



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 11:45 AM UTC

PDB ID : 8KD5 / pdb_00008kd5
EMDB ID : EMD-37125
Title : Rpd3S in complex with nucleosome with H3K36MLA modification and 187bp DNA, class2
Authors : Dong, S.; Li, H.; Wang, M.; Rasheed, N.; Zou, B.; Gao, X.; Guan, J.; Li, W.; Zhang, J.; Wang, C.; Zhou, N.; Shi, X.; Li, M.; Zhou, M.; Huang, J.; Li, H.; Zhang, Y.; Wong, K.H.; Chang, X.; Chao, W.C.H.; He, J.
Deposited on : 2023-08-09
Resolution : 2.90 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

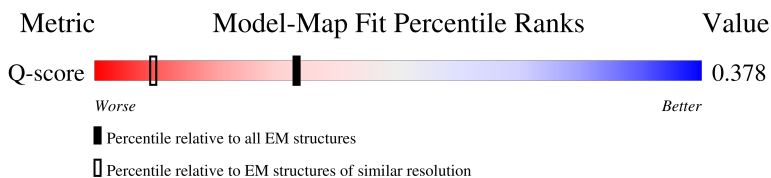
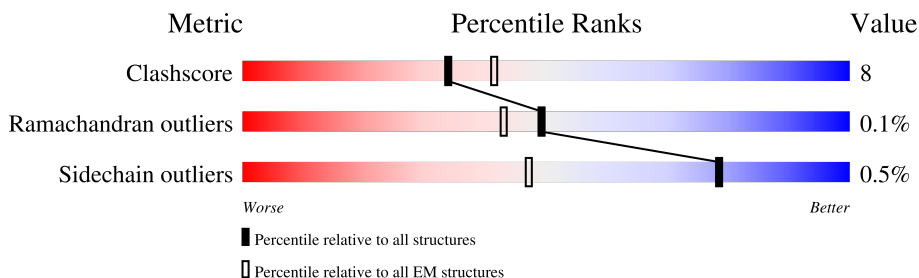
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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.



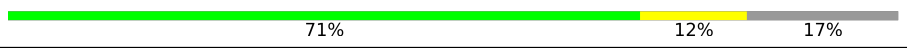
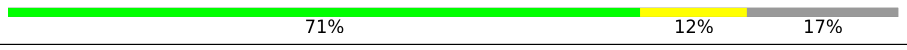
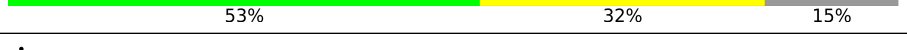
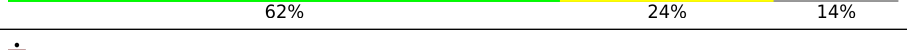
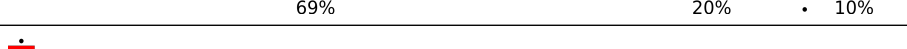
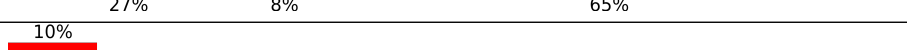
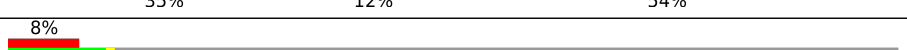
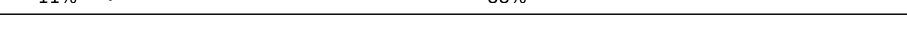
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	D	401	
1	F	401	
2	O	135	
2	S	135	

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Mol	Chain	Length	Quality of chain
3	P	102	
3	T	102	
4	Q	129	
4	U	129	
5	R	122	
5	V	122	
6	X	187	
7	Y	187	
8	A	433	
9	B	1544	
10	E	684	
10	G	684	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 26908 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 Chromatin modification-related protein EAF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	229	Total	C	N	O	S	0	0
			1867	1196	309	351	11		
1	F	191	Total	C	N	O	S	0	0
			1573	1016	260	288	9		

- Molecule 2 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	99	Total	C	N	O	S	0	0
			822	521	159	140	2		
2	S	98	Total	C	N	O	S	0	0
			811	515	155	139	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	110	ALA	CYS	engineered mutation	UNP A0A310TTQ1
S	110	ALA	CYS	engineered mutation	UNP A0A310TTQ1

- Molecule 3 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	79	Total	C	N	O	S	0	0
			637	403	124	109	1		
3	T	79	Total	C	N	O	S	0	0
			637	403	124	109	1		

- Molecule 4 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	Q	107	Total	C	N	O	0	0
			825	519	163	143		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	U	107	Total	C	N	O	0	0
			825	519	163	143		

- Molecule 5 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	93	Total	C	N	O	S	0	0
			730	460	131	137	2		
5	V	91	Total	C	N	O	S	0	0
			715	451	128	134	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	29	THR	SER	engineered mutation	UNP P02281
V	29	THR	SER	engineered mutation	UNP P02281

- Molecule 6 is a DNA chain called 187bp DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	159	Total	C	N	O	P	0	0
			3277	1550	616	952	159		

- Molecule 7 is a DNA chain called 187bp DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	160	Total	C	N	O	P	0	0
			3261	1548	591	962	160		

- Molecule 8 is a protein called Histone deacetylase RPD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	388	Total	C	N	O	S	0	0
			3073	1945	521	582	25		

- Molecule 9 is a protein called Transcriptional regulatory protein SIN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	539	Total	C	N	O	S	0	0
			4519	2908	758	838	15		

There are 9 discrepancies between the modelled and reference sequences:

