



Full wwPDB EM Validation Report ⓘ

Apr 25, 2026 – 10:54 PM EDT

PDB ID : 9PD3 / pdb_00009pd3
EMDB ID : EMD-71524
Title : NER dual incision complex - DuIS
Authors : Li, C.L.; Kim, J.; Yang, W.
Deposited on : 2025-06-30
Resolution : 3.30 Å(reported)
Based on initial models : 1l1o, 8ebt, 6sxa

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

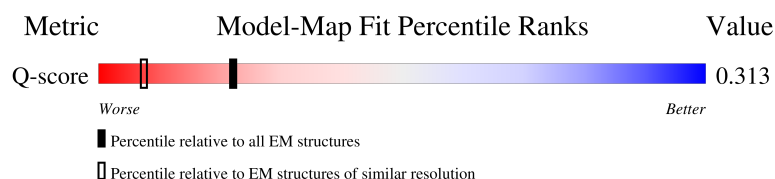
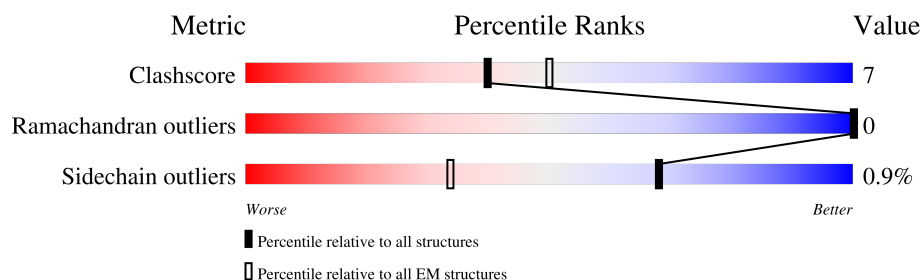
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	782	
2	B	768	
3	C	548	
4	D	462	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	395	
6	F	308	
7	G	71	
8	H	940	
9	K	273	
10	L	51	
11	M	53	
12	N	616	
13	O	270	
14	P	121	
15	Q	916	
16	R	295	
17	S	1186	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 35072 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 TFIIF basal transcription factor complex helicase XPB subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	613	Total	C	N	O	S	0	0
			4947	3159	856	902	30		

- Molecule 2 is a protein called General transcription and DNA repair factor IIF helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	702	Total	C	N	O	S	0	0
			5659	3622	985	1023	29		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	761	ASP	-	expression tag	UNP P18074
B	762	TYR	-	expression tag	UNP P18074
B	763	LYS	-	expression tag	UNP P18074
B	764	ASP	-	expression tag	UNP P18074
B	765	ASP	-	expression tag	UNP P18074
B	766	ASP	-	expression tag	UNP P18074
B	767	ASP	-	expression tag	UNP P18074
B	768	LYS	-	expression tag	UNP P18074

- Molecule 3 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	133	Total	C	N	O	S	0	0
			1076	684	185	200	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	428	Total	C	N	O	S	0	0
			3441	2218	597	613	13		

- Molecule 5 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	342	Total	C	N	O	S	0	0
			2677	1694	456	501	26		

- Molecule 6 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	255	Total	C	N	O	S	0	0
			2013	1289	333	372	19		

- Molecule 7 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	66	Total	C	N	O	S	0	0
			522	337	82	100	3		

- Molecule 8 is a protein called DNA repair protein complementing XP-C cells.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	17	Total	C	N	O	0	0
			131	80	27	24		

- Molecule 9 is a protein called DNA repair protein complementing XP-A cells.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	208	Total	C	N	O	S	0	0
			1716	1073	311	316	16		

- Molecule 10 is a DNA chain called DNA lesion strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	38	Total	C	N	O	P	0	0
			770	368	133	231	38		

- Molecule 11 is a DNA chain called DNA normal strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	32	Total	C	N	O	P	0	0
			665	315	126	192	32		

- Molecule 12 is a protein called Replication protein A 70 kDa DNA-binding subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	177	Total	C	N	O	S	0	0
			1459	918	252	278	11		

- Molecule 13 is a protein called Replication protein A 32 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	189	Total	C	N	O	S	0	0
			1485	937	254	286	8		

- Molecule 14 is a protein called Replication protein A 14 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	121	Total	C	N	O	S	0	0
			950	610	155	177	8		

- Molecule 15 is a protein called DNA repair endonuclease XPF.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	713	Total	C	N	O	S	0	0
			5461	3501	949	990	21		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	703	ASP	GLY	variant	UNP Q92889

- Molecule 16 is a protein called DNA excision repair protein ERCC-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	196	Total	C	N	O	S	0	0
			1400	901	240	255	4		

- Molecule 17 is a protein called DNA excision repair protein ERCC-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	83	Total	C	N	O	S	0	0
			685	427	115	140	3		

There are 3 discrepancies between the modelled and reference sequences:

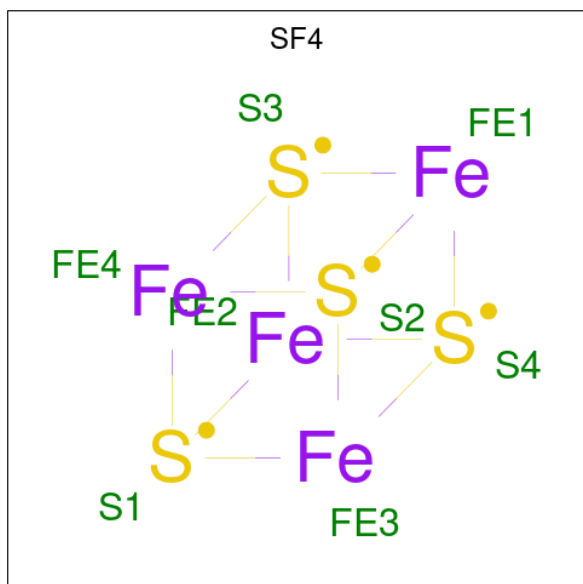
Chain	Residue	Modelled	Actual	Comment	Reference
S	812	ASN	ASP	conflict	UNP P28715

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
S	1053	ARG	GLY	variant	UNP P28715
S	1080	ARG	GLY	variant	UNP P28715

- Molecule 18 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

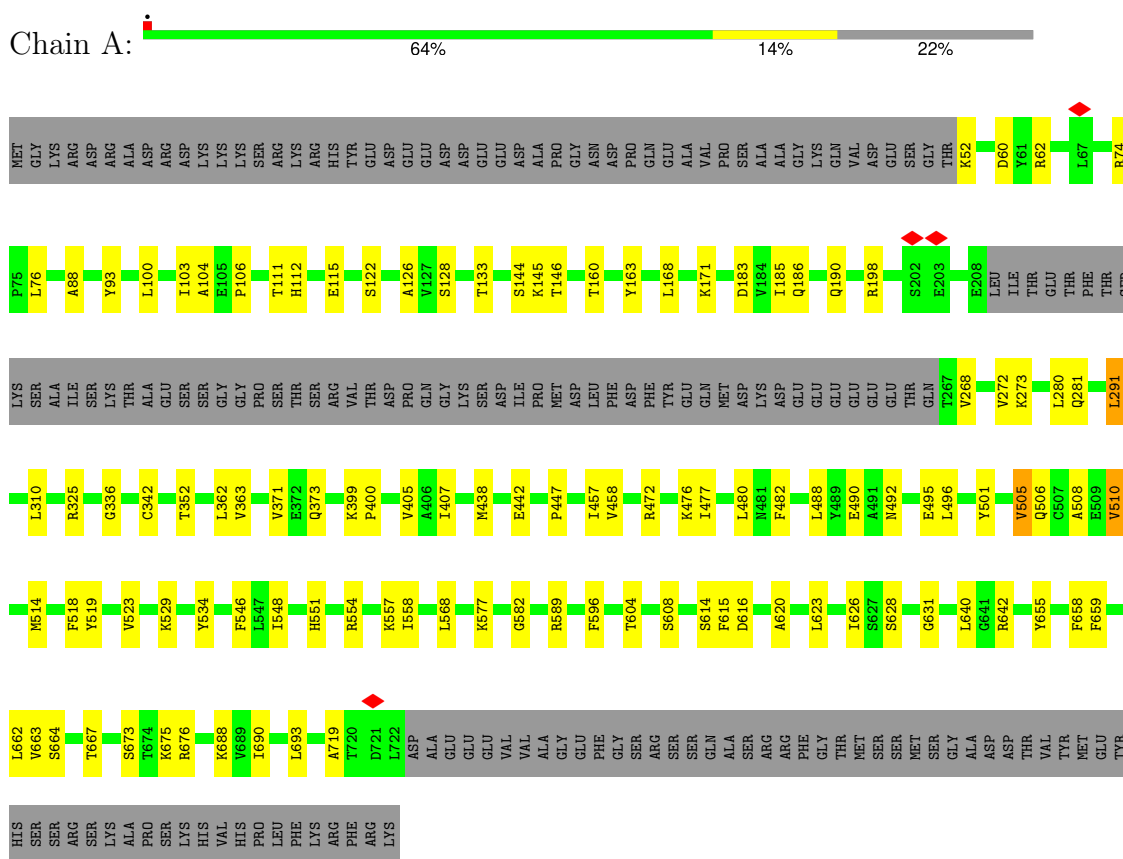
- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	E	3	Total	Zn	0
			3	3	
19	F	2	Total	Zn	0
			2	2	
19	K	1	Total	Zn	0
			1	1	
19	N	1	Total	Zn	0
			1	1	

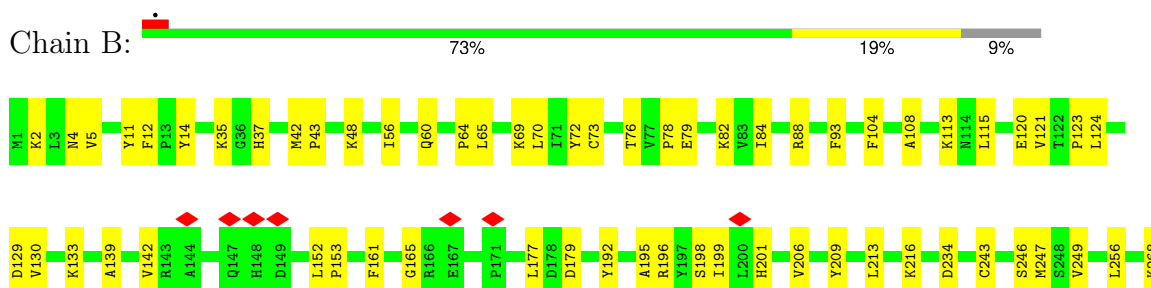
3 Residue-property plots

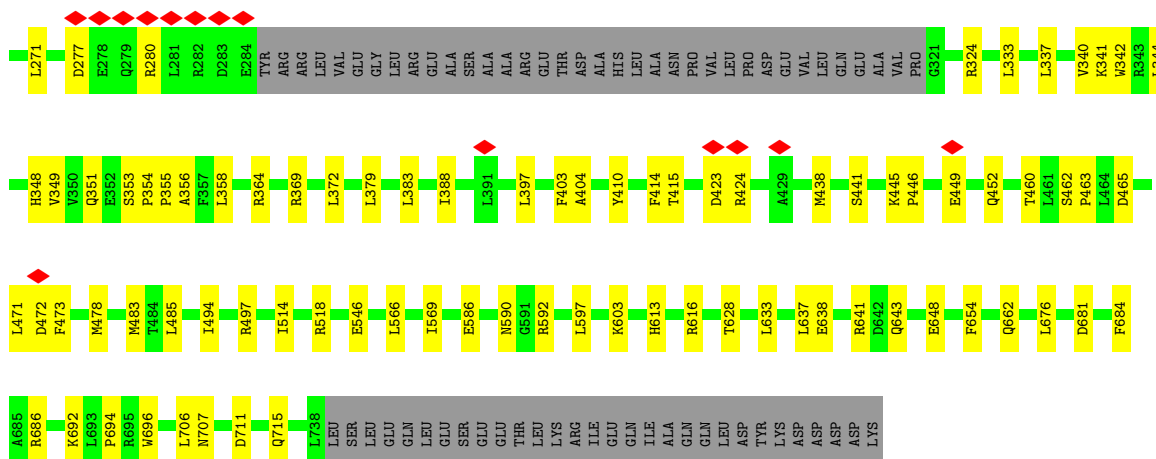
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

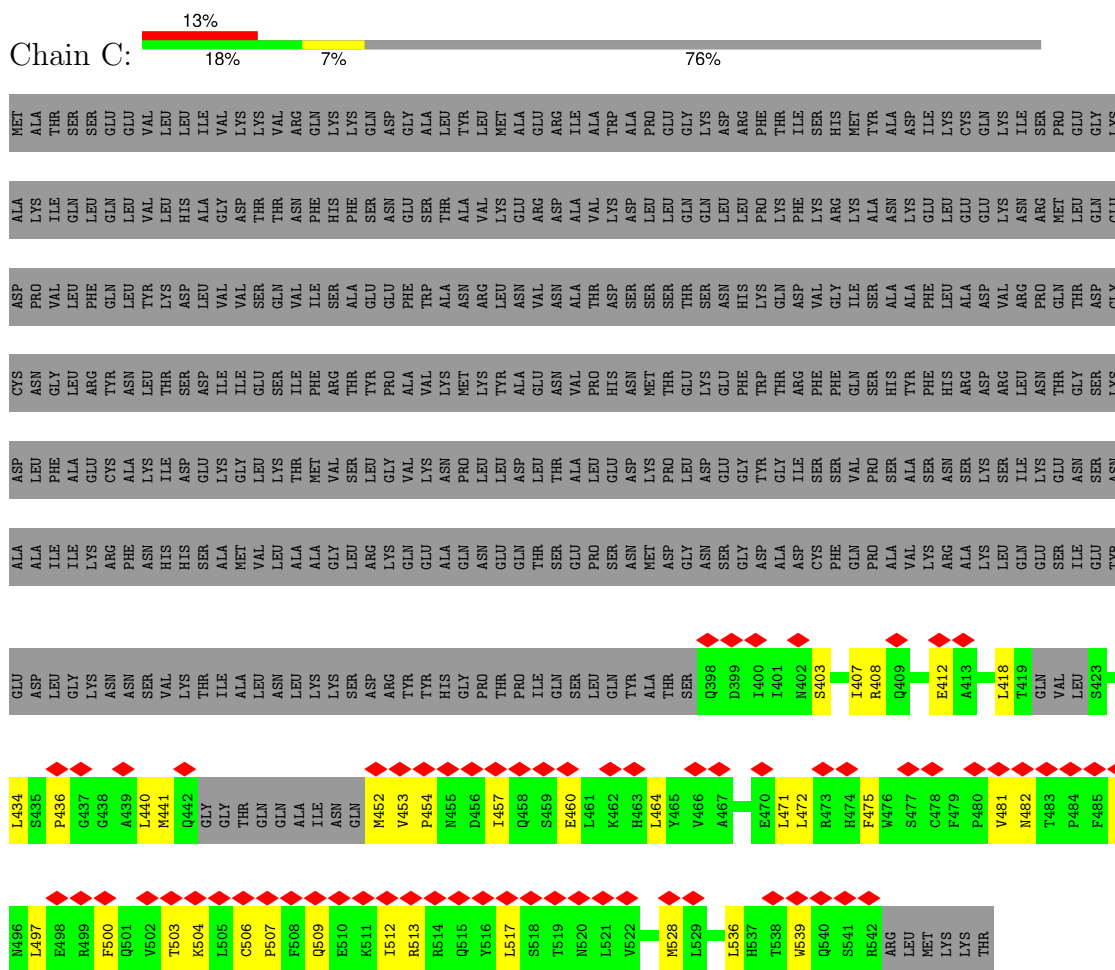


- Molecule 2: General transcription and DNA repair factor IHH helicase subunit XPD

