



Full wwPDB EM Validation Report ⓘ

Apr 28, 2026 – 01:18 pm BST

PDB ID : 28JM / pdb_000028jm
EMDB ID : EMD-56544
Title : Cryo-EM structure of the human holo-TFIIH and XPC initial encounter complex
Authors : de Martin Garrido, N.; Haste, C.A.F.; Feng, J.; Cronin, N.B.; Greber, B.J.
Deposited on : 2026-02-03
Resolution : 3.29 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:

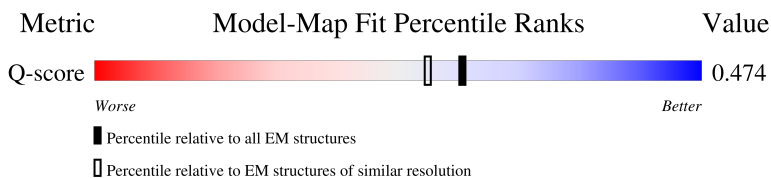
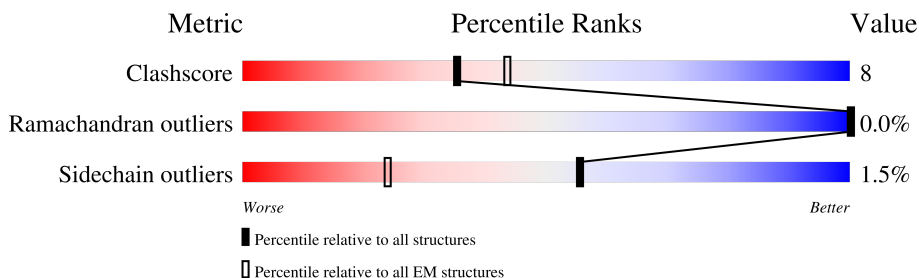
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.29 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	14466 (2.79 - 3.79)

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	<div><div></div><div>6%</div><div>83%</div><div>10%</div><div>7%</div></div>
6	F	308	<div><div></div><div>73%</div><div>12%</div><div>15%</div></div>
7	G	71	<div><div></div><div>39%</div><div>58%</div><div>32%</div><div>7%</div></div>
8	H	309	<div><div></div><div>28%</div><div>46%</div><div>21%</div><div>32%</div></div>
9	I	940	<div><div></div><div>99%</div></div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 25112 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	649	Total	C	N	O	S	0	0
			5246	3350	903	962	31		

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	760	Total	C	N	O	S	0	0
			6120	3907	1067	1117	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	374	Total	C	N	O	S	0	0
			3018	1919	525	560	14		

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	450	Total	C	N	O	S	0	0
			3592	2312	628	638	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	369	Total	C	N	O	S	0	0
			2893	1824	499	543	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	263	Total	C	N	O	S	0	0
			2066	1323	344	380	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	66	Total	C	N	O	S	0	0
			522	336	83	100	3		

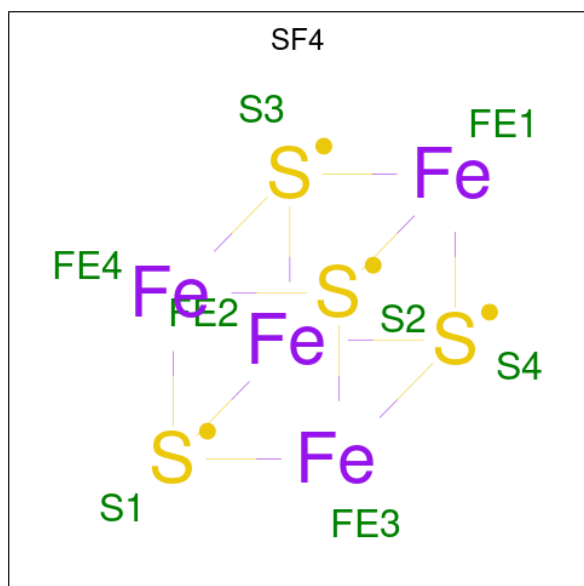
- Molecule 8 is a protein called CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	210	Total	C	N	O	S	0	0
			1592	986	281	316	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	6	Total	C	N	O		0	0
			48	32	6	10			

- Molecule 10 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

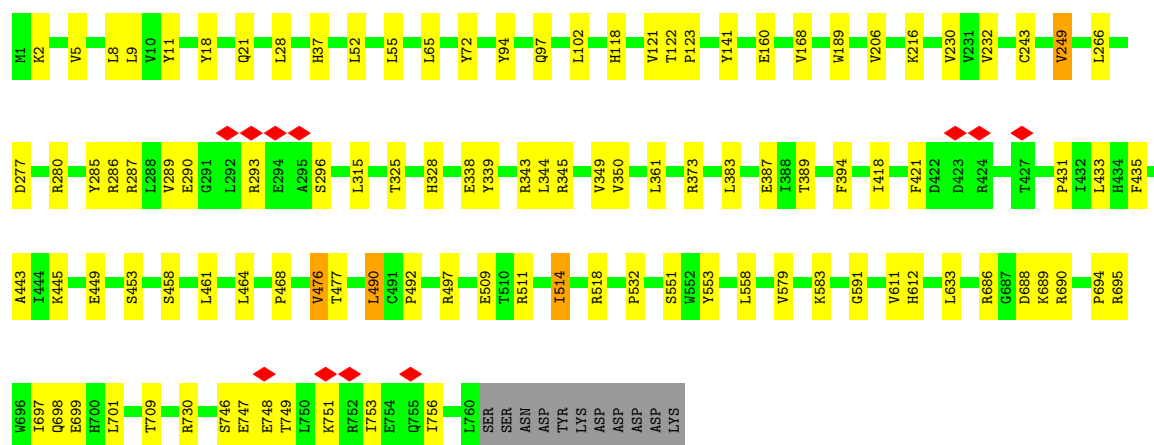
- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

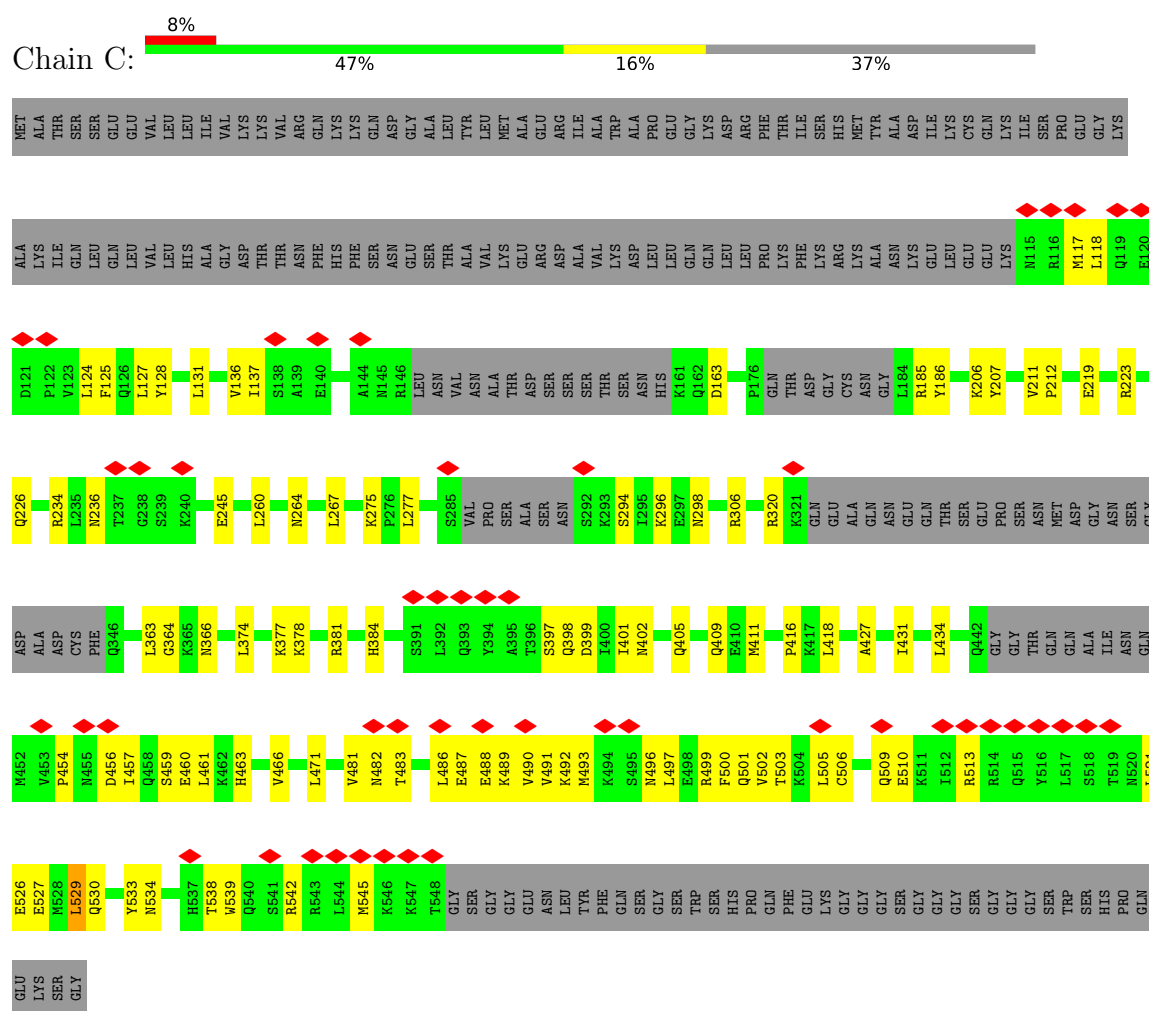
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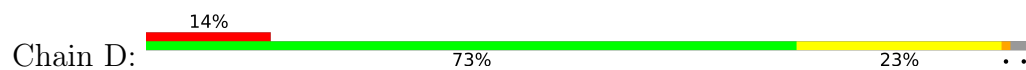
Mol	Chain	Residues	Atoms		AltConf
11	F	2	Total 2	Zn 2	0
11	H	2	Total 2	Zn 2	0

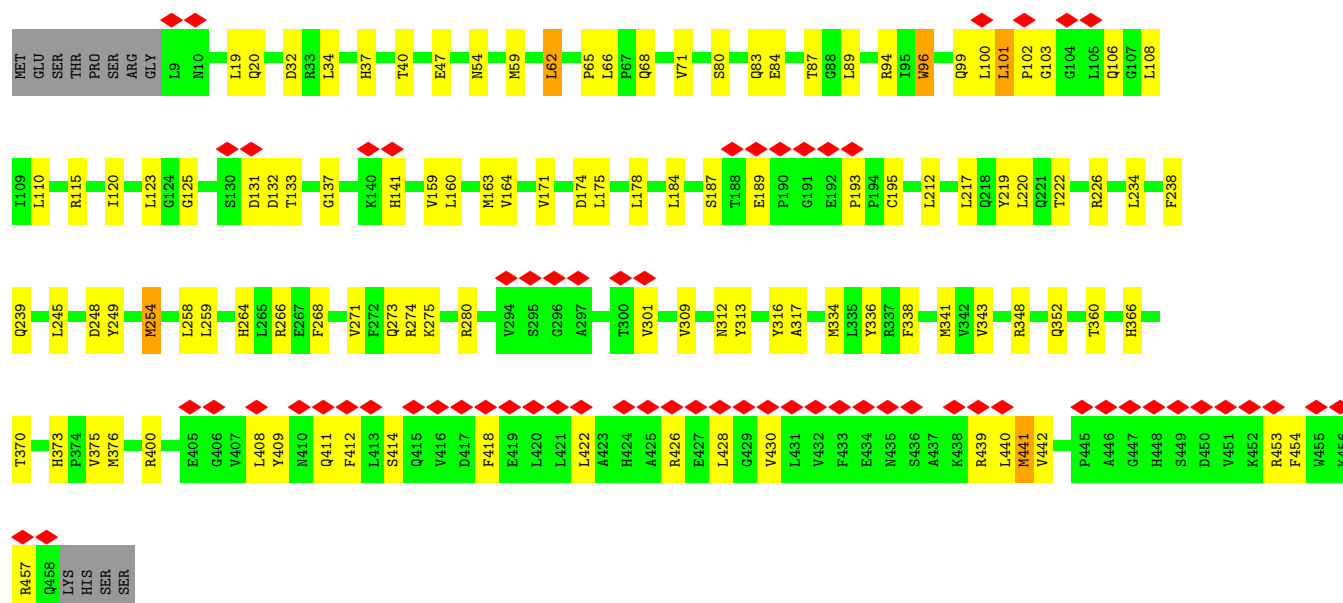


• Molecule 3: General transcription factor IIH subunit 1

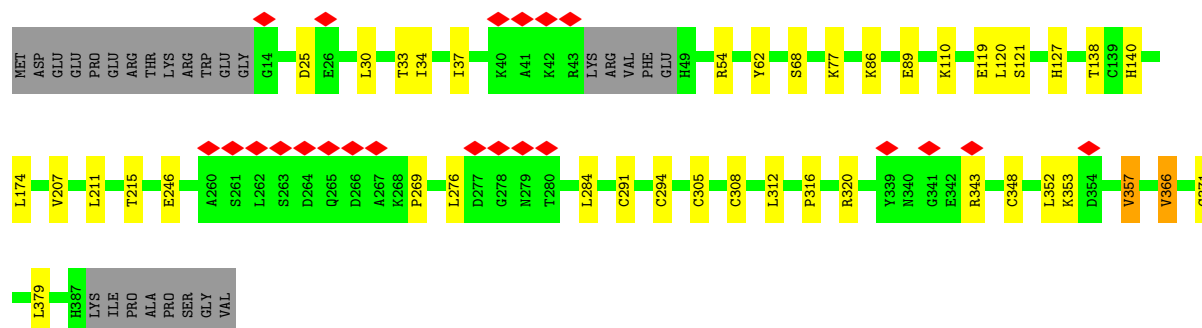
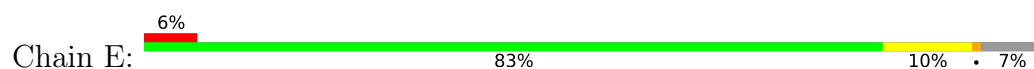