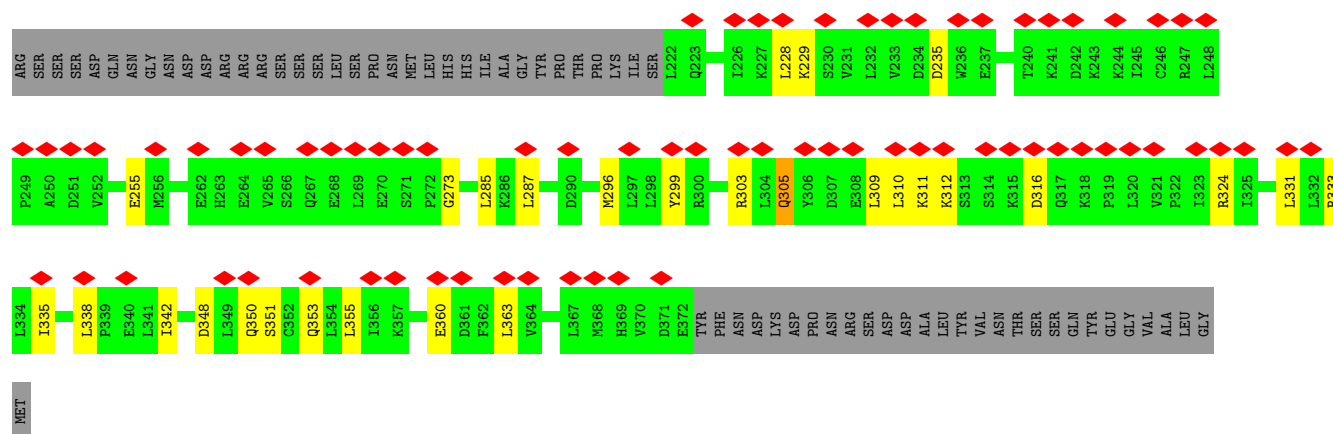
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	MET	-	initiating methionine	UNP P22579
B	-6	HIS	-	expression tag	UNP P22579
B	-5	HIS	-	expression tag	UNP P22579
B	-4	HIS	-	expression tag	UNP P22579
B	-3	HIS	-	expression tag	UNP P22579
B	-2	HIS	-	expression tag	UNP P22579
B	-1	HIS	-	expression tag	UNP P22579
B	0	HIS	-	expression tag	UNP P22579
B	1	HIS	-	expression tag	UNP P22579

- Molecule 10 is a protein called Transcriptional regulatory protein RCO1.

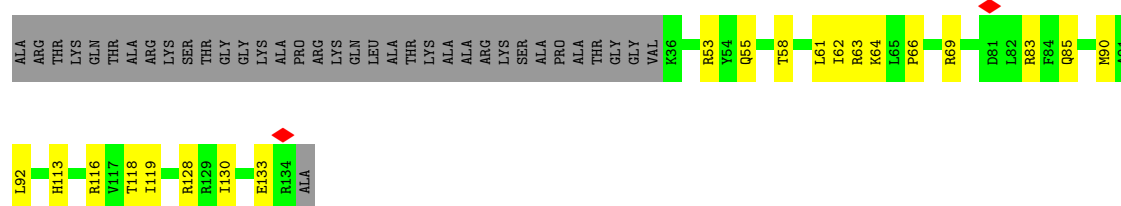
Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	317	Total	C	N	O	S	0	0
			2611	1661	455	478	17		
10	G	85	Total	C	N	O	S	0	0
			724	473	121	126	4		

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

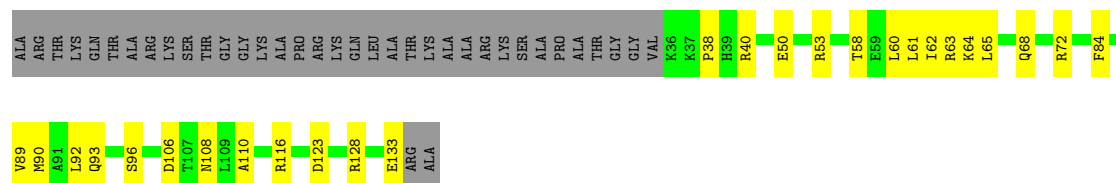
Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total	Zn	0
			1	1	



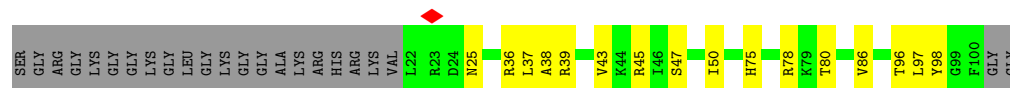
- Molecule 2: Histone H3



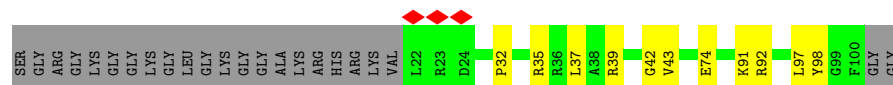
- Molecule 2: Histone H3



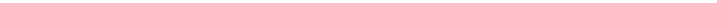
- Molecule 3: Histone H4



- Molecule 3: Histone H4

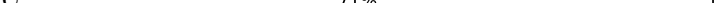


- Molecule 4: Histone H2A

Chain Q:  71% 12% 17%



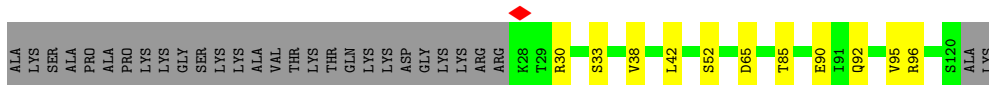
- Molecule 4: Histone H2A

Chain U:  71% 12% 17%

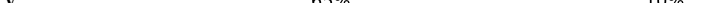


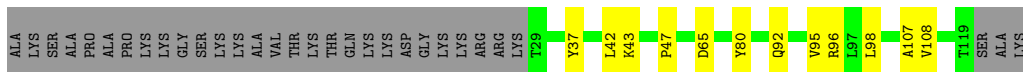
- Molecule 5: Histone H2B 1.1

Chain R:  67% 9% 24%

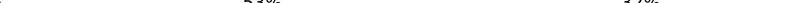


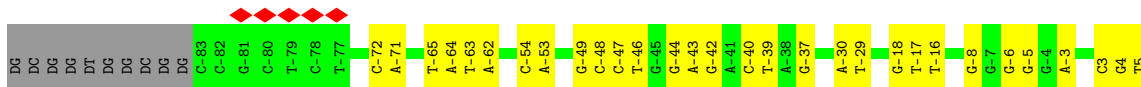
- Molecule 5: Histone H2B 1.1

Chain V:  65% 10% 25%

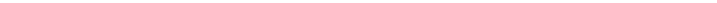


- Molecule 6: 187bp DNA

Chain X: 



- Molecule 7: 187bp DNA

Chain Y: 



Chain A:

69% 20% 10%

Residues (from left to right):

ALA, ASP, ASP, LEU, GLY, ASP, V404, E405, E406, D407, S408, Q419, D423, LEU, HIS, VAL, GLU, HIS, ASP, ASN, GLU, PHE, TYR

Residues (from left to right):

Y262, V267, V268, L269, S275, D279, R280, L281, N285, N293, C294, V295, V298, K299, G302, I303, R320, E325, T326, L329, N330, N331, L334, D335, P349, D350, Y351, K352, L353, E367, N375, K384, TYR, ALA, PRO, SER, VAL, GLN, LEU, ASN, HIS, THR, PRO, ARG, ASP

