



Full wwPDB EM Validation Report ⓘ

Jul 28, 2026 – 01:55 pm BST

PDB ID : 28KE / pdb_000028ke
EMDB ID : EMD-56573
Title : Cryo-EM structure of the human holo-TFIIH-XPC-XPA complex bound to bulky lesion-mimic DNA
Authors : de Martin Garrido, N.; Haste, C.A.F.; Feng, J.; Cronin, N.B.; Greber, B.J.
Deposited on : 2026-02-04
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

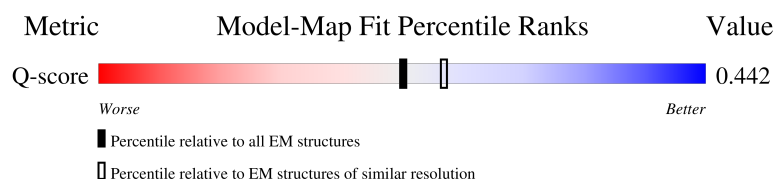
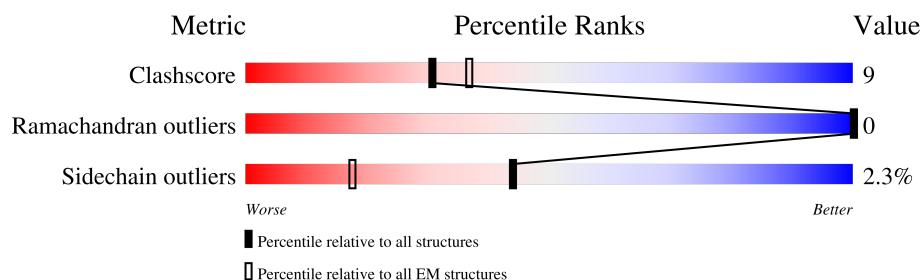
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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	797	
2	B	771	
3	C	591	
4	D	462	

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Mol	Chain	Length	Quality of chain
5	E	395	8%81%13%6%
6	F	308	71%13%16%
7	G	71	13%79%15%. .
8	H	309	24%13%11%76%
9	I	940	. .96%
10	N	273	29%42%20%37%
11	L	48	19%25%56%
12	M	69	14%13%72%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 24107 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 General transcription and DNA repair factor IIIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	625	Total	C	N	O	S	0	0
			5052	3227	877	919	29		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP P19447
A	-13	HIS	-	expression tag	UNP P19447
A	-12	HIS	-	expression tag	UNP P19447
A	-11	HIS	-	expression tag	UNP P19447
A	-10	HIS	-	expression tag	UNP P19447
A	-9	HIS	-	expression tag	UNP P19447
A	-8	GLU	-	expression tag	UNP P19447
A	-7	ASN	-	expression tag	UNP P19447
A	-6	LEU	-	expression tag	UNP P19447
A	-5	TYR	-	expression tag	UNP P19447
A	-4	PHE	-	expression tag	UNP P19447
A	-3	GLN	-	expression tag	UNP P19447
A	-2	SER	-	expression tag	UNP P19447
A	-1	ASN	-	expression tag	UNP P19447
A	0	ALA	-	expression tag	UNP P19447

- Molecule 2 is a protein called TFIIH basal transcription factor complex helicase XPD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	694	Total	C	N	O	S	0	0
			5600	3588	979	1004	29		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	761	SER	-	expression tag	UNP P18074

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Chain	Residue	Modelled	Actual	Comment	Reference
B	762	SER	-	expression tag	UNP P18074
B	763	ASN	-	expression tag	UNP P18074
B	764	ASP	-	expression tag	UNP P18074
B	765	TYR	-	expression tag	UNP P18074
B	766	LYS	-	expression tag	UNP P18074
B	767	ASP	-	expression tag	UNP P18074
B	768	ASP	-	expression tag	UNP P18074
B	769	ASP	-	expression tag	UNP P18074
B	770	ASP	-	expression tag	UNP P18074
B	771	LYS	-	expression tag	UNP P18074

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	152	Total	C	N	O	S	0	0
			1221	772	214	227	8		

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	549	GLY	-	expression tag	UNP P32780
C	550	SER	-	expression tag	UNP P32780
C	551	GLY	-	expression tag	UNP P32780
C	552	GLY	-	expression tag	UNP P32780
C	553	GLU	-	expression tag	UNP P32780
C	554	ASN	-	expression tag	UNP P32780
C	555	LEU	-	expression tag	UNP P32780
C	556	TYR	-	expression tag	UNP P32780
C	557	PHE	-	expression tag	UNP P32780
C	558	GLN	-	expression tag	UNP P32780
C	559	SER	-	expression tag	UNP P32780
C	560	GLY	-	expression tag	UNP P32780
C	561	SER	-	expression tag	UNP P32780
C	562	TRP	-	expression tag	UNP P32780
C	563	SER	-	expression tag	UNP P32780
C	564	HIS	-	expression tag	UNP P32780
C	565	PRO	-	expression tag	UNP P32780
C	566	GLN	-	expression tag	UNP P32780
C	567	PHE	-	expression tag	UNP P32780
C	568	GLU	-	expression tag	UNP P32780
C	569	LYS	-	expression tag	UNP P32780
C	570	GLY	-	expression tag	UNP P32780

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Chain	Residue	Modelled	Actual	Comment	Reference
C	571	GLY	-	expression tag	UNP P32780
C	572	GLY	-	expression tag	UNP P32780
C	573	SER	-	expression tag	UNP P32780
C	574	GLY	-	expression tag	UNP P32780
C	575	GLY	-	expression tag	UNP P32780
C	576	GLY	-	expression tag	UNP P32780
C	577	SER	-	expression tag	UNP P32780
C	578	GLY	-	expression tag	UNP P32780
C	579	GLY	-	expression tag	UNP P32780
C	580	GLY	-	expression tag	UNP P32780
C	581	SER	-	expression tag	UNP P32780
C	582	TRP	-	expression tag	UNP P32780
C	583	SER	-	expression tag	UNP P32780
C	584	HIS	-	expression tag	UNP P32780
C	585	PRO	-	expression tag	UNP P32780
C	586	GLN	-	expression tag	UNP P32780
C	587	PHE	-	expression tag	UNP P32780
C	588	GLU	-	expression tag	UNP P32780
C	589	LYS	-	expression tag	UNP P32780
C	590	SER	-	expression tag	UNP P32780
C	591	GLY	-	expression tag	UNP P32780

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	435	Total	C	N	O	S	0	0
			3490	2250	606	621	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	372	Total	C	N	O	S	0	0
			2923	1845	503	548	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	260	Total	C	N	O	S	0	0
			2045	1308	339	379	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	68	Total	C	N	O	S	0	0
			537	346	85	103	3		

- Molecule 8 is a protein called CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	75	Total	C	N	O	S	0	0
			642	408	107	126	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	41	Total	C	N	O	0	0
			322	200	58	64		

- Molecule 10 is a protein called DNA repair protein complementing XP-A cells.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	171	Total	C	N	O	S	0	0
			1441	903	254	271	13		

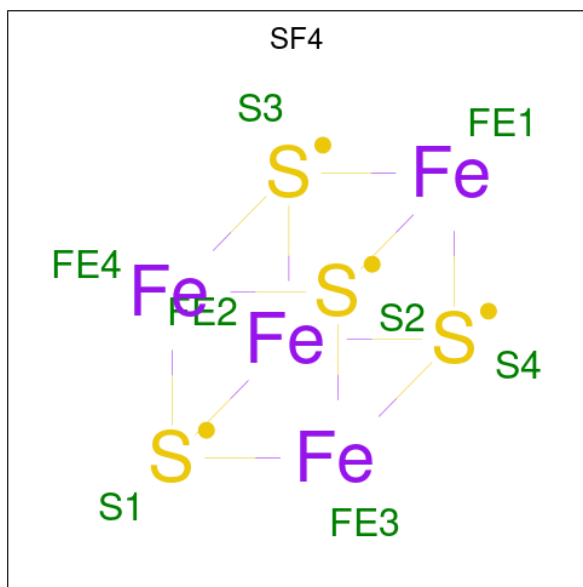
- Molecule 11 is a DNA chain called DNA lesion strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	21	Total	C	N	O	P	0	0
			415	199	71	124	21		

- Molecule 12 is a DNA chain called DNA non-lesion strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	19	Total	C	N	O	P	0	0
			405	190	80	116	19		

- Molecule 13 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

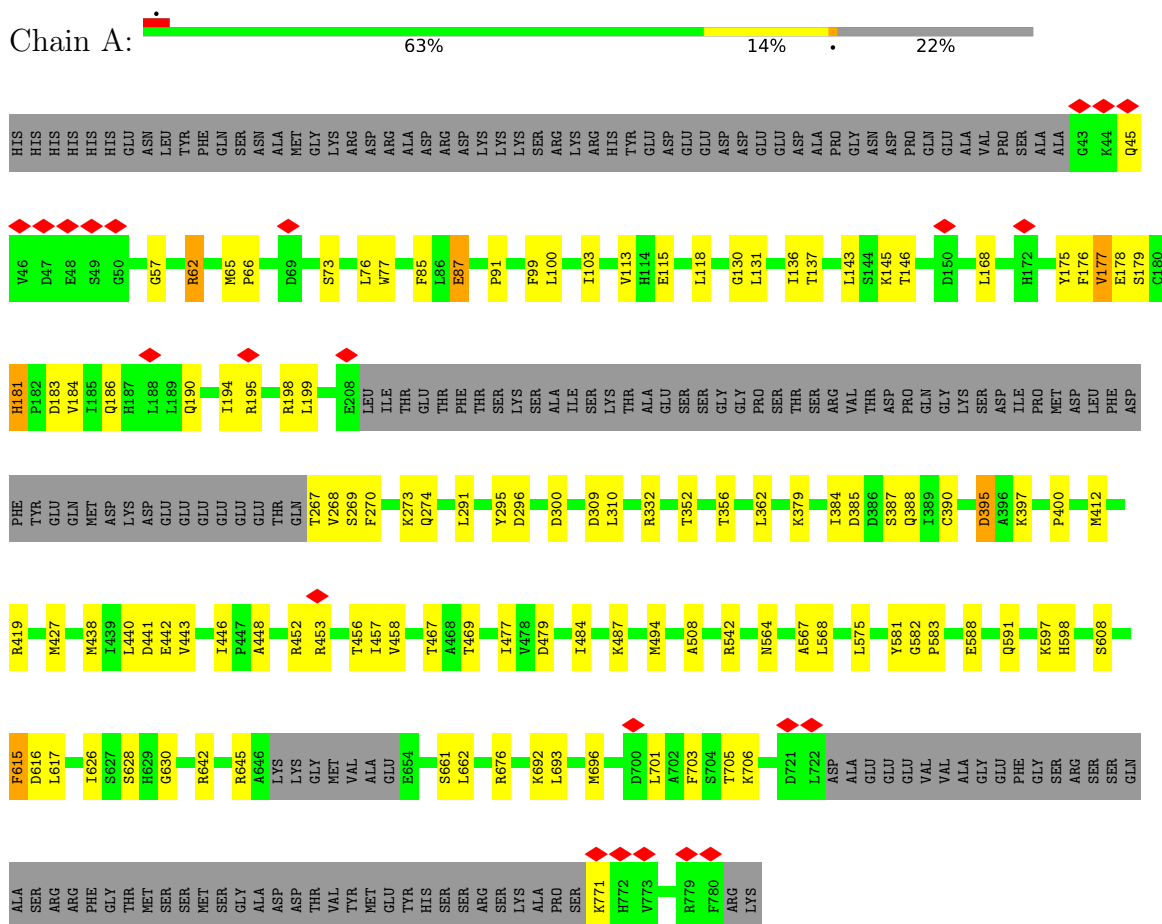
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

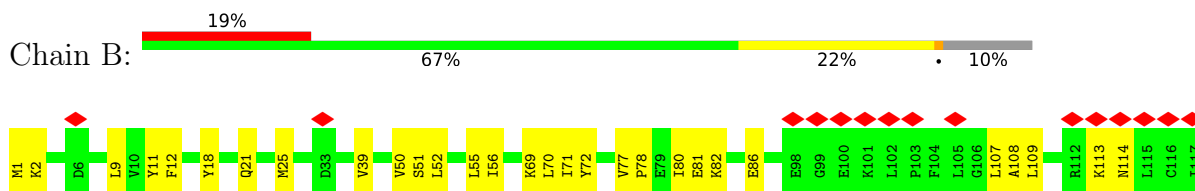
3 Residue-property plots

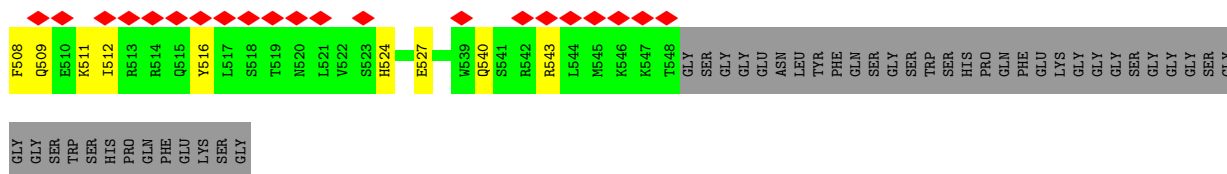
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