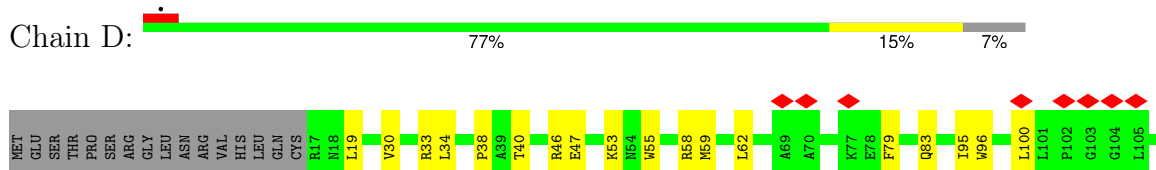




- Molecule 3: General transcription factor IIH subunit 1



- Molecule 4: General transcription factor IIH subunit 4, p52



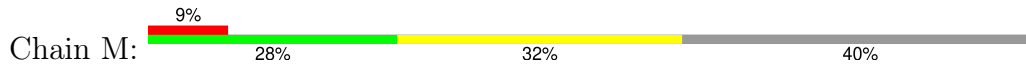
89% 7%

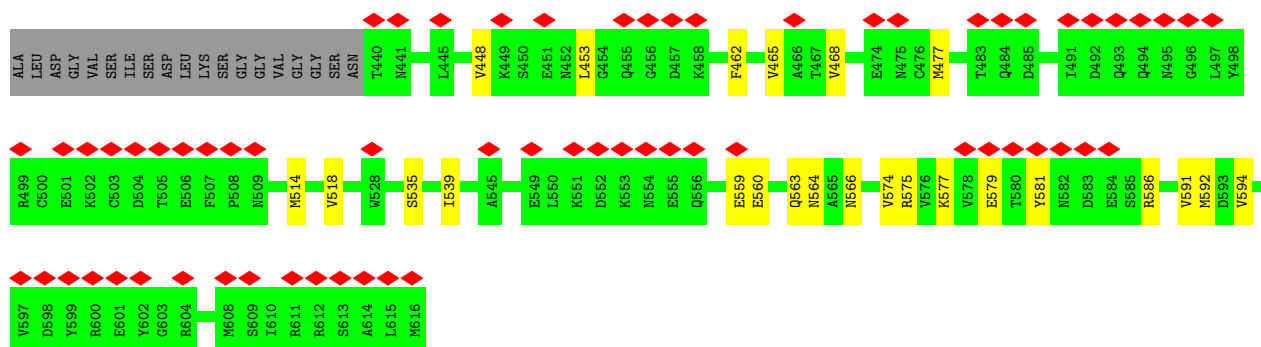


98%

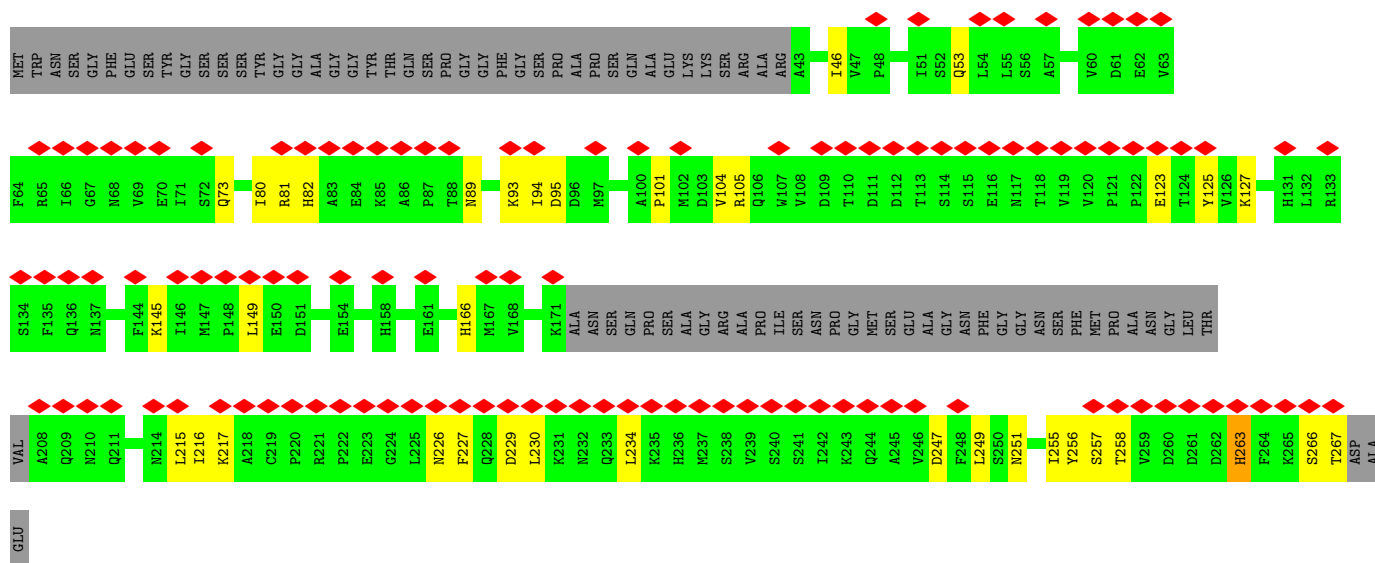
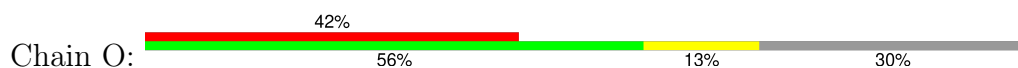


Chain K:

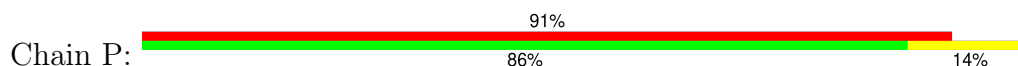




• Molecule 13: Replication protein A 32 kDa subunit

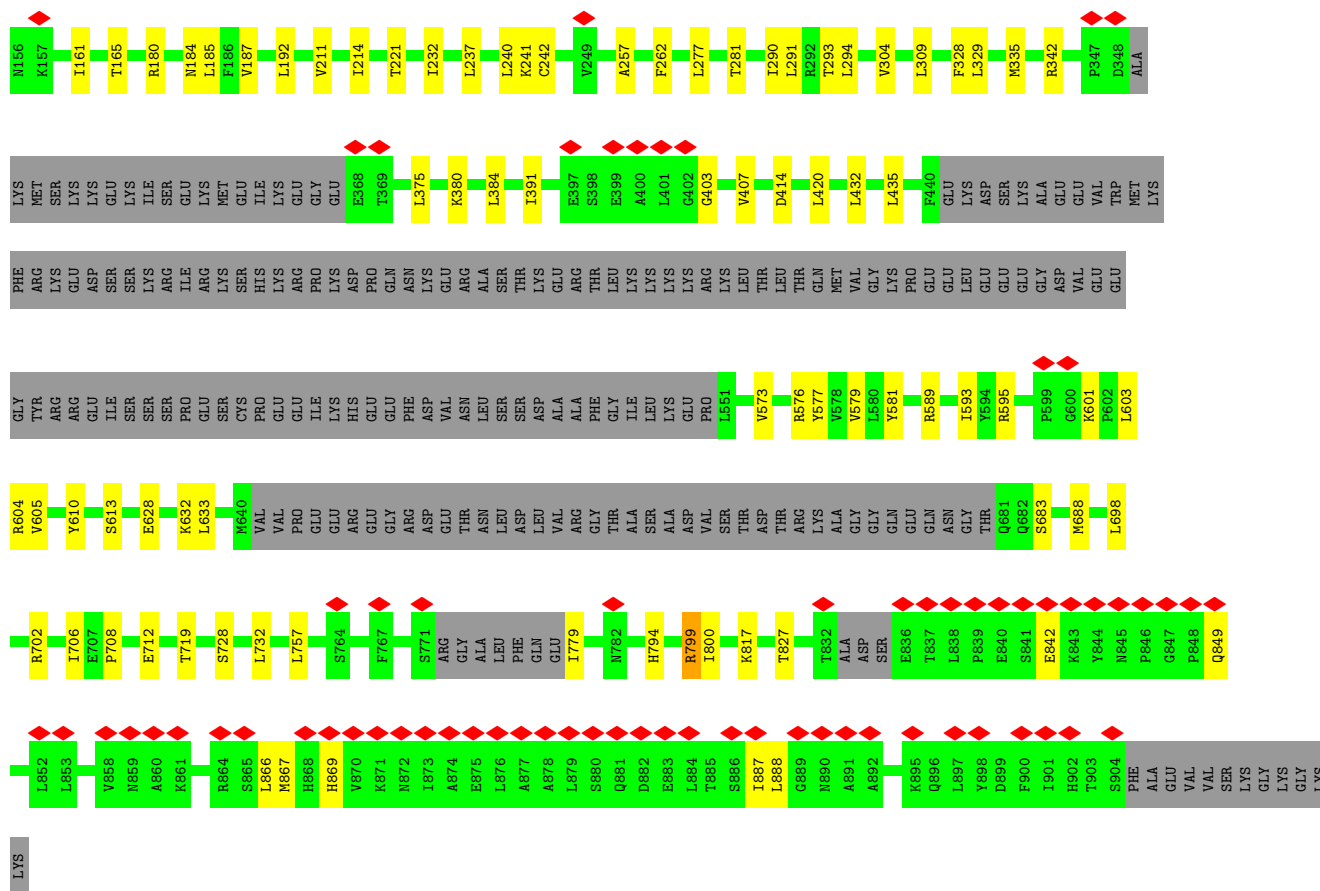


• Molecule 14: Replication protein A 14 kDa subunit

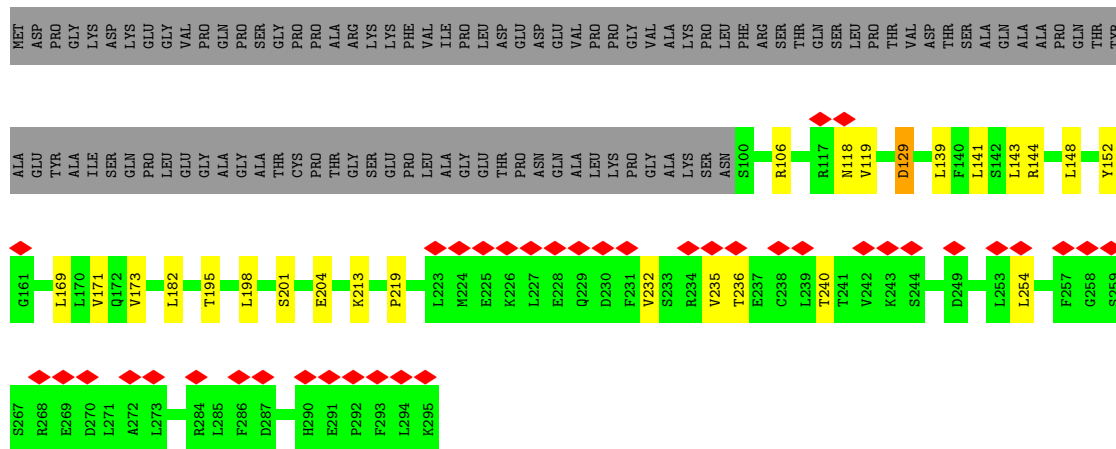


• Molecule 15: DNA repair endonuclease XPF





• Molecule 16: DNA excision repair protein ERCC-1



• Molecule 17: DNA excision repair protein ERCC-5





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	161019	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52.5	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.052	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	266.56, 266.56, 266.56	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.833, 0.833, 0.833	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, 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	A	0.08	0/5051	0.23	0/6822
2	B	0.09	0/5780	0.24	0/7821
3	C	0.11	0/1097	0.26	0/1480
4	D	0.08	0/3519	0.20	0/4765
5	E	0.09	0/2736	0.25	0/3706
6	F	0.11	0/2049	0.28	0/2776
7	G	0.07	0/528	0.19	0/713
8	H	0.16	0/133	0.31	0/180
9	K	0.09	0/1743	0.22	0/2322
10	L	0.16	0/860	0.35	0/1323
11	M	0.16	0/747	0.33	0/1153
12	N	0.07	0/1486	0.21	0/2001
13	O	0.10	0/1511	0.24	0/2051
14	P	0.06	0/970	0.18	0/1310
15	Q	0.09	0/5570	0.23	0/7583
16	R	0.09	0/1431	0.26	0/1968
17	S	0.09	0/695	0.24	0/929
All	All	0.09	0/35906	0.24	0/48903

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4947	0	4993	68	0
2	B	5659	0	5699	93	0
3	C	1076	0	1078	27	0
4	D	3441	0	3486	43	0
5	E	2677	0	2645	49	0
6	F	2013	0	2030	52	0
7	G	522	0	531	3	0
8	H	131	0	127	4	0
9	K	1716	0	1723	35	0
10	L	770	0	430	9	0
11	M	665	0	361	11	0
12	N	1459	0	1416	12	0
13	O	1485	0	1488	26	0
14	P	950	0	952	11	0
15	Q	5461	0	5326	61	0
16	R	1400	0	1292	20	0
17	S	685	0	662	20	0
18	B	8	0	0	0	0
19	E	3	0	0	0	0
19	F	2	0	0	0	0
19	K	1	0	0	0	0
19	N	1	0	0	0	0
All	All	35072	0	34239	490	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 7.