• Molecule 4: General transcription factor IIH subunit 4

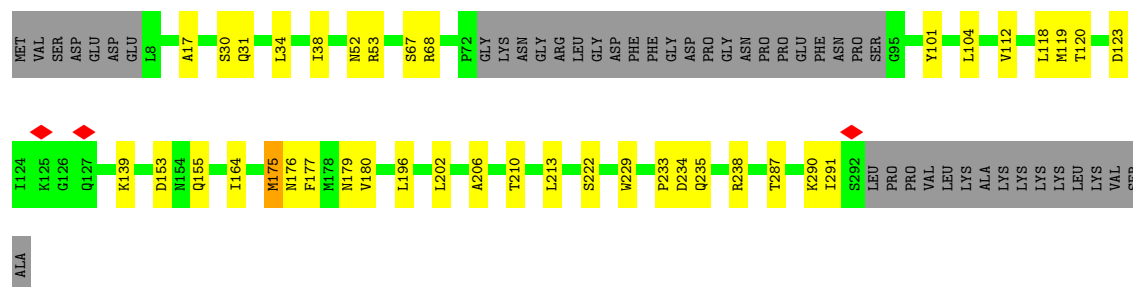




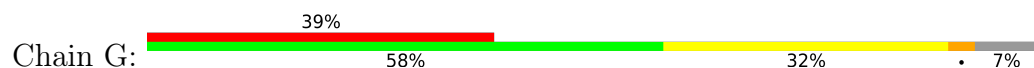
• Molecule 5: General transcription factor IIH subunit 2



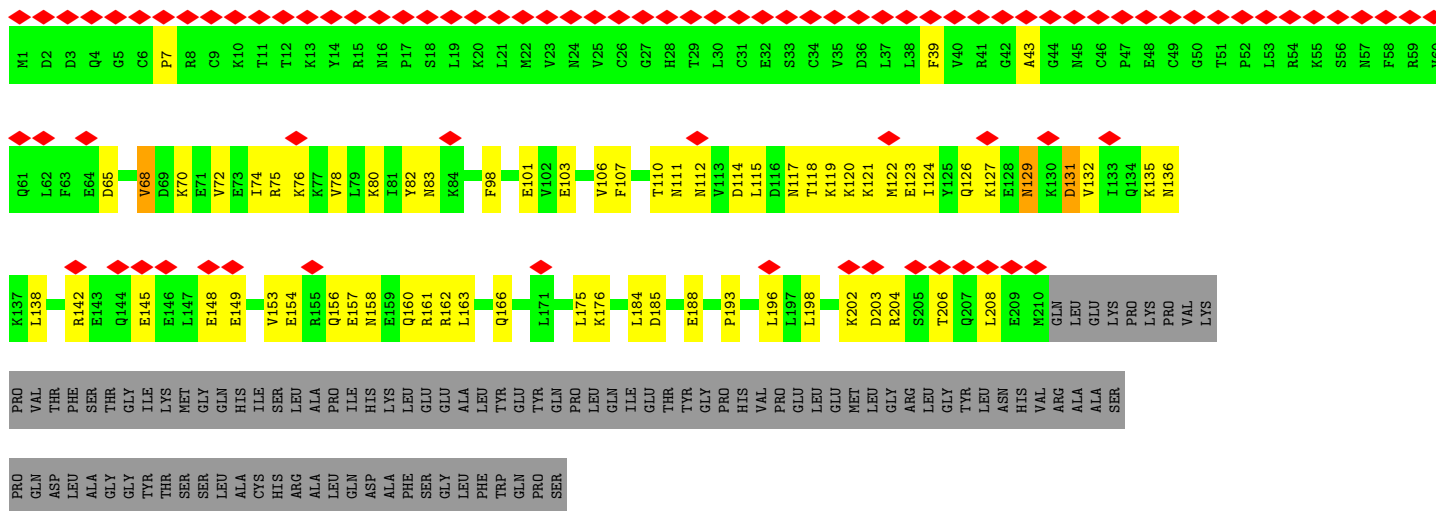
• Molecule 6: General transcription factor IIH subunit 3



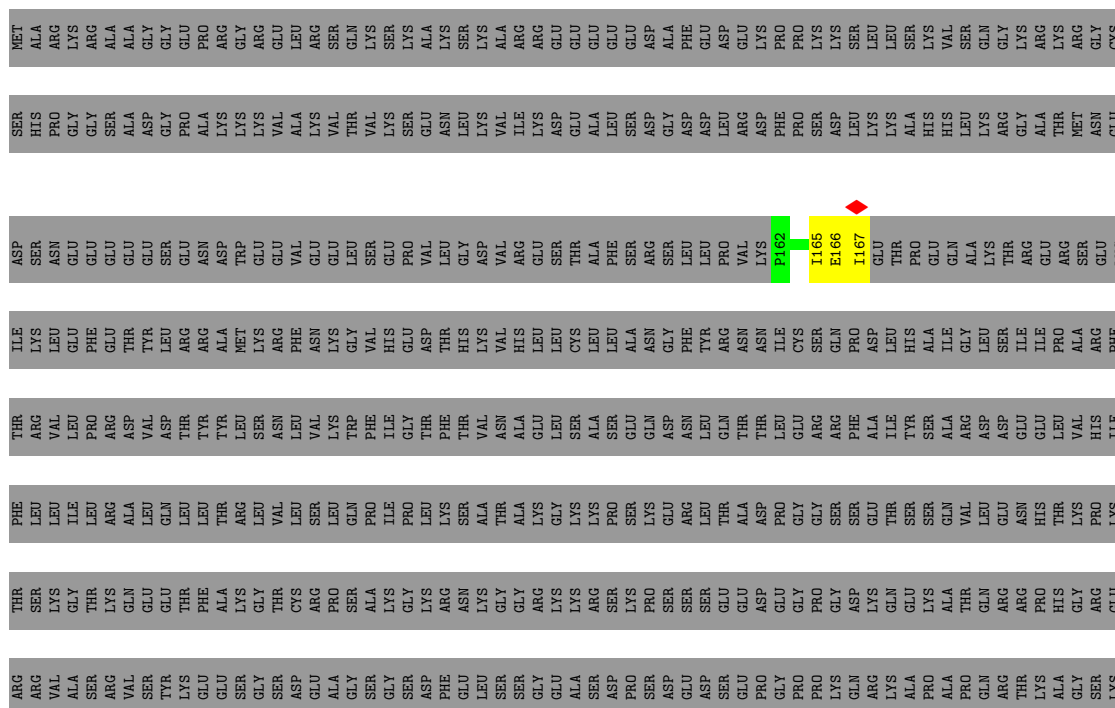
• Molecule 7: General transcription factor IIH subunit 5



- Molecule 8: CDK-activating kinase assembly factor MAT1



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



ALA	SER	TRP	ALA	ARG	VAL	LYS	VAL	PRO	GLU	THR	TRP	TRP	SER
SER	TRP	ALA	ARG	ALA	ARG	GLN	LYS	GLN	ALA	ALA	ALA	CYS	ALA
PRO	GLN	PRO	LYS	LEU	LEU	GLU	ILE	ILE	GLY	THR	THR	VAL	ARG
ASN	ASN	ASN	ASP	ASP	GLU	GLU	LEU	LEU	LEU	LEU	LEU	CYS	HIS
ARG	ARG	TRP	ILE	ASP	ILE	ASN	GLY	GLY	ARG	ARG	VAL	VAL	ARG
GLU	GLU	LYS	LYS	CYS	CYS	ASP	TYR	TYR	PRO	PRO	HIS	HIS	GLY
ASP	ASP	LEU	CYS	LEU	LEU	LEU	CYS	CYS	TYR	TYR	GLY	GLY	SER
GLU	GLU	LEU	VAL	VAL	VAL	GLY	ARG	ARG	GLN	GLN	VAL	VAL	HIS
GLU	GLU	ALA	GLN	GLN	GLN	LEU	GLY	GLY	SER	SER	THR	THR	LYS
LYS	LYS	ALA	ALA	PHE	PHE	PHE	GLU	GLU	ASP	GLU	GLY	GLY	ARG
GLN	GLN	GLY	ILE	ILE	ILE	GLY	ALA	ALA	PHE	PHE	GLN	GLN	ASP
LYS	LYS	LEU	LEU	LEU	THR	THR	VAL	VAL	TYR	MET	PRO	PRO	PRO
LEU	LEU	LEU	THR	THR	GLY	TRP	TYR	TYR	SER	ARG	THR	THR	SER
LYS	LYS	ILE	PHE	ASP	THR	GLN	SER	SER	ARG	GLU	THR	THR	SER
GLY	GLY	ARG	ASP	ASP	THR	GLU	GLY	GLY	LYS	LYS	LYS	LYS	PRO
GLY	GLY	GLU	PHE	PHE	PHE	GLU	GLU	GLU	ASP	ASP	THR	THR	ALA
PRO	PRO	ARG	HIS	HIS	HIS	GLU	CYS	CYS	ALA	LYS	LYS	LYS	ALA
LYS	LYS	LEU	GLY	GLY	GLY	TYR	VAL	VAL	VAL	VAL	VAL	VAL	SER
LYS	LYS	LEU	THR	THR	THR	GLN	ARG	ARG	ALA	ALA	ALA	ALA	SER
THR	THR	ARG	TYR	TYR	TYR	PRO	THR	THR	THR	THR	THR	THR	SER
LYS	LYS	ARG	SER	SER	SER	PRO	LEU	LEU	LEU	PHE	PRO	PRO	SER
ARG	ARG	TYR	HIS	HIS	HIS	VAL	HIS	SER	GLN	GLN	MET	MET	SER
GLU	GLU	GLY	PRO	PRO	PRO	ALA	SER	GLN	GLN	ASP	GLY	GLY	SER
LYS	LYS	PRO	VAL	VAL	VAL	VAL	ASP	ASP	ALA	ALA	THR	THR	SER
ALA	ALA	SER	THR	THR	THR	GLY	THR	ASP	THR	HIS	VAL	VAL	LYS
ALA	ALA	ALA	GLY	GLY	GLY	VAL	TRP	LYS	TRP	MET	ASP	VAL	GLY
ALA	ALA	ALA	TYR	TYR	TYR	VAL	LEU	LEU	ASP	ASP	GLY	GLY	GLY
SER	SER	ALA	ILE	ILE	ILE	PRO	LYS	PRO	GLN	GLN	ILE	ILE	LYS
HIS	HIS	LEU	VAL	VAL	VAL	ASN	LYS	LYS	PRO	PRO	ASP	ASP	MET
LEU	LEU	PRO	CYS	CYS	CYS	ASN	ALA	ALA	LEU	LEU	SER	SER	CYS
PHE	PHE	THR	GLU	GLU	GLU	GLU	ARG	ARG	PRO	THR	GLY	ASP	SER
PRO	PRO	THR	THR	THR	THR	PHE	VAL	VAL	THR	THR	THR	THR	ASP
GLU	GLU	GLY	PHE	PHE	PHE	GLY	VAL	VAL	VAL	ALA	TRP	GLY	GLY
GLU	GLU	GLY	ASP	ASP	ASP	ASN	ARG	ASN	ILE	ILE	VAL	VAL	GLU
GLN	GLN	LEU	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ASP	ALA	LYS
LEU	LEU	LEU	VAL	VAL	VAL	LEU	GLU	GLU	LEU	THR	THR	THR	LYS
			THR	THR	THR	PHE	VAL	LEU	PRO	ASN	GLN	ARG	ARG
			ALA	ALA	ALA	PRO	TYR	LEU	HIS	PRO	ARG	SER	ILE
			THR	THR	THR	SER	LYS	TYR	PRO	THR	THR	TRP	TRP
			GLY	GLY	GLY	MET	ASN	ARG	GLY	ASP	VAL	ASP	GLY
			ILE	ILE	ILE	GLY	PHE	GLY	LEU	VAL	TRP	ASP	ILE
			THR	THR	THR	ILE	THR	THR	GLY	LEU	TRP	GLN	ASP
			GLY	GLY	GLY	GLY	PHE	GLY	LYS	LYS	MET	GLN	GLY
			VAL	VAL	VAL	GLY	ARG	GLY	ARG	THR	THR	TRP	LYS
			ALA	ALA	ALA	ASN							