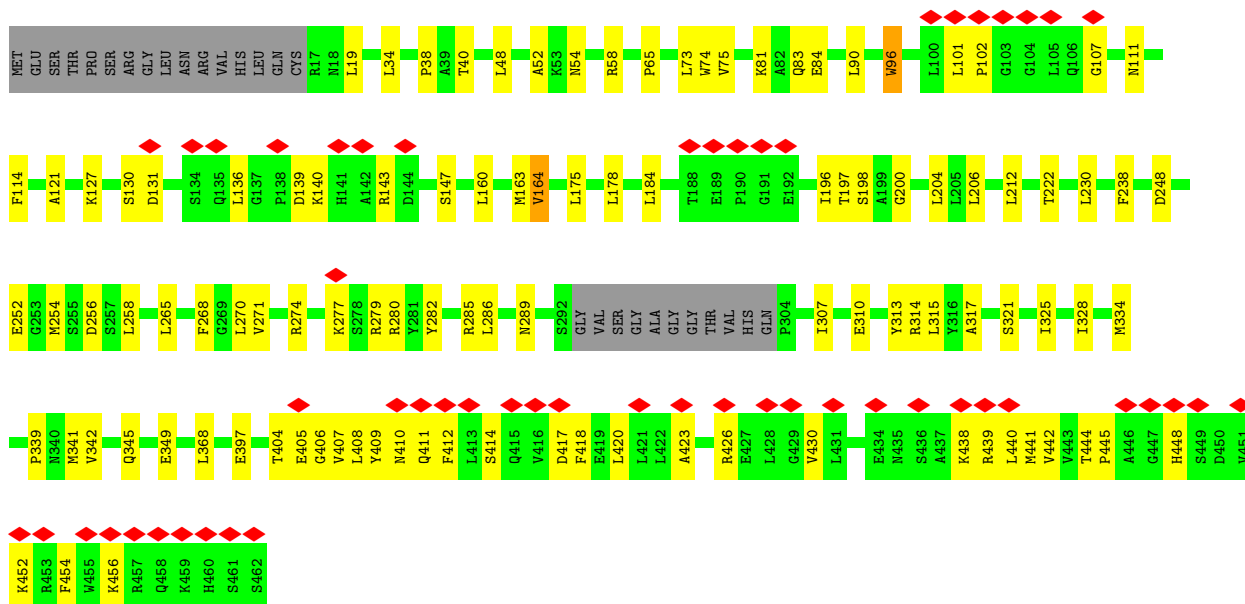


- Molecule 2: TFIIH basal transcription factor complex helicase XPD subunit

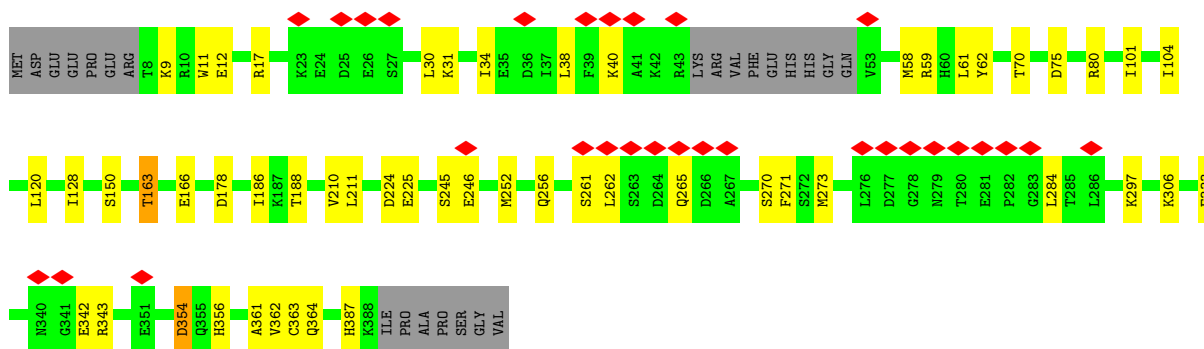
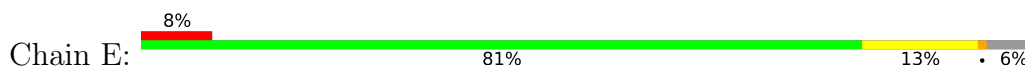




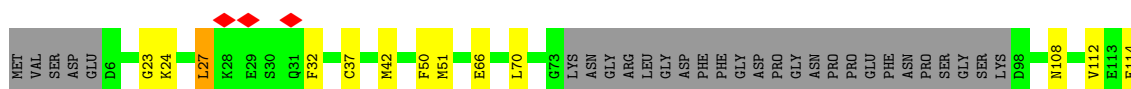
• Molecule 4: General transcription factor IIH subunit 4



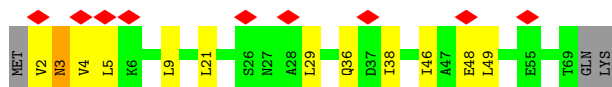
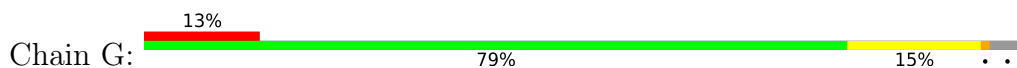
• Molecule 5: General transcription factor IIH subunit 2



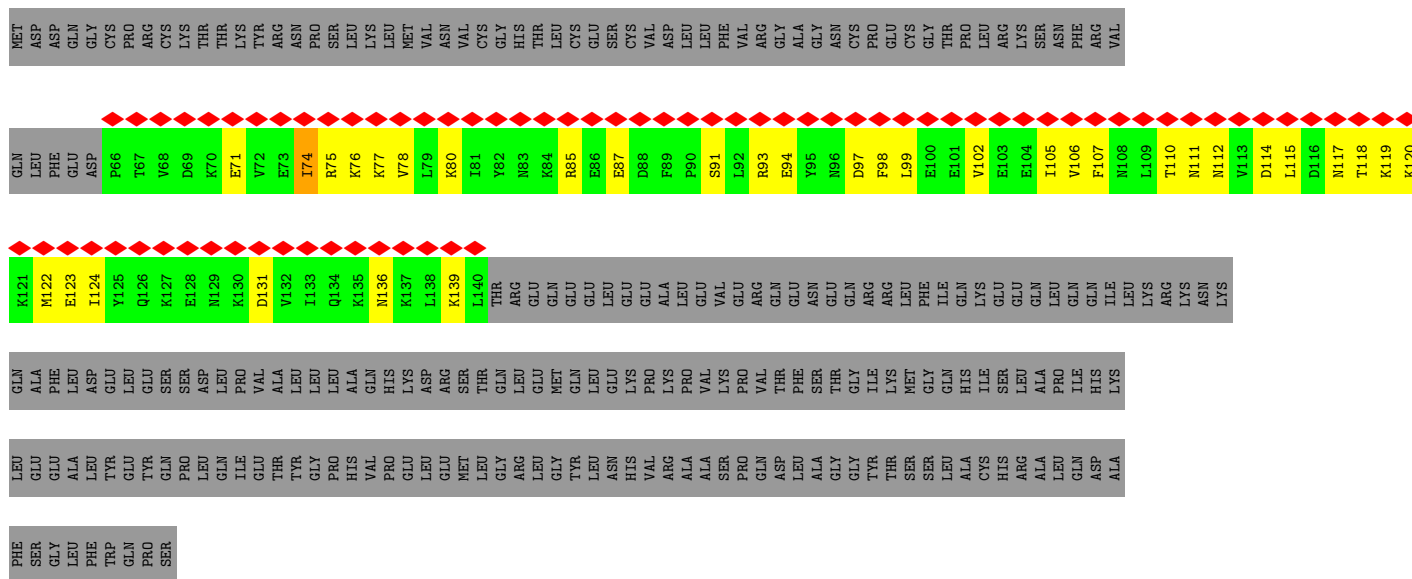
• Molecule 6: General transcription factor IIH subunit 3



- Molecule 7: General transcription factor IIH subunit 5

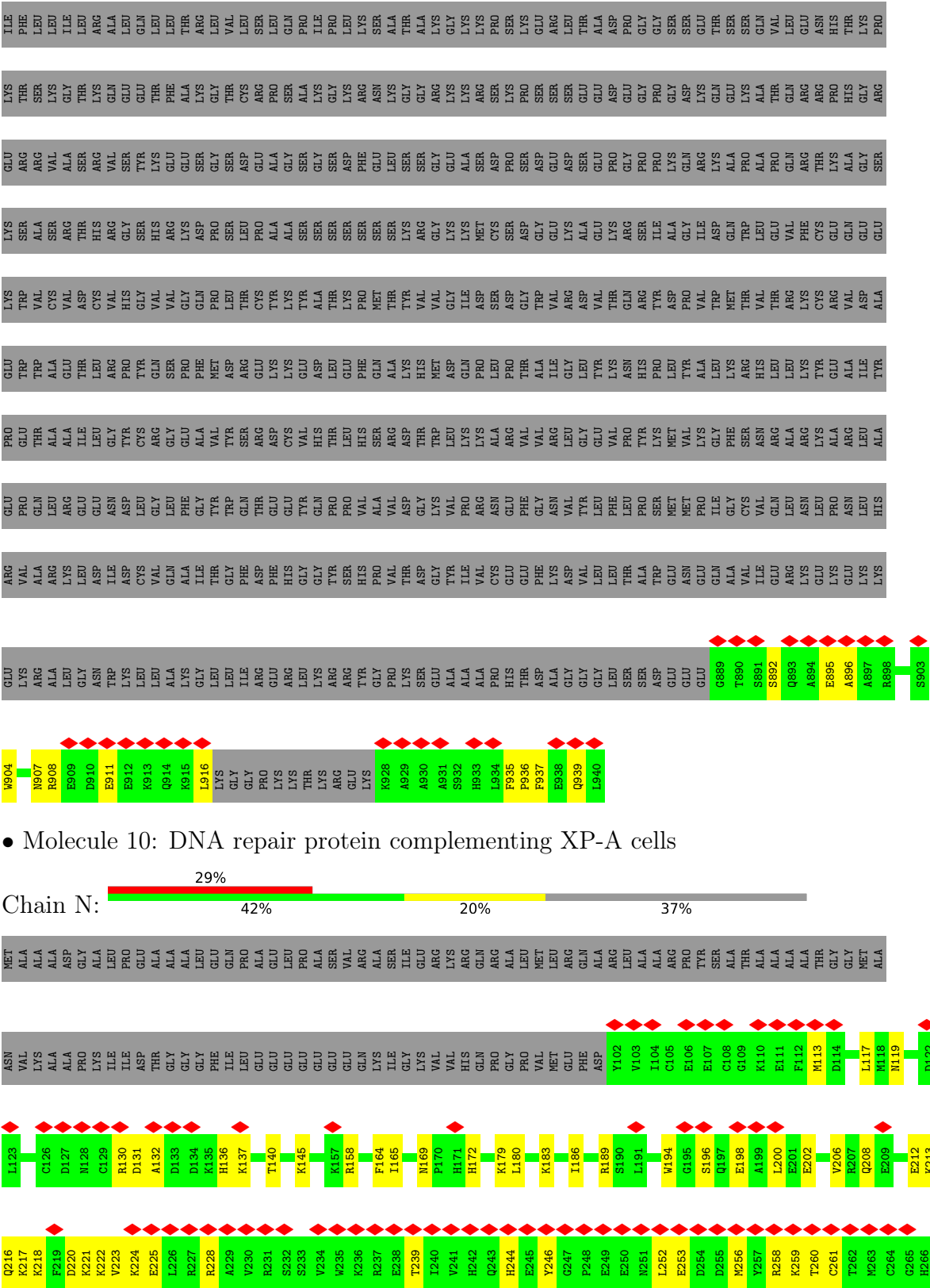


- Molecule 8: CDK-activating kinase assembly factor MAT1

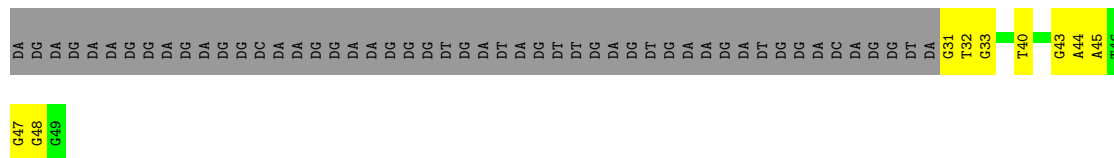


- Molecule 9: DNA repair protein complementing XP-C cells





- Molecule 12: DNA non-lesion strand



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43458	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0133	Depositor
Map size ($\text{\AA}$)	375.2, 375.2, 375.2	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.34, 1.34, 1.34	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.13	0/5159	0.28	0/6965
2	B	0.13	0/5720	0.30	0/7738
3	C	0.18	0/1244	0.45	0/1679
4	D	0.13	0/3572	0.29	0/4838
5	E	0.12	0/2987	0.26	0/4041
6	F	0.13	0/2082	0.27	0/2820
7	G	0.12	0/543	0.32	0/734
8	H	0.21	0/649	0.60	0/867
9	I	0.11	0/327	0.27	0/437
10	N	0.13	0/1469	0.33	0/1964
11	L	0.20	0/462	0.43	0/706
12	M	0.21	0/456	0.38	0/706
All	All	0.14	0/24670	0.31	0/33495

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	5052	0	5089	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5600	0	5653	109	0
3	C	1221	0	1238	31	0
4	D	3490	0	3534	82	0
5	E	2923	0	2892	34	0
6	F	2045	0	2060	24	0
7	G	537	0	546	18	0
8	H	642	0	660	34	0
9	I	322	0	309	10	0
10	N	1441	0	1425	40	0
11	L	415	0	236	9	0
12	M	405	0	215	7	0
13	B	8	0	0	0	0
14	E	3	0	0	0	0
14	F	2	0	0	0	0
14	N	1	0	0	0	0
All	All	24107	0	23857	429	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 9.