All (490) 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)
17:S:202:HIS:HE1	17:S:254:MET:HG3	1.08	1.17
17:S:202:HIS:CE1	17:S:254:MET:HG3	1.85	1.11
5:E:272:SER:HB3	5:E:275:HIS:HD2	1.18	1.08
5:E:272:SER:HB3	5:E:275:HIS:CD2	1.95	1.00
2:B:35:LYS:HD2	2:B:452:GLN:HE21	1.42	0.82
6:F:257:CYS:SG	6:F:258:HIS:N	2.54	0.81
4:D:148:LEU:HD21	4:D:284:THR:HA	1.63	0.80
2:B:35:LYS:HD2	2:B:452:GLN:NE2	1.97	0.80
17:S:202:HIS:CE1	17:S:254:MET:CG	2.64	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:VAL:HG21	1:A:280:LEU:HD22	1.66	0.78
1:A:111:THR:HG23	1:A:112:HIS:ND1	1.99	0.77
13:O:89:ASN:ND2	13:O:105:ARG:HD3	2.00	0.77
5:E:272:SER:CB	5:E:275:HIS:HD2	1.95	0.76
15:Q:779:ILE:HA	16:R:118:ASN:HD21	1.49	0.76
17:S:202:HIS:HE1	17:S:254:MET:CG	1.94	0.76
2:B:353:SER:HB2	2:B:356:ALA:HB3	1.68	0.76
2:B:35:LYS:CD	2:B:452:GLN:HE21	2.01	0.73
15:Q:757:LEU:HB3	15:Q:800:ILE:HG22	1.72	0.72
15:Q:779:ILE:HD12	16:R:118:ASN:ND2	2.04	0.72
8:H:903:SER:HB2	8:H:906:GLN:HE21	1.55	0.71
5:E:210:VAL:HG23	5:E:213:ARG:HH12	1.54	0.71
2:B:483:MET:HE2	2:B:485:LEU:HD21	1.73	0.70
2:B:546:GLU:OE2	17:S:240:LYS:NZ	2.25	0.70
1:A:568:LEU:HD13	1:A:608:SER:HB3	1.74	0.69
4:D:96:TRP:HB3	4:D:110:LEU:HD23	1.74	0.69
12:N:566:ASN:HB3	13:O:145:LYS:HE3	1.73	0.69
3:C:454:PRO:HD2	3:C:457:ILE:HD12	1.75	0.68
2:B:121:VAL:HG23	2:B:133:LYS:HB3	1.76	0.67
9:K:154:ASP:O	9:K:189:ARG:NH1	2.28	0.67
1:A:582:GLY:O	1:A:589:ARG:NH2	2.27	0.67
3:C:472:LEU:CD1	3:C:528:MET:HE2	2.25	0.66
9:K:25:ARG:HE	9:K:28:ILE:HD11	1.61	0.66
9:K:132:ALA:HA	9:K:136:HIS:HB2	1.78	0.65
13:O:217:LYS:HD3	13:O:266:SER:HB2	1.78	0.65
1:A:371:VAL:HG22	1:A:407:ILE:HG22	1.79	0.65
15:Q:403:GLY:O	15:Q:576:ARG:NH1	2.30	0.65
1:A:281:GLN:NE2	1:A:482:PHE:O	2.30	0.65
2:B:424:ARG:O	17:S:251:GLN:NE2	2.30	0.65
2:B:35:LYS:CD	2:B:452:GLN:NE2	2.60	0.64
9:K:160:PRO:O	9:K:189:ARG:NH2	2.30	0.64
2:B:586:GLU:O	2:B:590:ASN:ND2	2.31	0.63
4:D:19:LEU:HD23	4:D:47:GLU:HG3	1.81	0.63
1:A:62:ARG:HA	4:D:339:PRO:HG3	1.81	0.62
1:A:185:ILE:HD12	1:A:268:VAL:HG13	1.81	0.62
12:N:477:MET:HE2	12:N:514:MET:HE2	1.81	0.62
6:F:20:ILE:HG22	6:F:24:LYS:HE3	1.81	0.62
13:O:216:ILE:HG22	13:O:266:SER:HB3	1.81	0.62
15:Q:375:LEU:HD23	15:Q:432:LEU:HB3	1.81	0.62
13:O:247:ASP:O	13:O:251:ASN:ND2	2.28	0.61
15:Q:211:VAL:HG12	15:Q:605:VAL:HB	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:192:LEU:HD21	15:Q:633:LEU:HB3	1.83	0.61
15:Q:866:LEU:HD11	15:Q:888:LEU:HA	1.82	0.61
5:E:68:SER:HB3	5:E:143:PRO:HD3	1.81	0.61
5:E:159:MET:HB3	5:E:165:ARG:HE	1.66	0.60
15:Q:842:GLU:OE1	15:Q:849:GLN:NE2	2.34	0.60
16:R:182:LEU:HD21	16:R:198:LEU:HD21	1.82	0.60
15:Q:688:MET:HE1	15:Q:708:PRO:HB2	1.84	0.60
1:A:554:ARG:HE	5:E:77:LYS:HG2	1.67	0.59
2:B:603:LYS:HE3	10:L:59:DT:H5"	1.84	0.59
15:Q:779:ILE:HA	16:R:118:ASN:ND2	2.16	0.59
1:A:106:PRO:HG3	1:A:490:GLU:HG2	1.85	0.59
9:K:31:LYS:HB3	13:O:256:TYR:HB2	1.85	0.59
15:Q:706:ILE:HG22	15:Q:708:PRO:HD3	1.84	0.58
3:C:482:ASN:H	3:C:486:LEU:HD12	1.69	0.58
15:Q:125:SER:O	15:Q:155:LYS:NZ	2.32	0.58
17:S:202:HIS:NE2	17:S:250:VAL:HG12	2.18	0.58
9:K:27:SER:HA	9:K:30:ARG:HE	1.68	0.58
4:D:34:LEU:HB3	4:D:40:THR:HG21	1.84	0.57
12:N:574:VAL:HG22	12:N:591:VAL:HG12	1.85	0.57
3:C:403:SER:O	3:C:407:ILE:HG12	2.04	0.57
9:K:67:LYS:HE3	16:R:144:ARG:HH12	1.70	0.57
3:C:440:LEU:HD11	6:F:215:LEU:HD11	1.85	0.57
3:C:472:LEU:HD11	3:C:528:MET:HE2	1.86	0.57
6:F:13:ILE:HB	6:F:59:VAL:HG12	1.86	0.57
14:P:45:ASP:OD2	14:P:100:ASN:ND2	2.37	0.57
5:E:323:HIS:NE2	6:F:178:MET:HB3	2.20	0.57
1:A:198:ARG:O	1:A:273:LYS:NZ	2.38	0.57
4:D:143:ARG:HH21	4:D:147:SER:HB2	1.69	0.57
6:F:160:ARG:NH2	6:F:231:PHE:O	2.39	0.56
15:Q:214:ILE:HG12	17:S:360:GLU:HB2	1.87	0.56
17:S:205:LEU:HD12	17:S:206:THR:N	2.20	0.56
4:D:275:LYS:HB2	4:D:278:SER:HB2	1.88	0.56
6:F:68:ARG:HB2	6:F:118:LEU:HD12	1.87	0.56
1:A:447:PRO:HD3	1:A:480:LEU:HD21	1.86	0.56
5:E:255:PRO:HG3	5:E:312:LEU:HD13	1.88	0.56
6:F:43:VAL:HG11	6:F:224:LEU:HD21	1.88	0.56
15:Q:277:LEU:HD13	15:Q:281:THR:HB	1.88	0.55
15:Q:595:ARG:NH1	15:Q:601:LYS:O	2.38	0.55
6:F:13:ILE:HD13	6:F:162:LEU:HB3	1.88	0.55
15:Q:304:VAL:HG11	15:Q:435:LEU:HB3	1.88	0.55
4:D:421:LEU:HD21	4:D:455:TRP:HB2	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:255:CYS:SG	6:F:256:PHE:N	2.80	0.55
5:E:152:ALA:O	5:E:156:LEU:HB2	2.06	0.55
4:D:308:VAL:HB	4:D:316:TYR:HB2	1.89	0.55
6:F:248:HIS:O	6:F:248:HIS:ND1	2.40	0.55
13:O:226:ASN:ND2	13:O:229:ASP:OD2	2.39	0.55
2:B:616:ARG:O	2:B:676:LEU:N	2.38	0.55
5:E:59:ARG:NE	5:E:95:TYR:OH	2.40	0.55
2:B:42:MET:HB3	2:B:48:LYS:HD3	1.89	0.54
2:B:209:TYR:OH	2:B:234:ASP:O	2.24	0.54
2:B:681:ASP:HB3	2:B:684:PHE:HD2	1.70	0.54
2:B:246:SER:OG	2:B:247:MET:SD	2.60	0.54
2:B:35:LYS:CG	2:B:452:GLN:HE21	2.20	0.54
12:N:577:LYS:NZ	12:N:579:GLU:OE2	2.39	0.54
2:B:372:LEU:HD11	2:B:404:ALA:HB1	1.90	0.54
4:D:100:LEU:HD23	4:D:100:LEU:H	1.72	0.54
14:P:64:SER:H	14:P:86:GLN:NE2	2.06	0.54
15:Q:118:PHE:HA	15:Q:123:ILE:HD13	1.90	0.54
4:D:30:VAL:HG22	4:D:33:ARG:HH21	1.73	0.54
2:B:256:LEU:HD11	2:B:344:LEU:HD12	1.90	0.54
6:F:38:ILE:O	6:F:42:MET:HG2	2.08	0.54
15:Q:57:CYS:SG	15:Q:58:LEU:N	2.81	0.54
1:A:103:ILE:HA	1:A:126:ALA:HB2	1.89	0.53
4:D:59:MET:HG3	4:D:62:LEU:HD12	1.88	0.53
5:E:154:GLN:HA	5:E:157:LYS:HZ2	1.74	0.53
6:F:32:PHE:HA	6:F:36:LYS:HD2	1.90	0.53
17:S:202:HIS:CD2	17:S:250:VAL:HG12	2.42	0.53
2:B:445:LYS:HD3	2:B:472:ASP:HB3	1.91	0.53
9:K:115:SER:H	9:K:118:MET:HB3	1.74	0.53
6:F:273:SER:OG	6:F:282:CYS:SG	2.66	0.53
2:B:124:LEU:HD23	2:B:129:ASP:HB3	1.90	0.53
2:B:243:CYS:O	2:B:246:SER:OG	2.27	0.53
2:B:379:LEU:HD11	2:B:397:LEU:HG	1.88	0.53
3:C:464:LEU:HD22	3:C:504:LYS:HZ2	1.73	0.53
15:Q:143:CYS:SG	15:Q:144:GLN:N	2.80	0.53
2:B:88:ARG:NH2	2:B:179:ASP:OD2	2.41	0.53
4:D:291:SER:OG	6:F:53:ARG:NH1	2.42	0.53
14:P:64:SER:O	14:P:86:GLN:NE2	2.41	0.53
2:B:79:GLU:N	2:B:79:GLU:OE1	2.41	0.53
3:C:431:ILE:HG13	4:D:62:LEU:HD11	1.91	0.53
5:E:196:VAL:HB	5:E:211:LEU:HD21	1.89	0.53
11:M:51:DC:H2'	11:M:52:DT:H71	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:HIS:HD2	2:B:473:PHE:HB2	1.74	0.53
17:S:205:LEU:HD22	17:S:247:ILE:HG12	1.91	0.53
13:O:249:LEU:HB3	13:O:255:ILE:HG12	1.89	0.53
15:Q:328:PHE:HB3	15:Q:329:LEU:HD12	1.89	0.52
6:F:194:CYS:HB2	6:F:231:PHE:HE2	1.74	0.52
17:S:202:HIS:HA	17:S:205:LEU:HG	1.90	0.52
9:K:123:LEU:HD12	9:K:124:PRO:HD2	1.92	0.52
3:C:475:PHE:HB2	3:C:493:MET:SD	2.50	0.52
9:K:120:HIS:CD2	9:K:121:PHE:CE1	2.98	0.52
1:A:492:ASN:HB3	1:A:495:GLU:HG2	1.92	0.52
12:N:560:GLU:OE2	12:N:564:ASN:ND2	2.42	0.52
13:O:80:ILE:O	13:O:123:GLU:N	2.39	0.52
1:A:442:GLU:OE2	1:A:614:SER:OG	2.28	0.52
1:A:496:LEU:HD22	1:A:501:TYR:HD2	1.75	0.52
4:D:265:LEU:HD22	4:D:270:LEU:HD21	1.91	0.52
2:B:546:GLU:HA	17:S:237:LEU:HD21	1.91	0.51
3:C:464:LEU:HD13	3:C:504:LYS:HG2	1.92	0.51
9:K:162:LEU:HD23	9:K:185:GLN:HB3	1.93	0.51
13:O:125:TYR:HB3	13:O:149:LEU:HD12	1.92	0.51
15:Q:185:LEU:HB3	15:Q:187:VAL:HG22	1.93	0.51
12:N:581:TYR:HE1	12:N:586:ARG:HD3	1.76	0.51
1:A:514:MET:HE3	1:A:518:PHE:HB3	1.91	0.51
2:B:566:LEU:HG	2:B:592:ARG:HE	1.75	0.51
5:E:160:PRO:HG3	5:E:313:VAL:HG13	1.93	0.51
3:C:408:ARG:NH2	6:F:122:SER:O	2.40	0.51
11:M:63:DC:H2"	11:M:64:DG:C8	2.45	0.51
3:C:471:LEU:HD13	3:C:497:LEU:HD23	1.93	0.51
2:B:256:LEU:HD13	2:B:341:LYS:HG2	1.93	0.51
9:K:141:LYS:HE2	9:K:145:LYS:HD2	1.93	0.51
2:B:152:LEU:HG	2:B:153:PRO:HD2	1.93	0.51
5:E:252:MET:HB3	5:E:313:VAL:HG21	1.92	0.51
1:A:505:VAL:HG21	1:A:640:LEU:HD11	1.93	0.51
5:E:167:VAL:HB	5:E:196:VAL:HG22	1.93	0.51
1:A:457:ILE:HG13	1:A:458:VAL:HG23	1.93	0.51
5:E:195:ARG:HA	5:E:215:THR:HG22	1.92	0.51
15:Q:62:LEU:HB2	15:Q:133:VAL:HG12	1.92	0.51
15:Q:683:SER:O	15:Q:817:LYS:NZ	2.45	0.50
15:Q:799:ARG:HA	16:R:195:THR:HG22	1.92	0.50
1:A:623:LEU:HB3	1:A:659:PHE:HB2	1.94	0.50
2:B:351:GLN:N	2:B:351:GLN:OE1	2.44	0.50
12:N:448:VAL:HG13	12:N:453:LEU:HB3	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:462:SER:HB2	2:B:463:PRO:HD3	1.92	0.50
4:D:198:SER:HB2	4:D:358:GLY:HA3	1.93	0.50
5:E:257:HIS:CG	5:E:257:HIS:O	2.65	0.50
15:Q:595:ARG:HG2	15:Q:603:LEU:HD23	1.93	0.50
9:K:149:LEU:HD11	9:K:204:LYS:HG3	1.94	0.50
6:F:59:VAL:HG23	6:F:70:LEU:HB2	1.92	0.50
10:L:31:DC:H2"	10:L:32:DG:C8	2.46	0.50
15:Q:294:LEU:HD13	15:Q:309:LEU:HD22	1.94	0.50
2:B:249:VAL:HG21	2:B:403:PHE:HB2	1.94	0.50
13:O:101:PRO:HG3	14:P:5:MET:HE3	1.94	0.50
1:A:133:THR:OG1	1:A:160:THR:CG2	2.60	0.49
2:B:465:ASP:HA	2:B:478:MET:HE1	1.94	0.49
4:D:216:MET:HE2	4:D:237:LEU:HD21	1.94	0.49
15:Q:335:MET:SD	15:Q:335:MET:N	2.81	0.49
13:O:81:ARG:NH1	13:O:123:GLU:OE1	2.45	0.49
1:A:133:THR:OG1	1:A:160:THR:HG21	2.12	0.49
5:E:212:ALA:O	5:E:217:GLY:N	2.38	0.49
2:B:597:LEU:HD23	2:B:597:LEU:H	1.77	0.49
16:R:129:ASP:HB2	16:R:139:LEU:HD23	1.94	0.49
4:D:53:LYS:NZ	6:F:51:MET:O	2.41	0.49
12:N:575:ARG:HB2	12:N:592:MET:HE3	1.94	0.49
9:K:67:LYS:HZ2	16:R:148:LEU:HD13	1.76	0.49
13:O:82:HIS:HB3	13:O:93:LYS:HG3	1.95	0.49
1:A:472:ARG:NH2	11:M:59:DG:OP2	2.46	0.49
2:B:358:LEU:HD21	2:B:369:ARG:HB2	1.95	0.49
6:F:177:PHE:O	6:F:181:ILE:HG12	2.13	0.49
9:K:122:ASP:HB2	9:K:163:LYS:HE2	1.94	0.49
12:N:468:VAL:HG13	12:N:518:VAL:HG13	1.94	0.49
2:B:198:SER:HA	2:B:201:HIS:CE1	2.48	0.48
3:C:434:LEU:HD23	3:C:440:LEU:HD13	1.94	0.48
1:A:310:LEU:HD11	1:A:352:THR:HG23	1.95	0.48
2:B:333:LEU:HD13	2:B:397:LEU:HD11	1.95	0.48
2:B:460:THR:HG21	2:B:662:GLN:HA	1.95	0.48
4:D:396:LEU:HD21	8:H:908:ARG:HG3	1.95	0.48
6:F:181:ILE:HG21	6:F:206:ALA:HA	1.94	0.48
9:K:158:ARG:HH12	9:K:193:VAL:HG23	1.77	0.48
1:A:506:GLN:HB2	1:A:655:TYR:CG	2.48	0.48
1:A:128:SER:HA	1:A:163:TYR:CE1	2.49	0.48
1:A:615:PHE:H	1:A:642:ARG:HH12	1.62	0.48
2:B:354:PRO:HG2	2:B:355:PRO:HD3	1.96	0.48
5:E:94:GLU:HG3	5:E:236:VAL:HG11	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:31:LYS:HG2	13:O:257:SER:HB3	1.96	0.48
3:C:452:MET:HG2	3:C:453:VAL:HG12	1.94	0.48
11:M:53:DG:H2"	11:M:54:DA:C8	2.49	0.48
4:D:433:PHE:CE2	4:D:435:ASN:HB2	2.49	0.48
1:A:631:GLY:HA3	1:A:675:LYS:HE3	1.96	0.48
2:B:324:ARG:H	2:B:324:ARG:HD2	1.79	0.48
15:Q:712:GLU:OE1	15:Q:712:GLU:N	2.47	0.48
15:Q:849:GLN:HE21	15:Q:867:MET:HE3	1.78	0.48
1:A:74:ARG:HB2	1:A:145:LYS:HB3	1.96	0.47
1:A:447:PRO:HB2	1:A:476:LYS:HG2	1.96	0.47
2:B:478:MET:HE3	9:K:62:VAL:HG13	1.96	0.47
5:E:318:LEU:HB3	6:F:274:ILE:HD11	1.95	0.47
6:F:192:ASP:OD2	6:F:238:ARG:NH2	2.38	0.47
15:Q:237:LEU:O	15:Q:241:LYS:HG2	2.13	0.47
2:B:4:ASN:ND2	2:B:5:VAL:O	2.47	0.47
15:Q:81:VAL:HG22	15:Q:83:HIS:H	1.79	0.47
5:E:222:ILE:HG22	5:E:231:LEU:HD12	1.97	0.47
13:O:89:ASN:HD22	13:O:105:ARG:HD3	1.79	0.47
1:A:514:MET:HE1	1:A:534:TYR:HA	1.96	0.47
9:K:36:LEU:HD23	9:K:39:ARG:HH12	1.78	0.47
9:K:120:HIS:NE2	9:K:121:PHE:CZ	2.81	0.47
12:N:559:GLU:O	12:N:563:GLN:HG3	2.14	0.47
4:D:244:THR:HB	4:D:247:LYS:HB2	1.96	0.47
2:B:42:MET:HG2	2:B:48:LYS:HB2	1.96	0.47
3:C:509:GLN:O	3:C:513:ARG:HG2	2.15	0.47
4:D:265:LEU:HD13	4:D:270:LEU:HD11	1.97	0.47
4:D:412:PHE:HE1	4:D:421:LEU:HD12	1.80	0.47
1:A:160:THR:O	1:A:160:THR:HG22	2.14	0.47
1:A:168:LEU:HB2	1:A:291:LEU:HD22	1.96	0.47
1:A:548:ILE:HG21	1:A:577:LYS:HE3	1.97	0.47
10:L:29:DA:H2"	10:L:30:DA:C8	2.50	0.47
14:P:11:ARG:O	14:P:107:HIS:NE2	2.43	0.47
15:Q:391:ILE:HG21	15:Q:407:VAL:HG11	1.97	0.47
2:B:643:GLN:HG2	16:R:148:LEU:HD23	1.97	0.47
4:D:203:PHE:CZ	4:D:211:GLN:HB2	2.50	0.47
1:A:104:ALA:HA	1:A:122:SER:HB2	1.97	0.46
1:A:664:SER:O	1:A:667:THR:OG1	2.32	0.46
2:B:348:HIS:ND1	2:B:349:VAL:HG22	2.30	0.46
2:B:72:TYR:HB3	2:B:206:VAL:HG22	1.96	0.46
9:K:171:HIS:ND1	15:Q:242:CYS:SG	2.88	0.46
