Full wwPDB EM Validation Report (i)

Aug 5, 2026 – 08:31 AM EDT

PDB ID	:	8EBU / pdb_00008ebu
EMDB ID	:	EMD-27998
Title	:	XPC release from Core7-XPA-DNA (Cy5)
Authors	:	Kim, J.; Yang, W.
Deposited on	:	2022-08-31
Resolution	:	3.30 Å(reported)
Based on initial model	:	6RO4

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 (i) 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 (1)) were used in the production of this report:

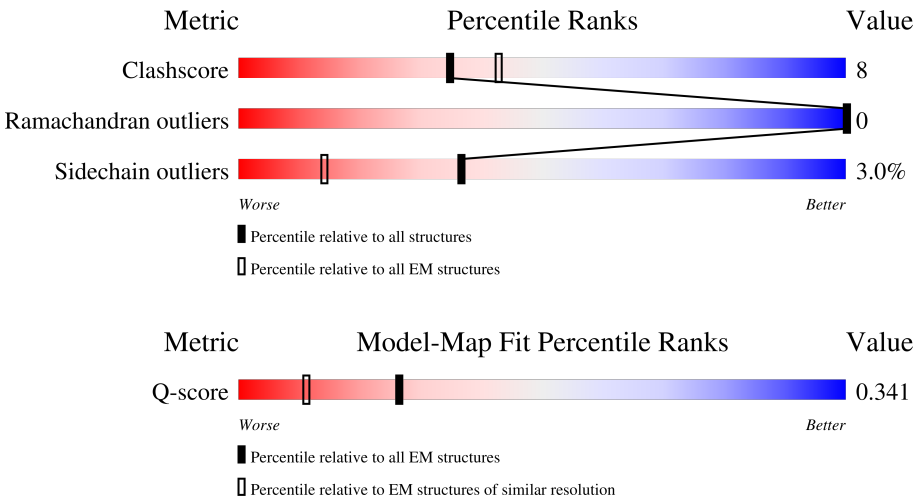
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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 <=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	56% 20% • 23%
2	B	768	66% 21% • 12%
3	C	548	7% 27% 5% 67%
4	D	462	77% 17% 6%

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Mol	Chain	Length	Quality of chain
5	E	417	5% 76% 15% 9%
6	F	308	68% 15% 16%
7	G	71	73% 20% 7%
8	H	950	96%
9	K	273	52% 10% 37%
10	L	24	8% 29% 71%
11	M	23	9% 65% 35%

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 23543 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 TFIIH basal transcription factor complex helicase XPB subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	604	4882	3119	845	889	29	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	677	5457	3502	948	978	29	0	0

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 IIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	179	1444	919	249	268	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	434	3483	2245	605	620	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	380	2989	1886	518	558	27	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-21	MET	-	expression tag	UNP Q13888
E	-20	GLY	-	expression tag	UNP Q13888
E	-19	SER	-	expression tag	UNP Q13888
E	-18	SER	-	expression tag	UNP Q13888
E	-17	HIS	-	expression tag	UNP Q13888
E	-16	HIS	-	expression tag	UNP Q13888
E	-15	HIS	-	expression tag	UNP Q13888
E	-14	HIS	-	expression tag	UNP Q13888
E	-13	HIS	-	expression tag	UNP Q13888
E	-12	HIS	-	expression tag	UNP Q13888
E	-11	SER	-	expression tag	UNP Q13888
E	-10	SER	-	expression tag	UNP Q13888
E	-9	GLY	-	expression tag	UNP Q13888
E	-8	LEU	-	expression tag	UNP Q13888
E	-7	GLU	-	expression tag	UNP Q13888
E	-6	VAL	-	expression tag	UNP Q13888
E	-5	LEU	-	expression tag	UNP Q13888
E	-4	PHE	-	expression tag	UNP Q13888
E	-3	GLN	-	expression tag	UNP Q13888
E	-2	GLY	-	expression tag	UNP Q13888
E	-1	PRO	-	expression tag	UNP Q13888
E	0	HIS	-	expression tag	UNP Q13888

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	258	2034	1301	337	377	19	0	0

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	H	38	303	189	54	60	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-9	MET	-	initiating methionine	UNP A0A024R2M8
H	-8	ASP	-	expression tag	UNP A0A024R2M8
H	-7	TYR	-	expression tag	UNP A0A024R2M8
H	-6	LYS	-	expression tag	UNP A0A024R2M8
H	-5	ASP	-	expression tag	UNP A0A024R2M8
H	-4	ASP	-	expression tag	UNP A0A024R2M8
H	-3	ASP	-	expression tag	UNP A0A024R2M8
H	-2	ASP	-	expression tag	UNP A0A024R2M8
H	-1	LYS	-	expression tag	UNP A0A024R2M8
H	0	HIS	-	expression tag	UNP A0A024R2M8
H	499	VAL	ALA	conflict	UNP A0A024R2M8

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	K	172	1450	908	255	273	14	0	0

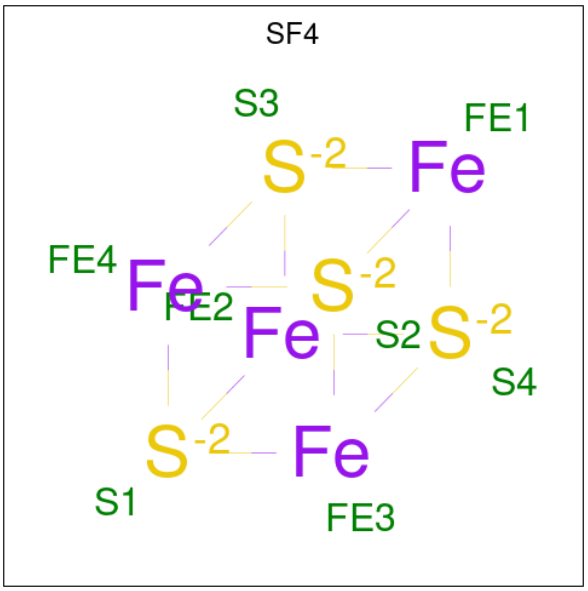
- Molecule 10 is a DNA chain called DNA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	L	24	496	235	92	145	24	0	0

- Molecule 11 is a DNA chain called DNA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	M	23	469	223	86	137	23	0	0

- Molecule 12 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

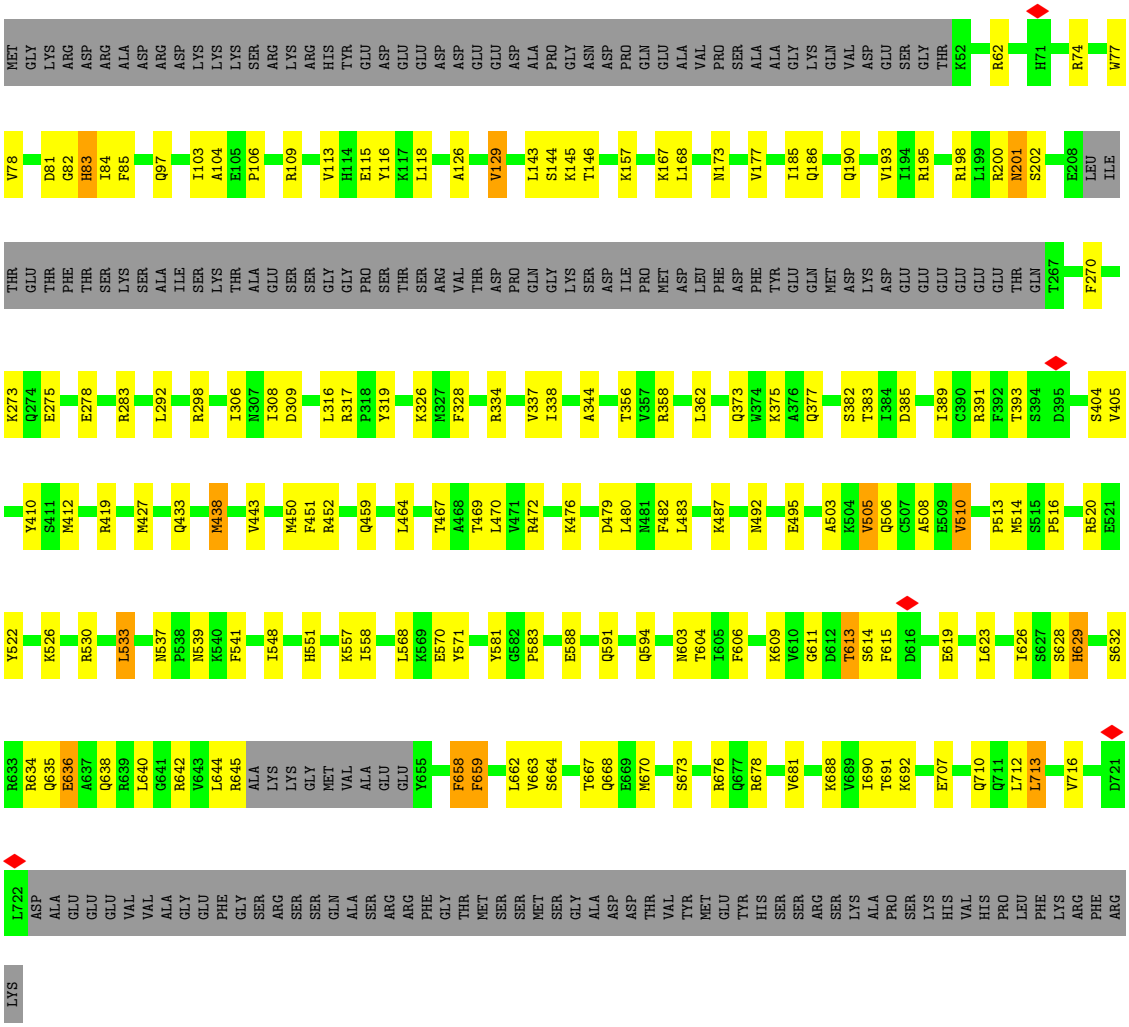
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
13	E	3	3	3	0
13	F	2	2	2	0
13	K	1	1	1	0

3 Residue-property plots (i)

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.

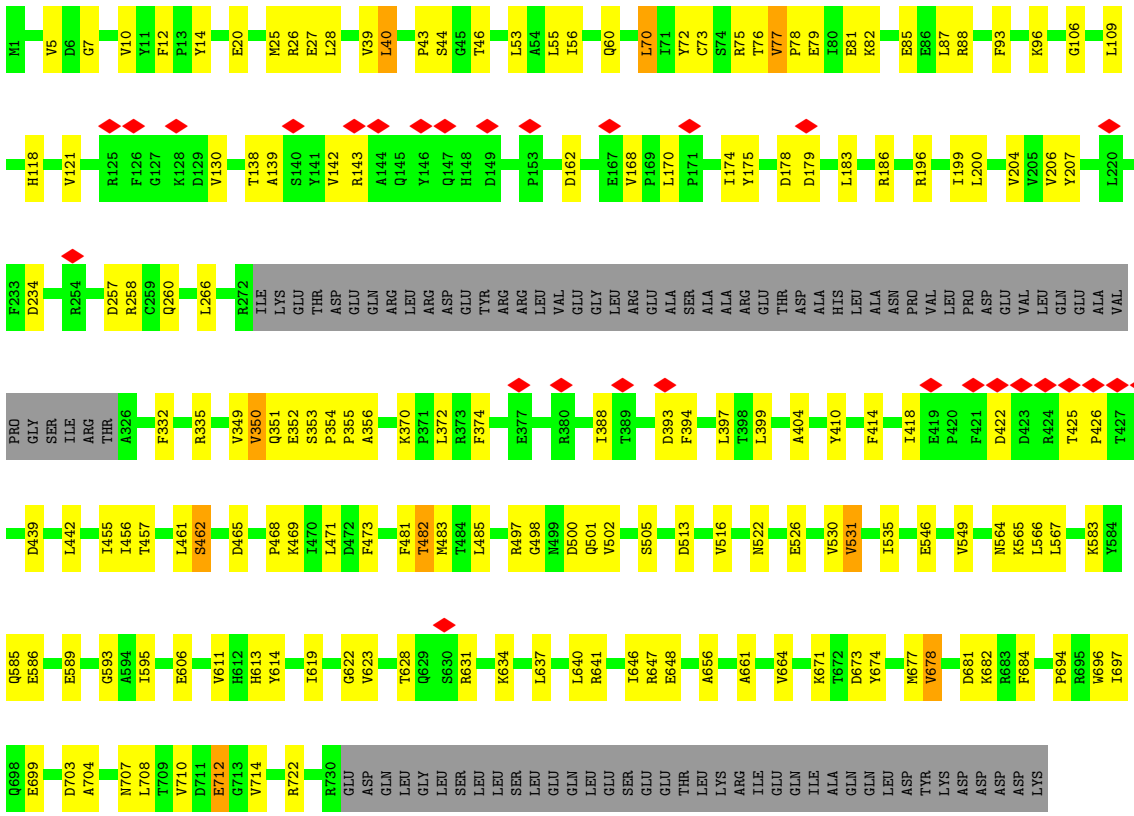
• Molecule 1: TFIIH basal transcription factor complex helicase XPB subunit