All (429) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:409:TYR:O	4:D:440:LEU:HA	1.54	1.08
4:D:441:MET:HE3	4:D:442:VAL:H	1.43	0.82
4:D:441:MET:HE3	4:D:442:VAL:N	1.99	0.78
3:C:506:CYS:HA	3:C:509:GLN:HE21	1.49	0.77
1:A:419:ARG:NH1	1:A:427:MET:SD	2.60	0.75
8:H:114:ASP:OD1	8:H:117:ASN:ND2	2.19	0.74
3:C:474:HIS:HB3	3:C:493:MET:HE2	1.69	0.73
3:C:426:ALA:HB1	6:F:222:SER:HB2	1.72	0.72
3:C:486:LEU:O	3:C:490:VAL:HG13	1.89	0.72
8:H:74:ILE:HA	8:H:77:LYS:HG2	1.70	0.72
2:B:224:GLU:O	2:B:227:ARG:NH1	2.23	0.71
7:G:4:VAL:HG22	10:N:271:GLU:HB2	1.73	0.71
1:A:91:PRO:HB3	5:E:38:LEU:HD21	1.74	0.70
6:F:118:LEU:HD23	6:F:119:MET:HG2	1.74	0.70
11:L:12:DC:H2'	11:L:13:DA:C8	2.27	0.69
7:G:3:ASN:HA	10:N:272:LYS:HA	1.75	0.69
2:B:253:ARG:HD3	2:B:431:PRO:HD2	1.75	0.68
1:A:356:THR:HG21	5:E:11:TRP:HE1	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:262:ASN:ND2	2:B:393:ASP:O	2.26	0.67
2:B:515:ALA:O	2:B:519:ASN:ND2	2.24	0.67
8:H:102:VAL:O	8:H:106:VAL:HG23	1.94	0.67
2:B:336:LEU:HD21	2:B:400:LEU:HD11	1.76	0.67
2:B:56:ILE:HG21	2:B:70:LEU:HD22	1.77	0.66
2:B:113:LYS:NZ	2:B:124:LEU:O	2.28	0.66
2:B:612:HIS:O	2:B:616:ARG:NH1	2.29	0.66
7:G:4:VAL:N	10:N:271:GLU:O	2.28	0.66
1:A:412:MET:O	1:A:419:ARG:NH2	2.29	0.66
3:C:489:LYS:O	3:C:493:MET:HG2	1.96	0.65
1:A:630:GLY:O	1:A:676:ARG:NH1	2.31	0.64
6:F:165:LYS:NZ	6:F:167:ALA:O	2.30	0.64
2:B:351:GLN:OE1	2:B:631:ARG:NH2	2.28	0.64
4:D:252:GLU:OE1	4:D:279:ARG:NH2	2.30	0.64
4:D:408:LEU:HD13	4:D:442:VAL:HG22	1.78	0.64
2:B:325:THR:HG22	2:B:328:HIS:H	1.63	0.63
2:B:419:GLU:O	2:B:431:PRO:HA	1.98	0.63
2:B:280:ARG:NH1	2:B:387:GLU:OE2	2.31	0.63
2:B:216:LYS:HG3	2:B:402:ASN:HD21	1.64	0.63
4:D:54:ASN:ND2	6:F:237:GLN:OE1	2.32	0.63
5:E:101:ILE:HG21	5:E:252:MET:HE1	1.81	0.63
2:B:71:ILE:HB	2:B:231:VAL:HG12	1.81	0.63
2:B:565:LYS:HD2	2:B:593:GLY:HA3	1.79	0.62
2:B:39:VAL:HG12	2:B:456:ILE:HB	1.81	0.62
4:D:143:ARG:HH21	4:D:147:SER:HB3	1.64	0.62
4:D:408:LEU:HA	4:D:441:MET:O	2.00	0.62
2:B:655:ASP:OD1	2:B:658:ARG:NH2	2.32	0.62
3:C:462:LYS:O	3:C:466:VAL:HG23	1.99	0.62
3:C:491:VAL:O	3:C:494:LYS:HG3	2.00	0.62
1:A:45:GLN:OE1	1:A:45:GLN:N	2.28	0.62
10:N:208:GLN:NE2	10:N:212:GLU:OE2	2.33	0.62
5:E:270:SER:O	5:E:297:LYS:NZ	2.33	0.61
2:B:405:THR:O	2:B:409:THR:OG1	2.16	0.61
4:D:408:LEU:HD11	4:D:440:LEU:HD12	1.81	0.61
1:A:452:ARG:NH2	1:A:479:ASP:OD2	2.33	0.61
3:C:508:PHE:HA	3:C:511:LYS:HG2	1.83	0.61
1:A:568:LEU:HD22	1:A:608:SER:HB3	1.81	0.61
5:E:256:GLN:HB3	6:F:250:ASP:HA	1.84	0.60
1:A:581:TYR:HD1	1:A:582:GLY:H	1.49	0.60
2:B:288:LEU:HD23	2:B:324:ARG:HG2	1.83	0.60
4:D:139:ASP:OD1	4:D:280:ARG:NH1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:258:ARG:NH2	10:N:260:THR:OG1	2.34	0.59
11:L:8:DC:H2'	11:L:9:DA:C8	2.37	0.59
2:B:252:THR:OG1	2:B:253:ARG:NH1	2.36	0.59
8:H:75:ARG:HG3	8:H:106:VAL:HG11	1.85	0.59
1:A:57:GLY:HA3	1:A:771:LYS:HG2	1.85	0.59
4:D:410:ASN:HB2	7:G:3:ASN:HD22	1.68	0.59
8:H:119:LYS:HA	8:H:122:MET:HG3	1.84	0.59
8:H:119:LYS:HD3	8:H:122:MET:SD	2.43	0.58
8:H:74:ILE:O	8:H:78:VAL:HG12	2.03	0.58
3:C:405:GLN:OE1	3:C:408:ARG:NH2	2.36	0.58
3:C:436:PRO:HG3	4:D:73:LEU:HD22	1.86	0.58
10:N:224:LYS:NZ	10:N:224:LYS:O	2.35	0.58
4:D:34:LEU:HG	4:D:40:THR:HG21	1.85	0.58
2:B:601:ARG:NH1	2:B:624:PRO:O	2.37	0.58
10:N:202:GLU:O	10:N:206:VAL:HG13	2.03	0.58
2:B:690:ARG:O	2:B:698:GLN:NE2	2.37	0.57
1:A:199:LEU:HD13	1:A:273:LYS:HG2	1.85	0.57
8:H:112:ASN:HA	8:H:115:LEU:HD21	1.87	0.57
7:G:3:ASN:HB3	10:N:270:TYR:CD2	2.39	0.57
1:A:494:MET:HA	1:A:494:MET:HE2	1.85	0.57
2:B:418:ILE:HD13	2:B:433:LEU:HB2	1.87	0.57
5:E:225:GLU:OE1	5:E:225:GLU:N	2.38	0.57
7:G:29:LEU:HD23	7:G:49:LEU:HD23	1.85	0.56
3:C:464:LEU:HD21	3:C:504:LYS:HE2	1.86	0.56
1:A:628:SER:OG	1:A:676:ARG:NH2	2.39	0.56
4:D:397:GLU:HA	9:I:904:TRP:HZ2	1.71	0.56
4:D:407:VAL:HA	7:G:5:LEU:O	2.06	0.56
2:B:1:MET:N	2:B:12:PHE:O	2.39	0.56
2:B:160:GLU:HG3	2:B:189:TRP:CD1	2.41	0.56
2:B:107:LEU:HD21	2:B:205:VAL:HG22	1.87	0.55
2:B:688:ASP:N	2:B:688:ASP:OD1	2.38	0.55
10:N:213:LYS:HD2	10:N:216:GLN:HE21	1.71	0.55
8:H:76:LYS:O	8:H:80:LYS:HG3	2.05	0.55
4:D:406:GLY:HA2	4:D:445:PRO:HD3	1.89	0.55
1:A:66:PRO:O	1:A:146:THR:OG1	2.21	0.55
1:A:195:ARG:HA	1:A:198:ARG:HD3	1.88	0.55
2:B:25:MET:HG2	2:B:55:LEU:HB2	1.88	0.55
2:B:195:ALA:O	2:B:199:ILE:HG23	2.07	0.55
2:B:253:ARG:NH1	2:B:430:ASN:OD1	2.39	0.55
4:D:407:VAL:O	4:D:442:VAL:HA	2.06	0.55
1:A:706:LYS:HE3	9:I:896:ALA:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:136:ASN:HA	8:H:139:LYS:HG2	1.89	0.55
5:E:224:ASP:N	5:E:224:ASP:OD1	2.38	0.54
4:D:409:TYR:HE1	7:G:4:VAL:HG12	1.71	0.54
5:E:75:ASP:OD2	5:E:80:ARG:NH2	2.41	0.54
11:L:13:DA:H2'	11:L:14:DT:H71	1.88	0.54
8:H:74:ILE:HG22	8:H:77:LYS:NZ	2.21	0.54
4:D:397:GLU:HA	9:I:904:TRP:CZ2	2.42	0.54
8:H:77:LYS:HA	8:H:80:LYS:HE2	1.90	0.54
10:N:172:HIS:O	12:M:31:DG:N2	2.41	0.54
1:A:661:SER:O	1:A:661:SER:OG	2.26	0.54
4:D:136:LEU:HD11	4:D:280:ARG:HB3	1.90	0.54
2:B:114:ASN:HB3	2:B:177:LEU:HD11	1.90	0.54
5:E:354:ASP:OD1	5:E:356:HIS:N	2.38	0.54
2:B:462:SER:HB3	2:B:463:PRO:HD3	1.90	0.54
10:N:165:ILE:HG22	10:N:180:LEU:HB2	1.89	0.54
1:A:385:ASP:OD1	1:A:387:SER:OG	2.25	0.53
1:A:542:ARG:NH1	1:A:703:PHE:O	2.41	0.53
1:A:615:PHE:HD1	1:A:616:ASP:H	1.56	0.53
10:N:158:ARG:O	10:N:189:ARG:NH1	2.42	0.53
4:D:285:ARG:O	4:D:289:ASN:ND2	2.40	0.53
6:F:116:LYS:O	6:F:120:THR:OG1	2.20	0.53
2:B:322:SER:HB3	8:H:99:LEU:HB3	1.91	0.53
6:F:66:GLU:OE2	6:F:66:GLU:N	2.42	0.53
8:H:85:ARG:NH1	8:H:87:GLU:OE1	2.41	0.53
1:A:379:LYS:NZ	1:A:384:ILE:O	2.42	0.53
4:D:420:LEU:HD13	4:D:454:PHE:HE2	1.74	0.53
10:N:217:LYS:O	10:N:221:LYS:HG2	2.09	0.53
2:B:70:LEU:HD23	2:B:204:VAL:HG22	1.91	0.52
2:B:584:TYR:OH	2:B:614:TYR:O	2.25	0.52
4:D:409:TYR:HD1	7:G:3:ASN:O	1.92	0.52
5:E:261:SER:OG	5:E:262:LEU:N	2.42	0.52
8:H:93:ARG:HH12	8:H:97:ASP:CG	2.17	0.52
4:D:341:MET:HG2	4:D:342:VAL:N	2.24	0.52
10:N:214:MET:O	10:N:218:LYS:HG2	2.10	0.52
2:B:335:ARG:HD3	8:H:75:ARG:NH2	2.25	0.52
2:B:363:GLN:HE22	2:B:364:ARG:HH21	1.58	0.52
10:N:213:LYS:O	10:N:216:GLN:HG3	2.10	0.52
3:C:416:PRO:HG3	6:F:112:VAL:HG21	1.89	0.52
11:L:16:DC:H2''	11:L:17:DC:C5	2.44	0.52
4:D:408:LEU:HD21	7:G:36:GLN:HG2	1.92	0.52
3:C:468:VAL:O	3:C:472:LEU:HD23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:117:ASN:O	8:H:120:LYS:HG2	2.09	0.51
8:H:93:ARG:NH1	8:H:93:ARG:O	2.43	0.51
1:A:176:PHE:HB3	1:A:269:SER:HB2	1.92	0.51
4:D:254:MET:HG2	4:D:258:LEU:HD22	1.93	0.51
2:B:627:TYR:HB2	11:L:21:DA:O4'	2.11	0.51
4:D:65:PRO:HB2	4:D:107:GLY:HA3	1.92	0.51
4:D:414:SER:OG	4:D:417:ASP:HB2	2.11	0.51
4:D:423:ALA:O	4:D:426:ARG:HG2	2.11	0.51
5:E:273:MET:N	5:E:273:MET:HE2	2.26	0.51
1:A:295:TYR:OH	1:A:300:ASP:OD2	2.27	0.51
1:A:469:THR:O	1:A:469:THR:OG1	2.28	0.51
2:B:439:ASP:HB3	2:B:442:LEU:HD23	1.93	0.51
11:L:5:DT:H2''	11:L:6:DT:O5'	2.11	0.51
1:A:181:HIS:O	1:A:184:VAL:HG22	2.12	0.50
1:A:706:LYS:HZ2	9:I:895:GLU:HB3	1.76	0.50
1:A:186:GLN:OE1	1:A:190:GLN:NE2	2.44	0.50
2:B:323:ILE:HD11	2:B:371:PRO:HG3	1.92	0.50
8:H:106:VAL:O	8:H:110:THR:HG23	2.12	0.50
4:D:101:LEU:HD12	4:D:102:PRO:HD2	1.92	0.50
3:C:524:HIS:HA	3:C:527:GLU:HG2	1.93	0.50
4:D:222:THR:HG22	4:D:222:THR:O	2.12	0.50
5:E:9:LYS:N	5:E:12:GLU:OE2	2.44	0.50
2:B:109:LEU:HD21	2:B:199:ILE:HG21	1.94	0.50
3:C:446:GLN:HG3	3:C:449:ILE:HB	1.94	0.50
10:N:196:SER:N	10:N:198:GLU:OE1	2.45	0.50
2:B:69:LYS:NZ	2:B:199:ILE:O	2.45	0.50
3:C:512:ILE:O	3:C:516:TYR:N	2.37	0.50
10:N:224:LYS:HE3	10:N:228:ARG:HH21	1.75	0.50
6:F:51:MET:HE1	6:F:232:LEU:HD21	1.94	0.49
4:D:130:SER:OG	4:D:131:ASP:N	2.45	0.49
10:N:258:ARG:HG3	10:N:269:THR:HG22	1.93	0.49
3:C:444:GLY:HA3	5:E:262:LEU:HD23	1.94	0.49
1:A:115:GLU:OE1	4:D:314:ARG:NH1	2.40	0.49
1:A:45:GLN:H	1:A:45:GLN:CD	2.20	0.49
2:B:52:LEU:HD11	2:B:72:TYR:HE2	1.77	0.49
2:B:324:ARG:HH22	8:H:93:ARG:NH1	2.10	0.49
3:C:487:GLU:O	3:C:490:VAL:HG22	2.13	0.49
4:D:197:THR:OG1	4:D:198:SER:N	2.46	0.49
12:M:32:DT:H2''	12:M:33:DG:H5'	1.93	0.49
2:B:72:TYR:OH	2:B:234:ASP:OD2	2.21	0.49
3:C:448:ALA:HA	3:C:451:GLN:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:48:LEU:HB3	4:D:52:ALA:HB3	1.94	0.49
2:B:493:MET:HG2	2:B:678:VAL:HG12	1.95	0.49
10:N:132:ALA:HA	10:N:136:HIS:HB2	1.95	0.49
4:D:409:TYR:CE1	7:G:4:VAL:HG12	2.47	0.49
8:H:131:ASP:OD1	8:H:131:ASP:N	2.43	0.49
5:E:245:SER:OG	5:E:246:GLU:N	2.46	0.48
4:D:175:LEU:HD13	4:D:268:PHE:HE1	1.78	0.48
5:E:333:GLU:HG3	5:E:356:HIS:HB3	1.95	0.48
4:D:405:GLU:HG3	4:D:445:PRO:HG3	1.94	0.48
7:G:48:GLU:OE2	7:G:48:GLU:N	2.31	0.48
1:A:310:LEU:HD11	1:A:352:THR:HG22	1.95	0.48
1:A:617:LEU:O	1:A:645:ARG:NH2	2.46	0.48
2:B:262:ASN:HB3	2:B:397:LEU:HD11	1.95	0.48
4:D:265:LEU:HD22	4:D:270:LEU:HD12	1.95	0.48
1:A:62:ARG:HG3	4:D:339:PRO:HA	1.96	0.48
4:D:411:GLN:HA	4:D:439:ARG:HB3	1.94	0.48
2:B:543:GLN:O	2:B:546:GLU:HG3	2.14	0.48
1:A:487:LYS:HB2	1:A:487:LYS:HE3	1.70	0.48
4:D:409:TYR:HA	7:G:3:ASN:O	2.14	0.48
2:B:416:ILE:HG13	2:B:435:PHE:HD1	1.78	0.48
3:C:540:GLN:O	3:C:543:ARG:HG2	2.14	0.48
4:D:334:MET:HE3	4:D:334:MET:HB3	1.77	0.48
5:E:361:ALA:O	5:E:364:GLN:NE2	2.38	0.48
1:A:385:ASP:HB3	1:A:388:GLN:HG3	1.96	0.47
2:B:78:PRO:O	2:B:81:GLU:HG3	2.13	0.47
2:B:196:ARG:O	2:B:199:ILE:HG12	2.14	0.47
2:B:255:THR:O	2:B:258:ARG:HG2	2.14	0.47
8:H:122:MET:SD	8:H:123:GLU:N	2.87	0.47
4:D:430:VAL:HB	4:D:444:THR:OG1	2.14	0.47
1:A:76:LEU:HD21	1:A:100:LEU:HD11	1.96	0.47
2:B:403:PHE:O	2:B:407:VAL:HG23	2.15	0.47
5:E:59:ARG:NE	5:E:166:GLU:OE2	2.42	0.47
1:A:73:SER:HB3	5:E:30:LEU:HD22	1.96	0.47
1:A:443:VAL:HG12	1:A:467:THR:HB	1.96	0.47
2:B:108:ALA:HA	2:B:206:VAL:HG22	1.96	0.47
2:B:236:ALA:H	2:B:458:SER:HB2	1.80	0.47
4:D:349:GLU:OE1	4:D:349:GLU:N	2.46	0.47
2:B:657:MET:HG3	2:B:692:LYS:HB2	1.96	0.47
3:C:502:VAL:HG23	3:C:503:THR:HG23	1.97	0.47
6:F:271:CYS:SG	6:F:284:THR:OG1	2.72	0.47
1:A:390:CYS:SG	1:A:400:PRO:HA	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:454:PRO:HD2	3:C:457:ILE:HD12	1.96	0.47
4:D:452:LYS:HG2	4:D:456:LYS:HE3	1.96	0.47
5:E:31:LYS:O	5:E:31:LYS:HD3	2.14	0.47
4:D:256:ASP:OD1	4:D:256:ASP:N	2.47	0.47