8:H:904:TRP:CD1	8:H:905:PRO:HD3	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:65:DT:H2''	11:M:66:DT:C6	2.50	0.46
16:R:106:ARG:NH2	16:R:152:TYR:OH	2.39	0.46
1:A:52:LYS:O	1:A:60:ASP:N	2.43	0.46
1:A:529:LYS:NZ	1:A:719:ALA:O	2.46	0.46
2:B:11:TYR:HB3	2:B:93:PHE:HE2	1.81	0.46
1:A:557:LYS:HB2	1:A:620:ALA:HA	1.97	0.46
2:B:78:PRO:O	2:B:82:LYS:HG2	2.16	0.46
2:B:84:ILE:HG13	2:B:108:ALA:HB2	1.98	0.46
1:A:325:ARG:HD2	5:E:19:TRP:HD1	1.80	0.46
1:A:626:ILE:HG22	1:A:662:LEU:HD12	1.96	0.46
2:B:69:LYS:NZ	2:B:199:ILE:O	2.35	0.46
13:O:53:GLN:NE2	14:P:112:PHE:O	2.49	0.46
15:Q:232:ILE:HG22	15:Q:291:LEU:HD11	1.98	0.46
15:Q:380:LYS:HD2	15:Q:581:TYR:CZ	2.51	0.46
3:C:494:LYS:HD2	3:C:536:LEU:HD23	1.98	0.46
11:M:56:DG:H2'	11:M:57:DT:H71	1.98	0.46
11:M:61:DA:C8	11:M:62:DT:H72	2.51	0.46
16:R:232:VAL:HA	16:R:235:VAL:HG12	1.97	0.46
1:A:362:LEU:HB3	1:A:438:MET:HG3	1.98	0.46
4:D:178:LEU:HD11	4:D:226:ARG:NH1	2.31	0.46
8:H:904:TRP:HE3	8:H:908:ARG:HH11	1.62	0.46
11:M:57:DT:H2''	11:M:58:DG:H8	1.80	0.46
15:Q:149:LEU:HD22	15:Q:161:ILE:HD13	1.98	0.46
6:F:115:ILE:HG13	6:F:119:MET:HE3	1.97	0.45
3:C:436:PRO:HA	3:C:441:MET:HG3	1.98	0.45
6:F:268:CYS:HB3	6:F:273:SER:H	1.82	0.45
2:B:638:GLU:OE1	2:B:641:ARG:NH2	2.50	0.45
4:D:373:HIS:CG	4:D:374:PRO:HD2	2.51	0.45
5:E:251:ARG:HB3	5:E:310:LEU:HD11	1.98	0.45
6:F:22:TRP:CE2	6:F:34:LEU:HD13	2.51	0.45
9:K:165:ILE:HB	9:K:180:LEU:HB2	1.97	0.45
16:R:143:LEU:HD12	16:R:173:VAL:HG13	1.98	0.45
2:B:139:ALA:HB3	2:B:142:VAL:HG23	1.99	0.45
15:Q:257:ALA:HA	15:Q:262:PHE:CG	2.52	0.45
1:A:519:TYR:HE2	7:G:19:PHE:HB2	1.82	0.45
3:C:434:LEU:HD13	6:F:229:TRP:CG	2.52	0.45
13:O:227:PHE:HD1	13:O:230:LEU:HD12	1.81	0.45
5:E:254:PHE:N	6:F:263:GLU:O	2.47	0.45
5:E:291:CYS:O	5:E:295:ARG:N	2.41	0.45
6:F:195:VAL:HG11	6:F:199:ASP:HA	1.99	0.45
15:Q:240:LEU:HD23	15:Q:240:LEU:HA	1.86	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:256:GLN:OE1	5:E:256:GLN:N	2.41	0.45
1:A:115:GLU:OE1	4:D:314:ARG:NH1	2.50	0.45
10:L:39:DC:C6	10:L:40:DT:H72	2.52	0.45
2:B:383:LEU:HD22	2:B:388:ILE:HD13	1.99	0.45
3:C:493:MET:HE3	3:C:493:MET:HB3	1.74	0.45
5:E:172:SER:HB2	5:E:201:LEU:HD12	1.99	0.45
13:O:226:ASN:HB3	13:O:263:HIS:CD2	2.52	0.45
1:A:76:LEU:HD21	1:A:100:LEU:HD11	1.99	0.44
5:E:66:ASP:HB3	5:E:71:MET:HE2	1.99	0.44
15:Q:407:VAL:HG12	15:Q:577:TYR:HB2	1.99	0.44
5:E:58:MET:HE3	5:E:317:HIS:ND1	2.31	0.44
5:E:252:MET:HE3	5:E:313:VAL:HG21	1.99	0.44
15:Q:290:ILE:HA	15:Q:293:THR:HG22	1.98	0.44
2:B:628:THR:HG21	10:L:54:DC:H2"	1.98	0.44
2:B:694:PRO:HB2	2:B:696:TRP:CD1	2.52	0.44
5:E:375:VAL:HA	5:E:379:LEU:HB3	1.99	0.44
1:A:508:ALA:HA	1:A:688:LYS:HG2	2.00	0.44
2:B:569:ILE:HG21	17:S:237:LEU:HD12	2.00	0.44
6:F:12:VAL:HG22	6:F:58:ALA:HB3	2.00	0.44
9:K:214:MET:HE3	9:K:214:MET:HB3	1.90	0.44
15:Q:147:PHE:O	15:Q:150:ARG:HG2	2.18	0.44
2:B:2:LYS:NZ	2:B:11:TYR:OH	2.50	0.44
2:B:192:TYR:OH	2:B:196:ARG:NH2	2.50	0.44
6:F:228:LEU:HA	6:F:232:LEU:HB2	1.98	0.44
9:K:117:LEU:HD12	9:K:125:THR:HB	1.99	0.44
15:Q:221:THR:HG23	15:Q:342:ARG:NH2	2.33	0.44
2:B:277:ASP:HA	2:B:280:ARG:HG2	2.00	0.44
13:O:53:GLN:OE1	13:O:166:HIS:NE2	2.50	0.44
2:B:209:TYR:HB3	2:B:213:LEU:HD21	2.00	0.44
4:D:409:TYR:OH	4:D:448:HIS:ND1	2.50	0.44
5:E:249:LEU:HB3	6:F:266:TYR:HB3	1.98	0.44
6:F:195:VAL:HG21	6:F:214:TYR:OH	2.16	0.44
13:O:258:THR:OG1	13:O:263:HIS:O	2.33	0.44
15:Q:628:GLU:OE1	15:Q:632:LYS:NZ	2.40	0.44
4:D:325:ILE:HD12	4:D:342:VAL:HG11	1.99	0.44
5:E:322:TYR:OH	6:F:274:ILE:HD12	2.18	0.44
2:B:637:LEU:HD13	2:B:648:GLU:HG3	1.99	0.43
5:E:292:PRO:HB2	6:F:264:ILE:HG23	1.99	0.43
10:L:47:DT:H2"	10:L:48:DT:H71	1.98	0.43
15:Q:728:SER:O	15:Q:732:LEU:N	2.42	0.43
2:B:64:PRO:HG2	2:B:65:LEU:HD22	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:423:ASP:OD1	2:B:423:ASP:N	2.50	0.43
3:C:408:ARG:O	3:C:412:GLU:HG2	2.18	0.43
14:P:55:LEU:HD23	14:P:81:CYS:HB3	2.00	0.43
1:A:88:ALA:HA	1:A:93:TYR:CD1	2.53	0.43
1:A:510:VAL:HB	1:A:690:ILE:HB	2.00	0.43
2:B:56:ILE:HG21	2:B:70:LEU:HD13	1.99	0.43
2:B:60:GLN:HE22	2:B:104:PHE:HE2	1.66	0.43
2:B:337:LEU:HA	2:B:340:VAL:HG22	1.99	0.43
5:E:182:ILE:HD12	5:E:182:ILE:H	1.84	0.43
5:E:323:HIS:HD2	6:F:182:PHE:CE2	2.37	0.43
6:F:112:VAL:HA	6:F:115:ILE:HG22	2.00	0.43
9:K:171:HIS:NE2	11:M:46:DC:OP2	2.52	0.43
14:P:28:VAL:HG22	14:P:68:GLU:HG3	2.01	0.43
15:Q:610:TYR:HB3	15:Q:613:SER:OG	2.18	0.43
1:A:336:GLY:HA3	1:A:488:LEU:HD13	1.99	0.43
2:B:711:ASP:OD1	2:B:715:GLN:NE2	2.47	0.43
5:E:319:ALA:HA	5:E:322:TYR:HD2	1.83	0.43
17:S:201:LYS:O	17:S:204:ILE:HG13	2.18	0.43
2:B:441:SER:HB3	2:B:471:LEU:HA	2.00	0.43
2:B:497:ARG:NH1	2:B:707:ASN:O	2.52	0.43
9:K:70:ASP:OD1	9:K:70:ASP:N	2.40	0.43
9:K:270:TYR:HE2	9:K:272:LYS:HE2	1.83	0.43
1:A:342:CYS:SG	1:A:642:ARG:NH2	2.91	0.43
2:B:115:LEU:HD21	2:B:177:LEU:HD22	2.00	0.43
6:F:247:VAL:HG13	6:F:248:HIS:CD2	2.54	0.43
13:O:95:ASP:OD2	14:P:9:ARG:NH1	2.50	0.43
15:Q:869:HIS:CE1	15:Q:887:ILE:HG22	2.53	0.43
4:D:309:VAL:N	4:D:376:MET:SD	2.84	0.43
6:F:165:LYS:HB2	6:F:203:LEU:HD11	2.00	0.43
15:Q:71:TYR:O	15:Q:75:GLN:HG2	2.19	0.43
1:A:183:ASP:OD1	1:A:183:ASP:N	2.52	0.43
4:D:415:GLN:O	4:D:419:GLU:HG2	2.19	0.43
5:E:156:LEU:HD23	5:E:165:ARG:HB3	2.01	0.43
6:F:174:TYR:CD1	6:F:202:LEU:HD21	2.54	0.43
15:Q:794:HIS:CD2	16:R:219:PRO:HB3	2.54	0.43
16:R:236:THR:O	16:R:240:THR:HB	2.18	0.43
4:D:46:ARG:NH1	6:F:53:ARG:HG2	2.34	0.42
6:F:193:ALA:HB1	6:F:203:LEU:HD13	2.00	0.42
15:Q:414:ASP:OD1	15:Q:414:ASP:N	2.52	0.42
9:K:148:TYR:HD1	9:K:200:LEU:HD21	1.84	0.42
1:A:186:GLN:O	1:A:190:GLN:HG2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:VAL:HB	1:A:407:ILE:HG12	2.01	0.42
2:B:410:TYR:HB3	2:B:414:PHE:CE1	2.55	0.42
2:B:415:THR:HB	2:B:438:MET:HE3	2.01	0.42
3:C:500:PHE:HA	3:C:503:THR:HG22	2.00	0.42
3:C:512:ILE:HG23	3:C:517:LEU:HB2	2.01	0.42
5:E:266:ASP:OD1	5:E:266:ASP:N	2.44	0.42
5:E:367:PHE:HB3	5:E:371:CYS:CB	2.49	0.42
14:P:74:THR:HG23	14:P:76:LYS:H	1.84	0.42
15:Q:17:GLU:O	15:Q:21:GLN:HG2	2.18	0.42
15:Q:420:LEU:HD21	15:Q:581:TYR:CD2	2.54	0.42
1:A:546:PHE:CD2	1:A:693:LEU:HD13	2.55	0.42
2:B:12:PHE:CE2	2:B:14:TYR:HB2	2.54	0.42
13:O:215:LEU:HG	13:O:234:LEU:HD21	2.01	0.42
15:Q:577:TYR:HD1	15:Q:604:ARG:HB3	1.85	0.42
17:S:225:GLU:OE1	17:S:227:ASP:N	2.51	0.42
2:B:123:PRO:HG2	2:B:124:LEU:HD12	2.02	0.42
6:F:213:LEU:HD22	6:F:243:LEU:HD13	2.02	0.42
13:O:46:ILE:HA	13:O:73:GLN:HB2	2.01	0.42
2:B:441:SER:O	2:B:445:LYS:HG2	2.19	0.42
2:B:494:ILE:HD12	2:B:706:LEU:HD12	2.01	0.42
9:K:213:LYS:O	9:K:216:GLN:HG3	2.20	0.42
12:N:462:PHE:CE1	12:N:574:VAL:HB	2.55	0.42
15:Q:589:ARG:O	15:Q:593:ILE:HG12	2.20	0.42
1:A:405:VAL:HG12	1:A:407:ILE:HG13	2.02	0.42
16:R:119:VAL:HG11	16:R:213:LYS:HG2	2.02	0.42
4:D:55:TRP:HH2	4:D:83:GLN:HG3	1.85	0.42
1:A:100:LEU:O	1:A:104:ALA:N	2.52	0.42
13:O:94:ILE:HD12	13:O:104:VAL:HG21	2.01	0.42
1:A:399:LYS:HA	1:A:400:PRO:HD3	1.89	0.41
1:A:628:SER:HB2	1:A:676:ARG:CZ	2.50	0.41
2:B:446:PRO:HA	2:B:449:GLU:HG2	2.01	0.41
3:C:506:CYS:HB2	3:C:507:PRO:HD3	2.01	0.41
4:D:38:PRO:HB3	4:D:121:ALA:HB2	2.02	0.41
15:Q:180:ARG:HG2	15:Q:184:ASN:ND2	2.35	0.41
1:A:551:HIS:HB2	1:A:558:ILE:HD11	2.00	0.41
6:F:145:HIS:NE2	6:F:149:LYS:HE3	2.34	0.41
9:K:117:LEU:HD11	9:K:130:ARG:HA	2.02	0.41
2:B:113:LYS:HB3	2:B:130:VAL:HG11	2.03	0.41
2:B:514:ILE:HG22	2:B:518:ARG:HG3	2.02	0.41
3:C:460:GLU:OE2	3:C:504:LYS:HE2	2.20	0.41
6:F:204:GLN:HG2	6:F:214:TYR:CZ	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:P:41:PHE:HZ	14:P:69:VAL:HG11	1.85	0.41
16:R:141:LEU:HD22	16:R:171:VAL:HG13	2.01	0.41
1:A:144:SER:O	1:A:146:THR:HG22	2.20	0.41
1:A:523:VAL:HG11	7:G:19:PHE:HD1	1.86	0.41
1:A:615:PHE:H	1:A:642:ARG:NH1	2.18	0.41
2:B:161:PHE:O	2:B:165:GLY:N	2.48	0.41
2:B:354:PRO:CG	2:B:355:PRO:HD3	2.51	0.41
3:C:464:LEU:HD22	3:C:504:LYS:NZ	2.34	0.41
7:G:38:ILE:HD11	7:G:44:PHE:HB2	2.02	0.41
9:K:188:LYS:HE3	9:K:188:LYS:HB3	1.86	0.41
13:O:127:LYS:HB2	13:O:149:LEU:HD21	2.01	0.41
15:Q:257:ALA:HA	15:Q:262:PHE:CD1	2.55	0.41
16:R:143:LEU:HD12	16:R:173:VAL:HA	2.02	0.41
2:B:628:THR:HA	2:B:633:LEU:HD23	2.03	0.41
15:Q:155:LYS:HA	15:Q:155:LYS:HD3	1.78	0.41
4:D:233:ILE:HG23	4:D:261:PHE:CZ	2.55	0.41
1:A:171:LYS:HB2	1:A:171:LYS:HE3	1.84	0.41
1:A:577:LYS:HD3	1:A:604:THR:HB	2.03	0.41
2:B:43:PRO:HB3	2:B:696:TRP:CD2	2.56	0.41
3:C:472:LEU:HB3	5:E:307:ILE:HG23	2.03	0.41
3:C:481:VAL:HB	3:C:539:TRP:CZ2	2.56	0.41
1:A:373:GLN:CD	1:A:616:ASP:H	2.28	0.41
2:B:342:TRP:HE1	2:B:364:ARG:HH11	1.69	0.41
2:B:462:SER:HB3	2:B:692:LYS:O	2.21	0.41
9:K:169:ASN:ND2	9:K:172:HIS:O	2.48	0.41
16:R:235:VAL:HG21	16:R:254:LEU:HD13	2.02	0.41
1:A:557:LYS:HB3	1:A:596:PHE:CZ	2.55	0.41
1:A:663:VAL:HG11	1:A:673:SER:HB2	2.02	0.41
2:B:342:TRP:HE1	2:B:364:ARG:NH1	2.18	0.41
4:D:95:ILE:HG22	4:D:110:LEU:HD22	2.03	0.41
5:E:59:ARG:NH2	5:E:166:GLU:OE1	2.51	0.41
5:E:251:ARG:HH21	6:F:278:PHE:HE2	1.69	0.41
5:E:313:VAL:HG12	5:E:314:SER:O	2.20	0.41
16:R:201:SER:HB3	16:R:204:GLU:HG2	2.03	0.41
17:S:353:LEU:H	17:S:353:LEU:HD23	1.84	0.41
5:E:151:ILE:O	5:E:154:GLN:HG2	2.20	0.41
6:F:190:LEU:HD12	6:F:235:GLN:HG2	2.03	0.41
12:N:535:SER:O	12:N:539:ILE:HG22	2.20	0.41
17:S:208:MET:HE3	17:S:243:LEU:HG	2.03	0.41
2:B:120:GLU:OE1	2:B:120:GLU:N	2.52	0.40
2:B:268:LYS:O	2:B:271:LEU:HG	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:686:ARG:NH2	10:L:53:DT:H5''	2.36	0.40
4:D:79:PHE:CG	6:F:240:GLN:HG2	2.56	0.40
4:D:232:GLU:HB3	4:D:258:LEU:HD21	2.02	0.40
4:D:384:PRO:HA	4:D:385:PRO:HD3	1.96	0.40
5:E:193:LYS:HE2	5:E:193:LYS:HB2	1.91	0.40
6:F:255:CYS:O	6:F:259:ARG:HD2	2.22	0.40
9:K:65:ALA:HA	9:K:66:PRO:HD3	1.94	0.40
11:M:65:DT:H2''	11:M:66:DT:C5	2.56	0.40
15:Q:32:LEU:HD23	15:Q:32:LEU:H	1.86	0.40
17:S:205:LEU:HD12	17:S:206:THR:HG23	2.02	0.40
17:S:209:LYS:NZ	17:S:240:LYS:HG3	2.36	0.40
10:L:42:DC:H2''	10:L:43:DA:H8	1.86	0.40
15:Q:34:VAL:HG12	15:Q:165:THR:HB	2.02	0.40
15:Q:698:LEU:O	15:Q:702:ARG:HG2	2.21	0.40
2:B:216:LYS:HE2	10:L:62:DG:N1	2.36	0.40
4:D:425:ALA:HB1	4:D:431:LEU:HB2	2.03	0.40
5:E:317:HIS:CD2	5:E:317:HIS:H	2.38	0.40
6:F:10:LEU:HD12	6:F:56:LYS:HD2	2.04	0.40
9:K:120:HIS:NE2	9:K:121:PHE:CE1	2.89	0.40
15:Q:112:ARG:NH1	15:Q:688:MET:HB3	2.35	0.40
16:R:141:LEU:HD12	16:R:169:LEU:HD11	2.03	0.40
2:B:73:CYS:HB3	2:B:209:TYR:HD1	1.86	0.40
2:B:195:ALA:O	2:B:199:ILE:HG23	2.22	0.40
5:E:314:SER:HB3	6:F:251:TYR:CD1	2.56	0.40
1:A:477:ILE:HD13	1:A:477:ILE:HA	1.96	0.40
4:D:58:ARG:NH2	6:F:241:LEU:HD23	2.36	0.40
4:D:155:ARG:NH2	4:D:267:GLU:O	2.55	0.40
4:D:226:ARG:HH22	4:D:264:HIS:HE1	1.70	0.40
9:K:32:ARG:NH1	13:O:267:THR:O	2.54	0.40
11:M:68:DA:H2''	11:M:69:DG:C8	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	609/782 (78%)	581 (95%)	28 (5%)	0	100	100
2	B	698/768 (91%)	676 (97%)	22 (3%)	0	100	100
3	C	127/548 (23%)	124 (98%)	3 (2%)	0	100	100
4	D	422/462 (91%)	413 (98%)	9 (2%)	0	100	100
5	E	336/395 (85%)	321 (96%)	15 (4%)	0	100	100
6	F	251/308 (82%)	243 (97%)	8 (3%)	0	100	100
7	G	64/71 (90%)	64 (100%)	0	0	100	100
8	H	15/940 (2%)	15 (100%)	0	0	100	100
9	K	200/273 (73%)	191 (96%)	9 (4%)	0	100	100
12	N	175/616 (28%)	171 (98%)	4 (2%)	0	100	100
13	O	185/270 (68%)	179 (97%)	6 (3%)	0	100	100
14	P	119/121 (98%)	117 (98%)	2 (2%)	0	100	100
15	Q	701/916 (76%)	678 (97%)	23 (3%)	0	100	100
16	R	194/295 (66%)	179 (92%)	15 (8%)	0	100	100
17	S	79/1186 (7%)	76 (96%)	3 (4%)	0	100	100
All	All	4175/7951 (52%)	4028 (96%)	147 (4%)	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	542/688 (79%)	538 (99%)	4 (1%)	76	80
2	B	614/672 (91%)	611 (100%)	3 (0%)	81	83
3	C	123/484 (25%)	122 (99%)	1 (1%)	73	79
4	D	374/399 (94%)	372 (100%)	2 (0%)	81	83