Chain A:



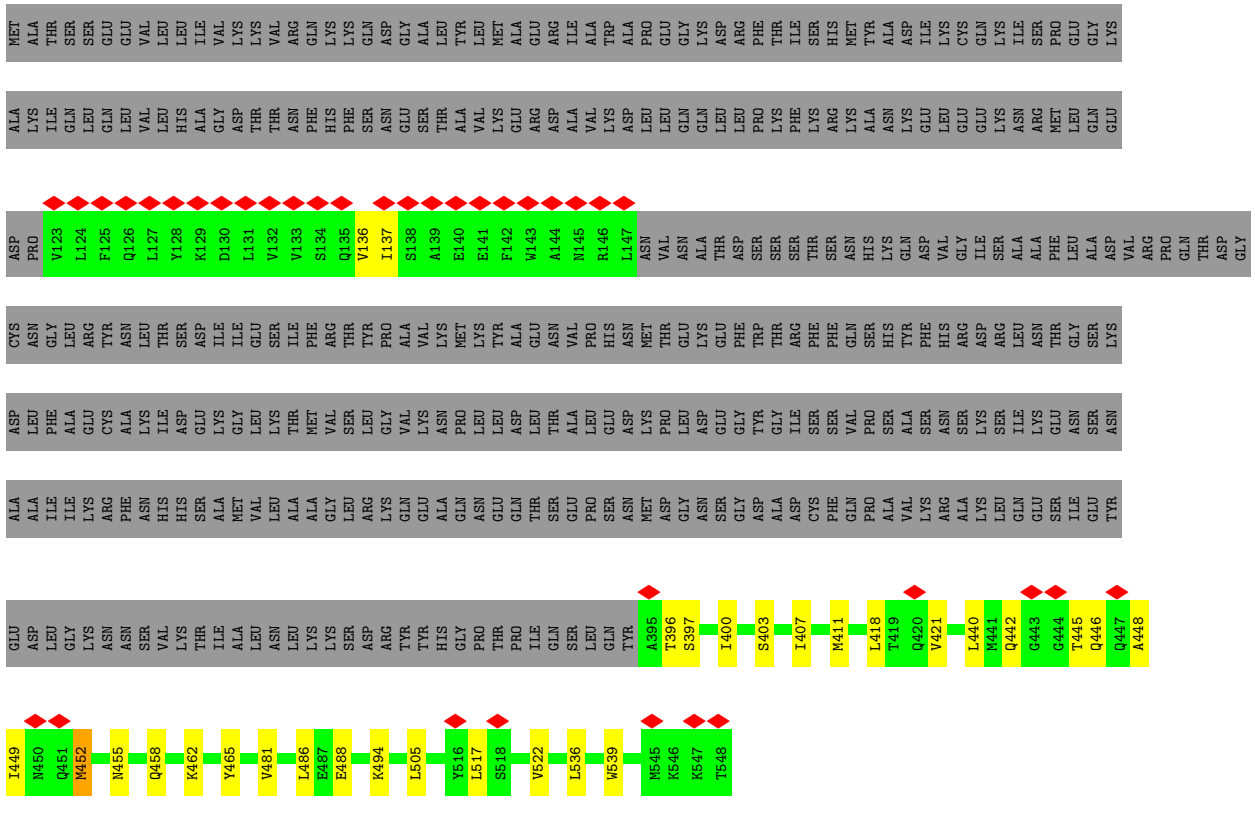
• Molecule 2: General transcription and DNA repair factor IIH helicase subunit XPD

Chain B:



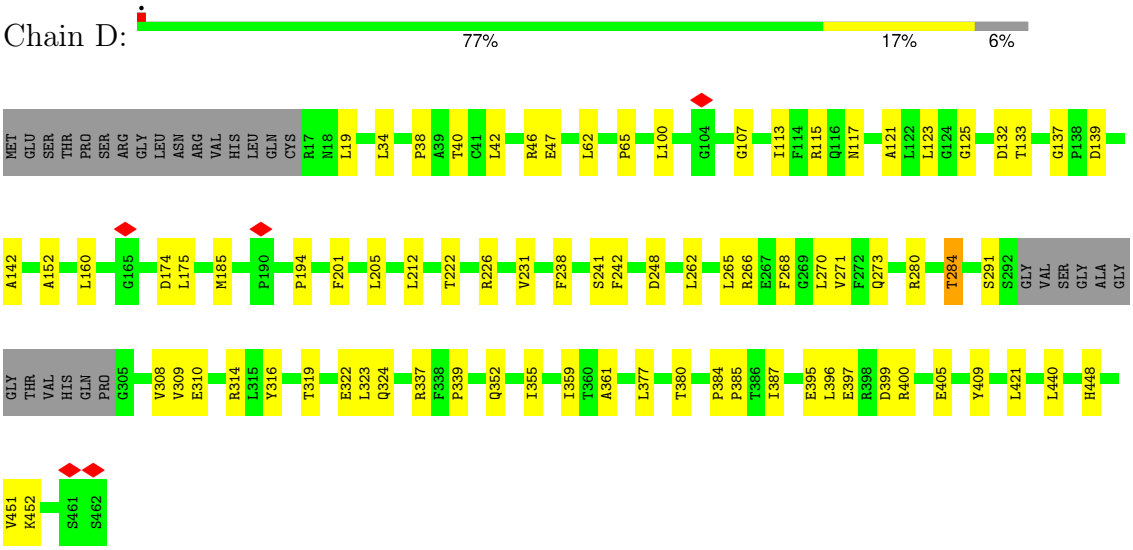
- Molecule 3: General transcription factor IIH subunit 1

Chain C: 7% 27% 5% 67%



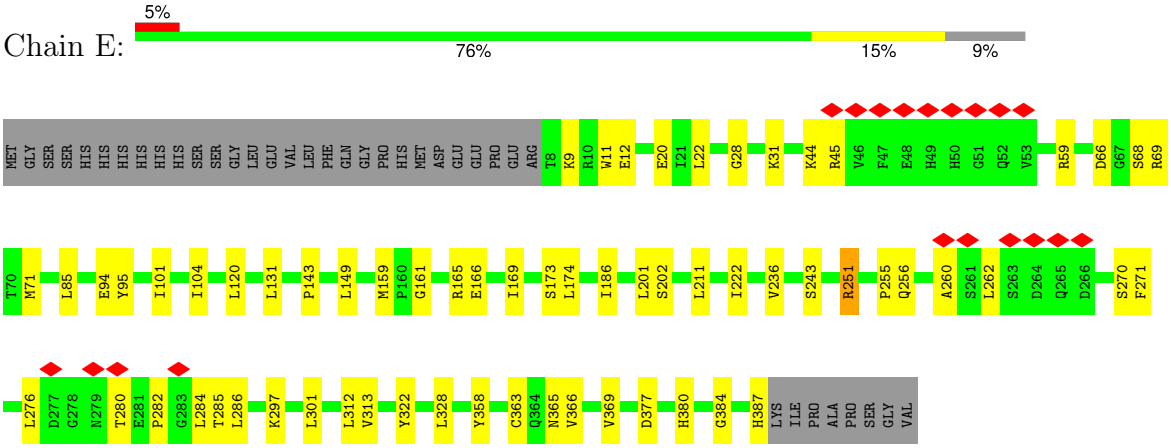
• Molecule 4: General transcription factor IIH subunit 4, p52

Chain D:



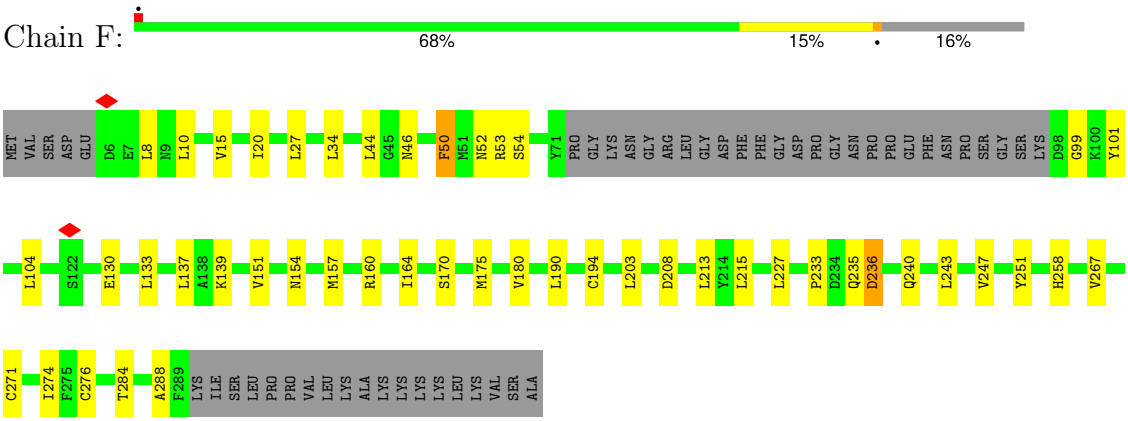
• Molecule 5: General transcription factor IIH subunit 2

Chain E:



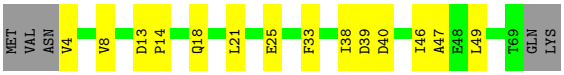
• Molecule 6: General transcription factor IIH subunit 3

Chain F:



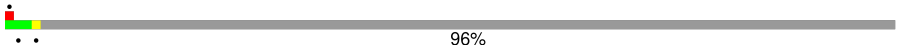
• Molecule 7: General transcription factor IIH subunit 5

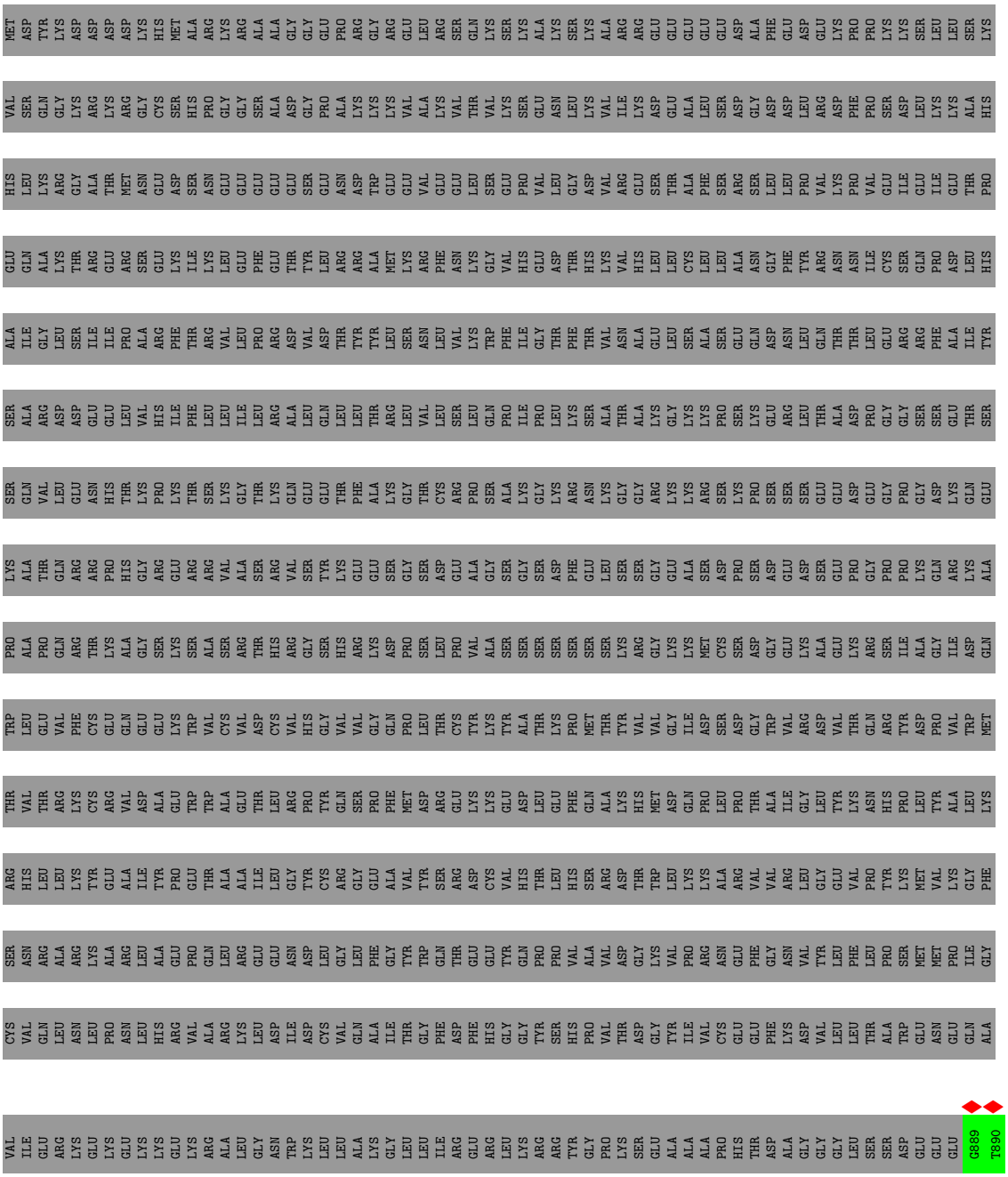
Chain G:

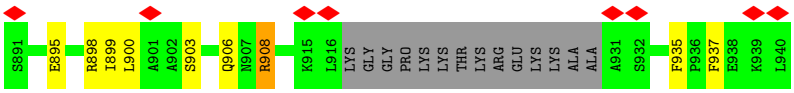


• Molecule 8: DNA repair protein complementing XP-C cells

Chain H:

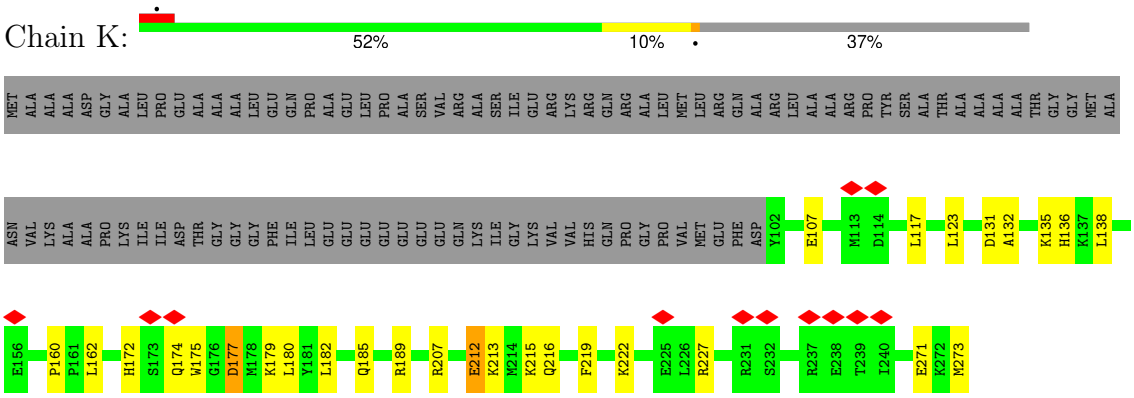






• Molecule 9: DNA repair protein complementing XP-A cells

Chain K:

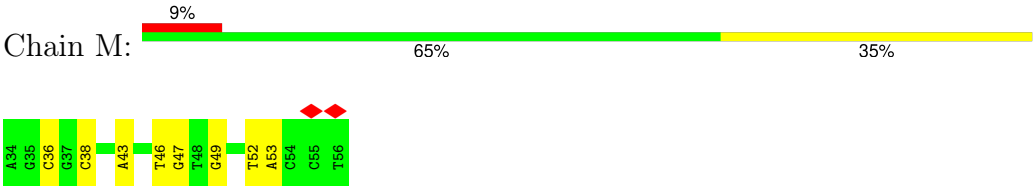


• Molecule 10: DNA1

Chain L:

• Molecule 11: DNA2

Chain M:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	136102	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 ($e^-/Å^2$)	54.1	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.750	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	373.5, 373.5, 373.5	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.245, 1.245, 1.245	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: ZN, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.12	0/4985	0.32	0/6734
2	B	0.11	0/5578	0.32	0/7551
3	C	0.10	0/1471	0.27	0/1986
4	D	0.10	0/3564	0.26	0/4827
5	E	0.11	0/3057	0.27	0/4136
6	F	0.09	0/2070	0.25	0/2803
7	G	0.10	0/528	0.29	0/713
8	H	0.11	0/308	0.43	0/411
9	K	0.08	0/1478	0.26	0/1974
10	L	0.19	0/556	0.40	0/857
11	M	0.16	0/525	0.31	0/807
All	All	0.11	0/24120	0.30	0/32799

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	4882	0	4923	108	0
2	B	5457	0	5499	107	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1444	0	1461	16	0
4	D	3483	0	3526	53	0
5	E	2989	0	2948	39	0
6	F	2034	0	2050	33	0
7	G	522	0	531	11	0
8	H	303	0	291	13	0
9	K	1450	0	1434	22	0
10	L	496	0	271	20	0
11	M	469	0	259	10	0
12	B	8	0	0	0	0
13	E	3	0	0	0	0
13	F	2	0	0	0	0
13	K	1	0	0	0	0
All	All	23543	0	23193	375	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 8.

