



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 06:20 PM EDT

PDB ID : 9PD4 / pdb_00009pd4
EMDB ID : EMD-71525
Title : NER dual incision complex - DuIM
Authors : Li, C.L.; Kim, J.; Yang, W.
Deposited on : 2025-06-30
Resolution : 3.40 Å(reported)
Based on initial models : 8ebt, 1l1o, 6sxa, 1jmc, 6tus

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:

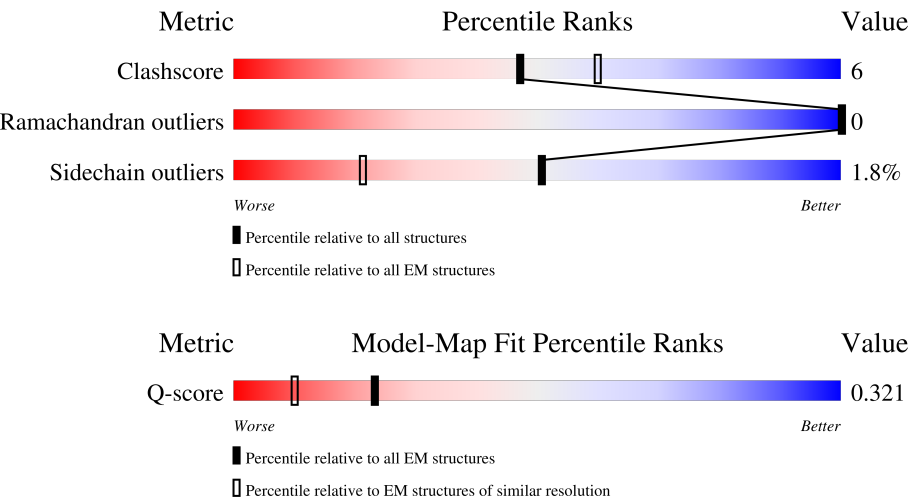
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.40 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.



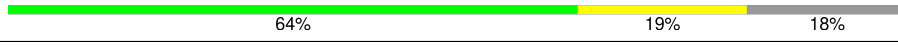
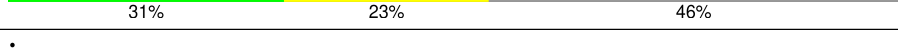
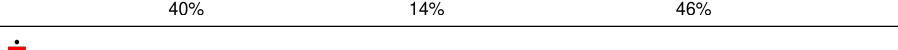
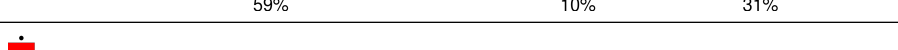
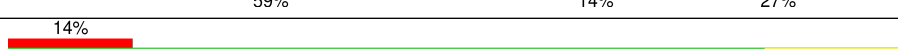
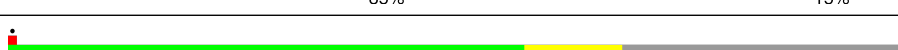
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	62%16%22%
2	B	768	77%15%7%
3	C	548	17%8%75%
4	D	462	77%17%6%

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Mol	Chain	Length	Quality of chain
5	E	395	
6	F	308	
7	G	71	
8	K	273	
9	L	93	
10	M	94	
11	N	616	
12	O	270	
13	P	121	
14	Q	916	
15	R	295	
16	S	1186	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 40053 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TFIIF basal transcription factor complex helicase XPB subunit.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	712	Total	C	N	O	S	0	0
			5745	3677	1001	1038	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	138	Total	C	N	O	S	0	0
			1130	718	196	209	7		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	343	Total	C	N	O	S	0	0
			2686	1697	457	506	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	254	Total	C	N	O	S	0	0
			2001	1280	332	370	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	65	Total	C	N	O	S	0	0
			515	332	81	99	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	209	Total	C	N	O	S	0	0
			1724	1078	309	321	16		

- Molecule 9 is a DNA chain called DNA (Cy5).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	50	Total	C	N	O	P	0	0
			1031	506	175	300	50		

- Molecule 10 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	51	Total	C	N	O	P	0	0
			1055	503	196	305	51		

- Molecule 11 is a protein called Replication protein A 70 kDa DNA-binding subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	427	Total	C	N	O	S	0	0
			3420	2154	583	666	17		

- Molecule 12 is a protein called Replication protein A 32 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	197	Total	C	N	O	S	0	0
			1538	968	262	300	8		

- Molecule 13 is a protein called Replication protein A 14 kDa subunit.

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

- Molecule 14 is a protein called DNA repair endonuclease XPF.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	632	Total	C	N	O	S	0	0
			5001	3204	866	909	22		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 15 is a protein called DNA excision repair protein ERCC-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	123	Total	C	N	O	S	0	0
			983	637	167	175	4		

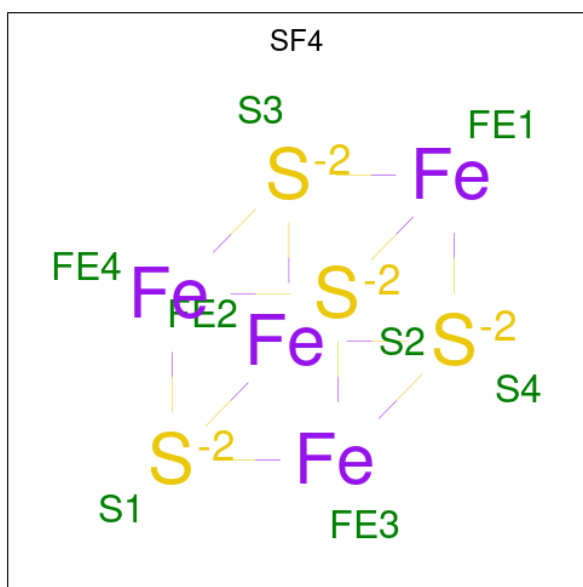
- Molecule 16 is a protein called DNA excision repair protein ERCC-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	466	Total	C	N	O	S	2	0
			3829	2440	653	723	13		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	812	ASN	ASP	engineered mutation	UNP P28715
S	1053	ARG	GLY	variant	UNP P28715
S	1080	ARG	GLY	variant	UNP P28715

- Molecule 17 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



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

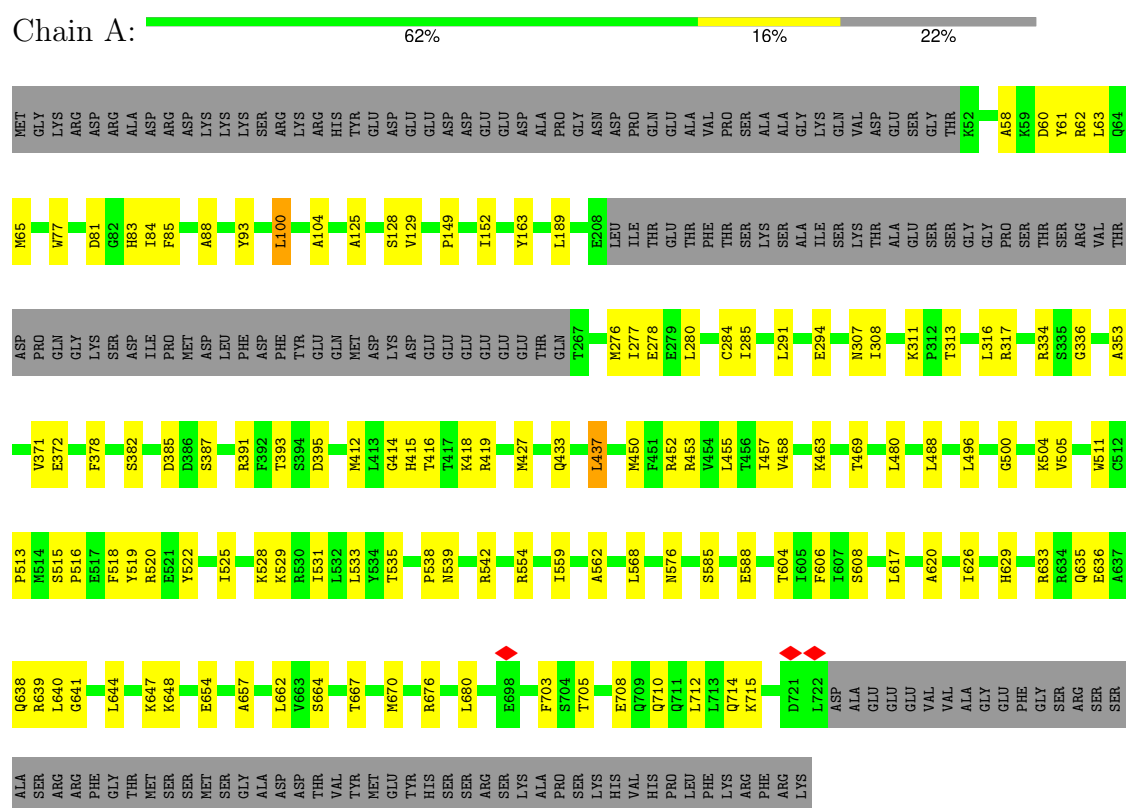
- Molecule 18 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

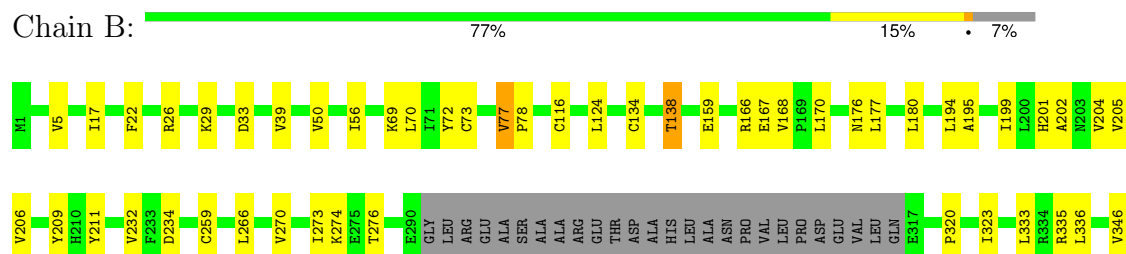
3 Residue-property plots

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

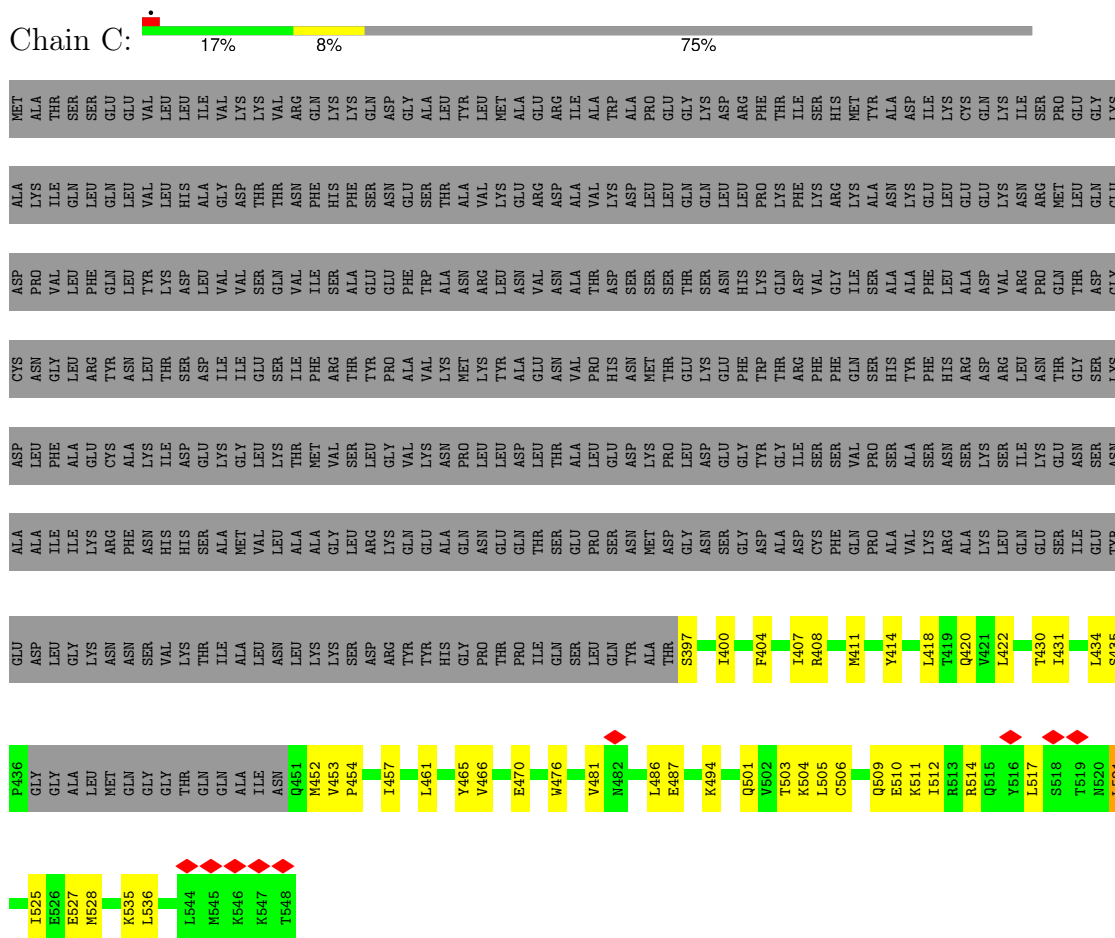
- Molecule 1: TFIIH basal transcription factor complex helicase XPB subunit



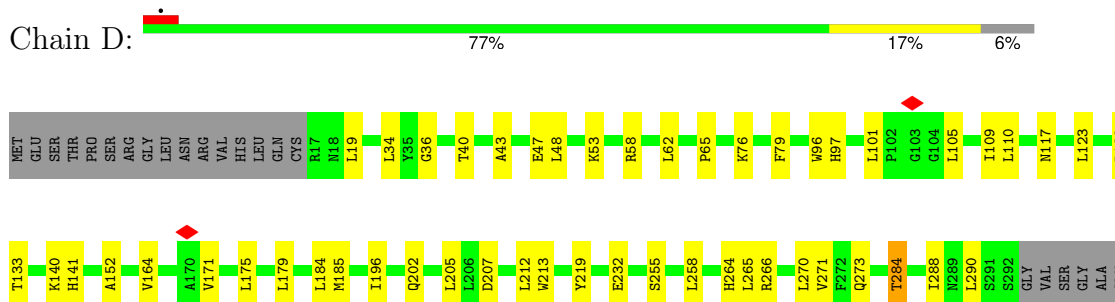
- Molecule 2: General transcription and DNA repair factor IIH helicase subunit XPD