8:H:71:GLU:O	8:H:74:ILE:HG13	2.15	0.47
8:H:91:SER:O	8:H:94:GLU:HG2	2.14	0.47
3:C:468:VAL:HB	3:C:500:PHE:HE1	1.79	0.47
3:C:428:SER:O	3:C:431:ILE:HG22	2.16	0.46
4:D:74:TRP:CE2	6:F:229:TRP:HH2	2.34	0.46
1:A:508:ALA:HB2	9:I:935:PHE:CZ	2.49	0.46
2:B:82:LYS:HE3	2:B:82:LYS:HB2	1.76	0.46
5:E:61:LEU:HB3	5:E:104:ILE:HG13	1.96	0.46
1:A:564:ASN:HD22	1:A:567:ALA:H	1.61	0.46
5:E:61:LEU:HD12	5:E:166:GLU:HB2	1.97	0.46
8:H:120:LYS:O	8:H:124:ILE:HG12	2.14	0.46
1:A:77:TRP:HB2	1:A:85:PHE:HB2	1.97	0.46
4:D:248:ASP:HB3	4:D:282:TYR:CZ	2.50	0.46
10:N:169:ASN:OD1	10:N:169:ASN:N	2.48	0.46
5:E:186:ILE:HG12	5:E:211:LEU:HD13	1.96	0.46
11:L:11:DC:H2'	11:L:12:DC:C6	2.50	0.46
2:B:463:PRO:HG2	2:B:654:PHE:CD1	2.50	0.46
2:B:487:ARG:HE	2:B:724:MET:HG3	1.80	0.46
1:A:705:THR:O	9:I:892:SER:OG	2.28	0.46
2:B:336:LEU:O	2:B:340:VAL:HG13	2.16	0.46
10:N:212:GLU:HA	10:N:215:LYS:HD2	1.98	0.46
2:B:530:VAL:HG21	2:B:714:VAL:HG13	1.97	0.46
4:D:143:ARG:HD2	4:D:143:ARG:HA	1.71	0.46
2:B:272:ARG:O	2:B:276:THR:HG22	2.16	0.46
2:B:495:ILE:HG22	2:B:504:ILE:HD11	1.98	0.46
10:N:220:ASP:O	10:N:223:VAL:HG12	2.14	0.46
10:N:253:GLU:O	10:N:256:MET:HB3	2.15	0.46
1:A:91:PRO:HB2	5:E:34:ILE:HD11	1.98	0.45
2:B:344:LEU:HD12	2:B:418:ILE:HD11	1.97	0.45
2:B:355:PRO:HD3	2:B:411:ALA:HB1	1.98	0.45
4:D:313:TYR:O	4:D:345:GLN:HG3	2.15	0.45
10:N:258:ARG:NH1	10:N:260:THR:OG1	2.50	0.45
1:A:395:ASP:HB2	1:A:397:LYS:HE3	1.99	0.45
2:B:18:TYR:HD2	2:B:21:GLN:HE21	1.63	0.45
2:B:263:LEU:HD13	2:B:333:LEU:HD11	1.98	0.45
2:B:285:TYR:O	2:B:289:VAL:N	2.46	0.45
4:D:277:LYS:H	4:D:277:LYS:HG2	1.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:104:ILE:O	5:E:120:LEU:HA	2.17	0.45
12:M:31:DG:H4'	12:M:32:DT:OP1	2.17	0.45
1:A:626:ILE:HG22	1:A:662:LEU:HD12	1.98	0.45
2:B:345:ARG:HG3	2:B:345:ARG:O	2.17	0.45
10:N:246:TYR:HD1	10:N:259:LYS:HB3	1.81	0.45
1:A:453:ARG:HA	1:A:456:THR:HG22	1.98	0.45
1:A:705:THR:HA	9:I:892:SER:HB3	1.98	0.45
3:C:422:LEU:HD21	6:F:225:GLN:HB2	1.99	0.45
4:D:212:LEU:HD11	4:D:286:LEU:HB3	1.98	0.45
1:A:362:LEU:HD23	1:A:438:MET:HE2	1.98	0.45
2:B:243:CYS:SG	2:B:443:ALA:HB3	2.57	0.45
2:B:372:LEU:HD13	2:B:404:ALA:HB1	1.98	0.45
8:H:136:ASN:HA	8:H:139:LYS:HE2	1.98	0.45
1:A:441:ASP:OD1	1:A:442:GLU:N	2.50	0.45
2:B:441:SER:HA	2:B:444:ILE:HG22	1.97	0.45
2:B:619:ILE:HA	2:B:678:VAL:HG23	1.98	0.44
5:E:178:ASP:OD1	5:E:178:ASP:N	2.48	0.44
10:N:164:PHE:CD2	10:N:179:LYS:HB3	2.52	0.44
1:A:296:ASP:HA	1:A:332:ARG:HG2	1.99	0.44
5:E:342:GLU:OE1	5:E:343:ARG:N	2.50	0.44
8:H:115:LEU:O	8:H:118:THR:HG22	2.18	0.44
9:I:936:PRO:HA	9:I:939:GLN:HG2	1.98	0.44
1:A:183:ASP:OD1	1:A:184:VAL:N	2.50	0.44
1:A:581:TYR:CD1	1:A:583:PRO:HD2	2.52	0.44
4:D:408:LEU:O	7:G:4:VAL:HA	2.17	0.44
4:D:412:PHE:CE1	7:G:2:VAL:HA	2.51	0.44
8:H:102:VAL:HA	8:H:105:ILE:HD12	1.99	0.44
2:B:585:GLN:HG3	2:B:614:TYR:CE1	2.53	0.44
3:C:524:HIS:O	3:C:527:GLU:HG2	2.17	0.44
4:D:140:LYS:HD2	4:D:274:ARG:HH12	1.83	0.44
4:D:448:HIS:O	4:D:448:HIS:ND1	2.49	0.44
10:N:131:ASP:O	10:N:136:HIS:N	2.49	0.44
1:A:99:PHE:O	1:A:103:ILE:HG22	2.17	0.44
2:B:343:ARG:HA	2:B:343:ARG:HD2	1.73	0.44
6:F:23:GLY:O	6:F:27:LEU:HD22	2.18	0.44
10:N:117:LEU:HG	10:N:130:ARG:HG3	1.98	0.44
1:A:113:VAL:N	4:D:310:GLU:OE2	2.47	0.44
1:A:309:ASP:OD1	1:A:310:LEU:N	2.51	0.44
2:B:620:MET:HE3	2:B:620:MET:HB3	1.73	0.44
10:N:137:LYS:O	10:N:183:LYS:HB2	2.18	0.44
1:A:457:ILE:HG23	1:A:458:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:81:LYS:O	4:D:84:GLU:HG2	2.18	0.44
10:N:217:LYS:HD3	12:M:40:DT:OP1	2.18	0.44
11:L:7:DC:H2'	11:L:8:DC:C6	2.52	0.44
2:B:320:PRO:HD3	2:B:370:LYS:NZ	2.33	0.43
3:C:399:ASP:OD1	6:F:24:LYS:NZ	2.47	0.43
1:A:168:LEU:HB2	1:A:291:LEU:HD11	1.98	0.43
2:B:133:LYS:HA	2:B:133:LYS:HD3	1.80	0.43
2:B:80:ILE:HG23	2:B:206:VAL:HG21	2.00	0.43
2:B:498:GLY:HA3	2:B:519:ASN:OD1	2.18	0.43
12:M:45:DA:C8	12:M:45:DA:H5'	2.53	0.43
1:A:642:ARG:HA	1:A:642:ARG:HD3	1.70	0.43
2:B:337:LEU:HA	2:B:340:VAL:HG22	2.00	0.43
2:B:354:PRO:HG2	2:B:411:ALA:HA	2.00	0.43
5:E:30:LEU:O	5:E:34:ILE:HG22	2.18	0.43
8:H:71:GLU:O	8:H:75:ARG:HD3	2.19	0.43
10:N:222:LYS:O	10:N:225:GLU:HG3	2.18	0.43
1:A:692:LYS:HB2	1:A:692:LYS:HE3	1.81	0.43
2:B:2:LYS:NZ	2:B:11:TYR:HB3	2.34	0.43
2:B:269:THR:HB	2:B:272:ARG:HH21	1.82	0.43
4:D:75:VAL:HG21	4:D:83:GLN:HG3	2.00	0.43
6:F:194:CYS:HB2	6:F:231:PHE:CE2	2.54	0.43
2:B:118:HIS:O	2:B:122:THR:HG23	2.19	0.43
1:A:356:THR:HG21	5:E:11:TRP:NE1	2.31	0.43
10:N:256:MET:HE3	10:N:258:ARG:HB2	2.01	0.43
1:A:143:LEU:HD12	1:A:143:LEU:HA	1.90	0.43
2:B:77:VAL:HG23	2:B:78:PRO:HD3	2.00	0.43
2:B:192:TYR:CZ	2:B:196:ARG:HD2	2.54	0.43
1:A:427:MET:HE2	1:A:427:MET:HB3	1.95	0.43
1:A:597:LYS:HE2	1:A:598:HIS:CE1	2.53	0.43
2:B:50:VAL:HG22	2:B:86:GLU:OE2	2.19	0.43
3:C:506:CYS:O	3:C:509:GLN:HG2	2.19	0.43
6:F:197:ASP:O	6:F:216:LYS:NZ	2.45	0.43
10:N:194:TRP:HD1	10:N:200:LEU:HD13	1.83	0.43
1:A:177:VAL:HG21	1:A:270:PHE:CZ	2.54	0.42
2:B:122:THR:N	2:B:123:PRO:HD2	2.34	0.42
10:N:113:MET:HE2	10:N:113:MET:HA	2.00	0.42
1:A:446:ILE:O	1:A:448:ALA:N	2.46	0.42
2:B:411:ALA:H	2:B:412:LYS:NZ	2.17	0.42
5:E:387:HIS:CD2	6:F:135:GLY:HA3	2.54	0.42
2:B:507:LYS:O	2:B:511:ARG:HG3	2.20	0.42
4:D:321:SER:O	4:D:325:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:32:PHE:CZ	6:F:37:CYS:HB2	2.54	0.42
1:A:118:LEU:HD23	1:A:118:LEU:HA	1.88	0.42
3:C:402:ASN:OD1	3:C:402:ASN:C	2.61	0.42
4:D:285:ARG:HG2	4:D:289:ASN:HD21	1.84	0.42
1:A:588:GLU:O	1:A:591:GLN:HG3	2.19	0.42
1:A:179:SER:O	1:A:267:THR:HA	2.19	0.42
1:A:575:LEU:HD23	1:A:575:LEU:HA	1.83	0.42
2:B:170:LEU:HD23	2:B:170:LEU:HA	1.90	0.42
2:B:370:LYS:HD2	2:B:374:PHE:HE1	1.85	0.42
4:D:197:THR:HG23	4:D:200:GLY:H	1.84	0.42
4:D:206:LEU:HD23	4:D:206:LEU:HA	1.85	0.42
4:D:307:ILE:HD11	4:D:328:ILE:HD11	2.01	0.42
5:E:40:LYS:HA	5:E:40:LYS:HD3	1.72	0.42
5:E:306:LYS:HB3	5:E:306:LYS:HE2	1.80	0.42
1:A:693:LEU:HD22	9:I:937:PHE:HE2	1.85	0.42
1:A:194:ILE:O	1:A:198:ARG:HG3	2.20	0.42
2:B:469:LYS:HG2	2:B:646:ILE:HD11	2.01	0.42
4:D:38:PRO:HB3	4:D:121:ALA:HB2	2.02	0.42
4:D:317:ALA:HB3	4:D:342:VAL:HG23	2.01	0.42
10:N:215:LYS:HG2	10:N:216:GLN:N	2.34	0.42
2:B:2:LYS:HG3	2:B:9:LEU:HD11	2.02	0.42
2:B:196:ARG:HE	2:B:220:LEU:HD22	1.85	0.42
2:B:688:ASP:O	2:B:692:LYS:HG2	2.19	0.42
4:D:58:ARG:HH12	6:F:241:LEU:HD11	1.85	0.42
5:E:271:PHE:CE1	5:E:284:LEU:HD13	2.54	0.42
7:G:46:ILE:HB	7:G:48:GLU:CD	2.45	0.42
1:A:542:ARG:HE	1:A:696:MET:HE3	1.85	0.41
1:A:693:LEU:HD12	1:A:696:MET:SD	2.60	0.41
2:B:270:VAL:O	2:B:273:ILE:HG22	2.20	0.41
2:B:320:PRO:HG2	2:B:323:ILE:CD1	2.50	0.41
2:B:324:ARG:HH22	8:H:93:ARG:HH11	1.68	0.41
8:H:98:PHE:O	8:H:102:VAL:HG12	2.20	0.41
8:H:119:LYS:O	8:H:122:MET:SD	2.78	0.41
12:M:47:DG:H2"	12:M:48:DG:C8	2.55	0.41
1:A:130:GLY:O	5:E:17:ARG:NH2	2.54	0.41
2:B:491:CYS:HB3	2:B:676:LEU:HD23	2.01	0.41
6:F:42:MET:HE3	6:F:108:ASN:CG	2.45	0.41
1:A:136:ILE:HG13	1:A:137:THR:N	2.35	0.41
4:D:90:LEU:HD23	4:D:96:TRP:CD2	2.55	0.41
4:D:412:PHE:H	4:D:418:PHE:HZ	1.68	0.41
1:A:178:GLU:HA	1:A:269:SER:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:19:LEU:HD21	4:D:238:PHE:HZ	1.85	0.41
4:D:111:ASN:HB3	4:D:114:PHE:HB3	2.01	0.41
4:D:438:LYS:HB2	4:D:438:LYS:HE2	1.73	0.41
10:N:252:LEU:HD12	10:N:252:LEU:HA	1.86	0.41
11:L:7:DC:H2'	11:L:8:DC:H6	1.86	0.41
12:M:43:DG:H2''	12:M:44:DA:H8	1.85	0.41
2:B:728:PHE:HE1	2:B:730:ARG:HH21	1.67	0.41
10:N:246:TYR:CD1	10:N:259:LYS:HB3	2.55	0.41
4:D:164:VAL:HA	4:D:196:ILE:HD11	2.03	0.41
4:D:368:LEU:HD23	4:D:368:LEU:HA	1.83	0.41
6:F:141:LEU:HD23	6:F:141:LEU:HA	1.87	0.41
8:H:74:ILE:HG22	8:H:77:LYS:HZ3	1.83	0.41
10:N:145:LYS:HB3	10:N:145:LYS:HE2	1.84	0.41
10:N:244:HIS:NE2	10:N:261:CYS:HB2	2.36	0.41
2:B:252:THR:O	2:B:255:THR:OG1	2.34	0.41
1:A:175:TYR:HE2	1:A:274:GLN:HG3	1.85	0.41
1:A:440:LEU:HD12	1:A:484:ILE:HD11	2.03	0.41
2:B:160:GLU:HG3	2:B:189:TRP:NE1	2.36	0.41
2:B:231:VAL:HG23	2:B:454:VAL:HA	2.01	0.41
2:B:634:LYS:HB3	2:B:634:LYS:HE3	1.82	0.41
4:D:160:LEU:HD23	4:D:160:LEU:HA	1.84	0.41
8:H:107:PHE:O	8:H:111:ASN:ND2	2.53	0.41
2:B:180:LEU:HB3	2:B:191:PRO:HB3	2.02	0.41
3:C:411:MET:HE2	3:C:411:MET:HA	2.01	0.41
3:C:497:LEU:HD12	3:C:497:LEU:HA	1.86	0.41
4:D:417:ASP:O	4:D:420:LEU:HG	2.21	0.41
6:F:108:ASN:N	6:F:108:ASN:HD22	2.17	0.41
4:D:163:MET:HE1	4:D:184:LEU:HB3	2.04	0.40
10:N:186:ILE:HD13	10:N:186:ILE:HA	1.87	0.40
1:A:65:MET:HG3	1:A:146:THR:OG1	2.20	0.40
2:B:412:LYS:H	2:B:412:LYS:HG2	1.65	0.40
4:D:404:THR:HG22	7:G:9:LEU:HB3	2.03	0.40
6:F:70:LEU:HD22	6:F:114:GLU:HB3	2.02	0.40
6:F:145:HIS:CE1	6:F:149:LYS:HE3	2.57	0.40
1:A:87:GLU:OE2	1:A:145:LYS:NZ	2.52	0.40
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.86	0.40
4:D:204:LEU:HD23	4:D:204:LEU:HA	1.77	0.40
4:D:438:LYS:HE3	7:G:38:ILE:O	2.22	0.40
5:E:58:MET:HG2	5:E:163:THR:HG22	2.04	0.40
9:I:907:ASN:OD1	9:I:908:ARG:N	2.53	0.40
2:B:485:LEU:HA	2:B:485:LEU:HD23	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:127:LYS:HD2	4:D:127:LYS:HA	1.73	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	617/797 (77%)	591 (96%)	26 (4%)	0	100	100
2	B	688/771 (89%)	660 (96%)	28 (4%)	0	100	100
3	C	150/591 (25%)	146 (97%)	4 (3%)	0	100	100
4	D	431/462 (93%)	420 (97%)	11 (3%)	0	100	100
5	E	368/395 (93%)	353 (96%)	15 (4%)	0	100	100
6	F	256/308 (83%)	247 (96%)	9 (4%)	0	100	100
7	G	66/71 (93%)	63 (96%)	3 (4%)	0	100	100
8	H	73/309 (24%)	72 (99%)	1 (1%)	0	100	100
9	I	37/940 (4%)	34 (92%)	3 (8%)	0	100	100
10	N	169/273 (62%)	161 (95%)	8 (5%)	0	100	100
All	All	2855/4917 (58%)	2747 (96%)	108 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	554/702 (79%)	545 (98%)	9 (2%)	55	69
2	B	606/675 (90%)	591 (98%)	15 (2%)	42	63
3	C	139/513 (27%)	136 (98%)	3 (2%)	45	65
4	D	378/399 (95%)	372 (98%)	6 (2%)	55	69
5	E	332/352 (94%)	321 (97%)	11 (3%)	33	58
6	F	231/272 (85%)	225 (97%)	6 (3%)	40	62
7	G	61/64 (95%)	59 (97%)	2 (3%)	33	58
8	H	75/283 (26%)	74 (99%)	1 (1%)	61	72
9	I	32/804 (4%)	30 (94%)	2 (6%)	16	44
10	N	161/233 (69%)	158 (98%)	3 (2%)	50	67
All	All	2569/4297 (60%)	2511 (98%)	58 (2%)	44	64

