:567:SER:O	13:Y:567:SER:OG	2.38	0.42
14:C:237:CYS:HB2	14:C:246:PRO:HG3	2.02	0.42
5:I:375:LEU:HD23	5:I:375:LEU:HA	1.91	0.42
2:E:116:LEU:HD12	2:E:116:LEU:HA	1.86	0.42
9:Q:3:LEU:HD13	9:Q:6:ILE:HB	2.00	0.42
1:B:146:LYS:H	1:B:146:LYS:HG3	1.70	0.42
5:I:326:CYS:SG	5:I:327:GLU:N	2.93	0.42
12:A:660:ASN:HA	12:A:663:LYS:HG2	2.02	0.42
1:B:206:ARG:HG2	1:B:208:TYR:CZ	2.55	0.42
12:A:73:ILE:HD13	12:A:73:ILE:HA	1.94	0.42
1:B:528:PHE:HB2	1:B:545:ILE:HD11	2.01	0.42
3:F:112:ASN:HB3	3:F:115:HIS:CD2	2.55	0.42
12:A:517:LEU:HD11	12:A:539:LEU:HD22	2.01	0.42
15:S:67:LYS:HA	15:S:67:LYS:HD3	1.81	0.42
13:Y:487:PRO:HA	13:Y:488:PRO:HD3	1.93	0.41
1:B:429:HIS:HD2	1:B:430:PRO:HD2	1.85	0.41
1:B:460:ARG:NH2	1:B:482:VAL:O	2.53	0.41
1:B:639:ASN:HD22	12:A:700:ARG:HH12	1.67	0.41
2:E:19:ILE:HD13	2:E:19:ILE:HA	1.88	0.41
2:E:81:PRO:O	2:E:93:ASN:ND2	2.42	0.41
5:I:85:GLU:HA	13:Y:577:GLU:HA	2.02	0.41
12:A:1168:LEU:HD22	12:A:1179:TYR:HD1	1.85	0.41
13:Y:92:ASP:O	13:Y:96:ASN:HB2	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1156:VAL:HG21	3:F:75:ARG:HG3	2.01	0.41
8:O:431:ASN:HB3	8:O:510:GLN:HA	2.03	0.41
1:B:1058:ARG:HD3	12:A:1239:HIS:CE1	2.55	0.41
12:A:288:SER:HB3	12:A:402:ILE:HG13	2.01	0.41
12:A:398:GLU:O	12:A:403:LYS:NZ	2.52	0.41
12:A:1235:ASN:O	12:A:1239:HIS:ND1	2.54	0.41
13:Y:287:ARG:HE	13:Y:287:ARG:HB2	1.74	0.41
15:S:102:THR:HB	15:S:122:LEU:HD12	2.02	0.41
9:Q:31:ILE:H	9:Q:31:ILE:HG13	1.65	0.41
14:C:87:GLN:HB3	14:C:137:GLN:HB3	2.02	0.41
1:B:1143:GLU:HB2	12:A:5:SER:HB3	2.01	0.41
8:O:327:ARG:HA	8:O:330:GLU:HB3	2.03	0.41
8:O:592:ARG:HA	8:O:673:ASN:HD21	1.85	0.41
8:O:747:ASP:N	8:O:747:ASP:OD1	2.54	0.41
8:O:822:ILE:HD13	8:O:822:ILE:HA	1.89	0.41
11:U:66:G:H2'	11:U:67:G:H8	1.85	0.41
15:S:129:LYS:HD3	15:S:129:LYS:HA	1.85	0.41
1:B:172:GLU:HG2	1:B:360:LEU:HG	2.03	0.41
2:E:30:ASN:N	2:E:30:ASN:OD1	2.50	0.41
9:R:31:ILE:HD13	9:R:31:ILE:HA	1.94	0.41
1:B:638:SER:O	12:A:700:ARG:NH2	2.47	0.41
1:B:1136:VAL:HG13	12:A:1224:ALA:HB2	2.02	0.41
1:B:1155:LYS:HD3	1:B:1155:LYS:HA	1.86	0.41
8:O:641:LYS:HD2	8:O:642:THR:HG23	2.03	0.41
14:C:129:GLN:H	14:C:137:GLN:HE22	1.67	0.41
1:B:309:TYR:O	1:B:313:HIS:HB3	2.20	0.41
1:B:521:ILE:HB	1:B:538:ALA:HB1	2.03	0.41
1:B:958:ASN:ND2	1:B:960:THR:O	2.54	0.41
2:E:1:MET:HG2	2:E:84:ILE:HD12	2.03	0.41
5:I:691:LEU:HB3	5:I:714:PRO:HB2	2.02	0.41
7:L:58:THR:HG1	7:L:114:ARG:H	1.67	0.41
12:A:237:GLU:O	12:A:241:GLN:CB	2.69	0.41
12:A:373:TYR:HA	12:A:393:SER:HB3	2.03	0.41
13:Y:287:ARG:HD2	13:Y:513:LEU:HD21	2.03	0.41
13:Y:367:LYS:HE3	13:Y:367:LYS:HB2	1.94	0.41
12:A:385:HIS:HD2	12:A:388:ASN:HD22	1.70	0.41
12:A:442:THR:HA	12:A:555:ILE:HD13	2.02	0.41
14:C:80:LEU:HB3	14:C:102:TYR:HB2	2.02	0.41
15:S:71:LYS:HE3	15:S:71:LYS:HB2	1.88	0.41
1:B:150:PRO:HG3	5:I:596:GLY:HA2	2.02	0.40
1:B:693:GLN:NE2	1:B:884:THR:OG1	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:713:ASP:HB3	5:I:730:LYS:HG2	2.03	0.40
15:S:252:ASP:OD1	15:S:252:ASP:N	2.49	0.40
1:B:1068:ASN:HA	1:B:1071:THR:HG22	2.03	0.40
2:E:129:GLN:O	3:F:70:LYS:NZ	2.47	0.40
14:C:45:SER:HA	14:C:137:GLN:HG3	2.04	0.40
1:B:11:GLN:HG3	1:B:664:PRO:HG2	2.03	0.40
1:B:131:PRO:HD2	1:B:366:PHE:HE2	1.86	0.40
1:B:1098:LYS:HE2	1:B:1098:LYS:HB2	1.93	0.40
5:I:24:ILE:H	5:I:24:ILE:HG13	1.73	0.40
7:L:49:ARG:HD3	7:L:49:ARG:HA	1.85	0.40
13:Y:78:ASN:ND2	13:Y:134:SER:OG	2.54	0.40
1:B:780:VAL:HG23	1:B:867:VAL:HB	2.04	0.40
1:B:1057:GLU:HG2	12:A:422:TRP:CZ2	2.57	0.40
7:L:92:ARG:HA	7:L:92:ARG:HD3	1.86	0.40
8:O:16:ASP:OD1	8:O:205:TYR:OH	2.33	0.40
8:O:484:LEU:HD13	8:O:486:ASN:HD21	1.86	0.40
8:O:775:PHE:O	8:O:780:PHE:N	2.53	0.40
9:Q:80:GLU:HA	9:Q:81:PRO:HD3	1.97	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1123/1164 (96%)	1046 (93%)	76 (7%)	1 (0%)	51	75
2	E	182/185 (98%)	164 (90%)	17 (9%)	1 (0%)	29	47
3	F	101/164 (62%)	95 (94%)	6 (6%)	0	100	100
4	G	149/161 (92%)	136 (91%)	13 (9%)	0	100	100
5	I	765/795 (96%)	715 (94%)	49 (6%)	1 (0%)	51	75
6	J	59/63 (94%)	56 (95%)	3 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	L	280/287 (98%)	267 (95%)	13 (5%)	0	100	100
8	O	820/844 (97%)	794 (97%)	26 (3%)	0	100	100
9	Q	122/129 (95%)	118 (97%)	4 (3%)	0	100	100
9	R	128/129 (99%)	121 (94%)	7 (6%)	0	100	100
10	K	87/710 (12%)	81 (93%)	6 (7%)	0	100	100
12	A	1268/1286 (99%)	1184 (93%)	84 (7%)	0	100	100
13	Y	592/631 (94%)	556 (94%)	36 (6%)	0	100	100
14	C	302/305 (99%)	278 (92%)	24 (8%)	0	100	100
15	S	152/259 (59%)	132 (87%)	19 (12%)	1 (1%)	22	39
All	All	6130/7112 (86%)	5743 (94%)	383 (6%)	4 (0%)	54	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	118	THR
5	I	482	PHE
1	B	1098	LYS
15	S	238	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1030/1064 (97%)	997 (97%)	33 (3%)	39	59
2	E	174/175 (99%)	168 (97%)	6 (3%)	37	58
3	F	94/151 (62%)	92 (98%)	2 (2%)	53	71
4	G	136/144 (94%)	130 (96%)	6 (4%)	28	47
5	I	735/755 (97%)	703 (96%)	32 (4%)	28	47
6	J	60/62 (97%)	55 (92%)	5 (8%)	11	20
7	L	269/272 (99%)	256 (95%)	13 (5%)	25	44