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	323811	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	0.088	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0109	Depositor
Map size (Å)	375.2, 375.2, 375.2	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: SF4, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.10	0/5358	0.27	0/7233
2	B	0.11	0/6247	0.29	0/8457
3	C	0.14	0/3075	0.37	0/4142
4	D	0.11	0/3676	0.28	0/4984
5	E	0.10	0/2957	0.27	0/4002
6	F	0.09	0/2103	0.24	0/2846
7	G	0.16	0/528	0.48	0/713
8	H	0.13	0/1609	0.36	0/2170
9	I	0.06	0/48	0.19	0/64
All	All	0.11	0/25601	0.30	0/34611

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	5246	0	5261	96	0
2	B	6120	0	6164	65	0
3	C	3018	0	3045	74	0
4	D	3592	0	3636	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	2893	0	2852	26	0
6	F	2066	0	2097	26	0
7	G	522	0	528	16	0
8	H	1592	0	1461	46	0
9	I	48	0	50	3	0
10	B	8	0	0	0	0
11	E	3	0	0	0	0
11	F	2	0	0	0	0
11	H	2	0	0	0	0
All	All	25112	0	25094	395	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (395) 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:408:LEU:HD11	4:D:440:LEU:HG	1.50	0.91
3:C:137:ILE:HG22	3:C:496:ASN:HD21	1.39	0.88
5:E:269:PRO:HB3	5:E:284:LEU:HD21	1.62	0.81
8:H:114:ASP:OD1	8:H:117:ASN:ND2	2.18	0.76
3:C:501:GLN:HG3	3:C:505:LEU:HD12	1.67	0.76
1:A:469:THR:HG23	1:A:471:VAL:H	1.52	0.75
4:D:62:LEU:O	4:D:115:ARG:NH1	2.20	0.75
3:C:234:ARG:HH21	3:C:236:ASN:HD22	1.35	0.74
5:E:294:CYS:SG	5:E:308:CYS:HB3	2.27	0.73
3:C:496:ASN:HA	3:C:499:ARG:HE	1.53	0.73
3:C:124:LEU:HD12	3:C:127:LEU:HD11	1.70	0.72
2:B:52:LEU:HD21	2:B:232:VAL:HG11	1.72	0.72
2:B:747:GLU:HG3	2:B:751:LYS:HE3	1.73	0.71
2:B:753:ILE:HA	2:B:756:ILE:HD12	1.72	0.70
1:A:513:PRO:O	1:A:539:ASN:ND2	2.26	0.69
4:D:37:HIS:HE1	4:D:239:GLN:HB2	1.58	0.69
1:A:632:SER:HB2	1:A:635:GLN:HB2	1.74	0.68
1:A:542:ARG:HE	1:A:696:MET:HE3	1.57	0.68
2:B:695:ARG:NH2	2:B:699:GLU:OE2	2.26	0.68
2:B:72:TYR:HB3	2:B:206:VAL:HG13	1.76	0.67
4:D:19:LEU:HB3	4:D:47:GLU:HG2	1.76	0.67
3:C:534:ASN:O	3:C:538:THR:HG23	1.95	0.67
2:B:230:VAL:HG13	2:B:453:SER:HB2	1.76	0.66
1:A:574:ARG:HH22	1:A:712:LEU:HD11	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:422:LEU:O	4:D:426:ARG:HG3	1.96	0.66
3:C:500:PHE:HE1	3:C:505:LEU:HD21	1.60	0.66
1:A:581:TYR:HD1	1:A:582:GLY:H	1.44	0.66
2:B:286:ARG:HH12	2:B:290:GLU:HB2	1.60	0.66
3:C:186:TYR:HB2	9:I:165:ILE:HG23	1.77	0.65
4:D:101:LEU:HG	4:D:103:GLY:H	1.61	0.65
5:E:77:LYS:HE3	5:E:77:LYS:HA	1.78	0.65
4:D:336:TYR:HB2	4:D:343:VAL:HB	1.78	0.65
7:G:16:MET:O	7:G:20:LEU:HG	1.96	0.65
3:C:294:SER:O	3:C:298:ASN:ND2	2.31	0.64
2:B:476:VAL:HG12	2:B:477:THR:HG23	1.78	0.64
3:C:459:SER:O	3:C:463:HIS:ND1	2.31	0.64
1:A:664:SER:HG	1:A:667:THR:HG1	1.40	0.64
1:A:166:VAL:HG12	1:A:179:SER:HB2	1.80	0.63
5:E:348:CYS:HB3	5:E:371:CYS:SG	2.37	0.63
8:H:202:LYS:O	8:H:206:THR:HG23	2.00	0.62
3:C:525:ILE:O	3:C:529:LEU:HD22	2.00	0.61
3:C:118:LEU:HD22	3:C:125:PHE:HA	1.81	0.61
8:H:75:ARG:NH1	8:H:103:GLU:OE2	2.23	0.61
8:H:78:VAL:HG11	8:H:106:VAL:HG22	1.82	0.61
1:A:581:TYR:O	1:A:589:ARG:NH2	2.33	0.61
4:D:120:ILE:HG23	4:D:125:GLY:HA3	1.82	0.61
6:F:68:ARG:HE	6:F:118:LEU:HD12	1.64	0.60
8:H:203:ASP:OD1	8:H:204:ARG:N	2.34	0.60
3:C:506:CYS:HA	3:C:509:GLN:HG2	1.82	0.60
7:G:55:GLU:O	7:G:59:GLU:HG3	2.01	0.60
4:D:87:THR:HG23	4:D:96:TRP:HZ3	1.66	0.60
4:D:163:MET:HE1	4:D:184:LEU:HD13	1.83	0.60
3:C:523:SER:O	3:C:526:GLU:HG3	2.02	0.59
4:D:266:ARG:HD2	4:D:273:GLN:HB2	1.85	0.59
2:B:277:ASP:OD2	2:B:280:ARG:NH1	2.34	0.59
4:D:54:ASN:HD21	6:F:233:PRO:HG3	1.68	0.59
5:E:379:LEU:HD11	6:F:180:VAL:HG12	1.84	0.59
3:C:411:MET:HA	3:C:411:MET:HE2	1.85	0.59
3:C:416:PRO:HG3	6:F:112:VAL:HG21	1.85	0.58
4:D:254:MET:HE3	4:D:258:LEU:HB3	1.85	0.58
5:E:121:SER:OG	5:E:127:HIS:NE2	2.34	0.58
8:H:149:GLU:O	8:H:153:VAL:HG13	2.03	0.58
4:D:131:ASP:OD1	4:D:131:ASP:N	2.36	0.58
1:A:664:SER:OG	1:A:667:THR:OG1	2.14	0.58
8:H:76:LYS:O	8:H:80:LYS:HG2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:234:ARG:O	3:C:306:ARG:NH2	2.37	0.58
4:D:132:ASP:OD1	4:D:132:ASP:N	2.36	0.58
4:D:309:VAL:H	4:D:376:MET:HE1	1.67	0.57
2:B:349:VAL:HA	2:B:418:ILE:O	2.04	0.57
2:B:730:ARG:NH2	3:C:366:ASN:OD1	2.37	0.57
1:A:636:GLU:O	1:A:640:LEU:HG	2.03	0.57
3:C:466:VAL:HG22	5:E:276:LEU:HD21	1.85	0.57
1:A:446:ILE:O	1:A:472:ARG:NH2	2.37	0.57
6:F:101:TYR:HB3	6:F:104:LEU:HG	1.87	0.57
7:G:29:LEU:HD12	7:G:56:ARG:HD2	1.87	0.57
8:H:131:ASP:N	8:H:131:ASP:OD2	2.32	0.57
2:B:325:THR:HG22	2:B:328:HIS:H	1.69	0.57
1:A:361:CYS:SG	1:A:362:LEU:N	2.78	0.56
1:A:565:VAL:HG12	1:A:569:LYS:HD2	1.87	0.56
3:C:461:LEU:HD11	3:C:521:LEU:HB3	1.86	0.56
1:A:647:LYS:HD3	1:A:648:LYS:HZ3	1.69	0.56
6:F:213:LEU:HD13	6:F:238:ARG:HD3	1.87	0.56
2:B:730:ARG:NH1	3:C:364:GLY:O	2.34	0.56
3:C:501:GLN:HA	3:C:505:LEU:HG	1.88	0.56
2:B:315:LEU:HD11	2:B:373:ARG:HH11	1.71	0.56
4:D:34:LEU:HD11	4:D:234:LEU:HD23	1.87	0.56
5:E:54:ARG:NH2	6:F:287:THR:OG1	2.39	0.56
8:H:83:ASN:O	8:H:136:ASN:ND2	2.39	0.56
1:A:577:LYS:HD2	1:A:604:THR:HB	1.88	0.56
4:D:254:MET:HE2	4:D:259:LEU:HD22	1.87	0.56
1:A:254:GLN:HA	1:A:257:LYS:HD2	1.89	0.55
8:H:68:VAL:O	8:H:72:VAL:HG12	2.07	0.55
1:A:517:GLU:HA	1:A:520:ARG:HD2	1.87	0.55
1:A:87:GLU:OE2	1:A:145:LYS:NZ	2.39	0.55
3:C:490:VAL:HA	3:C:493:MET:HE2	1.88	0.55
5:E:343:ARG:NH2	5:E:352:LEU:O	2.39	0.55
8:H:112:ASN:HA	8:H:115:LEU:HD21	1.89	0.55
1:A:60:ASP:OD2	1:A:62:ARG:NH2	2.39	0.55
7:G:19:PHE:CZ	7:G:60:LEU:HD22	2.42	0.55
8:H:82:TYR:HE2	8:H:122:MET:HE1	1.72	0.55
1:A:369:VAL:HG12	1:A:373:GLN:HE21	1.72	0.55
1:A:693:LEU:HD12	1:A:693:LEU:H	1.72	0.55
3:C:539:TRP:O	3:C:542:ARG:HG3	2.06	0.55
6:F:206:ALA:O	6:F:210:THR:OG1	2.20	0.55
3:C:418:LEU:HB3	4:D:123:LEU:HD22	1.89	0.54
8:H:106:VAL:O	8:H:110:THR:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:68:GLN:HG2	4:D:108:LEU:HG	1.90	0.54
2:B:5:VAL:HG23	2:B:8:LEU:HB3	1.90	0.54
4:D:40:THR:HG22	4:D:238:PHE:HD2	1.72	0.54
4:D:101:LEU:HD12	4:D:102:PRO:HD2	1.90	0.54
2:B:249:VAL:HG23	2:B:435:PHE:HB3	1.90	0.54
2:B:532:PRO:HA	5:E:174:LEU:HD13	1.90	0.54
3:C:457:ILE:O	3:C:460:GLU:HG3	2.08	0.54
2:B:339:TYR:OH	2:B:343:ARG:NH2	2.40	0.53
1:A:186:GLN:O	1:A:190:GLN:HG2	2.07	0.53
1:A:517:GLU:O	1:A:520:ARG:HG2	2.09	0.53
3:C:506:CYS:O	3:C:510:GLU:HG2	2.09	0.53
1:A:505:VAL:HA	1:A:657:ALA:HB3	1.89	0.53
3:C:489:LYS:HA	3:C:492:LYS:HE3	1.89	0.53
4:D:71:VAL:O	4:D:83:GLN:NE2	2.41	0.53
7:G:38:ILE:HG22	7:G:40:ASP:H	1.72	0.53
1:A:251:PHE:O	1:A:255:MET:HG3	2.08	0.53
1:A:428:GLU:O	1:A:432:THR:OG1	2.26	0.53
2:B:141:TYR:HE1	2:B:389:THR:HG22	1.73	0.53
5:E:316:PRO:O	5:E:320:ARG:HG3	2.09	0.53
4:D:20:GLN:HE21	4:D:89:LEU:HD11	1.74	0.53
1:A:81:ASP:OD2	4:D:336:TYR:OH	2.25	0.53
5:E:343:ARG:HA	5:E:352:LEU:HD12	1.91	0.52
1:A:703:PHE:CE1	1:A:712:LEU:HD22	2.44	0.52
4:D:193:PRO:O	4:D:195:CYS:N	2.43	0.52
1:A:179:SER:HB3	1:A:185:ILE:HD11	1.92	0.52
4:D:411:GLN:HB3	4:D:439:ARG:HB3	1.92	0.52
5:E:305:CYS:HB3	5:E:308:CYS:SG	2.49	0.52
1:A:596:PHE:HD1	1:A:602:ILE:HG22	1.74	0.52
1:A:666:ASP:OD2	4:D:400:ARG:NH2	2.43	0.52
5:E:357:VAL:HG13	5:E:366:VAL:HG23	1.91	0.52
4:D:248:ASP:OD1	4:D:248:ASP:N	2.43	0.52
8:H:107:PHE:O	8:H:111:ASN:ND2	2.42	0.52
8:H:82:TYR:CE2	8:H:122:MET:HE1	2.44	0.52
3:C:397:SER:O	3:C:401:ILE:HG12	2.10	0.51
1:A:492:ASN:HB3	1:A:495:GLU:HB3	1.92	0.51
8:H:74:ILE:O	8:H:78:VAL:HG12	2.10	0.51
3:C:411:MET:HG3	6:F:119:MET:HG2	1.92	0.51
3:C:488:GLU:O	3:C:491:VAL:HG22	2.10	0.51
8:H:154:GLU:O	8:H:157:GLU:HG3	2.11	0.51
2:B:28:LEU:HB3	2:B:55:LEU:HD22	1.93	0.51
3:C:226:GLN:HE22	9:I:167:ILE:HD13	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:219:GLU:OE2	3:C:223:ARG:NH2	2.37	0.51
1:A:408:SER:OG	1:A:409:THR:N	2.42	0.51
3:C:378:LYS:HB2	3:C:381:ARG:HD2	1.93	0.50
4:D:101:LEU:H	4:D:106:GLN:HA	1.76	0.50
1:A:360:ARG:NH1	1:A:433:GLN:OE1	2.45	0.50
2:B:285:TYR:O	2:B:289:VAL:HG22	2.12	0.50
1:A:273:LYS:HD2	1:A:276:MET:HE3	1.93	0.50
1:A:521:GLU:HG3	1:A:713:LEU:HD11	1.93	0.50
5:E:343:ARG:HH22	5:E:353:LYS:HD3	1.77	0.50
4:D:366:HIS:O	4:D:370:THR:OG1	2.26	0.50
1:A:178:GLU:HG2	1:A:269:SER:HB3	1.92	0.50
3:C:117:MET:SD	3:C:117:MET:N	2.84	0.50
1:A:590:MET:O	1:A:590:MET:HE3	2.11	0.50
2:B:497:ARG:HB2	2:B:709:THR:HG22	1.94	0.50
8:H:70:LYS:O	8:H:74:ILE:HG12	2.11	0.50
2:B:511:ARG:NH1	2:B:551:SER:HB2	2.26	0.50
8:H:118:THR:HA	8:H:121:LYS:HD2	1.93	0.50
3:C:398:GLN:O	3:C:402:ASN:ND2	2.45	0.49
4:D:418:PHE:HB3	4:D:441:MET:HE1	1.94	0.49
1:A:319:TYR:OH	1:A:344:ALA:O	2.29	0.49
1:A:531:ILE:O	1:A:535:THR:OG1	2.14	0.49
1:A:574:ARG:HH12	1:A:712:LEU:HD11	1.78	0.49
2:B:160:GLU:HG3	2:B:189:TRP:CD1	2.47	0.49
2:B:338:GLU:HG3	8:H:68:VAL:HG21	1.93	0.49
2:B:490:LEU:HD12	2:B:492:PRO:HD3	1.93	0.49
4:D:274:ARG:HG3	4:D:275:LYS:HG2	1.95	0.49
8:H:138:LEU:O	8:H:142:ARG:HG2	2.12	0.49
6:F:123:ASP:OD1	6:F:123:ASP:N	2.42	0.49
3:C:381:ARG:HA	3:C:384:HIS:ND1	2.27	0.49
6:F:30:SER:OG	6:F:31:GLN:N	2.46	0.49
1:A:497:GLN:HA	1:A:502:ILE:HG22	1.93	0.49
2:B:18:TYR:H	2:B:21:GLN:HE21	1.61	0.48
1:A:650:MET:HE1	1:A:653:GLU:HB3	1.95	0.48
2:B:509:GLU:H	2:B:509:GLU:CD	2.21	0.48
3:C:206:LYS:NZ	3:C:245:GLU:OE1	2.32	0.48
2:B:345:ARG:HG3	2:B:345:ARG:O	2.14	0.48
3:C:211:VAL:HB	3:C:212:PRO:HD3	1.95	0.48
3:C:427:ALA:O	3:C:431:ILE:HG12	2.13	0.48
4:D:258:LEU:HD23	4:D:258:LEU:HA	1.75	0.48
8:H:135:LYS:O	8:H:138:LEU:HG	2.14	0.48
1:A:198:ARG:NH2	8:H:185:ASP:OD1	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:222:THR:O	4:D:226:ARG:NH1	2.47	0.48
5:E:30:LEU:O	5:E:34:ILE:HG13	2.14	0.48
