



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 09:57 PM EDT

PDB ID : 8EBS / pdb_00008ebs
EMDB ID : EMD-27996
Title : Initial DNA-lesion (Cy5) binding by XPC and TFIIH
Authors : Kim, J.; Yang, W.
Deposited on : 2022-08-31
Resolution : 4.00 Å(reported)
Based on initial model : 6NMI

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:

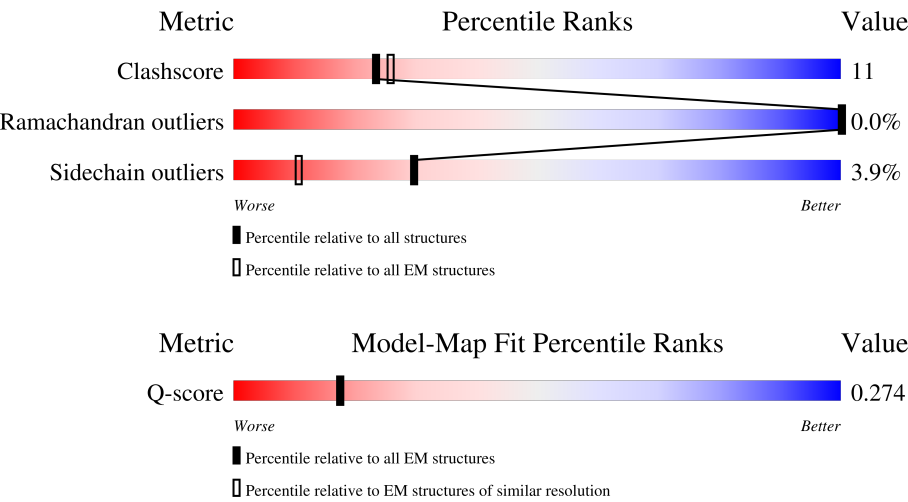
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
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 4.00 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.



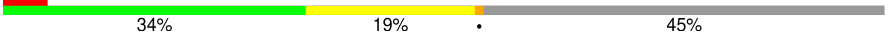
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	55% 22% • 22%
2	B	768	72% 27% ••
3	C	548	49% 15% • 35%
4	D	462	73% 23% ••

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Mol	Chain	Length	Quality of chain
5	E	417	
6	F	308	
7	G	71	
8	H	950	
9	I	417	
10	J	172	
11	L	52	
12	M	53	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 31035 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	611	Total	C	N	O	S	0	0
			4931	3149	854	898	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	760	Total	C	N	O	S	0	0
			6120	3907	1067	1117	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	358	Total	C	N	O	S	0	0
			2895	1835	505	542	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	446	Total	C	N	O	S	0	0
			3557	2289	620	635	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	355	Total	C	N	O	S	0	0
			2792	1760	483	522	27		

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
6	F	261	Total	C	N	O	S	0	0
			2057	1316	341	381	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	67	Total	C	N	O	S	0	0
			530	342	84	101	3		

- Molecule 8 is a protein called Xeroderma pigmentosum, complementation group C, isoform CRA_a.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	519	Total	C	N	O	S	0	0
			4264	2727	753	764	20		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-9	MET	-	expression tag	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 UV excision repair protein RAD23 homolog B.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	61	Total	C	N	O	S	0	0
			504	316	95	91	2		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	410	LEU	-	expression tag	UNP P54727
I	411	GLU	-	expression tag	UNP P54727
I	412	HIS	-	expression tag	UNP P54727
I	413	HIS	-	expression tag	UNP P54727
I	414	HIS	-	expression tag	UNP P54727
I	415	HIS	-	expression tag	UNP P54727
I	416	HIS	-	expression tag	UNP P54727
I	417	HIS	-	expression tag	UNP P54727

- Molecule 10 is a protein called Centrin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	149	Total	C	N	O	S	1	0
			1201	749	194	251	7		

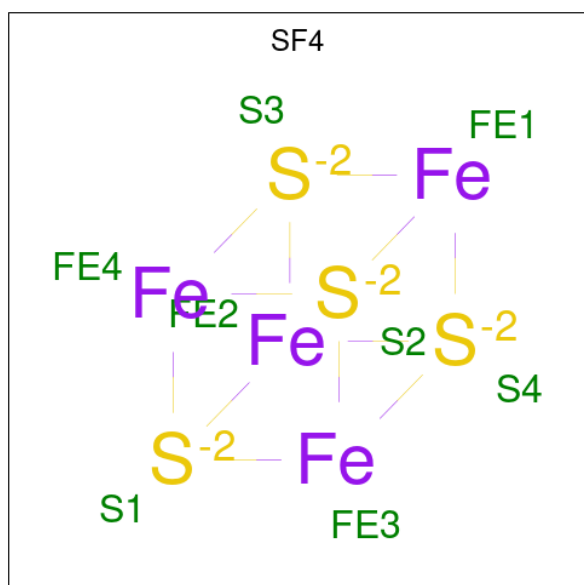
- Molecule 11 is a DNA chain called DNA (Cy5).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	52	Total	C	N	O	P	0	0
			1091	531	198	310	52		

- Molecule 12 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	53	Total	C	N	O	P	0	0
			1078	515	190	320	53		

- Molecule 13 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
14	E	3	Total	Zn	0
			3	3	

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Mol	Chain	Residues	Atoms		AltConf
14	F	2	Total	Zn	0
			2	2	

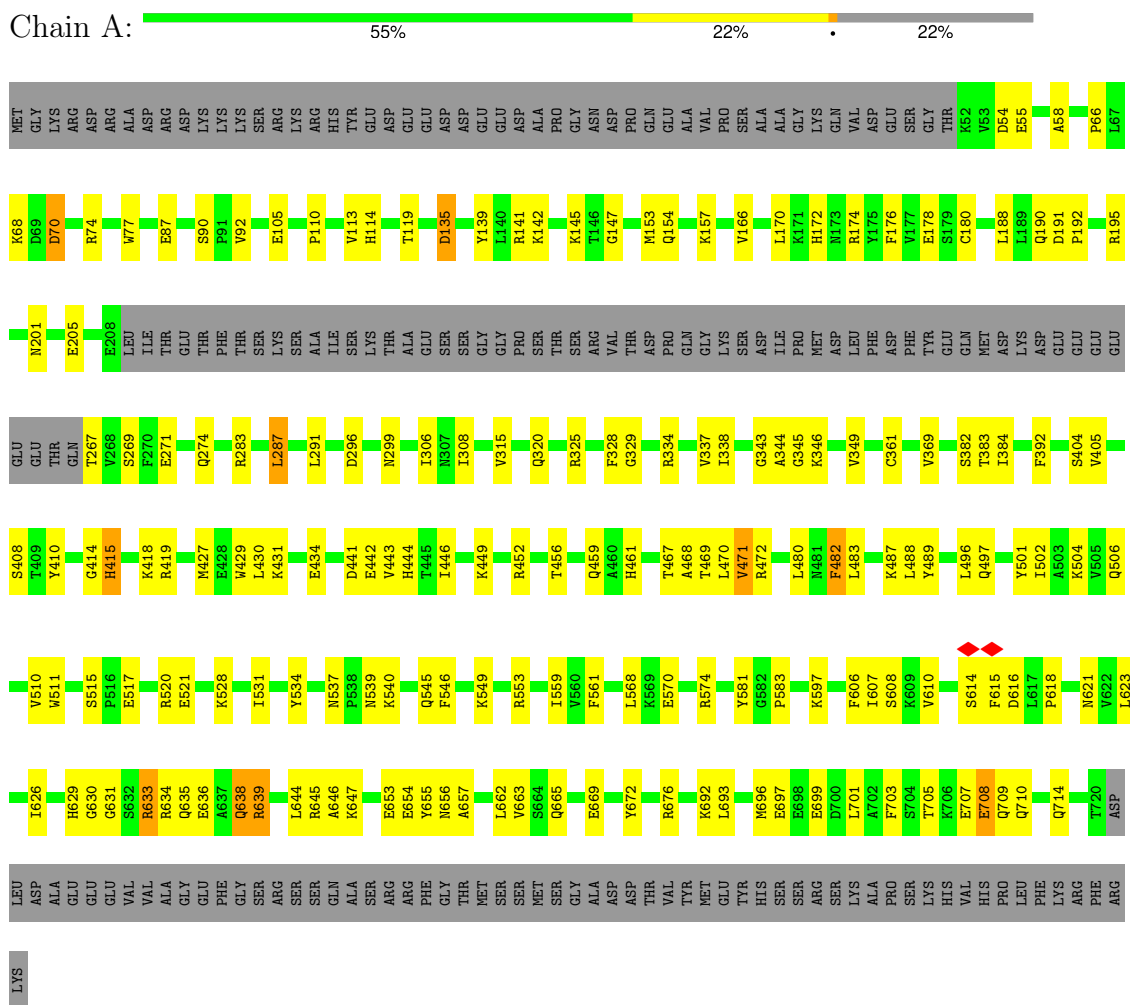
- Molecule 15 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
15	J	2	Total	Ca	0
			2	2	

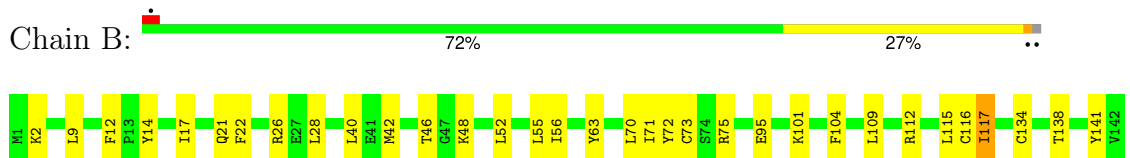
3 Residue-property plots

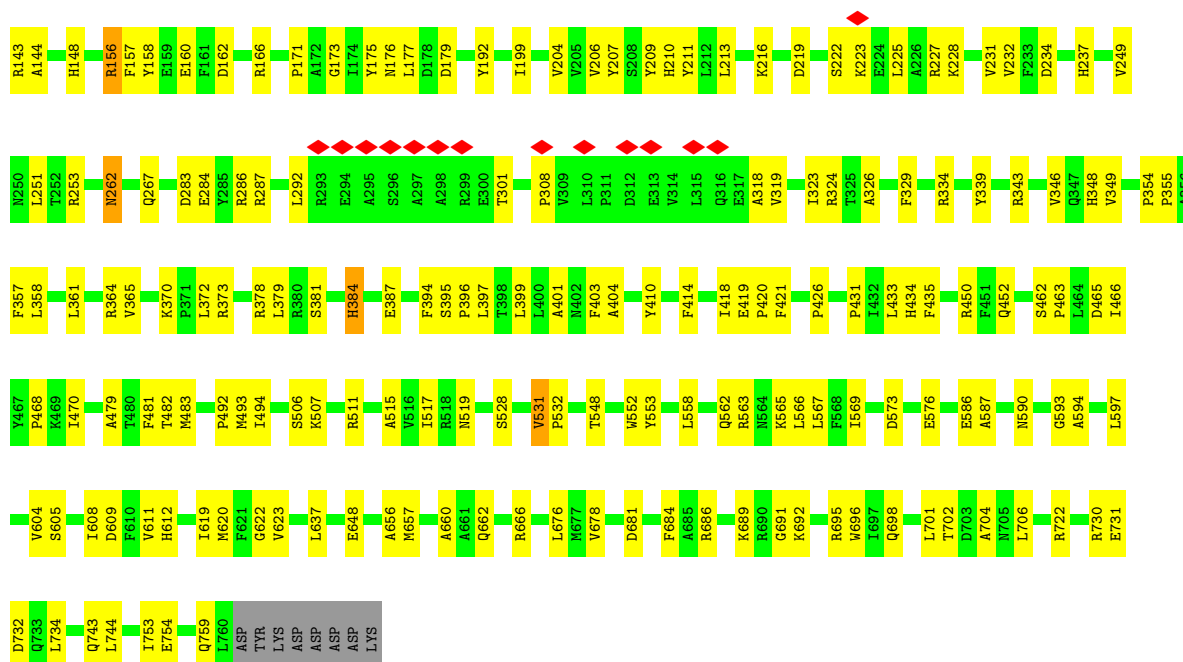
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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



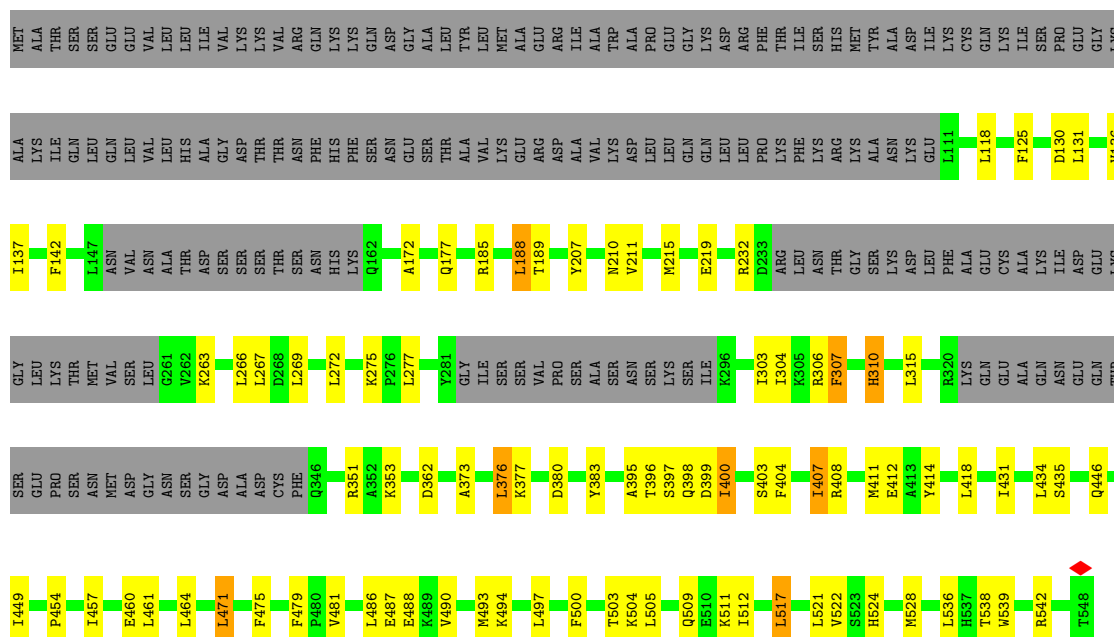
- Molecule 2: General transcription and DNA repair factor IIH helicase subunit XPD