Residues (from left to right):

MET, VAL, GLU, ALA, THR, PRO, PHE, ASP, PRO, ILE, THR, VAL, LYS, PRO, SER, D17, K18, R19, R20, V21, A36, G37, K41, P42, H43, R44, M47, I52, M53, N54, Y55, H78, I83, T90, P91, D92, E95, K103, F104, N105, D114, R136, G137, K138, V141, A146

Chain B:

27%

8%

65%

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	109319	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.593	Depositor
Minimum map value	-0.061	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	383.4, 383.4, 383.4	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.71, 0.71, 0.71	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: M3L, 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	D	0.19	0/1905	0.50	1/2573 (0.0%)
1	F	0.22	0/1605	0.59	0/2167
2	O	0.13	0/823	0.36	0/1106
2	S	0.12	0/812	0.32	0/1092
3	P	0.11	0/644	0.30	0/863
3	T	0.11	0/644	0.28	0/863
4	Q	0.15	0/835	0.37	0/1127
4	U	0.12	0/835	0.29	0/1127
5	R	0.15	0/741	0.37	0/997
5	V	0.12	0/726	0.30	0/978
6	X	0.17	0/3680	0.39	0/5682
7	Y	0.16	0/3653	0.35	0/5631
8	A	0.18	0/3147	0.42	0/4250
9	B	0.18	0/4621	0.43	0/6230
10	E	0.20	0/2674	0.51	0/3599
10	G	0.14	0/738	0.37	0/983
All	All	0.17	0/28083	0.42	1/39268 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	107	MET	CA-CB-CG	5.75	125.61	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1867	0	1862	53	0
1	F	1573	0	1598	23	0
2	O	822	0	874	21	0
2	S	811	0	861	21	0
3	P	637	0	681	15	0
3	T	637	0	681	11	0
4	Q	825	0	882	13	0
4	U	825	0	882	14	0
5	R	730	0	755	13	0
5	V	715	0	737	10	0
6	X	3277	0	1783	41	0
7	Y	3261	0	1796	32	0
8	A	3073	0	2937	77	0
9	B	4519	0	4482	89	0
10	E	2611	0	2589	75	0
10	G	724	0	737	8	0
11	A	1	0	0	0	0
All	All	26908	0	24137	417	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 (417) 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)
8:A:36:ALA:HB1	10:E:48:LEU:CD2	1.18	1.62
8:A:224:ILE:CG2	8:A:231:ASN:HA	1.48	1.40
8:A:36:ALA:CB	10:E:48:LEU:CD2	2.14	1.24
8:A:36:ALA:HB1	10:E:48:LEU:HD23	1.14	1.14
1:D:225:PRO:HG2	1:D:367:LEU:HD11	1.17	1.11
1:D:293:LEU:HD13	1:D:298:LEU:HD11	1.20	1.10
8:A:36:ALA:CB	10:E:48:LEU:HD22	1.79	1.09
8:A:224:ILE:HG21	8:A:231:ASN:HA	1.37	1.06
8:A:224:ILE:CG2	8:A:231:ASN:CA	2.35	1.04
8:A:224:ILE:HG22	8:A:231:ASN:HA	1.37	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:PRO:CG	1:D:367:LEU:HD11	1.88	1.02
8:A:224:ILE:HG22	8:A:231:ASN:CA	1.90	1.02
1:D:294:GLY:HA2	1:D:298:LEU:HD12	1.45	0.97
8:A:36:ALA:HB1	10:E:48:LEU:HD22	0.98	0.95
10:E:303:CYS:HB3	10:E:306:CYS:SG	2.10	0.90
8:A:224:ILE:HG22	8:A:231:ASN:N	1.86	0.89
8:A:36:ALA:CB	10:E:48:LEU:HD23	1.93	0.86
1:D:293:LEU:CD1	1:D:298:LEU:HD11	2.07	0.82
9:B:1010:LEU:HD21	9:B:1250:VAL:HG13	1.62	0.82
8:A:224:ILE:HG22	8:A:231:ASN:H	1.43	0.81
10:E:558:SER:O	10:E:561:VAL:HG22	1.83	0.79
9:B:799:ARG:HH22	10:E:395:ILE:H	1.34	0.76
10:E:325:ASN:HA	10:E:328:LYS:HB2	1.68	0.75
9:B:879:ILE:O	9:B:883:LEU:HG	1.85	0.75
9:B:883:LEU:HD23	9:B:890:THR:OG1	1.91	0.70
9:B:1268:LEU:HD13	9:B:1289:GLN:HE22	1.56	0.70
1:D:293:LEU:HD13	1:D:298:LEU:CD1	2.12	0.70
2:S:40:ARG:HH22	6:X:-8:DG:H21	1.40	0.69
8:A:224:ILE:HG23	8:A:231:ASN:HA	1.68	0.69
10:G:303:CYS:SG	10:G:306:CYS:N	2.61	0.69
10:E:321:LYS:O	10:E:325:ASN:ND2	2.27	0.68
10:E:395:ILE:O	10:E:397:LYS:NZ	2.26	0.68
10:E:540:THR:OG1	10:E:542:ILE:HG12	1.94	0.68
9:B:770:ARG:HG3	9:B:774:CYS:HB3	1.76	0.67
2:S:64:LYS:HE2	2:S:90:MET:HE1	1.78	0.66