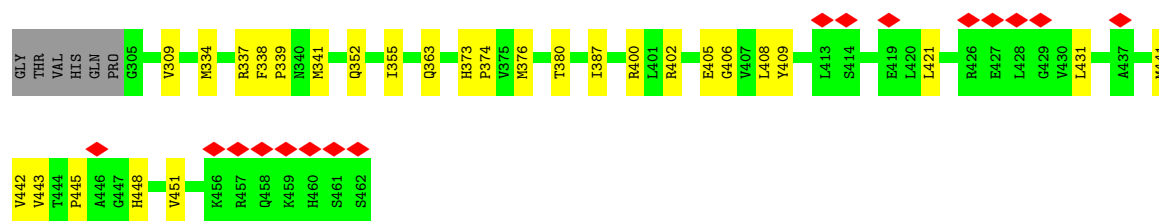


- Molecule 3: General transcription factor IIH subunit 1

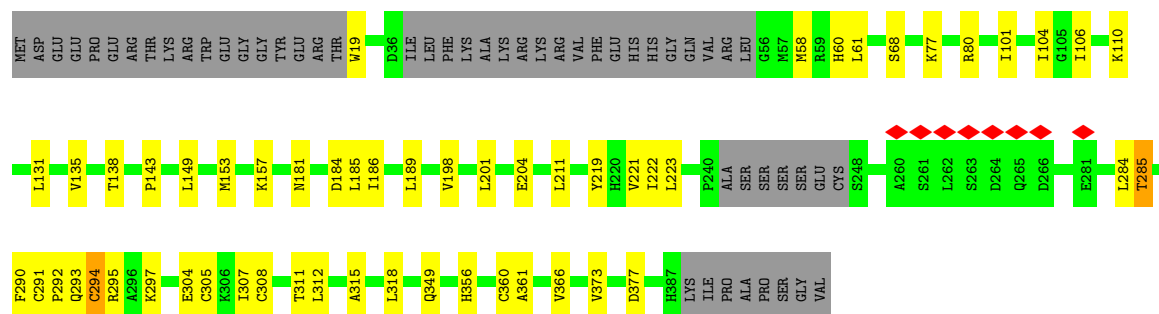


- Molecule 4: General transcription factor IIH subunit 4, p52

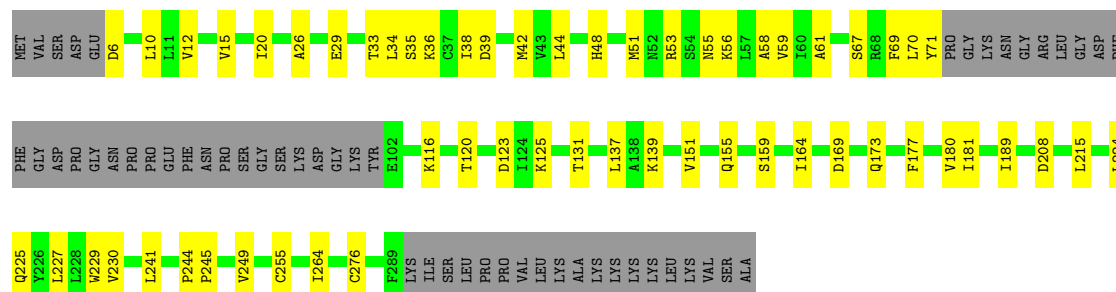




• Molecule 5: General transcription factor IIH subunit 2



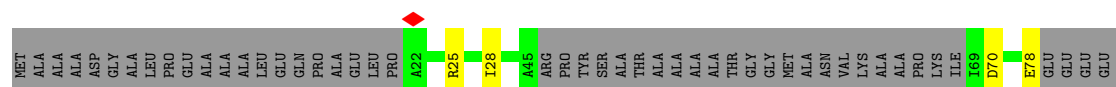
• Molecule 6: General transcription factor IIH subunit 3

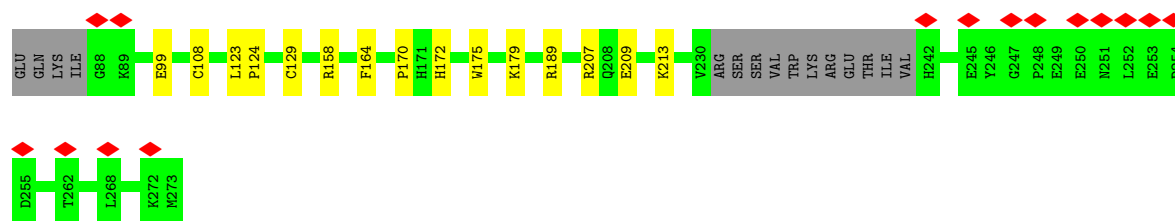


• Molecule 7: General transcription factor IIH subunit 5

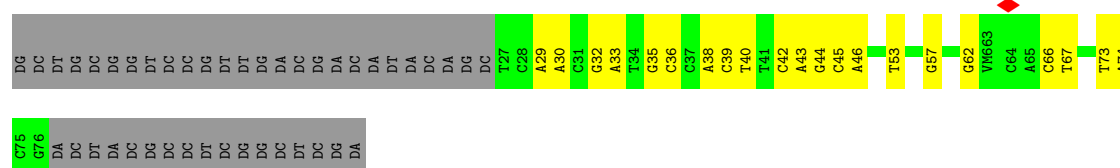
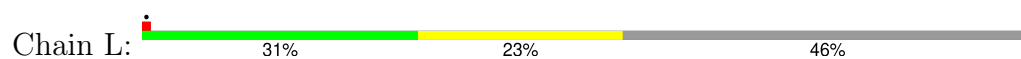


• Molecule 8: DNA repair protein complementing XP-A cells

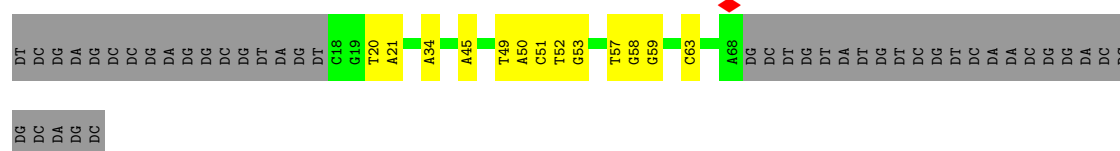




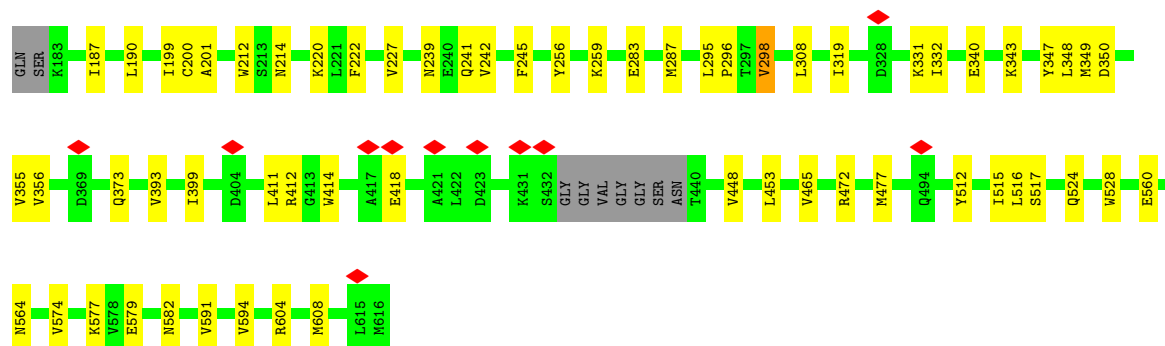
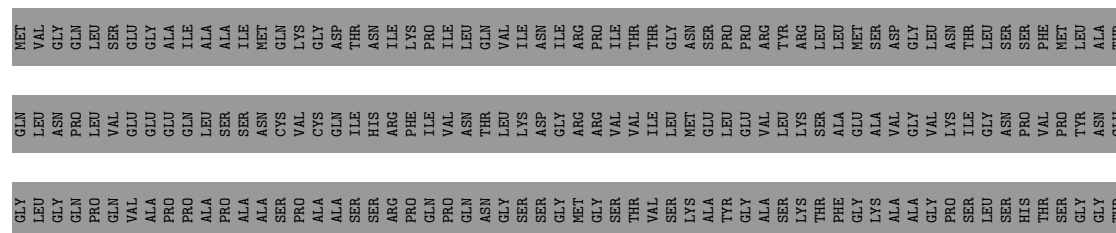
• Molecule 9: DNA (Cy5)



• Molecule 10: DNA



• Molecule 11: Replication protein A 70 kDa DNA-binding subunit



• Molecule 12: Replication protein A 32 kDa subunit

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	140332	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52.5	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.052	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	266.56, 266.56, 266.56	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.833, 0.833, 0.833	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, 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	0.09	0/5051	0.25	0/6822
2	B	0.09	0/5868	0.24	0/7941
3	C	0.10	0/1152	0.23	0/1553
4	D	0.08	0/3564	0.20	0/4827
5	E	0.08	0/2745	0.24	0/3718
6	F	0.09	0/2036	0.22	0/2758
7	G	0.09	0/521	0.26	0/703
8	K	0.08	0/1752	0.22	0/2335
9	L	0.16	0/1109	0.36	0/1704
10	M	0.16	0/1185	0.34	0/1829
11	N	0.09	0/3483	0.25	0/4702
12	O	0.11	0/1564	0.25	0/2124
13	P	0.08	0/970	0.26	0/1310
14	Q	0.08	0/5097	0.23	0/6916
15	R	0.08	0/1007	0.22	0/1370
16	S	0.08	0/3913	0.21	0/5275
All	All	0.09	0/41017	0.24	0/55887

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4947	0	4993	76	0
2	B	5745	0	5787	65	0
3	C	1130	0	1147	34	0
4	D	3483	0	3526	53	0
5	E	2686	0	2644	32	0
6	F	2001	0	2021	41	0
7	G	515	0	522	13	0
8	K	1724	0	1716	13	0
9	L	1031	0	554	15	0
10	M	1055	0	577	11	0
11	N	3420	0	3354	32	0
12	O	1538	0	1536	21	0
13	P	950	0	952	10	0
14	Q	5001	0	4971	59	0
15	R	983	0	993	15	0
16	S	3829	0	3743	31	0
17	B	8	0	0	0	0
18	E	3	0	0	0	0
18	F	2	0	0	0	0
18	K	1	0	0	0	0
18	N	1	0	0	0	0
All	All	40053	0	39036	470	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 6.