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ARG
1	A	87	GLU
1	A	177	VAL
1	A	181	HIS
1	A	268	VAL
1	A	395	ASP
1	A	477	ILE
1	A	615	PHE
1	A	701	LEU
2	B	51	SER
2	B	207	TYR
2	B	242	VAL
2	B	323	ILE
2	B	333	LEU
2	B	336	LEU
2	B	383	LEU
2	B	418	ILE
2	B	453	SER
2	B	466	ILE
2	B	471	LEU
2	B	531	VAL
2	B	567	LEU
2	B	632	ILE
2	B	709	THR

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Mol	Chain	Res	Type
3	C	424	SER
3	C	431	ILE
3	C	449	ILE
4	D	96	TRP
4	D	164	VAL
4	D	178	LEU
4	D	230	LEU
4	D	271	VAL
4	D	315	LEU
5	E	62	TYR
5	E	70	THR
5	E	128	ILE
5	E	150	SER
5	E	163	THR
5	E	188	THR
5	E	210	VAL
5	E	265	GLN
5	E	354	ASP
5	E	362	VAL
5	E	363	CYS
6	F	27	LEU
6	F	50	PHE
6	F	131	THR
6	F	147	MET
6	F	215	LEU
6	F	276	CYS
7	G	3	ASN
7	G	21	LEU
8	H	74	ILE
9	I	911	GLU
9	I	916	LEU
10	N	119	ASN
10	N	140	THR
10	N	239	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	HIS
1	A	97	GLN
1	A	154	GLN
1	A	187	HIS

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Mol	Chain	Res	Type
1	A	286	HIS
1	A	433	GLN
1	A	499	ASN
1	A	564	ASN
1	A	598	HIS
1	A	603	ASN
1	A	665	GLN
1	A	711	GLN
1	A	714	GLN
2	B	4	ASN
2	B	21	GLN
2	B	92	ASN
2	B	201	HIS
2	B	210	HIS
2	B	241	ASN
2	B	250	ASN
2	B	279	GLN
2	B	363	GLN
2	B	555	GLN
2	B	645	GLN
2	B	698	GLN
2	B	700	HIS
2	B	707	ASN
3	C	474	HIS
3	C	509	GLN
3	C	524	HIS
3	C	530	GLN
3	C	537	HIS
4	D	20	GLN
4	D	289	ASN
4	D	312	ASN
4	D	390	GLN
5	E	99	ASN
5	E	256	GLN
5	E	324	HIS
5	E	355	GLN
6	F	48	HIS
6	F	63	HIS
6	F	145	HIS
6	F	179	ASN
6	F	240	GLN
7	G	3	ASN

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Mol	Chain	Res	Type
8	H	111	ASN
8	H	129	ASN
9	I	914	GLN
10	N	120	HIS
10	N	210	ASN
10	N	216	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 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
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.

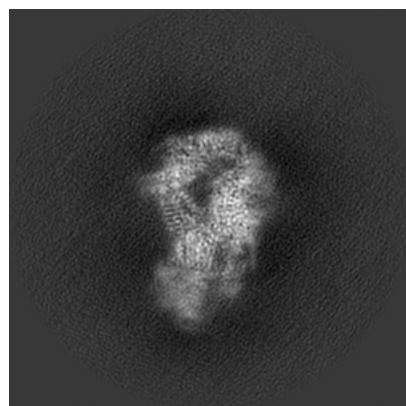
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56573. These allow visual inspection of the internal detail of the map and identification of artifacts.

