



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 03:55 PM UTC

PDB ID : 8C8H / pdb_00008c8h
EMDB ID : EMD-16476
Title : Cryo EM structure of the vaccinia complete RNA polymerase complex lacking the capping enzyme
Authors : Grimm, G.; Bartuli, J.; Fischer, U.
Deposited on : 2023-01-20
Resolution : 3.84 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:

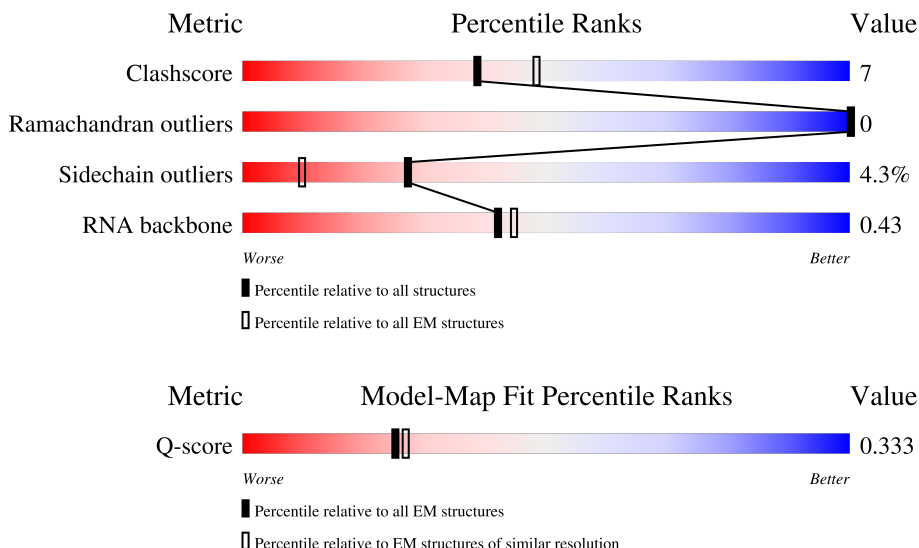
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.84 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	9033 (3.34 - 4.34)

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	B	1164	
2	E	185	
3	F	164	

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Mol	Chain	Length	Quality of chain
4	G	161	
5	I	795	
6	J	63	
7	Q	129	
7	R	129	
8	K	710	
9	U	72	
10	A	1286	
11	Y	631	
12	C	305	
13	S	259	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 41296 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 DNA-directed RNA polymerase 133 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1129	Total	C	N	O	S	0	0
			9091	5794	1554	1695	48		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	6	ASN	ASP	conflict	UNP Q76ZP7
B	343	PHE	TYR	variant	UNP Q76ZP7

- Molecule 2 is a protein called DNA-directed RNA polymerase 22 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	184	Total	C	N	O	S	0	0
			1495	966	248	276	5		

- Molecule 3 is a protein called DNA-directed RNA polymerase 19 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	103	Total	C	N	O	S	0	0
			849	545	148	153	3		

- Molecule 4 is a protein called DNA-directed RNA polymerase 18 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	153	Total	C	N	O	S	0	0
			1192	753	198	235	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	11	SER	PRO	variant	UNP P04310

- Molecule 5 is a protein called RNA polymerase-associated transcription-specificity factor

RAP94.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	669	Total	C	N	O	S	0	0
			5603	3669	896	1017	21		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	623	CYS	TYR	variant	UNP P68438
I	624	VAL	ILE	variant	UNP P68438

- Molecule 6 is a protein called DNA-directed RNA polymerase 7 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	61	Total	C	N	O	S	0	0
			490	310	88	88	4		

- Molecule 7 is a protein called Core protein E11.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	129	Total	C	N	O	S	1	0
			1056	689	165	197	5		
7	Q	124	Total	C	N	O	S	0	0
			1013	660	158	190	5		

- Molecule 8 is a protein called Early transcription factor 82 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	91	Total	C	N	O	S	0	0
			749	476	131	133	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	401	ARG	LYS	variant	UNP P20636

- Molecule 9 is a RNA chain called chr17.trna16-GlnTTG.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	U	63	Total	C	N	O	P	1	0
			1362	608	238	452	64		

- Molecule 10 is a protein called DNA-directed RNA polymerase 147 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	1268	Total	C	N	O	S	0	0
			10188	6556	1679	1908	45		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	THR	SER	variant	UNP P07392
A	1006	ASN	ASP	variant	UNP P07392
A	1007	ILE	HIS	variant	UNP P07392
A	1008	THR	SER	variant	UNP P07392
A	?	-	PHE	deletion	UNP P07392
A	1010	ARG	GLU	variant	UNP P07392
A	1012	GLU	LYS	variant	UNP P07392
A	1013	THR	GLN	variant	UNP P07392
A	1015	LYS	ARG	variant	UNP P07392
A	1024	ARG	LYS	variant	UNP P07392
A	1113	ASP	CYS	variant	UNP P07392

- Molecule 11 is a protein called Nucleoside triphosphatase I.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	539	Total	C	N	O	S	0	0
			4347	2789	738	797	23		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	342	LYS	ARG	variant	UNP P05807
Y	347	LYS	GLY	variant	UNP P05807
Y	568	LYS	ASN	variant	UNP P05807

- Molecule 12 is a protein called DNA-directed RNA polymerase 35 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	304	Total	C	N	O	S	0	0
			2484	1608	399	464	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	212	PHE	LEU	variant	UNP P24757

- Molecule 13 is a protein called DNA-directed RNA polymerase 30 kDa polypeptide.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	S	161	Total	C	N	O	P	S	0	0
			1311	820	211	273	3	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	20	ALA	THR	variant	UNP P21603

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

Mol	Chain	Residues	Atoms		AltConf
14	B	1	Total	Zn	0
			1	1	
14	I	1	Total	Zn	0
			1	1	
14	A	2	Total	Zn	0
			2	2	

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total	Mg	0
			1	1	

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		AltConf
16	B	26	Total	O	0
			26	26	
16	E	2	Total	O	0
			2	2	
16	F	1	Total	O	0
			1	1	
16	G	3	Total	O	0
			3	3	
16	I	4	Total	O	0
			4	4	
16	J	4	Total	O	0
			4	4	
16	K	1	Total	O	0
			1	1	

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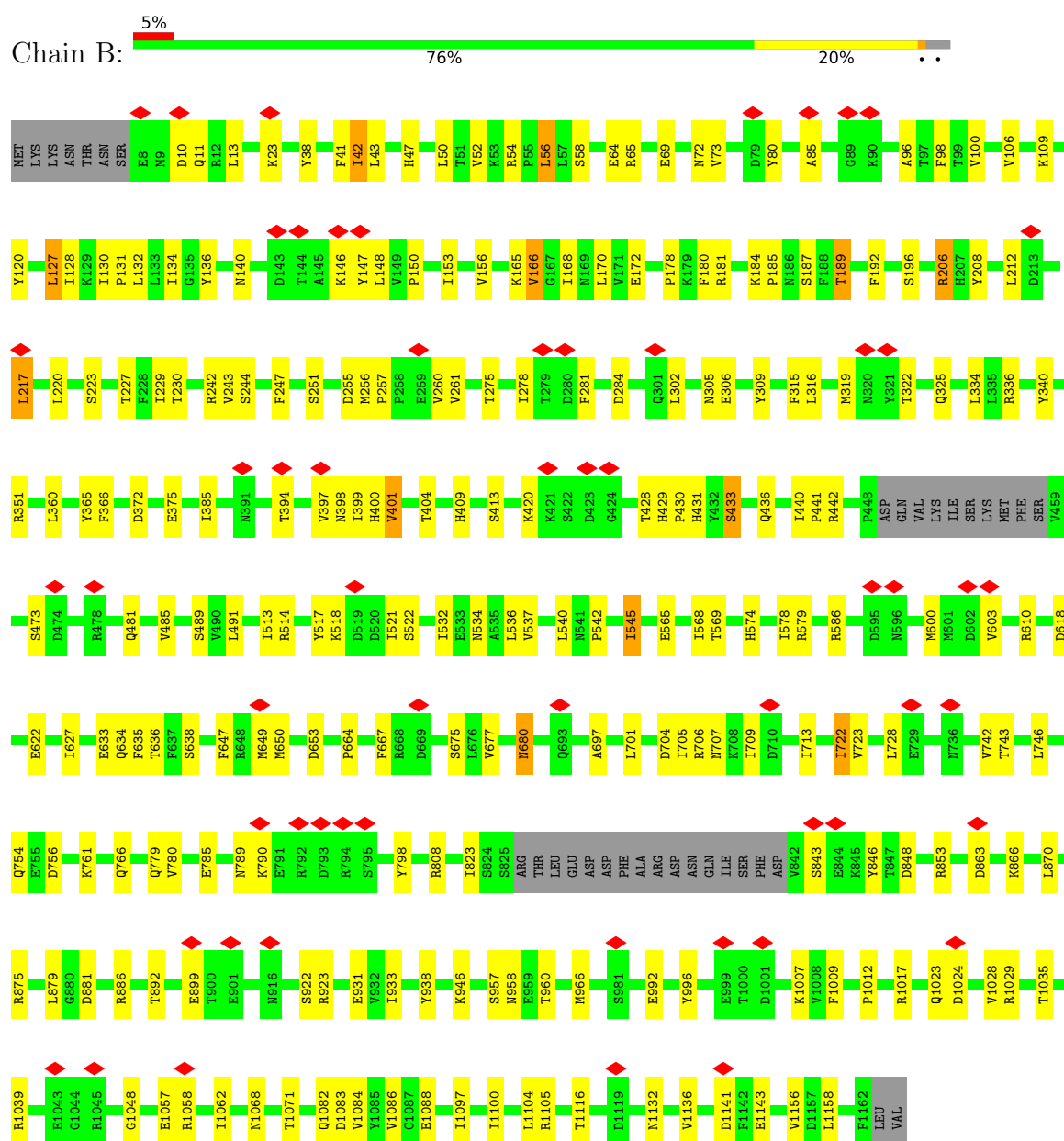
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Mol	Chain	Residues	Atoms		AltConf
16	A	17	Total 17	O 17	0
16	Y	1	Total 1	O 1	0
16	C	2	Total 2	O 2	0

3 Residue-property plots

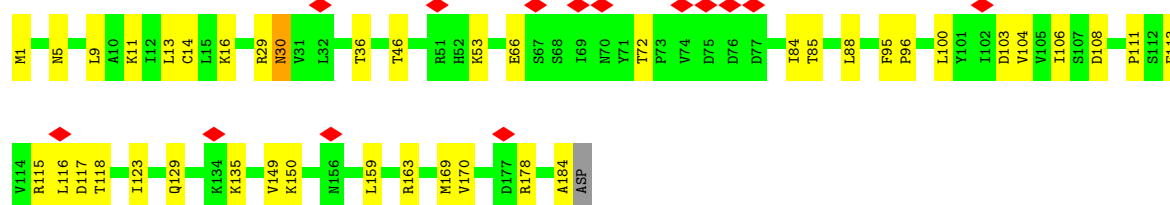
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: DNA-directed RNA polymerase 133 kDa polypeptide



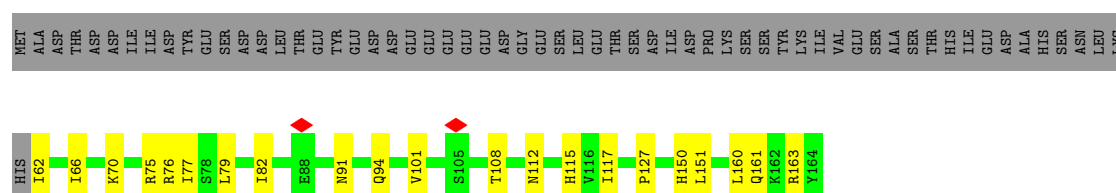
- Molecule 2: DNA-directed RNA polymerase 22 kDa subunit

Chain E: 



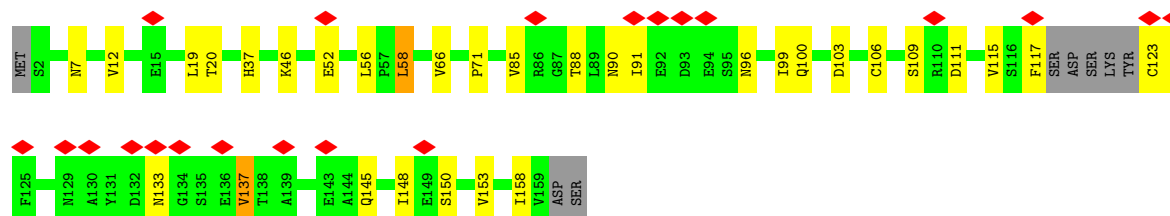
- Molecule 3: DNA-directed RNA polymerase 19 kDa subunit

Chain F: 



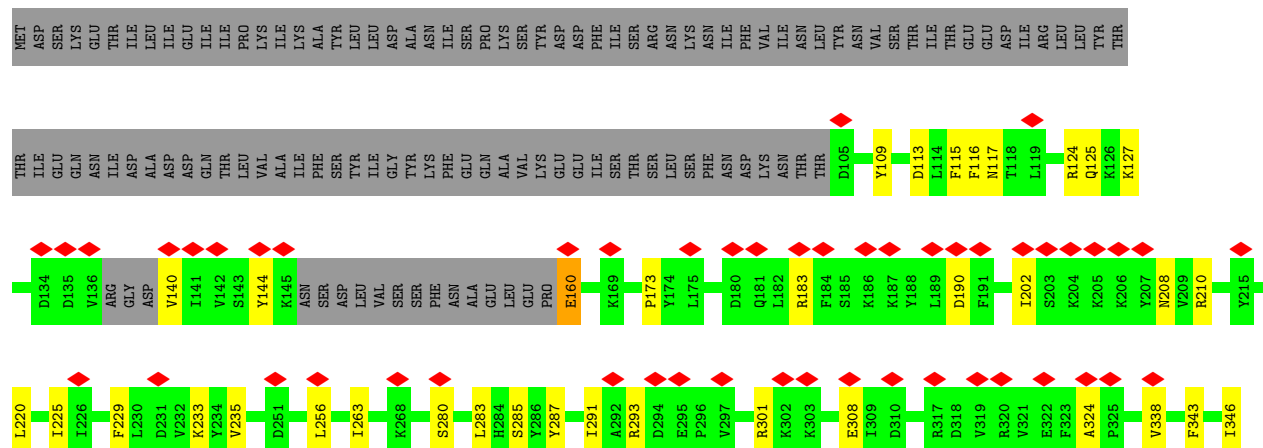
- Molecule 4: DNA-directed RNA polymerase 18 kDa subunit

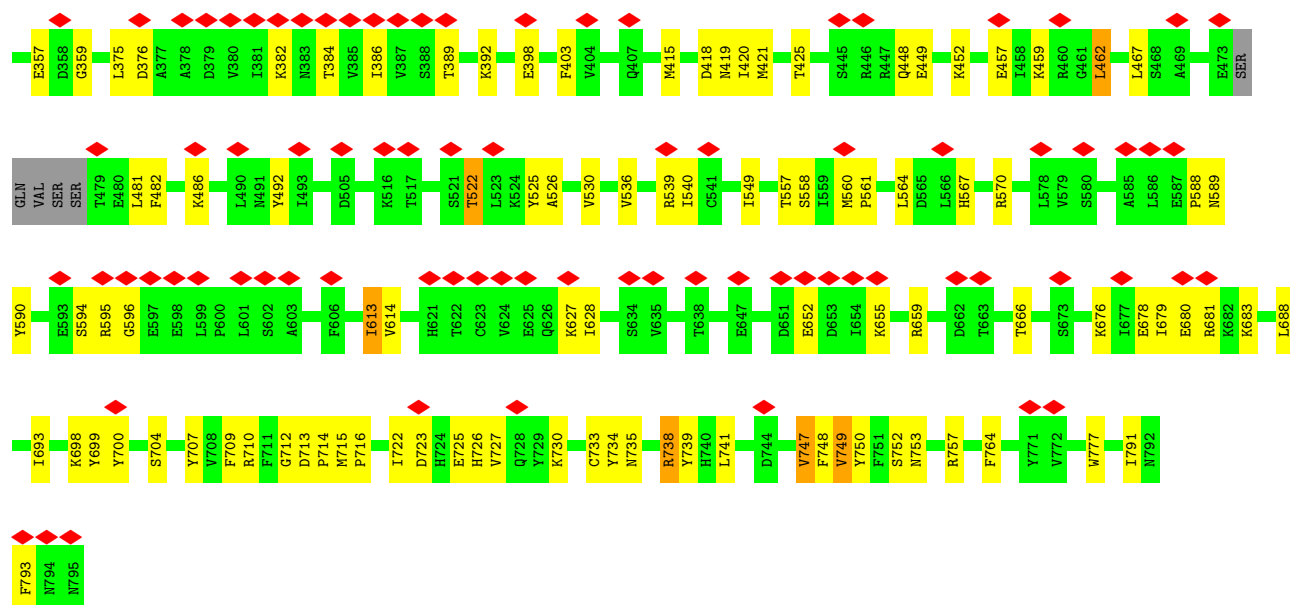
Chain G: 



- Molecule 5: RNA polymerase-associated transcription-specificity factor RAP94

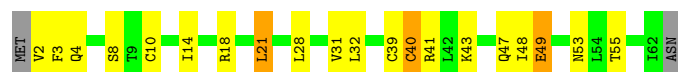
Chain I: 





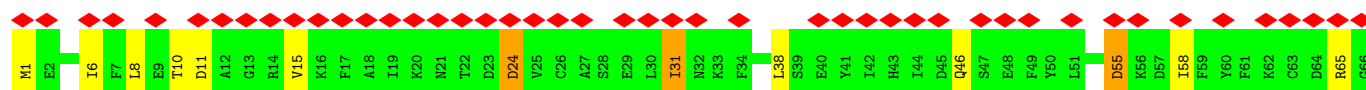
- Molecule 6: DNA-directed RNA polymerase 7 kDa subunit

Chain J: 65% 27% 5% .