All (375) 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)
4:D:396:LEU:HB3	8:H:908:ARG:HE	1.40	0.86
10:L:19:DG:H1	11:M:38:DC:H42	1.34	0.74
2:B:647:ARG:HH21	9:K:179:LYS:HE3	1.52	0.74
2:B:353:SER:HB2	2:B:356:ALA:HB3	1.71	0.73
1:A:692:LYS:HE2	8:H:906:GLN:HG3	1.71	0.73
1:A:419:ARG:HH11	1:A:427:MET:HG3	1.56	0.70
2:B:232:VAL:HG12	2:B:455:ILE:HB	1.72	0.70
1:A:510:VAL:HB	1:A:690:ILE:HB	1.71	0.70
4:D:400:ARG:NH2	7:G:13:ASP:OD2	2.26	0.69
4:D:291:SER:OG	6:F:53:ARG:NH2	2.26	0.69
1:A:615:PHE:HB2	1:A:642:ARG:HH22	1.59	0.68
2:B:352:GLU:OE2	2:B:631:ARG:NH1	2.29	0.65
1:A:77:TRP:HB2	1:A:85:PHE:HB2	1.78	0.65
1:A:356:THR:HG21	5:E:11:TRP:HE1	1.60	0.65
4:D:137:GLY:O	4:D:280:ARG:NH2	2.29	0.65
4:D:396:LEU:O	8:H:908:ARG:NH2	2.30	0.65
1:A:173:ASN:OD1	1:A:459:GLN:NE2	2.31	0.64
6:F:10:LEU:HB2	6:F:157:MET:HE2	1.78	0.64
2:B:5:VAL:HB	2:B:26:ARG:HH22	1.63	0.64
4:D:265:LEU:HD22	4:D:270:LEU:HD12	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:PRO:O	1:A:539:ASN:ND2	2.26	0.64
1:A:82:GLY:O	1:A:83:HIS:ND1	2.32	0.63
3:C:455:ASN:HA	3:C:458:GLN:HB2	1.80	0.63
5:E:260:ALA:HB3	5:E:286:LEU:HB3	1.80	0.63
1:A:526:LYS:O	1:A:530:ARG:NH1	2.32	0.62
3:C:481:VAL:HG13	3:C:486:LEU:HB2	1.80	0.62
1:A:198:ARG:HB3	1:A:202:SER:HB2	1.80	0.62
9:K:117:LEU:HD13	9:K:123:LEU:HD23	1.83	0.61
3:C:411:MET:HE3	6:F:34:LEU:HB3	1.81	0.61
1:A:337:VAL:HG21	1:A:480:LEU:HD21	1.80	0.61
2:B:505:SER:HB2	2:B:682:LYS:HG2	1.83	0.61
4:D:62:LEU:O	4:D:115:ARG:NH1	2.33	0.61
1:A:516:PRO:HG3	7:G:14:PRO:HB2	1.81	0.60
1:A:629:HIS:O	1:A:676:ARG:NH2	2.34	0.60
2:B:462:SER:HB3	2:B:694:PRO:HA	1.83	0.60
6:F:164:ILE:HG22	6:F:194:CYS:HB3	1.81	0.60
2:B:39:VAL:HG12	2:B:456:ILE:HB	1.82	0.60
2:B:109:LEU:HB2	2:B:207:TYR:HB3	1.83	0.60
2:B:564:ASN:OD1	5:E:69:ARG:NH2	2.35	0.60
1:A:278:GLU:OE2	1:A:452:ARG:NH2	2.35	0.60
2:B:75:ARG:NH2	2:B:606:GLU:O	2.34	0.60
1:A:514:MET:HA	1:A:537:ASN:HD21	1.65	0.60
4:D:405:GLU:HG2	7:G:8:VAL:HG22	1.84	0.60
2:B:43:PRO:HB3	2:B:696:TRP:CG	2.38	0.59
1:A:115:GLU:OE1	4:D:314:ARG:NH1	2.35	0.59
10:L:6:DG:H2'	10:L:7:DT:H71	1.84	0.59
2:B:641:ARG:NH1	9:K:177:ASP:OD2	2.36	0.58
2:B:88:ARG:HA	2:B:174:ILE:HD11	1.85	0.58
1:A:623:LEU:HB3	1:A:659:PHE:HB2	1.85	0.58
2:B:196:ARG:HH21	2:B:199:ILE:HD13	1.69	0.58
4:D:242:PHE:HB3	6:F:101:TYR:HE1	1.69	0.57
1:A:636:GLU:HG3	1:A:676:ARG:HE	1.69	0.57
2:B:468:PRO:HA	2:B:473:PHE:HB3	1.85	0.57
1:A:309:ASP:O	1:A:383:THR:OG1	2.21	0.57
2:B:677:MET:HE1	2:B:697:ILE:HD13	1.86	0.57
7:G:4:VAL:N	9:K:271:GLU:O	2.38	0.57
3:C:136:VAL:HG12	3:C:137:ILE:HG23	1.87	0.56
2:B:76:THR:OG1	2:B:79:GLU:OE1	2.22	0.56
1:A:514:MET:SD	1:A:537:ASN:ND2	2.78	0.56
2:B:628:THR:O	2:B:634:LYS:NZ	2.38	0.56
5:E:66:ASP:HB3	5:E:71:MET:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:11:DA:H2'	10:L:12:DG:C8	2.40	0.56
1:A:503:ALA:HB3	1:A:644:LEU:HA	1.87	0.56
4:D:355:ILE:HD13	4:D:395:GLU:HA	1.86	0.56
4:D:248:ASP:OD2	4:D:280:ARG:NH1	2.38	0.56
1:A:113:VAL:N	4:D:310:GLU:OE2	2.34	0.56
1:A:308:ILE:HD11	1:A:382:SER:HB2	1.88	0.56
4:D:132:ASP:OD1	4:D:133:THR:N	2.38	0.56
2:B:72:TYR:HB3	2:B:206:VAL:HG12	1.88	0.55
10:L:11:DA:H2'	10:L:12:DG:H8	1.71	0.55
2:B:485:LEU:HD11	2:B:671:LYS:HD2	1.88	0.55
2:B:372:LEU:HD12	2:B:404:ALA:HB1	1.89	0.55
1:A:505:VAL:HG11	1:A:640:LEU:HD11	1.89	0.55
3:C:494:LYS:HD2	3:C:536:LEU:HD23	1.87	0.55
3:C:400:ILE:HD11	6:F:20:ILE:HD13	1.88	0.55
9:K:172:HIS:HB3	9:K:175:TRP:HB2	1.89	0.55
2:B:482:THR:OG1	2:B:699:GLU:OE2	2.22	0.55
2:B:637:LEU:HD22	2:B:648:GLU:HG2	1.87	0.55
4:D:139:ASP:HB3	4:D:142:ALA:HB2	1.87	0.55
10:L:12:DG:H2'	10:L:13:DC:C6	2.42	0.55
2:B:497:ARG:NH2	2:B:707:ASN:O	2.40	0.55
4:D:396:LEU:HD13	8:H:908:ARG:HG3	1.88	0.55
2:B:350:VAL:HG11	2:B:631:ARG:HD3	1.89	0.55
5:E:243:SER:OG	6:F:288:ALA:O	2.21	0.55
4:D:421:LEU:HD11	4:D:451:VAL:HG13	1.88	0.54
1:A:375:LYS:HD3	1:A:391:ARG:HD3	1.89	0.54
6:F:151:VAL:HG21	6:F:157:MET:HB2	1.89	0.54
10:L:15:DG:H2'	10:L:16:DA:C8	2.42	0.54
1:A:522:TYR:HA	1:A:533:LEU:HD23	1.88	0.54
1:A:103:ILE:HA	1:A:126:ALA:HB2	1.89	0.54
4:D:352:GLN:HE22	4:D:397:GLU:HB2	1.72	0.54
7:G:39:ASP:OD1	7:G:40:ASP:N	2.40	0.54
1:A:508:ALA:HB2	8:H:935:PHE:CZ	2.43	0.54
6:F:267:VAL:HG22	6:F:274:ILE:HG12	1.90	0.54
3:C:418:LEU:HD22	4:D:123:LEU:HB3	1.89	0.54
1:A:356:THR:HG22	5:E:9:LYS:HG3	1.89	0.54
1:A:688:LYS:HD3	8:H:935:PHE:HE1	1.71	0.54
5:E:363:CYS:SG	5:E:365:ASN:ND2	2.81	0.54
1:A:581:TYR:HD2	1:A:583:PRO:HD2	1.73	0.53
2:B:422:ASP:H	2:B:426:PRO:HA	1.74	0.53
5:E:44:LYS:HD2	5:E:45:ARG:HG2	1.90	0.53
6:F:271:CYS:SG	6:F:284:THR:OG1	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:LEU:HD13	2:B:196:ARG:HH22	1.74	0.53
4:D:152:ALA:HB2	4:D:284:THR:HG21	1.91	0.53
1:A:613:THR:OG1	1:A:614:SER:N	2.42	0.53
4:D:310:GLU:HG3	4:D:316:TYR:HE1	1.73	0.53
2:B:703:ASP:OD1	2:B:703:ASP:N	2.42	0.53
6:F:190:LEU:HD11	6:F:235:GLN:HB3	1.90	0.53
1:A:628:SER:OG	1:A:635:GLN:OE1	2.26	0.53
2:B:77:VAL:HG13	2:B:78:PRO:HD3	1.89	0.53
1:A:664:SER:O	1:A:667:THR:OG1	2.25	0.53
3:C:462:LYS:HG3	5:E:276:LEU:HD22	1.90	0.52
2:B:28:LEU:HD23	2:B:55:LEU:HD23	1.90	0.52
5:E:387:HIS:HE1	6:F:139:LYS:HE3	1.74	0.52
9:K:207:ARG:NH1	10:L:17:DT:OP2	2.42	0.52
2:B:332:PHE:O	2:B:335:ARG:NH1	2.42	0.52
1:A:628:SER:OG	1:A:676:ARG:NH1	2.42	0.52
2:B:354:PRO:HG2	2:B:355:PRO:HD3	1.91	0.52
4:D:185:MET:HE2	4:D:194:PRO:HG2	1.90	0.52
4:D:399:ASP:HB2	8:H:908:ARG:HH22	1.75	0.52
6:F:52:ASN:ND2	6:F:54:SER:OG	2.42	0.52
1:A:326:LYS:O	1:A:334:ARG:NH2	2.42	0.52
5:E:174:LEU:HD21	5:E:202:SER:HB2	1.91	0.52
4:D:212:LEU:HD22	4:D:270:LEU:HD21	1.92	0.52
4:D:399:ASP:C	8:H:908:ARG:HH22	2.18	0.51
10:L:13:DC:H2'	10:L:14:DT:C6	2.45	0.51
1:A:492:ASN:HB3	1:A:495:GLU:HG2	1.91	0.51
2:B:500:ASP:HB2	2:B:502:VAL:HG22	1.93	0.51
4:D:113:ILE:O	4:D:117:ASN:ND2	2.41	0.51
2:B:12:PHE:HD1	2:B:14:TYR:H	1.59	0.51
2:B:139:ALA:H	2:B:142:VAL:HB	1.75	0.51
2:B:619:ILE:HA	2:B:678:VAL:HG22	1.92	0.51
3:C:440:LEU:HD13	6:F:215:LEU:HD11	1.93	0.51
5:E:201:LEU:HG	5:E:222:ILE:HD12	1.91	0.51
1:A:520:ARG:HG2	7:G:18:GLN:HB3	1.92	0.51
1:A:520:ARG:NH1	7:G:25:GLU:OE2	2.44	0.51
1:A:611:GLY:O	1:A:642:ARG:NH1	2.44	0.51
4:D:308:VAL:HB	4:D:316:TYR:HB2	1.92	0.51
2:B:589:GLU:OE2	2:B:614:TYR:OH	2.24	0.51
1:A:530:ARG:NH2	1:A:668:GLN:OE1	2.43	0.51
2:B:170:LEU:HD13	2:B:175:TYR:HE2	1.76	0.51
4:D:201:PHE:HB3	4:D:359:ILE:HD11	1.93	0.51
5:E:161:GLY:HA2	5:E:165:ARG:HH12	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:68:SER:HB3	5:E:143:PRO:HD3	1.92	0.51
5:E:186:ILE:HG12	5:E:211:LEU:HD13	1.92	0.51
1:A:678:ARG:HA	1:A:681:VAL:HG22	1.93	0.50
2:B:661:ALA:HA	2:B:664:VAL:HG12	1.93	0.50
5:E:85:LEU:HD22	5:E:131:LEU:HD22	1.93	0.50
1:A:167:LYS:HG2	1:A:292:LEU:HD11	1.94	0.50
2:B:43:PRO:HB2	2:B:483:MET:HE3	1.92	0.50
2:B:522:ASN:O	2:B:526:GLU:HG2	2.11	0.50
4:D:309:VAL:HG12	4:D:387:ILE:HD13	1.94	0.50
5:E:271:PHE:HD2	5:E:282:PRO:HB2	1.77	0.50
11:M:43:DA:H5'	11:M:43:DA:H8	1.77	0.50
1:A:84:ILE:HB	1:A:116:TYR:HB2	1.93	0.50
5:E:358:TYR:HE2	5:E:369:VAL:HG22	1.76	0.50
1:A:433:GLN:OE1	1:A:433:GLN:N	2.45	0.49
6:F:208:ASP:OD2	6:F:251:TYR:OH	2.30	0.49
9:K:138:LEU:HB3	9:K:180:LEU:HB3	1.94	0.49
9:K:219:PHE:HD1	9:K:222:LYS:HZ3	1.60	0.49
11:M:43:DA:H5'	11:M:43:DA:C8	2.47	0.49
5:E:255:PRO:HG3	5:E:312:LEU:HB3	1.94	0.49
9:K:107:GLU:OE2	9:K:135:LYS:NZ	2.44	0.49
1:A:450:MET:N	11:M:47:DG:OP1	2.39	0.49
2:B:258:ARG:HE	2:B:393:ASP:HA	1.78	0.49
3:C:488:GLU:N	3:C:488:GLU:OE1	2.45	0.49
4:D:262:LEU:HD11	4:D:271:VAL:HG11	1.94	0.49
1:A:309:ASP:OD1	1:A:309:ASP:N	2.45	0.49
3:C:448:ALA:O	3:C:452:MET:N	2.40	0.49
4:D:46:ARG:NH2	6:F:53:ARG:HE	2.11	0.49
1:A:62:ARG:HG3	4:D:339:PRO:HA	1.94	0.49
1:A:609:LYS:HB3	10:L:11:DA:H5'	1.94	0.49
1:A:710:GLN:HA	1:A:713:LEU:HD23	1.94	0.49
2:B:513:ASP:HB3	2:B:516:VAL:HG22	1.95	0.49
5:E:322:TYR:HB3	6:F:175:MET:HE3	1.93	0.49
1:A:77:TRP:CE2	1:A:145:LYS:HD3	2.48	0.49
2:B:708:LEU:HD12	2:B:712:GLU:HB2	1.93	0.49
1:A:317:ARG:HD3	1:A:319:TYR:HE1	1.77	0.48
1:A:568:LEU:HD11	1:A:606:PHE:HB3	1.94	0.48
2:B:56:ILE:HG21	2:B:70:LEU:HG	1.95	0.48
1:A:356:THR:HG21	5:E:11:TRP:NE1	2.28	0.48
2:B:234:ASP:HA	2:B:457:THR:HG23	1.94	0.48
9:K:182:LEU:HD23	9:K:185:GLN:HG3	1.96	0.48
1:A:338:ILE:HD13	1:A:464:LEU:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:44:LEU:HD22	6:F:227:LEU:HB3	1.94	0.48
10:L:16:DA:H2'	10:L:17:DT:C6	2.48	0.48
3:C:445:THR:HA	5:E:262:LEU:HD13	1.95	0.48
5:E:94:GLU:HG3	5:E:236:VAL:HG11	1.95	0.48
10:L:4:DT:H2"	10:L:5:DA:C8	2.48	0.48
1:A:690:ILE:HD13	8:H:937:PHE:HZ	1.78	0.48
2:B:640:LEU:HB3	2:B:646:ILE:HB	1.96	0.48
4:D:266:ARG:HD2	4:D:273:GLN:HB3	1.96	0.48
1:A:393:THR:O	1:A:393:THR:OG1	2.31	0.48
7:G:13:ASP:OD1	7:G:13:ASP:N	2.46	0.48
1:A:632:SER:HB3	11:M:49:DG:H5"	1.95	0.48
2:B:82:LYS:O	2:B:85:GLU:HG3	2.14	0.48
6:F:160:ARG:NH1	6:F:233:PRO:O	2.42	0.48
4:D:175:LEU:HD13	4:D:268:PHE:HE1	1.79	0.48