- Molecule 3: General transcription factor IIH subunit 1

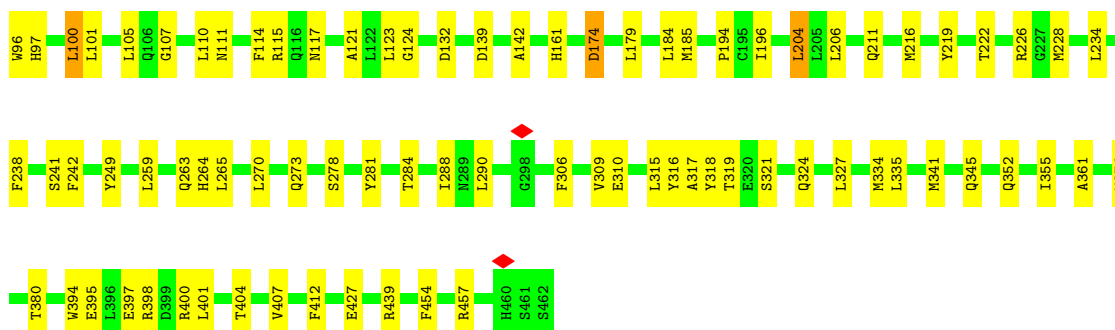
Chain C: 49% 15% 35%



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

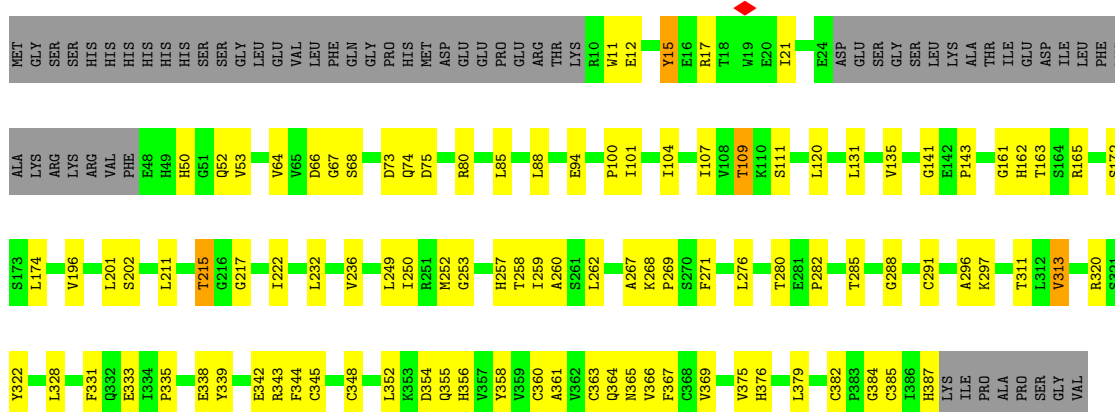
Chain D: 73% 23%





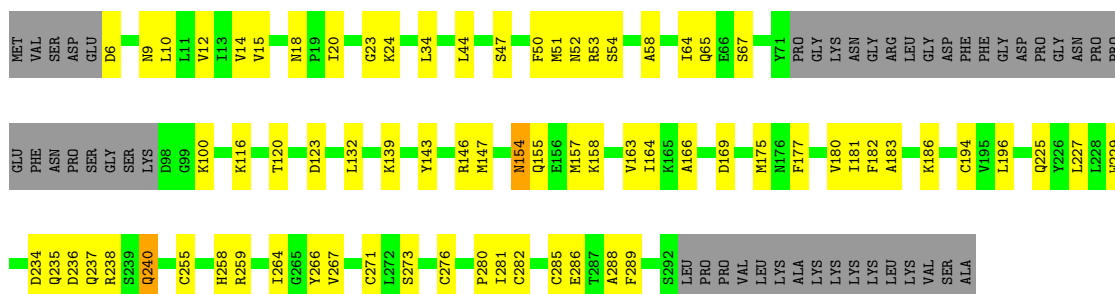
• Molecule 5: General transcription factor IIH subunit 2

Chain E: 61% 23% 15%



• Molecule 6: General transcription factor IIH subunit 3

Chain F: 61% 23% 15%



• Molecule 7: General transcription factor IIH subunit 5

Chain G: 58% 32% 6%



• Molecule 8: Xeroderma pigmentosum, complementation group C, isoform CRA_a



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	278447	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54.1	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.052	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	319.872, 319.872, 319.872	wwPDB
Map dimensions	384, 384, 384	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, CA, VM6, 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	0.14	0/5035	0.30	0/6800
2	B	0.10	0/6247	0.27	0/8457
3	C	0.11	0/2952	0.28	0/3983
4	D	0.14	0/3641	0.27	0/4934
5	E	0.11	0/2857	0.27	0/3870
6	F	0.11	0/2093	0.25	0/2833
7	G	0.17	0/536	0.30	0/724
8	H	0.11	0/4365	0.28	0/5906
9	I	0.10	0/515	0.31	0/696
10	J	0.09	0/1211	0.24	0/1605
11	L	0.18	0/1181	0.32	0/1820
12	M	0.18	0/1206	0.34	0/1857
All	All	0.12	0/31839	0.28	0/43485

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	4931	0	4978	122	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	6120	0	6164	122	0
3	C	2895	0	2886	66	0
4	D	3557	0	3596	72	0
5	E	2792	0	2735	60	0
6	F	2057	0	2079	55	0
7	G	530	0	539	14	0
8	H	4264	0	4254	141	0
9	I	504	0	497	17	0
10	J	1201	0	1184	27	0
11	L	1091	0	575	22	0
12	M	1078	0	599	23	0
13	B	8	0	0	0	0
14	E	3	0	0	0	0
14	F	2	0	0	0	0
15	J	2	0	0	0	0
All	All	31035	0	30086	670	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 11.