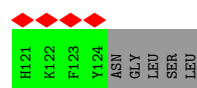
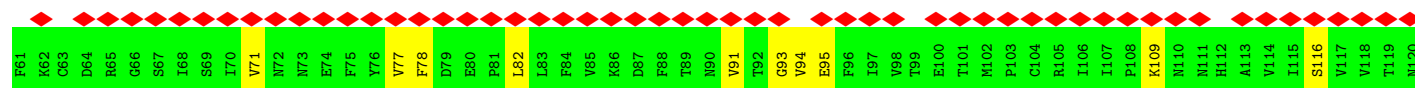
- Molecule 7: Core protein E11

Chain R: 73% 84% 14% .

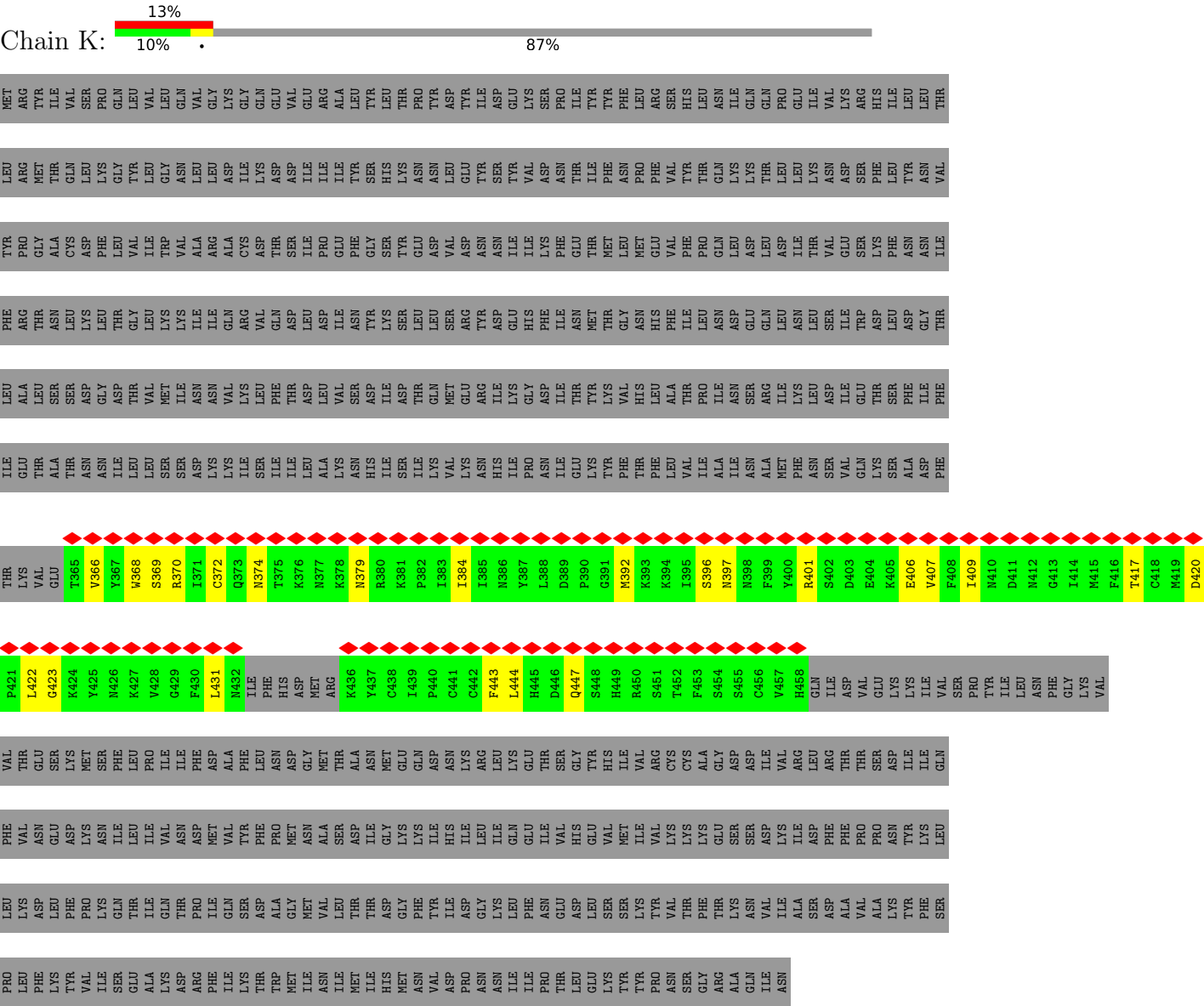


- Molecule 7: Core protein E11

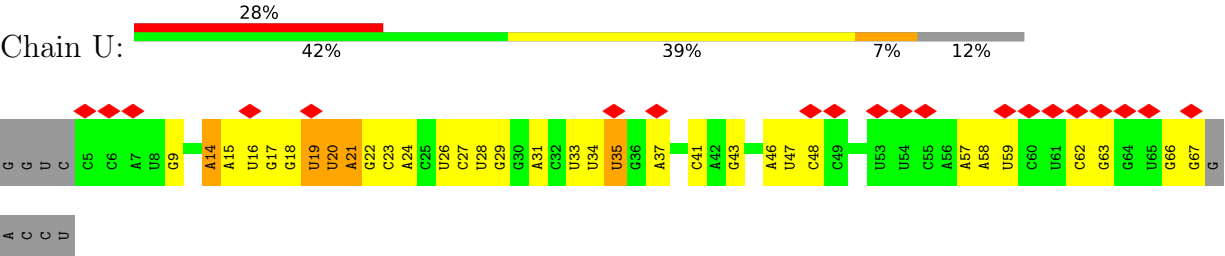
Chain Q: 91% 75% 19% . .



• Molecule 8: Early transcription factor 82 kDa subunit

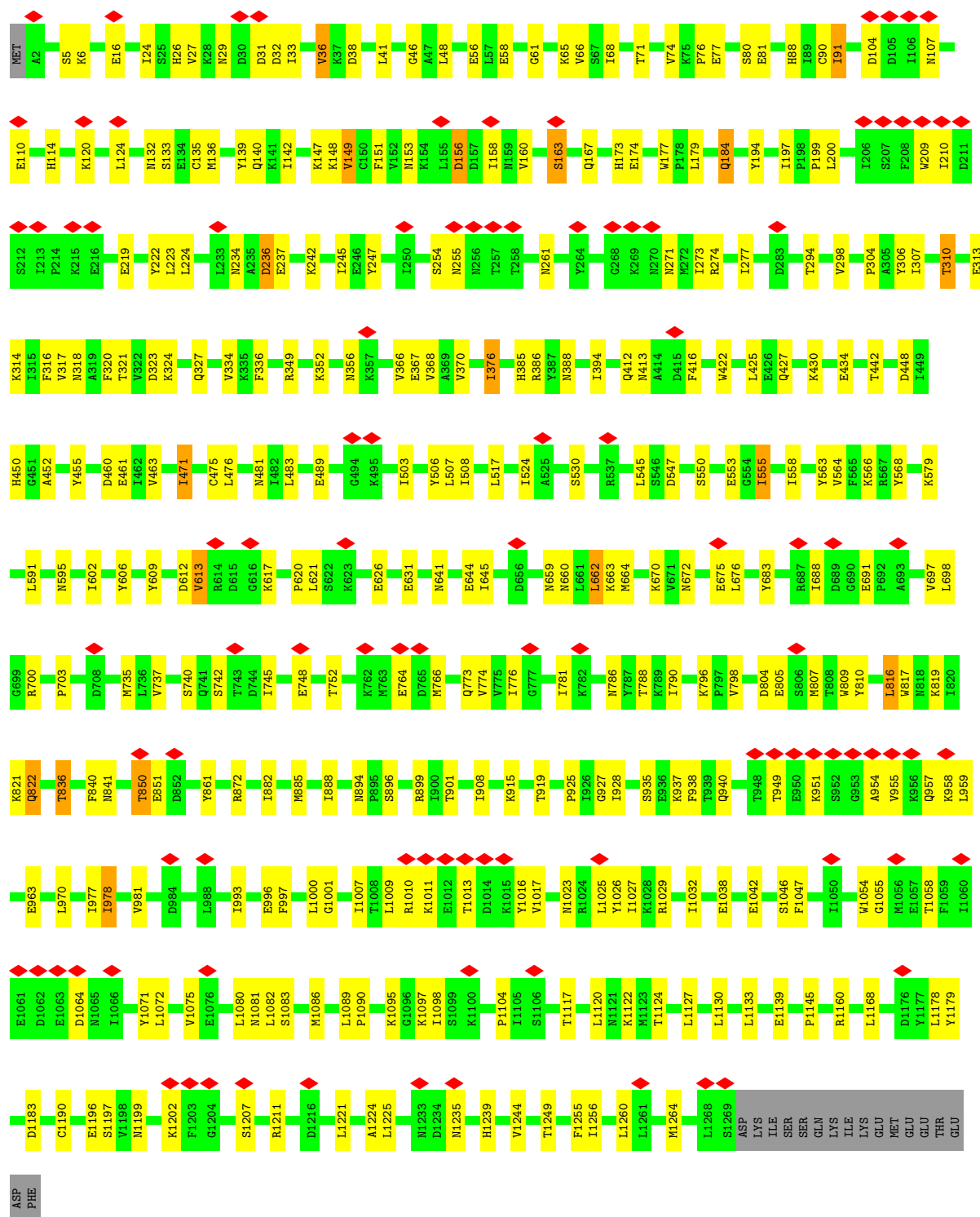


• Molecule 9: chr17.trna16-GlnTTG



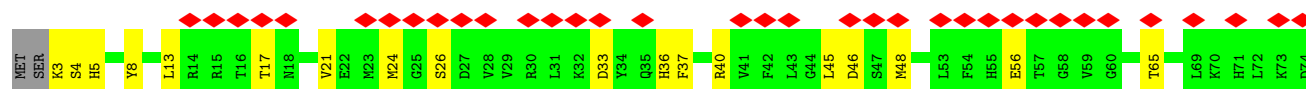
• Molecule 10: DNA-directed RNA polymerase 147 kDa polypeptide

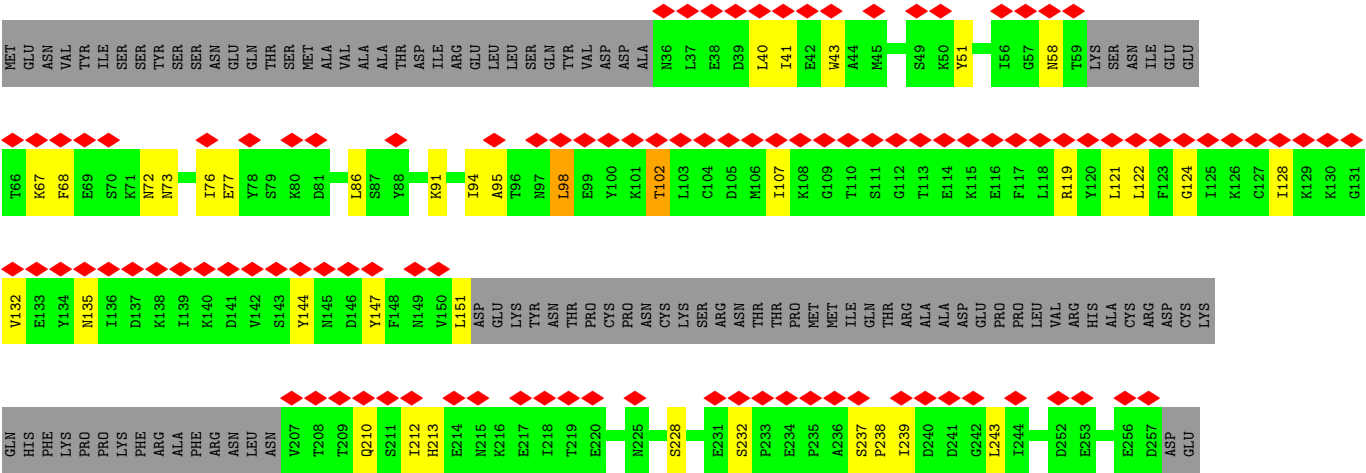




• Molecule 11: Nucleoside triphosphatase I

Chain Y:





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21338	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.345	Depositor
Minimum map value	-0.815	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	382.86002, 382.86002, 382.86002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0635, 1.0635, 1.0635	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, MG, 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	B	0.12	0/9281	0.34	0/12537
2	E	0.12	0/1522	0.37	1/2069 (0.0%)
3	F	0.13	0/863	0.33	0/1158
4	G	0.10	0/1209	0.31	0/1639
5	I	0.11	0/5733	0.33	0/7754
6	J	0.16	0/494	0.42	0/663
7	Q	0.09	0/1035	0.29	0/1402
7	R	0.08	0/1081	0.29	0/1463
8	K	0.07	0/767	0.33	0/1030
9	U	0.14	0/1521	0.42	0/2368
10	A	0.12	0/10394	0.36	0/14052
11	Y	0.09	0/4429	0.30	0/5960
12	C	0.12	0/2540	0.35	0/3440
13	S	0.09	0/1302	0.34	0/1749
All	All	0.11	0/42171	0.34	1/57284 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
10	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	14	CYS	N-CA-C	-6.19	104.94	113.18

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	A	147	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	9091	0	9146	156	0
2	E	1495	0	1548	26	0
3	F	849	0	874	15	0
4	G	1192	0	1181	18	0
5	I	5603	0	5659	87	0
6	J	490	0	530	12	0
7	Q	1013	0	998	13	0
7	R	1056	0	1056	13	0
8	K	749	0	727	9	0
9	U	1362	0	687	19	0
10	A	10188	0	10312	194	0
11	Y	4347	0	4415	67	0
12	C	2484	0	2470	37	0
13	S	1311	0	1268	31	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	I	1	0	0	0	0
15	A	1	0	0	0	0
16	A	17	0	0	2	0
16	B	26	0	0	0	0
16	C	2	0	0	0	0
16	E	2	0	0	0	0
16	F	1	0	0	0	0
16	G	3	0	0	0	0
16	I	4	0	0	0	0
16	J	4	0	0	0	0
16	K	1	0	0	0	0
16	Y	1	0	0	0	0
All	All	41296	0	40871	599	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 7.