7:Y:25:DG:OP1	9:B:1222:GLN:NE2	2.28	0.65
8:A:224:ILE:HG22	8:A:224:ILE:O	1.97	0.65
8:A:212:GLY:HA3	10:E:456:SER:HB3	1.78	0.64
8:A:367:GLU:OE2	10:E:435:ARG:NH1	2.30	0.64
10:E:432:GLU:O	10:E:435:ARG:NH2	2.30	0.64
9:B:1203:ALA:O	9:B:1207:VAL:HG23	1.98	0.63
10:E:498:ILE:HB	10:E:504:LEU:HD13	1.81	0.62
1:F:309:LEU:HA	1:F:312:LYS:HG2	1.80	0.62
1:D:225:PRO:HG2	1:D:367:LEU:CD1	2.12	0.62
1:D:225:PRO:HD2	1:D:363:LEU:HD12	1.81	0.61
8:A:220:GLU:H	8:A:223:ASP:HB2	1.64	0.61
9:B:799:ARG:HH12	10:E:394:SER:HA	1.65	0.61
4:Q:11:ARG:HH21	6:X:44:DT:H1'	1.65	0.61
8:A:248:ARG:NH1	8:A:293:ASN:OD1	2.34	0.61
8:A:150:HIS:HB3	8:A:166:ILE:HD12	1.83	0.60
1:D:22:MET:SD	1:D:101:ASN:ND2	2.71	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:29:ARG:NH2	5:V:37:TYR:OH	2.35	0.60
1:F:305:GLN:HE21	1:F:305:GLN:C	2.10	0.60
10:E:540:THR:OG1	10:E:542:ILE:CD1	2.49	0.60
4:U:54:VAL:HG22	5:V:107:ALA:HB1	1.84	0.60
8:A:221:LEU:HB3	8:A:375:ASN:HD21	1.67	0.59
3:T:32:PRO:HA	3:T:35:ARG:HB2	1.85	0.58
1:D:323:ILE:HG13	1:D:324:ARG:HD2	1.85	0.58
4:Q:16:THR:HA	7:Y:-43:DT:H5''	1.86	0.58
9:B:1002:TYR:O	9:B:1007:LYS:NZ	2.36	0.58
10:E:543:ASP:OD1	10:E:543:ASP:N	2.37	0.58
2:O:116:ARG:HD3	7:Y:-3:DG:H3'	1.85	0.57
8:A:78:HIS:HB2	8:A:83:ILE:HD11	1.84	0.57
9:B:810:ILE:HD12	9:B:919:LEU:HD22	1.86	0.57
2:O:113:HIS:NE2	2:S:123:ASP:OD2	2.27	0.57
1:D:335:ILE:HG21	1:D:363:LEU:HD21	1.86	0.57
4:Q:68:ASN:OD1	4:Q:71:ARG:NH2	2.35	0.57
1:F:17:PHE:HB2	1:F:96:ARG:HB3	1.87	0.57
3:P:39:ARG:NH1	3:P:43:VAL:O	2.36	0.57
9:B:1197:ASP:OD1	9:B:1197:ASP:N	2.38	0.57
2:S:108:ASN:ND2	3:T:42:GLY:O	2.37	0.56
4:U:41:GLU:OE1	4:U:41:GLU:N	2.32	0.56
10:E:540:THR:OG1	10:E:542:ILE:HD11	2.05	0.56
3:T:91:LYS:NZ	5:V:80:TYR:OH	2.38	0.56
9:B:706:VAL:HA	9:B:709:TYR:HB2	1.87	0.56
1:D:225:PRO:CB	1:D:367:LEU:HD11	2.35	0.56
8:A:257:LYS:HA	8:A:260:GLU:HG2	1.88	0.56
8:A:352:LYS:NZ	9:B:1176:SER:O	2.39	0.56
10:E:520:ILE:HG21	10:E:542:ILE:HG13	1.88	0.56
1:D:363:LEU:O	1:D:367:LEU:HG	2.06	0.56
5:R:30:ARG:HH11	5:R:30:ARG:HB3	1.70	0.55
8:A:20:ARG:H	8:A:20:ARG:HD3	1.71	0.55
1:D:303:ARG:NH2	10:E:287:LEU:O	2.39	0.55
9:B:1207:VAL:HG21	9:B:1232:TYR:OH	2.05	0.55
8:A:178:PRO:HA	8:A:202:ARG:HH21	1.71	0.55
9:B:863:TYR:O	9:B:867:ILE:HG12	2.05	0.55
10:E:440:CYS:HB3	10:E:445:THR:H	1.72	0.55
8:A:19:ARG:HG2	8:A:331:ASN:HD21	1.72	0.55
8:A:221:LEU:HD12	10:E:453:PRO:HB3	1.88	0.55
6:X:-47:DC:H2''	6:X:-46:DT:C5	2.42	0.55
8:A:90:THR:HG22	8:A:92:ASP:H	1.72	0.54
3:T:39:ARG:NH1	3:T:43:VAL:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:GLU:OE1	10:E:496:ARG:NH2	2.38	0.54
4:Q:54:VAL:HG21	5:R:95:VAL:HG11	1.89	0.54
2:S:90:MET:HE3	2:S:90:MET:HA	1.89	0.54
10:E:540:THR:OG1	10:E:542:ILE:CG1	2.54	0.54
2:O:58:THR:O	4:U:104:GLN:NE2	2.41	0.54
6:X:65:DA:H2''	6:X:66:DT:C2	2.43	0.54
10:E:545:ASN:HA	10:E:548:LYS:HE3	1.90	0.54
1:D:238:TYR:HA	1:D:242:ASP:HB2	1.89	0.54
8:A:186:ASP:HA	8:A:275:SER:HB3	1.90	0.54
1:D:228:LEU:HD13	1:D:332:LEU:HD21	1.90	0.54
3:T:92:ARG:HH22	5:V:98:LEU:HD23	1.73	0.54
8:A:41:LYS:O	8:A:44:ARG:NH1	2.38	0.54
1:D:304:LEU:HD22	1:D:397:VAL:HB	1.90	0.53
8:A:114:ASP:HB2	9:B:865:LYS:HD3	1.89	0.53
1:D:224:ILE:HB	1:D:229:LYS:HE3	1.90	0.53
9:B:872:ASP:HB2	9:B:875:ARG:HG3	1.91	0.53
2:O:85:GLN:HA	7:Y:-24:DG:H5''	1.89	0.53
2:S:116:ARG:HD3	6:X:-3:DA:H3'	1.91	0.53
4:U:99:ARG:HH11	4:U:99:ARG:HA	1.72	0.53
8:A:191:ASP:OD2	8:A:191:ASP:N	2.42	0.53
9:B:1157:ARG:HG2	9:B:1238:LYS:HB3	1.89	0.53
8:A:226:VAL:HG12	8:A:227:GLY:N	2.24	0.53