1:A:137:THR:HG23	1:A:153:MET:HE1	1.96	0.47
1:A:409:THR:HG22	1:A:412:MET:HB2	1.96	0.47
3:C:405:GLN:HE21	3:C:409:GLN:HE21	1.61	0.47
4:D:219:TYR:HH	4:D:264:HIS:HD1	1.62	0.47
7:G:20:LEU:O	7:G:23:LEU:HD12	2.15	0.47
4:D:19:LEU:HD23	4:D:47:GLU:HB2	1.97	0.47
2:B:511:ARG:O	2:B:511:ARG:HG3	2.14	0.47
3:C:399:ASP:HA	3:C:402:ASN:HD21	1.79	0.47
2:B:748:GLU:HA	2:B:751:LYS:HD2	1.96	0.47
1:A:373:GLN:NE2	1:A:614:SER:O	2.47	0.47
2:B:37:HIS:O	2:B:476:VAL:N	2.47	0.47
3:C:127:LEU:O	3:C:131:LEU:HD12	2.14	0.47
3:C:431:ILE:HG13	4:D:62:LEU:HD11	1.97	0.47
3:C:434:LEU:HD13	6:F:229:TRP:CD1	2.50	0.47
4:D:316:TYR:HD1	4:D:343:VAL:HG22	1.80	0.47
7:G:8:VAL:HG13	7:G:47:ALA:HB2	1.96	0.47
1:A:523:VAL:HG13	7:G:22:TYR:CE1	2.50	0.47
2:B:492:PRO:HB2	2:B:701:LEU:HD13	1.97	0.47
3:C:275:LYS:HD2	3:C:277:LEU:HD12	1.96	0.47
1:A:520:ARG:HB3	7:G:18:GLN:NE2	2.30	0.47
1:A:574:ARG:HA	1:A:574:ARG:HD3	1.63	0.47
3:C:124:LEU:HA	3:C:127:LEU:HG	1.96	0.46
1:A:198:ARG:NH1	8:H:188:GLU:OE1	2.48	0.46
3:C:489:LYS:O	3:C:492:LYS:HG2	2.16	0.46
4:D:428:LEU:HB2	4:D:430:VAL:HG22	1.97	0.46
3:C:136:VAL:HG11	3:C:500:PHE:HD2	1.79	0.46
1:A:574:ARG:NH2	1:A:712:LEU:HD11	2.29	0.46
2:B:694:PRO:HG2	2:B:697:ILE:HD12	1.97	0.46
6:F:153:ASP:OD1	6:F:153:ASP:N	2.48	0.46
2:B:418:ILE:HG12	2:B:433:LEU:HD12	1.97	0.46
1:A:420:SER:HB3	1:A:423:ALA:HB3	1.98	0.46
6:F:177:PHE:HD2	6:F:202:LEU:HD12	1.79	0.46
2:B:118:HIS:O	2:B:122:THR:HG23	2.15	0.46
5:E:246:GLU:HG2	6:F:290:LYS:HD2	1.98	0.46
6:F:34:LEU:O	6:F:38:ILE:HG12	2.15	0.46
6:F:52:ASN:OD1	6:F:53:ARG:N	2.49	0.46
1:A:506:GLN:HB2	1:A:655:TYR:CD1	2.51	0.46
1:A:619:GLU:HB3	1:A:645:ARG:HG3	1.96	0.46
1:A:647:LYS:HD3	1:A:647:LYS:HA	1.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:122:MET:HA	8:H:122:MET:HE2	1.98	0.45
1:A:425:ARG:HA	1:A:428:GLU:HG3	1.99	0.45
2:B:243:CYS:HB3	2:B:443:ALA:HB3	1.98	0.45
4:D:317:ALA:O	4:D:341:MET:HA	2.17	0.45
1:A:522:TYR:HE1	1:A:530:ARG:HD2	1.81	0.45
1:A:584:THR:HB	1:A:589:ARG:HH21	1.82	0.45
2:B:458:SER:HB3	2:B:461:LEU:HG	1.98	0.45
3:C:454:PRO:HB2	3:C:456:ASP:OD1	2.16	0.45
6:F:17:ALA:HB1	6:F:119:MET:HE1	1.99	0.45
8:H:175:LEU:HG	8:H:208:LEU:HD21	1.99	0.45
1:A:708:GLU:O	1:A:711:GLN:HG2	2.17	0.45
4:D:131:ASP:HB3	4:D:249:TYR:HD2	1.80	0.45
7:G:24:ASP:OD2	7:G:34:ILE:HG12	2.17	0.45
2:B:464:LEU:O	2:B:468:PRO:HD2	2.17	0.45
5:E:211:LEU:O	5:E:215:THR:OG1	2.31	0.45
1:A:659:PHE:CG	1:A:659:PHE:O	2.69	0.45
4:D:171:VAL:HG13	4:D:175:LEU:HD23	1.99	0.45
8:H:39:PHE:HA	8:H:43:ALA:HA	1.99	0.45
1:A:455:LEU:HD12	1:A:483:LEU:HB3	2.00	0.44
2:B:118:HIS:HB3	2:B:121:VAL:HG12	1.98	0.44
7:G:32:LYS:HA	7:G:32:LYS:HD2	1.62	0.44
8:H:153:VAL:O	8:H:156:GLN:HG3	2.16	0.44
8:H:158:ASN:O	8:H:162:ARG:HG2	2.17	0.44
2:B:633:LEU:HD12	2:B:633:LEU:HA	1.88	0.44
4:D:412:PHE:H	4:D:418:PHE:HZ	1.65	0.44
5:E:119:GLU:HG3	5:E:120:LEU:H	1.82	0.44
5:E:291:CYS:HB2	5:E:312:LEU:HD11	1.98	0.44
7:G:19:PHE:HZ	7:G:60:LEU:HD22	1.83	0.44
1:A:58:ALA:HB2	4:D:334:MET:HB3	1.99	0.44
3:C:296:LYS:HD2	3:C:296:LYS:HA	1.70	0.44
3:C:490:VAL:HA	3:C:493:MET:CE	2.46	0.44
4:D:408:LEU:HD13	4:D:442:VAL:HG22	1.99	0.44
8:H:98:PHE:HA	8:H:101:GLU:OE1	2.17	0.44
8:H:123:GLU:O	8:H:126:GLN:HG2	2.17	0.44
4:D:187:SER:HA	4:D:193:PRO:HB2	1.99	0.44
2:B:344:LEU:HG	2:B:431:PRO:HB2	1.99	0.44
1:A:52:LYS:HD2	1:A:52:LYS:HA	1.84	0.44
2:B:591:GLY:HA2	5:E:207:VAL:HG21	2.00	0.44
4:D:32:ASP:OD2	4:D:94:ARG:NH2	2.42	0.44
4:D:65:PRO:HG3	4:D:99:GLN:HE21	1.83	0.44
6:F:177:PHE:CD2	6:F:202:LEU:HD12	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:53:LEU:O	7:G:57:VAL:HG12	2.18	0.44
3:C:487:GLU:O	3:C:491:VAL:HG13	2.18	0.44
4:D:454:PHE:HA	4:D:457:ARG:HD2	2.00	0.43
5:E:86:LYS:O	5:E:89:GLU:HG2	2.18	0.43
7:G:46:ILE:HD12	7:G:48:GLU:HB2	2.00	0.43
8:H:145:GLU:O	8:H:148:GLU:HG3	2.18	0.43
1:A:510:VAL:HA	1:A:690:ILE:O	2.18	0.43
3:C:509:GLN:O	3:C:513:ARG:HG2	2.18	0.43
8:H:117:ASN:HA	8:H:120:LYS:HE3	2.00	0.43
2:B:2:LYS:HZ2	2:B:9:LEU:HD11	1.82	0.43
2:B:611:VAL:HG13	2:B:612:HIS:N	2.33	0.43
4:D:100:LEU:HA	4:D:106:GLN:HA	2.00	0.43
2:B:553:TYR:HB2	2:B:558:LEU:HD12	2.00	0.43
3:C:127:LEU:HD12	3:C:128:TYR:N	2.33	0.43
3:C:207:TYR:O	3:C:211:VAL:HG23	2.18	0.43
2:B:579:VAL:O	2:B:583:LYS:HG2	2.18	0.43
4:D:175:LEU:HD13	4:D:268:PHE:HE1	1.84	0.43
5:E:33:THR:O	5:E:37:ILE:HG12	2.18	0.43
6:F:175:MET:O	6:F:179:ASN:ND2	2.49	0.43
4:D:159:VAL:HG22	4:D:175:LEU:HD21	2.00	0.43
4:D:312:ASN:OD1	4:D:313:TYR:N	2.52	0.43
2:B:746:SER:O	2:B:749:THR:OG1	2.31	0.43
1:A:635:GLN:OE1	1:A:635:GLN:N	2.50	0.43
1:A:706:LYS:HA	1:A:709:GLN:HG2	2.00	0.43
4:D:220:LEU:HD11	4:D:234:LEU:HD13	2.00	0.43
4:D:348:ARG:O	4:D:352:GLN:HG2	2.19	0.43
7:G:9:LEU:O	7:G:10:ILE:HD13	2.19	0.43
1:A:520:ARG:O	1:A:523:VAL:HG23	2.19	0.42
1:A:531:ILE:HA	1:A:534:TYR:CE1	2.54	0.42
1:A:560:VAL:HG22	1:A:624:ILE:HB	2.00	0.42
4:D:59:MET:HG3	4:D:110:LEU:HD13	2.01	0.42
4:D:338:PHE:HB2	4:D:341:MET:O	2.19	0.42
1:A:627:SER:OG	1:A:628:SER:N	2.51	0.42
2:B:293:ARG:HA	2:B:293:ARG:HD3	1.87	0.42
3:C:500:PHE:CE1	3:C:505:LEU:HD21	2.48	0.42
4:D:245:LEU:HD23	4:D:245:LEU:HA	1.80	0.42
5:E:110:LYS:NZ	5:E:138:THR:O	2.50	0.42
1:A:385:ASP:HB3	1:A:388:GLN:HG3	2.01	0.42
1:A:578:PRO:HB2	1:A:592:ILE:HD11	2.01	0.42
3:C:471:LEU:HD21	3:C:497:LEU:HA	2.00	0.42
1:A:611:GLY:HA2	1:A:617:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:TYR:CD1	2:B:102:LEU:HD11	2.54	0.42
2:B:339:TYR:CD2	2:B:361:LEU:HD13	2.54	0.42
2:B:514:ILE:O	2:B:518:ARG:HG2	2.18	0.42
3:C:493:MET:HE2	3:C:493:MET:HB2	1.73	0.42
3:C:506:CYS:HA	3:C:509:GLN:CG	2.48	0.42
8:H:160:GLN:HA	8:H:163:LEU:HG	2.01	0.42
1:A:530:ARG:H	1:A:530:ARG:HG3	1.55	0.42
1:A:677:GLN:HG3	1:A:687:PHE:CD2	2.55	0.42
7:G:44:PHE:C	7:G:44:PHE:CD1	2.97	0.42
8:H:127:LYS:HD2	8:H:127:LYS:C	2.45	0.42
1:A:71:HIS:HB2	1:A:145:LYS:HG2	2.00	0.42
1:A:198:ARG:HE	8:H:184:LEU:HD21	1.85	0.42
2:B:11:TYR:CE2	2:B:97:GLN:HG2	2.55	0.42
2:B:11:TYR:HE2	2:B:97:GLN:HG2	1.84	0.42
8:H:163:LEU:O	8:H:166:GLN:HG3	2.20	0.42
4:D:189:GLU:HB2	4:D:193:PRO:HB3	2.01	0.42
1:A:414:GLY:O	1:A:453:ARG:NH1	2.53	0.42
1:A:588:GLU:O	1:A:591:GLN:HG2	2.20	0.42
3:C:185:ARG:HA	9:I:166:GLU:HG2	2.02	0.42
2:B:122:THR:N	2:B:123:PRO:HD2	2.34	0.42
3:C:234:ARG:HE	3:C:236:ASN:HB2	1.85	0.42
4:D:301:VAL:HG21	6:F:155:GLN:HE22	1.85	0.41
4:D:408:LEU:HD12	4:D:409:TYR:N	2.35	0.41
8:H:129:ASN:HB3	8:H:132:VAL:HG22	2.02	0.41
2:B:160:GLU:HG3	2:B:189:TRP:NE1	2.35	0.41
2:B:286:ARG:O	2:B:286:ARG:NH1	2.53	0.41
4:D:137:GLY:O	4:D:280:ARG:NH2	2.39	0.41
6:F:222:SER:O	6:F:222:SER:OG	2.38	0.41
8:H:74:ILE:HD11	8:H:110:THR:HG22	2.02	0.41
2:B:266:LEU:HG	2:B:394:PHE:HE2	1.85	0.41
2:B:690:ARG:O	2:B:698:GLN:NE2	2.53	0.41
3:C:486:LEU:O	3:C:490:VAL:HG13	2.20	0.41
3:C:260:LEU:HD23	3:C:260:LEU:HA	1.86	0.41
3:C:264:ASN:HB3	3:C:267:LEU:HD12	2.01	0.41
1:A:188:LEU:HD23	1:A:188:LEU:HA	1.81	0.41
1:A:703:PHE:CD1	1:A:708:GLU:HB3	2.55	0.41
2:B:383:LEU:HD23	2:B:383:LEU:HA	1.92	0.41
3:C:487:GLU:O	3:C:490:VAL:HG22	2.20	0.41
4:D:59:MET:HE3	4:D:66:LEU:HD21	2.03	0.41
6:F:196:LEU:HD23	6:F:196:LEU:HA	1.85	0.41
1:A:530:ARG:HA	1:A:533:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:LEU:O	1:A:644:LEU:HB2	2.21	0.41
4:D:212:LEU:HD23	4:D:212:LEU:HA	1.91	0.41
8:H:124:ILE:HA	8:H:127:LYS:HG3	2.02	0.41
8:H:157:GLU:CD	8:H:161:ARG:HH12	2.29	0.41
3:C:377:LYS:HA	3:C:377:LYS:HD3	1.80	0.41
6:F:176:ASN:O	6:F:180:VAL:HG13	2.20	0.41
1:A:265:THR:OG1	1:A:266:GLN:N	2.54	0.41
2:B:280:ARG:NE	2:B:387:GLU:OE2	2.54	0.41
3:C:502:VAL:HG23	3:C:503:THR:HG23	2.01	0.41
4:D:80:SER:O	4:D:84:GLU:HG2	2.21	0.41
4:D:133:THR:O	4:D:133:THR:OG1	2.36	0.41
4:D:373:HIS:HD2	4:D:375:VAL:H	1.69	0.41
8:H:65:ASP:O	8:H:68:VAL:HG22	2.20	0.41
8:H:193:PRO:HG2	8:H:196:LEU:HD12	2.03	0.41
1:A:260:GLU:OE2	2:B:686:ARG:NE	2.54	0.41
3:C:527:GLU:O	3:C:530:GLN:HG2	2.20	0.41
6:F:67:SER:O	6:F:139:LYS:NZ	2.53	0.41
6:F:234:ASP:CG	6:F:235:GLN:N	2.79	0.41
8:H:119:LYS:HA	8:H:119:LYS:HD2	1.88	0.41
1:A:94:LYS:HB3	1:A:94:LYS:HE3	1.69	0.40
1:A:517:GLU:HG2	1:A:518:PHE:HD1	1.86	0.40
1:A:534:TYR:HB3	1:A:667:THR:HG21	2.03	0.40
2:B:445:LYS:O	2:B:449:GLU:HG2	2.21	0.40
4:D:316:TYR:CD1	4:D:343:VAL:HG22	2.55	0.40
2:B:216:LYS:HE3	2:B:216:LYS:HB2	1.91	0.40
3:C:163:ASP:OD2	3:C:320:ARG:NH2	2.54	0.40
3:C:374:LEU:HD23	5:E:54:ARG:HA	2.02	0.40
3:C:501:GLN:OE1	3:C:533:TYR:OH	2.40	0.40
8:H:176:LYS:HA	8:H:176:LYS:HD2	1.72	0.40
1:A:382:SER:OG	1:A:383:THR:N	2.53	0.40
1:A:422:GLU:O	1:A:425:ARG:HG2	2.21	0.40
1:A:708:GLU:OE1	1:A:708:GLU:N	2.50	0.40
3:C:482:ASN:OD1	3:C:483:THR:HG23	2.21	0.40
4:D:453:ARG:HD3	4:D:457:ARG:NH2	2.35	0.40
5:E:86:LYS:HE2	5:E:86:LYS:HB3	1.86	0.40
1:A:277:ILE:O	1:A:280:LEU:HB3	2.21	0.40
1:A:541:PHE:O	1:A:545:GLN:HG3	2.21	0.40
2:B:688:ASP:OD1	2:B:689:LYS:N	2.55	0.40
3:C:481:VAL:HG13	3:C:481:VAL:O	2.21	0.40
4:D:160:LEU:HD23	4:D:160:LEU:HA	1.85	0.40
4:D:174:ASP:O	4:D:178:LEU:HG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:TRP:CD1	1:A:511:TRP:N	2.90	0.40
8:H:198:LEU:HG	8:H:202:LYS:HE3	2.04	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	643/797 (81%)	617 (96%)	26 (4%)	0	100	100
2	B	758/771 (98%)	735 (97%)	23 (3%)	0	100	100
3	C	362/591 (61%)	355 (98%)	7 (2%)	0	100	100
4	D	448/462 (97%)	432 (96%)	16 (4%)	0	100	100
5	E	365/395 (92%)	360 (99%)	5 (1%)	0	100	100
6	F	259/308 (84%)	254 (98%)	5 (2%)	0	100	100
7	G	64/71 (90%)	62 (97%)	2 (3%)	0	100	100
8	H	208/309 (67%)	185 (89%)	22 (11%)	1 (0%)	24	55
9	I	4/940 (0%)	4 (100%)	0	0	100	100
All	All	3111/4644 (67%)	3004 (97%)	106 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	7	PRO