4:D:377:LEU:HD13	6:F:154:ASN:HB3	1.96	0.47
2:B:722:ARG:NH1	5:E:201:LEU:O	2.47	0.47
10:L:18:DT:H1'	10:L:19:DG:C8	2.49	0.47
1:A:688:LYS:HD3	8:H:935:PHE:CE1	2.49	0.47
9:K:174:GLN:HA	10:L:23:DT:H73	1.96	0.47
1:A:308:ILE:O	1:A:358:ARG:NE	2.47	0.47
2:B:27:GLU:CD	2:B:40:LEU:HD11	2.39	0.47
2:B:106:GLY:N	2:B:174:ILE:HG22	2.29	0.47
2:B:349:VAL:HG12	2:B:350:VAL:HG22	1.97	0.47
4:D:34:LEU:HB3	4:D:40:THR:HG21	1.97	0.47
7:G:8:VAL:HG23	7:G:47:ALA:HB2	1.97	0.47
4:D:238:PHE:O	4:D:241:SER:OG	2.26	0.47
5:E:284:LEU:HD23	5:E:284:LEU:H	1.79	0.46
2:B:694:PRO:HB2	2:B:696:TRP:CD1	2.49	0.46
3:C:397:SER:O	3:C:400:ILE:HG22	2.15	0.46
5:E:251:ARG:HH11	5:E:251:ARG:HB3	1.79	0.46
5:E:255:PRO:HG2	5:E:301:LEU:HD11	1.97	0.46
4:D:222:THR:OG1	4:D:226:ARG:NH1	2.46	0.46
6:F:15:VAL:HG13	6:F:164:ILE:HD11	1.97	0.46
11:M:52:DT:H2"	11:M:53:DA:N7	2.30	0.46
3:C:403:SER:HB3	6:F:27:LEU:HD11	1.98	0.46
5:E:59:ARG:NH2	5:E:166:GLU:OE1	2.47	0.46
9:K:213:LYS:O	9:K:216:GLN:HG3	2.16	0.46
2:B:44:SER:OG	2:B:46:THR:O	2.26	0.46
2:B:530:VAL:HG11	2:B:714:VAL:HG13	1.98	0.46
5:E:377:ASP:O	5:E:380:HIS:NE2	2.49	0.46
6:F:213:LEU:HD11	6:F:243:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:178:ASP:OD1	2:B:179:ASP:N	2.49	0.45
1:A:298:ARG:HA	1:A:298:ARG:HH11	1.81	0.45
1:A:319:TYR:OH	1:A:344:ALA:HB1	2.15	0.45
9:K:132:ALA:HA	9:K:136:HIS:HB2	1.98	0.45
9:K:212:GLU:HA	9:K:215:LYS:HG2	1.97	0.45
1:A:634:ARG:NH2	1:A:638:GLN:OE1	2.50	0.45
2:B:25:MET:SD	2:B:55:LEU:HB2	2.57	0.45
1:A:506:GLN:HB3	1:A:658:PHE:HB3	1.97	0.45
1:A:306:ILE:HG21	1:A:404:SER:HB2	1.97	0.45
1:A:613:THR:O	1:A:642:ARG:NH1	2.50	0.45
2:B:199:ILE:HG13	2:B:200:LEU:HD22	1.98	0.45
2:B:622:GLY:HA2	2:B:681:ASP:HB2	1.97	0.45
4:D:452:LYS:HE3	9:K:273:MET:HG2	1.98	0.45
1:A:663:VAL:HG11	1:A:673:SER:HB2	1.99	0.45
6:F:236:ASP:OD1	6:F:236:ASP:N	2.46	0.45
1:A:201:ASN:O	1:A:201:ASN:ND2	2.50	0.45
1:A:588:GLU:O	1:A:591:GLN:HG3	2.17	0.45
1:A:626:ILE:HG22	1:A:662:LEU:HB2	1.98	0.45
2:B:60:GLN:HE21	2:B:70:LEU:HD23	1.82	0.45
5:E:143:PRO:HG3	5:E:173:SER:HB3	1.98	0.45
8:H:895:GLU:OE1	8:H:898:ARG:NH1	2.50	0.45
1:A:385:ASP:N	1:A:385:ASP:OD1	2.49	0.45
1:A:713:LEU:HA	1:A:716:VAL:HG12	1.98	0.45
2:B:79:GLU:HA	2:B:82:LYS:HG2	1.99	0.44
3:C:505:LEU:HD11	3:C:522:VAL:HG13	1.99	0.44
4:D:440:LEU:HD13	7:G:38:ILE:HG22	1.98	0.44
2:B:351:GLN:HB2	2:B:418:ILE:HD11	2.00	0.44
5:E:28:GLY:O	5:E:31:LYS:HG2	2.16	0.44
1:A:594:GLN:HG3	2:B:704:ALA:HB1	1.98	0.44
9:K:160:PRO:O	9:K:189:ARG:NH2	2.29	0.44
2:B:78:PRO:HA	2:B:81:GLU:HG2	2.00	0.44
9:K:131:ASP:HB3	9:K:135:LYS:HB3	1.98	0.44
2:B:5:VAL:HA	2:B:26:ARG:HH12	1.83	0.44
2:B:546:GLU:HA	2:B:549:VAL:HG22	1.98	0.44
4:D:19:LEU:HD23	4:D:47:GLU:HG3	2.00	0.44
2:B:585:GLN:HG3	2:B:614:TYR:CE1	2.53	0.44
8:H:899:ILE:O	8:H:903:SER:OG	2.28	0.44
2:B:43:PRO:HG2	2:B:483:MET:HB3	1.98	0.44
2:B:673:ASP:OD1	2:B:674:TYR:N	2.51	0.44
2:B:20:GLU:HG2	2:B:483:MET:HA	1.99	0.43
4:D:322:GLU:CD	4:D:337:ARG:HH22	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:266:LEU:HD21	2:B:394:PHE:HE1	1.82	0.43
2:B:498:GLY:HA2	2:B:710:VAL:HG23	2.00	0.43
4:D:34:LEU:HD23	4:D:231:VAL:HG13	1.99	0.43
9:K:117:LEU:HB3	9:K:123:LEU:HB3	1.99	0.43
1:A:362:LEU:HD23	1:A:438:MET:HG3	2.00	0.43
11:M:46:DT:H2"	11:M:47:DG:H8	1.83	0.43
1:A:106:PRO:HG3	1:A:109:ARG:HH11	1.84	0.43
2:B:40:LEU:HD12	2:B:481:PHE:HE2	1.83	0.43
4:D:384:PRO:HA	4:D:385:PRO:HD3	1.94	0.43
6:F:133:LEU:HD21	6:F:203:LEU:HD21	2.00	0.43
4:D:38:PRO:HB3	4:D:121:ALA:HB2	2.00	0.43
1:A:551:HIS:HB2	1:A:558:ILE:HD11	2.00	0.43
2:B:53:LEU:HD13	2:B:87:LEU:HD13	2.00	0.43
2:B:465:ASP:O	2:B:469:LYS:NZ	2.40	0.43
2:B:497:ARG:HG3	2:B:501:GLN:HA	2.01	0.43
1:A:195:ARG:HG2	1:A:198:ARG:NH2	2.34	0.43
1:A:480:LEU:HA	1:A:483:LEU:HB2	2.01	0.43
1:A:619:GLU:HG3	1:A:645:ARG:HG3	2.00	0.43
10:L:8:DC:H2"	10:L:9:DA:H8	1.84	0.43
1:A:104:ALA:HB2	1:A:118:LEU:HD23	2.00	0.43
9:K:179:LYS:N	11:M:36:DC:OP1	2.45	0.43
1:A:470:LEU:HD23	1:A:487:LYS:HE2	2.01	0.43
2:B:258:ARG:NE	2:B:393:ASP:HA	2.34	0.43
2:B:565:LYS:HD2	2:B:593:GLY:HA3	2.01	0.43
4:D:361:ALA:HB2	4:D:395:GLU:HB2	1.99	0.43
6:F:258:HIS:CE1	6:F:276:CYS:SG	2.81	0.43
9:K:162:LEU:HD22	9:K:185:GLN:HB3	2.00	0.43
1:A:636:GLU:HG3	1:A:676:ARG:NE	2.32	0.43
5:E:149:LEU:HD21	5:E:169:ILE:HD11	1.99	0.43
1:A:472:ARG:HH12	1:A:476:LYS:HD2	1.84	0.42
1:A:185:ILE:HD12	1:A:270:PHE:HE1	1.84	0.42
1:A:81:ASP:OD1	1:A:81:ASP:N	2.52	0.42
1:A:186:GLN:O	1:A:190:GLN:NE2	2.43	0.42
1:A:328:PHE:HB2	5:E:12:GLU:HA	2.02	0.42
6:F:130:GLU:OE1	6:F:170:SER:OG	2.29	0.42
2:B:143:ARG:NH1	2:B:162:ASP:OD2	2.52	0.42
2:B:410:TYR:HB3	2:B:414:PHE:CE1	2.55	0.42
2:B:354:PRO:CG	2:B:355:PRO:HD3	2.49	0.42
2:B:566:LEU:O	2:B:595:ILE:N	2.49	0.42
2:B:567:LEU:HD23	2:B:595:ILE:HB	2.01	0.42
2:B:623:VAL:HG12	2:B:656:ALA:HB1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:219:PHE:HA	9:K:222:LYS:HG2	2.02	0.42
10:L:9:DA:H2"	10:L:10:DC:O5'	2.18	0.42
1:A:200:ARG:HD3	1:A:200:ARG:HA	1.77	0.42
2:B:634:LYS:HA	2:B:637:LEU:HD12	2.01	0.42
10:L:14:DT:H2"	10:L:15:DG:C8	2.55	0.42
1:A:548:ILE:HD12	1:A:604:THR:HG21	2.01	0.42
10:L:15:DG:H2"	10:L:16:DA:OP1	2.19	0.42
1:A:412:MET:HG3	10:L:14:DT:H5"	2.01	0.42
1:A:144:SER:C	1:A:146:THR:H	2.27	0.41
5:E:95:TYR:CD2	5:E:104:ILE:HD11	2.55	0.41
1:A:450:MET:SD	11:M:46:DT:H4'	2.60	0.41
2:B:73:CYS:HA	2:B:207:TYR:O	2.21	0.41
5:E:256:GLN:CD	5:E:256:GLN:H	2.27	0.41
1:A:373:GLN:O	1:A:377:GLN:HG2	2.20	0.41
1:A:443:VAL:HG12	1:A:467:THR:HB	2.02	0.41
2:B:699:GLU:OE1	2:B:699:GLU:N	2.54	0.41
3:C:481:VAL:HB	3:C:539:TRP:CZ2	2.55	0.41
5:E:120:LEU:HD23	5:E:159:MET:HE3	2.01	0.41
5:E:285:THR:O	5:E:297:LYS:NZ	2.54	0.41
5:E:365:ASN:ND2	5:E:384:GLY:HA3	2.35	0.41
1:A:410:TYR:HB3	1:A:451:PHE:CE1	2.55	0.41
2:B:25:MET:HA	2:B:25:MET:HE2	2.02	0.41
2:B:40:LEU:HD13	2:B:40:LEU:HA	1.81	0.41
2:B:170:LEU:HD13	2:B:175:TYR:CE2	2.56	0.41
4:D:291:SER:HG	6:F:53:ARG:NH2	2.18	0.41
4:D:319:THR:OG1	4:D:324:GLN:OE1	2.38	0.41
4:D:409:TYR:OH	4:D:448:HIS:ND1	2.37	0.41
1:A:273:LYS:HG2	1:A:275:GLU:HG3	2.01	0.41
1:A:541:PHE:HA	1:A:571:TYR:OH	2.21	0.41
7:G:33:PHE:CG	7:G:49:LEU:HD21	2.56	0.41
10:L:14:DT:H2"	10:L:15:DG:H8	1.85	0.41
1:A:157:LYS:HE2	1:A:157:LYS:HB2	1.89	0.41
1:A:479:ASP:HA	1:A:482:PHE:CE2	2.56	0.41
2:B:70:LEU:HB2	2:B:204:VAL:HG12	2.02	0.41
4:D:125:GLY:O	6:F:99:GLY:HA3	2.21	0.41
1:A:74:ARG:HG2	1:A:143:LEU:HA	2.03	0.41
1:A:389:ILE:HD13	1:A:405:VAL:HB	2.02	0.41
1:A:670:MET:HE3	1:A:670:MET:HB3	1.93	0.41
2:B:183:LEU:HA	2:B:186:ARG:HG2	2.03	0.41
2:B:439:ASP:HB3	2:B:442:LEU:HD23	2.03	0.41
2:B:611:VAL:HG12	2:B:614:TYR:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:42:LEU:HD13	6:F:50:PHE:CZ	2.56	0.41
6:F:15:VAL:HG22	6:F:164:ILE:HD11	2.03	0.41
2:B:257:ASP:O	2:B:260:GLN:HG3	2.20	0.41
2:B:422:ASP:HB3	2:B:425:THR:O	2.21	0.41
4:D:65:PRO:HB2	4:D:107:GLY:HA3	2.03	0.41
2:B:5:VAL:HG23	2:B:7:GLY:H	1.86	0.41
2:B:40:LEU:O	2:B:461:LEU:HD12	2.21	0.41
2:B:56:ILE:HD13	2:B:56:ILE:HA	1.93	0.41
2:B:121:VAL:HG22	2:B:130:VAL:HG12	2.03	0.41
2:B:350:VAL:HG11	2:B:631:ARG:HH11	1.86	0.41
2:B:370:LYS:HG3	2:B:374:PHE:HE2	1.86	0.41
2:B:583:LYS:O	2:B:586:GLU:HG3	2.20	0.41
1:A:193:VAL:HG21	1:A:283:ARG:HE	1.85	0.41
2:B:93:PHE:HA	2:B:96:LYS:HG2	2.03	0.41
11:M:52:DT:H2"	11:M:53:DA:C8	2.56	0.41
4:D:160:LEU:HD12	4:D:323:LEU:HD21	2.03	0.40
10:L:23:DT:H6	10:L:23:DT:H2'	1.70	0.40
1:A:692:LYS:HG2	8:H:906:GLN:HE21	1.86	0.40
2:B:681:ASP:HB3	2:B:684:PHE:CD2	2.57	0.40
1:A:129:VAL:HG22	1:A:334:ARG:HH22	1.86	0.40
1:A:469:THR:HG21	1:A:638:GLN:HG3	2.03	0.40
5:E:270:SER:HB2	5:E:297:LYS:HD2	2.02	0.40
6:F:46:ASN:HB3	6:F:104:LEU:HD13	2.03	0.40
9:K:207:ARG:HA	9:K:207:ARG:HD3	1.95	0.40
6:F:137:LEU:HB3	6:F:180:VAL:HG11	2.04	0.40
1:A:557:LYS:HD3	1:A:603:ASN:HB2	2.03	0.40
2:B:531:VAL:HG13	2:B:535:ILE:HD11	2.03	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	598/782 (76%)	559 (94%)	39 (6%)	0	100	100
2	B	673/768 (88%)	644 (96%)	29 (4%)	0	100	100
3	C	175/548 (32%)	166 (95%)	9 (5%)	0	100	100
4	D	430/462 (93%)	426 (99%)	4 (1%)	0	100	100
5	E	378/417 (91%)	363 (96%)	15 (4%)	0	100	100
6	F	254/308 (82%)	250 (98%)	4 (2%)	0	100	100
7	G	64/71 (90%)	59 (92%)	5 (8%)	0	100	100
8	H	34/950 (4%)	30 (88%)	4 (12%)	0	100	100
9	K	170/273 (62%)	168 (99%)	2 (1%)	0	100	100
All	All	2776/4579 (61%)	2665 (96%)	111 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	536/688 (78%)	514 (96%)	22 (4%)	27	55
2	B	591/672 (88%)	572 (97%)	19 (3%)	34	60
3	C	163/484 (34%)	154 (94%)	9 (6%)	19	48
4	D	377/399 (94%)	372 (99%)	5 (1%)	61	74
5	E	338/371 (91%)	330 (98%)	8 (2%)	43	65
6	F	230/272 (85%)	225 (98%)	5 (2%)	45	66
7	G	59/64 (92%)	57 (97%)	2 (3%)	32	59
8	H	31/815 (4%)	29 (94%)	2 (6%)	15	43
9	K	162/233 (70%)	159 (98%)	3 (2%)	50	68
All	All	2487/3998 (62%)	2412 (97%)	75 (3%)	37	61