9:B:1214:LEU:HD23	9:B:1219:LEU:HD23	1.91	0.53
3:T:74:GLU:OE1	5:V:96:ARG:NH2	2.42	0.53
9:B:824:ASN:O	9:B:828:ILE:HG12	2.08	0.53
1:F:316:ASP:OD1	1:F:316:ASP:N	2.41	0.52
2:O:64:LYS:HE2	2:O:90:MET:HE1	1.89	0.52
4:Q:42:ARG:HE	5:R:85:THR:HB	1.73	0.52
2:S:62:ILE:O	2:S:93:GLN:NE2	2.43	0.52
9:B:936:LYS:HD3	9:B:1241:THR:HG22	1.92	0.52
9:B:883:LEU:HD21	9:B:894:VAL:HG21	1.92	0.52
9:B:692:TYR:O	10:E:554:LYS:NZ	2.43	0.52
1:F:287:LEU:HD12	10:G:333:VAL:CG2	2.40	0.52
8:A:189:HIS:NE2	8:A:218:THR:O	2.43	0.52
8:A:320:ARG:HD2	8:A:353:LEU:HA	1.92	0.52
9:B:962:LYS:HA	9:B:962:LYS:HE3	1.92	0.52
8:A:241:GLY:HA2	8:A:285:ASN:HB2	1.91	0.52
1:D:281:TYR:HA	10:E:335:ILE:HD11	1.92	0.51
2:O:130:ILE:HG12	2:S:106:ASP:HB3	1.92	0.51
6:X:31:DT:H2''	6:X:32:DG:H5''	1.91	0.51
9:B:1284:ILE:HD12	9:B:1284:ILE:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:61:LEU:HD12	3:T:37:LEU:HD23	1.91	0.51
8:A:279:ASP:O	9:B:800:LYS:NZ	2.35	0.51
2:O:55:GLN:O	4:U:81:ARG:NH2	2.44	0.51
2:S:128:ARG:HE	2:S:133:GLU:HB2	1.75	0.51
8:A:19:ARG:HD3	8:A:299:LYS:HD3	1.93	0.51
1:F:228:LEU:H	1:F:229:LYS:HD3	1.75	0.51
4:Q:103:ALA:HB2	3:T:97:LEU:HD11	1.92	0.51
9:B:831:LEU:HB2	9:B:895:LEU:HD13	1.93	0.51
1:F:335:ILE:HA	1:F:338:LEU:HG	1.92	0.51
2:O:119:ILE:HD12	3:P:50:ILE:HG12	1.93	0.51
5:R:30:ARG:HB3	5:R:30:ARG:NH1	2.26	0.51
6:X:-40:DC:H2'	6:X:-39:DT:H71	1.93	0.50
5:R:52:SER:HA	7:Y:-54:DA:H5''	1.93	0.50
9:B:1246:THR:O	9:B:1250:VAL:HG23	2.11	0.50
2:S:68:GLN:HG2	2:S:89:VAL:HG11	1.93	0.50
10:E:379:ILE:HD12	10:E:380:PRO:HD2	1.93	0.50
9:B:1227:SER:O	9:B:1231:ALA:HB2	2.12	0.50
10:E:507:GLU:N	10:E:507:GLU:OE2	2.45	0.50
8:A:19:ARG:HH12	8:A:302:GLY:HA2	1.77	0.49
10:E:558:SER:O	10:E:561:VAL:CG2	2.58	0.49
6:X:-6:DG:H2''	6:X:-5:DG:N7	2.26	0.49
9:B:893:VAL:HG11	10:E:62:SER:HB3	1.94	0.49
1:D:243:LYS:O	1:D:390:THR:OG1	2.23	0.49
1:F:296:MET:H	10:G:348:PRO:HB3	1.76	0.49
10:E:544:GLU:OE1	10:E:544:GLU:N	2.32	0.49
9:B:678:ASN:HB3	9:B:681:LEU:HD12	1.94	0.49
4:U:54:VAL:HG21	5:V:95:VAL:HG21	1.93	0.49
8:A:404:VAL:C	8:A:406:GLU:H	2.20	0.49
1:F:299:TYR:O	1:F:303:ARG:N	2.41	0.48
4:Q:29:ARG:NH1	5:R:33:SER:O	2.45	0.48
2:S:65:LEU:HA	2:S:68:GLN:HB2	1.94	0.48
1:F:305:GLN:NE2	1:F:309:LEU:HD23	2.27	0.48
9:B:666:VAL:O	10:G:548:LYS:NZ	2.45	0.48
8:A:36:ALA:CA	10:E:48:LEU:CD2	2.90	0.48
2:S:38:PRO:HB2	2:S:40:ARG:HG2	1.96	0.48
1:D:393:GLN:O	1:D:397:VAL:HG23	2.14	0.48
1:D:397:VAL:HG22	8:A:103:LYS:HB2	1.95	0.48
5:V:43:LYS:HE3	5:V:47:PRO:HA	1.95	0.48
9:B:781:GLU:OE2	9:B:781:GLU:N	2.47	0.48
10:E:456:SER:OG	10:E:457:PHE:N	2.47	0.48
10:E:476:LYS:HE3	10:E:490:LYS:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:103:LYS:C	8:A:105:ASN:H	2.22	0.48
9:B:686:LEU:HB3	10:E:547:ILE:HD12	1.95	0.48
9:B:1168:VAL:O	9:B:1172:ILE:HG13	2.13	0.48
1:F:348:ASP:O	1:F:351:SER:OG	2.31	0.48
9:B:1220:GLU:HB3	9:B:1223:TRP:HD1	1.77	0.48
1:D:254:VAL:HG13	1:D:331:LEU:HD22	1.96	0.48
2:O:63:ARG:HD3	6:X:17:DA:H4'	1.95	0.48
9:B:763:THR:HG23	9:B:780:ASP:HB3	1.96	0.48
10:E:275:CYS:HB3	10:E:278:CYS:HB3	1.96	0.48
1:F:273:GLY:HA2	10:E:556:TYR:HD2	1.78	0.47
10:E:441:ASP:HB3	10:E:463:LYS:HE3	1.96	0.47
1:D:222:LEU:HB2	1:D:356:ILE:HD11	1.96	0.47
8:A:141:VAL:HG11	8:A:329:LEU:HD22	1.96	0.47
8:A:404:VAL:C	8:A:406:GLU:N	2.72	0.47
9:B:773:MET:O	9:B:777:VAL:HG22	2.14	0.47
5:R:30:ARG:NH2	6:X:48:DG:N3	2.62	0.47
1:D:238:TYR:O	1:D:244:LYS:N	2.45	0.47
8:A:224:ILE:HG21	8:A:231:ASN:OD1	2.14	0.47