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	574/702 (82%)	571 (100%)	3 (0%)	81	83
2	B	664/675 (98%)	654 (98%)	10 (2%)	57	72
3	C	336/513 (66%)	333 (99%)	3 (1%)	70	78
4	D	388/399 (97%)	377 (97%)	11 (3%)	38	62
5	E	329/352 (94%)	323 (98%)	6 (2%)	51	70
6	F	234/272 (86%)	230 (98%)	4 (2%)	53	71
7	G	59/64 (92%)	57 (97%)	2 (3%)	32	59
8	H	158/283 (56%)	155 (98%)	3 (2%)	50	68
9	I	6/804 (1%)	6 (100%)	0	100	100
All	All	2748/4064 (68%)	2706 (98%)	42 (2%)	55	72

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	342	CYS
1	A	430	LEU
1	A	650	MET
2	B	65	LEU
2	B	168	VAL
2	B	249	VAL
2	B	287	ARG
2	B	296	SER
2	B	350	VAL
2	B	421	PHE
2	B	476	VAL
2	B	490	LEU
2	B	514	ILE
3	C	363	LEU
3	C	529	LEU
3	C	545	MET
4	D	62	LEU
4	D	96	TRP
4	D	101	LEU
4	D	141	HIS
4	D	164	VAL
4	D	217	LEU

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Mol	Chain	Res	Type
4	D	254	MET
4	D	271	VAL
4	D	360	THR
4	D	414	SER
4	D	441	MET
5	E	25	ASP
5	E	62	TYR
5	E	68	SER
5	E	140	HIS
5	E	357	VAL
5	E	366	VAL
6	F	120	THR
6	F	164	ILE
6	F	175	MET
6	F	291	ILE
7	G	32	LYS
7	G	44	PHE
8	H	68	VAL
8	H	129	ASN
8	H	131	ASP

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	97	GLN
1	A	132	GLN
1	A	181	HIS
1	A	281	GLN
1	A	373	GLN
1	A	595	ASN
1	A	625	GLN
1	A	629	HIS
2	B	21	GLN
2	B	154	HIS
2	B	262	ASN
2	B	402	ASN
2	B	434	HIS
2	B	501	GLN
2	B	662	GLN
2	B	733	GLN
2	B	743	GLN
3	C	213	HIS

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Mol	Chain	Res	Type
3	C	226	GLN
3	C	236	ASN
3	C	300	ASN
3	C	309	HIS
3	C	355	GLN
3	C	375	ASN
3	C	405	GLN
3	C	496	ASN
4	D	20	GLN
4	D	54	ASN
4	D	64	GLN
4	D	99	GLN
4	D	116	GLN
4	D	117	ASN
4	D	177	GLN
4	D	373	HIS
4	D	411	GLN
5	E	147	ASN
5	E	220	HIS
5	E	257	HIS
5	E	317	HIS
5	E	376	HIS
6	F	9	ASN
6	F	18	ASN
6	F	31	GLN
6	F	46	ASN
6	F	176	ASN
6	F	204	GLN
6	F	205	GLN
7	G	42	HIS
8	H	96	ASN
8	H	129	ASN
8	H	158	ASN
8	H	200	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
10	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
10	SF4	B	1000	2	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56544. These allow visual inspection of the internal detail of the map and identification of artifacts.