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	O	759/774 (98%)	720 (95%)	39 (5%)	24	41
9	Q	116/121 (96%)	108 (93%)	8 (7%)	15	27
9	R	122/121 (101%)	116 (95%)	6 (5%)	25	43
10	K	87/665 (13%)	80 (92%)	7 (8%)	12	21
12	A	1143/1157 (99%)	1089 (95%)	54 (5%)	26	45
13	Y	545/573 (95%)	529 (97%)	16 (3%)	42	62
14	C	286/287 (100%)	279 (98%)	7 (2%)	49	68
15	S	146/237 (62%)	143 (98%)	3 (2%)	53	71
All	All	5702/6558 (87%)	5465 (96%)	237 (4%)	33	49

All (237) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	52	VAL
1	B	56	LEU
1	B	58	SER
1	B	65	ARG
1	B	69	GLU
1	B	100	VAL
1	B	130	ILE
1	B	146	LYS
1	B	148	LEU
1	B	166	VAL
1	B	189	THR
1	B	196	SER
1	B	206	ARG
1	B	217	LEU
1	B	226	LYS
1	B	229	ILE
1	B	243	VAL
1	B	273	ARG
1	B	302	LEU
1	B	394	THR
1	B	433	SER
1	B	545	ILE
1	B	568	ILE
1	B	677	VAL
1	B	680	ASN
1	B	705	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	713	ILE
1	B	780	VAL
1	B	931	GLU
1	B	1028	VAL
1	B	1035	THR
1	B	1083	ASP
1	B	1097	ILE
2	E	30	ASN
2	E	72	THR
2	E	108	ASP
2	E	137	LEU
2	E	169	MET
2	E	170	VAL
3	F	77	ILE
3	F	117	ILE
4	G	12	VAL
4	G	20	THR
4	G	58	LEU
4	G	64	ASN
4	G	96	ASN
4	G	137	VAL
5	I	24	ILE
5	I	42	ILE
5	I	49	THR
5	I	51	THR
5	I	57	LEU
5	I	85	GLU
5	I	104	THR
5	I	220	LEU
5	I	235	VAL
5	I	253	ASN
5	I	256	LEU
5	I	285	SER
5	I	317	ARG
5	I	338	VAL
5	I	376	ASP
5	I	384	THR
5	I	386	ILE
5	I	389	THR
5	I	439	PHE
5	I	448	GLN
5	I	462	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	I	482	PHE
5	I	522	THR
5	I	558	SER
5	I	614	VAL
5	I	663	THR
5	I	666	THR
5	I	679	ILE
5	I	726	HIS
5	I	738	ARG
5	I	747	VAL
5	I	749	VAL
6	J	3	PHE
6	J	10	CYS
6	J	21	LEU
6	J	39	CYS
6	J	40	CYS
7	L	4	ILE
7	L	58	THR
7	L	61	LEU
7	L	63	LEU
7	L	82	LEU
7	L	92	ARG
7	L	136	LEU
7	L	165	VAL
7	L	170	ARG
7	L	182	LEU
7	L	201	VAL
7	L	217	THR
7	L	254	GLU
8	O	18	LEU
8	O	20	LYS
8	O	67	THR
8	O	99	ILE
8	O	103	VAL
8	O	131	PHE
8	O	153	THR
8	O	196	THR
8	O	203	VAL
8	O	242	LEU
8	O	245	GLN
8	O	270	VAL
8	O	299	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	O	326	ASP
8	O	327	ARG
8	O	339	VAL
8	O	351	LYS
8	O	402	THR
8	O	475	VAL
8	O	519	ARG
8	O	548	ARG
8	O	553	VAL
8	O	593	LYS
8	O	612	GLU
8	O	619	THR
8	O	622	ASP
8	O	635	LYS
8	O	640	ILE
8	O	651	GLN
8	O	653	THR
8	O	677	TRP
8	O	690	TYR
8	O	773	ARG
8	O	787	ASP
8	O	790	THR
8	O	804	THR
8	O	808	ARG
8	O	811	THR
8	O	837	VAL
9	R	20	LYS
9	R	24	ASP
9	R	31	ILE
9	R	55	ASP
9	R	114	VAL
9	R	125	ASN
10	K	366	VAL
10	K	369	SER
10	K	372	CYS
10	K	409	ILE
10	K	412	ASN
10	K	431	LEU
10	K	444	LEU
12	A	26	HIS
12	A	36	VAL
12	A	66	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	A	90	CYS
12	A	91	ILE
12	A	111	LEU
12	A	148	LYS
12	A	149	VAL
12	A	156	ASP
12	A	163	SER
12	A	179	LEU
12	A	184	GLN
12	A	236	ASP
12	A	261	ASN
12	A	283	ASP
12	A	310	THR
12	A	317	VAL
12	A	359	HIS
12	A	366	VAL
12	A	376	ILE
12	A	385	HIS
12	A	415	ASP
12	A	471	ILE
12	A	530	SER
12	A	536	MET
12	A	555	ILE
12	A	591	LEU
12	A	631	GLU
12	A	644	GLU
12	A	645	ILE
12	A	683	TYR
12	A	740	SER
12	A	773	GLN
12	A	798	VAL
12	A	816	LEU
12	A	822	GLN
12	A	836	THR
12	A	850	THR
12	A	901	THR
12	A	949	THR
12	A	957	GLN
12	A	959	LEU
12	A	961	PHE
12	A	1009	LEU