All (670) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:349:VAL:HA	2:B:418:ILE:O	1.76	0.85
6:F:271:CYS:SG	6:F:285:CYS:HB3	2.18	0.83
5:E:382:CYS:HB3	5:E:385:CYS:SG	2.20	0.82
10:J:57:MET:HB3	10:J:62:PHE:HB2	1.62	0.82
8:H:206:HIS:HE2	8:H:568:TYR:HH	1.22	0.81
1:A:178:GLU:HB3	1:A:269:SER:HB3	1.63	0.80
8:H:685:HIS:HA	12:M:26:DT:H3	1.48	0.79
3:C:481:VAL:HG11	3:C:487:GLU:HG3	1.67	0.77
2:B:420:PRO:HA	2:B:431:PRO:HA	1.67	0.76
4:D:50:SER:HB3	6:F:237:GLN:HE21	1.52	0.75
8:H:712:ASN:HD21	8:H:804:SER:H	1.31	0.75
1:A:306:ILE:HD13	1:A:404:SER:HB3	1.67	0.75
8:H:649:LEU:HD11	8:H:673:GLU:HB3	1.67	0.74
8:H:706:MET:HB3	8:H:729:ASP:HB3	1.71	0.71
6:F:255:CYS:O	6:F:259:ARG:N	2.17	0.71
8:H:237:ILE:HD11	8:H:305:ILE:HG23	1.73	0.71
4:D:317:ALA:O	4:D:341:MET:HA	1.90	0.70
1:A:172:HIS:HB2	1:A:174:ARG:HD3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:494:LYS:HD2	3:C:536:LEU:HD23	1.73	0.69
10:J:76:ILE:HG21	10:J:84:MET:HE3	1.74	0.69
6:F:282:CYS:HB3	6:F:285:CYS:SG	2.33	0.68
2:B:70:LEU:HB3	2:B:204:VAL:HG22	1.76	0.68
5:E:285:THR:O	5:E:297:LYS:NZ	2.27	0.67
1:A:653:GLU:HG2	1:A:655:TYR:H	1.59	0.67
1:A:274:GLN:NE2	1:A:456:THR:O	2.27	0.67
1:A:443:VAL:HG12	1:A:480:LEU:HD11	1.77	0.67
4:D:124:GLY:HA2	6:F:100:LYS:HB3	1.75	0.67
8:H:319:LEU:HB2	8:H:568:TYR:HD2	1.60	0.67
8:H:784:ARG:HH11	11:L:25:DA:H5'	1.60	0.66
5:E:211:LEU:O	5:E:215:THR:OG1	2.12	0.66
8:H:563:THR:HG22	8:H:565:PRO:HD2	1.77	0.66
4:D:222:THR:O	4:D:226:ARG:NH1	2.29	0.66
1:A:361:CYS:HB3	1:A:405:VAL:HG22	1.76	0.66
4:D:398:ARG:O	4:D:398:ARG:NH1	2.27	0.66
7:G:46:ILE:HG22	7:G:48:GLU:H	1.60	0.66
4:D:101:LEU:HB3	4:D:105:LEU:HB2	1.78	0.66
4:D:397:GLU:OE2	8:H:904:TRP:NE1	2.29	0.66
5:E:335:PRO:HG2	5:E:338:GLU:HB2	1.77	0.65
1:A:472:ARG:NH1	12:M:39:DA:OP2	2.29	0.65
3:C:475:PHE:HB2	3:C:493:MET:HG2	1.78	0.65
1:A:444:HIS:O	1:A:472:ARG:NH2	2.30	0.65
1:A:419:ARG:HA	11:L:24:DG:H5''	1.79	0.65
9:I:276:LEU:O	9:I:280:ARG:N	2.29	0.65
9:I:318:SER:O	9:I:321:GLN:NE2	2.30	0.64
6:F:10:LEU:HB2	6:F:157:MET:HE2	1.80	0.64
10:J:142:LEU:HA	10:J:145:MET:HE2	1.79	0.64
5:E:348:CYS:O	6:F:146:ARG:NH1	2.31	0.64
2:B:56:ILE:HG21	2:B:70:LEU:HD22	1.80	0.63
7:G:52:VAL:O	7:G:55:GLU:HB2	1.97	0.63
8:H:649:LEU:HD12	8:H:651:ARG:HG2	1.79	0.63
9:I:280:ARG:O	9:I:289:ARG:NH1	2.32	0.63
2:B:419:GLU:OE2	2:B:434:HIS:NE2	2.31	0.63
7:G:39:ASP:OD1	7:G:40:ASP:N	2.30	0.63
1:A:113:VAL:N	4:D:310:GLU:OE2	2.22	0.63
4:D:35:TYR:OH	4:D:93:LEU:O	2.15	0.63
5:E:339:TYR:O	5:E:343:ARG:NH1	2.32	0.63
8:H:825:TRP:O	8:H:829:GLN:NE2	2.29	0.63
8:H:754:ASN:OD1	8:H:758:ASN:N	2.31	0.62
6:F:255:CYS:SG	6:F:276:CYS:N	2.72	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:361:ALA:O	5:E:364:GLN:NE2	2.32	0.62
2:B:112:ARG:NH1	2:B:134:CYS:SG	2.72	0.62
2:B:702:THR:HG22	2:B:704:ALA:H	1.65	0.62
2:B:463:PRO:HG3	2:B:692:LYS:HE3	1.82	0.62
3:C:481:VAL:HG13	3:C:486:LEU:HB2	1.80	0.62
1:A:644:LEU:HD13	1:A:657:ALA:HB1	1.81	0.61
8:H:706:MET:SD	8:H:706:MET:N	2.73	0.61
2:B:734:LEU:HB3	2:B:743:GLN:HE22	1.66	0.61
4:D:34:LEU:HB3	4:D:40:THR:HG21	1.83	0.61
9:I:310:ASN:HB3	9:I:313:LEU:HB3	1.82	0.61
8:H:546:ASP:HB3	8:H:551:VAL:HB	1.82	0.61
8:H:798:ASP:OD2	8:H:800:HIS:NE2	2.34	0.61
1:A:58:ALA:HB2	4:D:334:MET:HB3	1.82	0.60
8:H:536:CYS:O	8:H:540:GLU:N	2.34	0.60
10:J:25:LEU:HD13	10:J:94:THR:HG21	1.82	0.60
3:C:210:ASN:HB3	3:C:215:MET:HG2	1.84	0.60
6:F:273:SER:OG	6:F:282:CYS:SG	2.59	0.60
8:H:834:ARG:HA	8:H:837:LYS:HD2	1.83	0.60
3:C:505:LEU:HD11	3:C:522:VAL:HG13	1.83	0.60
4:D:216:MET:HG3	4:D:290:LEU:HD21	1.83	0.60
5:E:363:CYS:SG	5:E:365:ASN:ND2	2.74	0.60
2:B:12:PHE:HD1	2:B:14:TYR:H	1.50	0.59
3:C:505:LEU:O	3:C:509:GLN:N	2.30	0.59
4:D:96:TRP:HB3	4:D:110:LEU:HD23	1.84	0.59
8:H:546:ASP:OD2	8:H:549:HIS:ND1	2.33	0.59
2:B:267:GLN:OE1	2:B:334:ARG:NH2	2.35	0.59
8:H:187:GLU:HB2	8:H:191:ARG:HH12	1.67	0.59
8:H:711:SER:O	8:H:715:ARG:N	2.22	0.59
1:A:170:LEU:O	1:A:461:HIS:NE2	2.32	0.59
6:F:9:ASN:ND2	6:F:234:ASP:OD2	2.35	0.59
9:I:293:GLN:NE2	9:I:330:GLU:O	2.35	0.59
2:B:222:SER:O	2:B:450:ARG:NH2	2.35	0.59
1:A:429:TRP:HE3	1:A:430:LEU:HD12	1.68	0.59
1:A:54:ASP:OD1	1:A:55:GLU:N	2.36	0.59
1:A:553:ARG:NH1	1:A:699:GLU:OE2	2.35	0.58
2:B:143:ARG:NH1	2:B:162:ASP:OD2	2.36	0.58
2:B:531:VAL:HG22	2:B:532:PRO:HD2	1.85	0.58
3:C:411:MET:HE3	6:F:34:LEU:HB3	1.85	0.58
5:E:68:SER:HB3	5:E:143:PRO:HD3	1.85	0.58
6:F:52:ASN:ND2	6:F:54:SER:OG	2.35	0.58
4:D:185:MET:HE2	4:D:194:PRO:HG2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:18:ASN:ND2	4:D:21:GLU:OE1	2.36	0.58
2:B:42:MET:HG2	2:B:48:LYS:HB3	1.85	0.58
2:B:730:ARG:NH1	3:C:362:ASP:O	2.36	0.58
4:D:30:VAL:HG22	4:D:33:ARG:HH21	1.68	0.58
5:E:342:GLU:OE1	5:E:344:PHE:N	2.36	0.58
8:H:903:SER:O	8:H:907:ASN:ND2	2.32	0.58
8:H:795:THR:N	8:H:807:VAL:O	2.27	0.58
2:B:262:ASN:HD22	2:B:394:PHE:HD1	1.50	0.58
1:A:597:LYS:HE2	1:A:618:PRO:HB3	1.85	0.58
2:B:622:GLY:HA2	2:B:681:ASP:HB2	1.86	0.58
1:A:70:ASP:OD1	1:A:70:ASP:N	2.35	0.58
2:B:249:VAL:HG11	2:B:403:PHE:HB2	1.86	0.58
2:B:517:ILE:HG23	2:B:548:THR:HG23	1.86	0.57
4:D:35:TYR:O	4:D:117:ASN:ND2	2.37	0.57
1:A:154:GLN:HA	1:A:157:LYS:HD2	1.86	0.57
1:A:329:GLY:HA3	1:A:334:ARG:HE	1.68	0.57
1:A:110:PRO:O	1:A:114:HIS:NE2	2.37	0.57
5:E:15:TYR:OH	5:E:17:ARG:NE	2.37	0.57
5:E:80:ARG:NH1	5:E:172:SER:OG	2.34	0.57
1:A:633:ARG:HA	1:A:676:ARG:HG3	1.85	0.57
2:B:176:ASN:OD1	2:B:177:LEU:N	2.37	0.57
4:D:401:LEU:HD21	7:G:57:VAL:HG11	1.87	0.57
9:I:282:GLN:O	9:I:286:GLN:N	2.36	0.57
1:A:431:LYS:O	1:A:459:GLN:NE2	2.37	0.57
2:B:2:LYS:HB3	2:B:9:LEU:HD11	1.86	0.57
2:B:284:GLU:OE1	2:B:287:ARG:NH1	2.38	0.57
3:C:414:TYR:HD2	6:F:116:LYS:HE3	1.68	0.57
5:E:161:GLY:HA2	5:E:165:ARG:HH22	1.69	0.57
1:A:631:GLY:H	1:A:676:ARG:NH1	2.03	0.57
8:H:907:ASN:OD1	8:H:908:ARG:NE	2.38	0.57
11:L:20:DC:H2'	11:L:21:DG:H8	1.69	0.57
4:D:206:LEU:O	4:D:211:GLN:NE2	2.32	0.57
5:E:345:CYS:HB2	5:E:352:LEU:HD21	1.87	0.57
8:H:208:VAL:HG22	9:I:317:ILE:HD13	1.86	0.57
1:A:174:ARG:NE	1:A:271:GLU:OE2	2.34	0.56
1:A:443:VAL:HG13	1:A:446:ILE:HD12	1.86	0.56
3:C:232:ARG:O	3:C:306:ARG:NH1	2.38	0.56
5:E:66:ASP:HA	5:E:109:THR:HG23	1.87	0.56
8:H:216:ASN:OD1	8:H:220:ARG:NH2	2.38	0.56
1:A:418:LYS:O	8:H:784:ARG:NH2	2.38	0.56
2:B:343:ARG:HG2	2:B:357:PHE:HE1	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:381:SER:O	2:B:384:HIS:ND1	2.38	0.56
6:F:154:ASN:OD1	6:F:154:ASN:N	2.37	0.56
9:I:292:ILE:HG21	9:I:328:LEU:HD13	1.87	0.56
1:A:471:VAL:HG23	1:A:634:ARG:HB3	1.87	0.56
4:D:101:LEU:HD22	4:D:105:LEU:HD12	1.86	0.56
8:H:258:VAL:HG11	8:H:550:GLY:HA2	1.87	0.56
3:C:137:ILE:HD11	3:C:142:PHE:HD1	1.70	0.56
10:J:47:THR:HB	10:J:83:LYS:HB3	1.88	0.56
1:A:308:ILE:HB	1:A:384:ILE:HB	1.86	0.56
1:A:570:GLU:HG3	1:A:574:ARG:HH12	1.71	0.56
2:B:292:LEU:HD11	2:B:318:ALA:HA	1.88	0.56
3:C:377:LYS:HB2	6:F:286:GLU:HG3	1.87	0.56
8:H:773:GLN:HE21	8:H:810:GLY:HA3	1.71	0.55
9:I:286:GLN:O	9:I:289:ARG:HG2	2.07	0.55
8:H:551:VAL:HG13	8:H:554:GLN:HB2	1.89	0.55
2:B:209:TYR:OH	2:B:234:ASP:O	2.24	0.55
4:D:31:LEU:HD12	4:D:94:ARG:HD3	1.88	0.55
6:F:6:ASP:HB3	6:F:155:GLN:HA	1.87	0.55
4:D:111:ASN:HB3	4:D:114:PHE:HB3	1.88	0.55
10:J:68:GLU:OE2	10:J:96:LYS:NZ	2.36	0.55
1:A:449:LYS:HG2	1:A:452:ARG:HH21	1.70	0.55
4:D:65:PRO:HB2	4:D:107:GLY:HA3	1.87	0.55
8:H:303:LEU:HD11	8:H:307:ARG:HE	1.71	0.55
8:H:663:THR:HG1	8:H:680:CYS:HG	1.53	0.55
1:A:630:GLY:H	1:A:676:ARG:HH12	1.53	0.55
1:A:636:GLU:OE2	1:A:639:ARG:NH2	2.40	0.55
2:B:421:PHE:HB2	2:B:426:PRO:HA	1.89	0.55
8:H:605:GLU:OE2	9:I:321:GLN:NE2	2.39	0.55
1:A:629:HIS:NE2	12:M:39:DA:O3'	2.40	0.55
10:J:55:VAL:O	10:J:59:ALA:N	2.40	0.55
1:A:540:LYS:HD3	1:A:626:ILE:HG23	1.88	0.55
1:A:672:TYR:OH	12:M:41:DT:OP1	2.25	0.55
2:B:681:ASP:HB3	2:B:684:PHE:HD2	1.72	0.55
5:E:100:PRO:HG3	5:E:320:ARG:HD2	1.88	0.55
8:H:728:ASN:OD1	8:H:729:ASP:N	2.35	0.55
12:M:43:DA:H2''	12:M:44:DG:C8	2.42	0.55
1:A:105:GLU:OE1	1:A:119:THR:OG1	2.24	0.54
5:E:174:LEU:HD21	5:E:202:SER:HB2	1.89	0.54
8:H:799:PHE:HD1	8:H:804:SER:HA	1.72	0.54
11:L:20:DC:H2'	11:L:21:DG:C8	2.41	0.54
2:B:372:LEU:HD11	2:B:404:ALA:HB1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:ARG:HH12	8:H:864:ARG:HD2	1.73	0.54
2:B:609:ASP:OD1	2:B:666:ARG:NH1	2.39	0.54
3:C:479:PHE:HE1	3:C:490:VAL:HG11	1.70	0.54
6:F:20:ILE:HG22	6:F:24:LYS:HE3	1.90	0.54
2:B:22:PHE:HD2	2:B:753:ILE:HG21	1.72	0.54
2:B:71:ILE:HB	2:B:231:VAL:HA	1.89	0.54
8:H:840:LYS:HA	8:H:843:ARG:HD2	1.89	0.54
12:M:24:DT:H2''	12:M:25:DA:N7	2.23	0.54
1:A:568:LEU:HD11	1:A:606:PHE:HB3	1.90	0.54
2:B:109:LEU:HB3	2:B:207:TYR:HB3	1.89	0.54
8:H:221:ASN:OD1	8:H:307:ARG:NH2	2.40	0.54
8:H:246:PRO:HG3	8:H:311:LEU:HD23	1.89	0.54
8:H:719:LEU:HD12	8:H:725:ARG:HH11	1.73	0.54
2:B:319:VAL:HG21	2:B:378:ARG:HG2	1.89	0.53
8:H:533:GLU:OE2	8:H:584:ARG:NH1	2.40	0.53
1:A:190:GLN:HA	1:A:195:ARG:HH21	1.73	0.53
1:A:634:ARG:NH2	1:A:635:GLN:OE1	2.39	0.53
4:D:273:GLN:NE2	4:D:278:SER:O	2.41	0.53
8:H:657:GLU:HG2	8:H:683:THR:HG22	1.88	0.53
1:A:635:GLN:O	1:A:638:GLN:NE2	2.41	0.53
3:C:376:LEU:HD13	3:C:376:LEU:H	1.73	0.53
6:F:44:LEU:HD22	6:F:227:LEU:HB3	1.89	0.53
8:H:707:VAL:O	8:H:729:ASP:HA	2.08	0.53
11:L:40:DG:H2''	11:L:41:DA:C8	2.44	0.53
2:B:219:ASP:HB3	2:B:223:LYS:HE3	1.90	0.53
8:H:536:CYS:O	8:H:540:GLU:CA	2.57	0.53
6:F:182:PHE:O	6:F:186:LYS:N	2.39	0.53
1:A:176:PHE:HB3	1:A:269:SER:HB2	1.89	0.53
8:H:195:LYS:HA	8:H:198:ASN:HD21	1.74	0.53
2:B:75:ARG:HH22	2:B:662:GLN:HE22	1.57	0.53
2:B:506:SER:O	2:B:511:ARG:NE	2.39	0.53
8:H:193:ALA:HA	8:H:196:ARG:HD2	1.90	0.53
8:H:194:MET:O	8:H:198:ASN:ND2	2.40	0.53
3:C:408:ARG:NH2	6:F:120:THR:O	2.39	0.53
3:C:461:LEU:HD22	3:C:521:LEU:HD13	1.91	0.53
6:F:65:GLN:NE2	6:F:123:ASP:O	2.42	0.53
10:J:122:SER:N	10:J:125:ASN:OD1	2.38	0.53
5:E:250:ILE:O	6:F:267:VAL:N	2.39	0.53
6:F:12:VAL:HG22	6:F:58:ALA:HB3	1.91	0.53
1:A:528:LYS:HE2	12:M:41:DT:H1'	1.91	0.52
2:B:569:ILE:HG12	2:B:597:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:PHE:HB3	1:A:408:SER:HB2	1.92	0.52
2:B:566:LEU:N	2:B:593:GLY:O	2.40	0.52
8:H:834:ARG:HH12	8:H:838:GLU:HG2	1.73	0.52
4:D:355:ILE:HD13	4:D:395:GLU:HA	1.91	0.52
1:A:66:PRO:HG2	1:A:147:GLY:HA3	1.91	0.52
5:E:201:LEU:HG	5:E:222:ILE:HD12	1.92	0.52
7:G:50:VAL:O	7:G:53:LEU:HB3	2.10	0.52
1:A:135:ASP:OD1	1:A:135:ASP:N	2.29	0.52
1:A:626:ILE:HG12	1:A:662:LEU:HD12	1.92	0.52
2:B:144:ALA:O	2:B:148:HIS:ND1	2.31	0.52
8:H:536:CYS:O	8:H:540:GLU:HA	2.10	0.52
8:H:313:THR:HG22	8:H:534:VAL:HG22	1.92	0.52
12:M:23:DC:H2''	12:M:24:DT:C5	2.45	0.52
2:B:515:ALA:O	2:B:519:ASN:ND2	2.30	0.52
8:H:758:ASN:HD21	8:H:792:GLN:HB2	1.74	0.52
2:B:42:MET:HB3	2:B:48:LYS:HD3	1.92	0.52
2:B:115:LEU:HD13	2:B:192:TYR:HA	1.92	0.52
2:B:71:ILE:HD12	2:B:231:VAL:HG22	1.92	0.51
6:F:281:ILE:HA	6:F:288:ALA:HA	1.92	0.51
8:H:794:ILE:HA	8:H:808:THR:HG22	1.92	0.51
11:L:9:DA:H2''	11:L:10:DC:H5''	1.91	0.51
1:A:74:ARG:NH1	1:A:142:LYS:O	2.40	0.51
1:A:581:TYR:CD2	1:A:583:PRO:HD2	2.46	0.51
2:B:604:VAL:HA	2:B:608:ILE:HD13	1.91	0.51
6:F:280:PRO:O	6:F:289:PHE:N	2.32	0.51
8:H:589:TRP:HA	8:H:593:THR:HB	1.93	0.51
3:C:131:LEU:HB3	3:C:137:ILE:HG12	1.91	0.51
5:E:342:GLU:OE1	5:E:343:ARG:N	2.42	0.51
2:B:410:TYR:HB3	2:B:414:PHE:CE2	2.46	0.51
3:C:177:GLN:HB2	3:C:185:ARG:O	2.11	0.51
3:C:400:ILE:HD11	6:F:20:ILE:HD13	1.91	0.51
3:C:471:LEU:HD22	3:C:497:LEU:HG	1.93	0.51
4:D:412:PHE:O	4:D:439:ARG:NH2	2.43	0.51
5:E:333:GLU:OE2	5:E:356:HIS:ND1	2.44	0.51
8:H:589:TRP:HZ3	8:H:597:ARG:HD2	1.76	0.51
2:B:605:SER:O	2:B:662:GLN:NE2	2.41	0.51
2:B:681:ASP:HB3	2:B:684:PHE:CD2	2.46	0.51
3:C:397:SER:O	3:C:399:ASP:N	2.44	0.51
6:F:67:SER:HB2	6:F:139:LYS:HD2	1.91	0.51
8:H:855:LEU:HD22	10:J:112:LEU:HD13	1.92	0.51
1:A:497:GLN:HB3	1:A:504:LYS:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:483:MET:HE2	2:B:696:TRP:HB2	1.93	0.51
2:B:493:MET:HE3	2:B:676:LEU:HD11	1.93	0.51
3:C:449:ILE:HG21	5:E:269:PRO:HG3	1.93	0.51
8:H:713:ARG:HE	8:H:714:ALA:N	2.08	0.51
1:A:329:GLY:O	1:A:334:ARG:NH1	2.43	0.51
2:B:620:MET:HE3	2:B:660:ALA:HA	1.92	0.51
3:C:503:THR:HG23	3:C:504:LYS:HG2	1.92	0.51
4:D:249:TYR:HB2	4:D:281:TYR:CZ	2.47	0.50
1:A:337:VAL:O	1:A:488:LEU:N	2.41	0.50
1:A:343:GLY:HA3	1:A:645:ARG:NE	2.26	0.50
2:B:216:LYS:HA	2:B:308:PRO:HD2	1.93	0.50
2:B:228:LYS:HA	2:B:452:GLN:HB2	1.93	0.50
2:B:326:ALA:HA	2:B:378:ARG:HH22	1.75	0.50
2:B:379:LEU:HD22	2:B:401:ALA:HB3	1.93	0.50
8:H:718:ARG:HG3	8:H:725:ARG:HA	1.91	0.50
8:H:805:HIS:NE2	12:M:29:DT:O4'	2.44	0.50
11:L:28:DA:H3'	11:L:29:DT:H71	1.93	0.50
1:A:415:HIS:HB2	1:A:419:ARG:HE	1.76	0.50
4:D:317:ALA:HB1	4:D:319:THR:HG22	1.94	0.50
8:H:654:LEU:HD22	11:L:34:DA:H5'	1.93	0.50
11:L:23:DT:H2''	11:L:24:DG:C8	2.46	0.50
3:C:431:ILE:O	3:C:435:SER:N	2.44	0.50
1:A:546:PHE:HB2	1:A:701:LEU:HD11	1.92	0.50
8:H:542:TRP:HZ2	8:H:617:ARG:HD3	1.74	0.50
8:H:685:HIS:HB2	8:H:690:TRP:CE2	2.47	0.50
8:H:797:PHE:HB2	12:M:27:DT:H72	1.94	0.50
2:B:349:VAL:HG22	2:B:419:GLU:HA	1.92	0.50
4:D:352:GLN:NE2	4:D:394:TRP:O	2.43	0.50
1:A:502:ILE:HA	1:A:646:ALA:HB2	1.93	0.50
1:A:520:ARG:HH22	8:H:864:ARG:HG2	1.77	0.50
6:F:236:ASP:OD1	6:F:236:ASP:N	2.45	0.49
9:I:285:PHE:CG	9:I:327:MET:HE1	2.46	0.49
2:B:619:ILE:HG12	2:B:678:VAL:HB	1.93	0.49
3:C:395:ALA:HB3	3:C:400:ILE:HD12	1.93	0.49
3:C:397:SER:O	3:C:400:ILE:HG22	2.13	0.49
11:L:36:DG:H2'	11:L:37:DT:C6	2.47	0.49
3:C:130:ASP:HB3	3:C:504:LYS:HE3	1.94	0.49
8:H:594:ARG:NH2	8:H:643:ASN:O	2.30	0.49
4:D:52:ALA:HB1	4:D:90:LEU:HD21	1.93	0.49
5:E:73:ASP:OD1	5:E:74:GLN:N	2.45	0.49
2:B:52:LEU:HD21	2:B:232:VAL:HG11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:ARG:NH1	2:B:158:TYR:OH	2.46	0.49
4:D:62:LEU:O	4:D:115:ARG:NH1	2.45	0.49
2:B:251:LEU:HD12	2:B:433:LEU:HD22	1.94	0.49
3:C:303:ILE:HA	3:C:306:ARG:HE	1.77	0.49
8:H:779:LEU:HD11	8:H:821:LEU:HG	1.93	0.49
2:B:21:GLN:NE2	2:B:46:THR:O	2.45	0.49
2:B:73:CYS:HB3	2:B:209:TYR:HD1	1.78	0.49
10:J:53:LEU:HD21	10:J:72:MET:HE2	1.93	0.49
10:J:110:PHE:CZ	10:J:121:ILE:HG13	2.47	0.49
1:A:325:ARG:HD2	5:E:15:TYR:HB3	1.95	0.49
2:B:553:TYR:HD2	3:C:303:ILE:HD13	1.78	0.49
3:C:188:LEU:H	3:C:188:LEU:HD23	1.78	0.49
4:D:319:THR:OG1	4:D:324:GLN:OE1	2.29	0.49
1:A:511:TRP:HB3	1:A:665:GLN:HG2	1.94	0.49
5:E:249:LEU:HG	6:F:266:TYR:HB3	1.93	0.49
1:A:531:ILE:HA	1:A:534:TYR:CE2	2.48	0.49
1:A:636:GLU:HB2	1:A:676:ARG:HD3	1.94	0.49
2:B:156:ARG:HG2	2:B:160:GLU:HG3	1.95	0.49
2:B:227:ARG:H	2:B:227:ARG:HD2	1.77	0.49
2:B:323:ILE:HB	2:B:329:PHE:HD1	1.77	0.49
5:E:85:LEU:HD12	5:E:135:VAL:HA	1.95	0.48
8:H:188:THR:O	8:H:192:ARG:HG2	2.12	0.48
3:C:303:ILE:HG12	3:C:306:ARG:HH11	1.77	0.48
3:C:446:GLN:HB3	5:E:262:LEU:HD12	1.94	0.48
4:D:204:LEU:HD22	4:D:327:LEU:HD21	1.95	0.48
1:A:515:SER:OG	1:A:517:GLU:OE1	2.29	0.48
2:B:323:ILE:O	2:B:378:ARG:NH1	2.46	0.48
3:C:538:THR:HG22	3:C:542:ARG:HE	1.78	0.48
8:H:303:LEU:HA	8:H:532:LEU:HD21	1.95	0.48
8:H:283:LEU:HD13	8:H:304:LEU:HD11	1.95	0.48
3:C:411:MET:HG3	6:F:34:LEU:HD23	1.96	0.48
3:C:488:GLU:N	3:C:488:GLU:OE1	2.46	0.48
1:A:296:ASP:HB3	1:A:299:ASN:HB2	1.96	0.48
2:B:26:ARG:NH1	2:B:754:GLU:OE2	2.46	0.48
5:E:358:TYR:HE1	5:E:369:VAL:HG22	1.76	0.48
11:L:3:DG:H2"	11:L:4:DT:C5	2.49	0.48