9:B:1253:ALA:HA	9:B:1256:LEU:HD13	1.96	0.47
10:E:303:CYS:SG	10:E:304:ASN:N	2.88	0.47
6:X:4:DG:H2''	6:X:5:DT:C5	2.49	0.47
6:X:46:DG:H2''	6:X:47:DA:N7	2.30	0.47
8:A:181:LEU:HD23	8:A:267:VAL:HG22	1.95	0.47
10:E:377:ASP:HA	10:E:462:SER:HA	1.96	0.47
8:A:52:ILE:HG12	8:A:326:THR:HG21	1.95	0.47
8:A:136:ARG:HH12	8:A:138:LYS:HD2	1.78	0.47
9:B:809:LYS:HG2	9:B:813:GLU:OE1	2.15	0.47
10:E:303:CYS:O	10:E:307:LYS:HG2	2.15	0.47
6:X:-18:DG:N2	7:Y:19:DC:O2	2.47	0.47
9:B:690:ASN:HB2	10:E:547:ILE:HG23	1.97	0.47
9:B:1266:MET:O	9:B:1270:VAL:HG23	2.15	0.47
9:B:849:PHE:HB3	9:B:887:PRO:HG2	1.97	0.46
9:B:963:LYS:O	9:B:967:LEU:N	2.48	0.46
1:D:251:ASP:OD1	1:D:251:ASP:N	2.38	0.46
1:D:300:ARG:NH1	10:E:268:GLN:OE1	2.42	0.46
1:F:80:HIS:ND1	1:F:89:ASP:OD2	2.45	0.46
3:P:75:HIS:NE2	5:R:90:GLU:OE1	2.48	0.46
4:U:68:ASN:OD1	4:U:71:ARG:NH2	2.44	0.46
10:E:33:LYS:HD2	10:E:35:ARG:HH21	1.80	0.46
1:D:294:GLY:CA	1:D:298:LEU:HD12	2.31	0.46
1:F:255:GLU:OE2	1:F:324:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:90:MET:HE2	2:O:90:MET:HA	1.97	0.46
1:F:285:LEU:HD21	1:F:331:LEU:HD11	1.98	0.46
2:S:50:GLU:HA	2:S:53:ARG:HG2	1.98	0.46
9:B:841:MET:HE1	9:B:846:LYS:HB2	1.98	0.46
1:D:288:TYR:O	1:D:292:CYS:HB3	2.16	0.46
5:R:65:ASP:OD2	3:T:98:TYR:OH	2.28	0.46
7:Y:-36:DT:H2''	7:Y:-35:DA:N7	2.30	0.46
7:Y:55:DT:H2''	7:Y:56:DC:C5	2.51	0.46
7:Y:78:DG:H2''	7:Y:79:DA:C8	2.51	0.46
3:P:98:TYR:OH	5:V:65:ASP:OD1	2.29	0.46
8:A:188:HIS:H	8:A:214:PHE:HE2	1.64	0.46
6:X:-37:DG:N2	7:Y:38:DT:O2	2.49	0.46
8:A:43:HIS:NE2	9:B:822:GLU:OE2	2.49	0.46
1:F:342:ILE:HD13	1:F:355:LEU:HD13	1.97	0.46
9:B:880:ILE:HA	9:B:883:LEU:HD12	1.97	0.46
1:D:227:LYS:HA	1:D:227:LYS:HD2	1.82	0.45
6:X:62:DG:H2''	6:X:63:DG:H5'	1.98	0.45
6:X:65:DA:H2''	6:X:66:DT:N3	2.29	0.45
1:D:257:VAL:HG22	1:D:373:TYR:CE2	2.51	0.45
8:A:103:LYS:C	8:A:105:ASN:N	2.74	0.45
9:B:904:GLU:HG3	10:E:43:ASN:HD22	1.82	0.45
1:F:80:HIS:NE2	7:Y:12:DT:OP1	2.49	0.45
2:O:63:ARG:HB2	2:O:66:PRO:HD2	1.98	0.45
10:E:35:ARG:HB2	10:E:39:LEU:HD23	1.99	0.45
10:E:548:LYS:HD2	10:G:551:PHE:HE2	1.80	0.45
1:F:287:LEU:HD12	10:G:333:VAL:HG23	1.98	0.45
5:R:30:ARG:NH2	6:X:49:DC:O4'	2.50	0.45
5:V:92:GLN:HG3	5:V:108:VAL:HG22	1.98	0.45
8:A:210:LYS:NZ	8:A:211:TYR:O	2.49	0.45
9:B:675:TYR:OH	9:B:712:SER:OG	2.34	0.45
3:P:78:ARG:HD3	6:X:28:DA:H3'	1.98	0.45
9:B:939:ASP:OD2	9:B:1241:THR:OG1	2.35	0.45
1:F:360:GLU:HA	1:F:363:LEU:HG	1.99	0.45
8:A:21:VAL:HG22	8:A:141:VAL:HB	1.97	0.45
10:E:45:ASN:N	10:E:45:ASN:OD1	2.50	0.45
2:S:92:LEU:O	2:S:96:SER:OG	2.32	0.45
8:A:55:TYR:HE2	8:A:334:LEU:HB3	1.82	0.45
10:E:263:CYS:HB2	10:E:272:PHE:CZ	2.52	0.45
2:O:69:ARG:NH1	3:P:25:ASN:OD1	2.50	0.45
8:A:179:ARG:NH1	8:A:262:TYR:O	2.50	0.45
8:A:350:ASP:OD1	8:A:350:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:304:ASN:HD22	10:E:348:PRO:HD3	1.81	0.45
10:E:378:LYS:NZ	10:E:441:ASP:OD2	2.50	0.45
1:D:290:ASP:HA	1:D:322:PRO:HG2	1.99	0.44
2:S:72:ARG:HH21	2:S:84:PHE:HB2	1.83	0.44
8:A:226:VAL:CG1	8:A:227:GLY:N	2.80	0.44
9:B:684:GLU:HG3	10:E:469:HIS:HD2	1.81	0.44
9:B:1303:ILE:HG12	9:B:1314:ILE:HG23	1.98	0.44
2:O:92:LEU:HG	3:P:86:VAL:HG11	1.99	0.44
6:X:-30:DA:H2'	6:X:-29:DT:H71	1.99	0.44
10:E:397:LYS:HB3	10:E:402:ASN:ND2	2.32	0.44
10:E:404:ASP:OD1	10:E:404:ASP:N	2.49	0.44
9:B:800:LYS:HB3	9:B:804:GLU:HB3	1.98	0.44
10:E:36:PRO:HD2	10:E:37:LYS:HE2	1.99	0.44
1:D:293:LEU:O	1:D:298:LEU:HD12	2.16	0.44
9:B:699:LEU:HD13	9:B:726:TYR:HD2	1.81	0.44