All (599) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:88:LEU:HD23	2:E:96:PRO:HG3	1.66	0.78
1:B:1097:ILE:HD12	1:B:1097:ILE:H	1.52	0.73
6:J:32:LEU:HD22	6:J:41:ARG:HG2	1.71	0.73
10:A:336:PHE:HB2	10:A:367:GLU:HB2	1.70	0.73
11:Y:406:ILE:O	11:Y:408:ASN:ND2	2.22	0.72
11:Y:268:GLU:HG2	11:Y:272:GLN:HE22	1.53	0.72
4:G:99:ILE:HB	4:G:106:CYS:HB2	1.70	0.72
5:I:715:MET:O	5:I:757:ARG:NH2	2.23	0.71
10:A:184:GLN:NE2	10:A:1224:ALA:O	2.24	0.71
6:J:2:VAL:HA	6:J:18:ARG:HD3	1.72	0.70
10:A:61:GLY:HA3	10:A:199:PRO:HB3	1.73	0.70
1:B:922:SER:HB2	10:A:670:LYS:HD3	1.74	0.70
1:B:1141:ASP:HB2	10:A:6:LYS:HB3	1.72	0.69
2:E:129:GLN:O	3:F:70:LYS:NZ	2.25	0.69
1:B:178:PRO:HB3	1:B:192:PHE:HB3	1.75	0.69
10:A:817:TRP:O	10:A:821:LYS:HB3	1.93	0.68
5:I:233:LYS:HB2	9:U:41:C:H5'	1.76	0.68
10:A:1075:VAL:O	10:A:1081:ASN:ND2	2.26	0.68
10:A:450:HIS:HD2	10:A:452:ALA:H	1.40	0.68
10:A:223:LEU:HD13	10:A:247:TYR:HA	1.75	0.68
12:C:25:GLY:O	12:C:29:LEU:HB2	1.93	0.68
1:B:761:LYS:HD2	1:B:899:GLU:HG3	1.75	0.67
4:G:117:PHE:HB3	4:G:123:CYS:HA	1.76	0.67
10:A:954:ALA:HB2	10:A:1104:PRO:HD2	1.75	0.67
11:Y:292:MET:HA	11:Y:295:THR:HG22	1.75	0.67
1:B:881:ASP:OD2	1:B:1017:ARG:NH2	2.28	0.66
1:B:325:GLN:HE22	5:I:749:VAL:HA	1.61	0.66
1:B:754:GLN:HE22	10:A:461:GLU:HG3	1.60	0.66
1:B:23:LYS:NZ	1:B:618:ASP:OD2	2.26	0.66
5:I:125:GLN:HE21	5:I:127:LYS:H	1.43	0.66
5:I:183:ARG:NH2	10:A:163:SER:OG	2.28	0.66
12:C:34:LEU:HD12	12:C:182:VAL:HG12	1.78	0.66
1:B:540:LEU:HD23	1:B:545:ILE:HD12	1.78	0.65
5:I:457:GLU:HB3	5:I:462:LEU:HD13	1.78	0.65
8:K:443:PHE:HB2	8:K:447:GLN:HE21	1.60	0.65
10:A:786:ASN:ND2	10:A:790:ILE:O	2.30	0.65
10:A:606:TYR:OH	10:A:626:GLU:OE2	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:710:ARG:HG2	5:I:716:PRO:HB3	1.78	0.64
10:A:996:GLU:O	10:A:1095:LYS:NZ	2.30	0.64
5:I:357:GLU:OE1	10:A:349:ARG:NH2	2.28	0.64
10:A:36:VAL:HG21	10:A:224:LEU:HB3	1.78	0.64
1:B:319:MET:HB3	1:B:322:THR:HB	1.79	0.63
1:B:610:ARG:NH2	1:B:622:GLU:OE1	2.31	0.63
10:A:764:GLU:HG3	10:A:928:ILE:HD12	1.81	0.63
2:E:13:LEU:HD23	2:E:16:LYS:HD3	1.81	0.63
11:Y:202:ARG:NH2	11:Y:228:GLY:O	2.30	0.63
3:F:112:ASN:HB3	3:F:115:HIS:HD2	1.63	0.62
1:B:675:SER:HA	1:B:728:LEU:HD11	1.80	0.62
1:B:1039:ARG:NH2	10:A:56:GLU:O	2.32	0.62
1:B:853:ARG:NH1	12:C:50:GLU:OE2	2.32	0.62
10:A:149:VAL:HG21	10:A:242:LYS:HB2	1.82	0.62
4:G:90:ASN:HD22	4:G:100:GLN:HG3	1.65	0.62
5:I:481:LEU:HD13	7:R:58:ILE:HD11	1.81	0.62
10:A:306:TYR:O	10:A:310:THR:OG1	2.18	0.61
10:A:153:ASN:ND2	10:A:156:ASP:OD1	2.34	0.61
1:B:514:ARG:HH12	5:I:753:ASN:HB2	1.65	0.61
5:I:173:PRO:HG3	10:A:158:ILE:HD13	1.82	0.61
11:Y:416:LYS:HA	11:Y:419:ARG:HD2	1.83	0.61
9:U:35:U:H3	11:Y:163:SER:HG	1.48	0.61
11:Y:278:GLU:HG2	11:Y:283:ILE:HD11	1.83	0.61
5:I:280:SER:HB3	5:I:283:LEU:HB2	1.82	0.61
13:S:94:ILE:HG22	13:S:95:ALA:H	1.66	0.61
1:B:542:PRO:HA	1:B:545:ILE:HD13	1.83	0.61
1:B:150:PRO:HG3	5:I:596:GLY:HA2	1.83	0.60
5:I:359:GLY:HA2	5:I:375:LEU:HD12	1.82	0.60
12:C:80:LEU:HB3	12:C:102:TYR:HB2	1.83	0.60
1:B:43:LEU:O	1:B:47:HIS:ND1	2.35	0.60
1:B:754:GLN:NE2	10:A:460:ASP:OD1	2.31	0.60
6:J:4:GLN:HB2	6:J:47:GLN:HE22	1.66	0.60
10:A:935:SER:HA	10:A:938:PHE:CE2	2.37	0.60
11:Y:476:ARG:HG2	11:Y:479:ARG:HH21	1.66	0.60
5:I:594:SER:H	6:J:53:ASN:HD22	1.49	0.60
10:A:304:PRO:HD2	10:A:307:ILE:HD12	1.83	0.60
1:B:208:TYR:OH	1:B:315:PHE:O	2.18	0.60
5:I:398:GLU:O	11:Y:547:SER:OG	2.17	0.60
3:F:91:ASN:HB2	10:A:430:LYS:HG3	1.84	0.59
11:Y:48:MET:O	11:Y:178:LYS:NZ	2.35	0.59
1:B:1071:THR:HG21	10:A:1244:VAL:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:808:ARG:HD2	12:C:168:ARG:HD2	1.83	0.59
2:E:11:LYS:NZ	2:E:103:ASP:OD2	2.35	0.59
5:I:589:ASN:HD21	12:C:134:LYS:HE2	1.66	0.59
1:B:1062:ILE:HD11	10:A:1239:HIS:HE1	1.67	0.59
3:F:101:VAL:HG21	3:F:108:THR:HG21	1.84	0.59
5:I:698:LYS:HA	5:I:793:PHE:HE2	1.68	0.59
9:U:14:A:N1	9:U:21:A:O2'	2.33	0.59
10:A:271:ASN:HB2	10:A:274:ARG:HG2	1.85	0.59
1:B:319:MET:HE1	1:B:536:LEU:H	1.68	0.59
10:A:978:ILE:HG13	10:A:1145:PRO:HA	1.84	0.59
1:B:431:HIS:HB3	1:B:701:LEU:HD21	1.84	0.58
10:A:1029:ARG:NH2	13:S:144:TYR:OH	2.36	0.58
6:J:21:LEU:HB3	6:J:31:VAL:HG21	1.84	0.58
9:U:35:U:N3	11:Y:163:SER:OG	2.37	0.58
7:R:55:ASP:OD1	7:R:55:ASP:N	2.35	0.58
1:B:680:ASN:HD21	1:B:957:SER:HA	1.68	0.58
10:A:475:CYS:SG	10:A:476:LEU:N	2.76	0.58
2:E:5:ASN:HB2	2:E:100:LEU:HB3	1.86	0.58
10:A:81:GLU:HG3	10:A:1225:LEU:HD21	1.85	0.58
5:I:392:LYS:NZ	10:A:219:GLU:OE2	2.27	0.58
1:B:569:THR:HG21	1:B:633:GLU:HG2	1.86	0.57
1:B:242:ARG:NH2	1:B:284:ASP:OD2	2.36	0.57
11:Y:412:SER:HB2	11:Y:443:SER:HB3	1.85	0.57
1:B:430:PRO:O	1:B:436:GLN:NE2	2.35	0.57
1:B:647:PHE:HA	1:B:650:MET:HE2	1.85	0.57
1:B:1057:GLU:HG2	10:A:422:TRP:CZ2	2.39	0.57
5:I:459:LYS:NZ	7:R:72:ASN:O	2.37	0.57
7:Q:4:VAL:HG11	7:Q:54:LYS:HE2	1.86	0.57
11:Y:483:HIS:HB3	11:Y:491:ARG:HG2	1.86	0.57
1:B:1097:ILE:HD11	1:B:1104:LEU:HD21	1.87	0.57
5:I:449:GLU:HA	5:I:452:LYS:HE2	1.86	0.57
10:A:156:ASP:OD1	10:A:156:ASP:N	2.38	0.57
5:I:492:TYR:HE1	5:I:549:ILE:HG23	1.69	0.57
11:Y:118:ASN:OD1	11:Y:121:ASN:ND2	2.37	0.57
1:B:636:THR:O	10:A:700:ARG:NH2	2.37	0.56
10:A:613:VAL:HG13	10:A:620:PRO:HG3	1.87	0.56
10:A:937:LYS:HG2	10:A:1178:LEU:HD11	1.86	0.56
1:B:41:PHE:CZ	1:B:366:PHE:HB3	2.41	0.56
11:Y:367:LYS:NZ	11:Y:510:ASP:OD2	2.35	0.56
1:B:1100:ILE:HG21	4:G:148:ILE:HG22	1.86	0.56
2:E:36:THR:HG23	2:E:53:LYS:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:112:ASN:HB3	3:F:115:HIS:CD2	2.40	0.56
1:B:11:GLN:HG3	1:B:664:PRO:HG2	1.88	0.56
5:I:594:SER:H	6:J:53:ASN:ND2	2.04	0.56
1:B:134:ILE:HD12	1:B:156:VAL:HG23	1.87	0.56
12:C:26:PHE:HD2	12:C:219:LEU:HD22	1.71	0.56
1:B:172:GLU:HG2	1:B:360:LEU:HG	1.88	0.56
1:B:766:GLN:O	12:C:58:HIS:NE2	2.37	0.56
7:Q:21:ASN:OD1	7:Q:21:ASN:N	2.37	0.55
1:B:242:ARG:O	5:I:738:ARG:NH2	2.40	0.55
1:B:409:HIS:NE2	5:I:415:MET:SD	2.77	0.55
10:A:804:ASP:H	10:A:807:MET:HE2	1.71	0.55
2:E:1:MET:SD	2:E:46:THR:OG1	2.64	0.55
7:Q:14:ARG:NH1	7:Q:95:GLU:OE1	2.40	0.55
10:A:1160:ARG:NH1	10:A:1183:ASP:OD1	2.38	0.55
5:I:418:ASP:OD1	5:I:425:THR:OG1	2.24	0.55
11:Y:124:PHE:HA	11:Y:127:ILE:HG12	1.89	0.55
1:B:309:TYR:OH	5:I:725:GLU:OE2	2.20	0.55
2:E:117:ASP:OD1	2:E:118:THR:N	2.40	0.55
4:G:19:LEU:HD11	4:G:66:VAL:HG21	1.89	0.55
7:R:104:CYS:SG	7:Q:116:SER:OG	2.64	0.55
1:B:709:ILE:HG23	1:B:870:LEU:HB2	1.89	0.55
7:Q:5:ASN:ND2	7:Q:50:TYR:O	2.34	0.55
2:E:111:PRO:HG2	2:E:113:PHE:HD2	1.71	0.54
10:A:385:HIS:HD2	10:A:388:ASN:HD22	1.54	0.54
13:S:102:THR:HB	13:S:122:LEU:HD12	1.88	0.54
1:B:180:PHE:O	1:B:351:ARG:NH2	2.41	0.54
9:U:31:A:OP2	11:Y:162:ARG:NH2	2.40	0.54
10:A:925:PRO:HB2	10:A:928:ILE:HG22	1.88	0.54
1:B:1088:GLU:OE2	1:B:1116:THR:OG1	2.23	0.54
1:B:372:ASP:OD2	1:B:420:LYS:NZ	2.32	0.54
1:B:1105:ARG:NH1	10:A:16:GLU:O	2.40	0.54
12:C:85:ARG:HG2	12:C:94:ILE:HG12	1.90	0.54
1:B:50:LEU:HD12	1:B:73:VAL:HG11	1.89	0.54
8:K:396:SER:O	8:K:397:ASN:ND2	2.41	0.54
10:A:822:GLN:O	10:A:822:GLN:NE2	2.40	0.54
1:B:649:MET:HG3	5:I:613:ILE:HG13	1.90	0.53
1:B:255:ASP:O	1:B:574:HIS:ND1	2.40	0.53
5:I:382:LYS:HD3	13:S:238:PRO:HG3	1.90	0.53
10:A:376:ILE:HD12	10:A:425:LEU:HD13	1.90	0.53
1:B:156:VAL:HG12	1:B:166:VAL:HG13	1.90	0.53
13:S:41:ILE:HD13	13:S:121:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:109:SER:OG	4:G:111:ASP:OD1	2.26	0.53
7:R:6:ILE:HG21	7:R:38:LEU:HD21	1.91	0.53
10:A:700:ARG:NE	16:A:1406:HOH:O	2.39	0.53
11:Y:457:ASP:OD2	11:Y:496:HIS:NE2	2.37	0.53
1:B:109:LYS:HD2	5:I:683:LYS:HD2	1.90	0.53
12:C:10:ILE:HB	12:C:198:PHE:HB2	1.89	0.53
11:Y:361:LEU:HD11	11:Y:403:VAL:HG11	1.91	0.53
1:B:722:ILE:HD12	1:B:723:VAL:HG23	1.89	0.52
10:A:236:ASP:N	10:A:236:ASP:OD1	2.41	0.52
10:A:1010:ARG:HG3	10:A:1017:VAL:HB	1.90	0.52
10:A:71:THR:HG23	10:A:237:GLU:HG2	1.91	0.52
11:Y:504:ASN:OD1	11:Y:504:ASN:N	2.39	0.52
5:I:109:TYR:O	5:I:113:ASP:HB2	2.08	0.52
10:A:24:ILE:HG13	10:A:197:ILE:HG13	1.92	0.52
10:A:313:GLU:HG2	10:A:370:VAL:HA	1.91	0.52
11:Y:92:ASP:O	11:Y:96:ASN:HB2	2.10	0.52
12:C:12:VAL:HG21	12:C:298:ILE:HG12	1.92	0.52
10:A:659:ASN:HB3	10:A:662:LEU:HB2	1.92	0.52
10:A:851:GLU:OE1	10:A:899:ARG:NE	2.41	0.52
1:B:1057:GLU:HG2	10:A:422:TRP:HZ2	1.74	0.52
1:B:127:LEU:HD12	5:I:419:ASN:HB3	1.91	0.52
11:Y:268:GLU:O	11:Y:272:GLN:NE2	2.43	0.52
5:I:117:ASN:HA	5:I:210:ARG:HD3	1.91	0.52
7:Q:28:SER:O	7:Q:32:ASN:ND2	2.43	0.52
12:C:11:VAL:HG22	12:C:197:THR:HG23	1.92	0.52
5:I:557:THR:HA	5:I:560:MET:HE3	1.91	0.51
10:A:46:GLY:N	10:A:56:GLU:OE2	2.36	0.51
10:A:167:GLN:NE2	16:A:1405:HOH:O	2.38	0.51
1:B:212:LEU:HD13	1:B:220:LEU:HD13	1.92	0.51
6:J:8:SER:HB2	6:J:43:LYS:HE2	1.93	0.51
4:G:145:GLN:HB2	4:G:153:VAL:HG12	1.91	0.51
7:R:46:GLN:HA	7:R:65:ARG:HG3	1.92	0.51
11:Y:278:GLU:HG3	11:Y:289:LEU:HB2	1.91	0.51
1:B:798:TYR:OH	1:B:843:SER:OG	2.29	0.51
4:G:7:ASN:O	5:I:293:ARG:NH2	2.44	0.51
5:I:713:ASP:HB2	5:I:726:HIS:HE1	1.76	0.51
1:B:257:PRO:HG2	1:B:260:VAL:HG23	1.92	0.51
10:A:140:GLN:OE1	10:A:153:ASN:ND2	2.43	0.51
10:A:376:ILE:HB	10:A:394:ILE:HD11	1.92	0.51
1:B:545:ILE:HG13	1:B:578:ILE:HD11	1.93	0.51
10:A:1027:ILE:HG23	10:A:1032:ILE:HG13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:741:LEU:HB3	5:I:777:TRP:HZ2	1.76	0.51
11:Y:165:TYR:CE1	11:Y:200:LEU:HB2	2.46	0.51
1:B:399:ILE:HD11	5:I:539:ARG:HD2	1.93	0.50
5:I:709:PHE:O	5:I:734:TYR:OH	2.29	0.50
13:S:40:LEU:HD11	13:S:124:GLY:HA3	1.93	0.50
1:B:433:SER:OG	1:B:697:ALA:O	2.28	0.50
1:B:1062:ILE:HD11	10:A:1239:HIS:CE1	2.47	0.50
5:I:116:PHE:O	5:I:210:ARG:NH1	2.45	0.50
9:U:33:U:H2'	9:U:35:U:C6	2.45	0.50
1:B:170:LEU:O	1:B:360:LEU:N	2.36	0.50
1:B:634:GLN:O	1:B:638:SER:OG	2.22	0.50
1:B:1156:VAL:HG21	3:F:75:ARG:HG3	1.92	0.50
8:K:420:ASP:HB3	8:K:423:GLY:HA2	1.92	0.50
1:B:534:ASN:OD1	1:B:579:ARG:NH1	2.43	0.50
1:B:1132:ASN:ND2	1:B:1136:VAL:O	2.42	0.50
2:E:16:LYS:NZ	2:E:150:LYS:O	2.45	0.50
10:A:104:ASP:N	10:A:104:ASP:OD1	2.43	0.50
11:Y:411:PHE:O	11:Y:445:SER:OG	2.22	0.50
2:E:16:LYS:HD2	2:E:95:PHE:HZ	1.76	0.50
5:I:208:ASN:HB2	5:I:229:PHE:CZ	2.46	0.50
10:A:993:ILE:HG12	13:S:51:TYR:HD2	1.77	0.50
3:F:76:ARG:NH2	10:A:919:THR:O	2.45	0.50
10:A:41:LEU:HB2	10:A:200:LEU:HD12	1.93	0.50
10:A:74:VAL:HG21	10:A:151:PHE:HE1	1.77	0.50
11:Y:283:ILE:HG13	11:Y:286:PHE:HA	1.94	0.50
13:S:43:TRP:NE1	13:S:135:ASN:OD1	2.45	0.50
3:F:161:GLN:HG3	3:F:163:ARG:HG3	1.94	0.50
10:A:174:GLU:HG3	10:A:177:TRP:CH2	2.47	0.50
5:I:713:ASP:HB3	5:I:730:LYS:HG2	1.93	0.49
5:I:723:ASP:OD1	5:I:723:ASP:N	2.44	0.49
10:A:742:SER:HA	10:A:745:ILE:HG12	1.93	0.49
10:A:1023:ASN:HD22	10:A:1025:LEU:H	1.60	0.49
13:S:40:LEU:HD22	13:S:128:ILE:HD12	1.94	0.49
5:I:699:TYR:OH	5:I:714:PRO:O	2.30	0.49
8:K:401:ARG:NH1	8:K:406:GLU:OE2	2.45	0.49
10:A:1055:GLY:HA3	13:S:94:ILE:HB	1.93	0.49
1:B:863:ASP:OD1	1:B:863:ASP:N	2.44	0.49
11:Y:401:PHE:HB3	11:Y:408:ASN:HD22	1.78	0.49
9:U:66:G:H2'	9:U:67:G:H8	1.78	0.49
10:A:76:PRO:HB3	10:A:245:ILE:HG12	1.95	0.49
10:A:90:CYS:HB2	10:A:139:TYR:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:314:LYS:HD3	10:A:427:GLN:HB2	1.93	0.49
10:A:978:ILE:HG12	10:A:1130:LEU:HD11	1.94	0.49
5:I:676:LYS:HD2	5:I:683:LYS:HD3	1.94	0.49
10:A:872:ARG:HB2	10:A:882:ILE:HD11	1.94	0.49
10:A:1000:LEU:HB3	10:A:1090:PRO:HA	1.93	0.49
11:Y:366:VAL:HA	11:Y:369:ILE:HG22	1.94	0.49
1:B:223:SER:HB3	1:B:230:THR:HG23	1.94	0.49
10:A:29:ASN:ND2	10:A:33:ILE:O	2.28	0.49
10:A:672:ASN:OD1	10:A:675:GLU:HG2	2.12	0.49
1:B:754:GLN:NE2	10:A:461:GLU:HG3	2.26	0.49
10:A:612:ASP:HA	10:A:617:LYS:HD2	1.94	0.49
12:C:39:ILE:HG13	12:C:173:VAL:HG21	1.95	0.49
1:B:491:LEU:HG	1:B:667:PHE:HB3	1.93	0.49
5:I:627:LYS:NZ	5:I:628:ILE:O	2.46	0.49
5:I:750:TYR:CZ	5:I:752:SER:HB3	2.48	0.49
1:B:892:THR:OG1	10:A:416:PHE:O	2.29	0.48
9:U:62:C:H2'	9:U:63:G:H8	1.77	0.48
11:Y:165:TYR:HE1	11:Y:200:LEU:HB2	1.77	0.48
1:B:64:GLU:HG3	1:B:106:VAL:HG22	1.95	0.48
10:A:955:VAL:HG11	10:A:977:ILE:HG21	1.95	0.48
1:B:140:ASN:OD1	1:B:140:ASN:N	2.45	0.48
9:U:28:U:H2'	9:U:29:G:C8	2.48	0.48
1:B:704:ASP:HB3	1:B:707:ASN:HB2	1.96	0.48
1:B:1083:ASP:OD1	1:B:1083:ASP:N	2.38	0.48
5:I:482:PHE:HB2	5:I:486:LYS:HE3	1.96	0.48
10:A:805:GLU:HG2	10:A:810:TYR:CZ	2.49	0.48
1:B:1058:ARG:NH1	10:A:764:GLU:OE2	2.47	0.48
1:B:399:ILE:HG22	1:B:400:HIS:H	1.78	0.48
1:B:442:ARG:NH2	1:B:489:SER:O	2.47	0.48
10:A:107:ASN:HB3	10:A:110:GLU:HG2	1.96	0.48
10:A:334:VAL:HA	10:A:368:VAL:HG12	1.96	0.48
1:B:875:ARG:HH12	1:B:1024:ASP:CG	2.21	0.48
2:E:115:ARG:NH1	2:E:159:LEU:HD13	2.29	0.48
11:Y:387:PRO:HB3	11:Y:397:LEU:HD22	1.96	0.48
12:C:32:TRP:HB3	12:C:184:ARG:HG3	1.96	0.48
10:A:688:ILE:HD11	10:A:737:VAL:HA	1.95	0.47
4:G:88:THR:O	4:G:100:GLN:N	2.42	0.47
7:R:31:ILE:HG22	7:R:68:ILE:HD13	1.97	0.47
10:A:481:ASN:ND2	12:C:268:ASN:O	2.37	0.47
1:B:256:MET:HE1	1:B:340:TYR:HB2	1.97	0.47
1:B:746:LEU:HB2	1:B:1009:PHE:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:933:ILE:HD13	1:B:966:MET:HE1	1.97	0.47
8:K:374:ASN:HD22	8:K:379:ASN:HA	1.77	0.47
9:U:66:G:H2'	9:U:67:G:C8	2.49	0.47
1:B:722:ILE:HG21	1:B:938:TYR:CZ	2.49	0.47
4:G:91:ILE:H	4:G:133:ASN:ND2	2.13	0.47
10:A:77:GLU:HG3	10:A:1221:LEU:HD22	1.96	0.47
11:Y:46:ASP:H	11:Y:552:GLU:CD	2.22	0.47
1:B:275:THR:HG23	1:B:281:PHE:CD2	2.50	0.47
4:G:58:LEU:HB3	10:A:1255:PHE:HB3	1.97	0.47
9:U:27:C:H2'	9:U:28:U:C6	2.49	0.47
5:I:403:PHE:CE2	5:I:467:LEU:HD13	2.49	0.47
10:A:442:THR:HA	10:A:555:ILE:HD13	1.95	0.47
1:B:13:LEU:HD22	1:B:627:ILE:HD11	1.96	0.47
11:Y:384:VAL:O	11:Y:442:PHE:N	2.41	0.47
5:I:735:ASN:HD21	5:I:748:PHE:HB3	1.80	0.47
11:Y:85:VAL:HG12	11:Y:141:ASP:HB3	1.97	0.47
11:Y:371:VAL:HG21	11:Y:461:LEU:HD21	1.97	0.47
8:K:407:VAL:HG22	8:K:417:THR:HG22	1.96	0.47
1:B:96:ALA:HB3	1:B:128:ILE:HB	1.97	0.46
5:I:722:ILE:H	5:I:726:HIS:HD2	1.61	0.46
9:U:62:C:H2'	9:U:63:G:C8	2.50	0.46
11:Y:21:VAL:HG12	11:Y:36:HIS:CD2	2.50	0.46
12:C:233:LYS:O	12:C:244:TYR:N	2.48	0.46
13:S:95:ALA:HB1	13:S:98:LEU:HD23	1.98	0.46
1:B:184:LYS:HB2	1:B:187:SER:HB3	1.97	0.46
1:B:404:THR:HB	13:S:243:LEU:HD21	1.96	0.46
1:B:779:GLN:HE21	1:B:866:LYS:HD2	1.79	0.46
8:K:368:TRP:CZ2	8:K:370:ARG:HD2	2.50	0.46
2:E:115:ARG:HH11	2:E:159:LEU:HD13	1.81	0.46
6:J:28:LEU:HD23	6:J:28:LEU:HA	1.80	0.46
1:B:181:ARG:HB3	1:B:189:THR:HG22	1.97	0.46
5:I:680:GLU:O	5:I:681:ARG:HG2	2.15	0.46
11:Y:268:GLU:HG3	11:Y:502:LEU:HD22	1.97	0.46