All (470) 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)
5:E:291:CYS:HB3	5:E:312:LEU:HD21	1.57	0.86
15:R:141:LEU:HB3	15:R:171:VAL:HG12	1.64	0.80
6:F:10:LEU:HG	6:F:56:LYS:HB2	1.67	0.75
12:O:69:VAL:HG11	12:O:169:LEU:HD13	1.72	0.71
3:C:400:ILE:HD11	6:F:20:ILE:HD12	1.74	0.69
4:D:408:LEU:HB2	4:D:442:VAL:HG22	1.72	0.69
5:E:68:SER:HB3	5:E:143:PRO:HD3	1.74	0.69
12:O:104:VAL:HG12	12:O:141:LEU:HB3	1.74	0.69
1:A:500:GLY:O	1:A:648:LYS:NZ	2.25	0.68
11:N:477:MET:SD	11:N:512:TYR:OH	2.50	0.68
14:Q:86:ARG:NH2	14:Q:104:GLY:O	2.27	0.68
16:S:69:ARG:NH1	16:S:986:ALA:O	2.28	0.67
14:Q:85:PRO:HB3	14:Q:106:VAL:HB	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:685:VAL:HB	14:Q:717:ILE:HB	1.77	0.66
1:A:505:VAL:HG12	1:A:657:ALA:HB3	1.77	0.66
4:D:171:VAL:HB	4:D:175:LEU:HD21	1.78	0.65
1:A:58:ALA:HB2	4:D:334:MET:HB3	1.78	0.65
2:B:232:VAL:HG12	2:B:455:ILE:HB	1.79	0.65
3:C:411:MET:HG3	6:F:34:LEU:HD23	1.77	0.65
2:B:77:VAL:HG23	2:B:78:PRO:HD3	1.77	0.64
11:N:332:ILE:HG13	11:N:343:LYS:HD3	1.78	0.64
5:E:294:CYS:SG	5:E:305:CYS:HB2	2.37	0.64
14:Q:409:ILE:HB	14:Q:554:ILE:HG12	1.78	0.64
12:O:53:GLN:HE21	13:P:114:PRO:HD2	1.62	0.64
4:D:36:GLY:O	4:D:117:ASN:ND2	2.30	0.63
14:Q:12:MET:HB3	14:Q:571:HIS:HE1	1.63	0.63
15:R:129:ASP:OD1	15:R:156:ARG:NH1	2.31	0.63
2:B:637:LEU:HD13	2:B:648:GLU:HG3	1.80	0.63
1:A:528:LYS:HD3	10:M:63:DC:H4'	1.80	0.63
3:C:418:LEU:HD22	4:D:123:LEU:HB3	1.79	0.62
4:D:288:ILE:O	6:F:53:ARG:NH2	2.32	0.62
15:R:178:PRO:HB2	15:R:182:LEU:HD23	1.80	0.62
5:E:304:GLU:HA	5:E:311:THR:HA	1.82	0.62
2:B:361:LEU:HD12	2:B:367:ILE:HD12	1.82	0.62
1:A:629:HIS:O	1:A:676:ARG:NH1	2.33	0.62
1:A:515:SER:HB3	1:A:518:PHE:HB2	1.82	0.61
3:C:461:LEU:HD22	3:C:521:LEU:HD13	1.81	0.61
6:F:15:VAL:HG22	6:F:164:ILE:HD11	1.81	0.61
6:F:159:SER:HB2	6:F:189:ILE:HD12	1.82	0.61
16:S:808:THR:HG22	16:S:810:ASP:H	1.64	0.61
11:N:574:VAL:HG22	11:N:591:VAL:HG12	1.80	0.61
11:N:414:TRP:NE1	11:N:418:GLU:OE2	2.33	0.61
12:O:207:VAL:HG12	12:O:211:GLN:HE21	1.65	0.61
4:D:19:LEU:HB2	4:D:213:TRP:HZ2	1.65	0.61
4:D:402:ARG:HB2	7:G:11:GLU:HB3	1.81	0.61
14:Q:94:SER:HA	14:Q:97:ARG:HD3	1.81	0.61
5:E:349:GLN:NE2	6:F:71:TYR:O	2.34	0.61
1:A:308:ILE:HD11	1:A:382:SER:HB2	1.83	0.61
6:F:12:VAL:HG22	6:F:58:ALA:HB3	1.83	0.61
2:B:441:SER:HA	2:B:444:ILE:HG22	1.83	0.60
5:E:181:ASN:ND2	5:E:184:ASP:OD1	2.35	0.60
1:A:311:LYS:HZ2	1:A:313:THR:HG1	1.47	0.60
3:C:430:THR:HG21	6:F:225:GLN:HB3	1.83	0.60
6:F:208:ASP:HB2	6:F:249:VAL:HG11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:45:DA:OP1	11:N:582:ASN:ND2	2.35	0.59
1:A:635:GLN:OE1	1:A:639:ARG:NH2	2.36	0.59
4:D:309:VAL:H	4:D:376:MET:HE1	1.67	0.59
6:F:67:SER:O	6:F:139:LYS:NZ	2.33	0.59
11:N:331:LYS:HB3	11:N:340:GLU:HB3	1.83	0.59
1:A:418:LYS:NZ	9:L:42:DC:OP1	2.37	0.58
4:D:152:ALA:HB2	4:D:284:THR:HG21	1.84	0.58
1:A:414:GLY:O	1:A:453:ARG:NH2	2.36	0.58
1:A:284:CYS:HB2	1:A:291:LEU:HD13	1.85	0.58
11:N:393:VAL:HG11	11:N:399:ILE:HD11	1.86	0.58
2:B:39:VAL:HG12	2:B:456:ILE:HB	1.84	0.58
7:G:31:LYS:HG2	7:G:32:LYS:H	1.69	0.58
4:D:265:LEU:HD22	4:D:270:LEU:HD22	1.84	0.57
14:Q:211:VAL:HG12	14:Q:605:VAL:HB	1.85	0.57
1:A:568:LEU:HD11	1:A:606:PHE:HB3	1.86	0.57
3:C:452:MET:SD	3:C:452:MET:N	2.77	0.57
7:G:34:ILE:HD13	7:G:45:VAL:HG23	1.87	0.57
5:E:315:ALA:HB1	5:E:318:LEU:HB2	1.87	0.57
10:M:34:DA:OP1	11:N:214:ASN:ND2	2.37	0.57
2:B:72:TYR:HB3	2:B:206:VAL:HG12	1.85	0.57
7:G:24:ASP:HB2	7:G:34:ILE:HG13	1.86	0.57
15:R:130:TYR:HB2	15:R:138:ALA:HB3	1.87	0.56
2:B:601:ARG:HD3	9:L:57:DG:H21	1.68	0.56
1:A:278:GLU:OE2	1:A:452:ARG:NH2	2.38	0.56
1:A:450:MET:HG3	1:A:453:ARG:HH21	1.71	0.56
2:B:69:LYS:NZ	2:B:202:ALA:O	2.38	0.56
11:N:190:LEU:HD11	11:N:199:ILE:HD13	1.87	0.56
1:A:277:ILE:O	1:A:280:LEU:HG	2.05	0.56
14:Q:216:VAL:HG13	14:Q:379:PRO:HB2	1.88	0.56
1:A:554:ARG:HH21	5:E:77:LYS:HB3	1.71	0.56
9:L:45:DC:H2"	9:L:46:DA:C5	2.41	0.56
5:E:186:ILE:HG12	5:E:211:LEU:HD13	1.87	0.55
1:A:626:ILE:HG22	1:A:662:LEU:HB2	1.88	0.55
1:A:61:TYR:HB2	1:A:65:MET:HE2	1.87	0.55
3:C:431:ILE:O	3:C:435:SER:N	2.39	0.55
4:D:409:TYR:HH	4:D:448:HIS:HD1	1.54	0.55
2:B:70:LEU:HD12	2:B:204:VAL:HG13	1.88	0.55
1:A:525:ILE:HG12	1:A:529:LYS:HB2	1.88	0.55
14:Q:114:LEU:HD23	14:Q:148:ILE:HD13	1.89	0.55
14:Q:637:LYS:HA	14:Q:640:MET:HE2	1.88	0.55
4:D:219:TYR:OH	4:D:264:HIS:ND1	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:187:ILE:HD11	11:N:201:ALA:HB2	1.87	0.55
14:Q:129:THR:O	14:Q:159:GLY:HA2	2.06	0.55
12:O:84:GLU:HG2	12:O:91:VAL:HB	1.89	0.54
2:B:259:CYS:HB2	2:B:396:PRO:HB2	1.89	0.54
12:O:126:VAL:HB	12:O:146:ILE:HD11	1.90	0.54
14:Q:570:LEU:HD11	14:Q:587:PHE:HE1	1.71	0.54
2:B:619:ILE:HA	2:B:678:VAL:HG23	1.89	0.54
2:B:513:ASP:HB3	2:B:516:VAL:HG22	1.89	0.54
5:E:58:MET:SD	5:E:60:HIS:NE2	2.80	0.54
14:Q:177:HIS:NE2	14:Q:636:GLU:OE1	2.41	0.54
3:C:487:GLU:OE1	3:C:487:GLU:N	2.38	0.54
4:D:309:VAL:HG22	4:D:387:ILE:HD13	1.89	0.54
1:A:317:ARG:HH22	1:A:496:LEU:HD22	1.72	0.54
3:C:476:TRP:CH2	3:C:535:LYS:HG2	2.43	0.53
4:D:101:LEU:HB2	4:D:105:LEU:HB2	1.90	0.53
5:E:198:VAL:HB	5:E:219:TYR:HD1	1.71	0.53
1:A:519:TYR:HE2	7:G:19:PHE:HB2	1.73	0.53
2:B:354:PRO:HG3	2:B:415:THR:HA	1.90	0.53
11:N:448:VAL:HG13	11:N:453:LEU:HB3	1.91	0.53
4:D:409:TYR:HB2	4:D:441:MET:SD	2.49	0.53
5:E:285:THR:HG23	5:E:297:LYS:HD2	1.90	0.53
15:R:143:LEU:HB3	15:R:175:VAL:HG23	1.91	0.53
12:O:130:GLY:HA2	12:O:144:PHE:CD2	2.44	0.53
2:B:333:LEU:HD12	2:B:378:ARG:HH12	1.72	0.53
2:B:361:LEU:HB3	2:B:367:ILE:HB	1.91	0.53
1:A:372:GLU:HG2	1:A:391:ARG:HH11	1.74	0.53
11:N:577:LYS:NZ	11:N:579:GLU:OE2	2.41	0.53
1:A:705:THR:OG1	1:A:708:GLU:OE1	2.24	0.53
2:B:649:ASN:ND2	9:L:53:DT:O2	2.42	0.53
3:C:422:LEU:HD12	6:F:224:LEU:HD23	1.89	0.53
11:N:560:GLU:OE2	11:N:564:ASN:ND2	2.41	0.53
6:F:215:LEU:HD22	6:F:230:VAL:HG21	1.90	0.53
16:S:295:ILE:HD11	16:S:349:GLN:HB3	1.89	0.53
14:Q:35:CYS:HB3	14:Q:39:LEU:HB2	1.91	0.52
9:L:39:DC:H2'	9:L:40:DT:C6	2.44	0.52
14:Q:386:GLU:HA	14:Q:389:LYS:HE3	1.91	0.52
2:B:526:GLU:HG3	2:B:714:VAL:HG21	1.91	0.52
14:Q:149:LEU:HD13	14:Q:185:LEU:HA	1.91	0.52
13:P:61:GLU:OE2	13:P:86:GLN:NE2	2.43	0.52
2:B:417:ILE:HD12	2:B:632:ILE:HD13	1.92	0.52
6:F:255:CYS:SG	6:F:276:CYS:N	2.82	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:57:DT:C2	10:M:58:DG:C8	2.97	0.52
2:B:448:PHE:HE1	2:B:454:VAL:HG11	1.75	0.52
8:K:99:GLU:N	8:K:99:GLU:OE1	2.41	0.52
1:A:568:LEU:HD22	1:A:608:SER:HB2	1.91	0.52
14:Q:687:ASP:OD1	14:Q:688:MET:N	2.43	0.52
14:Q:735:SER:HB2	14:Q:741:LEU:HB2	1.92	0.52
1:A:520:ARG:HG2	7:G:18:GLN:HB3	1.92	0.51
4:D:421:LEU:HD11	4:D:451:VAL:HG13	1.92	0.51
1:A:336:GLY:HA3	1:A:488:LEU:HD13	1.91	0.51
1:A:371:VAL:HG21	1:A:393:THR:HG21	1.91	0.51
11:N:348:LEU:HB2	11:N:356:VAL:HG12	1.92	0.51
3:C:512:ILE:HG23	3:C:517:LEU:HB2	1.93	0.51
4:D:179:LEU:HD22	4:D:184:LEU:HD12	1.93	0.51
5:E:110:LYS:NZ	5:E:138:THR:O	2.37	0.51
5:E:149:LEU:HB2	5:E:185:LEU:HD21	1.92	0.51
2:B:320:PRO:HB2	2:B:323:ILE:HG22	1.93	0.51
8:K:108:CYS:HB3	8:K:129:CYS:SG	2.50	0.51
14:Q:303:CYS:HB3	14:Q:342:ARG:HH21	1.76	0.51
2:B:653:THR:HG22	2:B:692:LYS:HD2	1.93	0.51
3:C:481:VAL:HA	3:C:486:LEU:HD12	1.91	0.51
12:O:106:GLN:HB2	12:O:143:ALA:HB3	1.92	0.51
5:E:153:MET:HG3	5:E:157:LYS:HD2	1.91	0.51
2:B:416:ILE:HG12	2:B:435:PHE:HD1	1.76	0.51
2:B:439:ASP:HB3	2:B:442:LEU:HD23	1.92	0.51
2:B:571:THR:O	2:B:577:THR:OG1	2.28	0.51
1:A:77:TRP:HB2	1:A:85:PHE:HB2	1.92	0.50
2:B:361:LEU:O	2:B:366:CYS:N	2.45	0.50
14:Q:640:MET:HB3	16:S:283:SER:HB3	1.93	0.50
1:A:562:ALA:HB3	1:A:568:LEU:HD13	1.94	0.50
2:B:655:ASP:OD1	2:B:658:ARG:NH2	2.44	0.50
14:Q:728:SER:O	14:Q:732:LEU:N	2.35	0.50
16:S:209:LYS:HG2	16:S:213:LYS:HE3	1.93	0.50
2:B:170:LEU:HD22	2:B:201:HIS:HB2	1.93	0.50
7:G:46:ILE:HG22	7:G:49:LEU:HD22	1.93	0.50
16:S:2:GLY:N	16:S:810:ASP:OD1	2.45	0.50
2:B:56:ILE:HG21	2:B:70:LEU:HG	1.94	0.50
4:D:164:VAL:HA	4:D:196:ILE:HD11	1.93	0.50
5:E:204:GLU:HG3	5:E:219:TYR:HE2	1.76	0.50
16:S:27:LEU:HB3	16:S:807:ILE:HG22	1.93	0.50
4:D:232:GLU:HB3	4:D:258:LEU:HD21	1.94	0.50
16:S:266:TYR:O	16:S:270:GLY:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:408:LEU:HG	14:Q:578:VAL:HG12	1.92	0.49
5:E:61:LEU:O	5:E:104:ILE:HA	2.12	0.49
14:Q:302:ASP:OD1	14:Q:303:CYS:N	2.44	0.49
1:A:311:LYS:NZ	1:A:313:THR:OG1	2.32	0.49
2:B:346:VAL:HG22	2:B:348:HIS:H	1.78	0.49
6:F:137:LEU:HB3	6:F:180:VAL:HG11	1.93	0.49
12:O:223:GLU:O	12:O:258:THR:OG1	2.29	0.49
1:A:559:ILE:HD13	1:A:617:LEU:HD12	1.95	0.49
3:C:494:LYS:HD2	3:C:536:LEU:HD23	1.95	0.49
8:K:170:PRO:HB3	15:R:117:ARG:HH22	1.78	0.49
1:A:455:LEU:HD12	1:A:463:LYS:HD3	1.95	0.49
8:K:172:HIS:HB3	8:K:175:TRP:HD1	1.78	0.49
13:P:12:ILE:HB	13:P:16:MET:HB2	1.95	0.49
1:A:419:ARG:HH11	1:A:427:MET:HE3	1.78	0.49
2:B:354:PRO:HB2	2:B:355:PRO:HD3	1.95	0.49
3:C:397:SER:O	3:C:400:ILE:HG22	2.13	0.49
6:F:59:VAL:HG12	6:F:70:LEU:HD12	1.95	0.49
11:N:373:GLN:O	11:N:412:ARG:NH1	2.44	0.48
5:E:201:LEU:HD23	5:E:222:ILE:HG12	1.94	0.48
2:B:569:ILE:HD13	16:S:237:LEU:HD13	1.94	0.48
11:N:190:LEU:HD11	11:N:199:ILE:HG21	1.94	0.48
2:B:637:LEU:HD22	2:B:648:GLU:HA	1.96	0.48
4:D:43:ALA:O	4:D:47:GLU:HG2	2.13	0.48
9:L:38:DA:H2'	9:L:39:DC:C6	2.49	0.48
14:Q:37:ARG:HB2	14:Q:589:ARG:HH11	1.78	0.48
4:D:431:LEU:HA	4:D:443:VAL:HG12	1.95	0.48
10:M:49:DT:H2''	10:M:50:DA:C8	2.49	0.48
14:Q:786:SER:HA	15:R:211:THR:HG21	1.96	0.48
3:C:414:TYR:OH	6:F:39:ASP:OD1	2.27	0.48
1:A:633:ARG:HG2	1:A:676:ARG:HA	1.95	0.48
4:D:132:ASP:OD1	4:D:133:THR:N	2.46	0.47
2:B:589:GLU:OE2	2:B:614:TYR:OH	2.29	0.47
6:F:38:ILE:O	6:F:42:MET:HG3	2.15	0.47
14:Q:763:PRO:HG3	14:Q:804:PRO:HB2	1.95	0.47
16:S:77:ASP:OD1	16:S:790:ALA:N	2.41	0.47
11:N:220:LYS:HB2	11:N:239:ASN:HA	1.95	0.47
14:Q:91:GLU:HG2	14:Q:92:ILE:HG23	1.94	0.47
2:B:725:ALA:HB1	5:E:221:VAL:HG21	1.96	0.47
3:C:434:LEU:HD13	6:F:229:TRP:CD2	2.50	0.47
4:D:288:ILE:HG22	6:F:53:ARG:HH22	1.79	0.47
6:F:177:PHE:O	6:F:181:ILE:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:472:ARG:HB2	11:N:517:SER:HB3	1.97	0.47
16:S:793:GLN:HE21	16:S:797:LEU:HG	1.79	0.47
1:A:641:GLY:HA2	1:A:644:LEU:HB2	1.95	0.47
9:L:32:DG:H2"	9:L:33:DA:H8	1.79	0.47
2:B:195:ALA:O	2:B:199:ILE:HG23	2.15	0.47
2:B:350:VAL:O	2:B:351:GLN:NE2	2.48	0.47
3:C:503:THR:HG23	3:C:504:LYS:HG2	1.97	0.47
14:Q:168:ALA:HA	14:Q:171:PHE:HD2	1.79	0.47
14:Q:709:VAL:HG21	14:Q:825:ALA:HB1	1.97	0.47
4:D:97:HIS:CE1	4:D:109:ILE:HG23	2.50	0.47
13:P:72:ARG:O	13:P:80:LEU:N	2.34	0.47
14:Q:588:VAL:O	14:Q:592:GLU:HG2	2.15	0.47
16:S:930:PRO:O	16:S:934:GLU:HG2	2.14	0.47
1:A:62:ARG:HA	4:D:339:PRO:HG3	1.97	0.47
11:N:212:TRP:NE1	11:N:214:ASN:OD1	2.48	0.47
12:O:226:ASN:OD1	12:O:227:PHE:N	2.47	0.47
14:Q:153:ARG:NE	14:Q:647:GLU:O	2.26	0.47
1:A:84:ILE:HG21	1:A:100:LEU:HD11	1.97	0.46
2:B:209:TYR:OH	2:B:234:ASP:O	2.30	0.46
14:Q:423:TYR:HE1	14:Q:428:ALA:HB2	1.80	0.46
3:C:434:LEU:HD13	6:F:229:TRP:CG	2.50	0.46
1:A:128:SER:OG	1:A:294:GLU:OE2	2.30	0.46
2:B:73:CYS:HB3	2:B:209:TYR:HD1	1.81	0.46
5:E:294:CYS:SG	5:E:307:ILE:HB	2.55	0.46
15:R:137:CYS:SG	15:R:167:ARG:HG2	2.55	0.46
16:S:189:GLU:OE2	16:S:242:TYR:OH	2.28	0.46
16:S:32:SER:HA	16:S:35:LEU:HB2	1.97	0.46
1:A:100:LEU:O	1:A:104:ALA:N	2.47	0.46
1:A:531:ILE:O	1:A:535:THR:OG1	2.33	0.46
10:M:20:DT:H2"	10:M:21:DA:C8	2.51	0.46
11:N:524:GLN:HE21	12:O:168:VAL:HG12	1.80	0.46
12:O:133:ARG:HE	12:O:142:VAL:HG22	1.81	0.46