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	VAL
1	A	83	HIS
1	A	97	GLN
1	A	129	VAL
1	A	168	LEU
1	A	177	VAL
1	A	201	ASN
1	A	316	LEU
1	A	438	MET
1	A	505	VAL
1	A	510	VAL
1	A	533	LEU
1	A	570	GLU
1	A	613	THR
1	A	629	HIS
1	A	636	GLU
1	A	658	PHE
1	A	659	PHE
1	A	691	THR
1	A	707	GLU
1	A	712	LEU
1	A	713	LEU
2	B	10	VAL
2	B	40	LEU
2	B	70	LEU
2	B	77	VAL
2	B	118	HIS
2	B	138	THR
2	B	168	VAL
2	B	350	VAL
2	B	388	ILE
2	B	397	LEU
2	B	399	LEU
2	B	434	HIS
2	B	462	SER
2	B	471	LEU
2	B	482	THR
2	B	531	VAL
2	B	613	HIS
2	B	678	VAL
2	B	712	GLU
3	C	396	THR
3	C	407	ILE

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Mol	Chain	Res	Type
3	C	421	VAL
3	C	442	GLN
3	C	446	GLN
3	C	449	ILE
3	C	452	MET
3	C	465	TYR
3	C	517	LEU
4	D	100	LEU
4	D	174	ASP
4	D	205	LEU
4	D	284	THR
4	D	380	THR
5	E	20	GLU
5	E	22	LEU
5	E	101	ILE
5	E	251	ARG
5	E	280	THR
5	E	313	VAL
5	E	328	LEU
5	E	366	VAL
6	F	8	LEU
6	F	50	PHE
6	F	236	ASP
6	F	240	GLN
6	F	247	VAL
7	G	21	LEU
7	G	46	ILE
8	H	900	LEU
8	H	908	ARG
9	K	177	ASP
9	K	212	GLU
9	K	227	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	GLN
1	A	307	ASN
1	A	499	ASN
1	A	595	ASN
1	A	656	ASN
2	B	92	ASN

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Mol	Chain	Res	Type
2	B	238	ASN
2	B	402	ASN
2	B	519	ASN
2	B	560	ASN
2	B	729	HIS
3	C	509	GLN
4	D	97	HIS
4	D	352	GLN
5	E	365	ASN
6	F	52	ASN
6	F	65	GLN
6	F	145	HIS
6	F	179	ASN
6	F	260	ASN
7	G	27	ASN
7	G	42	HIS
9	K	210	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 6 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	$\#\|Z\| > 2$
12	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
12	SF4	B	1000	2	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation (i)

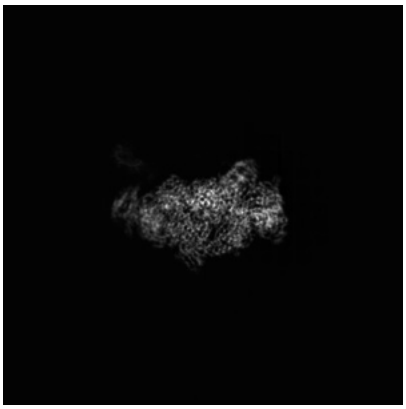
This section contains visualisations of the EMDB entry EMD-27998. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

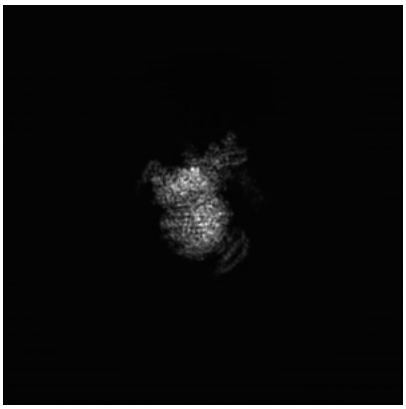
6.1 Orthogonal projections (i)

6.1.1 Primary map

X

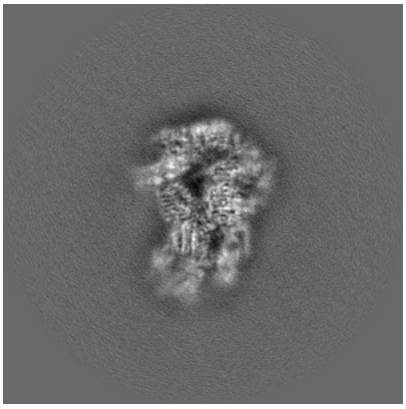


Y

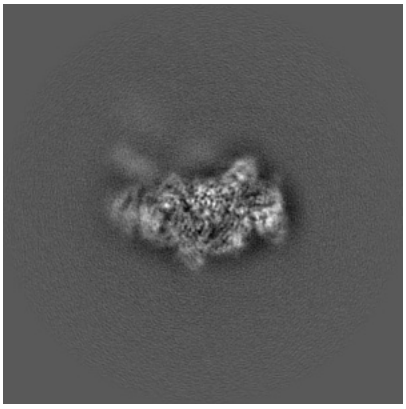


Z

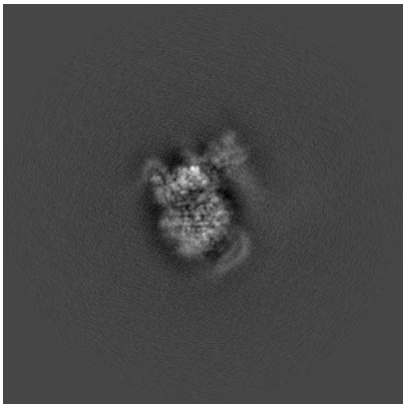
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

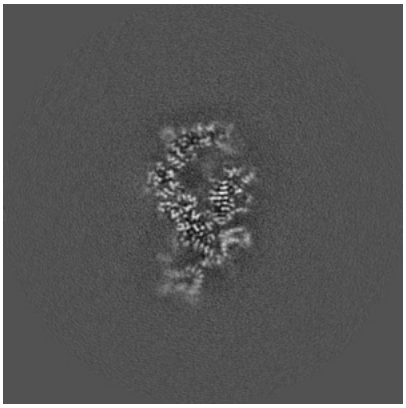
6.2.1 Primary map

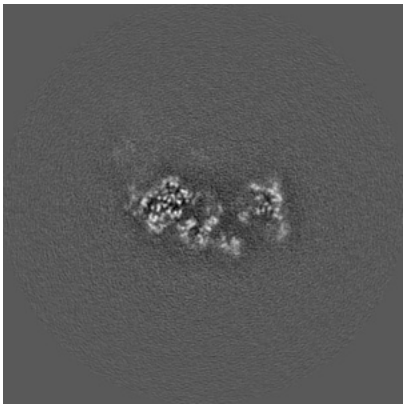
X Index: 150

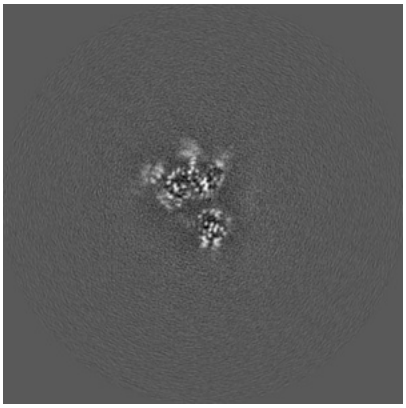
Y Index: 150

Z Index: 150

6.2.2 Raw map


X Index: 150


Y Index: 150


Z Index: 150

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

6.3 Largest variance slices (i)

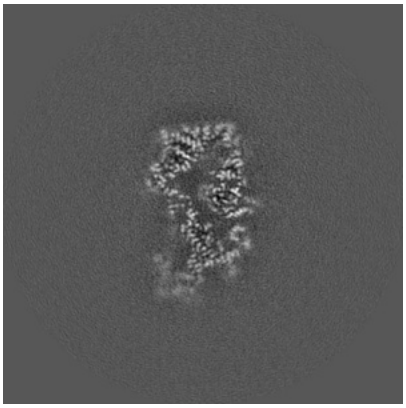
6.3.1 Primary map

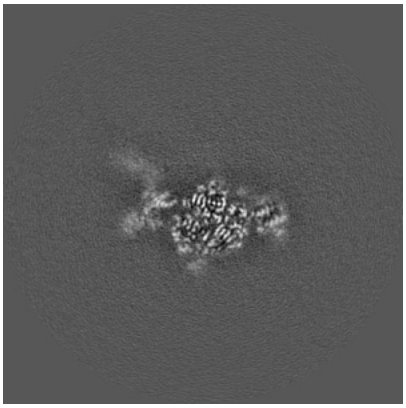
X Index: 146

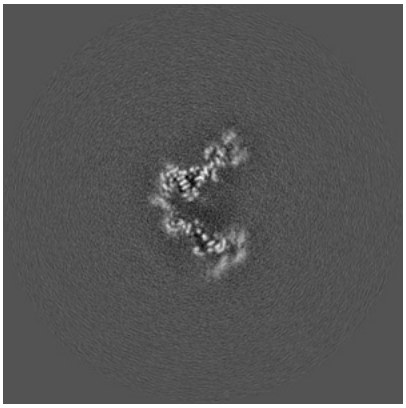
Y Index: 165

Z Index: 174

6.3.2 Raw map


X Index: 146


Y Index: 165

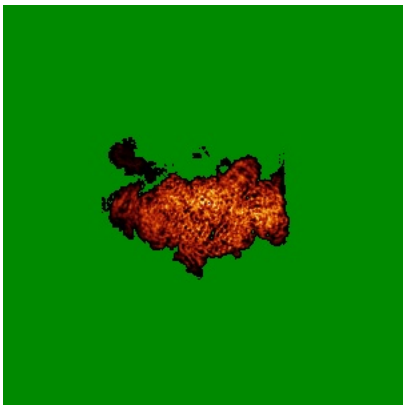

Z Index: 174

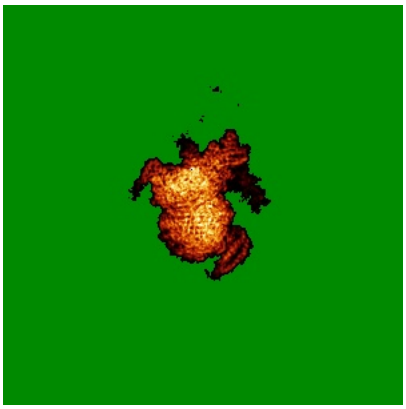
The images above show the largest variance slices of the map in three orthogonal directions.