2:B:637:LEU:HD13	2:B:648:GLU:HB2	1.95	0.48
1:A:410:TYR:O	1:A:414:GLY:N	2.44	0.48
1:A:506:GLN:N	1:A:657:ALA:O	2.34	0.48
3:C:232:ARG:HD3	3:C:306:ARG:HD2	1.96	0.48
8:H:572:ILE:HG12	8:H:578:VAL:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:787:ASP:N	8:H:787:ASP:OD1	2.46	0.48
8:H:831:VAL:O	8:H:834:ARG:HG3	2.13	0.48
9:I:306:ILE:HA	9:I:310:ASN:HB2	1.96	0.48
3:C:471:LEU:HD13	3:C:497:LEU:HD23	1.96	0.48
5:E:291:CYS:HB3	5:E:296:ALA:H	1.78	0.47
8:H:773:GLN:HE22	8:H:775:ASN:HB2	1.79	0.47
8:H:845:LEU:HD21	10:J:168:LYS:HE3	1.95	0.47
1:A:714:GLN:HG2	8:H:861:LEU:HD12	1.96	0.47
3:C:454:PRO:HD2	3:C:457:ILE:HD12	1.97	0.47
2:B:507:LYS:O	2:B:511:ARG:N	2.47	0.47
8:H:260:TRP:O	8:H:264:THR:OG1	2.27	0.47
8:H:317:LEU:HA	8:H:530:GLN:HG2	1.95	0.47
2:B:562:GLN:OE1	3:C:310:HIS:NE2	2.47	0.47
7:G:20:LEU:HD22	7:G:53:LEU:HD11	1.94	0.47
10:J:50:VAL:HA	10:J:84:MET:HE1	1.97	0.47
1:A:361:CYS:O	1:A:405:VAL:HA	2.14	0.47
1:A:504:LYS:HB3	1:A:654:GLU:O	2.15	0.47
3:C:407:ILE:HB	6:F:23:GLY:HA2	1.96	0.47
5:E:260:ALA:HB1	5:E:267:ALA:HA	1.96	0.47
8:H:294:ASP:OD1	8:H:297:GLU:N	2.42	0.47
1:A:345:GLY:O	1:A:349:VAL:N	2.43	0.47
3:C:136:VAL:HG11	3:C:500:PHE:HB2	1.97	0.47
3:C:512:ILE:HG23	3:C:517:LEU:HB2	1.96	0.47
8:H:229:LEU:HB3	8:H:304:LEU:HD13	1.96	0.47
8:H:684:LEU:HD11	8:H:704:TYR:HD1	1.80	0.47
2:B:171:PRO:O	2:B:175:TYR:OH	2.22	0.47
2:B:657:MET:HG3	2:B:692:LYS:HB3	1.97	0.47
4:D:42:LEU:HG	4:D:242:PHE:CZ	2.50	0.47
4:D:79:PHE:CG	6:F:240:GLN:HB3	2.50	0.47
8:H:206:HIS:NE2	8:H:568:TYR:OH	2.23	0.47
8:H:904:TRP:O	8:H:907:ASN:ND2	2.47	0.47
1:A:502:ILE:HG22	1:A:645:ARG:HH12	1.79	0.47
4:D:139:ASP:HB3	4:D:142:ALA:HB2	1.96	0.47
4:D:46:ARG:HH12	6:F:53:ARG:HE	1.60	0.47
1:A:470:LEU:HD12	1:A:487:LYS:HE2	1.96	0.47
5:E:67:GLY:N	5:E:109:THR:O	2.44	0.47
11:L:14:DT:H2''	11:L:15:DG:C8	2.50	0.47
2:B:346:VAL:HG12	2:B:348:HIS:H	1.80	0.46
1:A:441:ASP:OD1	1:A:442:GLU:N	2.47	0.46
6:F:164:ILE:HG22	6:F:194:CYS:HB3	1.97	0.46
12:M:36:DC:H2'	12:M:37:DG:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:THR:HG23	1:A:708:GLU:HB2	1.96	0.46
1:A:634:ARG:HG3	1:A:635:GLN:N	2.29	0.46
7:G:34:ILE:HG23	7:G:45:VAL:HG22	1.96	0.46
1:A:692:LYS:HD3	8:H:906:GLN:HG2	1.98	0.46
2:B:162:ASP:OD1	2:B:166:ARG:NE	2.45	0.46
5:E:80:ARG:HD3	5:E:201:LEU:HD22	1.98	0.46
6:F:183:ALA:O	6:F:186:LYS:HB3	2.16	0.46
12:M:42:DC:H2''	12:M:43:DA:C8	2.51	0.46
1:A:496:LEU:HD22	1:A:501:TYR:HD2	1.81	0.46
2:B:339:TYR:HE1	2:B:364:ARG:HD2	1.79	0.46
4:D:96:TRP:H	4:D:96:TRP:CD1	2.33	0.46
8:H:711:SER:OG	8:H:713:ARG:NH1	2.48	0.46
2:B:73:CYS:HB3	2:B:209:TYR:CD1	2.51	0.46
2:B:573:ASP:HB3	2:B:576:GLU:HB3	1.98	0.46
1:A:510:VAL:HB	1:A:662:LEU:HD23	1.98	0.46
4:D:38:PRO:HB3	4:D:121:ALA:HB2	1.97	0.46
10:J:33:ILE:HA	10:J:60:LEU:HD11	1.98	0.46
1:A:191:ASP:CG	1:A:283:ARG:HE	2.24	0.45
4:D:66:LEU:HD13	4:D:74:TRP:HH2	1.81	0.45
8:H:748:ASP:HB2	8:H:750:LYS:HE3	1.97	0.45
8:H:597:ARG:HG2	8:H:598:VAL:H	1.81	0.45
8:H:776:LEU:HB2	8:H:779:LEU:HB2	1.99	0.45
1:A:170:LEU:HB3	1:A:461:HIS:CD2	2.51	0.45
2:B:552:TRP:HB3	2:B:558:LEU:HB2	1.97	0.45
2:B:587:ALA:HB3	2:B:594:ALA:HB2	1.98	0.45
2:B:623:VAL:HG12	2:B:656:ALA:HB1	1.98	0.45
4:D:19:LEU:HD21	4:D:238:PHE:HE1	1.82	0.45
6:F:158:LYS:HD3	6:F:235:GLN:HE22	1.81	0.45
10:J:162:PHE:HA	10:J:165:ILE:HG12	1.98	0.45
1:A:325:ARG:HG2	5:E:12:GLU:HA	1.98	0.45
2:B:162:ASP:HA	2:B:166:ARG:HE	1.81	0.45
3:C:307:PHE:O	3:C:310:HIS:ND1	2.45	0.45
2:B:12:PHE:HE1	2:B:14:TYR:HB2	1.81	0.45
4:D:454:PHE:N	4:D:457:ARG:HH21	2.15	0.45
9:I:290:GLN:NE2	9:I:294:GLN:OE1	2.46	0.45
9:I:299:LEU:HG	9:I:303:LEU:HD13	1.98	0.45
10:J:126:LEU:HG	10:J:142:LEU:HD22	1.98	0.45
3:C:434:LEU:HD13	6:F:229:TRP:CD2	2.51	0.45
3:C:524:HIS:NE2	3:C:528:MET:SD	2.89	0.45
4:D:407:VAL:HG22	7:G:6:LYS:HB3	1.98	0.45
5:E:375:VAL:HA	5:E:379:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:718:ARG:HH11	8:H:728:ASN:HB3	1.80	0.45
12:M:49:DG:H2''	12:M:50:DA:C8	2.52	0.45
2:B:466:ILE:HG12	2:B:470:ILE:HG13	1.99	0.45
4:D:265:LEU:HD22	4:D:270:LEU:HD12	1.99	0.45
5:E:365:ASN:HD21	5:E:384:GLY:HA3	1.81	0.45
1:A:70:ASP:OD2	1:A:74:ARG:NH2	2.50	0.45
2:B:283:ASP:HA	2:B:286:ARG:HD2	1.99	0.45
8:H:285:ARG:O	8:H:289:ILE:HG13	2.17	0.45
8:H:645:PRO:HB3	8:H:678:ARG:HG2	1.99	0.45
2:B:179:ASP:OD1	3:C:351:ARG:NH2	2.49	0.45
1:A:139:TYR:CZ	5:E:21:ILE:HB	2.52	0.45
1:A:338:ILE:HG23	1:A:489:TYR:HB3	1.98	0.45
1:A:419:ARG:NH1	1:A:427:MET:HG3	2.31	0.45
3:C:373:ALA:HA	5:E:53:VAL:HA	1.99	0.45
5:E:252:MET:HG2	5:E:311:THR:HB	1.98	0.45
4:D:174:ASP:OD1	4:D:174:ASP:N	2.36	0.44
4:D:309:VAL:HG22	4:D:315:LEU:HD22	2.00	0.44
8:H:192:ARG:HH22	8:H:195:LYS:HG3	1.81	0.44
11:L:42:DT:H2''	11:L:43:DA:C8	2.52	0.44
1:A:545:GLN:HE21	1:A:549:LYS:HE3	1.81	0.44
2:B:482:THR:HB	2:B:695:ARG:CZ	2.48	0.44
2:B:686:ARG:HD2	2:B:689:LYS:HE3	1.98	0.44
4:D:97:HIS:NE2	4:D:111:ASN:HA	2.32	0.44
10:J:56:ALA:O	10:J:59:ALA:HB3	2.17	0.44
2:B:253:ARG:HB2	2:B:431:PRO:HG2	1.99	0.44
2:B:479:ALA:HB2	2:B:759:GLN:HG2	1.98	0.44
4:D:78:GLU:HG3	4:D:79:PHE:CD2	2.52	0.44
5:E:111:SER:HA	5:E:141:GLY:HA3	1.99	0.44
6:F:18:ASN:HD22	6:F:64:ILE:HD11	1.82	0.44
8:H:582:THR:OG1	8:H:597:ARG:NH2	2.50	0.44
4:D:259:LEU:O	4:D:263:GLN:HG2	2.17	0.44
11:L:31:DT:H6	11:L:31:DT:H2'	1.63	0.44
1:A:480:LEU:HA	1:A:483:LEU:HB2	1.99	0.44
2:B:567:LEU:HD23	2:B:567:LEU:H	1.82	0.44
3:C:263:LYS:O	3:C:267:LEU:HB2	2.17	0.44
4:D:335:LEU:HD11	4:D:345:GLN:HB2	1.99	0.44
5:E:258:THR:N	5:E:288:GLY:O	2.50	0.44
6:F:177:PHE:CE2	6:F:181:ILE:HD11	2.53	0.44
1:A:703:PHE:HB3	1:A:709:GLN:HG2	2.00	0.44
2:B:354:PRO:N	2:B:355:PRO:HD2	2.33	0.44
3:C:136:VAL:HG12	3:C:137:ILE:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:238:PRO:HB2	8:H:240:ARG:HG2	2.00	0.44
1:A:714:GLN:HE22	8:H:858:ARG:HA	1.83	0.44
4:D:309:VAL:HB	4:D:376:MET:HE1	2.00	0.44
7:G:36:GLN:HG2	7:G:37:ASP:O	2.18	0.44
8:H:653:LEU:HD11	8:H:659:ILE:HG23	1.99	0.44
8:H:837:LYS:HA	8:H:840:LYS:HE3	1.99	0.44
11:L:31:DT:H1'	11:L:32:DA:C5	2.53	0.44
2:B:462:SER:HB2	2:B:463:PRO:HD3	1.99	0.44
6:F:14:VAL:HB	6:F:163:VAL:HG22	1.99	0.44
6:F:235:GLN:HA	6:F:238:ARG:HD2	2.00	0.44
8:H:753:ARG:HB3	8:H:757:GLY:HA2	2.00	0.44
1:A:561:PHE:CD2	1:A:623:LEU:HD11	2.53	0.43
1:A:607:ILE:HD13	1:A:615:PHE:HZ	1.83	0.43
3:C:207:TYR:O	3:C:211:VAL:HG22	2.18	0.43
8:H:664:ALA:HB2	8:H:680:CYS:SG	2.58	0.43
1:A:308:ILE:HG13	1:A:382:SER:HB3	2.00	0.43
2:B:104:PHE:O	2:B:173:GLY:N	2.51	0.43
8:H:196:ARG:HH11	12:M:23:DC:P	2.40	0.43
8:H:261:PHE:HE1	8:H:301:ILE:HG22	1.83	0.43
8:H:569:VAL:HG12	8:H:581:VAL:HG23	1.98	0.43
8:H:663:THR:O	8:H:663:THR:OG1	2.34	0.43
8:H:718:ARG:CZ	8:H:724:LEU:HD12	2.48	0.43
12:M:10:DA:H2''	12:M:11:DG:C8	2.54	0.43
1:A:68:LYS:NZ	1:A:141:ARG:O	2.42	0.43
1:A:467:THR:OG1	1:A:468:ALA:N	2.51	0.43
3:C:380:ASP:HA	3:C:383:TYR:CD2	2.54	0.43
3:C:431:ILE:HG13	6:F:225:GLN:HE22	1.83	0.43
4:D:306:PHE:HB2	4:D:318:TYR:HB2	2.00	0.43
8:H:584:ARG:HH11	8:H:585:TYR:HE1	1.66	0.43
8:H:684:LEU:HD11	8:H:704:TYR:CD1	2.52	0.43
11:L:18:DT:H2''	11:L:19:DG:C8	2.53	0.43
1:A:87:GLU:HG3	1:A:90:SER:HB2	2.01	0.43
8:H:745:VAL:HG22	8:H:769:ILE:HB	1.99	0.43
10:J:58:ARG:HE	10:J:63:GLU:HG2	1.83	0.43
5:E:271:PHE:HD2	5:E:282:PRO:HB2	1.83	0.43
8:H:542:TRP:CZ2	8:H:617:ARG:HD3	2.52	0.43
1:A:581:TYR:HA	1:A:608:SER:OG	2.18	0.43
4:D:34:LEU:HD21	4:D:234:LEU:HB2	2.01	0.43
5:E:196:VAL:O	5:E:217:GLY:HA3	2.18	0.43
5:E:322:TYR:HB3	6:F:175:MET:HE3	1.99	0.43
8:H:282:THR:O	8:H:286:ARG:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:719:LEU:HA	8:H:725:ARG:HH12	1.83	0.43
1:A:320:GLN:NE2	1:A:344:ALA:O	2.49	0.43
1:A:537:ASN:HD21	1:A:539:ASN:HB2	1.83	0.43
8:H:688:ASP:OD1	8:H:688:ASP:N	2.49	0.43
2:B:109:LEU:HD22	2:B:199:ILE:HD11	2.01	0.43
5:E:387:HIS:CD2	6:F:132:LEU:HD13	2.54	0.43
12:M:36:DC:H2'	12:M:37:DG:C8	2.54	0.43
1:A:201:ASN:N	1:A:205:GLU:O	2.32	0.43
1:A:338:ILE:HG12	1:A:488:LEU:HB2	2.00	0.43
12:M:33:DC:H2''	12:M:34:DA:C8	2.54	0.43
2:B:12:PHE:CE1	2:B:14:TYR:HB2	2.54	0.42
8:H:743:PRO:HB2	8:H:768:PRO:HA	2.01	0.42
8:H:759:VAL:HG11	8:H:768:PRO:HD3	2.01	0.42
10:J:95:GLN:NE2	10:J:99:GLU:OE2	2.52	0.42
1:A:697:GLU:CD	1:A:697:GLU:H	2.27	0.42
2:B:691:GLY:HA2	2:B:698:GLN:HE22	1.84	0.42
5:E:335:PRO:HA	5:E:355:GLN:O	2.19	0.42
8:H:303:LEU:HD22	8:H:315:LEU:HB2	2.00	0.42
10:J:38:ASP:HA	10:J:41:ASP:HB3	2.01	0.42
1:A:517:GLU:H	1:A:517:GLU:CD	2.24	0.42
4:D:59:MET:HE2	4:D:110:LEU:HG	2.00	0.42
4:D:400:ARG:HH21	7:G:13:ASP:CG	2.27	0.42
8:H:632:GLN:HB3	8:H:633:PRO:HD3	2.02	0.42
8:H:848:TRP:NE1	10:J:145:MET:HB3	2.35	0.42
9:I:279:LEU:HA	9:I:282:GLN:HB2	2.01	0.42
1:A:191:ASP:O	1:A:195:ARG:HG3	2.20	0.42
1:A:192:PRO:HA	1:A:195:ARG:HD2	2.02	0.42
1:A:291:LEU:H	1:A:482:PHE:HZ	1.67	0.42
2:B:370:LYS:HA	2:B:373:ARG:HD3	2.01	0.42
3:C:263:LYS:HG2	3:C:353:LYS:HE3	2.02	0.42
4:D:226:ARG:HB2	4:D:228:MET:HE2	2.00	0.42
5:E:131:LEU:O	5:E:135:VAL:HG23	2.19	0.42
5:E:311:THR:HG22	5:E:313:VAL:HG22	2.01	0.42
7:G:44:PHE:HD1	7:G:44:PHE:HA	1.75	0.42
8:H:761:LEU:HD12	8:H:761:LEU:HA	1.91	0.42
1:A:714:GLN:NE2	8:H:858:ARG:HA	2.34	0.42
2:B:569:ILE:HB	3:C:304:ILE:HG23	2.01	0.42
3:C:269:LEU:HD23	3:C:272:LEU:HD12	2.01	0.42
4:D:179:LEU:HD22	4:D:184:LEU:HD12	2.00	0.42
8:H:711:SER:H	8:H:714:ALA:HB3	1.83	0.42
8:H:754:ASN:N	8:H:758:ASN:O	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:ASN:HD21	1:A:647:LYS:HD2	1.84	0.42
2:B:209:TYR:HB3	2:B:213:LEU:HD12	2.01	0.42
2:B:249:VAL:HG13	2:B:399:LEU:HD11	2.02	0.42
8:H:779:LEU:HB3	8:H:811:TYR:CE2	2.54	0.42
8:H:784:ARG:NH1	11:L:25:DA:H5'	2.31	0.42
1:A:470:LEU:HD23	1:A:470:LEU:HA	1.88	0.42
2:B:319:VAL:O	2:B:324:ARG:NE	2.53	0.42
8:H:677:SER:HB3	8:H:680:CYS:SG	2.59	0.42
1:A:180:CYS:HA	1:A:267:THR:HG22	2.02	0.42
2:B:141:TYR:CZ	2:B:387:GLU:HA	2.55	0.42
2:B:528:SER:O	2:B:565:LYS:HE2	2.20	0.42
2:B:586:GLU:O	2:B:590:ASN:HB2	2.20	0.42
4:D:132:ASP:N	4:D:132:ASP:OD1	2.50	0.42
5:E:345:CYS:SG	5:E:367:PHE:HA	2.60	0.42
6:F:18:ASN:ND2	6:F:64:ILE:HD11	2.35	0.42
8:H:300:HIS:O	8:H:304:LEU:HG	2.19	0.42
8:H:613:PRO:HA	8:H:615:MET:HE2	2.02	0.42
8:H:638:ILE:HD12	12:M:16:DC:H3'	2.01	0.42
10:J:53:LEU:HD13	10:J:84:MET:HE2	2.01	0.42
1:A:633:ARG:HB3	1:A:676:ARG:HA	2.02	0.42
4:D:100:LEU:H	4:D:100:LEU:HD13	1.85	0.42
6:F:169:ASP:OD1	6:F:169:ASP:N	2.53	0.42
1:A:77:TRP:CE2	1:A:145:LYS:HD2	2.55	0.42
2:B:222:SER:HA	2:B:225:LEU:HD12	2.02	0.42
3:C:418:LEU:HD22	4:D:123:LEU:HB3	2.01	0.42
4:D:310:GLU:HG3	4:D:316:TYR:HE1	1.85	0.42
1:A:693:LEU:HB2	1:A:696:MET:SD	2.60	0.41
2:B:40:LEU:HB3	2:B:481:PHE:HE1	1.85	0.41
3:C:460:GLU:O	3:C:464:LEU:HG	2.20	0.41
4:D:241:SER:HA	4:D:288:ILE:HA	2.02	0.41
5:E:331:PHE:H	5:E:376:HIS:HE1	1.68	0.41
8:H:207:LYS:HD3	8:H:602:TRP:CD2	2.55	0.41
11:L:40:DG:C2	12:M:17:DG:C2	3.08	0.41
2:B:28:LEU:HD23	2:B:55:LEU:HD23	2.02	0.41
3:C:275:LYS:HE3	3:C:277:LEU:HD11	2.01	0.41
3:C:457:ILE:HG12	3:C:511:LYS:HE2	2.03	0.41
4:D:46:ARG:HH22	6:F:53:ARG:NE	2.18	0.41
6:F:143:TYR:CE1	6:F:147:MET:HE3	2.55	0.41
8:H:703:PRO:HB3	8:H:731:GLY:HA3	2.01	0.41
2:B:465:ASP:C	2:B:468:PRO:HD2	2.45	0.41
2:B:637:LEU:HD22	2:B:648:GLU:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:722:ARG:HH22	5:E:75:ASP:HB3	1.85	0.41
3:C:538:THR:O	3:C:542:ARG:HG3	2.21	0.41
5:E:94:GLU:HG3	5:E:236:VAL:HG11	2.01	0.41
3:C:408:ARG:O	3:C:412:GLU:HB2	2.19	0.41
4:D:95:ILE:HG23	4:D:114:PHE:CE2	2.55	0.41
4:D:273:GLN:HE21	4:D:278:SER:HB3	1.86	0.41
8:H:195:LYS:HA	8:H:198:ASN:ND2	2.35	0.41
3:C:118:LEU:HB3	3:C:125:PHE:HD1	1.84	0.41
4:D:91:SER:N	4:D:96:TRP:HE1	2.18	0.41
7:G:37:ASP:HB2	7:G:43:VAL:HG12	2.03	0.41
8:H:697:VAL:HA	8:H:738:THR:HG22	2.03	0.41
10:J:113:PHE:HA	10:J:129:VAL:HG21	2.03	0.41
11:L:31:DT:H1'	11:L:32:DA:C6	2.56	0.41
12:M:34:DA:H2''	12:M:35:DG:C8	2.56	0.41
2:B:134:CYS:O	2:B:138:THR:N	2.54	0.41
3:C:266:LEU:O	3:C:267:LEU:HD23	2.20	0.41
4:D:306:PHE:HZ	4:D:324:GLN:HG2	1.86	0.41
8:H:685:HIS:HB3	8:H:689:THR:HB	2.02	0.41
8:H:776:LEU:HD12	8:H:779:LEU:HD22	2.03	0.41
10:J:48:ILE:O	10:J:83:LYS:HA	2.20	0.41
10:J:35:GLU:O	10:J:39:LEU:HG	2.20	0.41
2:B:262:ASN:HD21	2:B:397:LEU:HD22	1.86	0.41
10:J:146:ILE:O	10:J:150:ASP:N	2.54	0.41
12:M:23:DC:OP2	12:M:23:DC:H2'	2.21	0.41
1:A:328:PHE:CD2	5:E:12:GLU:HB3	2.56	0.41
1:A:614:SER:OG	11:L:22:DC:OP1	2.30	0.41
3:C:481:VAL:HB	3:C:539:TRP:CZ2	2.56	0.41
4:D:46:ARG:HE	4:D:46:ARG:HB3	1.55	0.41
5:E:162:HIS:CD2	5:E:163:THR:HG23	2.55	0.41
6:F:180:VAL:O	6:F:183:ALA:HB3	2.21	0.41
6:F:282:CYS:HB2	6:F:289:PHE:CZ	2.56	0.41
8:H:818:LYS:O	8:H:822:LEU:HG	2.21	0.41
10:J:98:SER:HA	10:J:101:ASP:OD2	2.21	0.41
1:A:707:GLU:HG3	1:A:710:GLN:HE21	1.86	0.41
2:B:249:VAL:HB	2:B:435:PHE:HB3	2.03	0.41
5:E:257:HIS:CD2	5:E:259:ILE:HD11	2.56	0.41
6:F:15:VAL:HG13	6:F:164:ILE:HD11	2.03	0.41
6:F:47:SER:O	6:F:51:MET:HG3	2.21	0.41
7:G:9:LEU:HA	7:G:43:VAL:O	2.21	0.41
7:G:17:LYS:O	7:G:21:LEU:HG	2.21	0.41
11:L:3:DG:H2''	11:L:4:DT:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:LYS:N	1:A:656:ASN:OD1	2.54	0.40
1:A:663:VAL:HG13	1:A:669:GLU:HG2	2.03	0.40
1:A:153:MET:HB3	1:A:157:LYS:HE3	2.03	0.40
1:A:610:VAL:HG23	1:A:615:PHE:HE1	1.85	0.40
5:E:331:PHE:CD1	5:E:360:CYS:HA	2.55	0.40
8:H:594:ARG:NH2	8:H:644:HIS:HA	2.36	0.40
8:H:660:TYR:N	8:H:680:CYS:O	2.54	0.40
8:H:712:ASN:HD22	12:M:28:DA:H4'	1.86	0.40
1:A:369:VAL:HG21	1:A:615:PHE:HA	2.04	0.40
2:B:117:ILE:HB	2:B:157:PHE:CE2	2.56	0.40
2:B:494:ILE:HD12	2:B:706:LEU:HD12	2.02	0.40
4:D:96:TRP:HA	4:D:110:LEU:HA	2.03	0.40
4:D:219:TYR:OH	4:D:264:HIS:ND1	2.50	0.40
4:D:376:MET:HE2	4:D:376:MET:HB3	1.97	0.40
5:E:64:VAL:HG22	5:E:107:ILE:HB	2.03	0.40
5:E:104:ILE:C	5:E:120:LEU:HD12	2.47	0.40
5:E:348:CYS:SG	6:F:146:ARG:HD3	2.61	0.40
8:H:549:HIS:HB2	8:H:551:VAL:HG23	2.04	0.40
8:H:637:ALA:HB3	8:H:640:LEU:HG	2.04	0.40
8:H:698:ARG:HE	8:H:739:GLU:HG3	1.85	0.40
9:I:289:ARG:HB2	9:I:328:LEU:HA	2.03	0.40
12:M:13:DT:H2''	12:M:14:DA:C8	2.56	0.40
1:A:188:LEU:HG	1:A:287:LEU:HG	2.04	0.40
2:B:395:SER:N	2:B:396:PRO:HD2	2.37	0.40
2:B:563:ARG:HH21	3:C:172:ALA:HB1	1.87	0.40
4:D:361:ALA:HB2	4:D:395:GLU:HB2	2.02	0.40
8:H:209:HIS:ND1	9:I:299:LEU:HD11	2.37	0.40
8:H:287:PHE:CZ	8:H:301:ILE:HG23	2.56	0.40
8:H:695:ARG:NH2	8:H:738:THR:O	2.38	0.40
8:H:734:GLY:H	8:H:737:GLN:CD	2.29	0.40
2:B:72:TYR:HB3	2:B:206:VAL:HG13	2.04	0.40
2:B:95:GLU:HG2	2:B:101:LYS:HA	2.03	0.40
2:B:492:PRO:HB2	2:B:701:LEU:HD13	2.04	0.40
5:E:232:LEU:O	5:E:236:VAL:HG23	2.21	0.40
5:E:253:GLY:HA2	6:F:264:ILE:HA	2.02	0.40
6:F:166:ALA:HB2	6:F:196:LEU:HD12	2.02	0.40
11:L:28:DA:H2'	11:L:29:DT:C6	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	607/782 (78%)	580 (96%)	27 (4%)	0	100	100
2	B	758/768 (99%)	749 (99%)	9 (1%)	0	100	100
3	C	348/548 (64%)	336 (97%)	11 (3%)	1 (0%)	36	70
4	D	444/462 (96%)	437 (98%)	7 (2%)	0	100	100
5	E	351/417 (84%)	340 (97%)	11 (3%)	0	100	100
6	F	257/308 (83%)	248 (96%)	9 (4%)	0	100	100
7	G	65/71 (92%)	61 (94%)	4 (6%)	0	100	100
8	H	511/950 (54%)	497 (97%)	14 (3%)	0	100	100
9	I	59/417 (14%)	54 (92%)	5 (8%)	0	100	100
10	J	148/172 (86%)	144 (97%)	4 (3%)	0	100	100
All	All	3548/4895 (72%)	3446 (97%)	101 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	398	GLN