16:S:788:MET:HE3	16:S:788:MET:HB3	1.86	0.46
8:K:123:LEU:HD12	8:K:124:PRO:HD2	1.98	0.46
14:Q:135:ARG:HG2	14:Q:137:HIS:CE1	2.51	0.46
16:S:276:VAL:HG22	16:S:292:ILE:HG12	1.97	0.46
1:A:353:ALA:HB1	1:A:437:LEU:HD11	1.98	0.46
1:A:511:TRP:HB3	1:A:670:MET:HE1	1.97	0.46
2:B:211:TYR:OH	9:L:62:DG:OP1	2.27	0.46
4:D:400:ARG:HH21	7:G:16:MET:HE2	1.80	0.46
11:N:295:LEU:HD13	11:N:296:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:ASN:OD1	2:B:177:LEU:N	2.44	0.46
14:Q:62:LEU:HD21	14:Q:145:GLU:HB3	1.97	0.46
2:B:29:LYS:NZ	2:B:33:ASP:OD2	2.38	0.45
4:D:185:MET:SD	4:D:185:MET:N	2.89	0.45
16:S:810:ASP:OD2	16:S:812:ASN:ND2	2.49	0.45
1:A:505:VAL:HG21	1:A:640:LEU:HD11	1.98	0.45
7:G:17:LYS:HE2	7:G:43:VAL:HG13	1.99	0.45
1:A:81:ASP:N	1:A:81:ASP:OD1	2.49	0.45
3:C:408:ARG:NH2	6:F:120:THR:O	2.46	0.45
3:C:420:GLN:O	6:F:36:LYS:NZ	2.37	0.45
10:M:52:DT:H2''	10:M:53:DG:H5'	1.98	0.45
11:N:200:CYS:HB3	11:N:256:TYR:CE1	2.51	0.45
11:N:259:LYS:HB3	11:N:283:GLU:HG3	1.99	0.45
1:A:393:THR:OG1	1:A:395:ASP:OD1	2.30	0.45
12:O:95:ASP:OD2	13:P:9:ARG:NH2	2.48	0.45
14:Q:756:VAL:HG23	14:Q:799:ARG:HB2	1.99	0.45
16:S:846:LEU:HA	16:S:850:LYS:HD2	1.98	0.45
2:B:159:GLU:N	2:B:159:GLU:OE1	2.48	0.45
3:C:505:LEU:O	3:C:509:GLN:N	2.45	0.45
4:D:205:LEU:HD23	4:D:363:GLN:HB3	1.99	0.45
4:D:409:TYR:OH	4:D:448:HIS:ND1	2.46	0.45
11:N:241:GLN:O	11:N:245:PHE:HB2	2.16	0.45
12:O:135:PHE:O	12:O:136:GLN:HG3	2.17	0.45
2:B:422:ASP:HB2	2:B:425:THR:OG1	2.17	0.45
3:C:506:CYS:O	3:C:510:GLU:HG2	2.16	0.45
9:L:44:DG:H2''	9:L:45:DC:C5	2.51	0.45
14:Q:687:ASP:OD2	14:Q:689:ARG:NH2	2.50	0.45
1:A:378:PHE:O	1:A:382:SER:OG	2.28	0.45
1:A:385:ASP:OD2	1:A:387:SER:OG	2.35	0.45
2:B:335:ARG:HH11	16:S:149:LEU:HG	1.81	0.44
3:C:476:TRP:HH2	3:C:535:LYS:HG2	1.82	0.44
4:D:255:SER:H	4:D:258:LEU:HD12	1.81	0.44
14:Q:226:GLN:HE22	14:Q:613:SER:HA	1.82	0.44
14:Q:720:PRO:HG3	14:Q:823:PRO:HA	2.00	0.44
16:S:959:ARG:NH2	16:S:974:ASP:OD2	2.48	0.44
1:A:412:MET:HA	1:A:415:HIS:CE1	2.53	0.44
2:B:124:LEU:HD12	2:B:124:LEU:H	1.82	0.44
5:E:292:PRO:HG2	6:F:264:ILE:HD11	2.00	0.44
8:K:158:ARG:O	8:K:189:ARG:NH2	2.50	0.44
14:Q:760:GLU:HG2	14:Q:803:CYS:SG	2.57	0.44
4:D:202:GLN:HB3	4:D:363:GLN:HE22	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:15:LEU:HD12	14:Q:19:GLU:HB3	1.99	0.44
14:Q:381:TRP:HB3	14:Q:423:TYR:CZ	2.52	0.44
16:S:290:ILE:HG13	16:S:347:ALA:HA	1.99	0.44
1:A:412:MET:HE2	1:A:412:MET:HB2	1.75	0.44
2:B:166:ARG:HG3	2:B:167:GLU:HG2	1.98	0.44
3:C:521:LEU:O	3:C:525:ILE:HG13	2.18	0.44
15:R:106:ARG:HH11	15:R:156:ARG:HH21	1.65	0.44
16:S:251:GLN:HA	16:S:254:MET:HG2	1.98	0.44
4:D:48:LEU:O	4:D:53:LYS:HE3	2.17	0.44
12:O:125:TYR:HB3	12:O:149:LEU:HD12	1.99	0.44
1:A:703:PHE:CE2	1:A:712:LEU:HD12	2.52	0.44
2:B:724:MET:HE2	2:B:724:MET:HB2	1.76	0.44
14:Q:806:PRO:HA	14:Q:809:THR:HG22	1.99	0.44
1:A:88:ALA:HA	1:A:93:TYR:CD1	2.53	0.44
1:A:311:LYS:NZ	1:A:313:THR:HG1	2.12	0.44
2:B:535:ILE:HB	2:B:595:ILE:HG12	1.99	0.44
4:D:65:PRO:HB2	4:D:101:LEU:HD21	2.00	0.44
4:D:140:LYS:HG3	4:D:141:HIS:ND1	2.32	0.44
5:E:291:CYS:SG	5:E:294:CYS:N	2.83	0.44
16:S:182:ASN:HD22	16:S:185:ALA:HB2	1.83	0.44
1:A:307:ASN:HD22	1:A:307:ASN:H	1.65	0.44
2:B:654:PHE:HA	2:B:692:LYS:HD3	1.99	0.44
6:F:131:THR:O	6:F:173:GLN:NE2	2.51	0.44
10:M:58:DG:H2"	10:M:59:DG:H8	1.83	0.44
12:O:57:ALA:HB3	12:O:139:LYS:HE2	2.00	0.44
12:O:260:ASP:OD1	12:O:263:HIS:ND1	2.51	0.44
16:S:30:ASP:OD1	16:S:30:ASP:N	2.45	0.44
1:A:60:ASP:HB3	4:D:337:ARG:HB3	1.99	0.43
3:C:422:LEU:HD13	6:F:225:GLN:HG2	2.00	0.43
5:E:349:GLN:HE21	6:F:69:PHE:HB3	1.83	0.43
13:P:41:PHE:HZ	13:P:69:VAL:HG21	1.83	0.43
1:A:416:THR:HG22	1:A:453:ARG:HH12	1.83	0.43
2:B:674:TYR:CD1	2:B:724:MET:HE3	2.52	0.43
6:F:48:HIS:HA	6:F:51:MET:HG2	2.00	0.43
7:G:17:LYS:HZ3	7:G:21:LEU:HD11	1.82	0.43
3:C:511:LYS:HA	3:C:514:ARG:HD2	2.01	0.43
6:F:61:ALA:HB2	6:F:70:LEU:HD11	1.99	0.43
4:D:405:GLU:HG2	7:G:8:VAL:HG22	2.00	0.43
14:Q:30:ASP:N	14:Q:30:ASP:OD1	2.51	0.43
14:Q:801:LEU:HD22	15:R:186:ALA:HB1	1.99	0.43
1:A:504:LYS:HE3	1:A:654:GLU:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:454:PRO:HD2	3:C:457:ILE:HD12	2.00	0.43
5:E:106:ILE:HD13	5:E:131:LEU:HD21	2.01	0.43
16:S:789:GLU:HG3	16:S:791:GLU:H	1.82	0.43
5:E:153:MET:HE2	5:E:189:LEU:HD23	2.01	0.43
14:Q:754:ARG:NH2	15:R:190:ILE:O	2.51	0.43
15:R:171:VAL:HG11	15:R:185:LEU:HD13	2.01	0.43
1:A:516:PRO:HA	7:G:18:GLN:HG3	2.01	0.43
14:Q:113:ILE:HA	14:Q:116:VAL:HG12	2.01	0.43
16:S:837:TYR:HA	16:S:840:PHE:CE2	2.53	0.43
5:E:360:CYS:SG	5:E:361:ALA:N	2.92	0.43
5:E:373:VAL:O	5:E:377:ASP:HB2	2.19	0.43
1:A:149:PRO:HG2	1:A:152:ILE:HG22	1.99	0.43
8:K:25:ARG:O	8:K:28:ILE:HG22	2.19	0.43
12:O:79:ILE:HB	12:O:125:TYR:CE1	2.54	0.43
14:Q:136:ALA:HB1	14:Q:185:LEU:HD11	2.01	0.43
14:Q:726:ARG:HG3	14:Q:758:LEU:HD21	2.00	0.43
2:B:134:CYS:O	2:B:138:THR:OG1	2.33	0.43
3:C:476:TRP:CZ2	5:E:293:GLN:HB3	2.54	0.43
4:D:373:HIS:CG	4:D:374:PRO:HD2	2.54	0.43
8:K:209:GLU:O	8:K:213:LYS:HG2	2.19	0.43
14:Q:136:ALA:HB2	14:Q:163:ALA:HB1	2.01	0.43
14:Q:562:ASP:OD1	14:Q:565:ALA:N	2.52	0.43
12:O:147:MET:HE3	12:O:147:MET:HB2	1.98	0.42
15:R:187:LYS:HA	15:R:190:ILE:HG22	2.01	0.42
1:A:65:MET:HE3	4:D:339:PRO:HD3	2.01	0.42
1:A:522:TYR:HA	1:A:533:LEU:HG	2.02	0.42
1:A:640:LEU:HD22	1:A:680:LEU:HD13	2.01	0.42
4:D:212:LEU:HB3	4:D:290:LEU:HD13	2.01	0.42
4:D:406:GLY:HA2	4:D:445:PRO:HD3	2.01	0.42
6:F:44:LEU:HD22	6:F:227:LEU:HB3	2.00	0.42
2:B:358:LEU:HD13	2:B:369:ARG:HG2	2.02	0.42
4:D:76:LYS:HB2	4:D:79:PHE:HD2	1.84	0.42
6:F:26:ALA:O	6:F:29:GLU:HG3	2.18	0.42
8:K:70:ASP:H	8:K:78:GLU:HG2	1.84	0.42
9:L:35:DG:H2'	9:L:36:DC:C6	2.53	0.42
2:B:653:THR:HG23	2:B:689:LYS:HG2	2.02	0.42
5:E:293:GLN:HB2	5:E:308:CYS:SG	2.59	0.42
8:K:172:HIS:HB3	8:K:175:TRP:CD1	2.54	0.42
10:M:51:DC:H2''	10:M:52:DT:C6	2.54	0.42
11:N:347:TYR:HB3	11:N:355:VAL:HG13	2.01	0.42
14:Q:135:ARG:HG2	14:Q:137:HIS:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:523:LEU:HD13	2:B:710:VAL:HG13	2.01	0.42
3:C:466:VAL:O	3:C:470:GLU:HG2	2.20	0.42
4:D:338:PHE:HB2	4:D:341:MET:HB3	2.02	0.42
14:Q:153:ARG:HA	14:Q:153:ARG:HD3	1.79	0.42
4:D:34:LEU:HD12	4:D:40:THR:HG21	2.00	0.42
8:K:164:PHE:CD1	8:K:179:LYS:HD2	2.55	0.42
1:A:712:LEU:HA	1:A:715:LYS:HG2	2.02	0.42
2:B:70:LEU:HB3	2:B:204:VAL:HG22	2.01	0.42
2:B:486:ALA:HB2	2:B:733:GLN:HA	2.01	0.42
6:F:244:PRO:HA	6:F:245:PRO:HD3	1.90	0.42
11:N:287:MET:HE2	11:N:287:MET:HB2	1.98	0.42
12:O:54:LEU:HD22	12:O:132:LEU:HD22	2.02	0.42
12:O:237:MET:HE3	12:O:237:MET:HB2	1.95	0.42
2:B:351:GLN:O	2:B:417:ILE:HA	2.20	0.42
6:F:33:THR:HG23	6:F:35:SER:H	1.85	0.42
16:S:263:ARG:HG2	16:S:273:LEU:HD22	2.01	0.42
1:A:125:ALA:O	1:A:129:VAL:HG23	2.20	0.41
1:A:585:SER:HB2	1:A:588:GLU:HB3	2.02	0.41
1:A:664:SER:O	1:A:667:THR:OG1	2.38	0.41
4:D:19:LEU:HB2	4:D:213:TRP:CZ2	2.52	0.41
5:E:80:ARG:HD2	5:E:201:LEU:HD13	2.01	0.41
9:L:73:DT:H2''	9:L:74:DA:C8	2.55	0.41
16:S:871:CYS:O	16:S:875:MET:HG2	2.19	0.41
1:A:576:ASN:O	1:A:576:ASN:ND2	2.53	0.41
2:B:180:LEU:HD22	2:B:194:LEU:HD11	2.02	0.41
3:C:527:GLU:OE2	5:E:295:ARG:HB3	2.20	0.41
4:D:207:ASP:OD1	4:D:207:ASP:N	2.52	0.41
13:P:12:ILE:HG22	13:P:107:HIS:CE1	2.55	0.41
13:P:90:ASP:OD1	13:P:90:ASP:N	2.52	0.41
2:B:613:HIS:ND1	2:B:613:HIS:O	2.54	0.41
3:C:431:ILE:HD11	4:D:62:LEU:HD11	2.01	0.41
3:C:465:TYR:CE1	3:C:525:ILE:HG12	2.55	0.41
6:F:123:ASP:HB2	6:F:125:LYS:HE3	2.01	0.41
6:F:48:HIS:O	6:F:55:ASN:ND2	2.50	0.41
9:L:29:DA:H2''	9:L:30:DA:C8	2.55	0.41
10:M:52:DT:H2''	10:M:53:DG:H8	1.85	0.41
11:N:227:VAL:HG11	11:N:298:VAL:HA	2.02	0.41
1:A:469:THR:HG21	1:A:638:GLN:HG3	2.03	0.41
1:A:710:GLN:HE22	1:A:714:GLN:HE21	1.67	0.41
2:B:424:ARG:HA	2:B:424:ARG:HD2	1.66	0.41
3:C:422:LEU:CD1	6:F:225:GLN:HG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:69:PHE:CE1	6:F:139:LYS:HB3	2.56	0.41
9:L:45:DC:H2''	9:L:46:DA:N7	2.36	0.41
13:P:11:ARG:NH1	13:P:99:TYR:OH	2.54	0.41
15:R:110:ASN:ND2	15:R:130:TYR:HH	2.18	0.41
4:D:171:VAL:HG21	4:D:175:LEU:HD11	2.02	0.41
4:D:266:ARG:HG3	4:D:273:GLN:HG3	2.02	0.41
14:Q:222:MET:HE2	14:Q:342:ARG:NH2	2.36	0.41
16:S:849:ASN:HB3	16:S:885:GLY:HA2	2.03	0.41
4:D:19:LEU:HD23	4:D:47:GLU:HG3	2.02	0.41
4:D:58:ARG:NH2	6:F:241:LEU:HD13	2.36	0.41
10:M:58:DG:C2	10:M:59:DG:C5	3.09	0.41
11:N:222:PHE:HD1	11:N:242:VAL:HG22	1.84	0.41
14:Q:688:MET:HA	14:Q:691:PHE:HD2	1.86	0.41
1:A:457:ILE:HG23	1:A:458:VAL:HG13	2.02	0.41
2:B:270:VAL:O	2:B:274:LYS:HG2	2.21	0.41
3:C:505:LEU:HD11	3:C:522:VAL:HG12	2.02	0.41
4:D:96:TRP:HB3	4:D:110:LEU:HD23	2.01	0.41
6:F:6:ASP:HB3	6:F:155:GLN:HG2	2.03	0.41
6:F:169:ASP:OD1	6:F:169:ASP:N	2.54	0.41
7:G:46:ILE:HD12	7:G:46:ILE:HA	1.94	0.41
11:N:350:ASP:HA	11:N:411:LEU:HD21	2.02	0.41
13:P:53:ILE:HG12	13:P:79:ILE:HB	2.03	0.41
14:Q:307:LEU:HD13	14:Q:339:ALA:HB1	2.02	0.41
14:Q:729:ILE:O	14:Q:733:ILE:HG12	2.20	0.41
16:S:774:GLU:O	16:S:778:LEU:HG	2.21	0.41
1:A:620:ALA:O	1:A:647:LYS:NZ	2.54	0.41
2:B:22:PHE:HE2	2:B:26:ARG:HH21	1.69	0.41
9:L:66:DC:H2''	9:L:67:DT:C5	2.56	0.41
14:Q:646:ARG:HG2	14:Q:647:GLU:H	1.85	0.41
15:R:177:ASP:OD1	15:R:177:ASP:N	2.52	0.41
1:A:513:PRO:HG2	1:A:539:ASN:HD22	1.86	0.40
1:A:636:GLU:OE1	1:A:676:ARG:NE	2.54	0.40
16:S:253:GLU:O	16:S:257:GLN:HG3	2.22	0.40
5:E:290:PHE:CE2	5:E:297:LYS:HE2	2.56	0.40
8:K:207:ARG:NH1	9:L:43:DA:OP1	2.54	0.40
2:B:694:PRO:HB2	2:B:696:TRP:CD1	2.56	0.40
11:N:308:LEU:HD21	11:N:319:ILE:HD11	2.03	0.40
11:N:604:ARG:O	11:N:608:MET:HG2	2.21	0.40
14:Q:335:MET:HE3	14:Q:335:MET:HB3	1.98	0.40
1:A:284:CYS:SG	1:A:285:ILE:N	2.94	0.40
2:B:273:ILE:O	2:B:276:THR:OG1	2.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:352:GLN:HA	4:D:355:ILE:HG22	2.02	0.40
8:K:213:LYS:HA	8:K:213:LYS:HD2	1.93	0.40
14:Q:254:LEU:O	14:Q:258:ILE:HG13	2.22	0.40
1:A:294:GLU:HG2	1:A:334:ARG:HB3	2.03	0.40
1:A:538:PRO:O	1:A:542:ARG:HG3	2.22	0.40
11:N:472:ARG:HE	11:N:528:TRP:HZ3	1.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	609/782 (78%)	574 (94%)	35 (6%)	0	100	100
2	B	708/768 (92%)	686 (97%)	22 (3%)	0	100	100
3	C	134/548 (24%)	131 (98%)	3 (2%)	0	100	100
4	D	430/462 (93%)	425 (99%)	5 (1%)	0	100	100
5	E	337/395 (85%)	325 (96%)	12 (4%)	0	100	100
6	F	250/308 (81%)	245 (98%)	5 (2%)	0	100	100
7	G	63/71 (89%)	57 (90%)	6 (10%)	0	100	100
8	K	201/273 (74%)	194 (96%)	7 (4%)	0	100	100
11	N	423/616 (69%)	412 (97%)	11 (3%)	0	100	100
12	O	193/270 (72%)	189 (98%)	4 (2%)	0	100	100
13	P	119/121 (98%)	117 (98%)	2 (2%)	0	100	100
14	Q	616/916 (67%)	601 (98%)	15 (2%)	0	100	100
15	R	121/295 (41%)	116 (96%)	5 (4%)	0	100	100
16	S	456/1186 (38%)	443 (97%)	13 (3%)	0	100	100
All	All	4660/7011 (66%)	4515 (97%)	145 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	542/688 (79%)	531 (98%)	11 (2%)	48	65
2	B	623/672 (93%)	603 (97%)	20 (3%)	34	58
3	C	131/484 (27%)	125 (95%)	6 (5%)	24	50
4	D	377/399 (94%)	374 (99%)	3 (1%)	73	77
5	E	307/352 (87%)	298 (97%)	9 (3%)	37	60
6	F	227/272 (84%)	225 (99%)	2 (1%)	70	76
7	G	58/64 (91%)	57 (98%)	1 (2%)	53	67
8	K	188/233 (81%)	188 (100%)	0	100	100
11	N	379/530 (72%)	373 (98%)	6 (2%)	55	68
12	O	178/228 (78%)	176 (99%)	2 (1%)	65	74
13	P	106/106 (100%)	104 (98%)	2 (2%)	50	66
14	Q	535/816 (66%)	529 (99%)	6 (1%)	65	74
15	R	107/252 (42%)	104 (97%)	3 (3%)	38	60
16	S	418/1050 (40%)	415 (99%)	3 (1%)	76	78
All	All	4176/6146 (68%)	4102 (98%)	74 (2%)	51	67