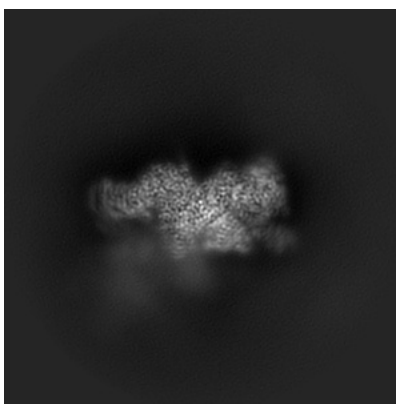
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

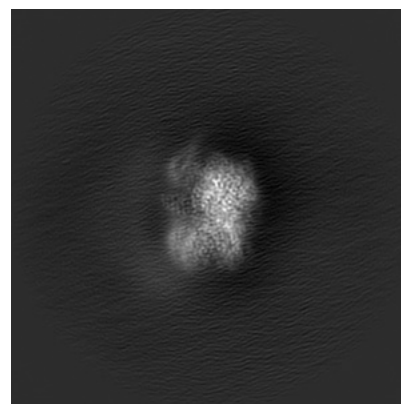
6.1.1 Primary map



X

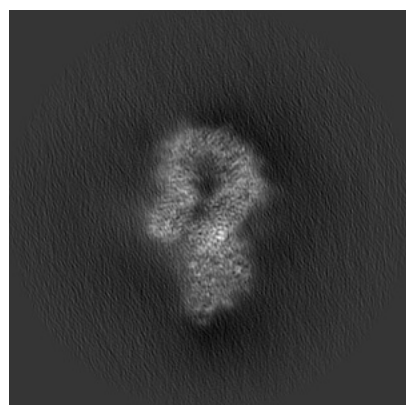


Y

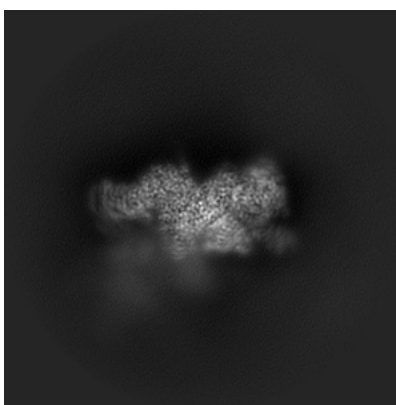


Z

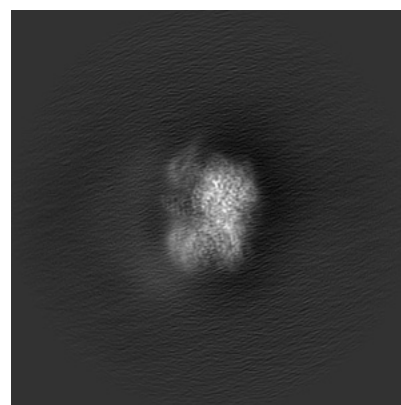
6.1.2 Raw map



X



Y

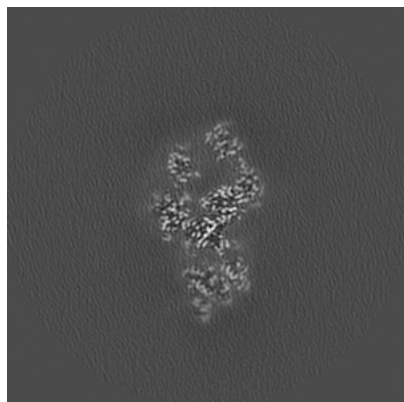


Z

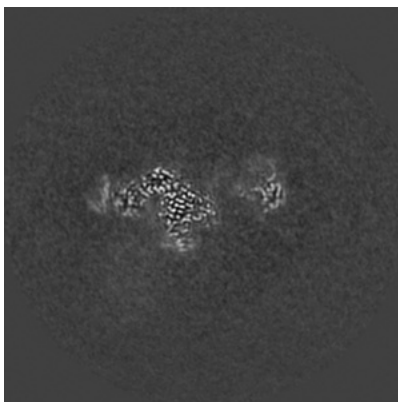
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

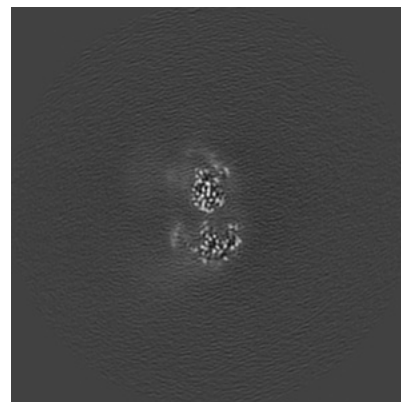
6.2.1 Primary map



X Index: 140

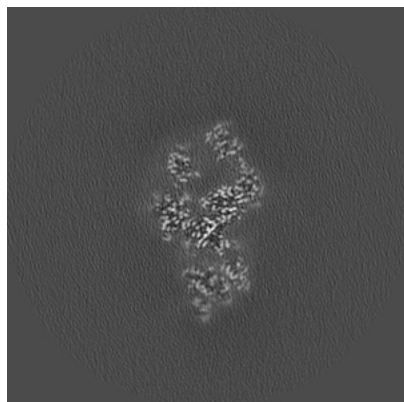


Y Index: 140

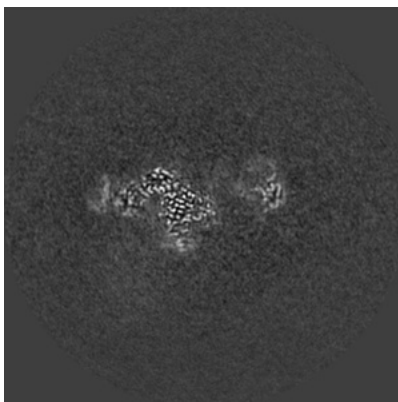


Z Index: 140

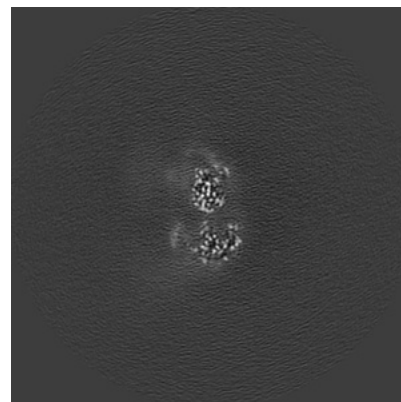
6.2.2 Raw map



X Index: 140



Y Index: 140



Z Index: 140

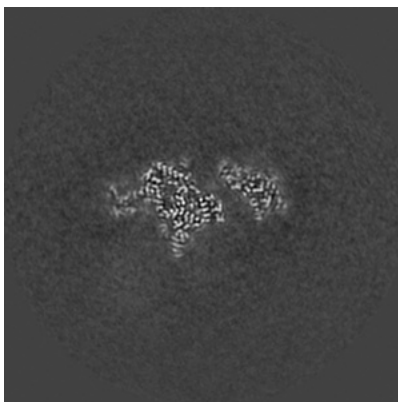
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

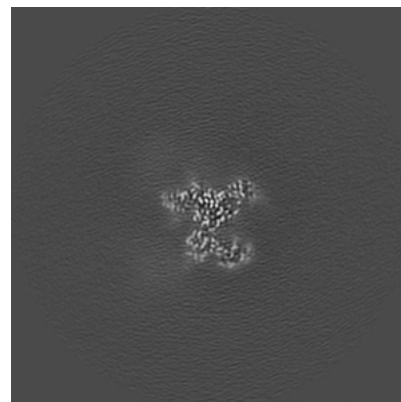
6.3.1 Primary map



X Index: 148

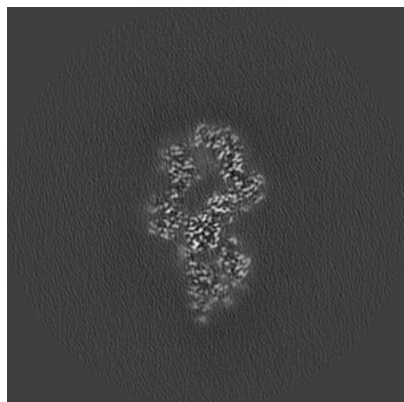


Y Index: 148

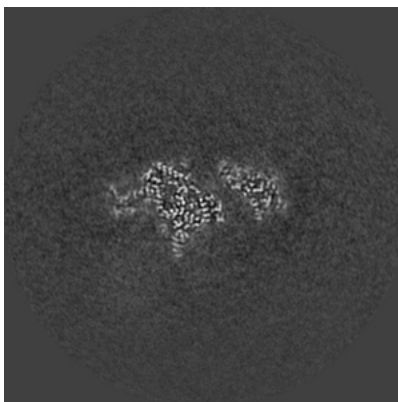


Z Index: 124

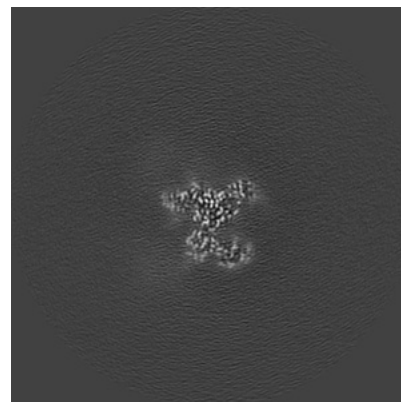
6.3.2 Raw map



X Index: 145



Y Index: 148

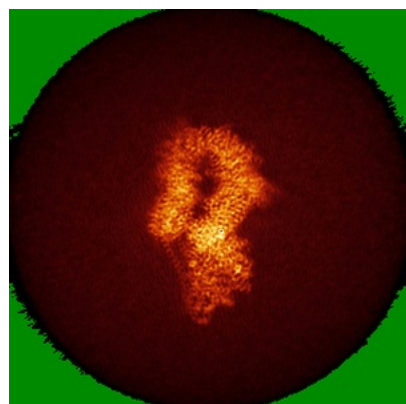


Z Index: 124

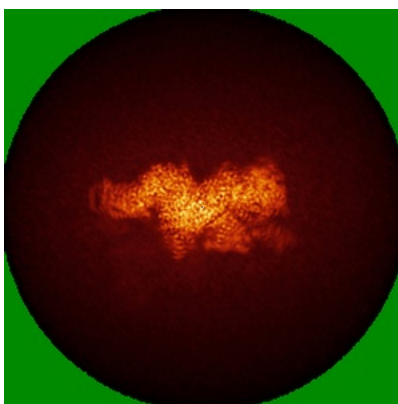
The images above show the largest variance slices of the map in three orthogonal directions.

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

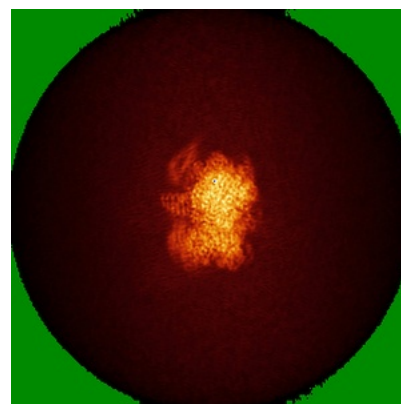
6.4.1 Primary map



X

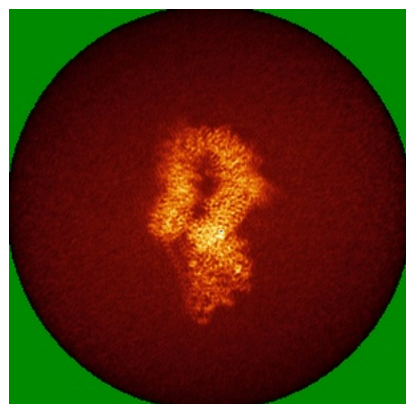


Y

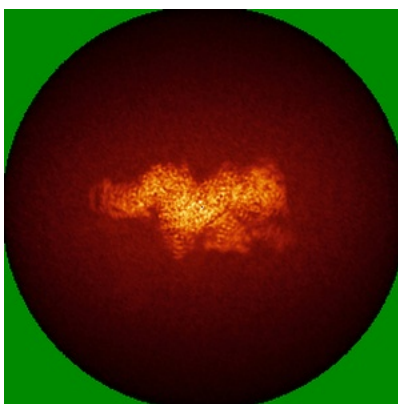


Z

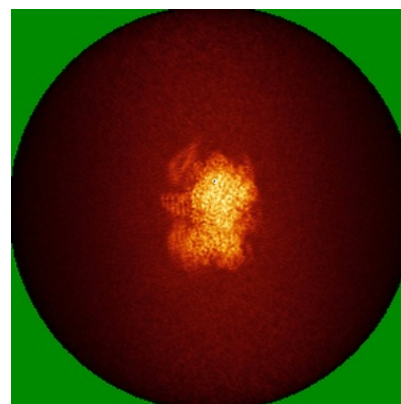
6.4.2 Raw map



X



Y



Z

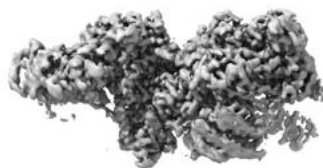
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

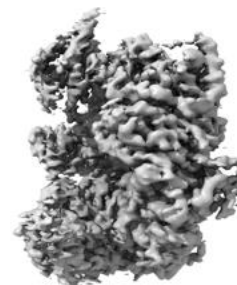
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0109. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

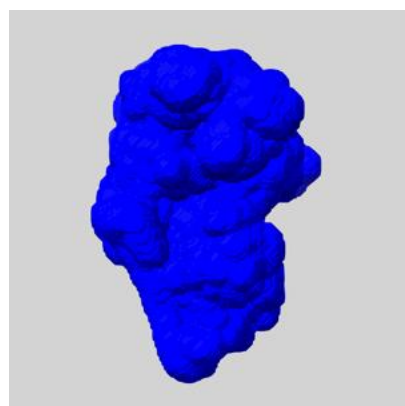
6.6 Mask visualisation [i](#)