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	306/352 (87%)	301 (98%)	5 (2%)	55	72
6	F	228/272 (84%)	223 (98%)	5 (2%)	45	66
7	G	59/64 (92%)	59 (100%)	0	100	100
8	H	12/804 (2%)	11 (92%)	1 (8%)	10	34
9	K	187/233 (80%)	186 (100%)	1 (0%)	81	83
12	N	160/530 (30%)	158 (99%)	2 (1%)	61	74
13	O	172/228 (75%)	171 (99%)	1 (1%)	78	81
14	P	106/106 (100%)	106 (100%)	0	100	100
15	Q	564/816 (69%)	557 (99%)	7 (1%)	63	75
16	R	132/252 (52%)	131 (99%)	1 (1%)	73	79
17	S	78/1050 (7%)	78 (100%)	0	100	100
All	All	3657/6950 (53%)	3624 (99%)	33 (1%)	68	78

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	291	LEU
1	A	505	VAL
1	A	510	VAL
1	A	658	PHE
2	B	76	THR
2	B	613	HIS
2	B	654	PHE
3	C	418	LEU
4	D	148	LEU
4	D	222	THR
5	E	101	ILE
5	E	155	THR
5	E	254	PHE
5	E	284	LEU
5	E	328	LEU
6	F	37	CYS
6	F	59	VAL
6	F	60	ILE
6	F	119	MET
6	F	164	ILE
8	H	904	TRP
9	K	175	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	N	465	VAL
12	N	594	VAL
13	O	263	HIS
15	Q	93	THR
15	Q	384	LEU
15	Q	573	VAL
15	Q	579	VAL
15	Q	719	THR
15	Q	799	ARG
15	Q	827	THR
16	R	129	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	545	GLN
1	A	629	HIS
1	A	677	GLN
2	B	452	GLN
3	C	524	HIS
3	C	534	ASN
4	D	273	GLN
4	D	366	HIS
5	E	220	HIS
8	H	906	GLN
14	P	86	GLN
15	Q	52	HIS
15	Q	286	GLN
16	R	118	ASN
17	S	202	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
18	SF4	B	1000	2	0,12,12	-	-	-		