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LEU
1	A	83	HIS
1	A	100	LEU
1	A	163	TYR
1	A	189	LEU
1	A	276	MET
1	A	316	LEU
1	A	433	GLN

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Mol	Chain	Res	Type
1	A	437	LEU
1	A	480	LEU
1	A	604	THR
2	B	5	VAL
2	B	17	ILE
2	B	50	VAL
2	B	77	VAL
2	B	116	CYS
2	B	138	THR
2	B	168	VAL
2	B	205	VAL
2	B	266	LEU
2	B	336	LEU
2	B	458	SER
2	B	462	SER
2	B	531	VAL
2	B	545	MET
2	B	571	THR
2	B	581	LEU
2	B	611	VAL
2	B	613	HIS
2	B	654	PHE
2	B	724	MET
3	C	404	PHE
3	C	407	ILE
3	C	453	VAL
3	C	501	GLN
3	C	521	LEU
3	C	528	MET
4	D	271	VAL
4	D	284	THR
4	D	380	THR
5	E	19	TRP
5	E	101	ILE
5	E	135	VAL
5	E	223	LEU
5	E	284	LEU
5	E	285	THR
5	E	294	CYS
5	E	356	HIS
5	E	366	VAL
6	F	116	LYS

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Mol	Chain	Res	Type
6	F	151	VAL
7	G	43	VAL
11	N	298	VAL
11	N	349	MET
11	N	465	VAL
11	N	515	ILE
11	N	516	LEU
11	N	594	VAL
12	O	46	ILE
12	O	118	THR
13	P	74	THR
13	P	96	LEU
14	Q	91	GLU
14	Q	110	THR
14	Q	175	PHE
14	Q	579	VAL
14	Q	641	VAL
14	Q	758	LEU
15	R	127	ILE
15	R	168	VAL
15	R	173	VAL
16	S	83	LEU
16	S	255	ASN
16	S	941	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	307	ASN
1	A	499	ASN
1	A	576	ASN
1	A	594	GLN
1	A	714	GLN
2	B	21	GLN
2	B	201	HIS
2	B	203	ASN
2	B	402	ASN
2	B	562	GLN
2	B	649	ASN
2	B	662	GLN
4	D	20	GLN
4	D	415	GLN

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Mol	Chain	Res	Type
5	E	147	ASN
5	E	376	HIS
6	F	48	HIS
6	F	52	ASN
6	F	65	GLN
6	F	173	GLN
6	F	185	GLN
6	F	225	GLN
6	F	260	ASN
7	G	54	GLN
8	K	120	HIS
8	K	197	GLN
11	N	241	GLN
11	N	420	GLN
11	N	524	GLN
12	O	68	ASN
12	O	89	ASN
12	O	209	GLN
12	O	211	GLN
12	O	244	GLN
14	Q	83	HIS
14	Q	137	HIS
14	Q	215	HIS
14	Q	226	GLN
14	Q	286	GLN
14	Q	296	GLN
14	Q	419	GLN
14	Q	555	HIS
14	Q	571	HIS
15	R	146	HIS
15	R	149	HIS
16	S	37	GLN
16	S	176	GLN
16	S	182	ASN
16	S	202	HIS
16	S	231	GLN
16	S	251	GLN
16	S	349	GLN
16	S	793	GLN
16	S	802	GLN
16	S	812	ASN
16	S	842	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	S	843	GLN
16	S	897	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
17	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
17	SF4	B	1000	2	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