1:B:132:LEU:HD23	1:B:140:ASN:HD22	1.81	0.46
1:B:185:PRO:HB3	13:S:77:GLU:CD	2.41	0.46
9:U:57:A:O2'	9:U:59:U:OP2	2.25	0.46
10:A:31:ASP:HB3	10:A:33:ILE:HG13	1.97	0.46
10:A:90:CYS:HB2	10:A:139:TYR:HE1	1.81	0.46
11:Y:8:TYR:HB3	11:Y:45:LEU:HD21	1.98	0.46
12:C:154:ILE:O	12:C:158:LEU:HG	2.15	0.46
1:B:429:HIS:HD2	1:B:430:PRO:HD2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:116:LEU:HD11	2:E:163:ARG:NH2	2.31	0.46
10:A:489:GLU:OE1	10:A:506:TYR:OH	2.33	0.46
10:A:676:LEU:HD23	10:A:676:LEU:HA	1.81	0.46
4:G:52:GLU:O	5:I:301:ARG:NH2	2.49	0.46
10:A:609:TYR:HB2	13:S:147:TYR:HB3	1.98	0.46
11:Y:386:GLU:HG2	11:Y:444:SER:H	1.81	0.46
1:B:242:ARG:HB3	5:I:739:TYR:CD2	2.50	0.46
5:I:160:GLU:N	5:I:160:GLU:OE1	2.49	0.46
2:E:135:LYS:HA	2:E:135:LYS:HE2	1.98	0.45
5:I:338:VAL:HG22	10:A:48:LEU:HD12	1.98	0.45
12:C:25:GLY:HA3	12:C:223:LEU:HD21	1.97	0.45
2:E:178:ARG:NH2	10:A:1190:CYS:O	2.35	0.45
10:A:349:ARG:HB2	10:A:352:LYS:HB2	1.96	0.45
12:C:34:LEU:HD21	12:C:184:ARG:HB3	1.98	0.45
12:C:242:SER:HB2	12:C:254:ASN:H	1.81	0.45
1:B:600:MET:HA	1:B:603:VAL:HG22	1.98	0.45
10:A:816:LEU:HD12	10:A:819:LYS:HE3	1.98	0.45
10:A:1097:LYS:HG3	13:S:58:ASN:ND2	2.32	0.45
7:R:10:THR:HG22	7:R:91:VAL:HG22	1.97	0.45
9:U:15:A:H2'	9:U:58:A:H61	1.81	0.45
10:A:273:ILE:HA	10:A:277:ILE:HD12	1.98	0.45
2:E:66:GLU:HB2	2:E:85:THR:HA	1.99	0.45
3:F:79:LEU:HA	3:F:82:ILE:HG22	1.99	0.45
12:C:236:ASN:HD22	12:C:246:PRO:HA	1.81	0.45
1:B:789:ASN:ND2	1:B:823:ILE:O	2.50	0.45
10:A:1054:TRP:HE1	13:S:91:LYS:N	2.15	0.45
1:B:147:TYR:HE1	5:I:595:ARG:HA	1.81	0.45
10:A:1260:LEU:HG	10:A:1264:MET:HE3	1.98	0.45
11:Y:375:ILE:HG21	11:Y:406:ILE:HD13	1.98	0.45
1:B:473:SER:HA	10:A:735:MET:HE2	1.98	0.45
5:I:735:ASN:ND2	5:I:747:VAL:O	2.50	0.45
12:C:232:ILE:HD12	12:C:279:MET:HE3	1.99	0.45
1:B:206:ARG:HG2	1:B:208:TYR:CZ	2.52	0.45
1:B:653:ASP:OD1	1:B:653:ASP:N	2.50	0.45
10:A:1001:GLY:HA3	13:S:72:ASN:ND2	2.31	0.45
10:A:1038:GLU:OE1	13:S:119:ARG:NH2	2.44	0.45
10:A:1055:GLY:O	10:A:1071:TYR:N	2.35	0.45
10:A:1168:LEU:HD22	10:A:1179:TYR:HD1	1.81	0.45
11:Y:202:ARG:NH1	11:Y:227:LEU:HA	2.32	0.45
13:S:68:PHE:HD2	13:S:73:ASN:HD22	1.65	0.45
1:B:257:PRO:O	1:B:261:VAL:HG23	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:723:VAL:O	1:B:886:ARG:NH2	2.43	0.44
2:E:29:ARG:HD3	2:E:106:ILE:HA	1.99	0.44
10:A:997:PHE:HZ	13:S:76:ILE:HG12	1.83	0.44
11:Y:254:LYS:HD3	11:Y:478:ILE:HG21	1.99	0.44
11:Y:424:ALA:O	11:Y:428:GLN:HG3	2.17	0.44
10:A:133:SER:HA	10:A:136:MET:HE2	1.99	0.44
12:C:78:GLY:O	12:C:104:ILE:N	2.50	0.44
1:B:875:ARG:NH1	1:B:1024:ASP:OD2	2.46	0.44
10:A:660:ASN:HA	10:A:663:LYS:HG2	1.99	0.44
10:A:796:LYS:HB2	10:A:841:ASN:HB2	1.99	0.44
13:S:243:LEU:H	13:S:243:LEU:HD12	1.81	0.44
1:B:992:GLU:HB3	1:B:1007:LYS:HD3	1.98	0.44
4:G:46:LYS:HE3	4:G:103:ASP:OD2	2.16	0.44
5:I:561:PRO:HG2	5:I:564:LEU:HD13	1.99	0.44
5:I:567:HIS:HA	5:I:570:ARG:HG2	2.00	0.44
10:A:1207:SER:O	10:A:1211:ARG:HG3	2.18	0.44
11:Y:33:ASP:OD1	11:Y:33:ASP:N	2.45	0.44
2:E:123:ILE:HG12	3:F:66:ILE:HD11	2.00	0.44
5:I:713:ASP:OD1	5:I:713:ASP:N	2.50	0.44
10:A:254:SER:OG	10:A:255:ASN:N	2.50	0.44
10:A:1064:ASP:OD1	10:A:1064:ASP:N	2.51	0.44
7:Q:9:GLU:N	7:Q:93:GLY:O	2.48	0.44
1:B:80:TYR:HE1	1:B:85:ALA:HB2	1.83	0.44
1:B:996:TYR:CZ	12:C:192:PRO:HB3	2.53	0.44
10:A:547:ASP:OD2	10:A:841:ASN:ND2	2.44	0.44
11:Y:362:LYS:HB3	11:Y:362:LYS:HE3	1.78	0.44
1:B:38:TYR:OH	1:B:131:PRO:O	2.31	0.44
5:I:652:GLU:HG2	5:I:655:LYS:HD3	1.99	0.44
7:R:1:MET:HE3	7:R:1:MET:HB2	1.82	0.44
7:R:24:ASP:OD1	7:R:24:ASP:N	2.48	0.44
11:Y:295:THR:HG23	11:Y:296:PHE:CD2	2.53	0.44
1:B:178:PRO:HG3	1:B:334:LEU:HD22	1.99	0.44
9:U:15:A:H2'	9:U:58:A:N6	2.33	0.44
1:B:72:ASN:OD1	1:B:72:ASN:N	2.51	0.43
4:G:137:VAL:HG11	4:G:158:ILE:HD13	2.00	0.43
5:I:712:GLY:HA3	5:I:733:CYS:SG	2.58	0.43
7:Q:52:VAL:HG11	7:Q:78:PHE:CE1	2.53	0.43
5:I:522:THR:HG22	5:I:525:TYR:HB3	2.00	0.43
10:A:563:TYR:OH	12:C:272:GLU:OE1	2.25	0.43
10:A:1097:LYS:HG3	13:S:58:ASN:HD21	1.83	0.43
12:C:246:PRO:HD2	12:C:250:MET:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:TYR:HD1	1:B:153:ILE:HG22	1.83	0.43
5:I:722:ILE:H	5:I:726:HIS:CD2	2.36	0.43
7:R:11:ASP:OD1	7:R:11:ASP:N	2.50	0.43
7:Q:10:THR:HG22	7:Q:91:VAL:HG22	2.01	0.43
11:Y:266:LYS:HD3	11:Y:363:GLU:HB3	1.99	0.43
12:C:188:ILE:HB	12:C:199:PHE:HB2	2.00	0.43
1:B:532:ILE:HD12	1:B:537:VAL:HG21	2.00	0.43
3:F:151:LEU:HD23	3:F:151:LEU:HA	1.87	0.43
1:B:136:TYR:CD1	1:B:153:ILE:HG22	2.53	0.43
6:J:32:LEU:HB3	6:J:41:ARG:NH1	2.34	0.43
11:Y:289:LEU:HA	11:Y:292:MET:HG2	2.00	0.43
1:B:946:LYS:HB2	1:B:946:LYS:HE2	1.79	0.43
10:A:591:LEU:HD23	10:A:591:LEU:HA	1.86	0.43
10:A:691:GLU:HG2	10:A:951:LYS:HE2	2.01	0.43
10:A:807:MET:SD	10:A:894:ASN:ND2	2.92	0.43
10:A:993:ILE:HD11	10:A:1032:ILE:HG22	2.00	0.43
10:A:1130:LEU:HG	10:A:1133:LEU:HD12	2.01	0.43
1:B:756:ASP:CG	1:B:923:ARG:HH22	2.26	0.43
4:G:85:VAL:HG12	8:K:384:ILE:HB	2.00	0.43
10:A:65:LYS:HB2	10:A:194:TYR:HB3	2.00	0.43
10:A:323:ASP:OD1	10:A:323:ASP:N	2.52	0.43
10:A:764:GLU:HG2	10:A:1235:ASN:HD22	1.84	0.43
12:C:203:TYR:HB2	12:C:206:PHE:CE1	2.54	0.43
10:A:1196:GLU:OE2	10:A:1202:LYS:N	2.49	0.43
10:A:748:GLU:O	10:A:752:THR:OG1	2.21	0.43
10:A:958:LYS:HB3	10:A:963:GLU:HB2	2.00	0.43
10:A:1097:LYS:HA	13:S:58:ASN:HD21	1.83	0.43
12:C:226:ASN:HB3	12:C:257:MET:HE1	2.01	0.43
1:B:481:GLN:HB3	1:B:485:VAL:HG23	2.01	0.42
3:F:82:ILE:HG21	3:F:150:HIS:HB3	2.01	0.42
9:U:22:G:O6	9:U:23:C:N4	2.52	0.42
1:B:875:ARG:HH21	1:B:1023:GLN:HB2	1.83	0.42
10:A:88:HIS:NE2	10:A:120:LYS:HE2	2.34	0.42
10:A:294:THR:HG22	10:A:566:LYS:NZ	2.34	0.42
10:A:388:ASN:HA	10:A:412:GLN:HG2	2.00	0.42
10:A:621:LEU:HA	10:A:1029:ARG:NH1	2.34	0.42
7:Q:3:LEU:HD13	7:Q:6:ILE:HB	2.01	0.42
11:Y:82:ILE:HD11	11:Y:130:ILE:HD11	2.00	0.42
1:B:54:ARG:NH1	1:B:375:GLU:OE2	2.44	0.42
5:I:526:ALA:O	5:I:530:VAL:HG23	2.19	0.42
5:I:678:GLU:HG2	5:I:683:LYS:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:997:PHE:CE1	10:A:1098:ILE:HG12	2.55	0.42
12:C:102:TYR:CD2	12:C:111:VAL:HG12	2.54	0.42
1:B:147:TYR:CE1	5:I:595:ARG:HD3	2.55	0.42
4:G:56:LEU:HD12	4:G:71:PRO:HD2	2.00	0.42
10:A:1011:LYS:HD3	10:A:1016:TYR:CE2	2.55	0.42
10:A:809:TRP:CE2	10:A:861:TYR:HB2	2.55	0.42
12:C:52:TRP:HB3	12:C:141:LEU:HD21	2.02	0.42
13:S:67:LYS:HA	13:S:67:LYS:HD3	1.82	0.42
13:S:212:ILE:HG22	13:S:213:HIS:CD2	2.55	0.42
4:G:115:VAL:HA	4:G:124:PHE:O	2.20	0.42
10:A:508:ILE:HG23	10:A:545:LEU:HD21	2.02	0.42
10:A:602:ILE:HD11	13:S:151:LEU:HD23	2.00	0.42
10:A:1007:ILE:HD13	10:A:1089:LEU:HD23	2.01	0.42
7:Q:6:ILE:HD13	7:Q:38:LEU:HD21	2.00	0.42
11:Y:65:THR:OG1	11:Y:182:LEU:HD21	2.19	0.42
2:E:30:ASN:OD1	2:E:30:ASN:N	2.52	0.42
3:F:62:ILE:HD12	3:F:62:ILE:HA	1.90	0.42
5:I:392:LYS:HB3	10:A:222:TYR:CE1	2.54	0.42
10:A:318:ASN:HD22	10:A:320:PHE:HD1	1.68	0.42
10:A:840:PHE:HZ	10:A:908:ILE:HG23	1.85	0.42
10:A:1023:ASN:HB3	10:A:1026:TYR:HD2	1.85	0.42
11:Y:13:LEU:HD11	11:Y:37:PHE:HE1	1.84	0.42
1:B:10:ASP:OD1	1:B:10:ASP:N	2.52	0.42
1:B:251:SER:O	1:B:336:ARG:NH1	2.53	0.42
5:I:115:PHE:CD2	5:I:263:ILE:HD12	2.55	0.42
8:K:392:MET:HE1	8:K:407:VAL:HG23	2.01	0.42
10:A:142:ILE:HD13	10:A:160:VAL:HG21	2.01	0.42
10:A:970:LEU:HD12	10:A:1197:SER:HA	2.02	0.42
12:C:85:ARG:NH2	12:C:91:ASP:O	2.52	0.42
1:B:120:TYR:OH	5:I:420:ILE:HG12	2.20	0.42
1:B:513:ILE:HD12	1:B:532:ILE:HD11	2.02	0.42
10:A:463:VAL:HG11	10:A:664:MET:HG2	2.02	0.42
10:A:774:VAL:HG12	10:A:781:ILE:HB	2.02	0.42
11:Y:167:PHE:O	11:Y:171:THR:OG1	2.36	0.42
11:Y:384:VAL:HG11	11:Y:397:LEU:HD21	2.02	0.42
1:B:217:LEU:HD12	1:B:217:LEU:HA	1.79	0.42
5:I:287:TYR:O	5:I:291:ILE:HG12	2.20	0.42
5:I:588:PRO:HG2	5:I:590:TYR:CE2	2.55	0.42
10:A:385:HIS:CD2	10:A:388:ASN:HD22	2.37	0.42
1:B:846:TYR:CE2	1:B:848:ASP:HB2	2.55	0.41
5:I:398:GLU:OE2	11:Y:3:LYS:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:91:ILE:H	10:A:91:ILE:HG12	1.51	0.41
10:A:850:THR:O	10:A:850:THR:OG1	2.34	0.41
11:Y:4:SER:HB2	11:Y:543:GLU:OE1	2.20	0.41
5:I:124:ARG:HA	5:I:124:ARG:HD3	1.84	0.41
10:A:507:LEU:HD11	10:A:564:VAL:HG21	2.01	0.41
10:A:595:ASN:HD21	10:A:641:ASN:HD21	1.68	0.41
10:A:766:MET:HB3	10:A:927:GLY:HA3	2.01	0.41
11:Y:86:LYS:HD2	11:Y:145:ASN:HD22	1.86	0.41
11:Y:223:LEU:HG	11:Y:565:LEU:HD21	2.03	0.41
1:B:168:ILE:O	1:B:365:TYR:OH	2.30	0.41
1:B:413:SER:OG	13:S:239:ILE:HD11	2.19	0.41
1:B:680:ASN:ND2	1:B:957:SER:HA	2.33	0.41
1:B:992:GLU:OE1	10:A:579:LYS:HD3	2.21	0.41
2:E:111:PRO:HG2	2:E:113:PHE:CD2	2.54	0.41
5:I:190:ASP:HA	5:I:202:ILE:HG12	2.02	0.41
10:A:550:SER:HB3	10:A:553:GLU:OE1	2.20	0.41
10:A:1042:GLU:O	10:A:1046:SER:OG	2.21	0.41
1:B:518:LYS:O	1:B:522:SER:OG	2.30	0.41
1:B:1029:ARG:NH1	1:B:1048:GLY:O	2.53	0.41
10:A:132:ASN:HB3	10:A:135:CYS:HB3	2.02	0.41
10:A:316:PHE:O	10:A:321:THR:OG1	2.37	0.41
10:A:1127:LEU:HD12	10:A:1127:LEU:HA	1.82	0.41
1:B:56:LEU:HD12	1:B:56:LEU:HA	1.82	0.41
3:F:127:PRO:HB2	10:A:1256:ILE:HG13	2.02	0.41
10:A:517:LEU:O	10:A:524:ILE:N	2.31	0.41
11:Y:426:PHE:O	11:Y:431:ASN:ND2	2.54	0.41
1:B:132:LEU:HD12	1:B:132:LEU:HA	1.86	0.41
1:B:165:LYS:HD3	1:B:428:THR:HA	2.02	0.41
1:B:398:ASN:O	1:B:401:VAL:HG22	2.20	0.41
1:B:440:ILE:HB	1:B:441:PRO:HD3	2.01	0.41
1:B:1158:LEU:HD12	1:B:1158:LEU:HA	1.83	0.41
5:I:144:TYR:HB2	9:U:33:U:H4'	2.02	0.41
6:J:14:ILE:HG21	6:J:40:CYS:HB3	2.03	0.41
10:A:32:ASP:O	10:A:38:ASP:HB3	2.21	0.41
10:A:981:VAL:HG13	10:A:1120:LEU:HB3	2.01	0.41
1:B:42:ILE:HG23	1:B:43:LEU:N	2.35	0.41
1:B:278:ILE:HD12	1:B:281:PHE:HD1	1.85	0.41
1:B:517:TYR:O	1:B:521:ILE:HG12	2.20	0.41
9:U:28:U:H2'	9:U:29:G:H8	1.83	0.41
10:A:471:ILE:HD12	10:A:568:TYR:HE1	1.86	0.41
10:A:483:LEU:HD21	10:A:503:ILE:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:26:SER:N	11:Y:100:ARG:O	2.52	0.41
11:Y:324:LYS:HB3	11:Y:364:LYS:NZ	2.35	0.41
12:C:83:LEU:HD23	12:C:141:LEU:HD12	2.02	0.41
1:B:244:SER:HB3	1:B:247:PHE:H	1.85	0.41
2:E:184:ALA:HB3	10:A:114:HIS:ND1	2.35	0.41
10:A:612:ASP:OD2	13:S:147:TYR:OH	2.35	0.41
10:A:788:THR:HG22	10:A:885:MET:HE2	2.02	0.41
7:Q:3:LEU:HD11	7:Q:51:LEU:HD23	2.03	0.41
12:C:278:ASP:OD2	12:C:280:THR:OG1	2.37	0.41
1:B:315:PHE:CD2	1:B:316:LEU:HG	2.56	0.41
1:B:706:ARG:HD3	6:J:55:THR:HG21	2.03	0.41
1:B:1143:GLU:HB2	10:A:5:SER:HB3	2.02	0.41
2:E:84:ILE:HA	2:E:95:PHE:O	2.20	0.41
4:G:37:HIS:HB3	4:G:150:SER:HB2	2.03	0.41
5:I:225:ILE:HG12	10:A:173:HIS:HA	2.03	0.41
5:I:791:ILE:HD13	5:I:791:ILE:HA	1.96	0.41
7:R:8:LEU:HB2	7:R:15:VAL:HG22	2.02	0.41
10:A:209:TRP:CE2	10:A:210:ILE:HG12	2.56	0.41
10:A:324:LYS:O	10:A:327:GLN:HG3	2.21	0.41
10:A:993:ILE:HG12	13:S:51:TYR:CD2	2.55	0.41
10:A:1007:ILE:HG22	10:A:1086:MET:HE1	2.02	0.41
11:Y:24:MET:HE3	11:Y:24:MET:HB3	1.88	0.41
11:Y:86:LYS:O	11:Y:90:ILE:HG13	2.21	0.41
11:Y:243:ASP:O	11:Y:254:LYS:NZ	2.35	0.41
11:Y:245:VAL:HB	11:Y:254:LYS:HB3	2.02	0.41
12:C:79:PHE:HA	12:C:103:ILE:HA	2.02	0.41
1:B:635:PHE:CZ	10:A:703:PRO:HG2	2.55	0.41
1:B:879:LEU:HD23	1:B:879:LEU:HA	1.88	0.41
9:U:19:U:H4'	9:U:20:U:OP2	2.21	0.41
10:A:273:ILE:HG12	10:A:277:ILE:HD12	2.02	0.41
10:A:386:ARG:NH2	10:A:448:ASP:OD1	2.54	0.41
10:A:1047:PHE:O	13:S:86:LEU:N	2.52	0.41
2:E:9:LEU:HD13	2:E:100:LEU:HD11	2.03	0.40
2:E:184:ALA:HB3	10:A:114:HIS:CE1	2.56	0.40
5:I:343:PHE:HA	5:I:346:ILE:HG12	2.03	0.40
5:I:704:SER:HA	5:I:707:TYR:HD2	1.86	0.40
5:I:734:TYR:HB3	5:I:764:PHE:CE1	2.57	0.40
10:A:65:LYS:HD2	10:A:194:TYR:CG	2.56	0.40
10:A:807:MET:HA	10:A:896:SER:OG	2.21	0.40
7:Q:39:SER:O	7:Q:109:LYS:NZ	2.45	0.40
11:Y:381:LYS:HD2	11:Y:432:THR:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:40:VAL:HG22	12:C:141:LEU:HD23	2.02	0.40
12:C:176:ILE:HD12	12:C:176:ILE:HA	1.90	0.40
1:B:42:ILE:HG23	1:B:43:LEU:H	1.86	0.40
1:B:958:ASN:ND2	1:B:960:THR:O	2.54	0.40
2:E:149:VAL:HG13	2:E:159:LEU:HD23	2.02	0.40
5:I:375:LEU:HD23	5:I:375:LEU:HA	1.90	0.40
6:J:2:VAL:HB	6:J:49:GLU:HG3	2.04	0.40
10:A:234:ASN:ND2	11:Y:557:THR:O	2.49	0.40
1:B:385:ILE:HG12	1:B:397:VAL:HB	2.04	0.40
1:B:1068:ASN:HA	1:B:1071:THR:HG22	2.03	0.40
5:I:324:ALA:HB2	10:A:356:ASN:HD22	1.87	0.40
7:R:6:ILE:HG12	7:R:96:PHE:CD2	2.56	0.40
10:A:434:GLU:OE2	10:A:1249:THR:OG1	2.24	0.40
10:A:609:TYR:HB2	13:S:147:TYR:CB	2.51	0.40
10:A:836:THR:HB	10:A:888:ILE:HD11	2.04	0.40
10:A:915:LYS:O	10:A:919:THR:OG1	2.37	0.40
11:Y:5:HIS:HD2	11:Y:555:TRP:CZ3	2.39	0.40
11:Y:36:HIS:NE2	11:Y:40:ARG:HD2	2.36	0.40
1:B:73:VAL:HG22	1:B:98:PHE:HB3	2.02	0.40
1:B:306:GLU:HG3	5:I:693:ILE:HG21	2.02	0.40
3:F:160:LEU:HD23	3:F:160:LEU:HA	1.98	0.40
5:I:659:ARG:HD3	5:I:700:TYR:CE1	2.56	0.40
5:I:723:ASP:O	5:I:727:VAL:HG23	2.21	0.40
10:A:455:TYR:HB2	10:A:558:ILE:HD13	2.03	0.40
1:B:565:GLU:O	1:B:586:ARG:NH2	2.49	0.40
1:B:743:THR:HA	1:B:1012:PRO:HA	2.04	0.40
1:B:1082:GLN:HE22	10:A:58:GLU:HA	1.86	0.40
10:A:413:ASN:ND2	10:A:940:GLN:HE22	2.19	0.40
10:A:697:VAL:HG12	10:A:698:LEU:HG	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1123/1164 (96%)	1047 (93%)	76 (7%)	0	100	100
2	E	182/185 (98%)	165 (91%)	17 (9%)	0	100	100
3	F	101/164 (62%)	95 (94%)	6 (6%)	0	100	100
4	G	149/161 (92%)	139 (93%)	10 (7%)	0	100	100
5	I	661/795 (83%)	615 (93%)	46 (7%)	0	100	100
6	J	59/63 (94%)	56 (95%)	3 (5%)	0	100	100
7	Q	122/129 (95%)	118 (97%)	4 (3%)	0	100	100
7	R	128/129 (99%)	121 (94%)	7 (6%)	0	100	100
8	K	87/710 (12%)	81 (93%)	6 (7%)	0	100	100
10	A	1266/1286 (98%)	1190 (94%)	76 (6%)	0	100	100
11	Y	533/631 (84%)	502 (94%)	31 (6%)	0	100	100
12	C	302/305 (99%)	281 (93%)	21 (7%)	0	100	100
13	S	152/259 (59%)	132 (87%)	20 (13%)	0	100	100
All	All	4865/5981 (81%)	4542 (93%)	323 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1030/1064 (97%)	990 (96%)	40 (4%)	28	53
2	E	174/175 (99%)	168 (97%)	6 (3%)	32	56
3	F	94/151 (62%)	91 (97%)	3 (3%)	34	56
4	G	136/144 (94%)	131 (96%)	5 (4%)	30	54
5	I	637/755 (84%)	611 (96%)	26 (4%)	27	52
6	J	60/62 (97%)	53 (88%)	7 (12%)	5	22
7	Q	116/121 (96%)	108 (93%)	8 (7%)	14	41
7	R	122/121 (101%)	116 (95%)	6 (5%)	22	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	K	87/665 (13%)	80 (92%)	7 (8%)	11	36
10	A	1139/1157 (98%)	1084 (95%)	55 (5%)	23	48
11	Y	490/573 (86%)	474 (97%)	16 (3%)	33	56
12	C	286/287 (100%)	276 (96%)	10 (4%)	32	55
13	S	146/237 (62%)	141 (97%)	5 (3%)	32	56
All	All	4517/5512 (82%)	4323 (96%)	194 (4%)	27	50