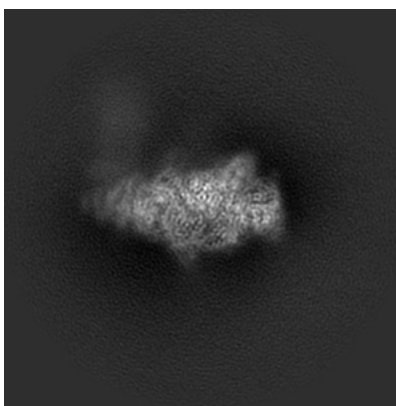
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

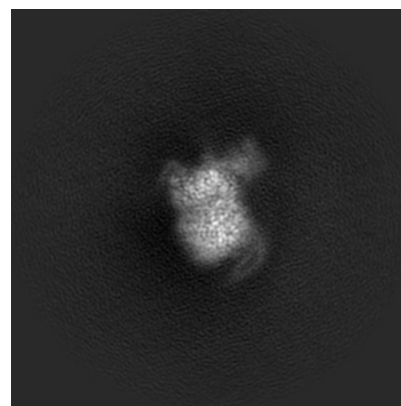
6.1.1 Primary map



X

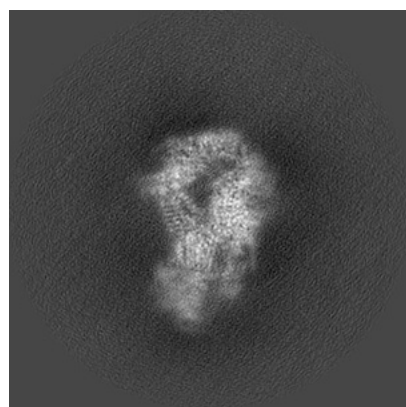


Y

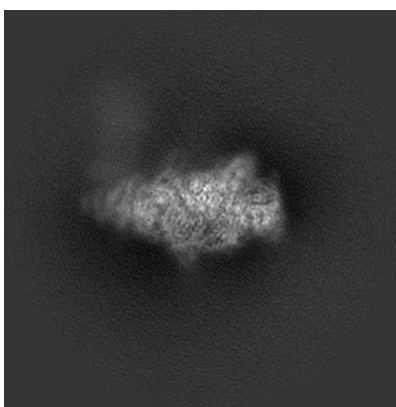


Z

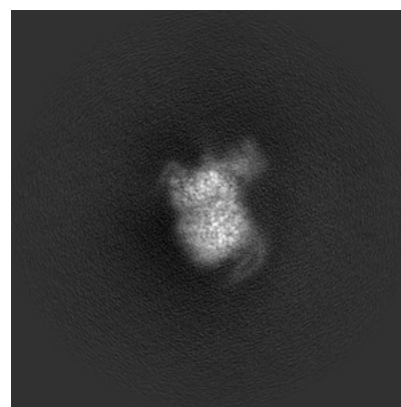
6.1.2 Raw map



X



Y

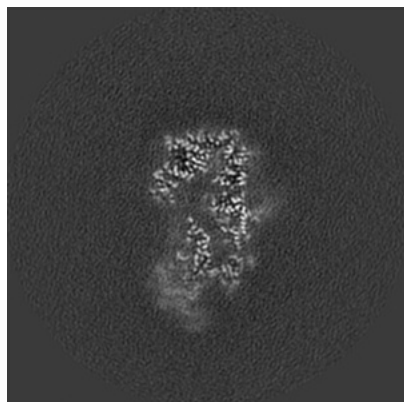


Z

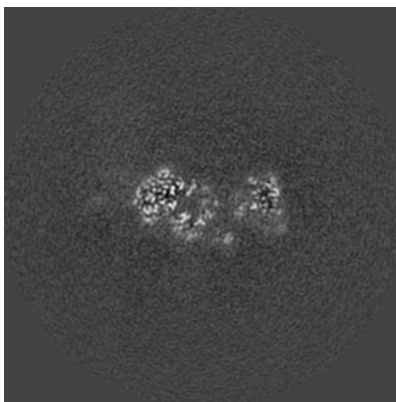
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

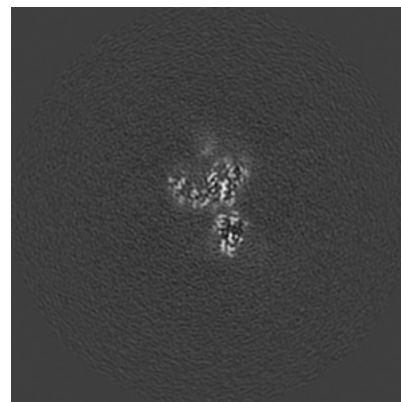
6.2.1 Primary map



X Index: 140

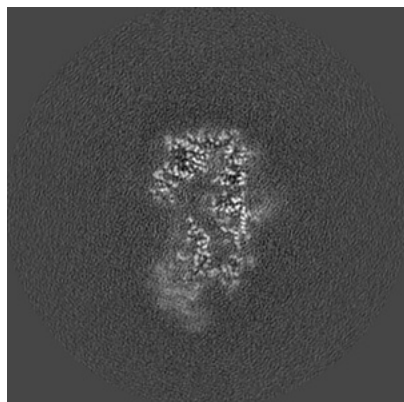


Y Index: 140

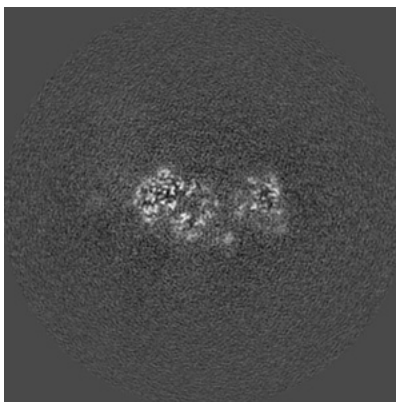


Z Index: 140

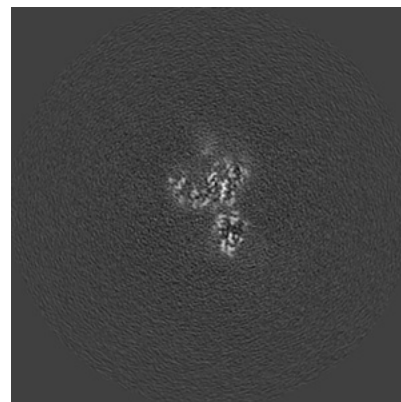
6.2.2 Raw map



X Index: 140



Y Index: 140

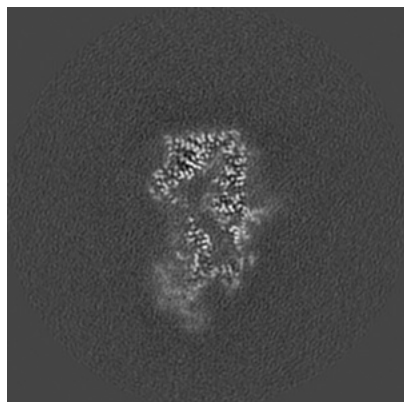


Z Index: 140

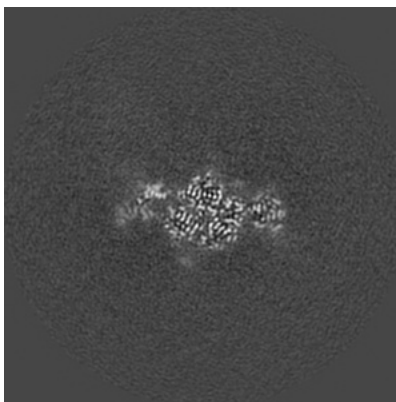
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

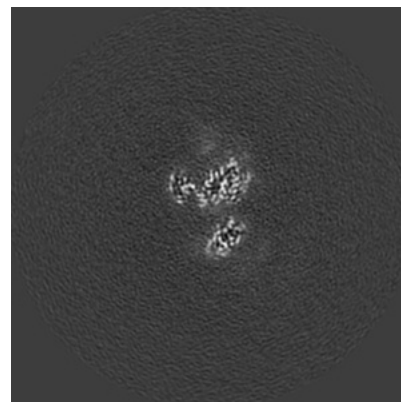
6.3.1 Primary map



X Index: 141

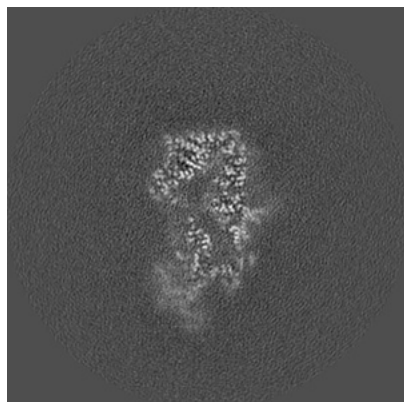


Y Index: 154

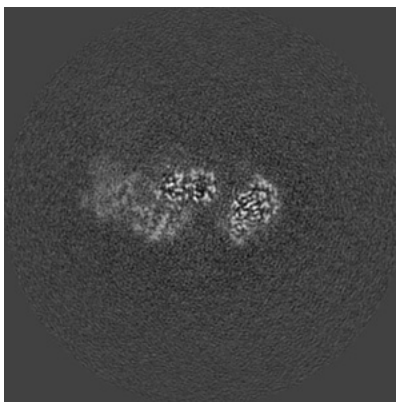


Z Index: 144

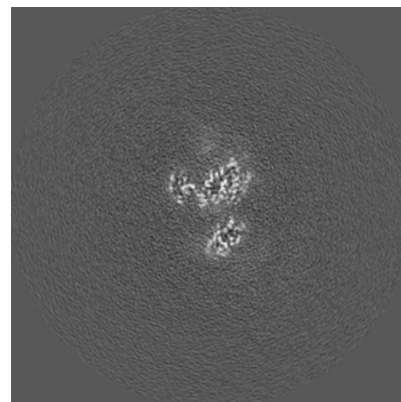
6.3.2 Raw map



X Index: 141



Y Index: 126

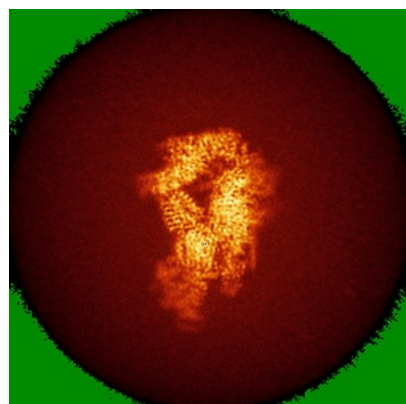


Z Index: 144

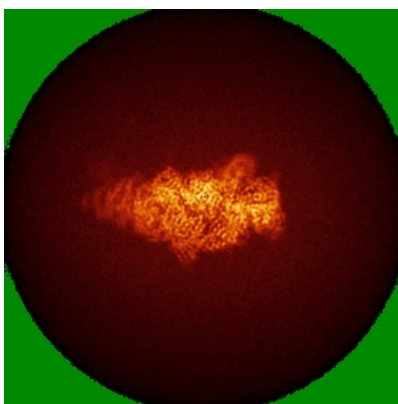
The images above show the largest variance slices of the map in three orthogonal directions.

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

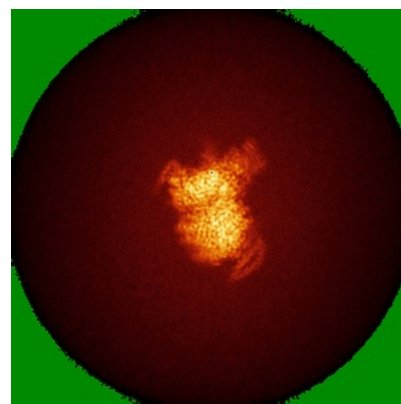
6.4.1 Primary map



X

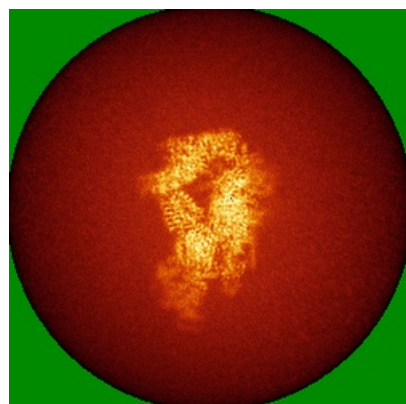


Y

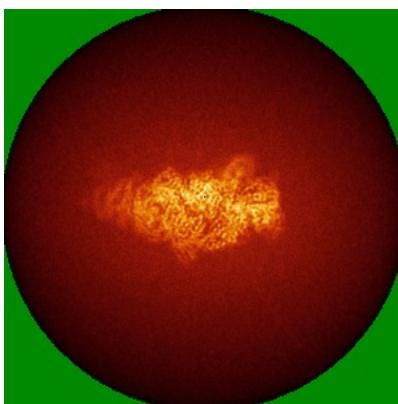


Z

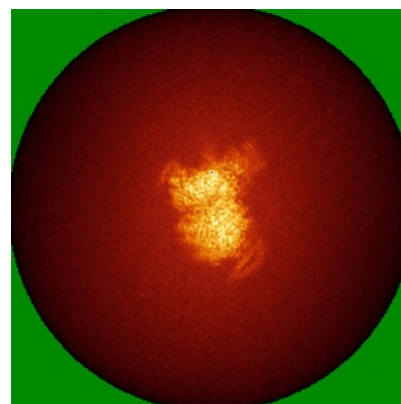
6.4.2 Raw map



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.