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

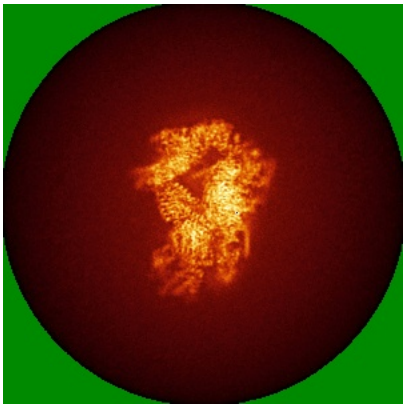
6.4.1 Primary map

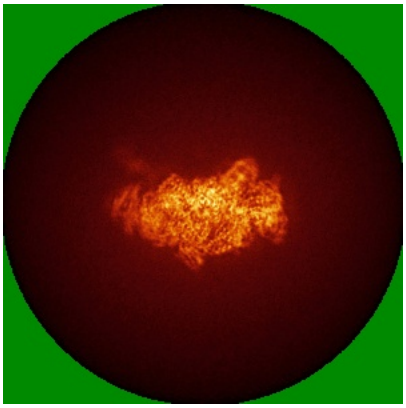
X

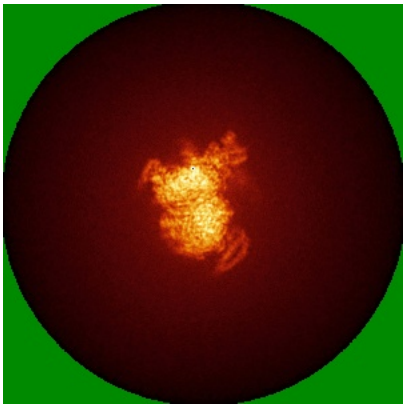

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

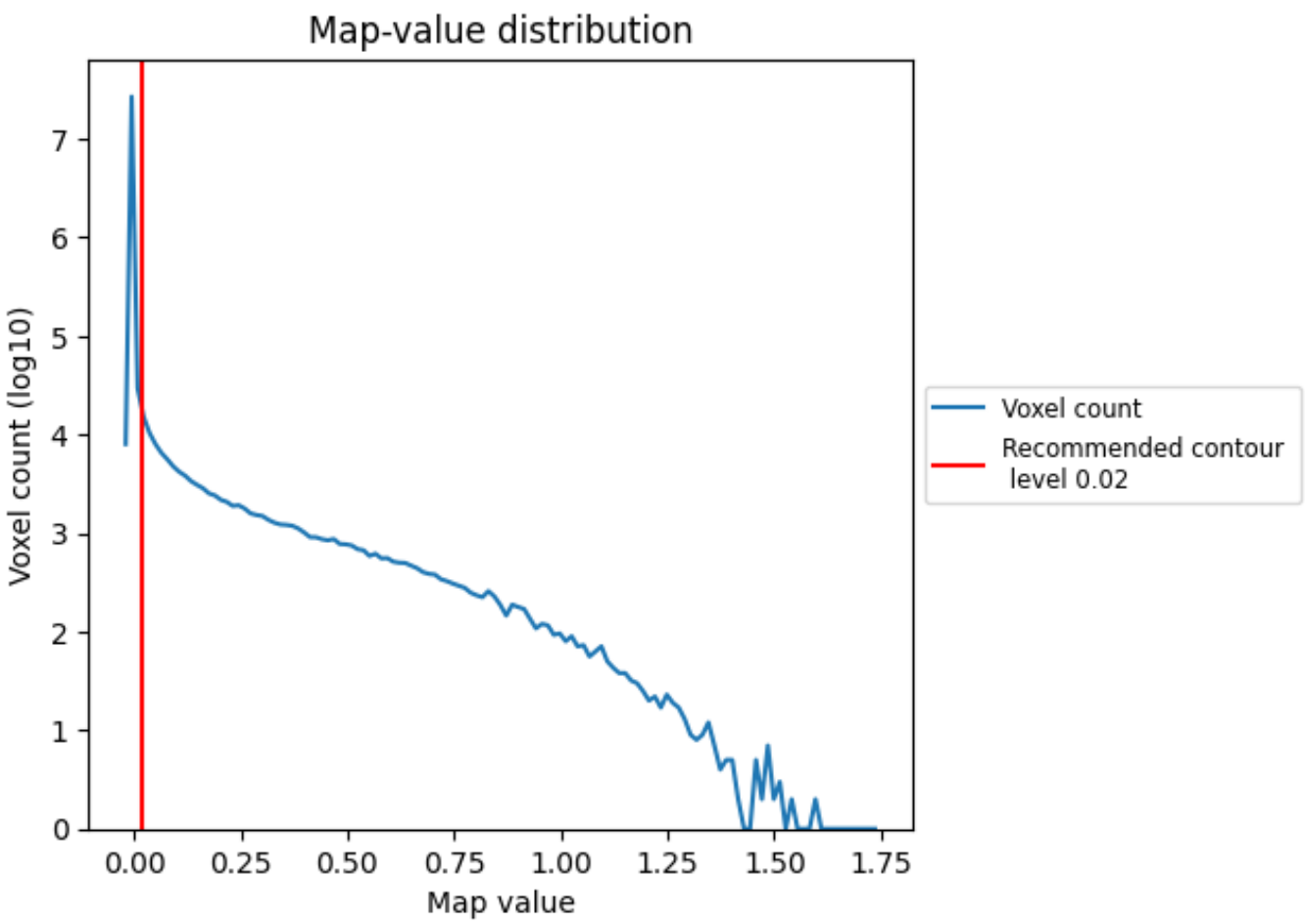
6.6 Mask visualisation (i)

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

7 Map analysis (i)

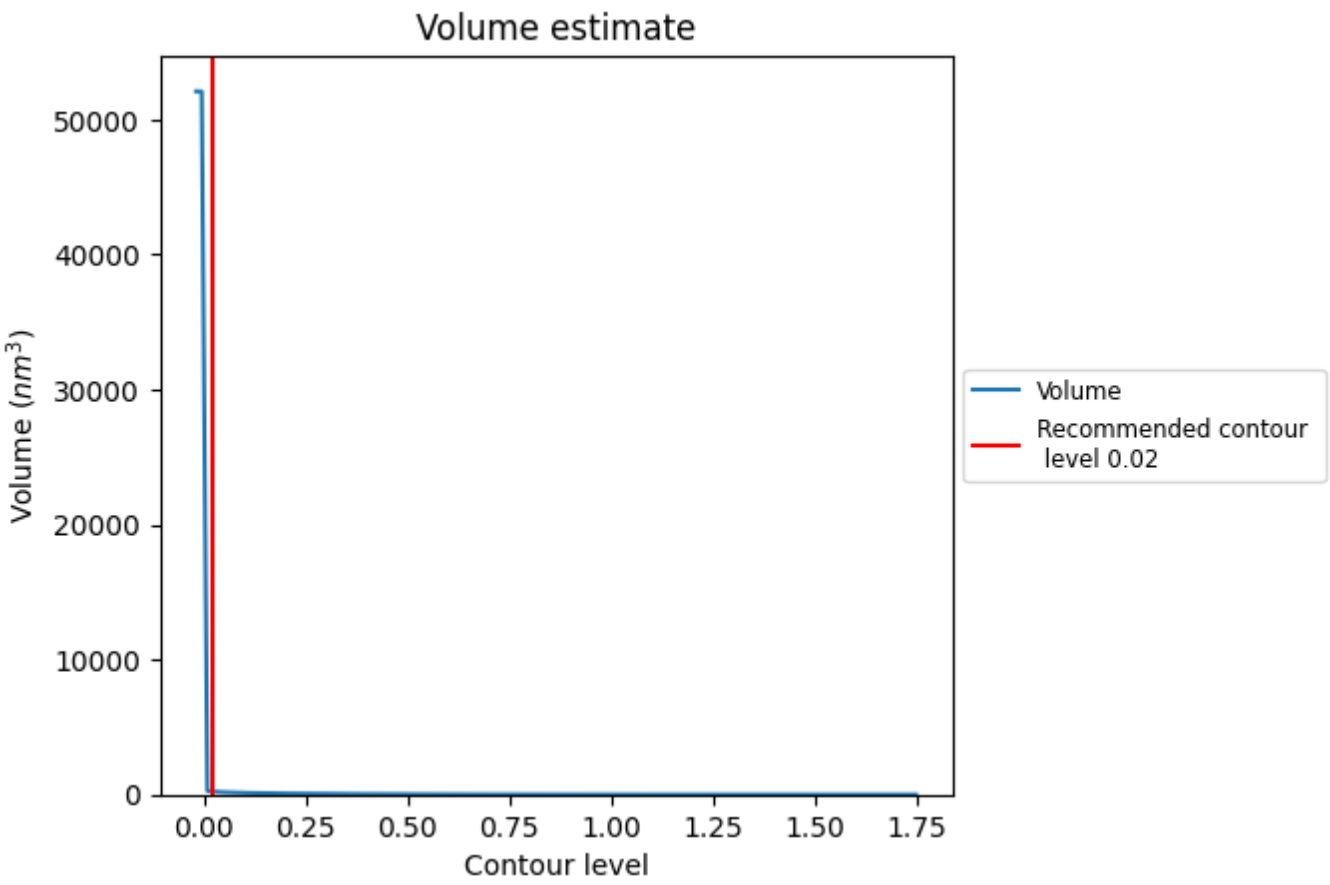
This section contains the results of statistical analysis of the map.

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.

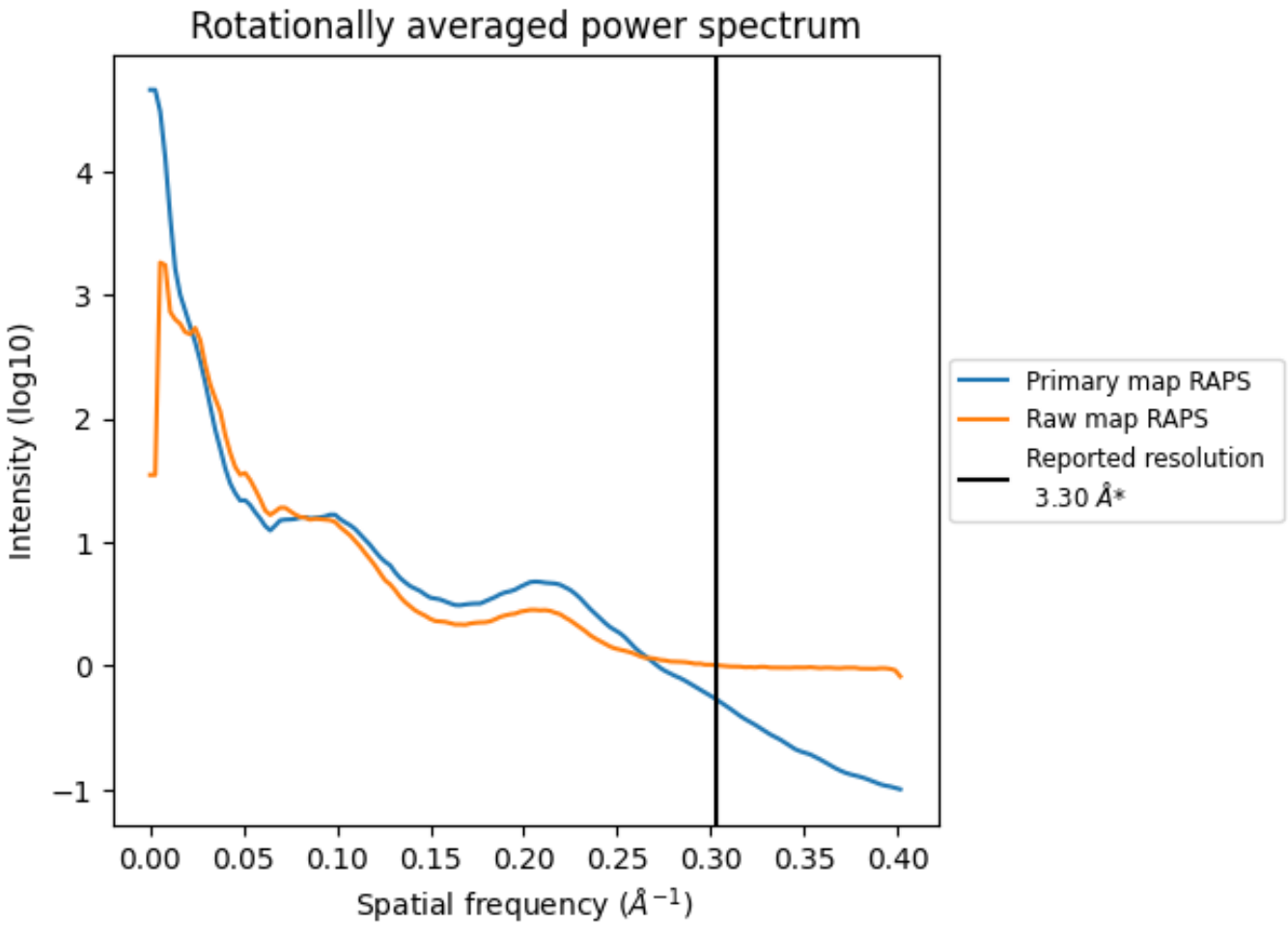
7.2 Volume estimate (i)



The volume at the recommended contour level is 232 nm^3; this corresponds to an approximate mass of 209 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)