All (194) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	42	ILE
1	B	52	VAL
1	B	56	LEU
1	B	58	SER
1	B	65	ARG
1	B	69	GLU
1	B	100	VAL
1	B	127	LEU
1	B	130	ILE
1	B	146	LYS
1	B	148	LEU
1	B	166	VAL
1	B	189	THR
1	B	196	SER
1	B	206	ARG
1	B	217	LEU
1	B	227	THR
1	B	229	ILE
1	B	243	VAL
1	B	302	LEU
1	B	305	ASN
1	B	394	THR
1	B	401	VAL
1	B	433	SER
1	B	545	ILE
1	B	568	ILE
1	B	677	VAL
1	B	680	ASN
1	B	705	ILE
1	B	713	ILE

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Mol	Chain	Res	Type
1	B	722	ILE
1	B	742	VAL
1	B	780	VAL
1	B	785	GLU
1	B	790	LYS
1	B	931	GLU
1	B	1028	VAL
1	B	1035	THR
1	B	1084	VAL
1	B	1086	VAL
2	E	30	ASN
2	E	72	THR
2	E	104	VAL
2	E	108	ASP
2	E	169	MET
2	E	170	VAL
3	F	77	ILE
3	F	94	GLN
3	F	117	ILE
4	G	12	VAL
4	G	20	THR
4	G	58	LEU
4	G	96	ASN
4	G	137	VAL
5	I	140	VAL
5	I	160	GLU
5	I	220	LEU
5	I	235	VAL
5	I	256	LEU
5	I	285	SER
5	I	308	GLU
5	I	376	ASP
5	I	384	THR
5	I	386	ILE
5	I	389	THR
5	I	421	MET
5	I	448	GLN
5	I	462	LEU
5	I	522	THR
5	I	536	VAL
5	I	540	ILE
5	I	558	SER