1:D:296:MET:HE2	1:D:341:LEU:HD21	1.99	0.44
7:Y:-48:DC:H2''	7:Y:-47:DT:C5	2.53	0.44
10:G:320:LYS:NZ	10:G:324:SER:OG	2.51	0.44
10:E:282:PHE:HZ	10:E:347:ASN:HB3	1.82	0.44
1:D:380:ASN:OD1	1:D:389:ASN:ND2	2.51	0.44
4:U:12:ALA:HB3	6:X:-42:DG:H4'	2.00	0.44
6:X:-72:DC:H2''	6:X:-71:DA:C8	2.53	0.44
6:X:14:DT:H2''	6:X:15:DT:C6	2.53	0.44
10:G:355:ASN:N	10:G:355:ASN:OD1	2.49	0.44
4:U:63:LEU:HD22	5:V:42:LEU:HD13	2.00	0.44
6:X:28:DA:H2''	6:X:29:DG:H5''	1.99	0.44
9:B:779:ASN:HD22	9:B:782:TRP:CD1	2.36	0.44
9:B:915:VAL:HG22	10:E:35:ARG:H	1.83	0.44
10:E:322:ILE:HA	10:E:325:ASN:HD21	1.83	0.44
6:X:11:DC:H2''	6:X:12:DG:C8	2.53	0.44
7:Y:44:DC:H2''	7:Y:45:DC:C5	2.53	0.44
9:B:1141:ASN:HD21	9:B:1262:THR:HG23	1.83	0.44
1:D:309:LEU:HD13	1:D:320:LEU:HD21	2.00	0.43
2:S:108:ASN:HB2	3:T:43:VAL:HG22	1.99	0.43
6:X:21:DG:H2'	6:X:22:DT:H71	2.00	0.43
8:A:335:ASP:OD1	8:A:335:ASP:N	2.50	0.43
9:B:1283:GLN:H	9:B:1283:GLN:HG2	1.61	0.43
1:D:356:ILE:O	1:D:360:GLU:HG2	2.17	0.43
9:B:967:LEU:HG	9:B:969:PRO:HD2	1.99	0.43
9:B:1205:LYS:O	9:B:1209:ARG:HG3	2.18	0.43
1:D:293:LEU:HD11	1:D:326:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:62:ILE:HD11	3:P:37:LEU:HD11	2.01	0.43
2:O:113:HIS:CE1	2:S:110:ALA:HB1	2.53	0.43
8:A:224:ILE:CG2	8:A:224:ILE:O	2.66	0.43
8:A:349:PRO:HB3	9:B:921:GLN:HG2	1.99	0.43
2:O:61:LEU:HD22	3:P:36:ARG:HB3	1.99	0.43
4:Q:75:LYS:HD3	6:X:58:DC:H5"	2.01	0.43
2:S:60:LEU:HD13	2:S:93:GLN:HG2	1.99	0.43
10:E:419:LYS:HD3	10:E:451:CYS:HB3	2.01	0.43
8:A:171:ILE:HA	8:A:174:LEU:HD12	2.01	0.43
9:B:779:ASN:HB2	9:B:782:TRP:HD1	1.83	0.43
1:F:310:LEU:HD12	1:F:311:LYS:NZ	2.33	0.43
2:O:128:ARG:HE	2:O:133:GLU:HB2	1.83	0.43
9:B:681:LEU:HD13	10:E:418:TYR:HE2	1.83	0.43
9:B:956:LYS:HD2	9:B:1316:TYR:CD2	2.54	0.43
9:B:1029:ILE:HD13	9:B:1032:SER:HB3	2.00	0.43
1:F:98:ARG:HD2	1:F:100:TYR:H	1.84	0.43
4:Q:63:LEU:HD22	5:R:42:LEU:HD13	2.01	0.43
6:X:-54:DC:H2"	6:X:-53:DA:C8	2.54	0.43
6:X:-17:DT:H2"	6:X:-16:DT:C6	2.54	0.42
7:Y:24:DA:H2"	7:Y:25:DG:C8	2.54	0.42
8:A:44:ARG:HA	8:A:47:MET:HE3	2.01	0.42
9:B:1140:ALA:HB1	9:B:1144:ILE:HB	2.01	0.42
3:P:47:SER:HA	6:X:7:DC:H5"	2.01	0.42
6:X:-65:DT:H2"	6:X:-64:DA:C8	2.54	0.42
7:Y:81:DC:H2"	7:Y:82:DG:C8	2.54	0.42
7:Y:-8:DC:H2"	7:Y:-7:DG:C8	2.54	0.42
9:B:1274:ASN:OD1	9:B:1274:ASN:N	2.53	0.42
2:O:118:THR:HG1	3:P:45:ARG:HE	1.65	0.42
6:X:-49:DG:H2"	6:X:-48:DC:H5"	2.01	0.42
7:Y:45:DC:H2"	7:Y:46:DA:N7	2.33	0.42
8:A:294:CYS:O	8:A:298:VAL:HG12	2.18	0.42
9:B:987:ASP:HB3	9:B:1208:LEU:HD11	2.00	0.42
1:D:20:PRO:HD2	1:D:102:GLU:HG2	2.01	0.42
1:D:360:GLU:O	1:D:364:VAL:HG12	2.18	0.42
9:B:702:LEU:O	9:B:706:VAL:HG23	2.20	0.42
9:B:864:LYS:HG2	9:B:880:ILE:HG12	2.01	0.42
9:B:953:SER:O	9:B:957:VAL:HG13	2.19	0.42
9:B:1268:LEU:HD13	9:B:1289:GLN:NE2	2.30	0.42
2:O:53:ARG:NH1	6:X:-65:DT:OP1	2.53	0.42
7:Y:12:DT:H2"	7:Y:13:DT:C5	2.55	0.42
8:A:405:GLU:HG3	8:A:408:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:128:ARG:NH2	2:O:133:GLU:O	2.53	0.42
3:P:38:ALA:HB1	3:P:43:VAL:HB	2.02	0.42
7:Y:18:DC:H6	7:Y:18:DC:H2'	1.71	0.42
8:A:151:HIS:NE2	8:A:188:HIS:O	2.49	0.42
8:A:251:PHE:CE1	8:A:294:CYS:HB3	2.55	0.42
8:A:404:VAL:O	8:A:406:GLU:N	2.53	0.42
9:B:679:LYS:HD3	9:B:679:LYS:HA	1.89	0.42
9:B:840:ASN:OD1	9:B:840:ASN:N	2.47	0.42
9:B:1168:VAL:HA	9:B:1171:GLU:HB3	2.01	0.42
10:E:511:LYS:H	10:E:511:LYS:HG2	1.72	0.42
1:D:299:TYR:CZ	10:E:351:PHE:HD2	2.37	0.42
1:F:235:ASP:OD2	1:F:333:ARG:NH2	2.52	0.42
7:Y:71:DT:H2''	7:Y:72:DG:C8	2.54	0.42