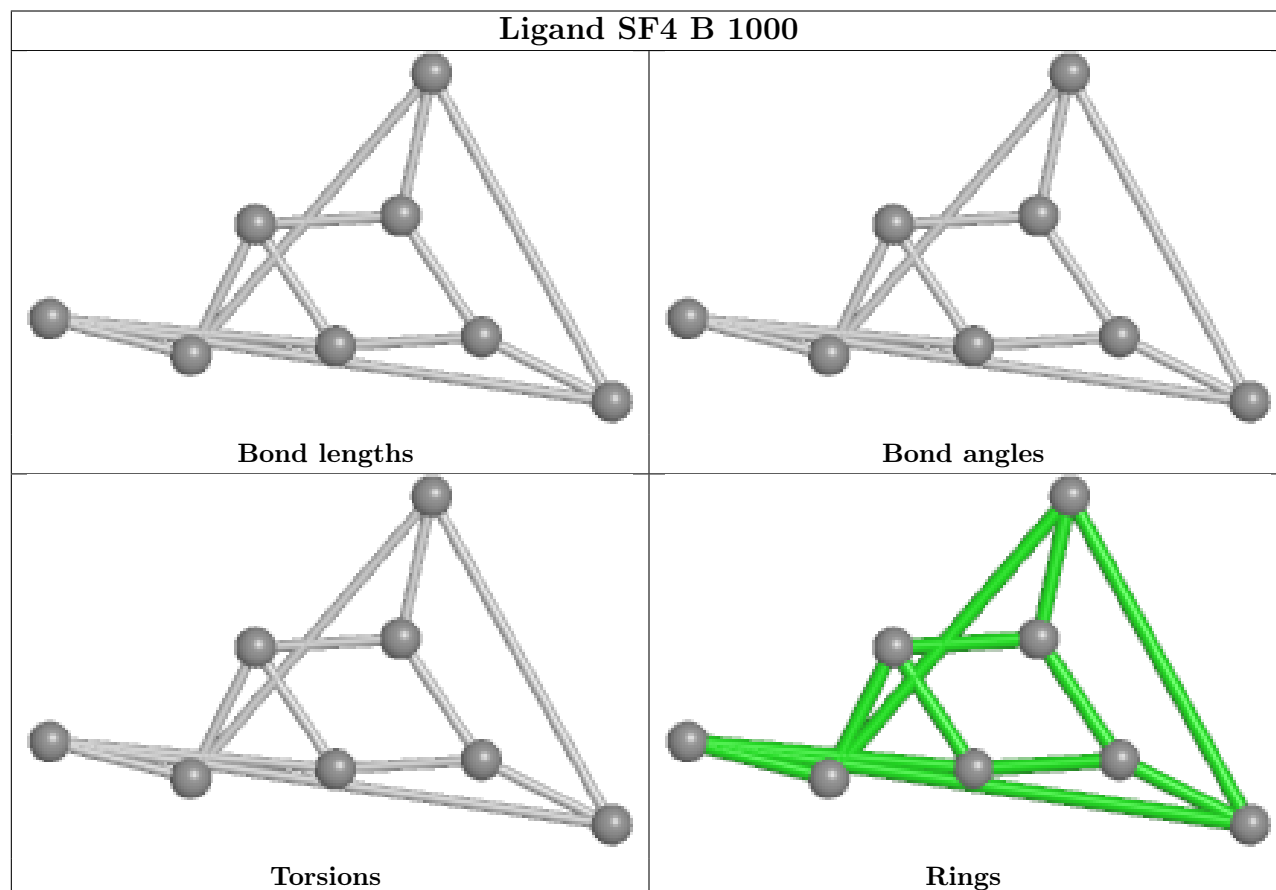
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

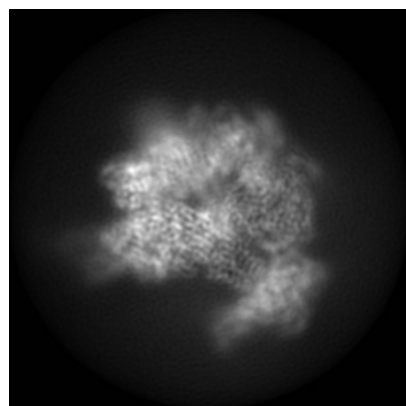
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71525. These allow visual inspection of the internal detail of the map and identification of artifacts.

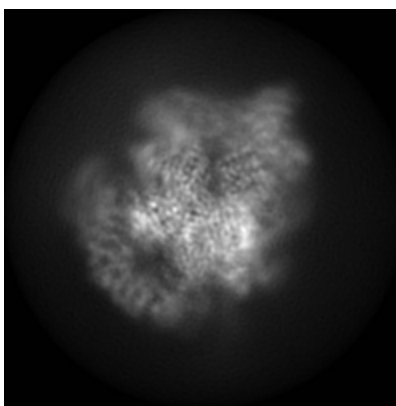
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

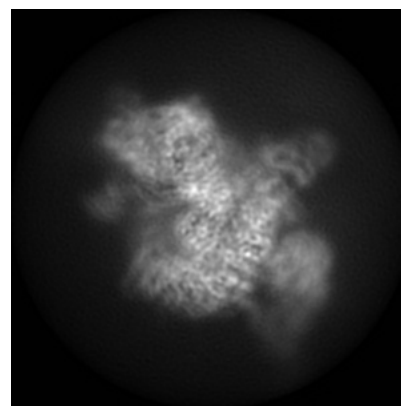
6.1.1 Primary map



X

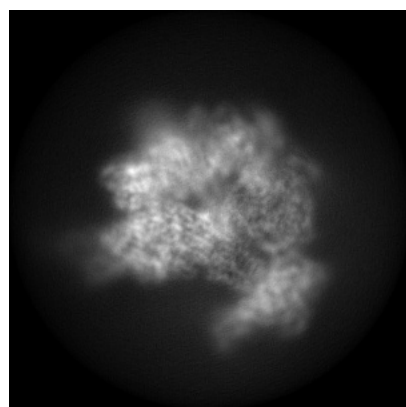


Y

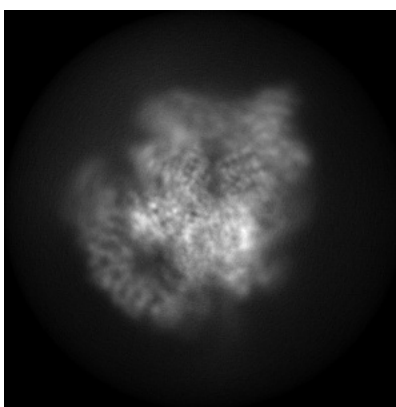


Z

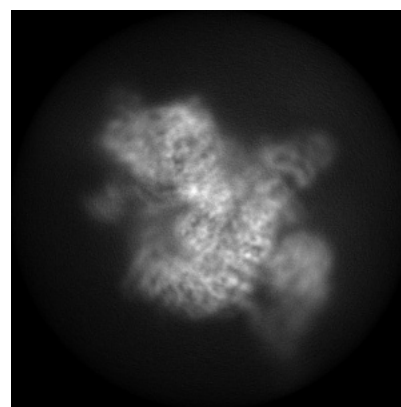
6.1.2 Raw map



X



Y

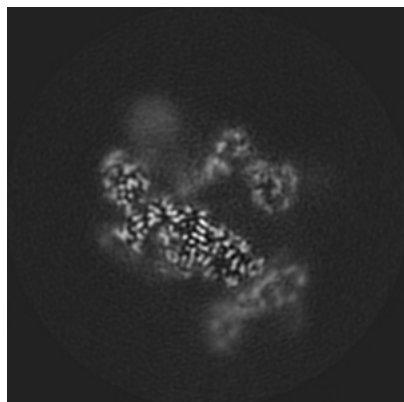


Z

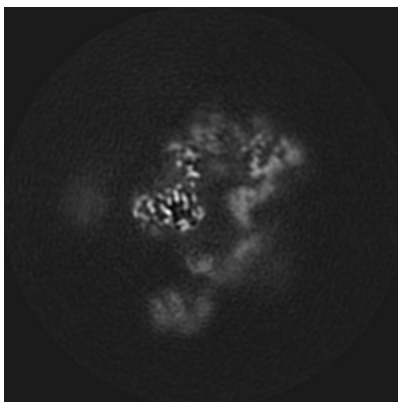
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

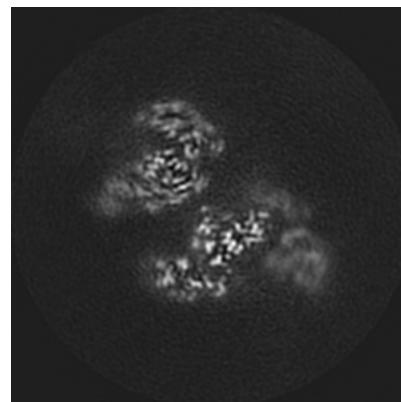
6.2.1 Primary map



X Index: 160

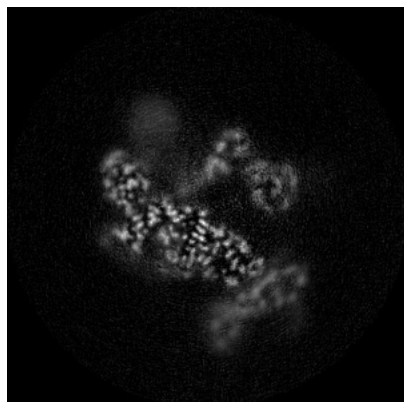


Y Index: 160

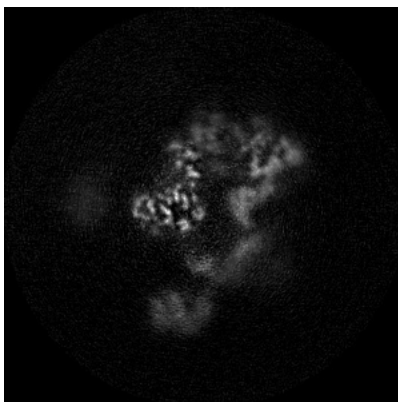


Z Index: 160

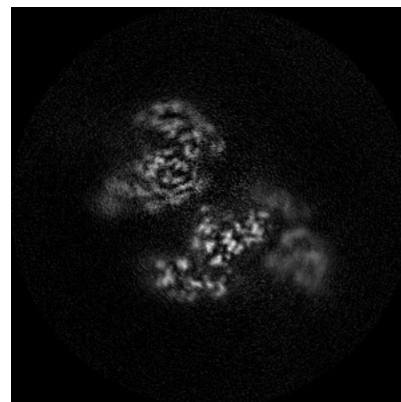
6.2.2 Raw map



X Index: 160



Y Index: 160

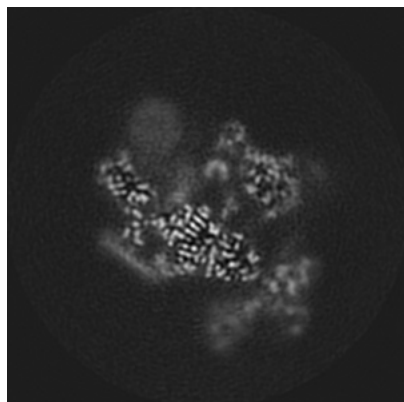


Z Index: 160

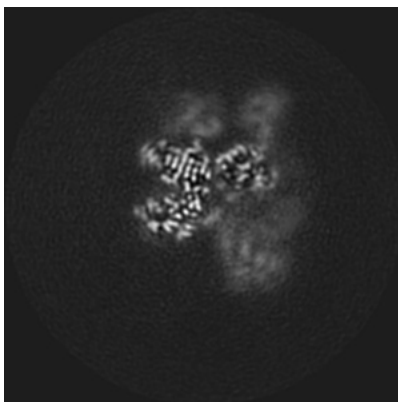
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

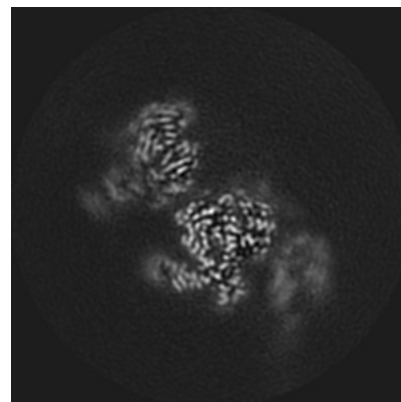
6.3.1 Primary map



X Index: 153

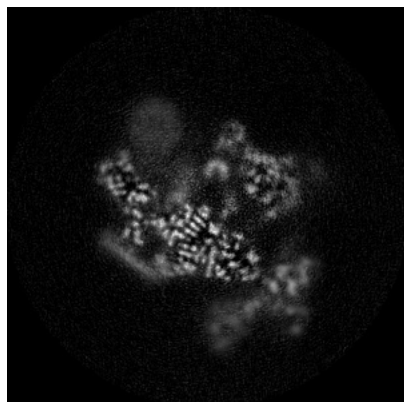


Y Index: 134

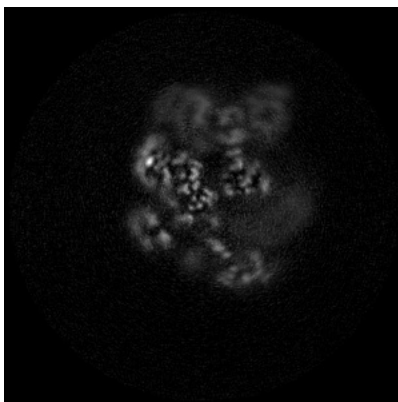


Z Index: 147

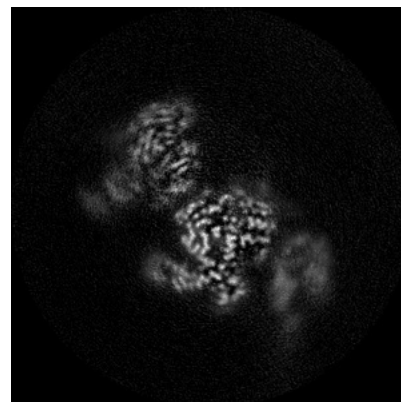
6.3.2 Raw map



X Index: 153



Y Index: 120

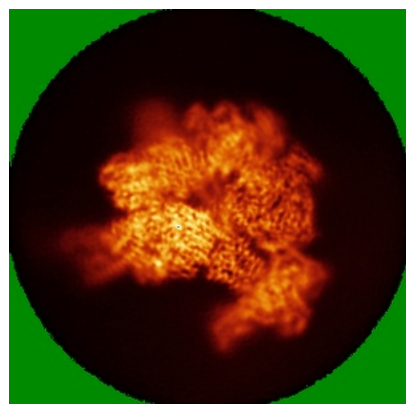


Z Index: 146

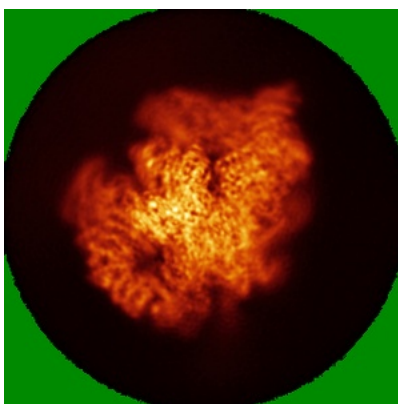
The images above show the largest variance slices of the map in three orthogonal directions.