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Mol	Chain	Res	Type
5	I	613	ILE
5	I	614	VAL
5	I	666	THR
5	I	679	ILE
5	I	688	LEU
5	I	738	ARG
5	I	747	VAL
5	I	749	VAL
6	J	3	PHE
6	J	10	CYS
6	J	21	LEU
6	J	39	CYS
6	J	40	CYS
6	J	48	ILE
6	J	49	GLU
7	R	24	ASP
7	R	31	ILE
7	R	55	ASP
7	R	114	VAL
7	R	117	VAL
7	R	125	ASN
8	K	366	VAL
8	K	369	SER
8	K	372	CYS
8	K	409	ILE
8	K	422	LEU
8	K	431	LEU
8	K	444	LEU
10	A	26	HIS
10	A	27	VAL
10	A	36	VAL
10	A	66	VAL
10	A	68	ILE
10	A	80	SER
10	A	91	ILE
10	A	124	LEU
10	A	148	LYS
10	A	149	VAL
10	A	156	ASP
10	A	163	SER
10	A	179	LEU
10	A	184	GLN

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Mol	Chain	Res	Type
10	A	236	ASP
10	A	261	ASN
10	A	298	VAL
10	A	310	THR
10	A	317	VAL
10	A	366	VAL
10	A	376	ILE
10	A	471	ILE
10	A	530	SER
10	A	555	ILE
10	A	613	VAL
10	A	631	GLU
10	A	644	GLU
10	A	645	ILE
10	A	662	LEU
10	A	683	TYR
10	A	740	SER
10	A	773	GLN
10	A	776	ILE
10	A	798	VAL
10	A	816	LEU
10	A	822	GLN
10	A	836	THR
10	A	850	THR
10	A	901	THR
10	A	949	THR
10	A	957	GLN
10	A	959	LEU
10	A	978	ILE
10	A	1009	LEU
10	A	1013	THR
10	A	1058	THR
10	A	1072	LEU
10	A	1080	LEU
10	A	1082	LEU
10	A	1083	SER
10	A	1117	THR
10	A	1122	LYS
10	A	1124	THR
10	A	1139	GLU
10	A	1199	ASN
7	Q	14	ARG

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Mol	Chain	Res	Type
7	Q	21	ASN
7	Q	38	LEU
7	Q	44	ILE
7	Q	71	VAL
7	Q	77	VAL
7	Q	82	LEU
7	Q	94	VAL
11	Y	17	THR
11	Y	56	GLU
11	Y	171	THR
11	Y	188	VAL
11	Y	218	VAL
11	Y	219	ASP
11	Y	276	LEU
11	Y	283	ILE
11	Y	394	ILE
11	Y	398	LEU
11	Y	415	THR
11	Y	423	VAL
11	Y	441	VAL
11	Y	464	THR
11	Y	486	THR
11	Y	504	ASN
12	C	18	LEU
12	C	29	LEU
12	C	103	ILE
12	C	108	THR
12	C	149	VAL
12	C	175	THR
12	C	211	CYS
12	C	234	VAL
12	C	239	GLU
12	C	247	GLU
13	S	98	LEU
13	S	102	THR
13	S	107	ILE
13	S	132	VAL
13	S	210	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (114) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	40	ASN
1	B	169	ASN
1	B	221	ASN
1	B	232	ASN
1	B	301	GLN
1	B	313	HIS
1	B	325	GLN
1	B	387	ASN
1	B	389	HIS
1	B	429	HIS
1	B	431	HIS
1	B	639	ASN
1	B	681	HIS
1	B	736	ASN
1	B	766	GLN
1	B	858	GLN
1	B	971	GLN
1	B	1040	GLN
1	B	1068	ASN
2	E	92	HIS
2	E	125	ASN
2	E	129	GLN
2	E	168	ASN
3	F	94	GLN
3	F	115	HIS
4	G	17	HIS
4	G	90	ASN
4	G	133	ASN
4	G	145	GLN
4	G	157	ASN
5	I	110	ASN
5	I	125	GLN
5	I	239	ASN
5	I	253	ASN
5	I	348	ASN
5	I	419	ASN
5	I	448	GLN
5	I	567	HIS
5	I	589	ASN
5	I	724	HIS
5	I	726	HIS
5	I	728	GLN
5	I	735	ASN

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Mol	Chain	Res	Type
5	I	740	HIS
5	I	776	GLN
5	I	781	ASN
5	I	795	ASN
6	J	47	GLN
6	J	51	GLN
6	J	53	ASN
6	J	57	GLN
7	R	110	ASN
7	R	125	ASN
8	K	374	ASN
8	K	397	ASN
8	K	412	ASN
8	K	447	GLN
10	A	167	GLN
10	A	183	HIS
10	A	309	ASN
10	A	318	ASN
10	A	333	GLN
10	A	359	HIS
10	A	381	GLN
10	A	385	HIS
10	A	388	ASN
10	A	428	ASN
10	A	450	HIS
10	A	513	ASN
10	A	538	HIS
10	A	548	HIS
10	A	589	ASN
10	A	611	ASN
10	A	636	ASN
10	A	641	ASN
10	A	685	GLN
10	A	741	GLN
10	A	881	ASN
10	A	932	GLN
10	A	940	GLN
10	A	957	GLN
10	A	1023	ASN
10	A	1116	GLN
10	A	1169	ASN
10	A	1233	ASN

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Mol	Chain	Res	Type
10	A	1235	ASN
10	A	1239	HIS
7	Q	43	HIS
7	Q	46	GLN
7	Q	120	ASN
11	Y	5	HIS
11	Y	71	HIS
11	Y	78	ASN
11	Y	117	GLN
11	Y	144	HIS
11	Y	145	ASN
11	Y	166	ASN
11	Y	177	HIS
11	Y	236	ASN
11	Y	272	GLN
11	Y	391	GLN
11	Y	408	ASN
11	Y	542	ASN
12	C	27	ASN
12	C	129	GLN
12	C	137	GLN
12	C	171	ASN
12	C	229	ASN
12	C	236	ASN
12	C	260	ASN
13	S	55	ASN
13	S	58	ASN
13	S	72	ASN
13	S	73	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	U	61/72 (84%)	17 (27%)	2 (3%)

All (17) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	U	9	G
9	U	14	A
9	U	16	U

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Mol	Chain	Res	Type
9	U	17	G
9	U	18	G
9	U	19	U
9	U	20	U
9	U	21	A
9	U	24	A
9	U	26	U
9	U	34	U
9	U	35	U
9	U	37	A
9	U	43	G
9	U	46	A
9	U	47	U
9	U	48	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	U	18	G
9	U	20	U

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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	SEP	S	237	13	8,9,10	1.63	1 (12%)	7,12,14	1.18	1 (14%)
13	SEP	S	232	13	8,9,10	1.63	1 (12%)	7,12,14	1.81	2 (28%)
13	SEP	S	228	13	8,9,10	1.61	1 (12%)	7,12,14	1.32	1 (14%)

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	SEP	S	237	13	-	0/6/8/10	-
13	SEP	S	232	13	-	2/6/8/10	-
13	SEP	S	228	13	-	4/6/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	S	232	SEP	P-O1P	3.56	1.61	1.50
13	S	237	SEP	P-O1P	3.54	1.61	1.50
13	S	228	SEP	P-O1P	3.51	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	S	232	SEP	OG-CB-CA	4.04	112.08	108.14
13	S	228	SEP	OG-CB-CA	2.91	110.98	108.14
13	S	237	SEP	OG-CB-CA	2.47	110.55	108.14
13	S	232	SEP	OG-P-O1P	2.18	112.32	106.44

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	S	228	SEP	CB-OG-P-O2P
13	S	228	SEP	CB-OG-P-O3P
13	S	228	SEP	CB-OG-P-O1P
13	S	232	SEP	CB-OG-P-O1P
13	S	228	SEP	CA-CB-OG-P
13	S	232	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

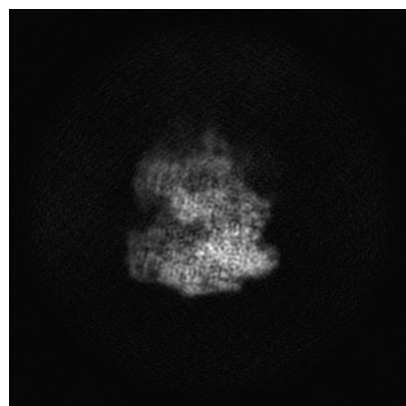
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16476. These allow visual inspection of the internal detail of the map and identification of artifacts.

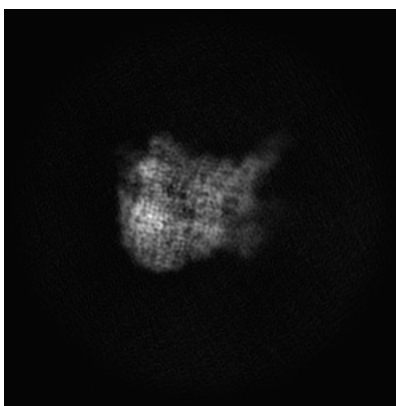
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

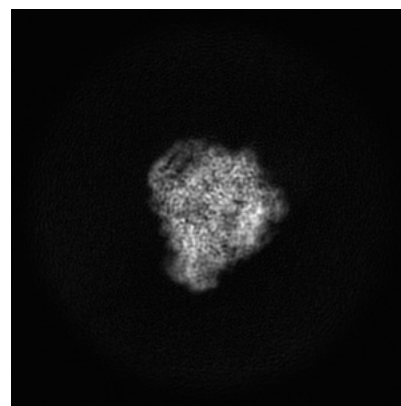
6.1.1 Primary map



X

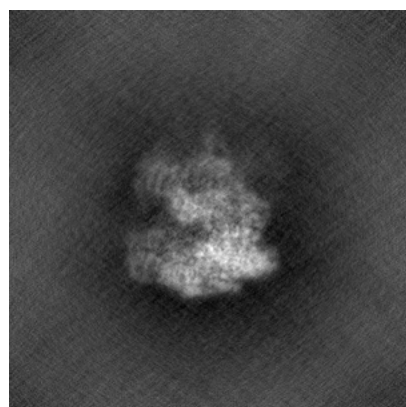


Y

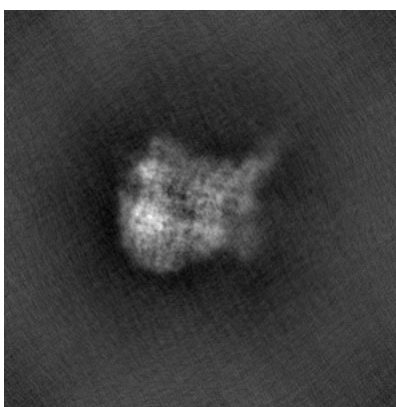


Z

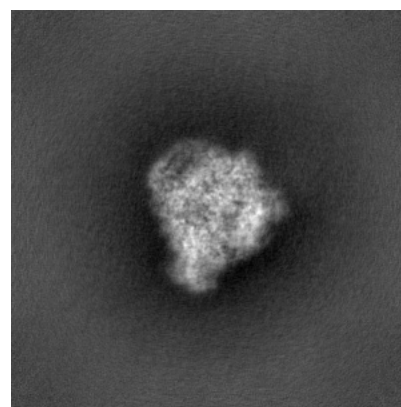
6.1.2 Raw map



X



Y

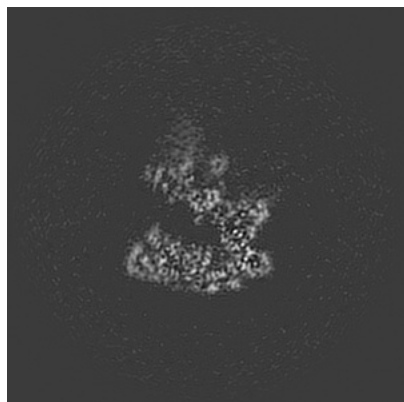


Z

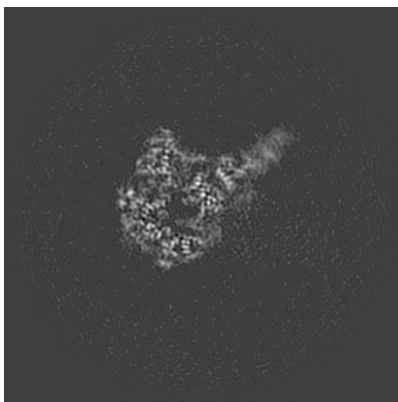
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