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	540/688 (78%)	520 (96%)	20 (4%)	30	52
2	B	664/672 (99%)	644 (97%)	20 (3%)	36	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	320/484 (66%)	306 (96%)	14 (4%)	25	48
4	D	384/399 (96%)	373 (97%)	11 (3%)	37	58
5	E	317/371 (85%)	302 (95%)	15 (5%)	23	46
6	F	233/272 (86%)	229 (98%)	4 (2%)	53	68
7	G	60/64 (94%)	52 (87%)	8 (13%)	4	18
8	H	457/815 (56%)	432 (94%)	25 (6%)	19	44
9	I	57/336 (17%)	55 (96%)	2 (4%)	32	54
10	J	130/152 (86%)	126 (97%)	4 (3%)	35	56
All	All	3162/4253 (74%)	3039 (96%)	123 (4%)	30	51

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ASP
1	A	92	VAL
1	A	135	ASP
1	A	166	VAL
1	A	287	LEU
1	A	315	VAL
1	A	346	LYS
1	A	383	THR
1	A	415	HIS
1	A	434	GLU
1	A	469	THR
1	A	471	VAL
1	A	482	PHE
1	A	521	GLU
1	A	559	ILE
1	A	616	ASP
1	A	633	ARG
1	A	638	GLN
1	A	639	ARG
1	A	708	GLU
2	B	17	ILE
2	B	63	TYR
2	B	116	CYS
2	B	117	ILE
2	B	156	ARG
2	B	210	HIS