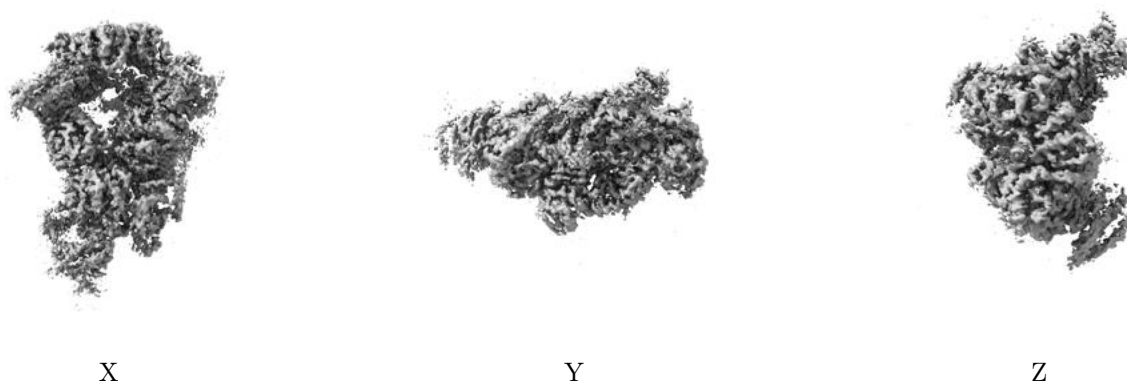
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0133. 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.

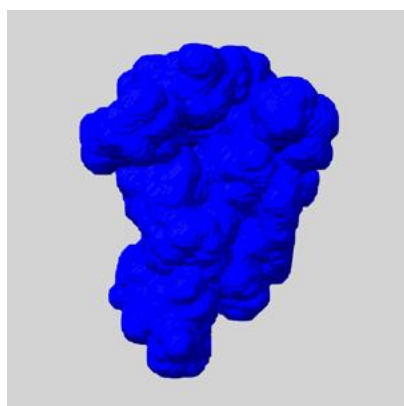
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

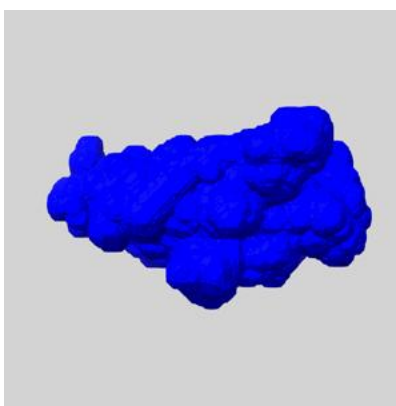
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

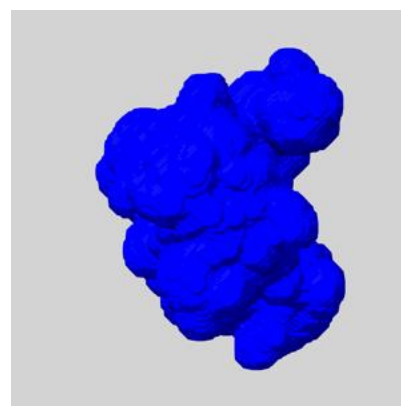
6.6.1 emd_56573_msk_1.map [i](#)



X



Y

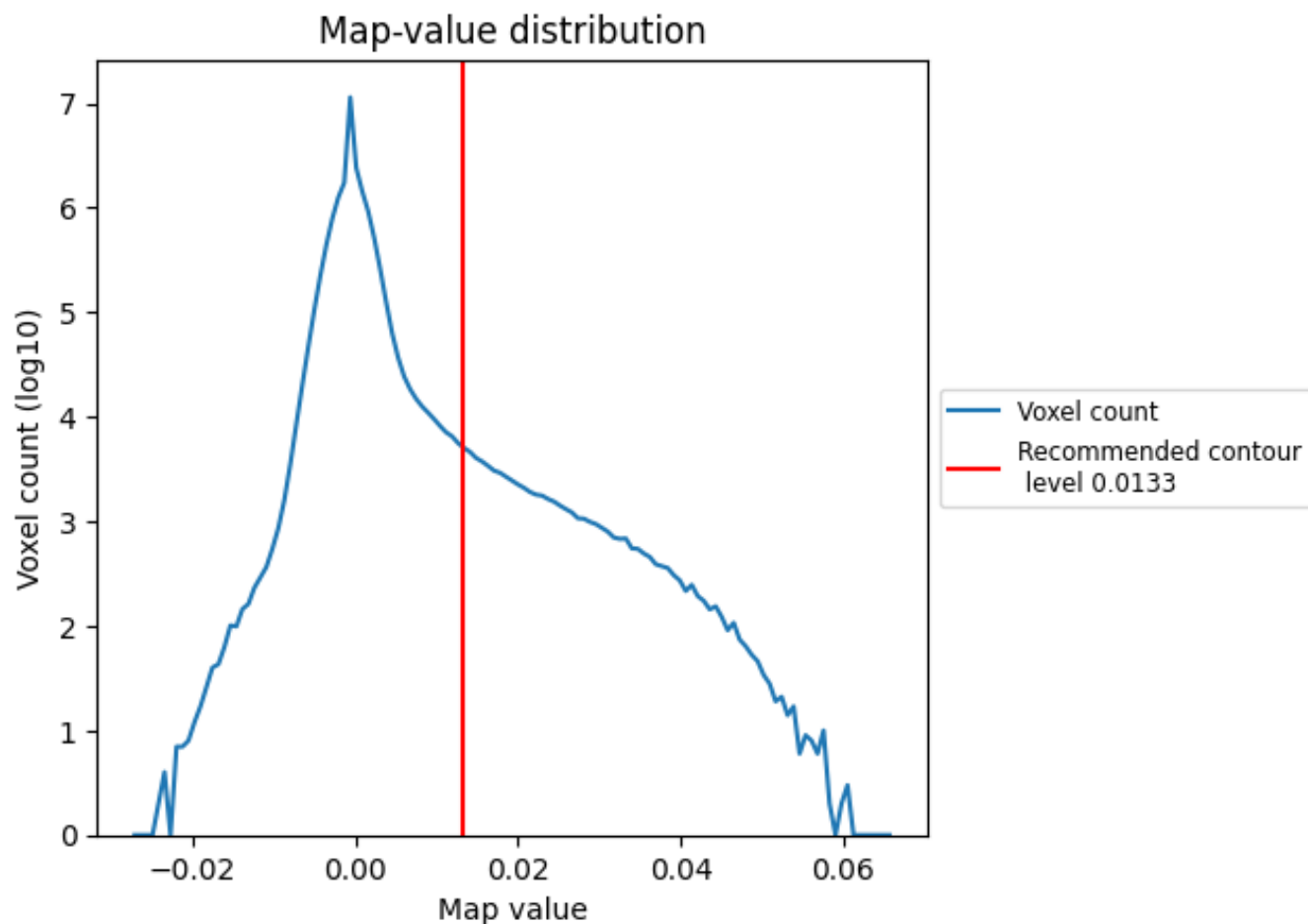


Z

7 Map analysis [i](#)

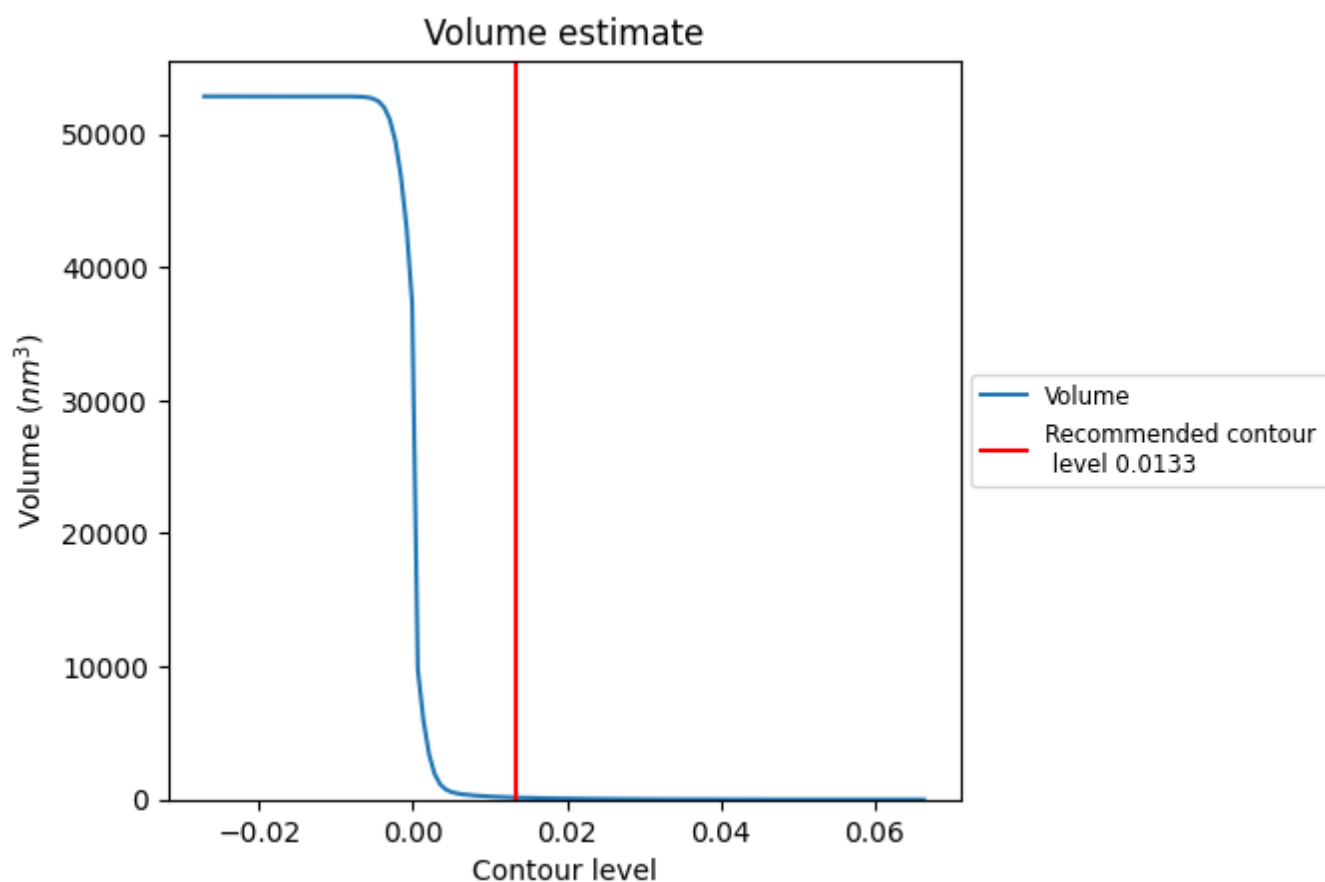
This section contains the results of statistical analysis of the map.

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.

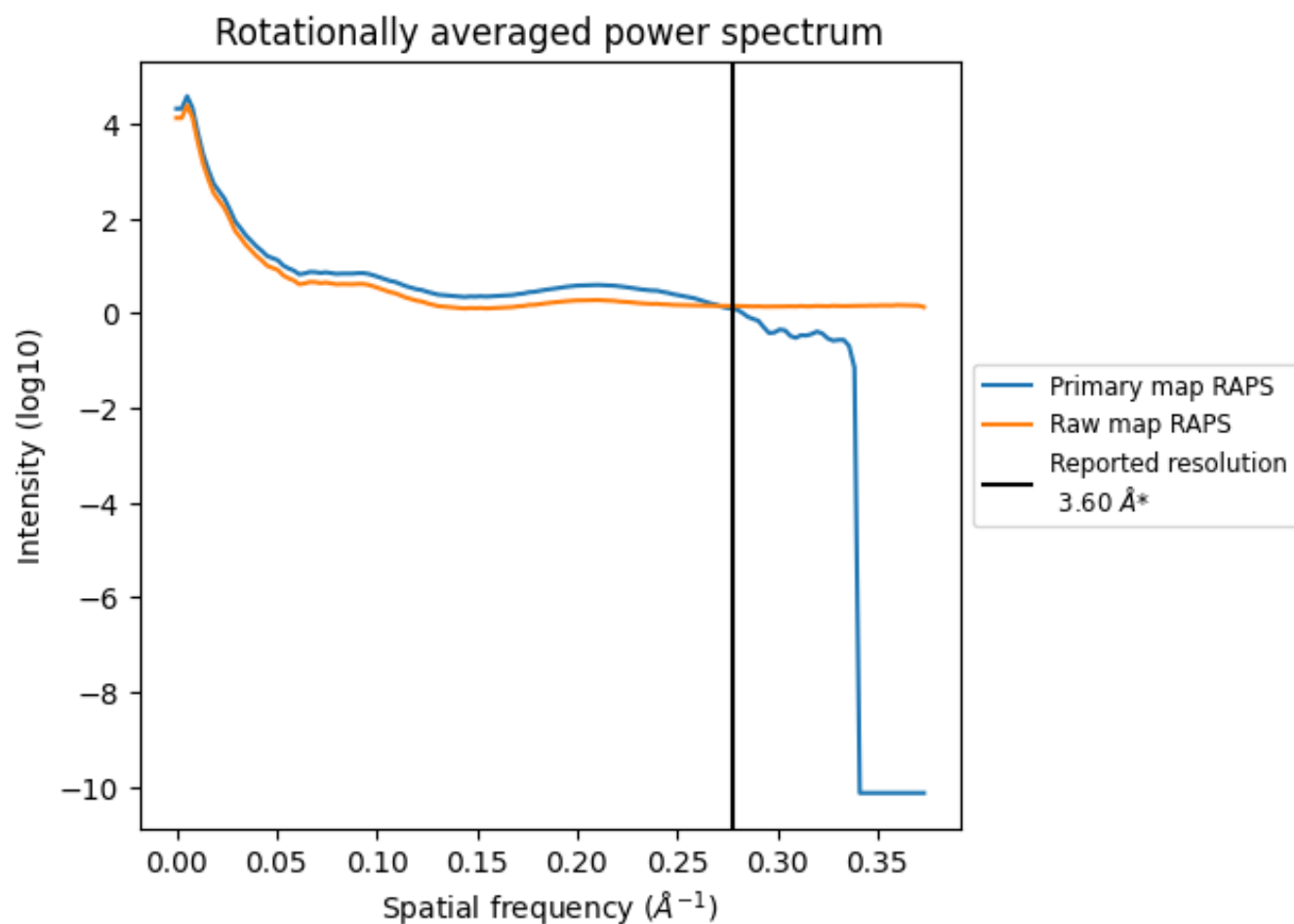
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 151 nm³; this corresponds to an approximate mass of 137 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 ⓘ