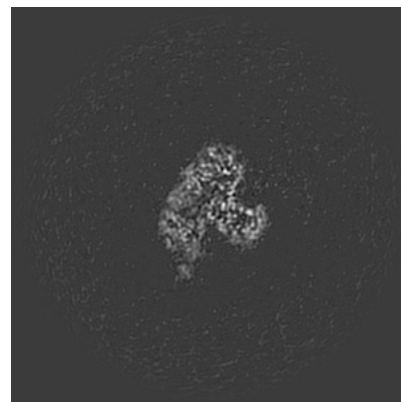
6.2.1 Primary map



X Index: 180

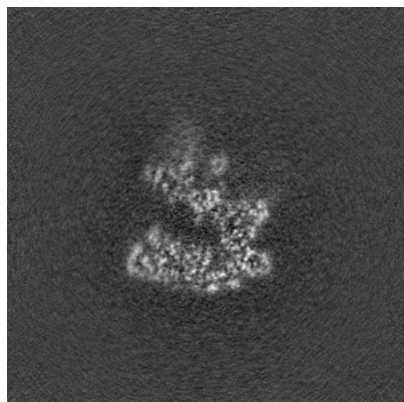


Y Index: 180

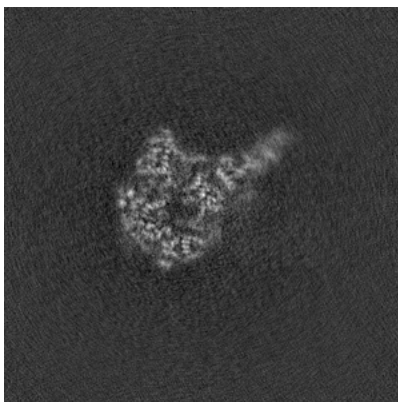


Z Index: 180

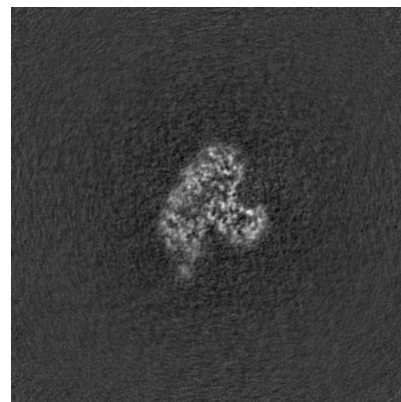
6.2.2 Raw map



X Index: 180



Y Index: 180

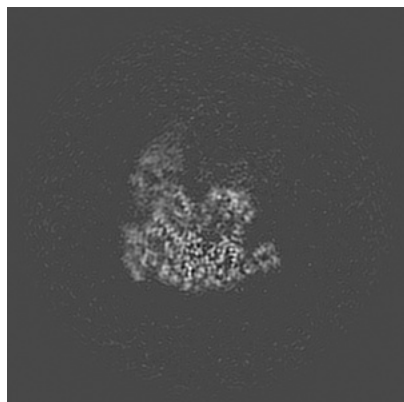


Z Index: 180

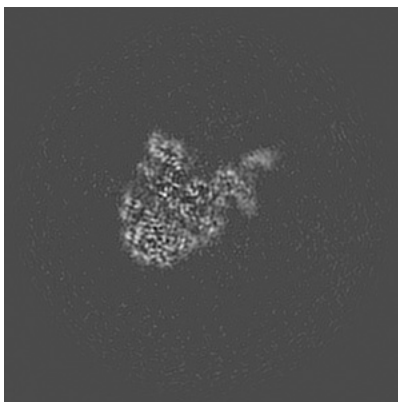
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

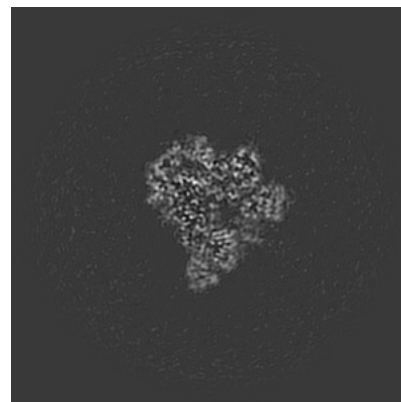
6.3.1 Primary map



X Index: 163

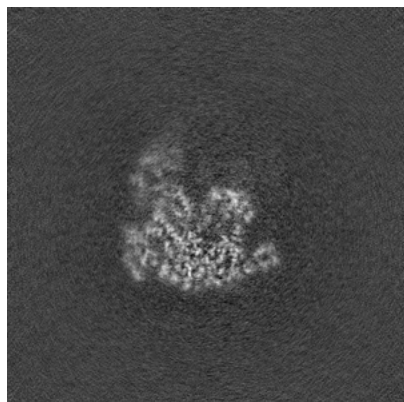


Y Index: 194

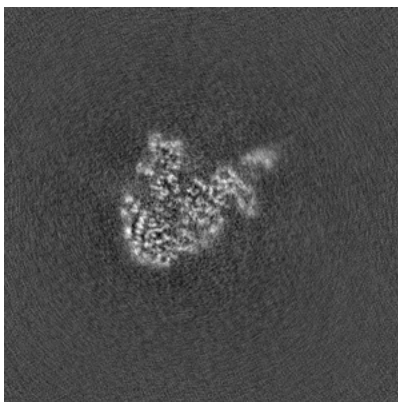


Z Index: 137

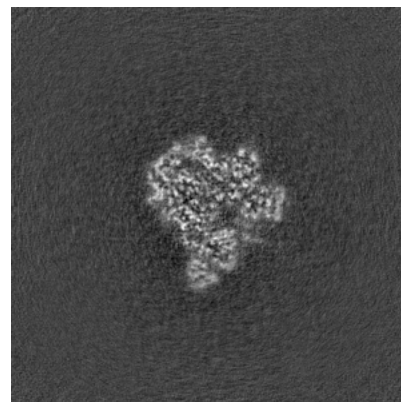
6.3.2 Raw map



X Index: 163



Y Index: 192

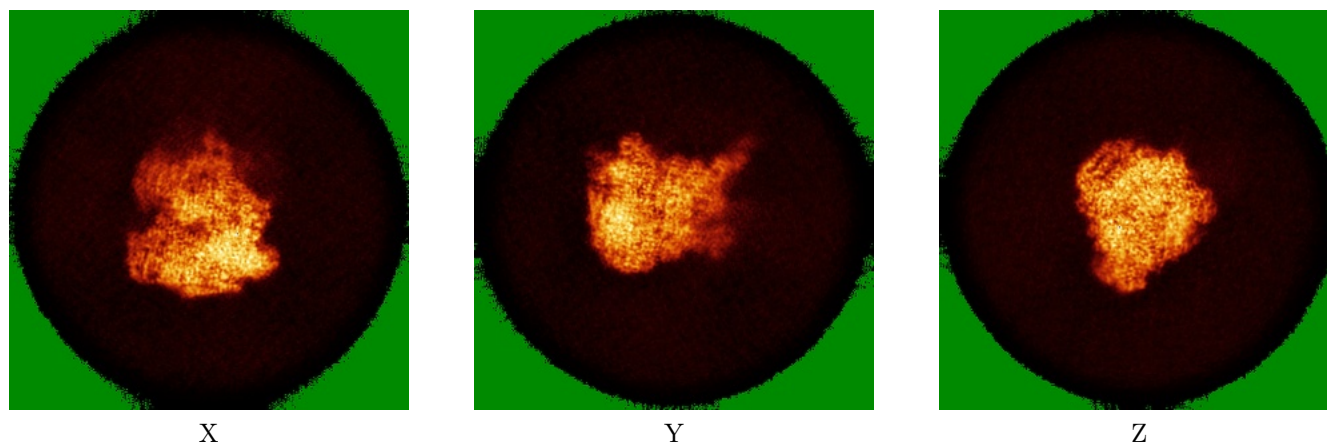


Z Index: 138

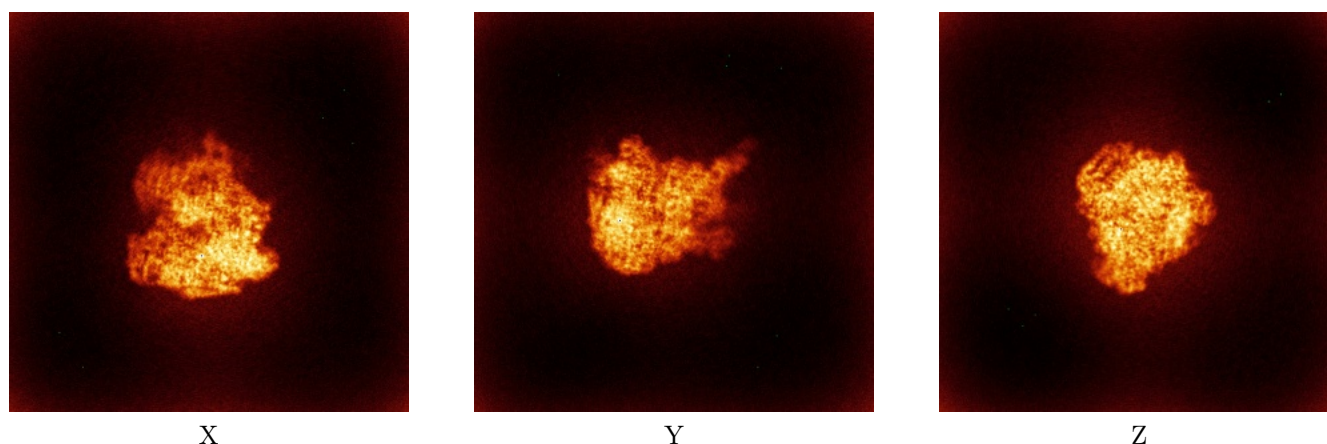
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

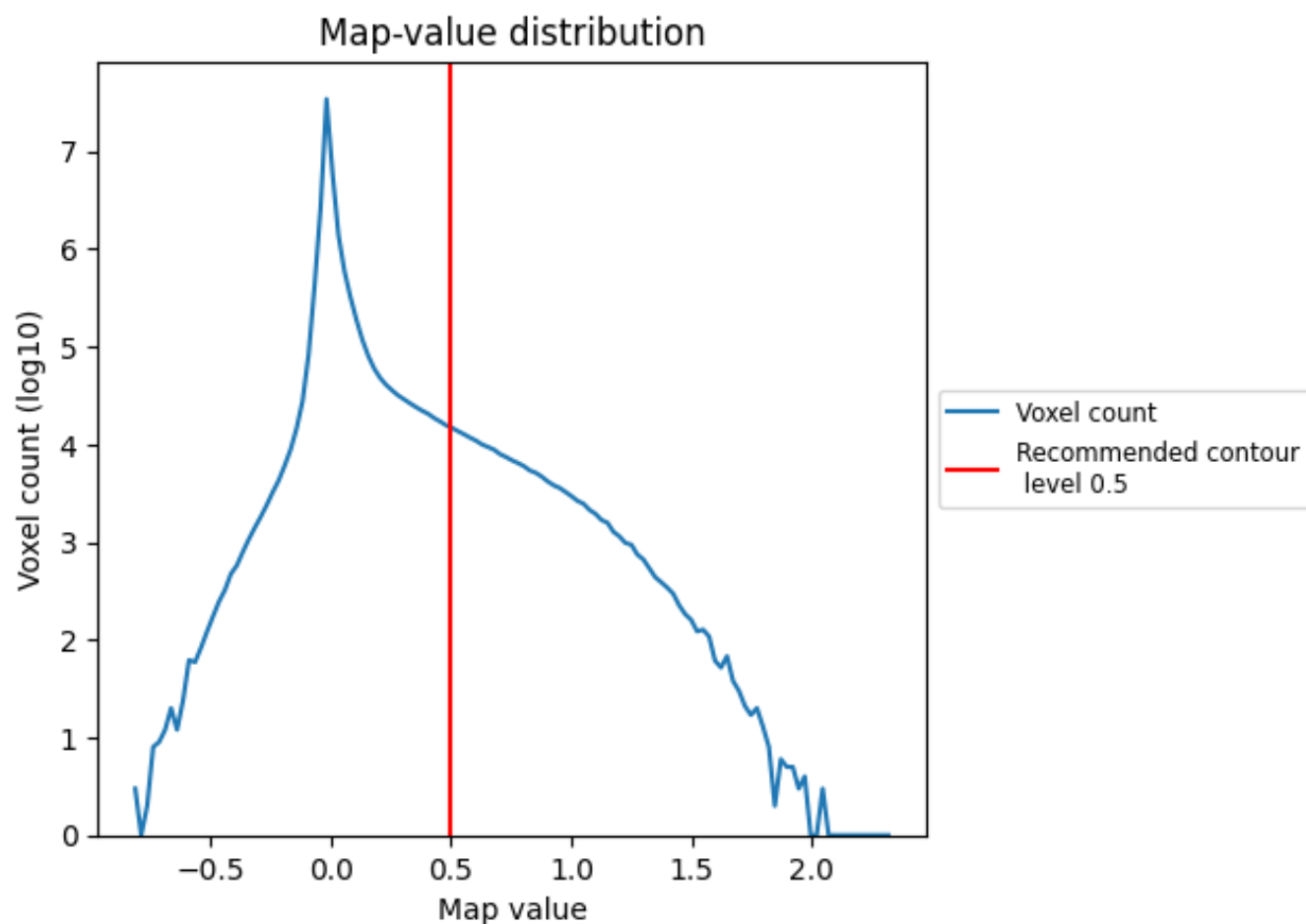
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