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Mol	Chain	Res	Type
2	B	211	TYR
2	B	237	HIS
2	B	262	ASN
2	B	301	THR
2	B	358	LEU
2	B	361	LEU
2	B	365	VAL
2	B	384	HIS
2	B	531	VAL
2	B	611	VAL
2	B	612	HIS
2	B	731	GLU
2	B	732	ASP
2	B	744	LEU
3	C	188	LEU
3	C	189	THR
3	C	219	GLU
3	C	307	PHE
3	C	310	HIS
3	C	315	LEU
3	C	376	LEU
3	C	396	THR
3	C	400	ILE
3	C	403	SER
3	C	404	PHE
3	C	407	ILE
3	C	471	LEU
3	C	517	LEU
4	D	75	VAL
4	D	100	LEU
4	D	161	HIS
4	D	174	ASP
4	D	196	ILE
4	D	204	LEU
4	D	284	THR
4	D	321	SER
4	D	380	THR
4	D	404	THR
4	D	427	GLU
5	E	11	TRP
5	E	15	TYR
5	E	50	HIS

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Mol	Chain	Res	Type
5	E	52	GLN
5	E	88	LEU
5	E	101	ILE
5	E	109	THR
5	E	215	THR
5	E	268	LYS
5	E	276	LEU
5	E	280	THR
5	E	313	VAL
5	E	328	LEU
5	E	354	ASP
5	E	366	VAL
6	F	50	PHE
6	F	154	ASN
6	F	240	GLN
6	F	258	HIS
7	G	4	VAL
7	G	6	LYS
7	G	9	LEU
7	G	38	ILE
7	G	44	PHE
7	G	49	LEU
7	G	59	GLU
7	G	62	ASP
8	H	167	ILE
8	H	189	TYR
8	H	568	TYR
8	H	588	VAL
8	H	634	LEU
8	H	636	THR
8	H	649	LEU
8	H	659	ILE
8	H	660	TYR
8	H	663	THR
8	H	666	ILE
8	H	688	ASP
8	H	708	LYS
8	H	713	ARG
8	H	787	ASP
8	H	790	CYS
8	H	791	VAL
8	H	799	PHE

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Mol	Chain	Res	Type
8	H	813	VAL
8	H	826	GLU
8	H	828	GLU
8	H	829	GLN
8	H	834	ARG
8	H	841	GLU
8	H	855	LEU
9	I	285	PHE
9	I	299	LEU
10	J	63	GLU
10	J	93	MET
10	J	116	ASP
10	J	168	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	537	ASN
1	A	598	HIS
1	A	638	GLN
1	A	710	GLN
1	A	714	GLN
2	B	37	HIS
2	B	304	HIS
2	B	560	ASN
2	B	698	GLN
2	B	700	HIS
3	C	182	ASN
3	C	402	ASN
3	C	482	ASN
4	D	117	ASN
4	D	273	GLN
5	E	103	GLN
5	E	127	HIS
5	E	275	HIS
5	E	365	ASN
6	F	52	ASN
6	F	65	GLN
6	F	187	GLN
6	F	258	HIS
6	F	260	ASN
7	G	64	ASN

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Mol	Chain	Res	Type
8	H	198	ASN
8	H	644	HIS
8	H	685	HIS
8	H	712	ASN
8	H	773	GLN
8	H	847	ASN
8	H	906	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	$\# Z > 2$
13	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
13	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.

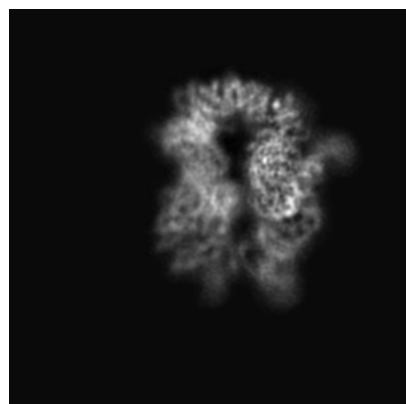
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27996. These allow visual inspection of the internal detail of the map and identification of artifacts.

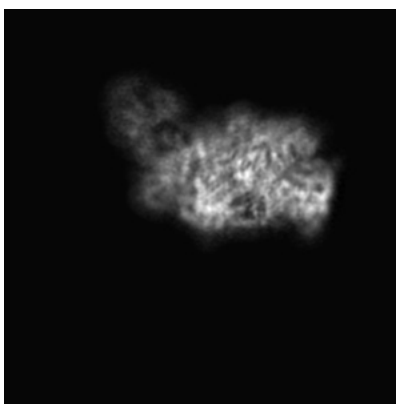
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

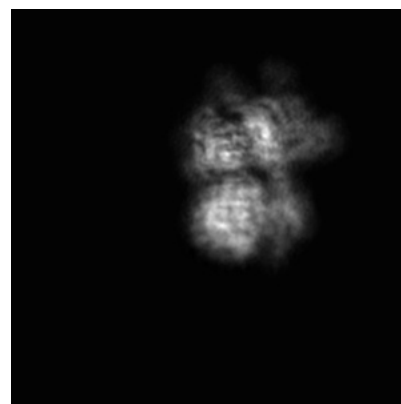
6.1.1 Primary map



X

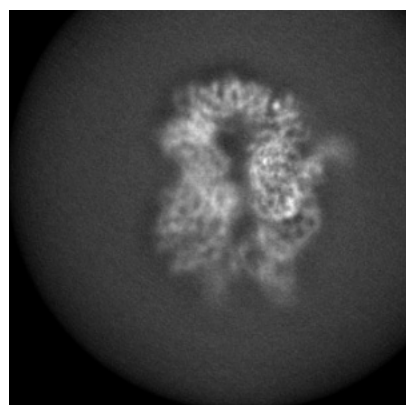


Y

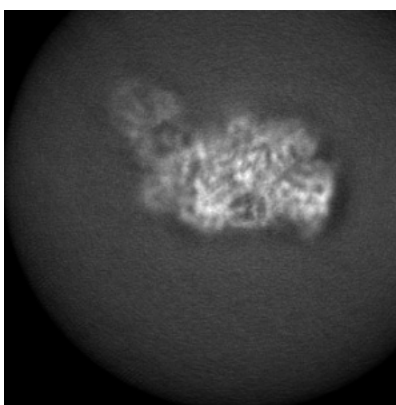


Z

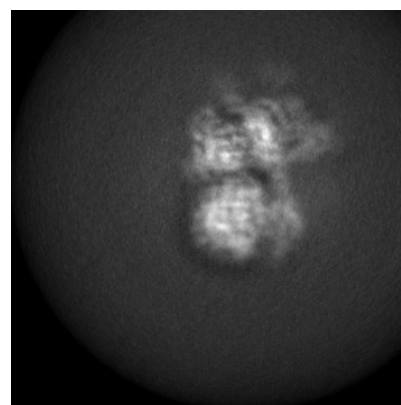
6.1.2 Raw map



X



Y

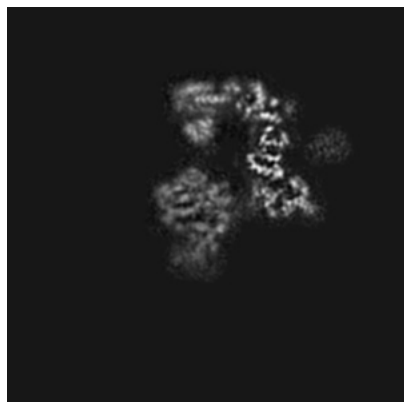


Z

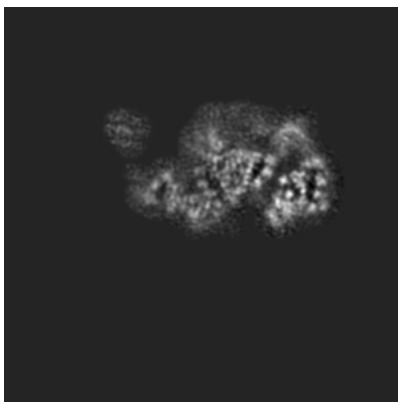
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

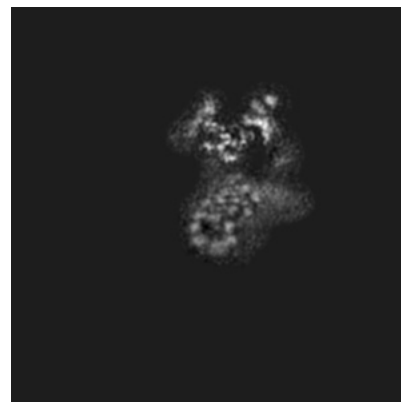
6.2.1 Primary map



X Index: 192

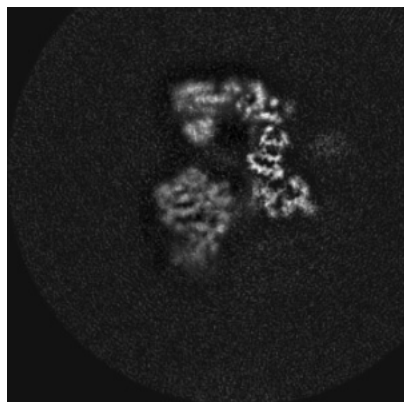


Y Index: 192

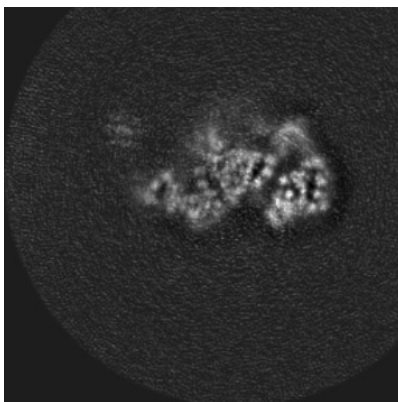


Z Index: 192

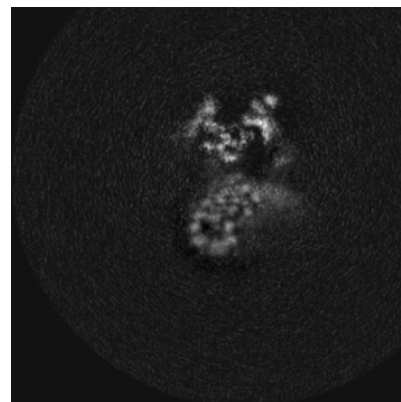
6.2.2 Raw map



X Index: 192



Y Index: 192

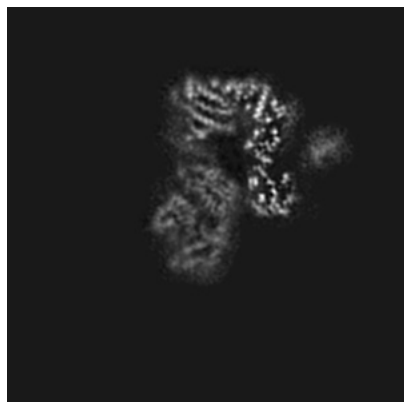


Z Index: 192

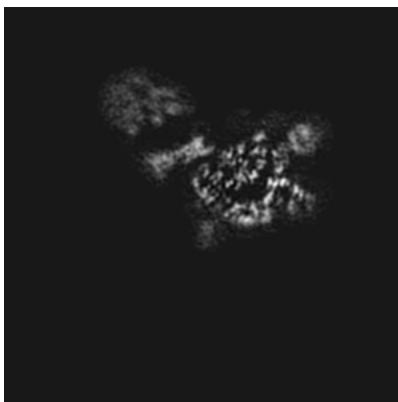
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

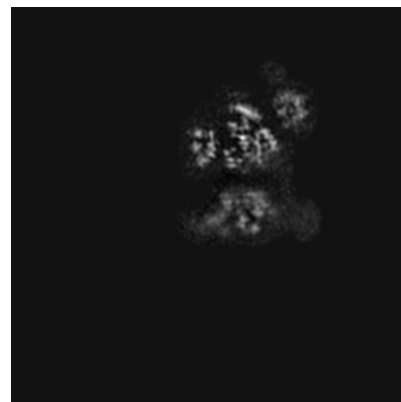
6.3.1 Primary map



X Index: 205

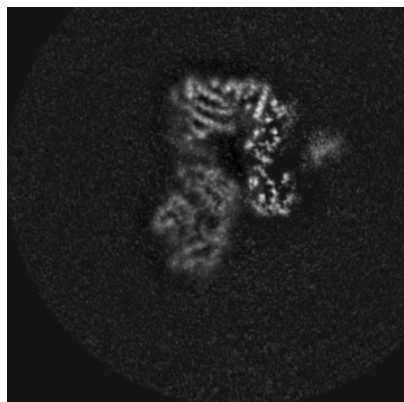


Y Index: 260

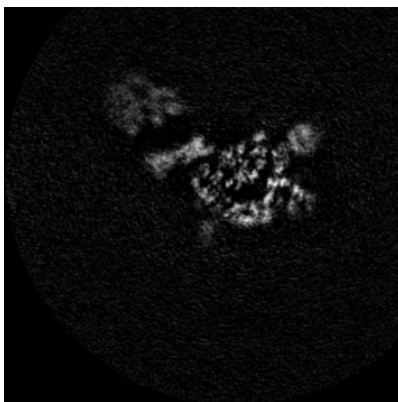


Z Index: 226

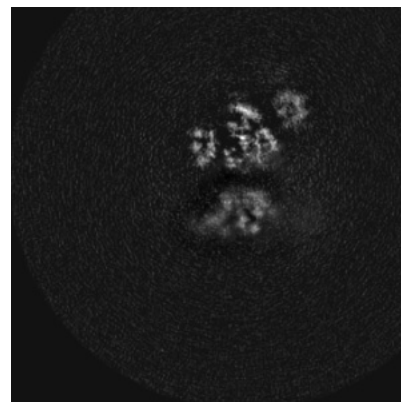
6.3.2 Raw map



X Index: 205



Y Index: 260

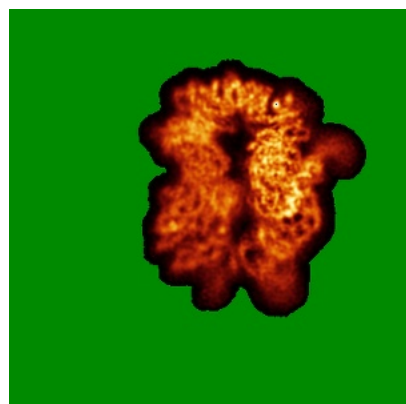


Z Index: 226

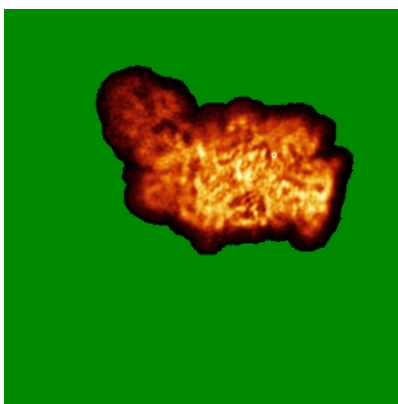
The images above show the largest variance slices of the map in three orthogonal directions.