12	A	1013	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	A	1014	ASP
12	A	1058	THR
12	A	1080	LEU
12	A	1082	LEU
12	A	1083	SER
12	A	1117	THR
12	A	1124	THR
12	A	1139	GLU
12	A	1199	ASN
9	Q	14	ARG
9	Q	17	PHE
9	Q	21	ASN
9	Q	44	ILE
9	Q	51	LEU
9	Q	71	VAL
9	Q	77	VAL
9	Q	94	VAL
13	Y	15	ARG
13	Y	54	PHE
13	Y	171	THR
13	Y	219	ASP
13	Y	280	LYS
13	Y	398	LEU
13	Y	415	THR
13	Y	423	VAL
13	Y	441	VAL
13	Y	457	ASP
13	Y	464	THR
13	Y	486	THR
13	Y	504	ASN
13	Y	531	PHE
13	Y	573	ASN
13	Y	627	LEU
14	C	18	LEU
14	C	108	THR
14	C	149	VAL
14	C	175	THR
14	C	211	CYS
14	C	234	VAL
14	C	247	GLU
15	S	102	THR
15	S	130	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	S	132	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	40	ASN
1	B	169	ASN
1	B	301	GLN
1	B	325	GLN
1	B	387	ASN
1	B	429	HIS
1	B	639	ASN
1	B	681	HIS
1	B	693	GLN
1	B	858	GLN
1	B	971	GLN
1	B	1040	GLN
1	B	1110	ASN
2	E	125	ASN
2	E	129	GLN
2	E	168	ASN
3	F	115	HIS
4	G	64	ASN
4	G	100	GLN
4	G	133	ASN
4	G	145	GLN
5	I	46	ASN
5	I	99	ASN
5	I	253	ASN
5	I	271	HIS
5	I	329	GLN
5	I	348	ASN
5	I	419	ASN
5	I	448	GLN
5	I	489	ASN
5	I	501	ASN
5	I	589	ASN
5	I	726	HIS
5	I	728	GLN
5	I	735	ASN
5	I	740	HIS
5	I	776	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	I	795	ASN
6	J	47	GLN
6	J	51	GLN
6	J	53	ASN
7	L	7	ASN
7	L	46	GLN
7	L	229	GLN
7	L	276	ASN
8	O	147	ASN
8	O	404	ASN
8	O	463	ASN
8	O	509	ASN
8	O	521	GLN
8	O	601	ASN
8	O	630	ASN
8	O	634	ASN
8	O	678	GLN
9	R	125	ASN
10	K	374	ASN
10	K	397	ASN
10	K	447	GLN
12	A	137	GLN
12	A	167	GLN
12	A	309	ASN
12	A	381	GLN
12	A	388	ASN
12	A	548	HIS
12	A	589	ASN
12	A	611	ASN
12	A	636	ASN
12	A	641	ASN
12	A	686	GLN
12	A	741	GLN
12	A	932	GLN
12	A	940	GLN
12	A	941	GLN
12	A	947	HIS
12	A	957	GLN
12	A	994	ASN
12	A	1023	ASN
12	A	1116	GLN
12	A	1142	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	A	1169	ASN
12	A	1239	HIS
9	Q	43	HIS
13	Y	78	ASN
13	Y	144	HIS
13	Y	208	HIS
13	Y	236	ASN
13	Y	272	GLN
13	Y	391	GLN
13	Y	408	ASN
14	C	129	GLN
14	C	171	ASN
14	C	236	ASN
14	C	260	ASN
15	S	58	ASN
15	S	72	ASN
15	S	73	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	U	56/72 (77%)	11 (19%)	0

All (11) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	U	9	G
11	U	14	A
11	U	16	U
11	U	17	G
11	U	24	A
11	U	26	U
11	U	37	A
11	U	43	G
11	U	46	A
11	U	47	U
11	U	48	C

There are no RNA pucker outliers to report.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	SEP	S	228	15	8,9,10	1.52	1 (12%)	8,12,14	1.56	2 (25%)
15	SEP	S	237	15	8,9,10	1.53	1 (12%)	8,12,14	1.60	2 (25%)
15	SEP	S	232	15	8,9,10	1.55	1 (12%)	8,12,14	1.53	2 (25%)

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
15	SEP	S	228	15	-	4/5/8/10	-
15	SEP	S	237	15	-	3/5/8/10	-
15	SEP	S	232	15	-	4/5/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	S	232	SEP	P-O1P	3.39	1.61	1.50
15	S	228	SEP	P-O1P	3.33	1.61	1.50
15	S	237	SEP	P-O1P	3.31	1.61	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	S	237	SEP	P-OG-CB	-3.16	109.60	118.30
15	S	228	SEP	OG-CB-CA	2.93	111.00	108.14
15	S	232	SEP	OG-CB-CA	2.82	110.89	108.14
15	S	237	SEP	OG-CB-CA	2.79	110.86	108.14
15	S	228	SEP	P-OG-CB	-2.76	110.69	118.30
15	S	232	SEP	P-OG-CB	-2.56	111.25	118.30