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

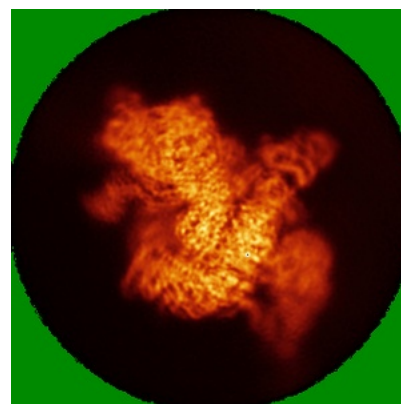
6.4.1 Primary map



X

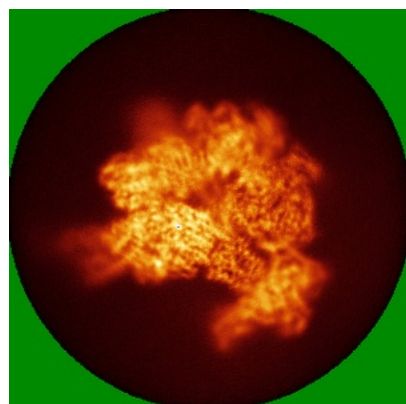


Y

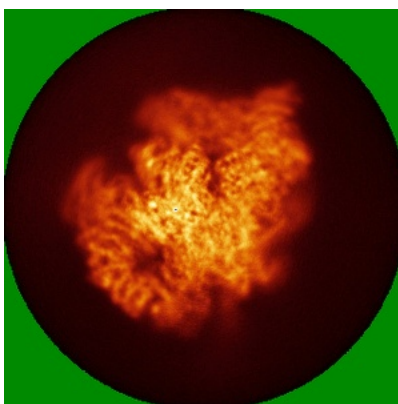


Z

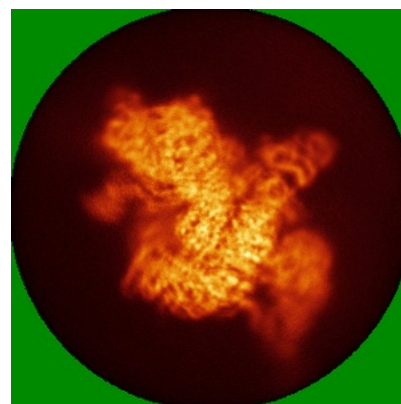
6.4.2 Raw map



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.

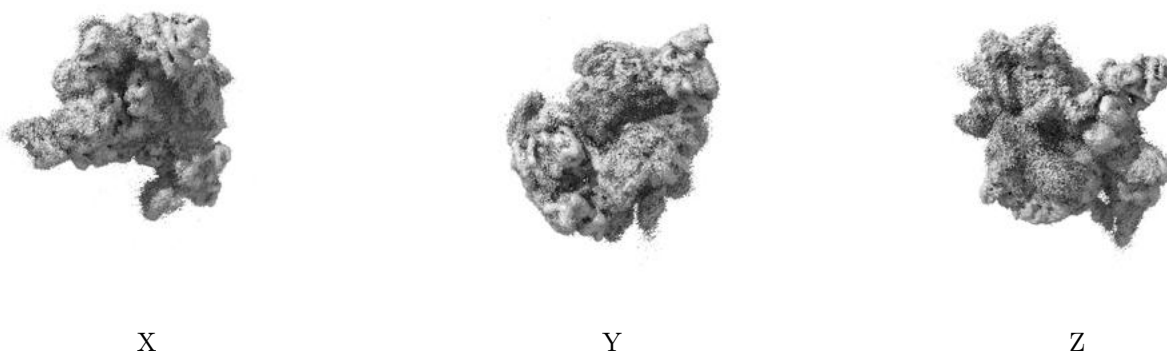
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. 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.

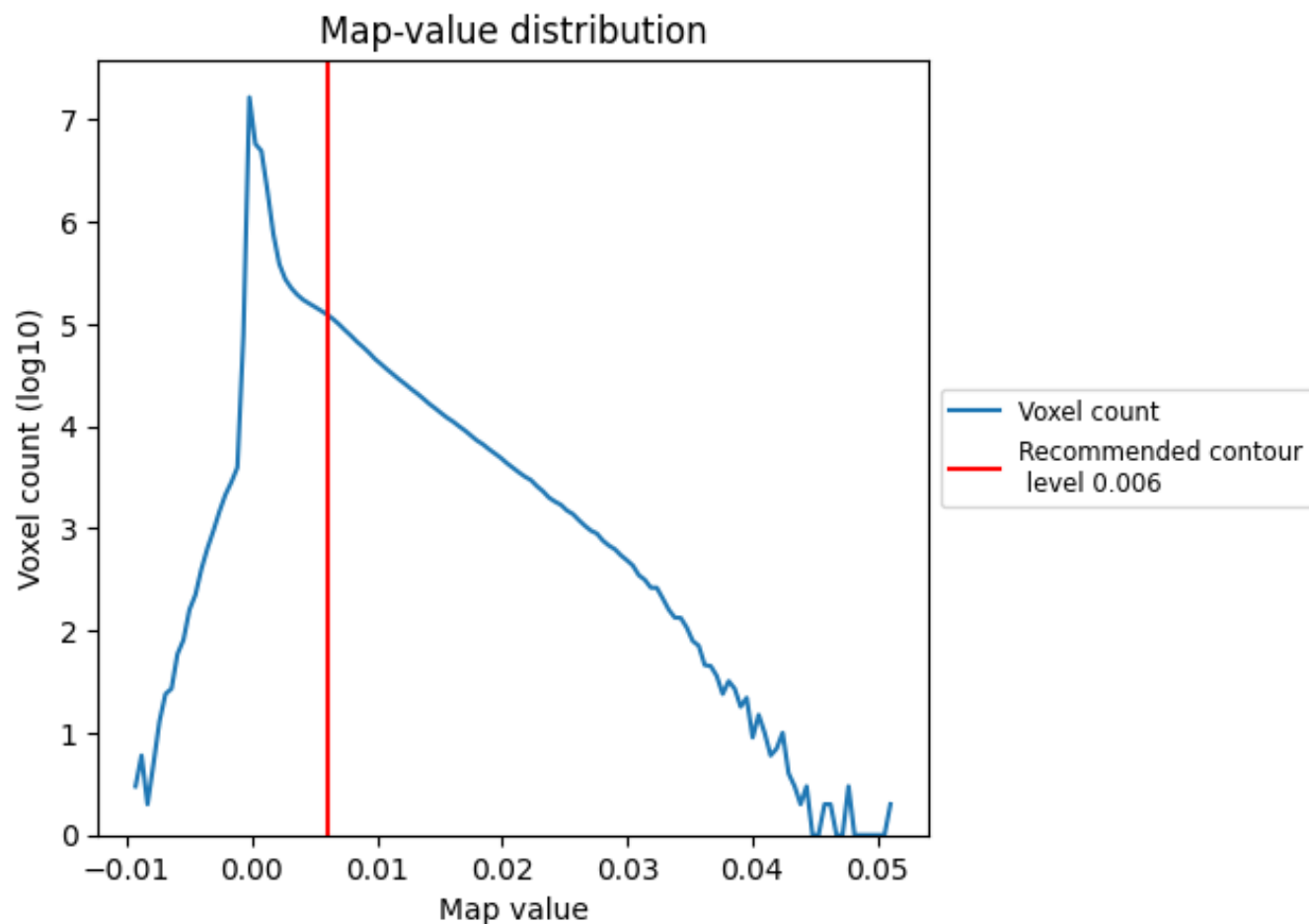
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

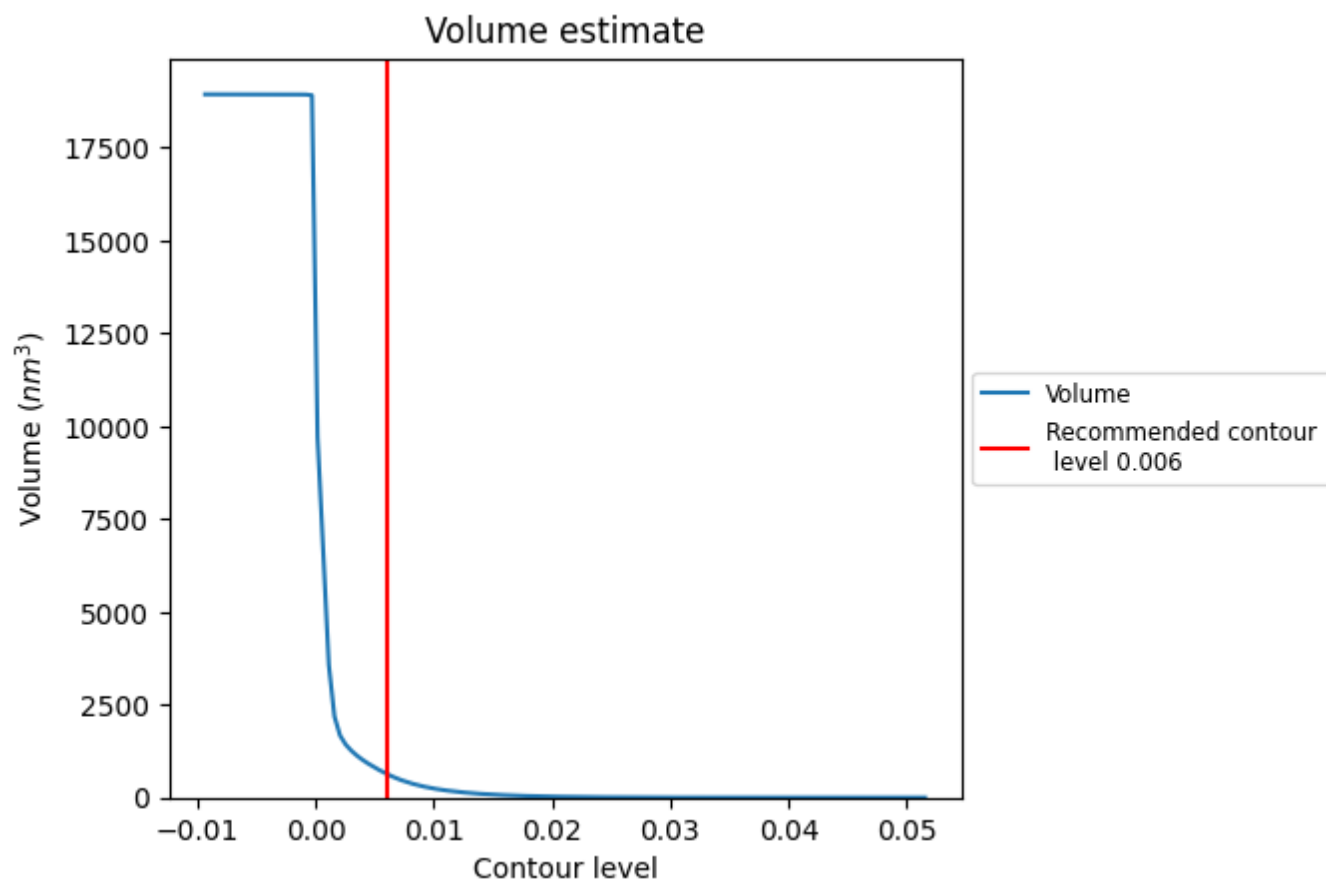
This section contains the results of statistical analysis of the map.

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.

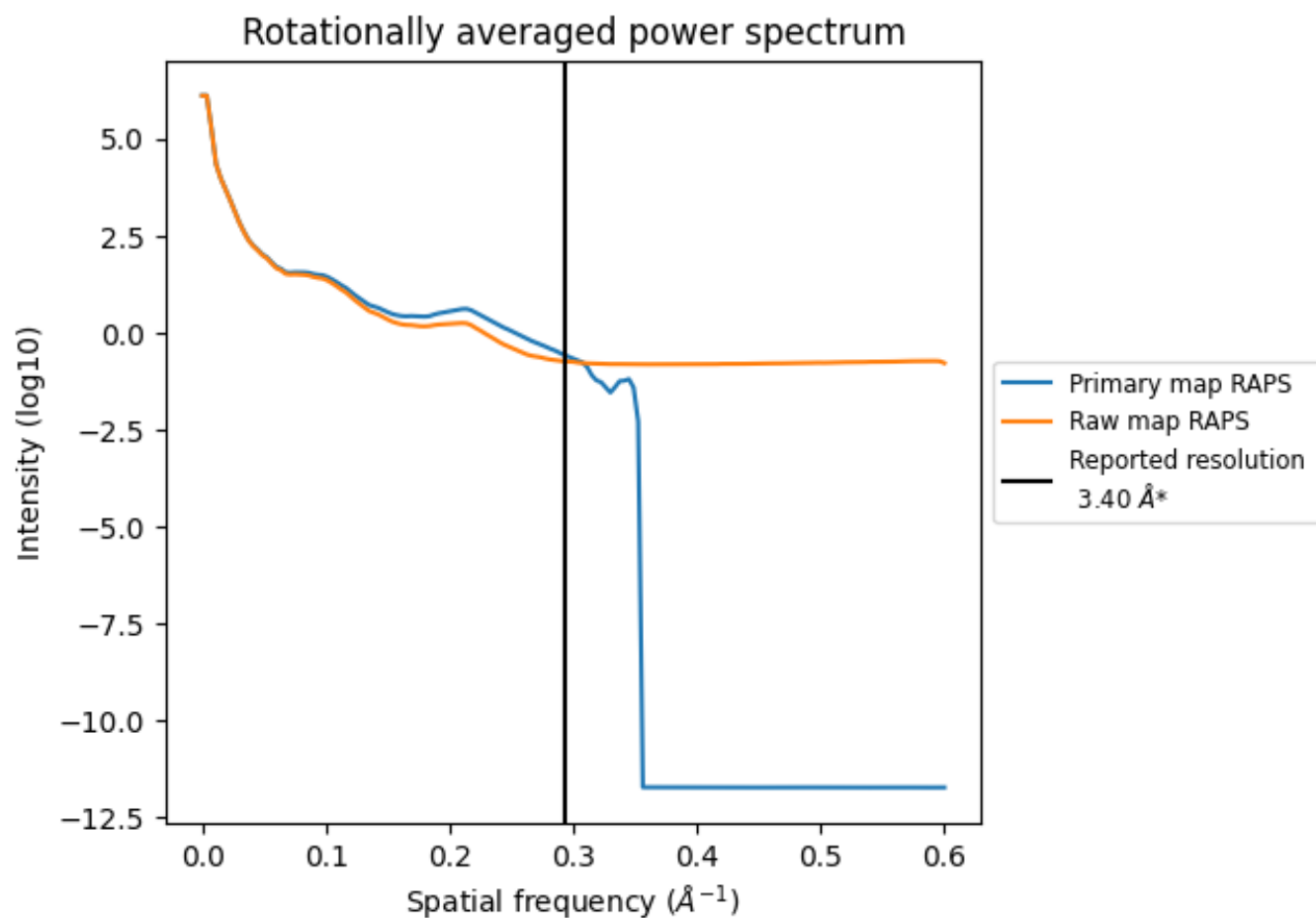
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 642 nm³; this corresponds to an approximate mass of 580 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 ⓘ