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

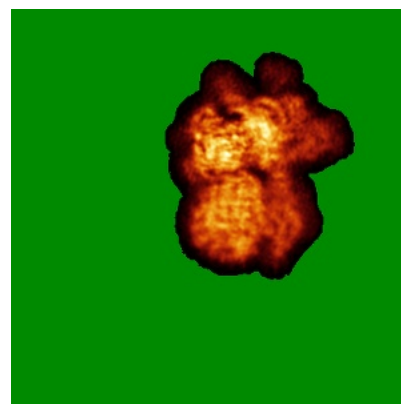
6.4.1 Primary map



X

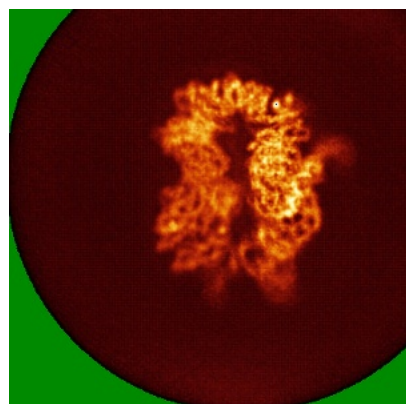


Y

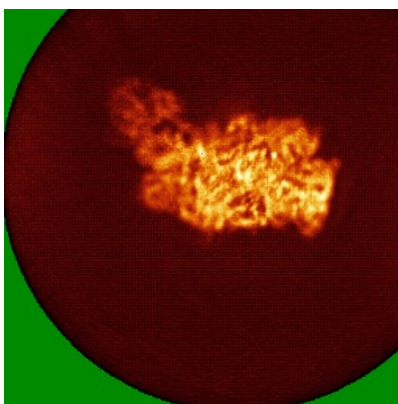


Z

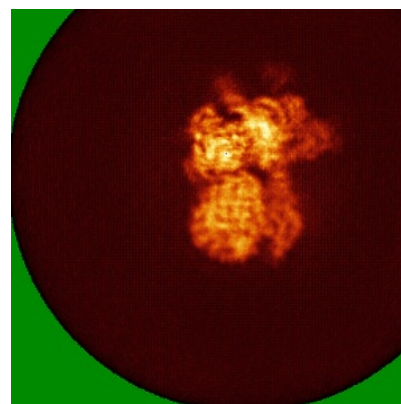
6.4.2 Raw map



X



Y

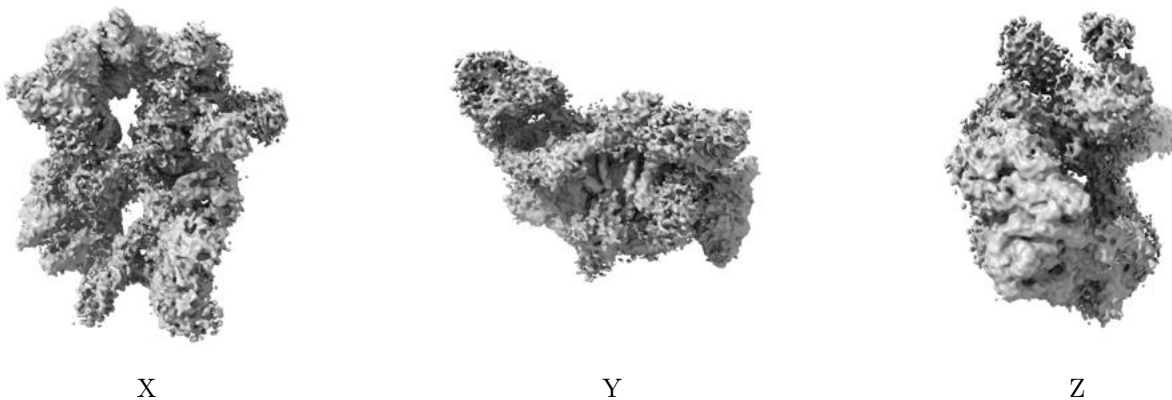


Z

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

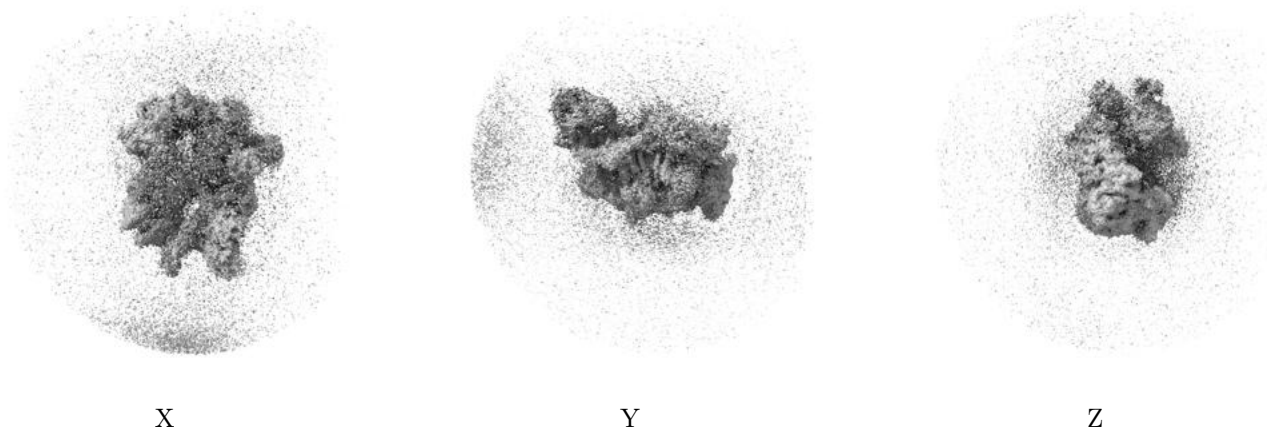
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. 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



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.

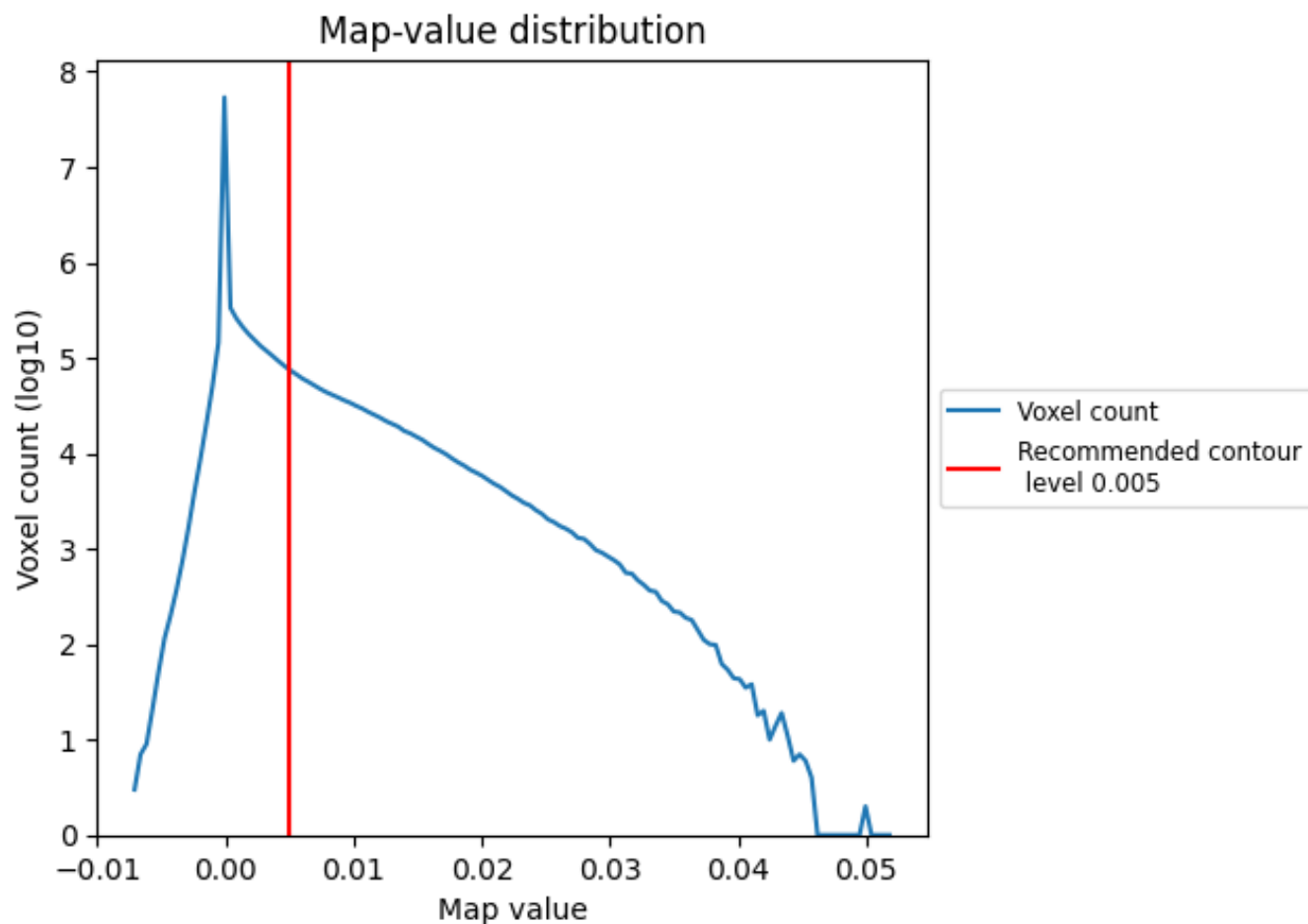
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

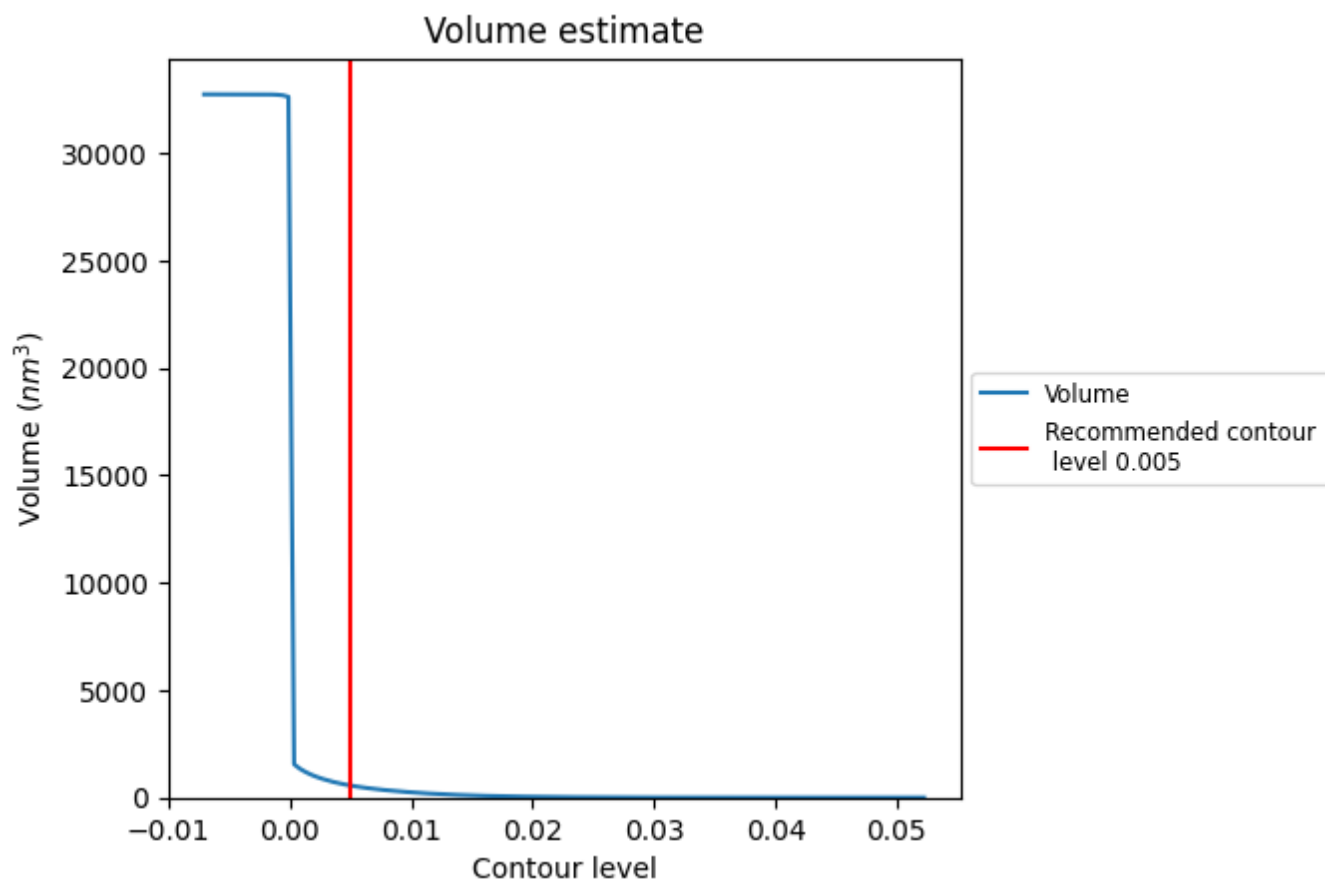
This section contains the results of statistical analysis of the map.

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.