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	S	228	SEP	CB-OG-P-O2P
15	S	228	SEP	CB-OG-P-O3P
15	S	232	SEP	CA-CB-OG-P
15	S	232	SEP	CB-OG-P-O2P
15	S	232	SEP	CB-OG-P-O3P
15	S	237	SEP	CB-OG-P-O2P
15	S	237	SEP	CB-OG-P-O3P
15	S	228	SEP	CB-OG-P-O1P
15	S	232	SEP	CB-OG-P-O1P
15	S	237	SEP	CB-OG-P-O1P
15	S	228	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

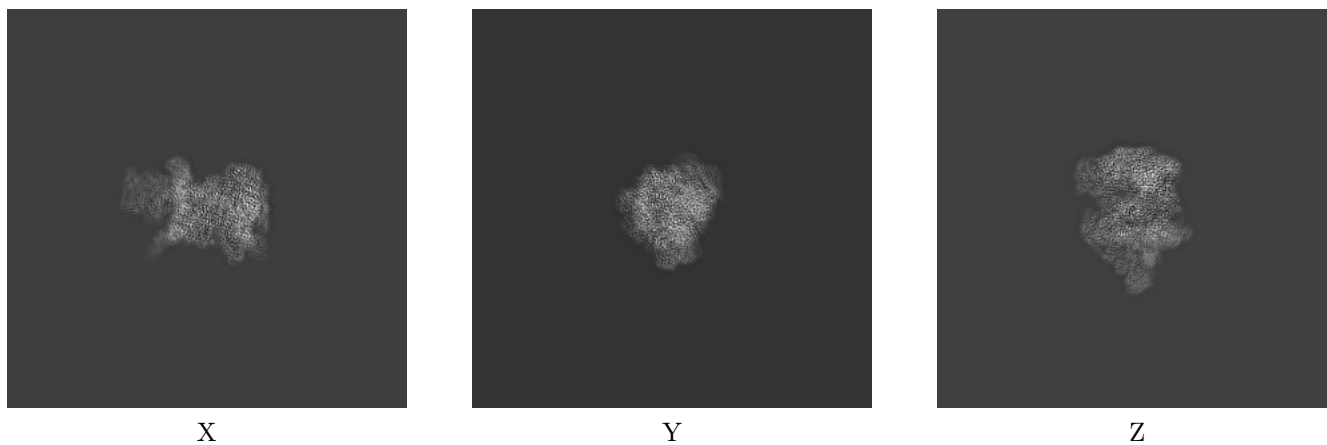
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4868. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

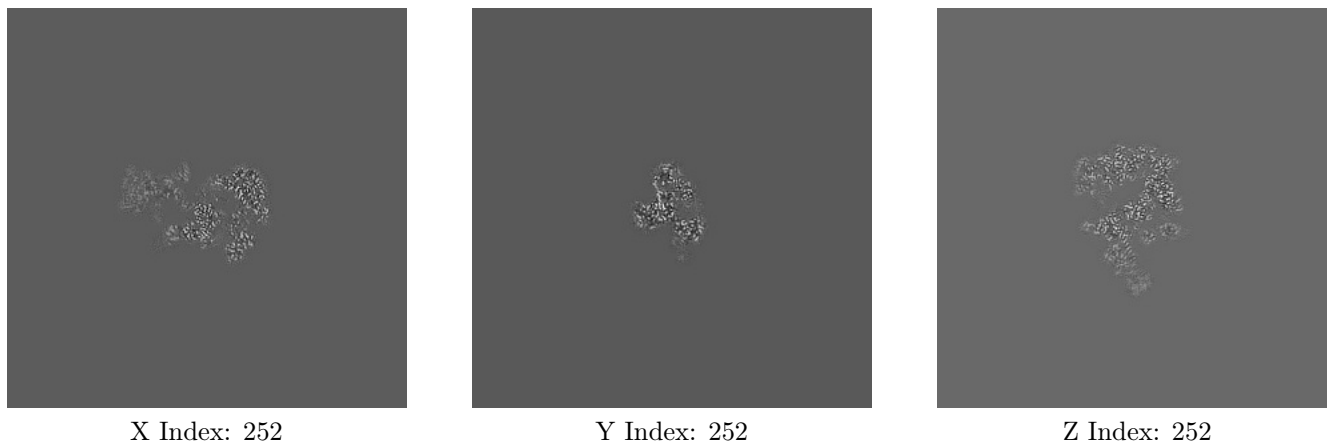
6.1.1 Primary map



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

6.2 Central slices [i](#)

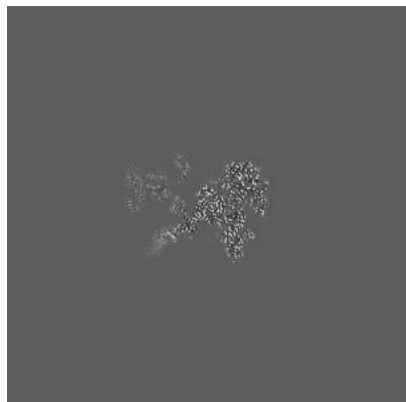
6.2.1 Primary map



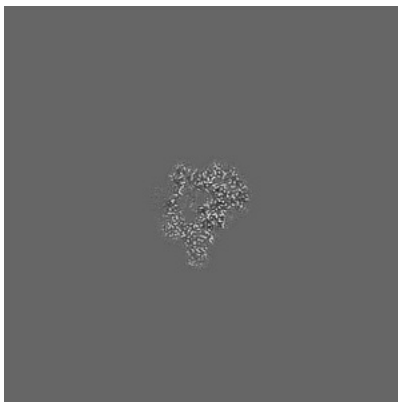
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 262



Y Index: 302

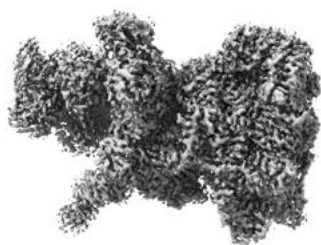


Z Index: 248

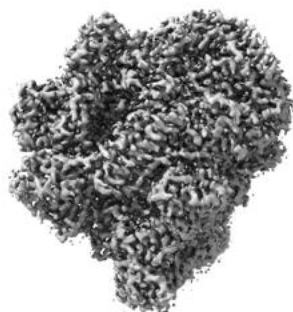
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