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

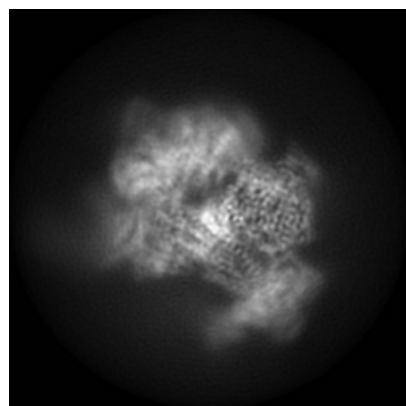
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71524. These allow visual inspection of the internal detail of the map and identification of artifacts.

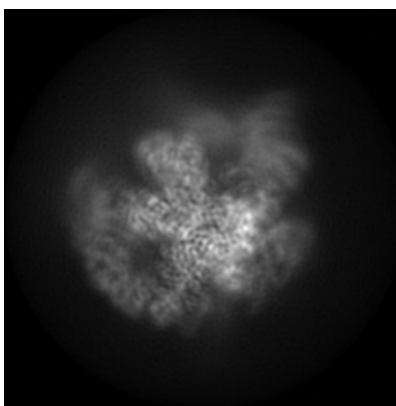
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

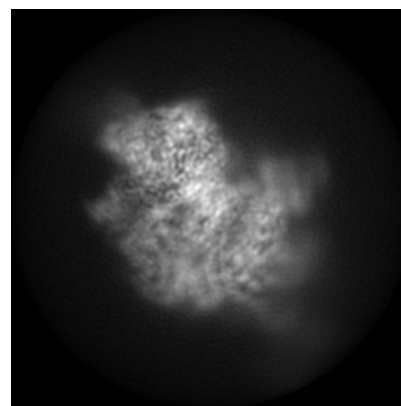
6.1.1 Primary map



X

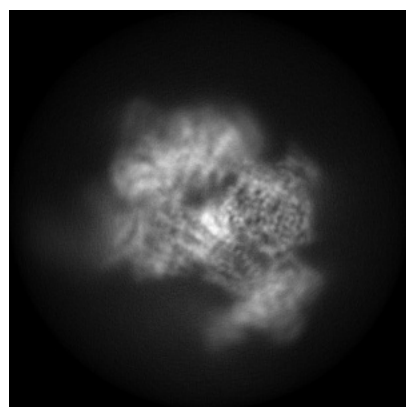


Y

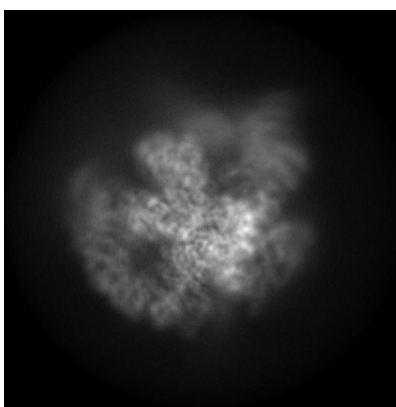


Z

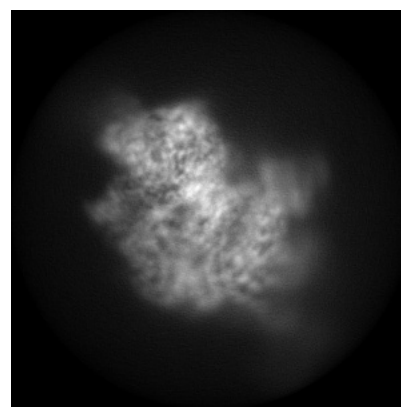
6.1.2 Raw map



X



Y

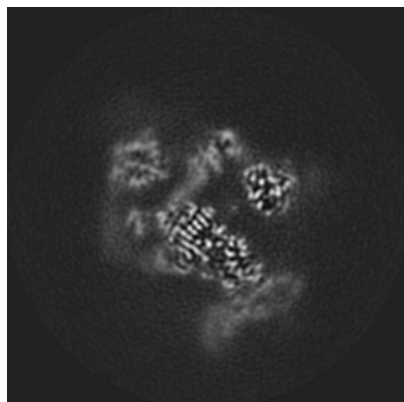


Z

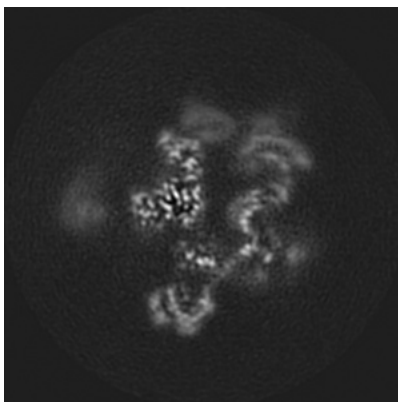
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

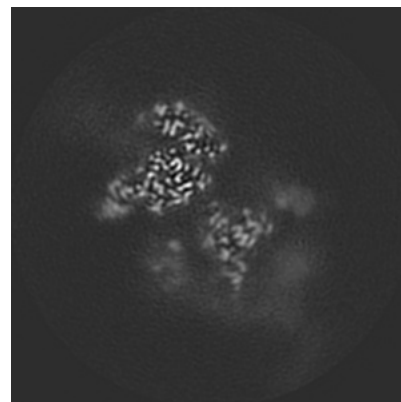
6.2.1 Primary map



X Index: 160

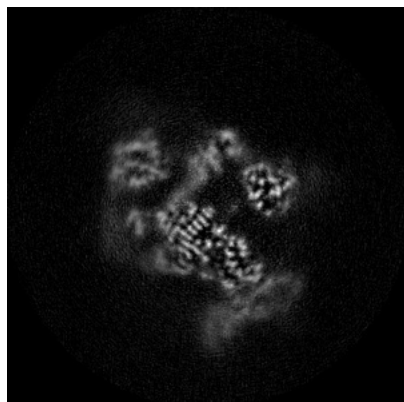


Y Index: 160

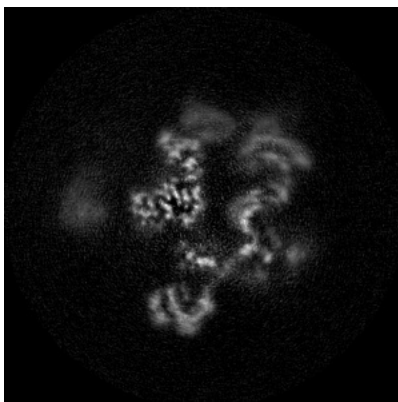


Z Index: 160

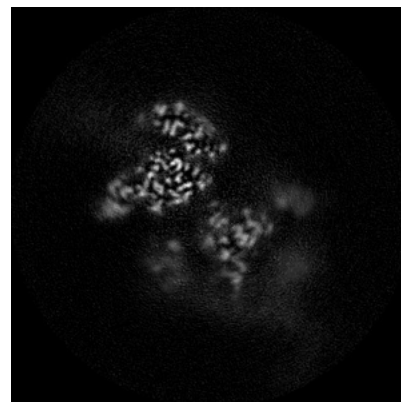
6.2.2 Raw map



X Index: 160



Y Index: 160

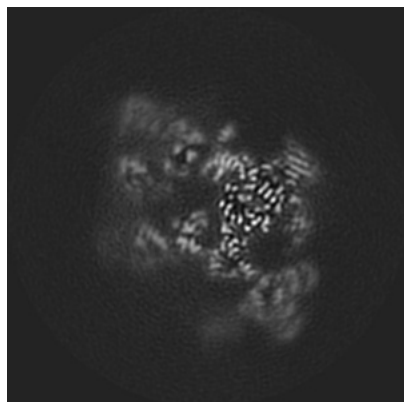


Z Index: 160

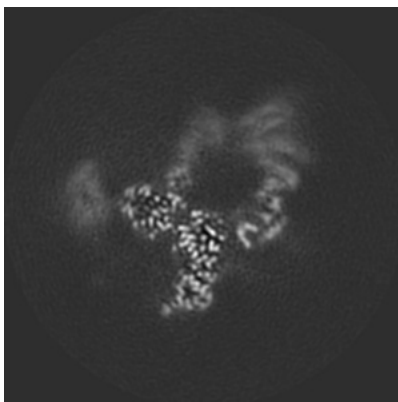
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

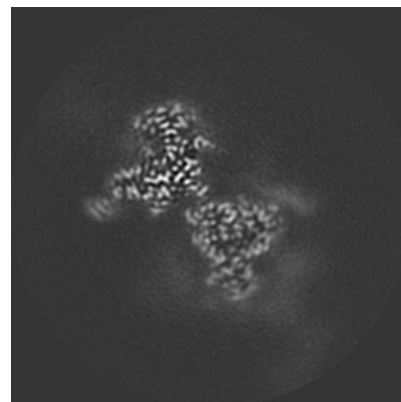
6.3.1 Primary map



X Index: 143

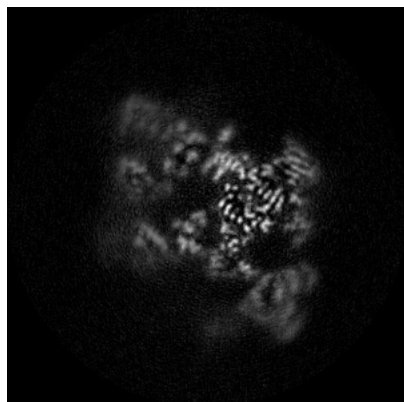


Y Index: 173

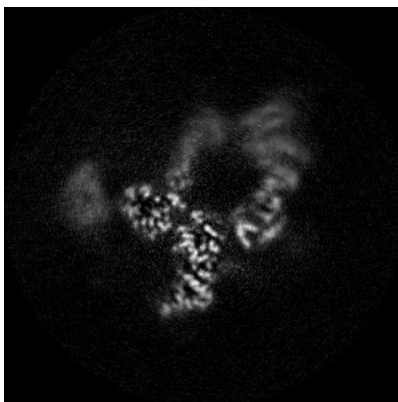


Z Index: 153

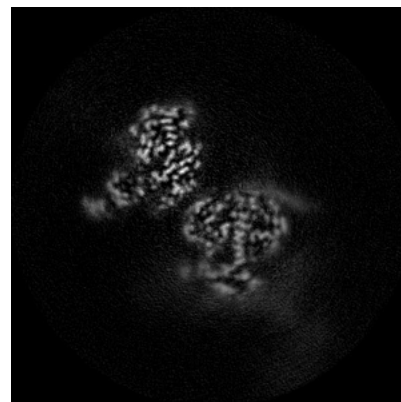
6.3.2 Raw map



X Index: 142



Y Index: 172

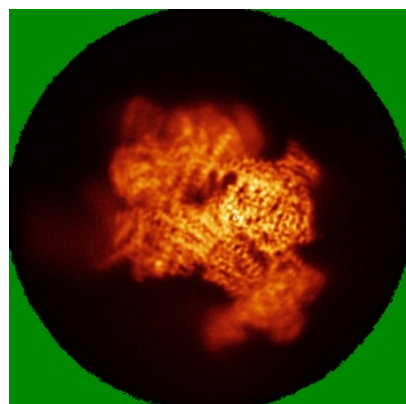


Z Index: 146

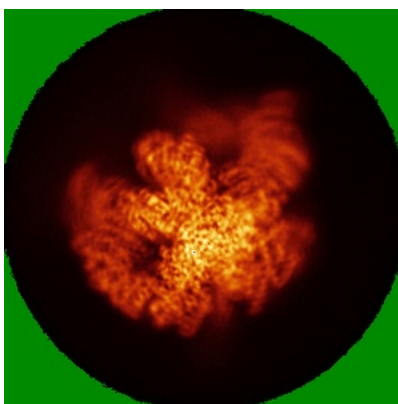
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