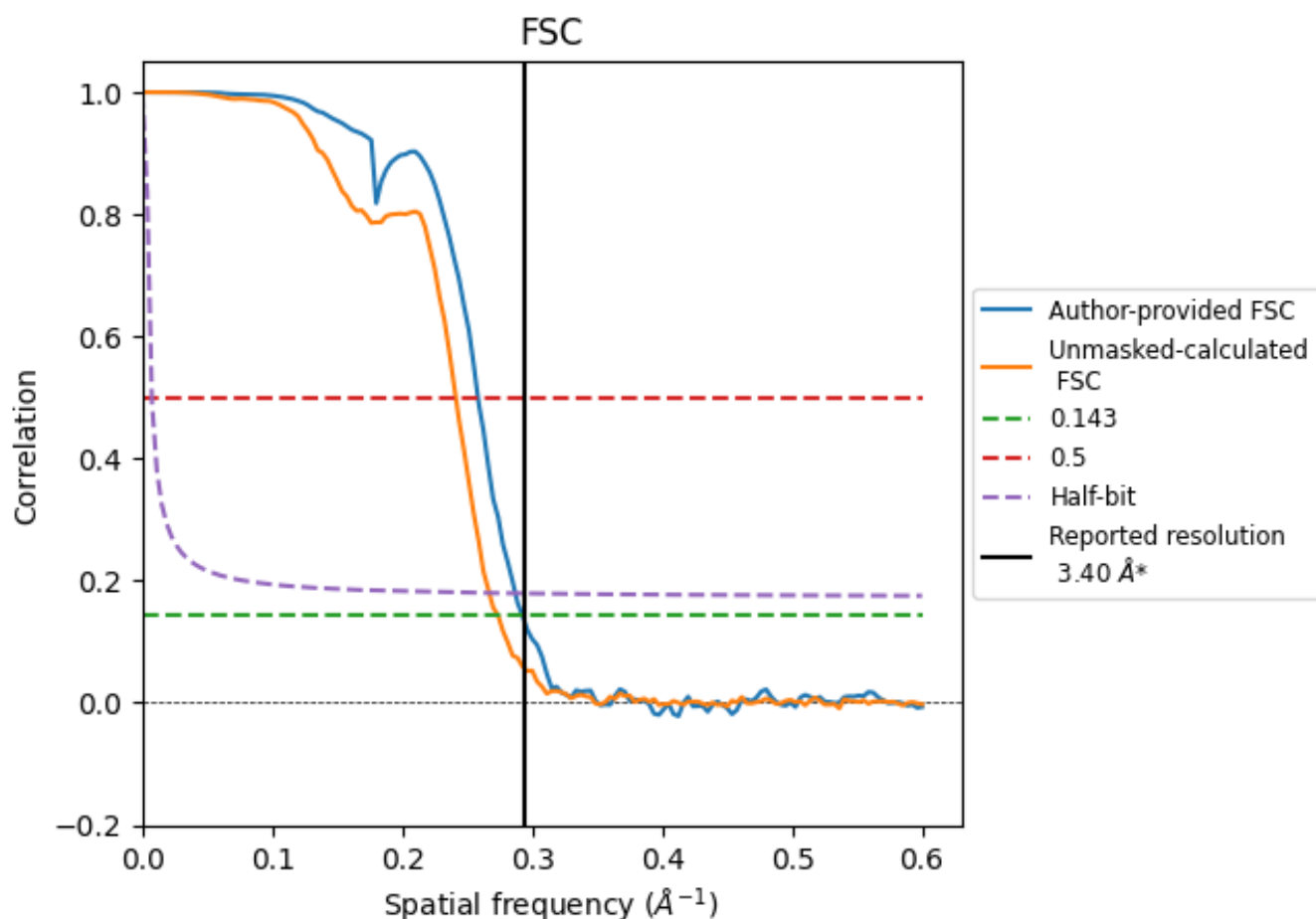


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

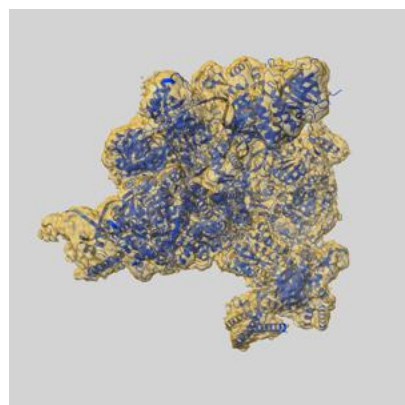
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.42	3.87	3.48
Unmasked-calculated*	3.65	4.14	3.75

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

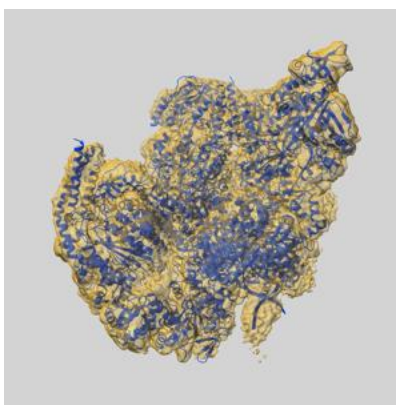
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71525 and PDB model 9PD4. Per-residue inclusion information can be found in section [3](#) on page [8](#).

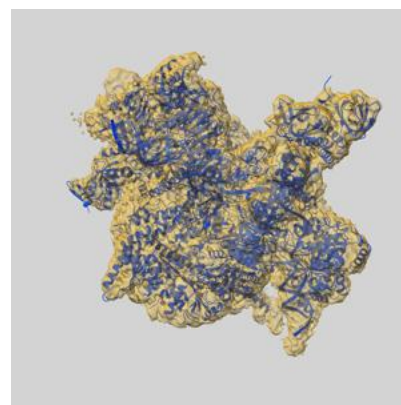
9.1 Map-model overlay [i](#)



X



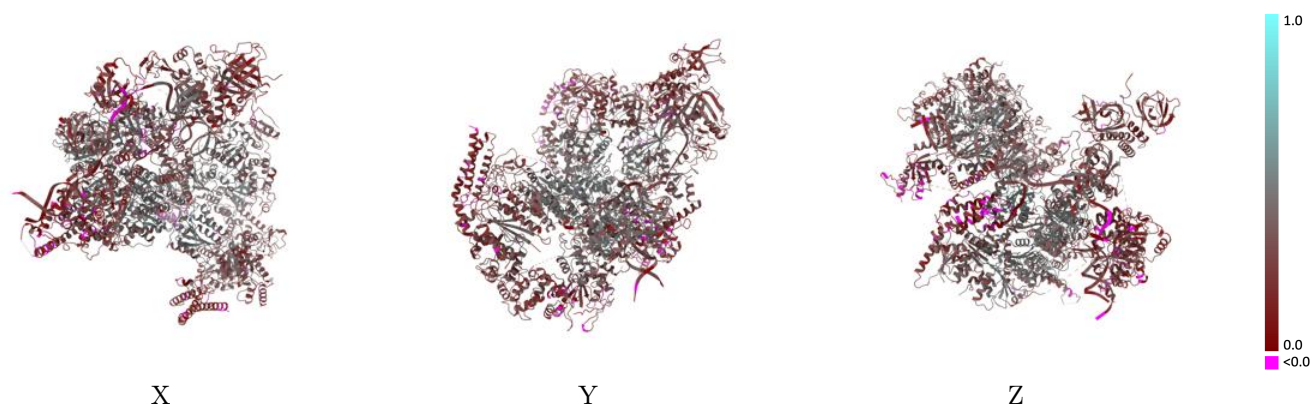
Y



Z

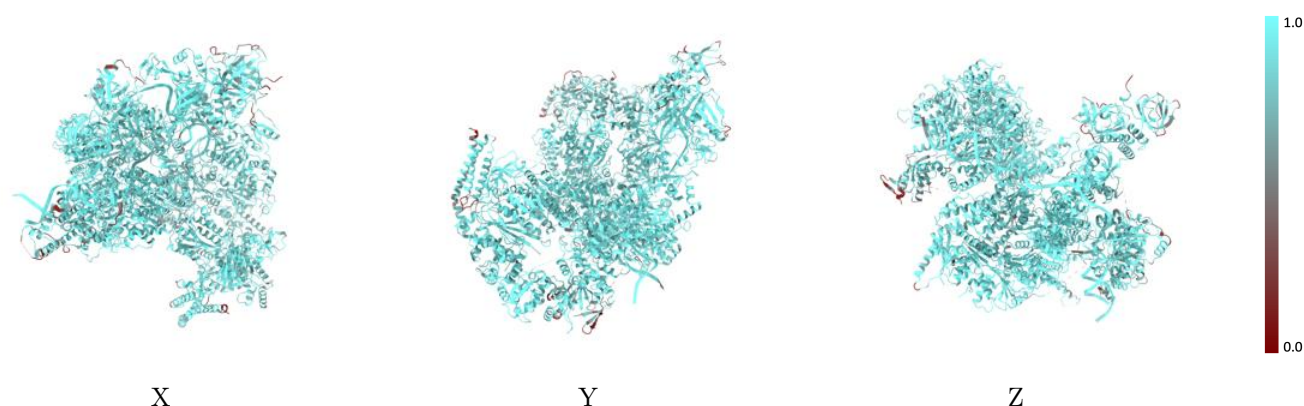
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



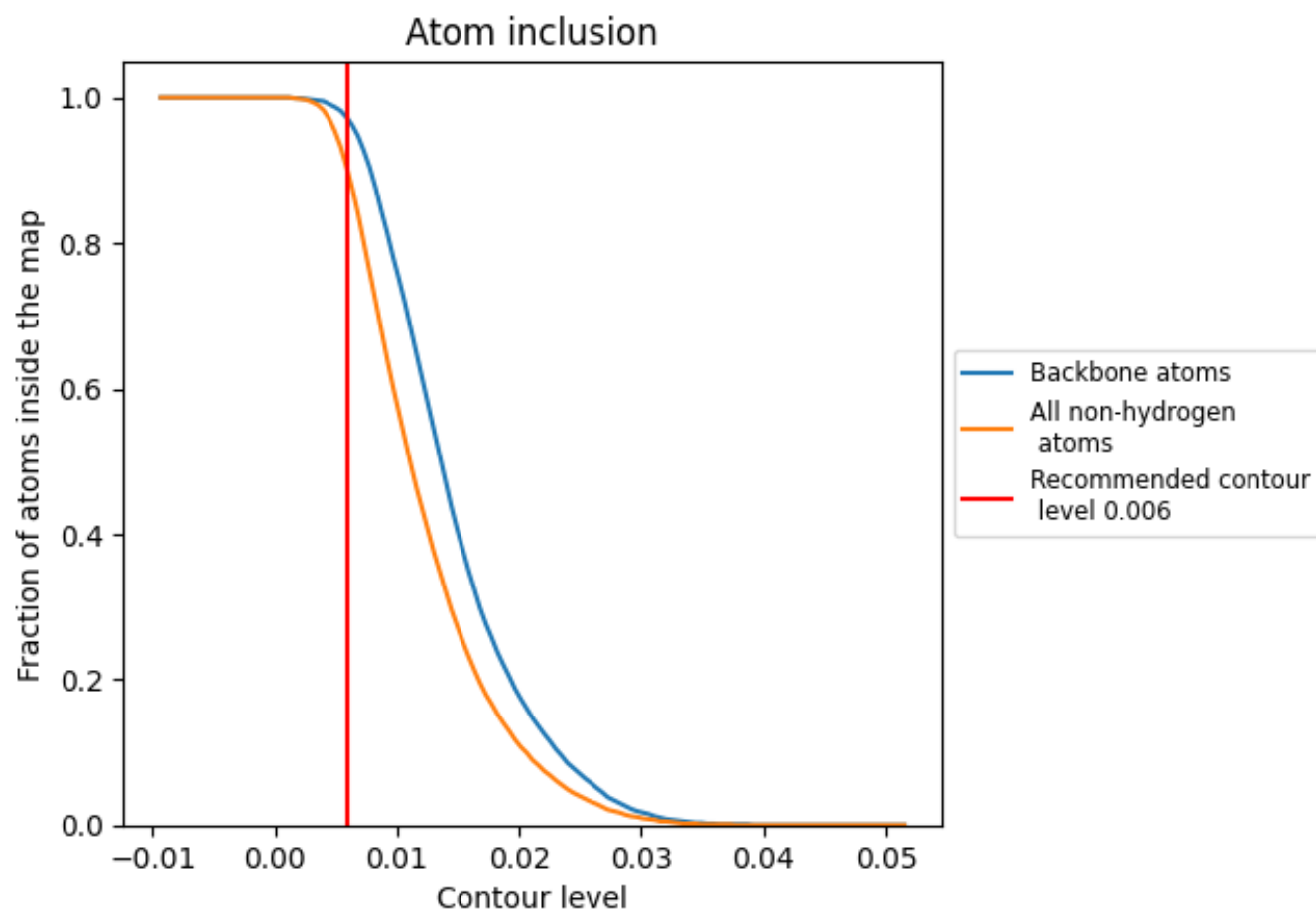
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8990	0.3210
A	0.9130	0.3840
B	0.9590	0.4220
C	0.8180	0.1760
D	0.8700	0.2880
E	0.8950	0.3540
F	0.9100	0.3060
G	0.8670	0.2990
K	0.8420	0.2660
L	0.9490	0.2710
M	0.9260	0.2660
N	0.9030	0.2620
O	0.8470	0.3000
P	0.7430	0.2250
Q	0.9450	0.3420
R	0.9710	0.4410
S	0.8300	0.2260