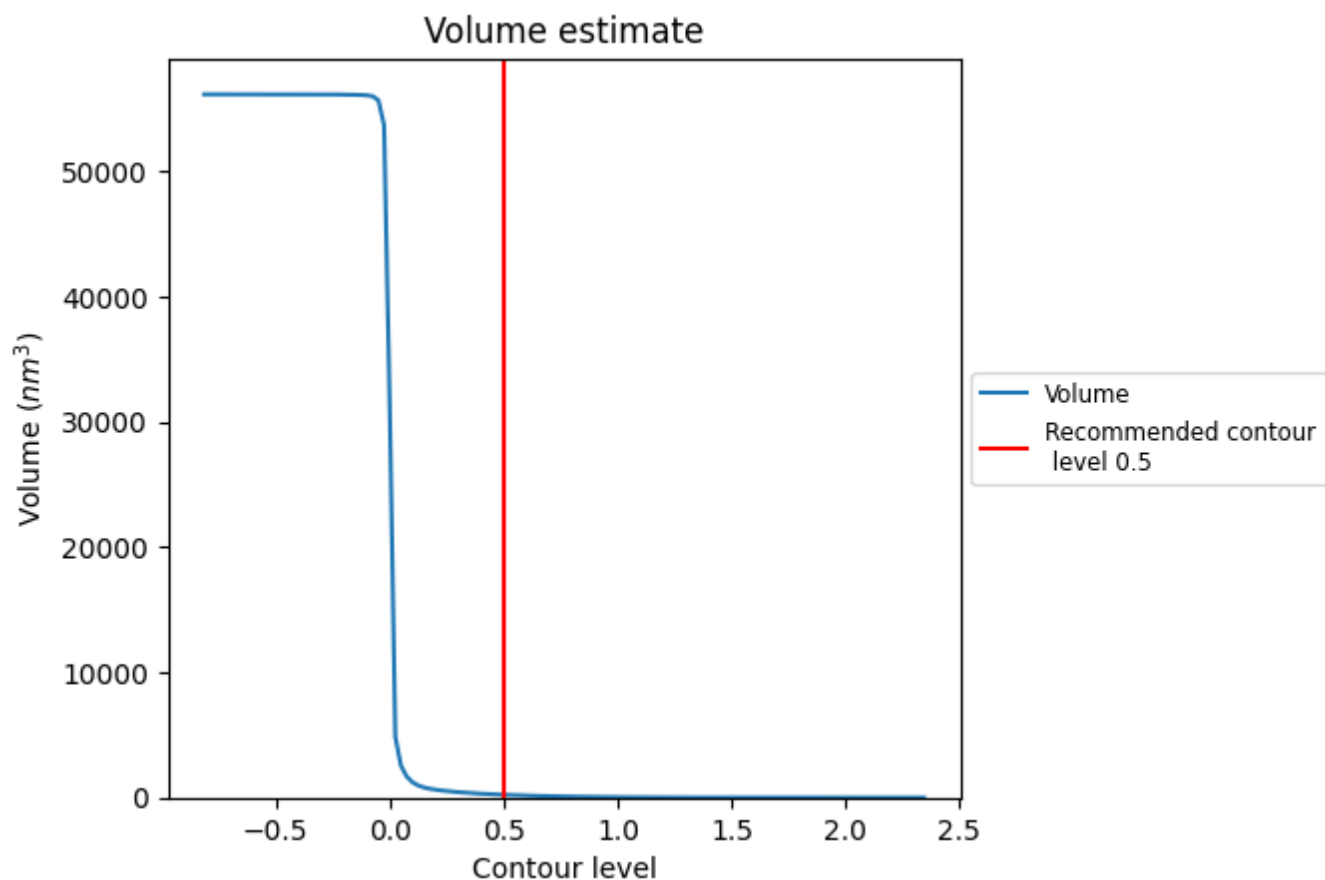
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

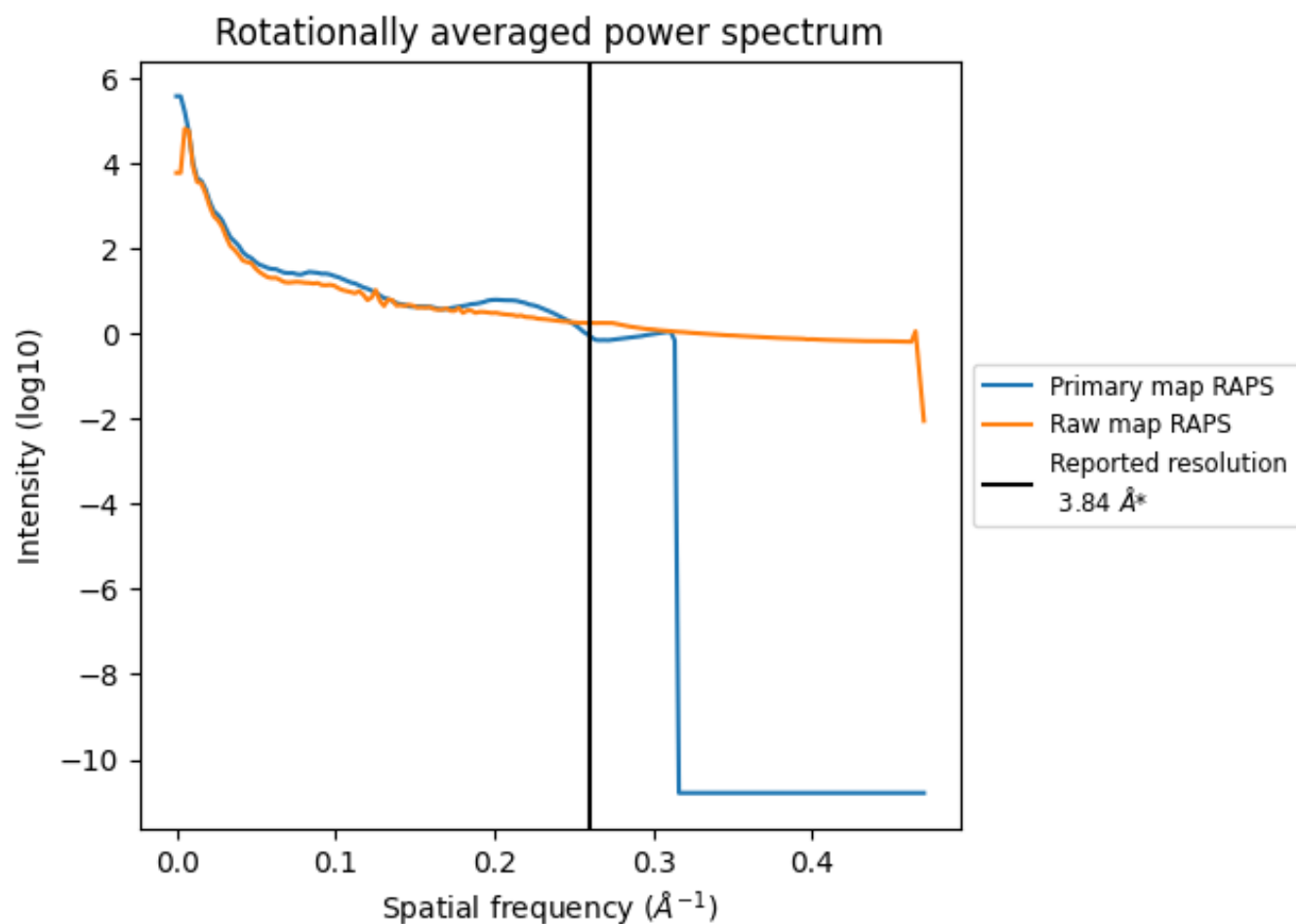
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 221 nm³; this corresponds to an approximate mass of 199 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 ⓘ

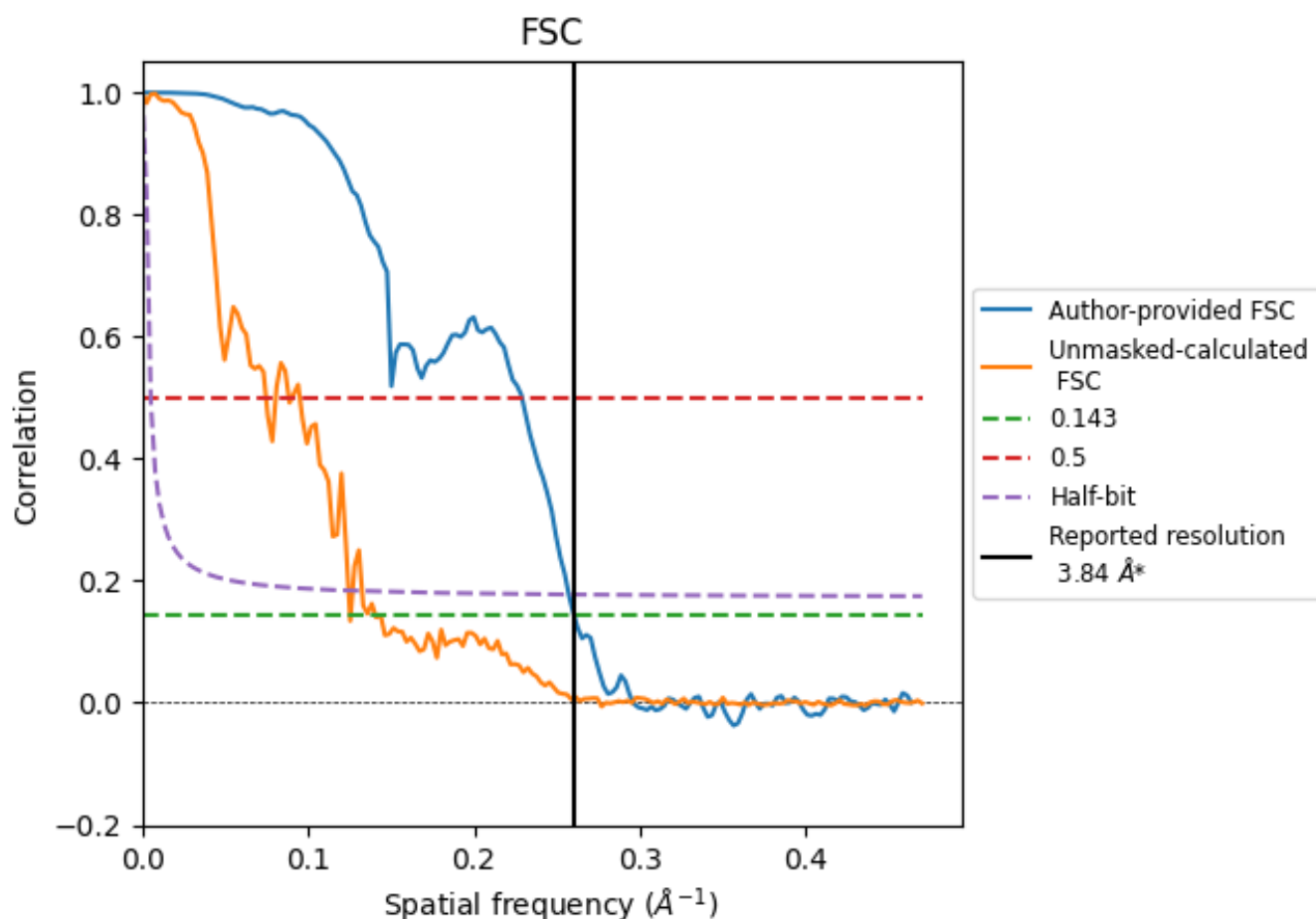


*Reported resolution corresponds to spatial frequency of 0.260 $\text{\AA}^{-1}$

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 0.260 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.84	-	-
Author-provided FSC curve	3.84	4.37	3.89
Unmasked-calculated*	7.99	13.39	8.05

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.99 differs from the reported value 3.84 by more than 10 %

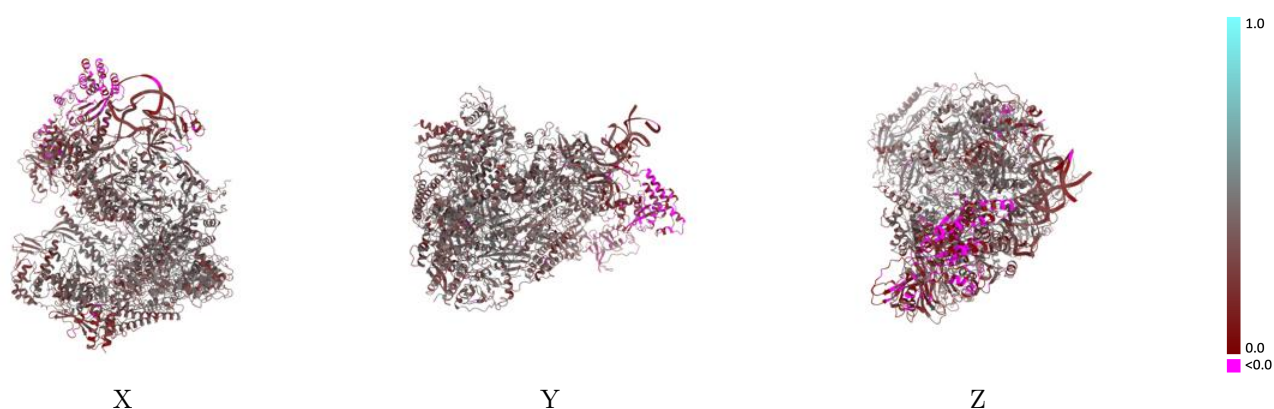
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16476 and PDB model 8C8H. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

This section was not generated.

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

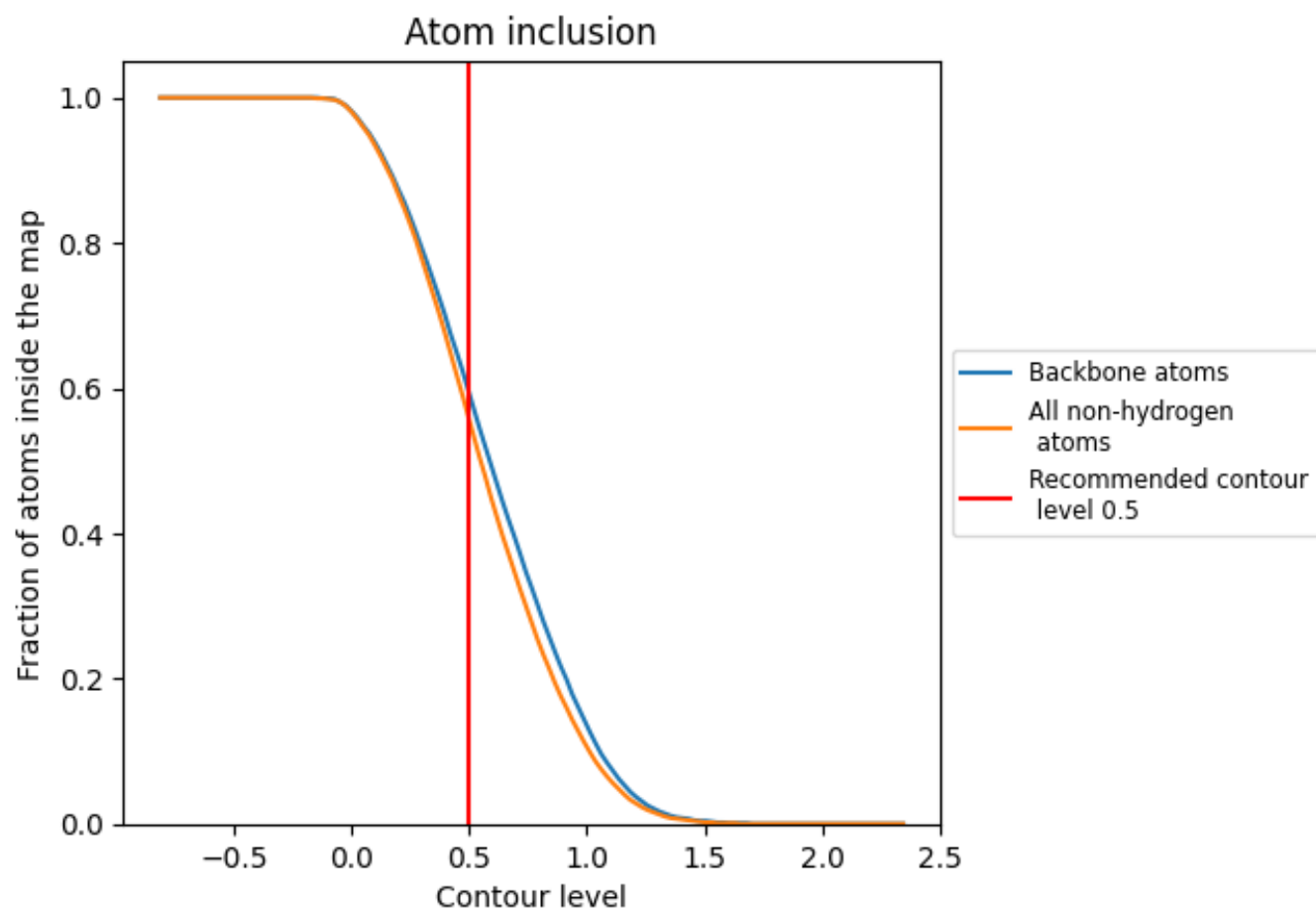


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 56% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5550	 0.3330
A	 0.6760	 0.3790
B	 0.6940	 0.3930
C	 0.6610	 0.3610
E	 0.6870	 0.3790
F	 0.7370	 0.3870
G	 0.6330	 0.3450
I	 0.5730	 0.3320
J	 0.6900	 0.3770
K	 0.0080	 0.1850
Q	 0.0810	 0.1460
R	 0.2580	 0.2560
S	 0.3100	 0.2700
U	 0.5140	 0.2520
Y	 0.1930	 0.1790