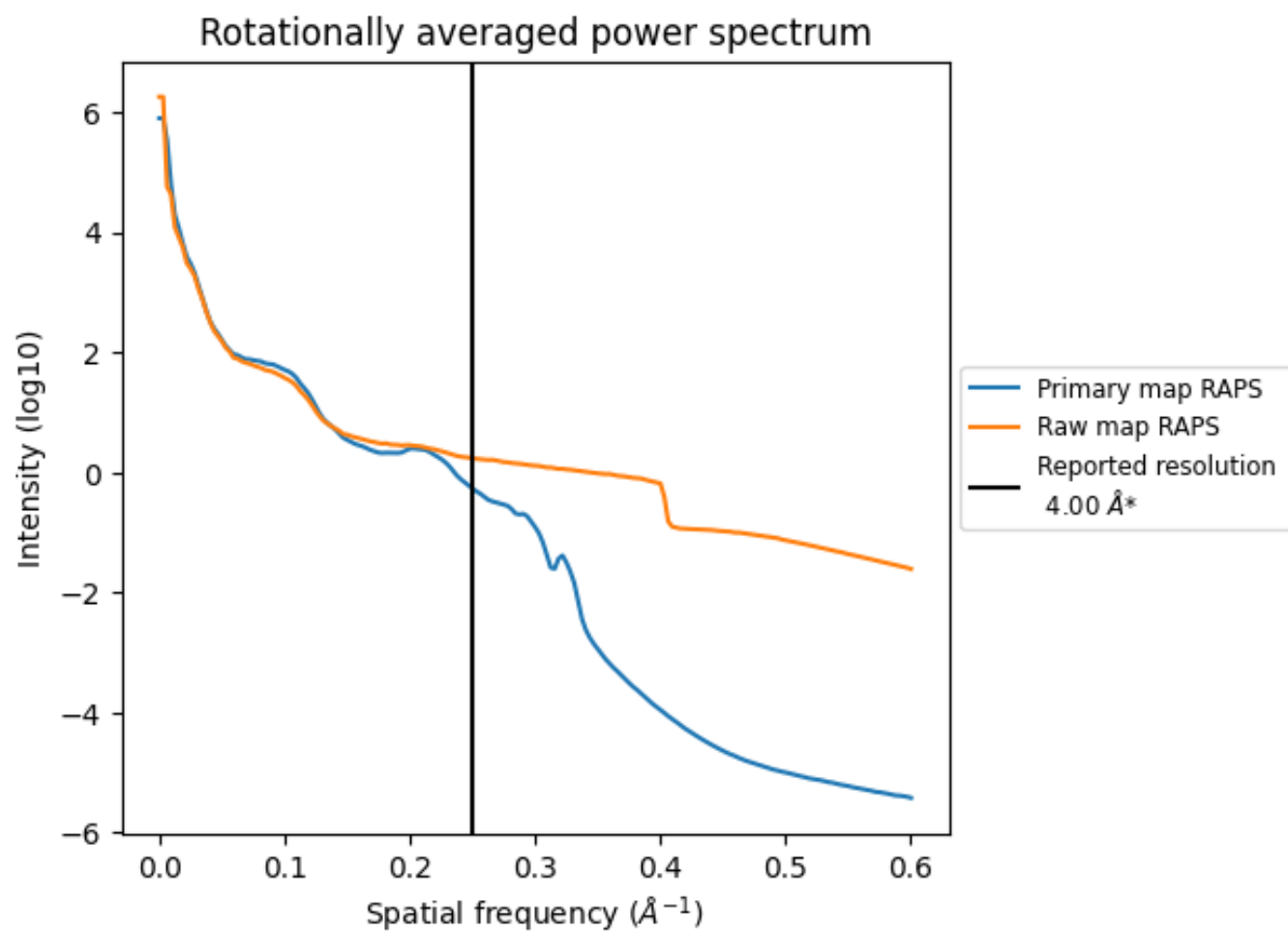
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 558 nm³; this corresponds to an approximate mass of 504 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 ⓘ

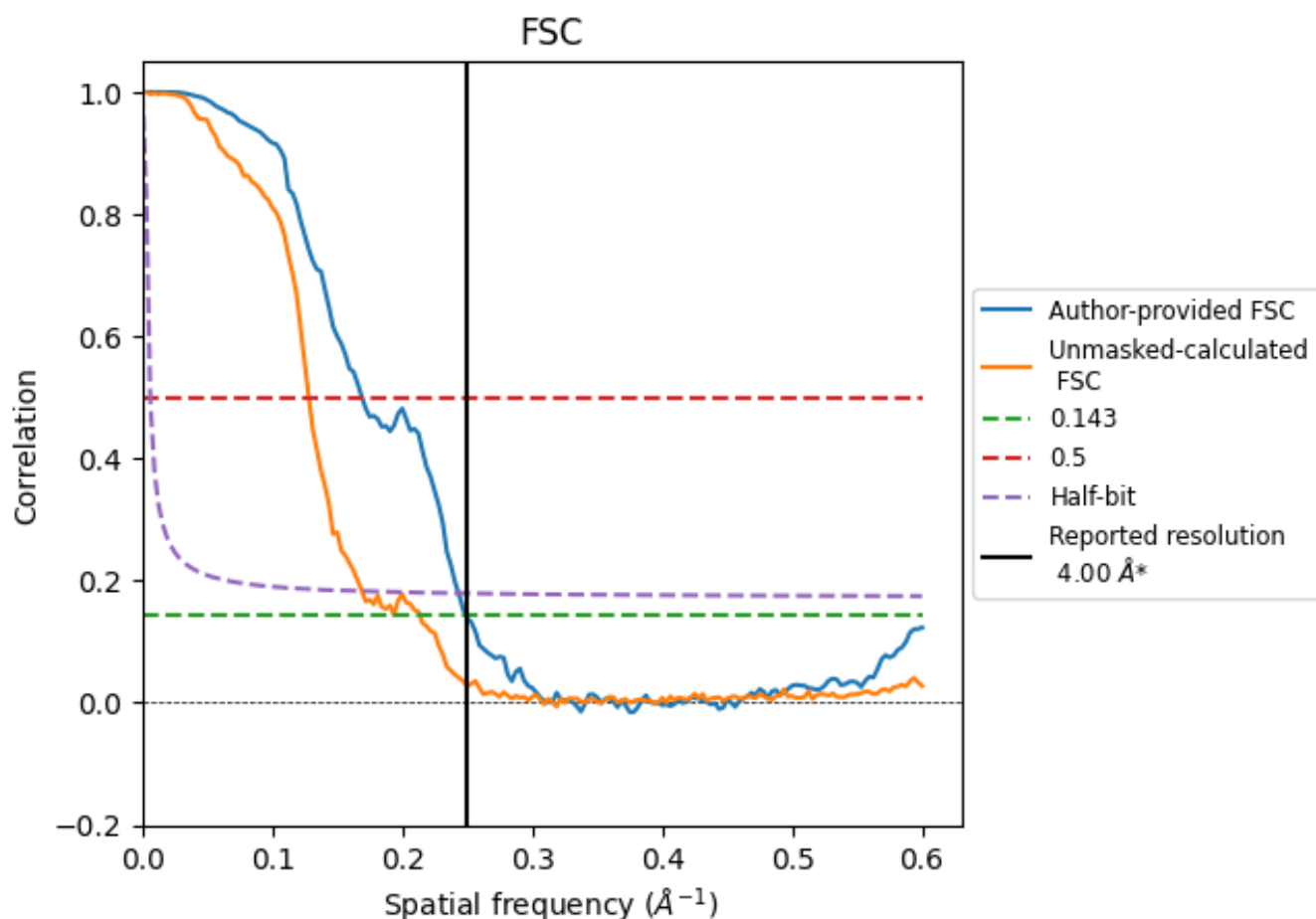


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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 0.250 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

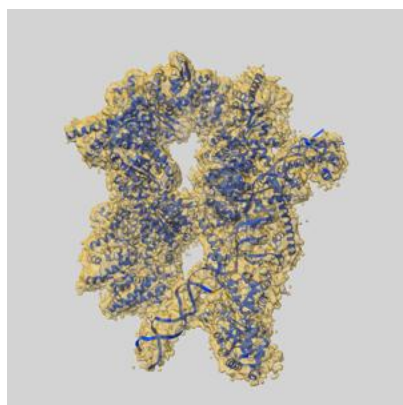
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	4.02	5.91	4.11
Unmasked-calculated*	5.16	7.81	5.91

*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 5.16 differs from the reported value 4.0 by more than 10 %

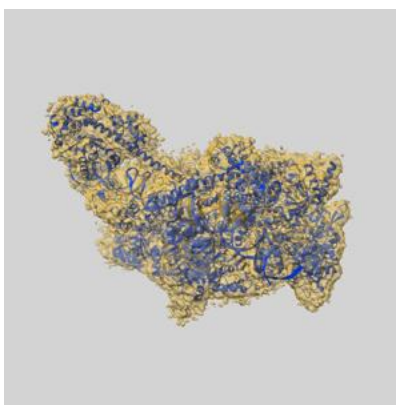
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27996 and PDB model 8EBS. Per-residue inclusion information can be found in section [3](#) on page [9](#).

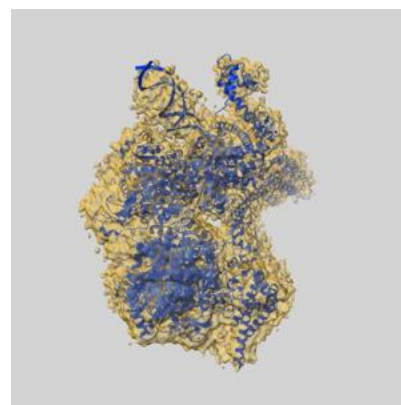
9.1 Map-model overlay [i](#)



X



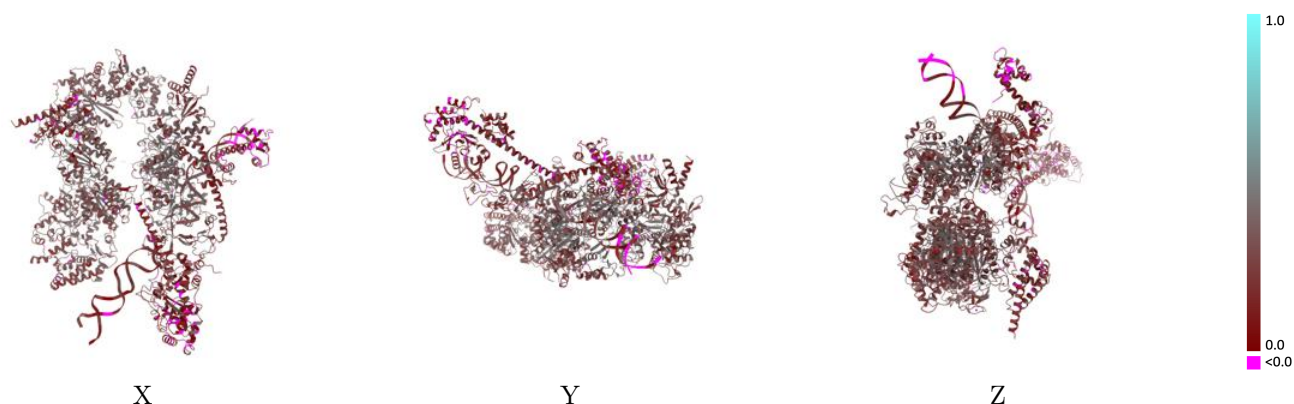
Y



Z

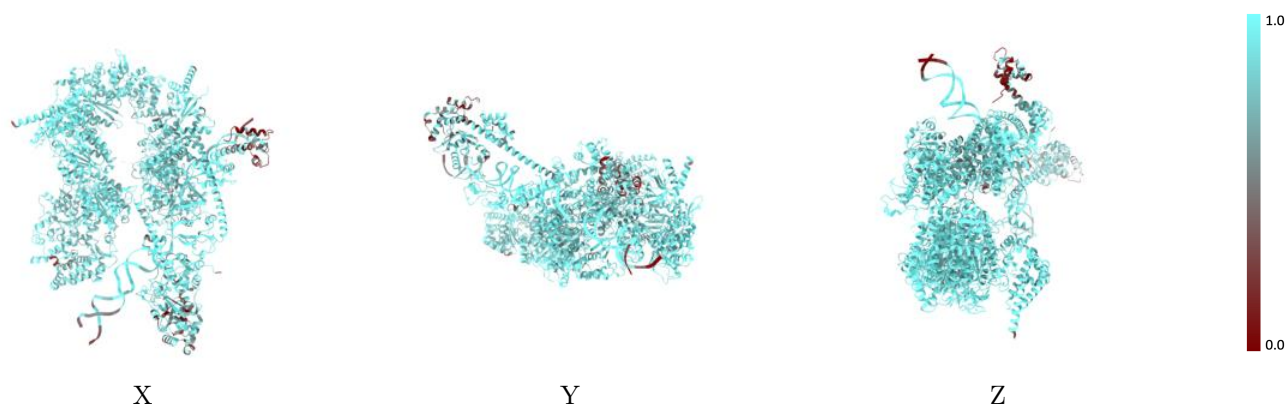
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



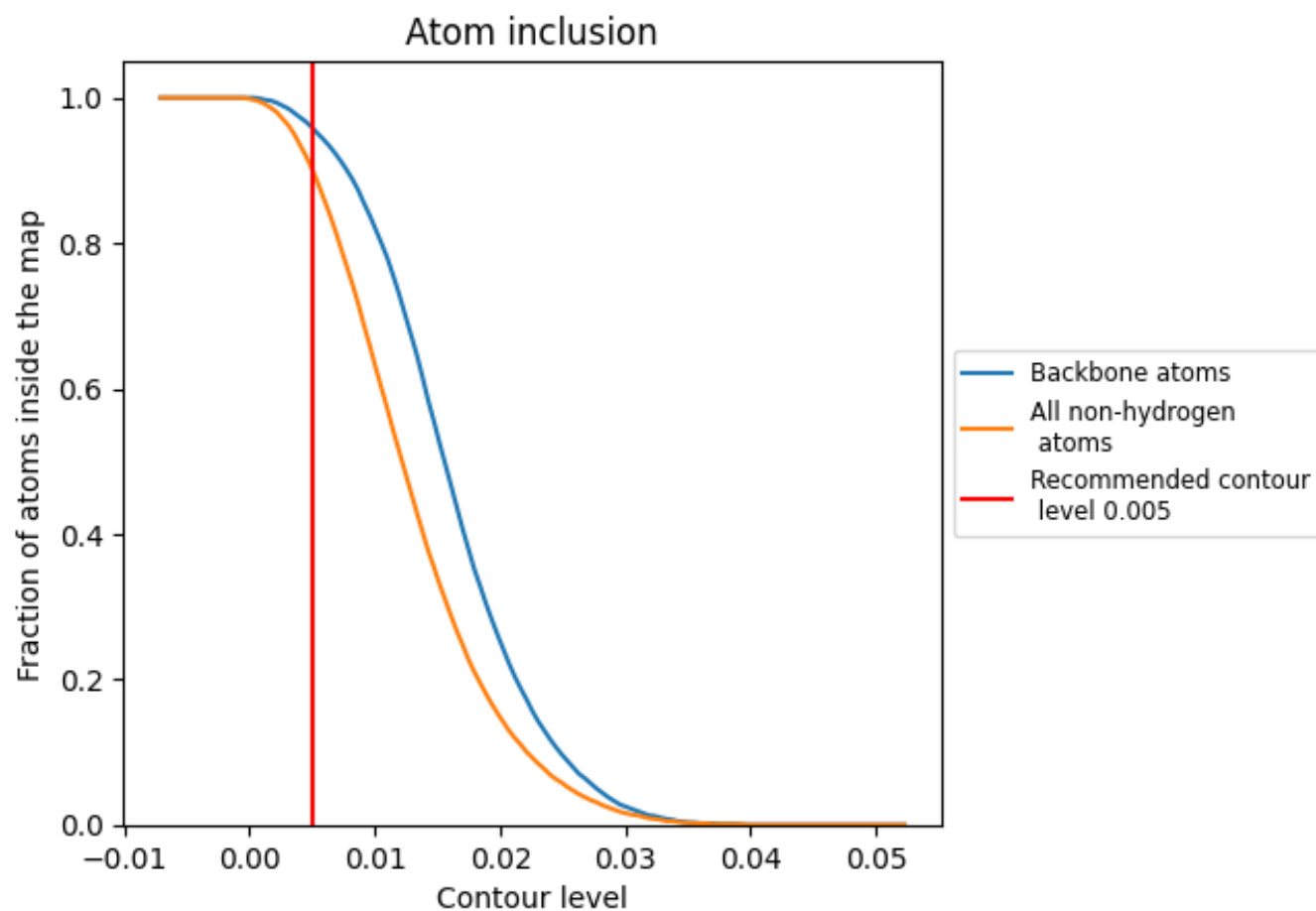
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 90% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9020	0.2740
A	0.9080	0.3470
B	0.9360	0.2840
C	0.9370	0.2440
D	0.9440	0.3090
E	0.9560	0.3100
F	0.9550	0.3240
G	0.8940	0.3090
H	0.8270	0.1970
I	0.8610	0.1750
J	0.6360	0.1410
L	0.8550	0.2090
M	0.8590	0.2110

1.0

0.0

<0.0