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

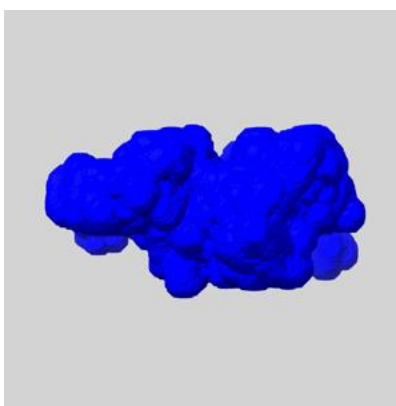
A mask typically either:

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

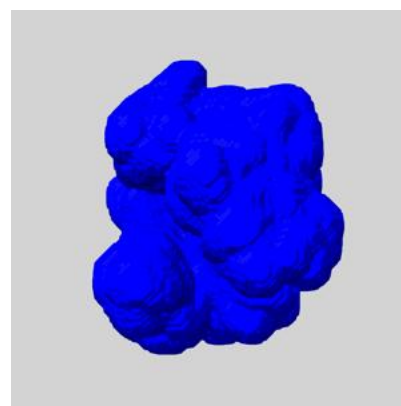
6.6.1 emd_56544_msk_1.map [i](#)



X



Y

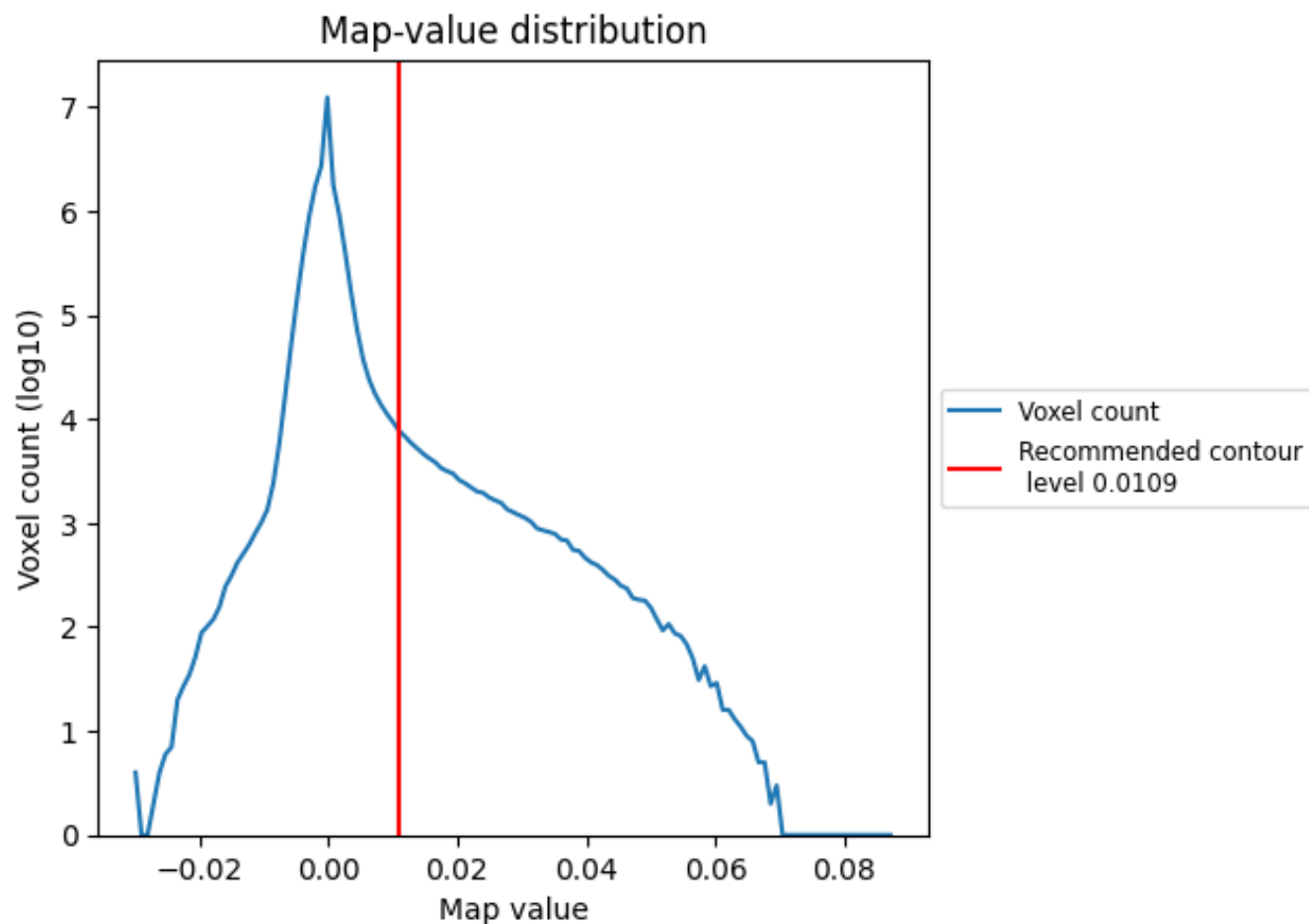


Z

7 Map analysis [i](#)

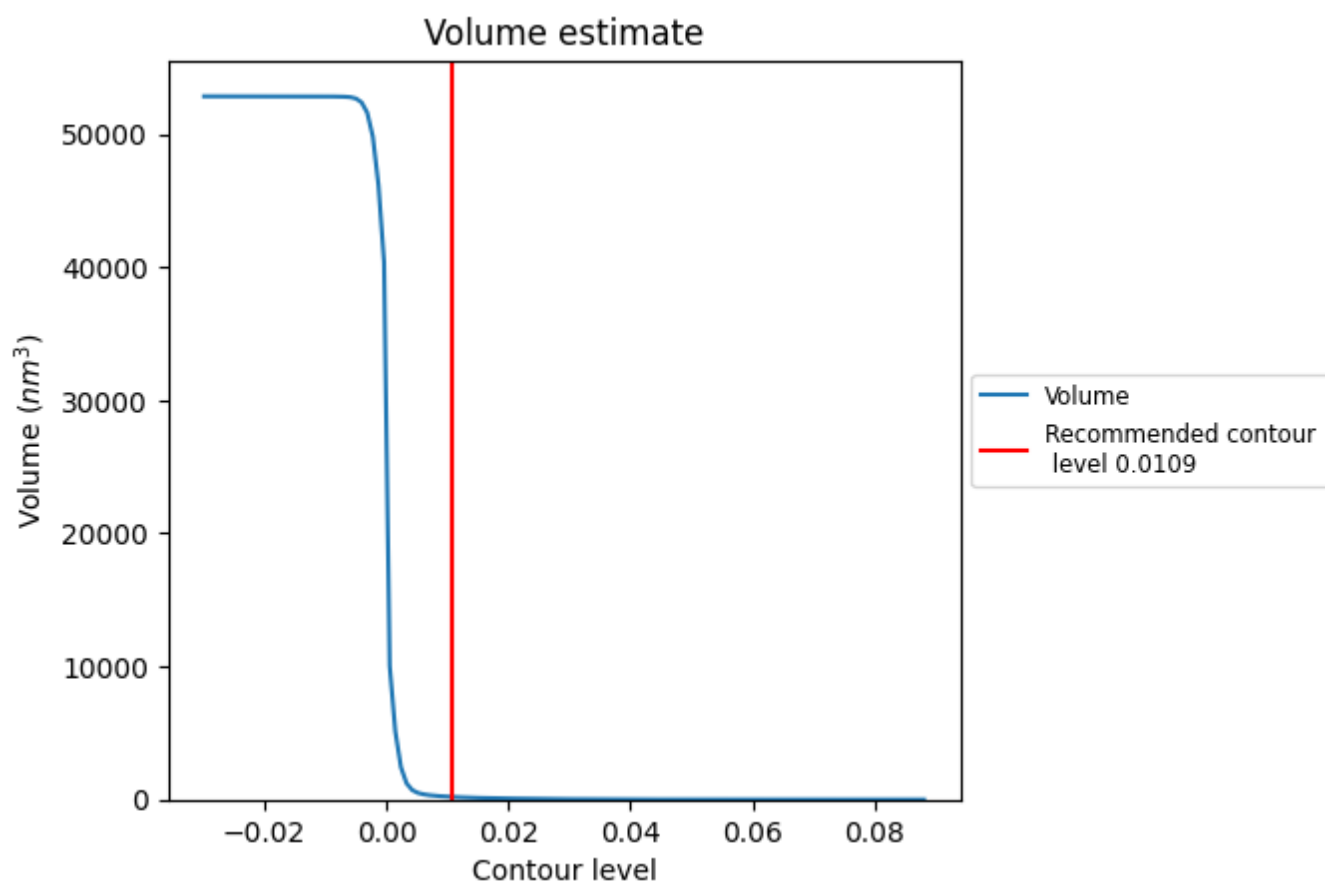
This section contains the results of statistical analysis of the map.

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.

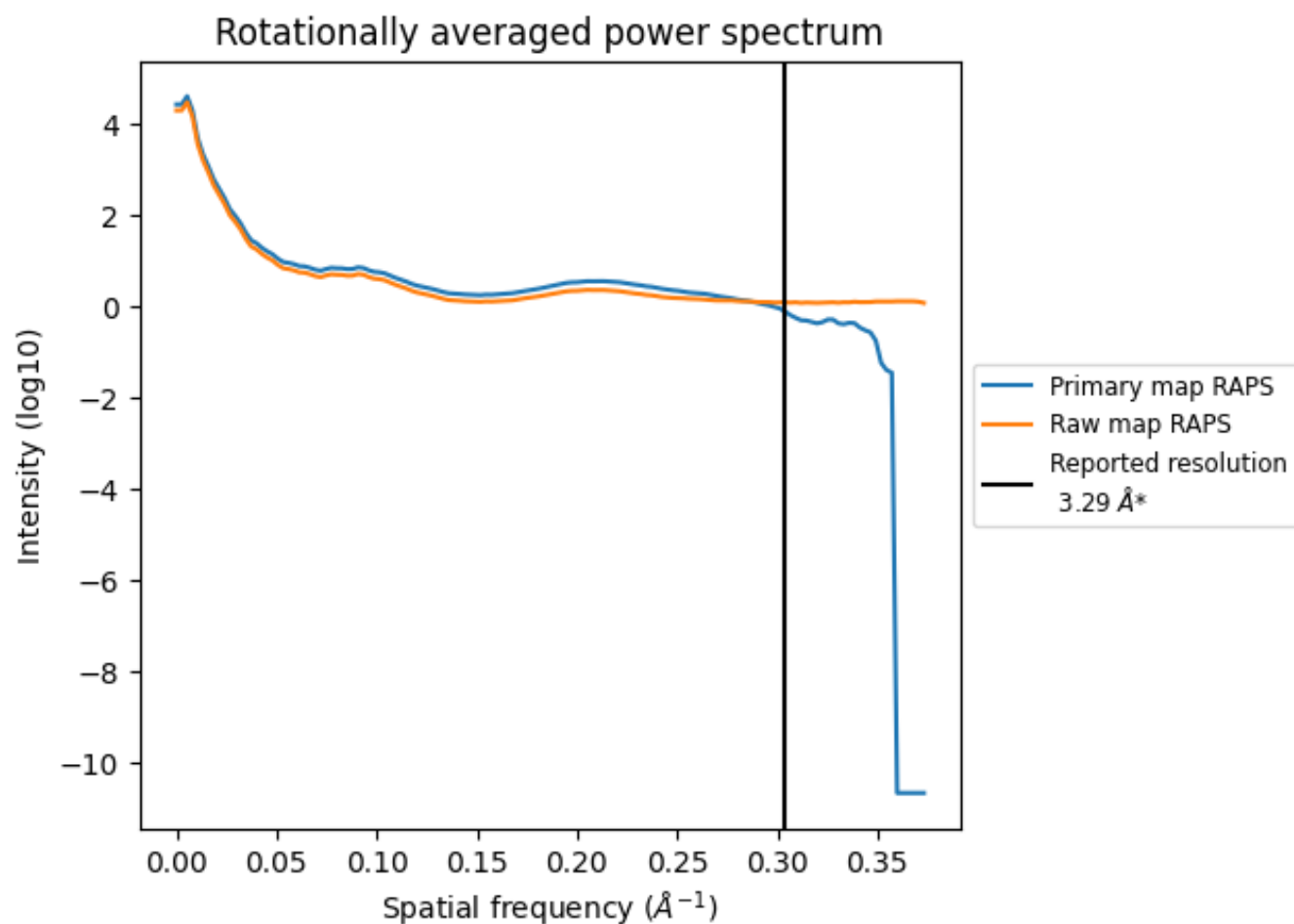
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 195 nm³; this corresponds to an approximate mass of 176 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 ⓘ