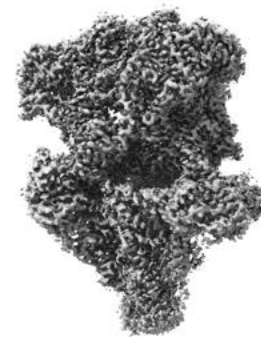
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

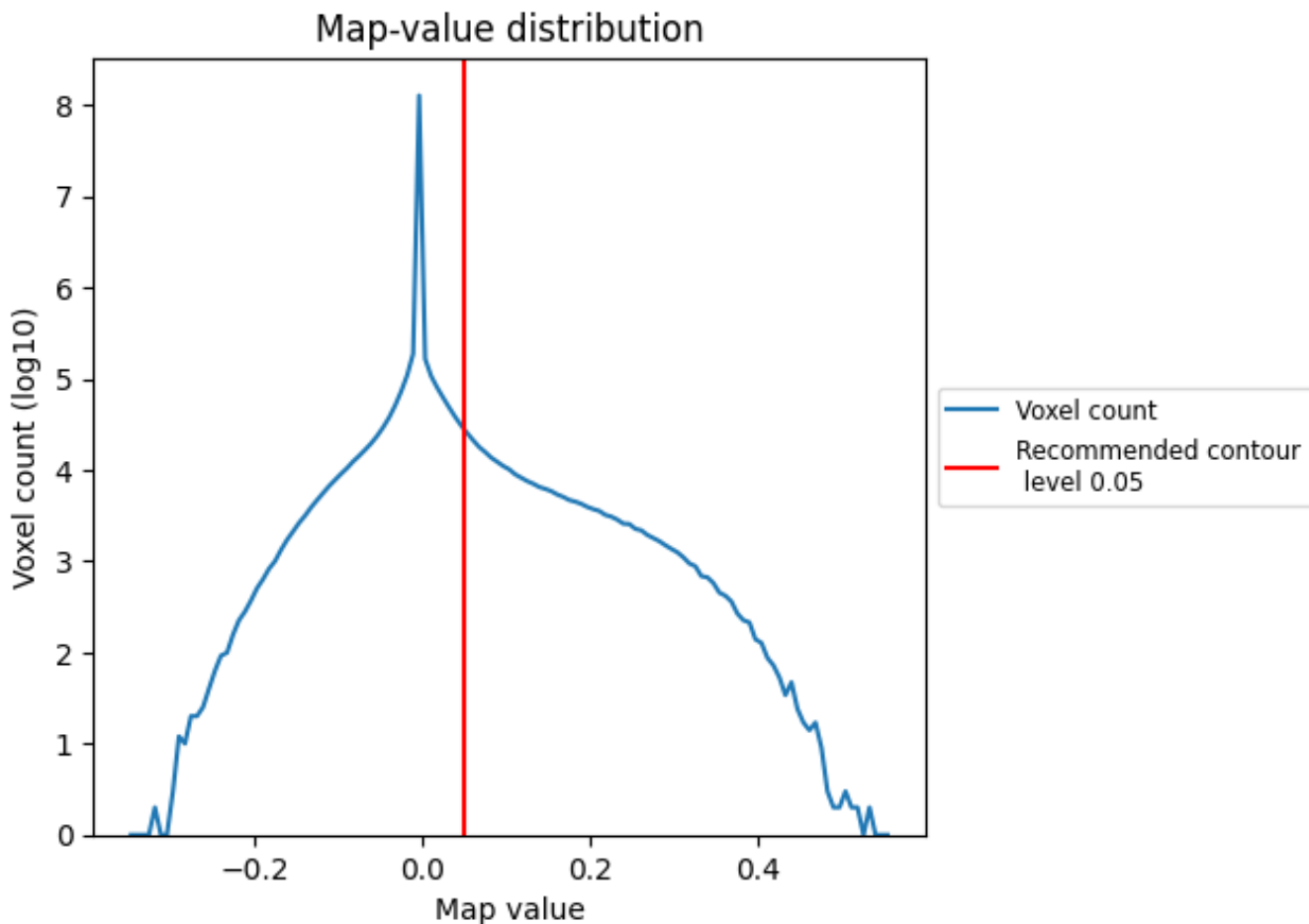
6.5 Mask visualisation

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

7 Map analysis [i](#)

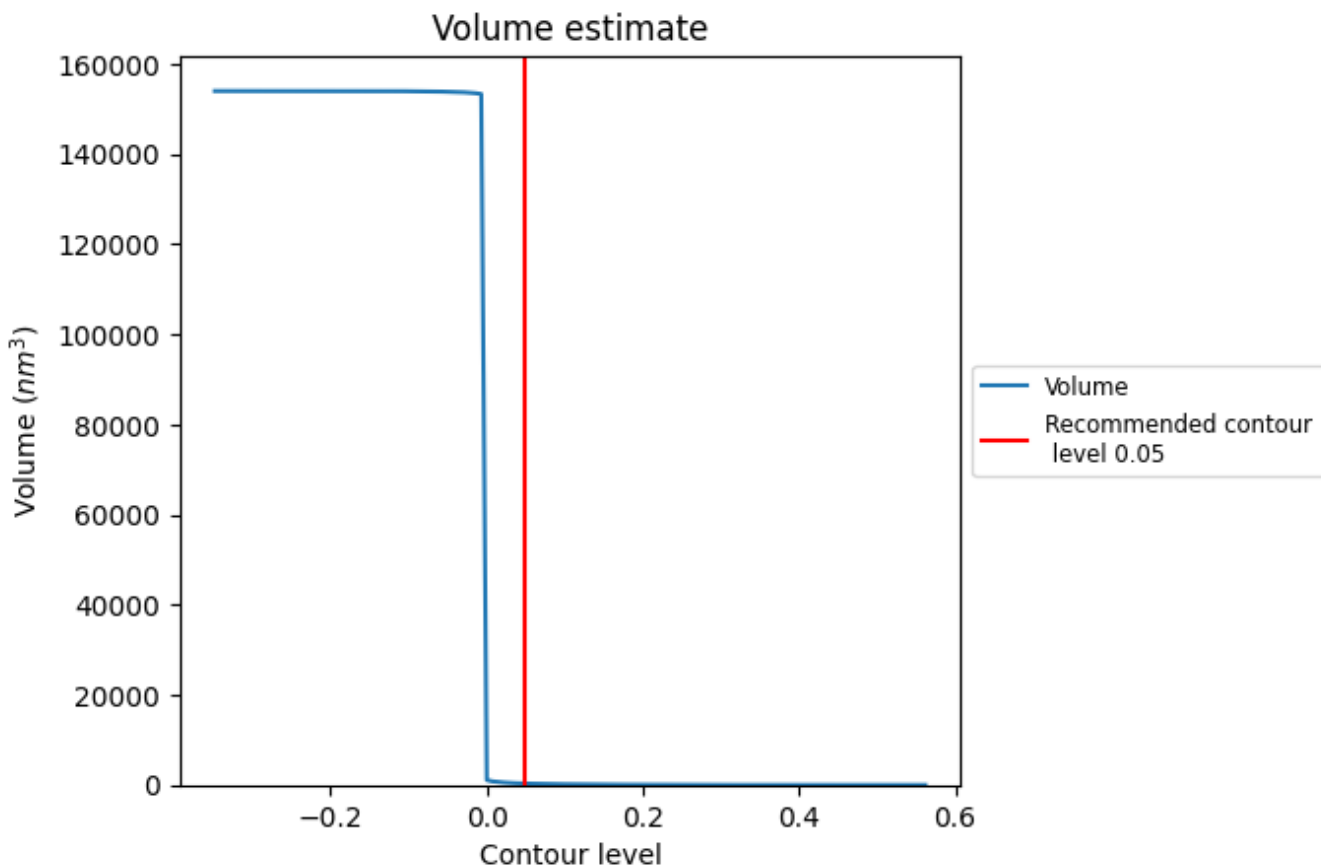
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