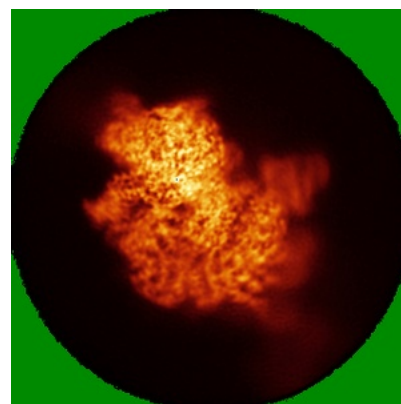
6.4.1 Primary map



X

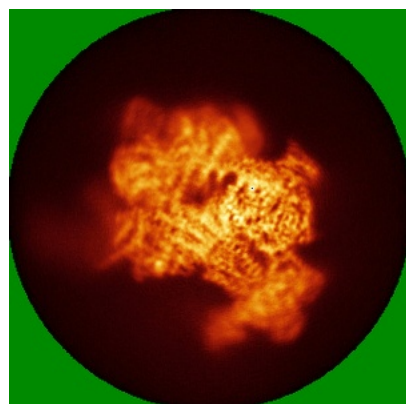


Y

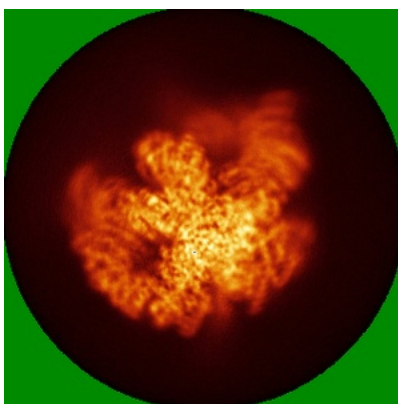


Z

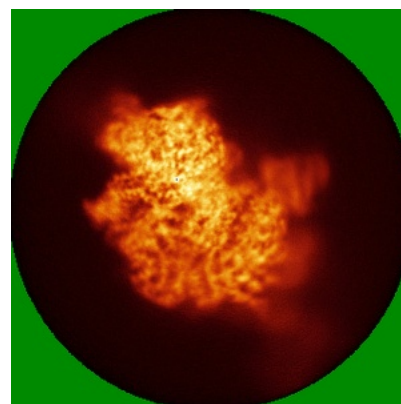
6.4.2 Raw map



X



Y



Z

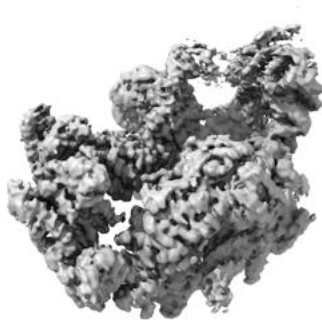
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

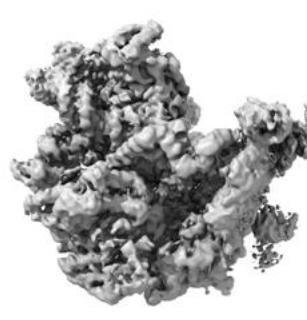
6.5.1 Primary map



X



Y



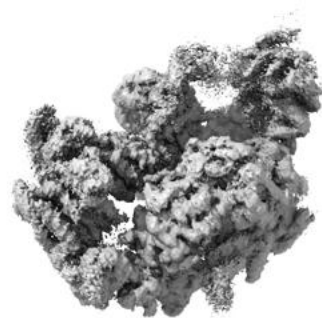
Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

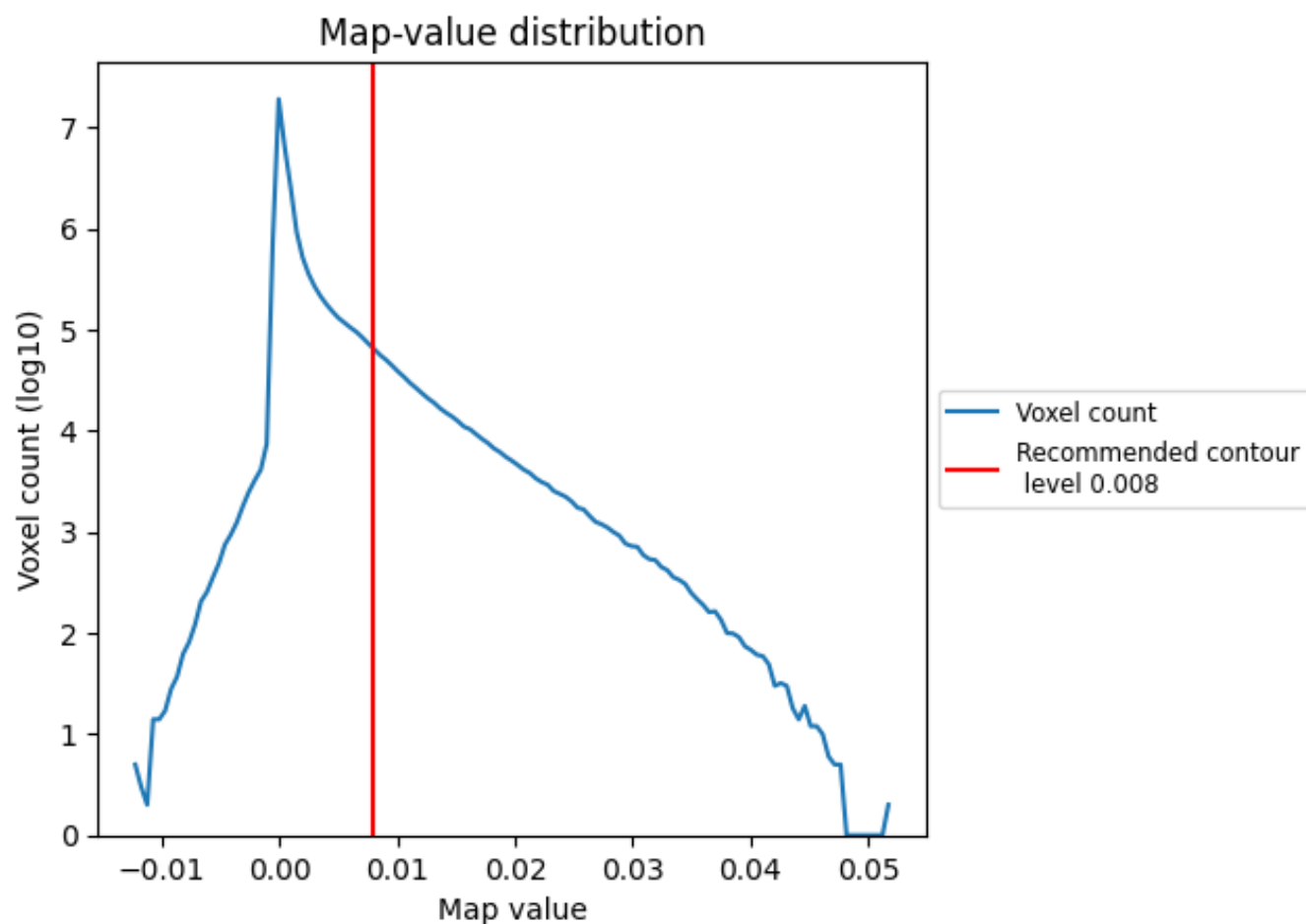
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

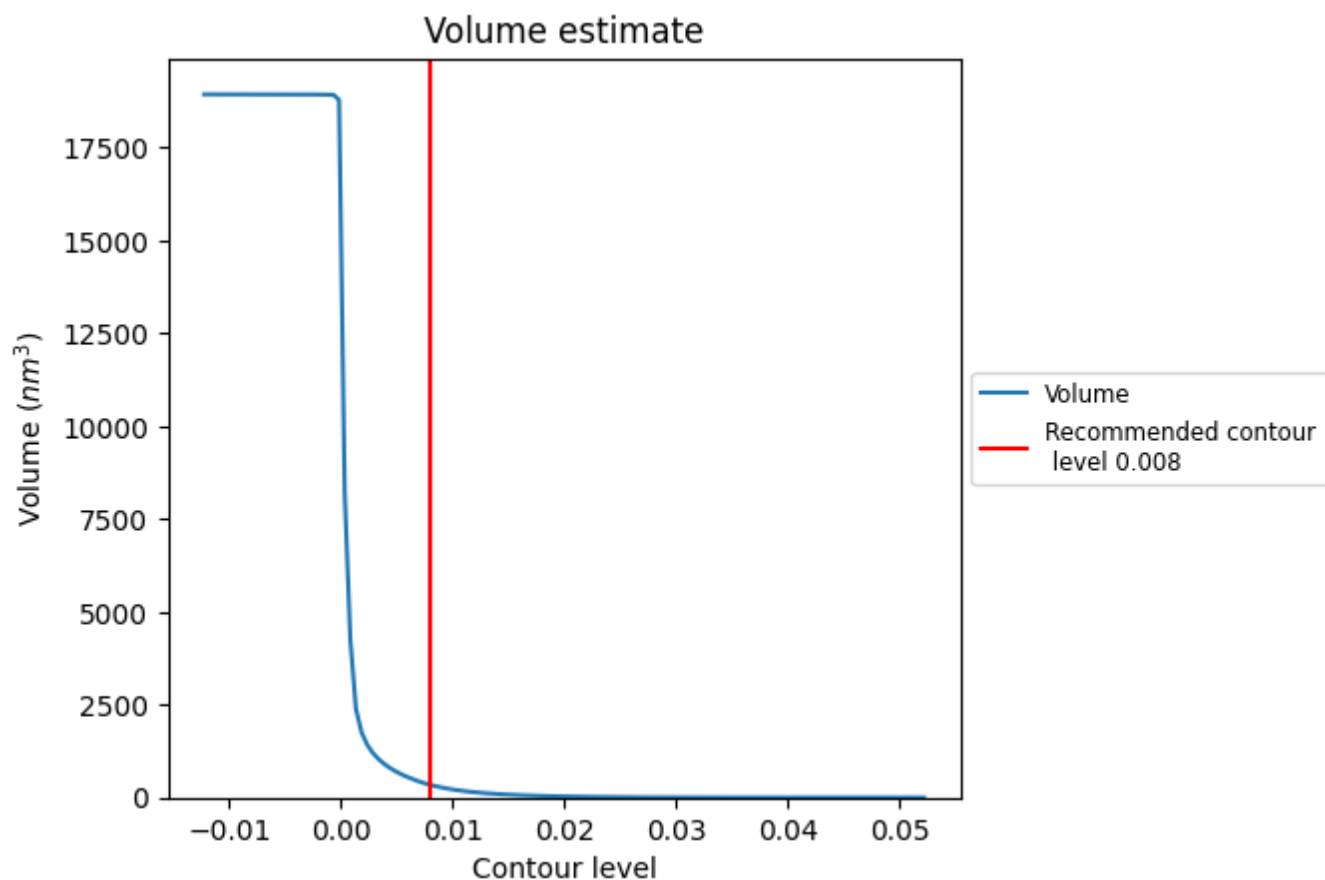
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

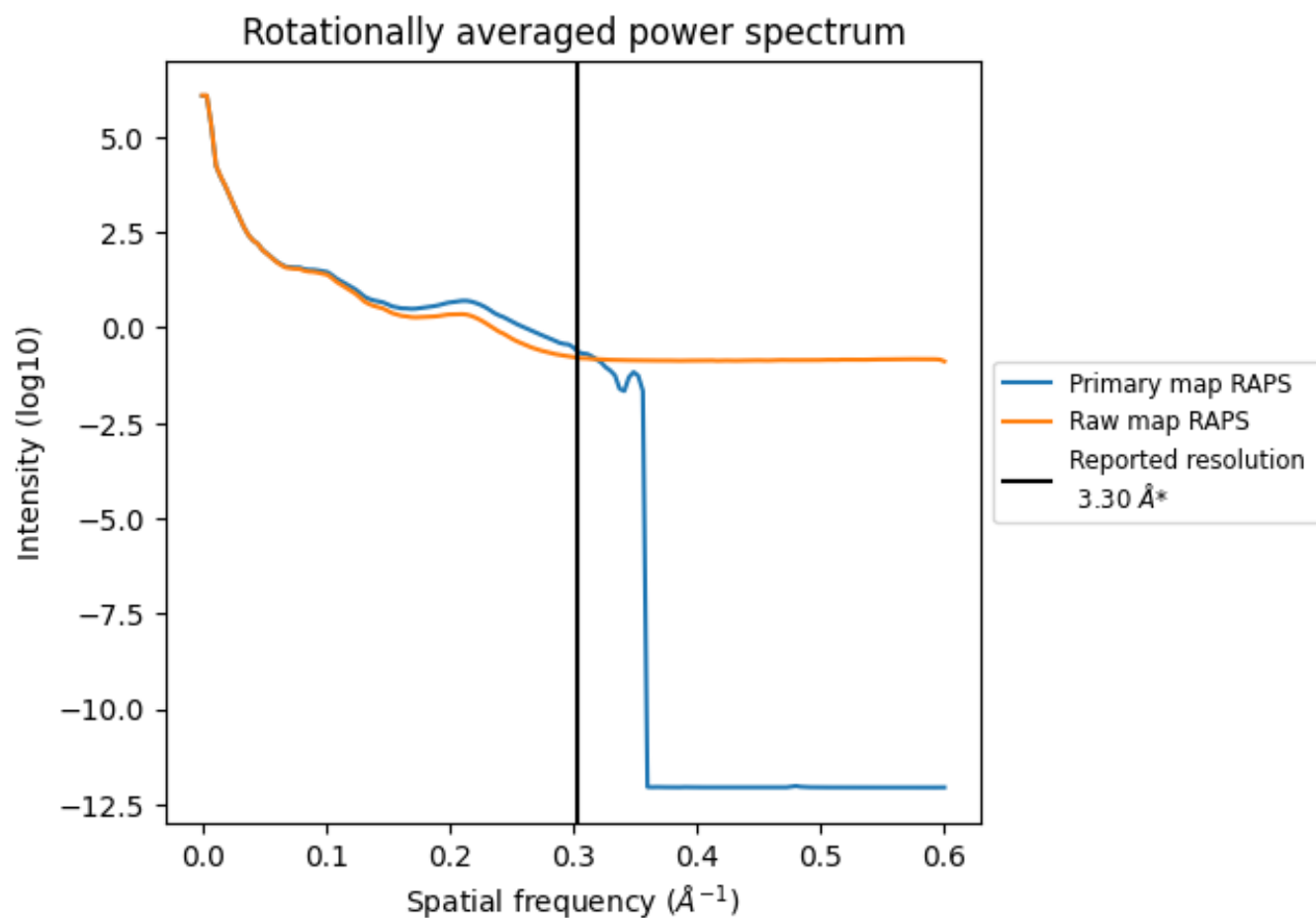
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 343 nm³; this corresponds to an approximate mass of 310 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 ⓘ