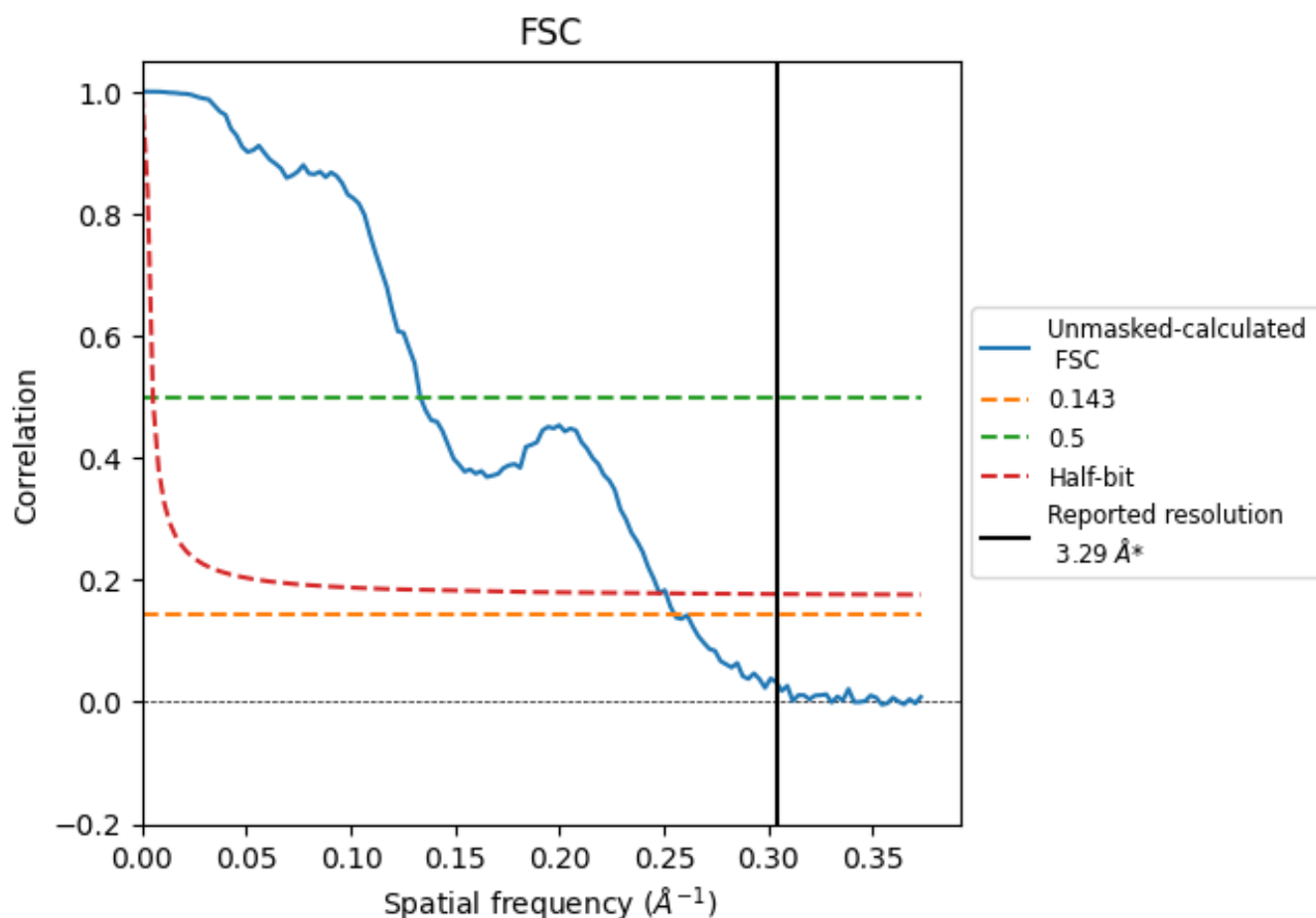


*Reported resolution corresponds to spatial frequency of 0.304 Å⁻¹

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 0.304 Å⁻¹

8.2 Resolution estimates [i](#)

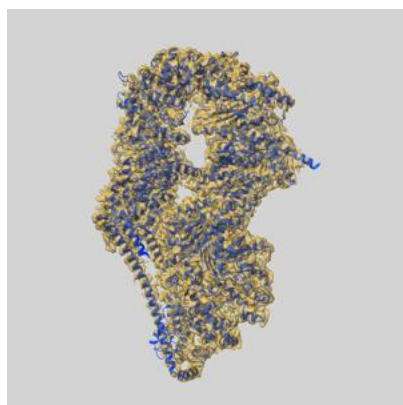
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.29	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.92	7.51	3.98

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.92 differs from the reported value 3.29 by more than 10 %

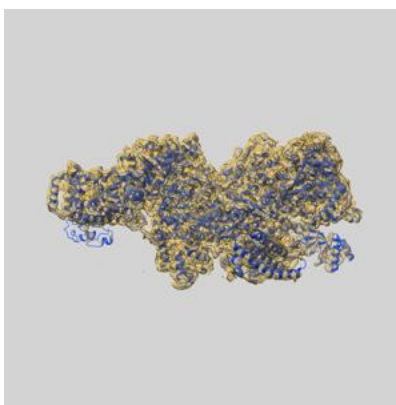
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-56544 and PDB model 28JM. Per-residue inclusion information can be found in section [3](#) on page [9](#).

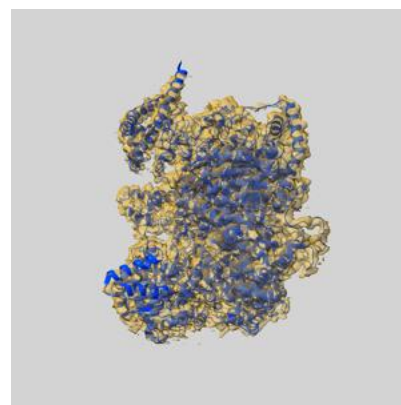
9.1 Map-model overlay [i](#)



X



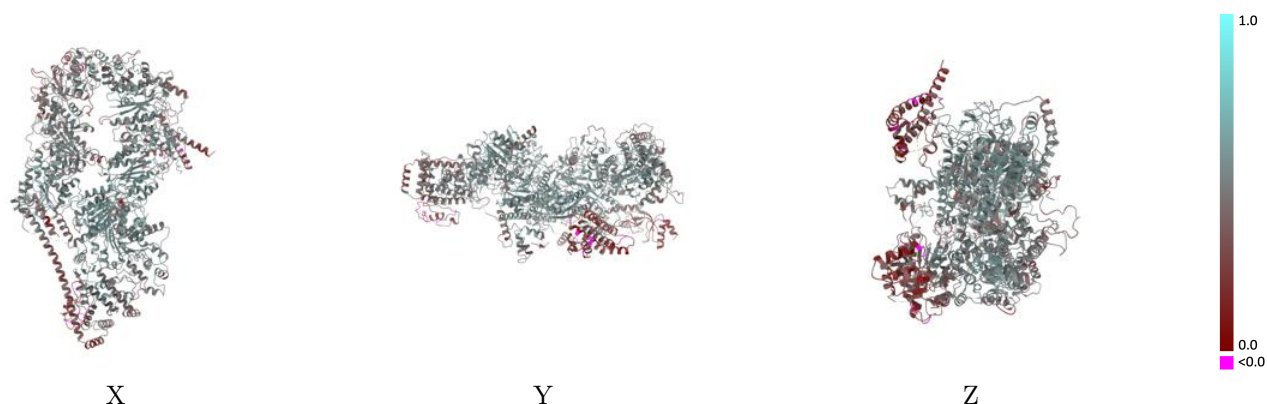
Y



Z

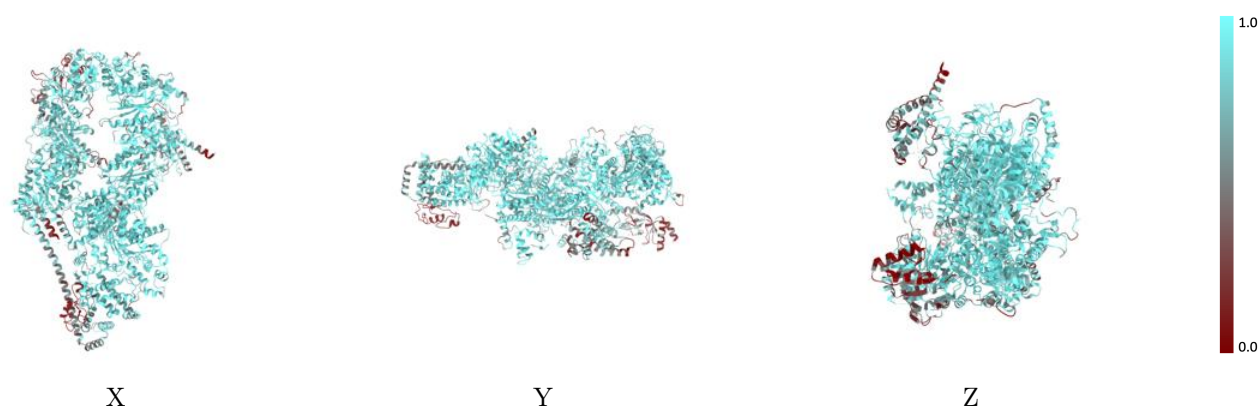
The images above show the 3D surface view of the map at the recommended contour level 0.0109 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



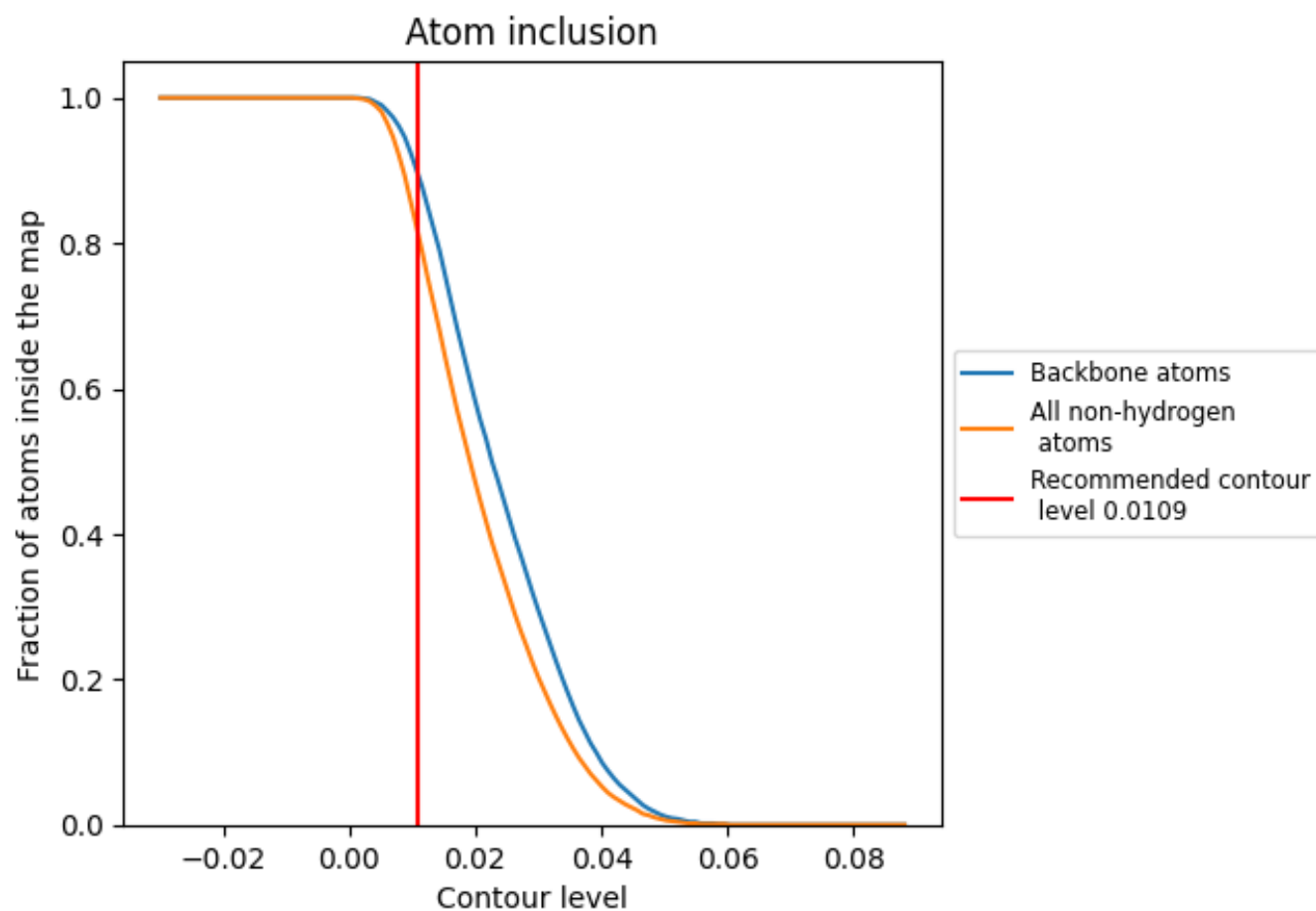
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0109).

9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 82% 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 (0.0109) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8150	<div></div> 0.4740
A	<div></div> 0.8480	<div></div> 0.4860
B	<div></div> 0.9110	<div></div> 0.5300
C	<div></div> 0.7300	<div></div> 0.3970
D	<div></div> 0.7600	<div></div> 0.4500
E	<div></div> 0.8820	<div></div> 0.5220
F	<div></div> 0.9150	<div></div> 0.5330
G	<div></div> 0.4990	<div></div> 0.2870
H	<div></div> 0.4770	<div></div> 0.3270
I	<div></div> 0.7290	<div></div> 0.3350

1.0

0.0

<0.0