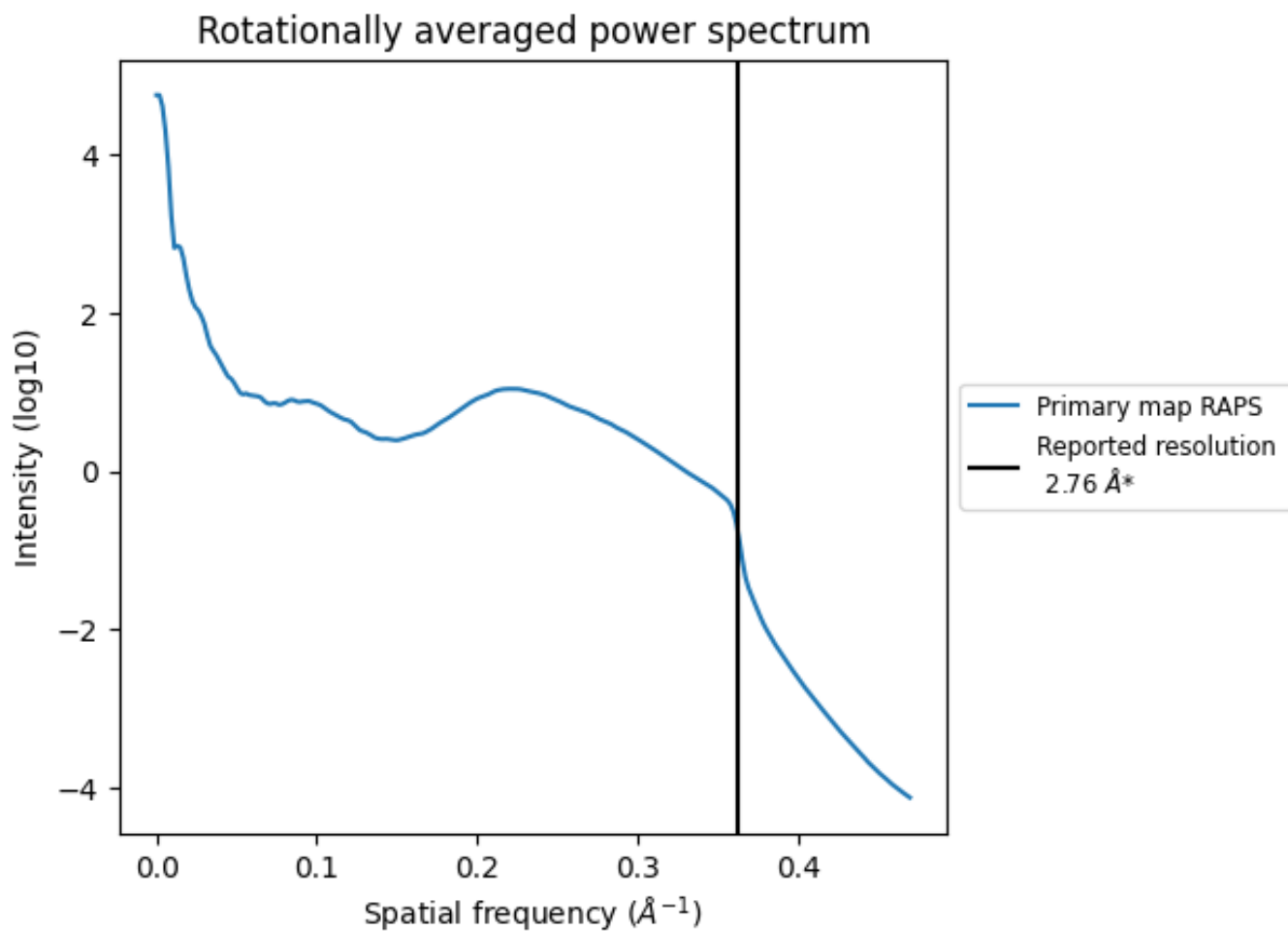
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 314 nm³; this corresponds to an approximate mass of 284 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](#)