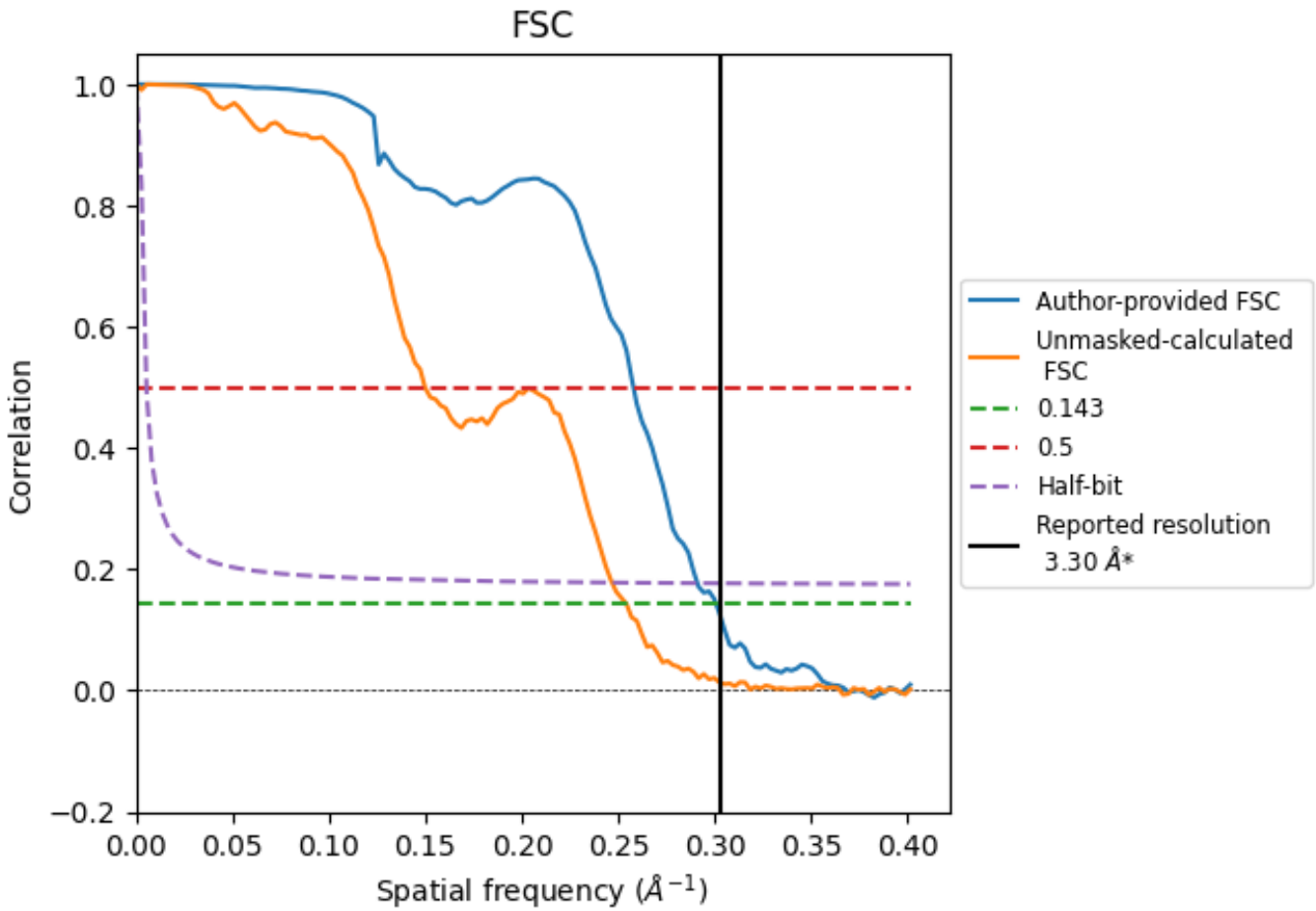


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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 Å^{-1}

8.2 Resolution estimates (i)

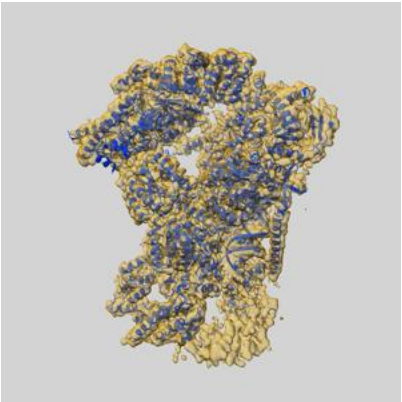
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.88	3.43
Unmasked-calculated*	3.93	6.67	4.05

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.93 differs from the reported value 3.3 by more than 10 %

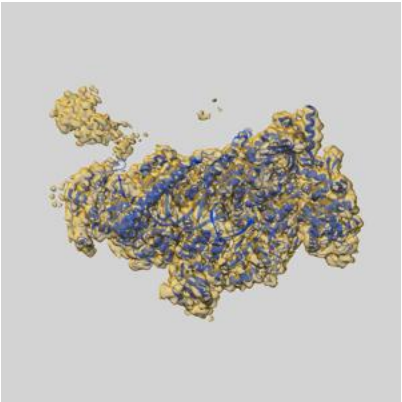
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-27998 and PDB model 8EBU. Per-residue inclusion information can be found in section 3 on page 8.

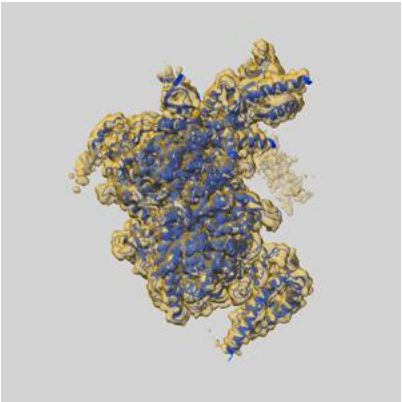
9.1 Map-model overlay (i)



X



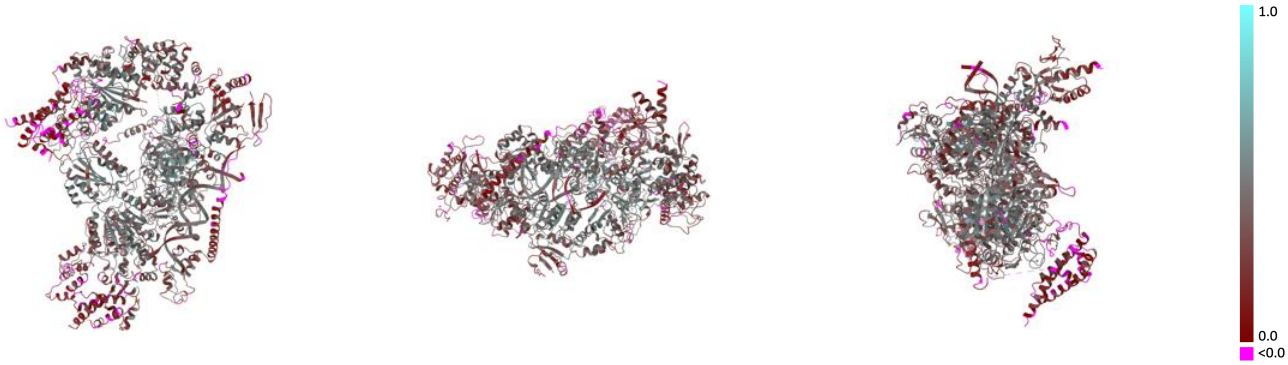
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

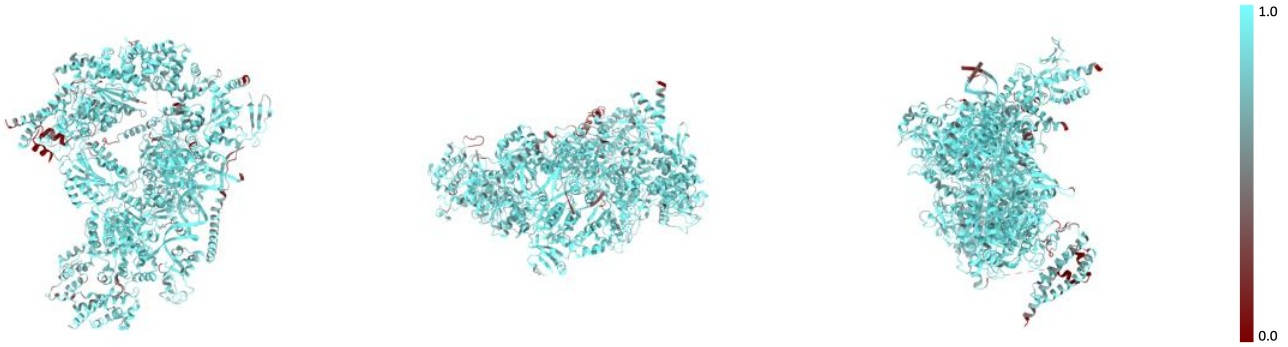
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

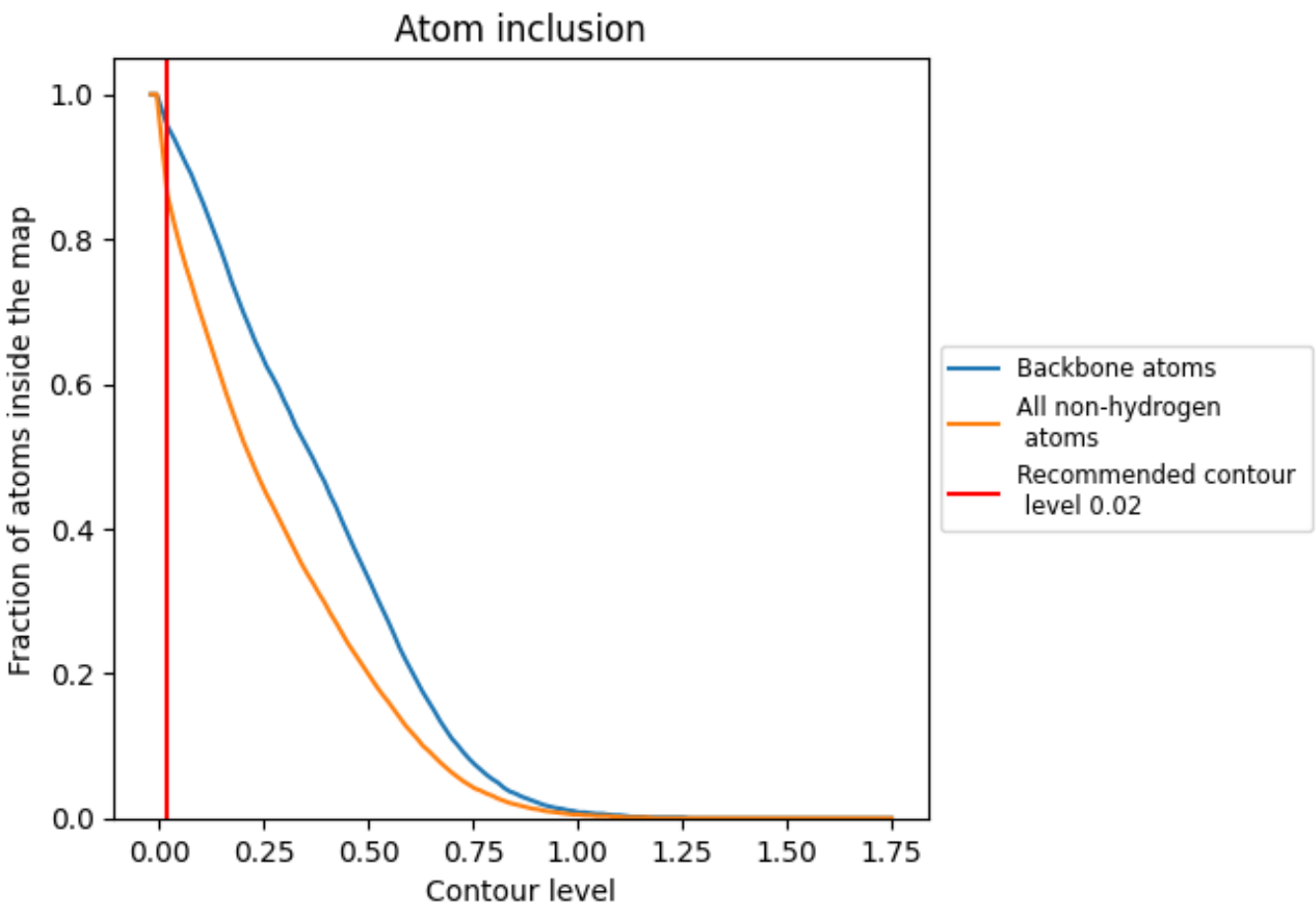
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8610	0.3410
A	0.9200	0.4140
B	0.8580	0.3000
C	0.6590	0.1360
D	0.8860	0.3500
E	0.8730	0.3950
F	0.9060	0.4180
G	0.8960	0.3780
H	0.6340	0.2020
K	0.7520	0.2230
L	0.8950	0.3610
M	0.8740	0.3680