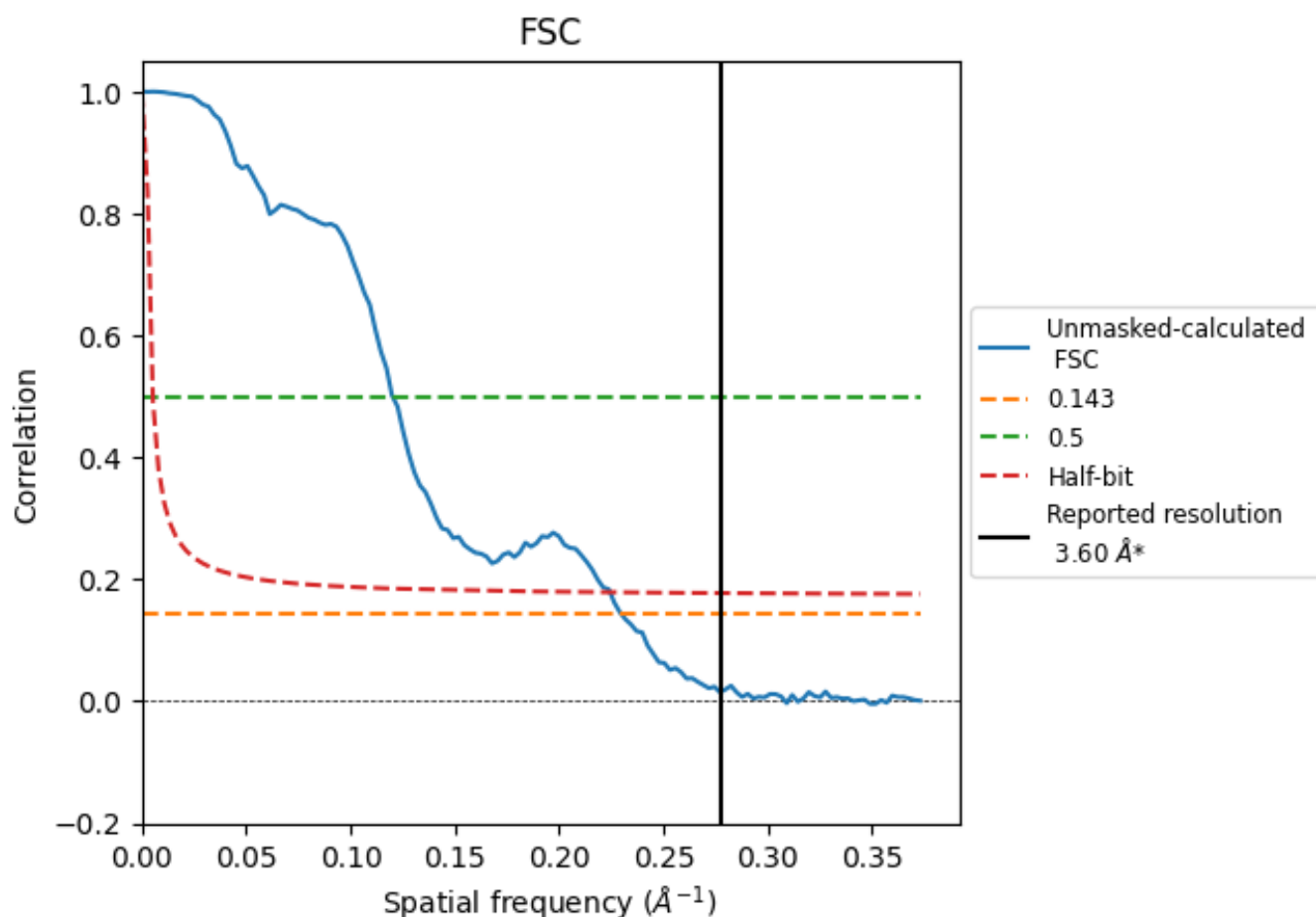


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

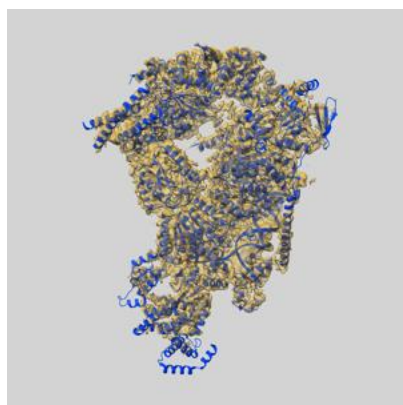
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.35	8.32	4.45

*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 4.35 differs from the reported value 3.6 by more than 10 %

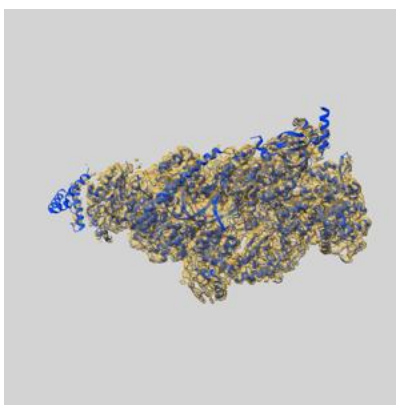
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-56573 and PDB model 28KE. Per-residue inclusion information can be found in section 3 on page 9.

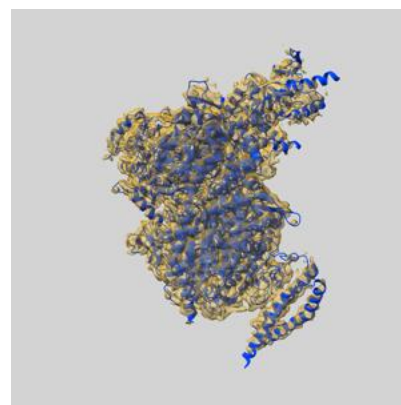
9.1 Map-model overlay [i](#)



X



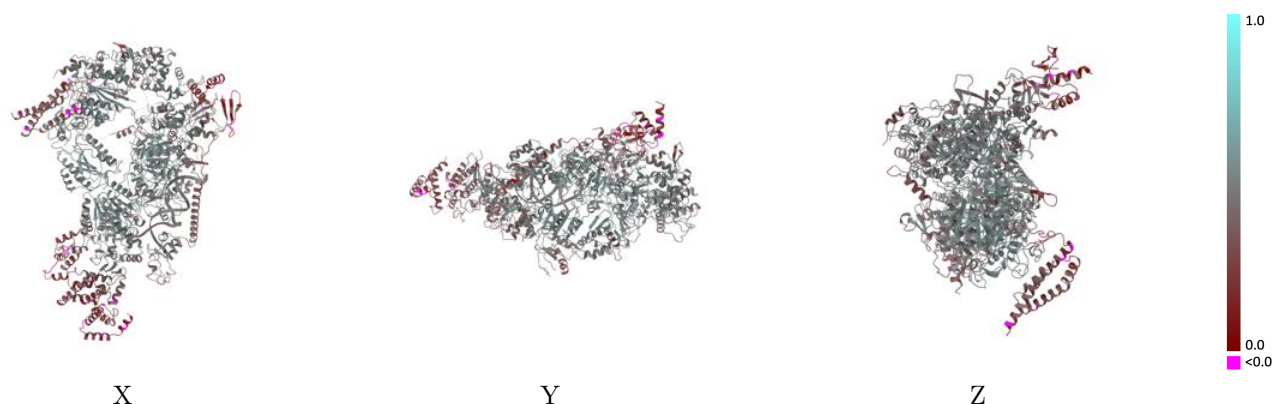
Y



Z

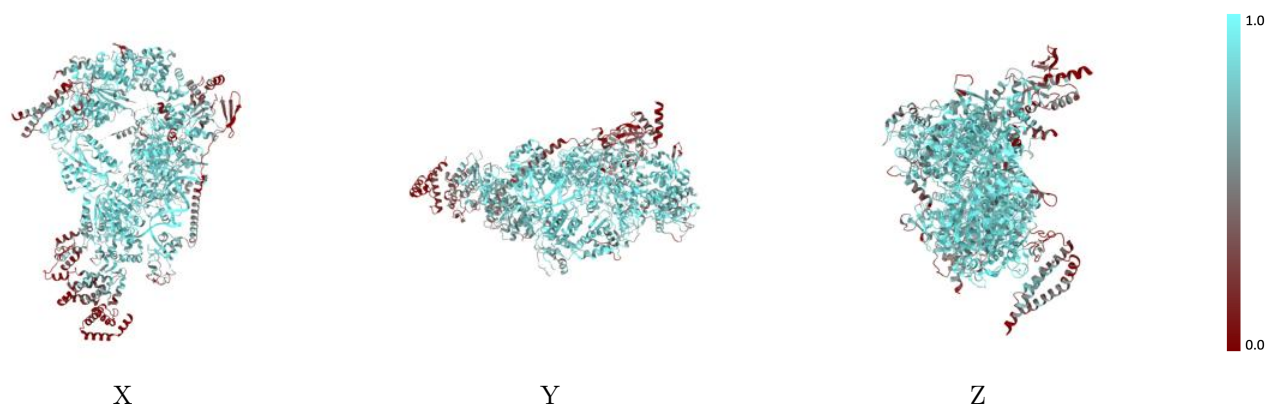
The images above show the 3D surface view of the map at the recommended contour level 0.0133 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



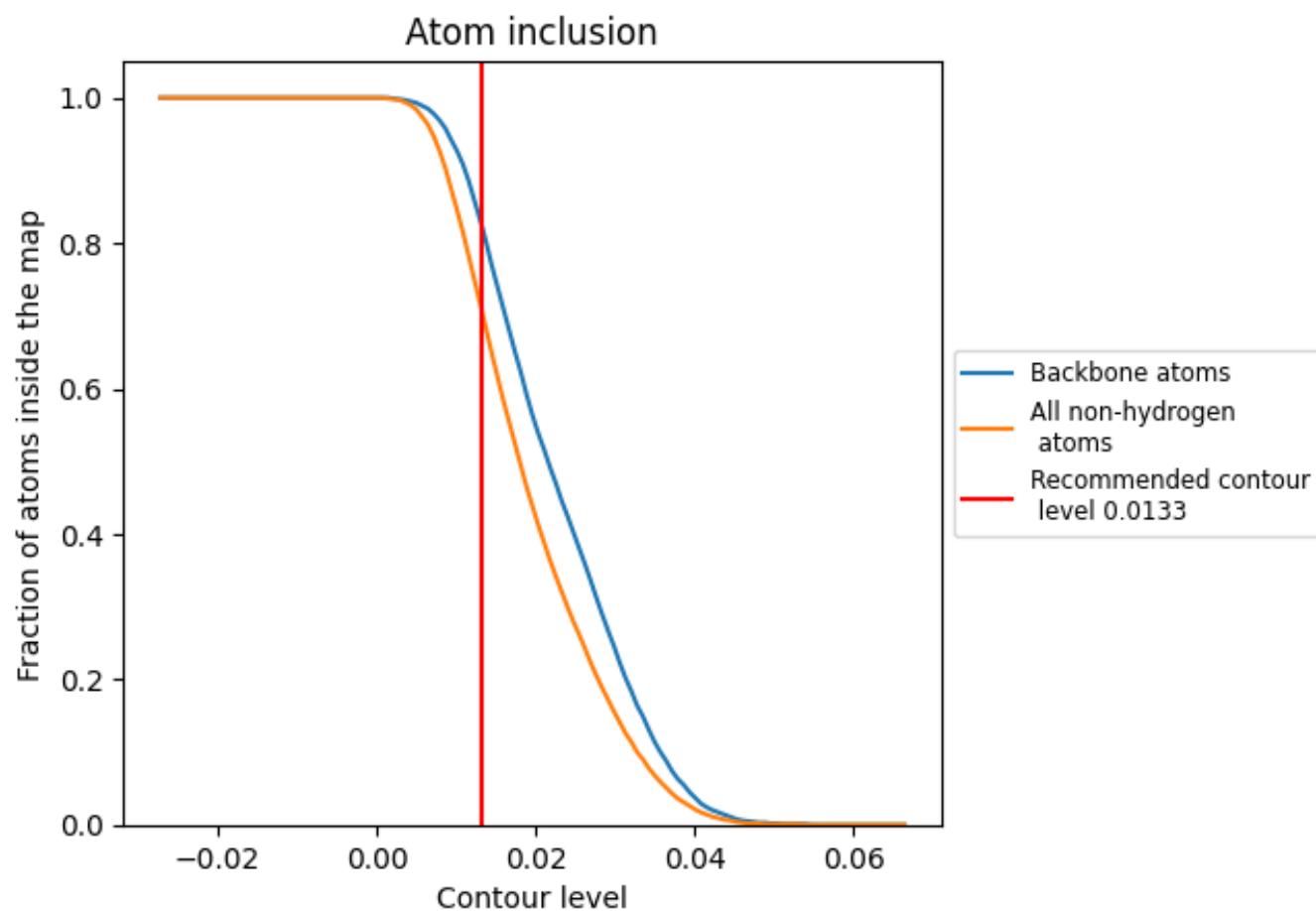
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0133).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 70% 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 (0.0133) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7050	0.4420
A	0.8250	0.5010
B	0.6570	0.4020
C	0.4700	0.3310
D	0.7290	0.4500
E	0.8090	0.4990
F	0.8460	0.5110
G	0.6910	0.4310
H	0.0510	0.1950
I	0.3600	0.4240
L	0.9180	0.4630
M	0.8990	0.4460
N	0.4530	0.3570

1.0

0.0

<0.0