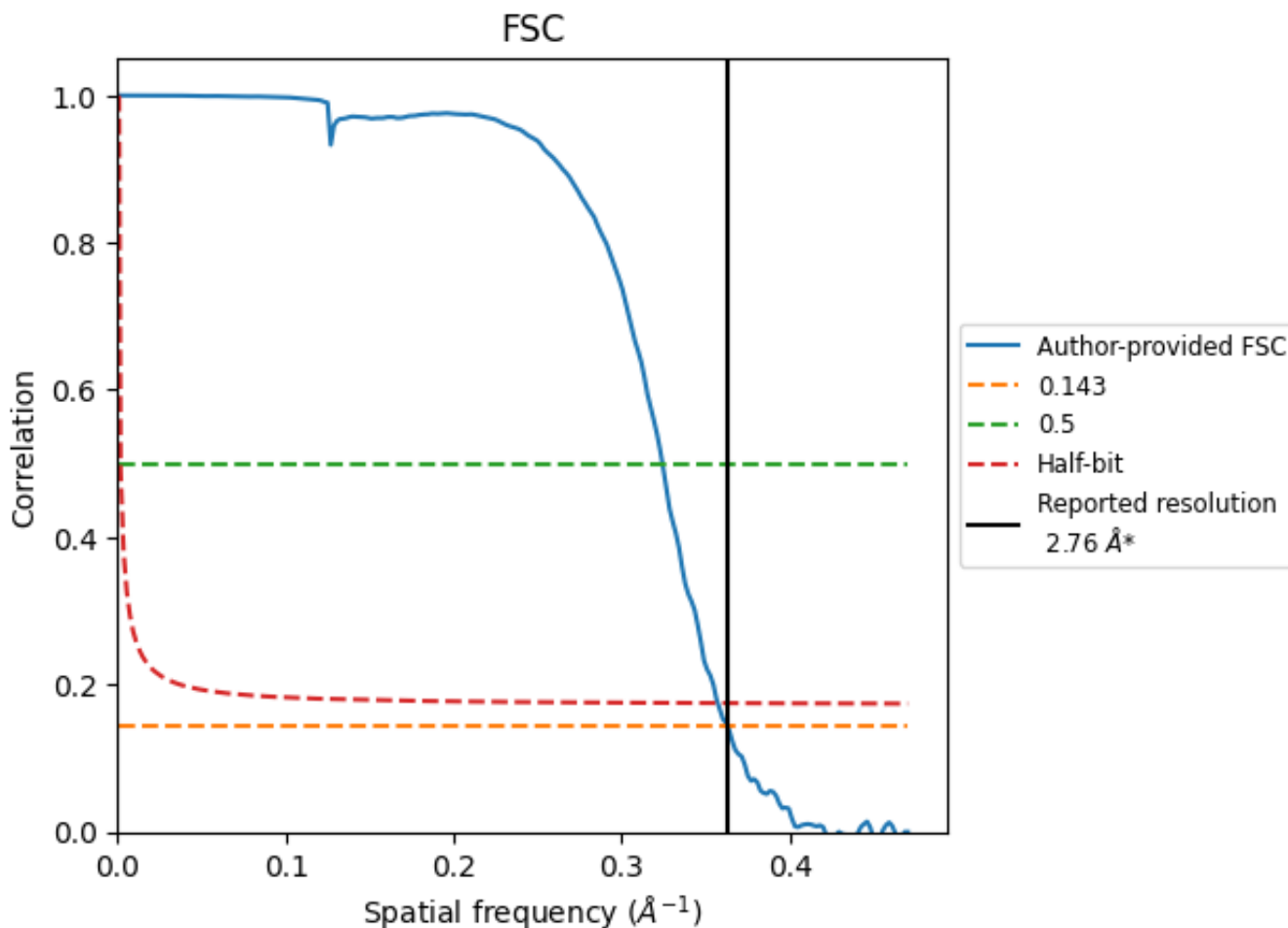


*Reported resolution corresponds to spatial frequency of 0.362\AA^{-1}

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 0.362 Å⁻¹

8.2 Resolution estimates [i](#)

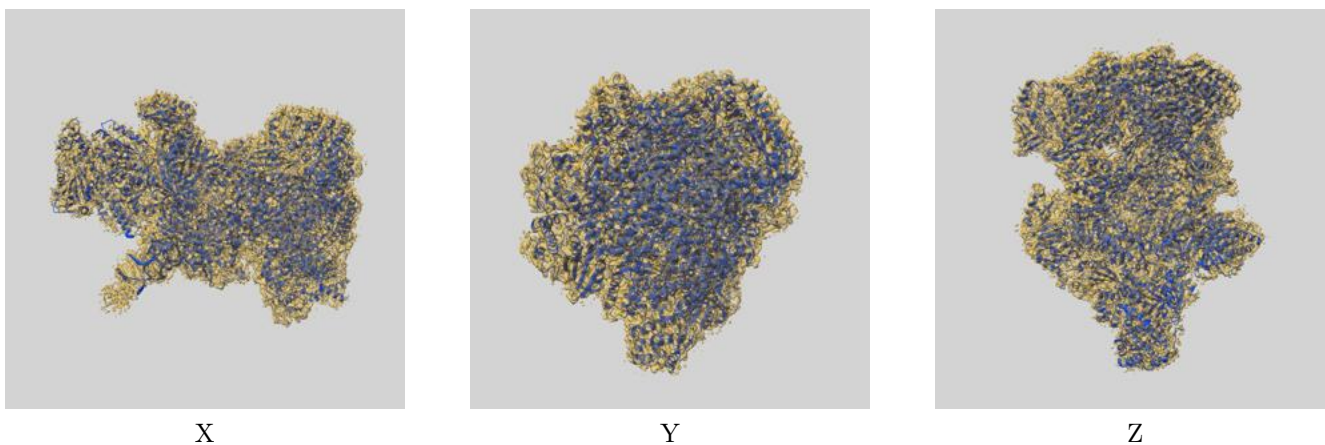
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.76	-	-
Author-provided FSC curve	2.76	3.08	2.80
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

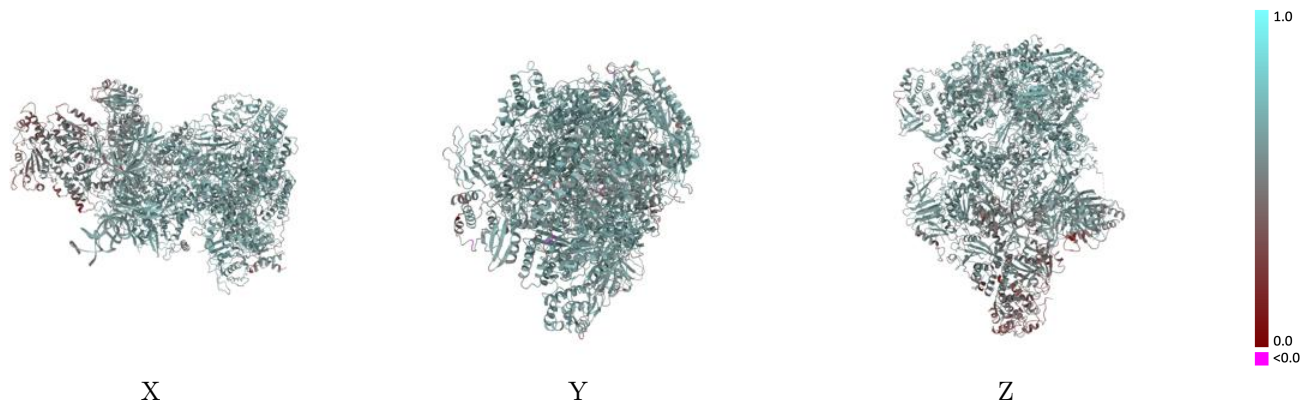
This section contains information regarding the fit between EMDB map EMD-4868 and PDB model 6RFL. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