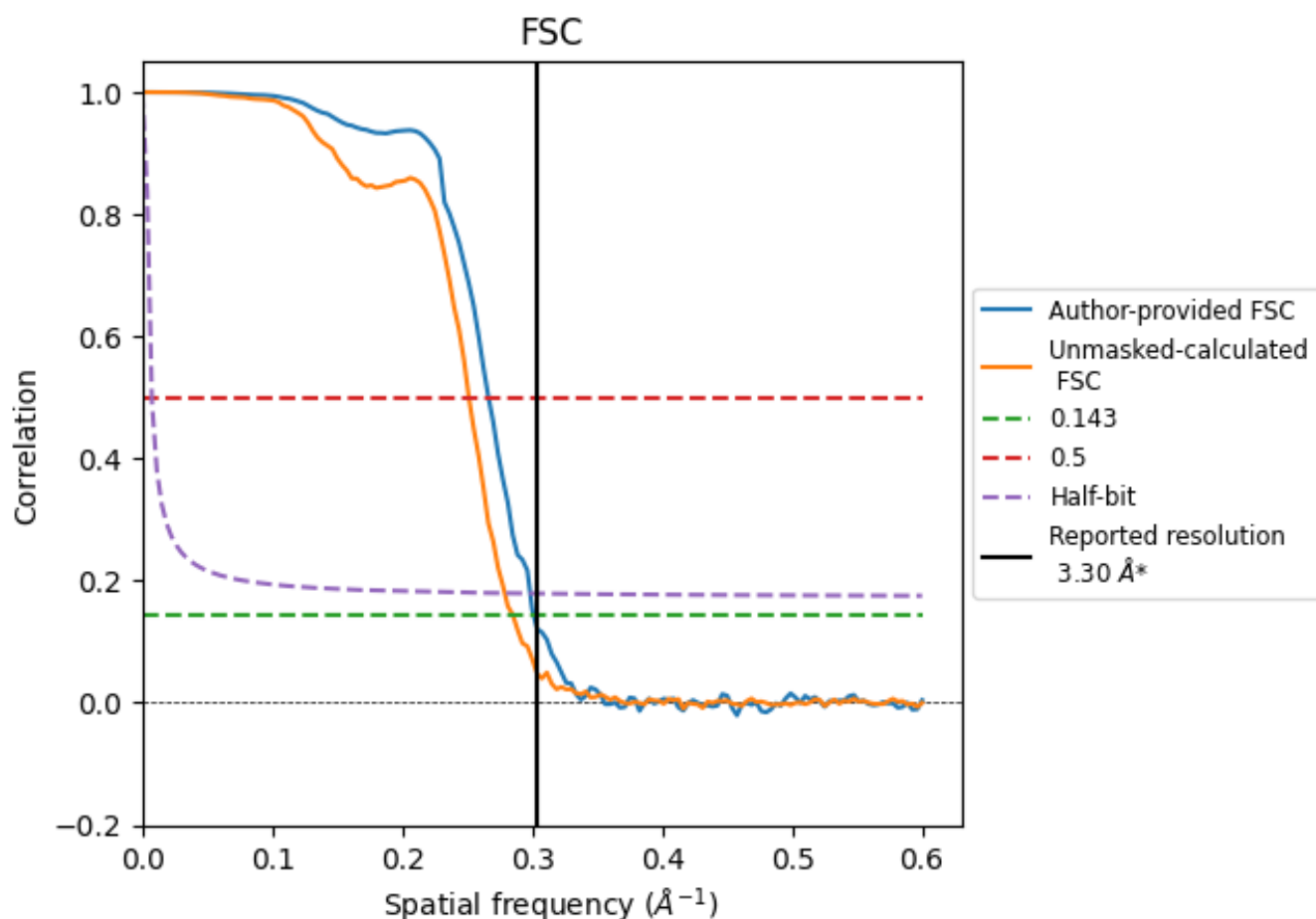


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 $0.303 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

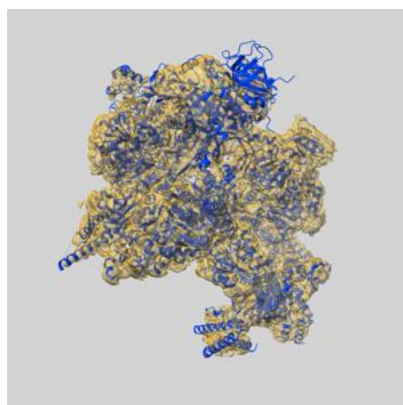
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.75	3.35
Unmasked-calculated*	3.51	3.98	3.58

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

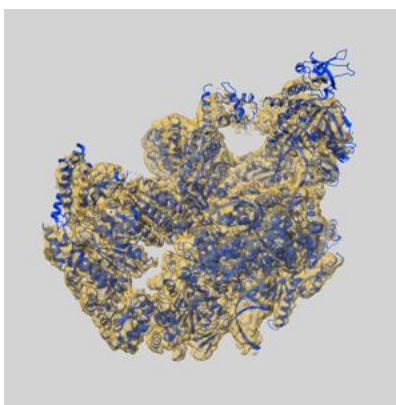
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71524 and PDB model 9PD3. Per-residue inclusion information can be found in section [3](#) on page [8](#).

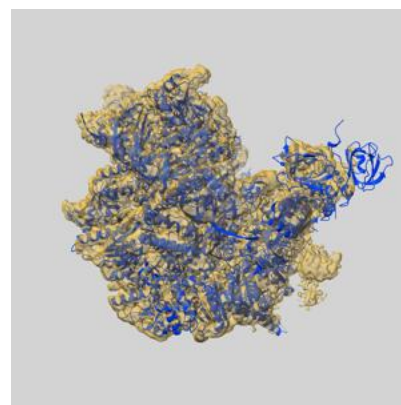
9.1 Map-model overlay [i](#)



X



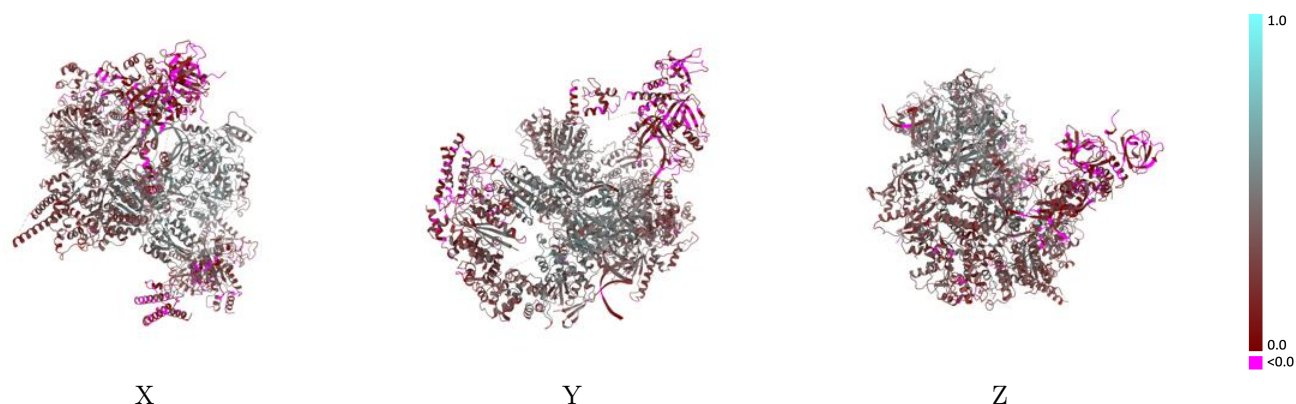
Y



Z

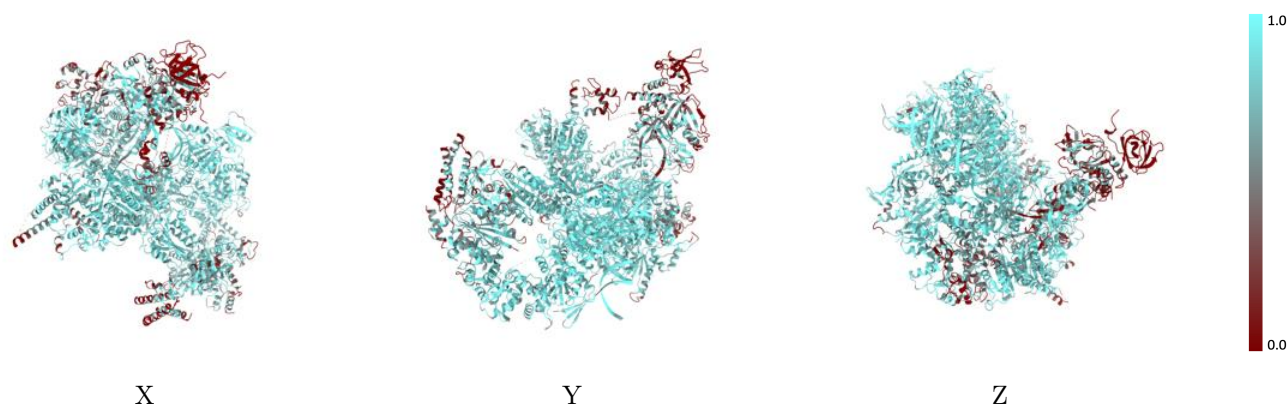
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



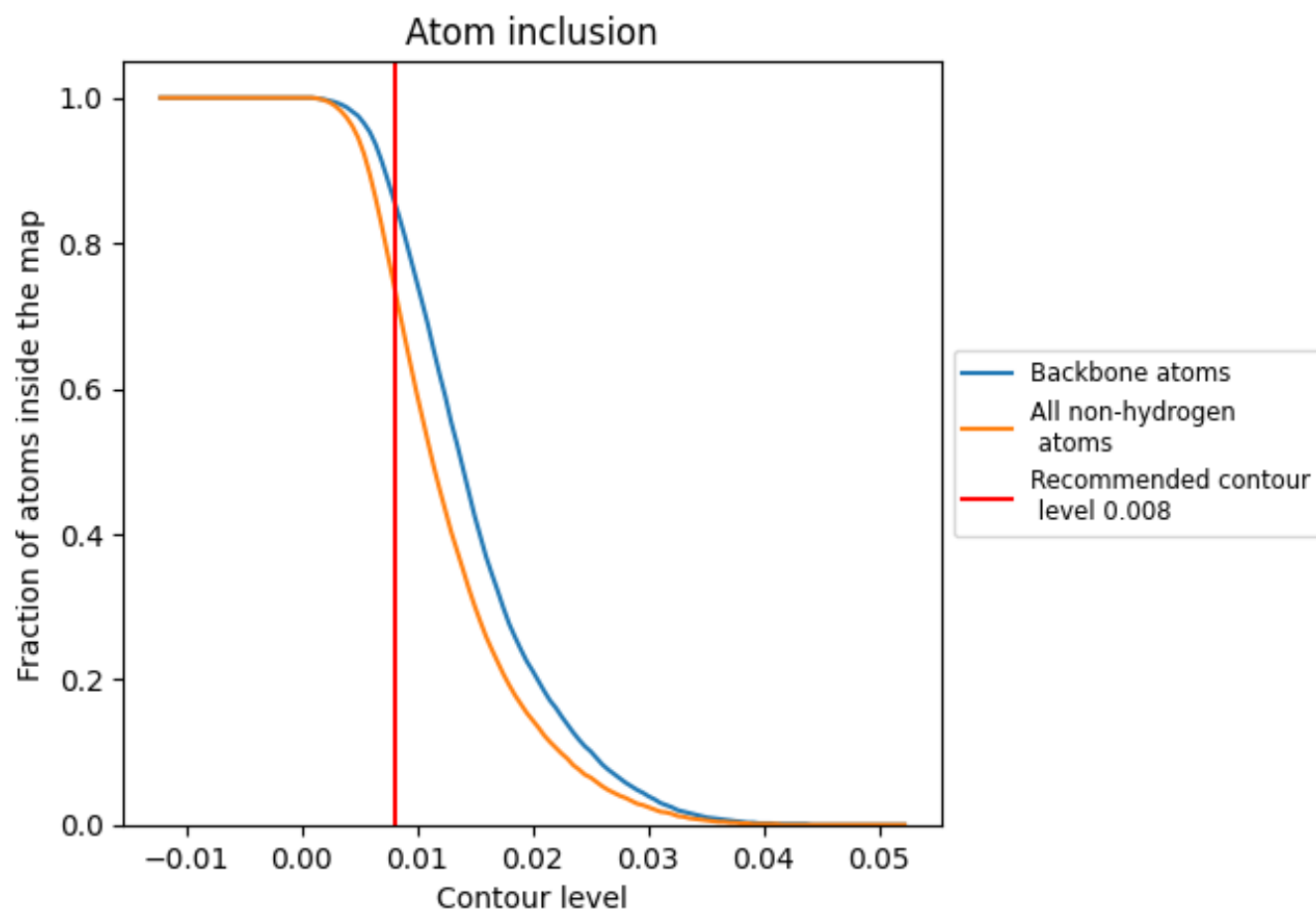
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 74% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7400	 0.3130
A	 0.9080	 0.4680
B	 0.8390	 0.3650
C	 0.3960	 0.1320
D	 0.8150	 0.3490
E	 0.7580	 0.3290
F	 0.7070	 0.2630
G	 0.8610	 0.4080
H	 0.5870	 0.4140
K	 0.7630	 0.2740
L	 0.9320	 0.3400
M	 0.7970	 0.3090
N	 0.5580	 0.1230
O	 0.3250	 0.0890
P	 0.0920	 0.0380
Q	 0.7640	 0.3080
R	 0.6720	 0.3030
S	 0.6840	 0.2820