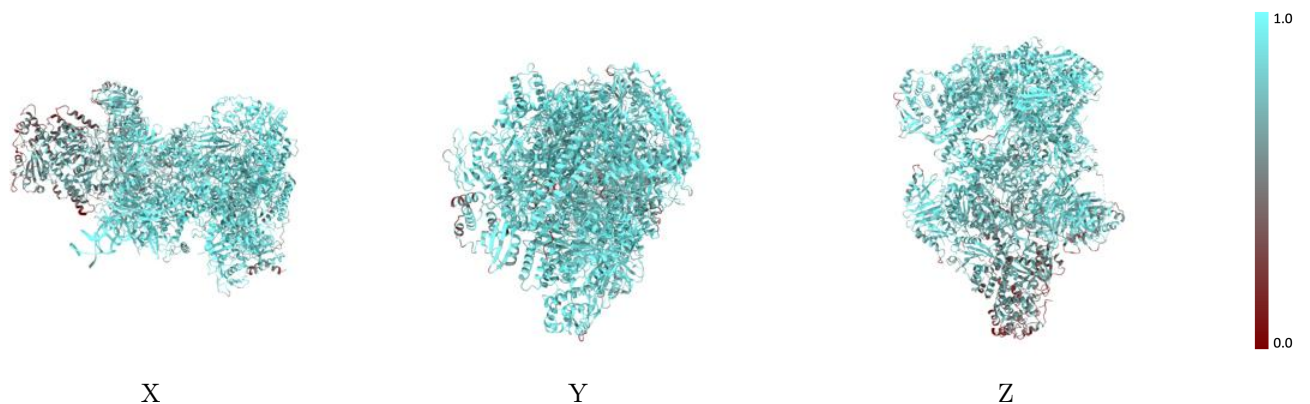
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



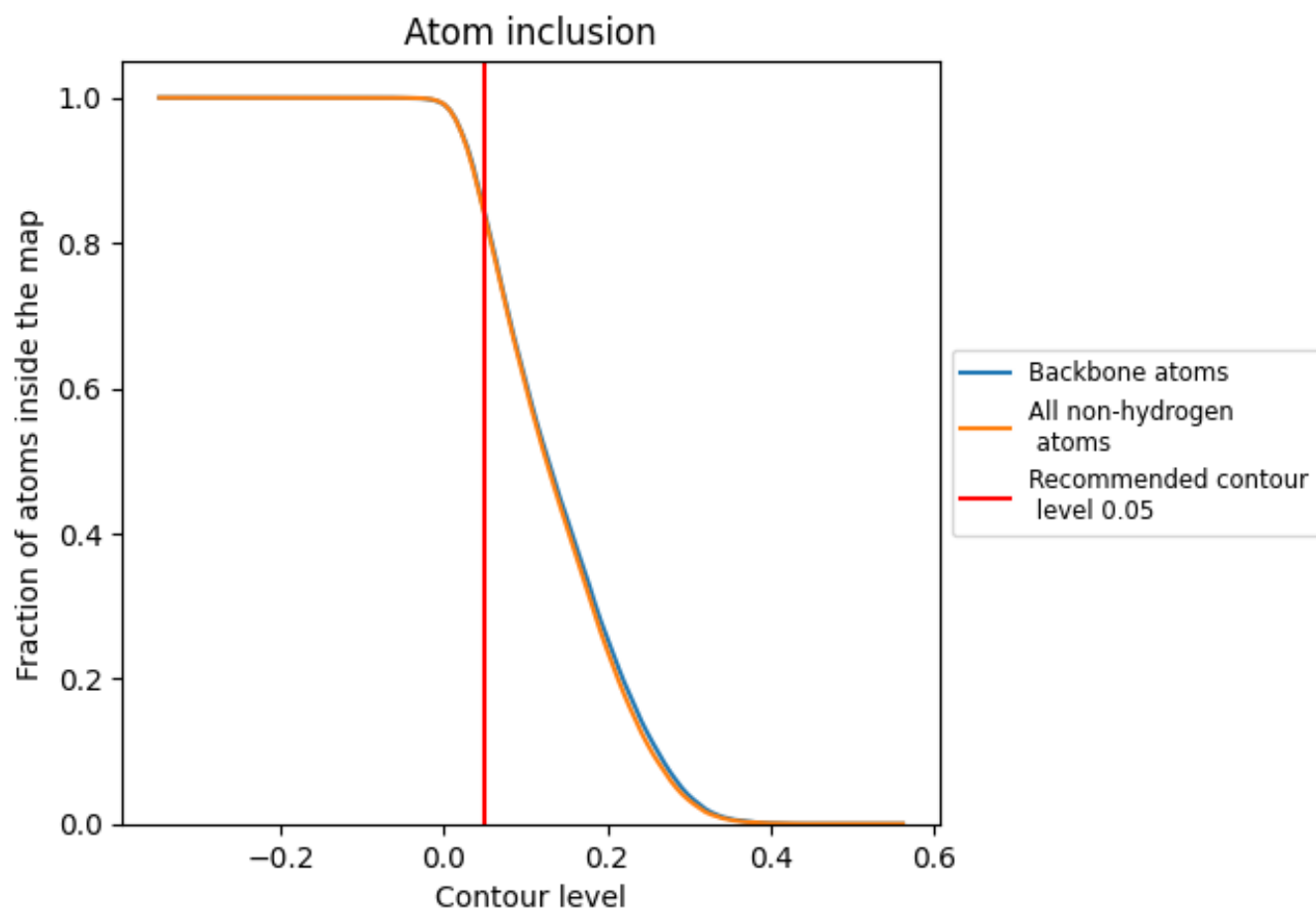
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).



































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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8386	 0.5720
A	 0.9092	 0.6090
B	 0.9240	 0.6120
C	 0.9147	 0.6000
E	 0.9085	 0.5940
F	 0.9422	 0.6250
G	 0.8994	 0.5960
I	 0.8349	 0.5680
J	 0.9439	 0.6110
K	 0.8381	 0.5710
L	 0.5189	 0.4060
O	 0.7178	 0.5210
Q	 0.7874	 0.5500
R	 0.8383	 0.5670
S	 0.6677	 0.5120
U	 0.9305	 0.5630
Y	 0.8058	 0.5610