1:D:245:ILE:HG22	1:D:302:GLU:HG2	2.02	0.42
1:D:300:ARG:HA	1:D:303:ARG:HG2	2.00	0.42
4:Q:30:VAL:HG11	4:Q:51:LEU:HB3	2.02	0.42
4:U:16:THR:HA	6:X:-43:DA:H5''	2.01	0.42
6:X:67:DT:H2''	6:X:68:DC:C5	2.55	0.42
10:E:61:ARG:HA	10:E:61:ARG:HD3	1.81	0.42
9:B:943:LEU:HD13	10:E:428:TRP:HD1	1.85	0.41
9:B:1218:ASP:N	9:B:1218:ASP:OD1	2.53	0.41
3:P:36:ARG:NH1	7:Y:-13:DA:OP2	2.42	0.41
7:Y:-58:DG:H2''	7:Y:-57:DC:C5	2.55	0.41
7:Y:35:DC:H2''	7:Y:36:DC:C5	2.54	0.41
7:Y:49:DC:H2''	7:Y:50:DA:C8	2.55	0.41
8:A:209:HIS:HE1	8:A:235:ASN:HD22	1.68	0.41
8:A:267:VAL:HG23	8:A:303:ILE:HD11	2.02	0.41
1:D:338:LEU:HD23	1:D:338:LEU:HA	1.95	0.41
7:Y:3:DT:H2''	7:Y:4:DC:C5	2.55	0.41
8:A:53:MET:HE2	8:A:419:GLN:HB2	2.03	0.41
1:D:332:LEU:HD23	1:D:332:LEU:HA	1.86	0.41
2:O:83:ARG:HE	3:P:80:THR:HB	1.85	0.41
3:T:37:LEU:HD23	3:T:37:LEU:HA	1.91	0.41
10:E:438:MET:HB3	10:E:457:PHE:CE2	2.56	0.41
3:P:97:LEU:HD11	4:U:103:ALA:HB2	2.01	0.41
1:D:347:MET:SD	1:D:352:CYS:HB2	2.61	0.41
7:Y:24:DA:OP1	9:B:1221:HIS:N	2.54	0.41
9:B:692:TYR:CG	9:B:702:LEU:HD22	2.56	0.41
6:X:37:DC:H2''	6:X:38:DG:C8	2.56	0.41
4:U:28:GLY:HA3	6:X:-44:DG:H3'	2.02	0.41
6:X:35:DT:H2''	6:X:36:DA:N7	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:172:GLU:OE1	8:A:175:ARG:NH1	2.52	0.41
8:A:209:HIS:HE1	8:A:235:ASN:ND2	2.19	0.41
10:E:408:ASP:OD1	10:E:408:ASP:N	2.44	0.41
6:X:-63:DT:H2''	6:X:-62:DA:C8	2.55	0.41
9:B:681:LEU:HD13	10:E:418:TYR:CE2	2.56	0.41
9:B:756:LYS:H	9:B:756:LYS:HG2	1.72	0.41
9:B:818:ASP:HA	9:B:821:ILE:HB	2.03	0.41
9:B:932:GLY:HA2	9:B:935:PHE:HB2	2.02	0.41
9:B:1165:ASN:HA	9:B:1168:VAL:HG22	2.03	0.41
4:Q:63:LEU:HD11	5:R:38:VAL:HG13	2.03	0.41
4:Q:88:ARG:HB2	4:Q:108:LEU:HD21	2.03	0.41
7:Y:-57:DC:H2''	7:Y:-56:DC:C5	2.57	0.41
7:Y:-32:DC:H2''	7:Y:-31:DA:H8	1.86	0.41
1:D:22:MET:SD	1:D:22:MET:N	2.94	0.40
1:D:234:ASP:OD1	10:E:496:ARG:NH1	2.54	0.40
1:D:393:GLN:HB3	8:A:103:LYS:CG	2.52	0.40
1:D:395:GLU:OE1	9:B:788:TRP:NE1	2.53	0.40
7:Y:34:DT:H2''	7:Y:35:DC:C6	2.56	0.40
8:A:243:ASP:OD2	8:A:243:ASP:N	2.49	0.40
10:E:315:SER:C	10:E:316:MET:HE3	2.46	0.40
1:D:236:TRP:O	1:D:240:THR:OG1	2.39	0.40
1:D:293:LEU:O	1:D:298:LEU:CD1	2.69	0.40
4:U:90:ASP:HB3	4:U:93:LEU:HB2	2.03	0.40
9:B:1170:LYS:HB2	9:B:1170:LYS:HE2	1.90	0.40
9:B:1213:ARG:HA	9:B:1216:ASN:HB2	2.03	0.40
4:Q:81:ARG:HB2	2:S:58:THR:HG21	2.03	0.40
7:Y:12:DT:H6	7:Y:12:DT:H2'	1.78	0.40
9:B:812:GLU:OE1	9:B:812:GLU:N	2.54	0.40
1:F:350:GLN:HA	1:F:353:GLN:HB3	2.04	0.40
5:R:92:GLN:HE21	5:R:96:ARG:HH22	1.69	0.40
2:S:63:ARG:HD3	7:Y:17:DA:H4'	2.02	0.40
6:X:3:DC:H2''	6:X:4:DG:C8	2.57	0.40
6:X:24:DC:H6	6:X:24:DC:H2'	1.75	0.40
6:X:61:DC:H2''	6:X:62:DG:H5''	2.02	0.40
7:Y:-38:DC:H2''	7:Y:-37:DG:C8	2.56	0.40
8:A:269:LEU:HD21	8:A:295:VAL:HG22	2.04	0.40
10:E:311:PHE:HD1	10:E:311:PHE:HA	1.78	0.40
10:E:390:SER:OG	10:E:391:TYR:N	2.54	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	D	223/401 (56%)	205 (92%)	18 (8%)	0	100	100
1	F	185/401 (46%)	172 (93%)	13 (7%)	0	100	100
2	O	97/135 (72%)	95 (98%)	2 (2%)	0	100	100
2	S	96/135 (71%)	95 (99%)	1 (1%)	0	100	100
3	P	77/102 (76%)	76 (99%)	1 (1%)	0	100	100
3	T	77/102 (76%)	76 (99%)	1 (1%)	0	100	100
4	Q	105/129 (81%)	103 (98%)	2 (2%)	0	100	100
4	U	105/129 (81%)	104 (99%)	1 (1%)	0	100	100
5	R	91/122 (75%)	90 (99%)	1 (1%)	0	100	100
5	V	89/122 (73%)	89 (100%)	0	0	100	100
8	A	384/433 (89%)	366 (95%)	15 (4%)	3 (1%)	16	44
9	B	533/1544 (34%)	517 (97%)	16 (3%)	0	100	100
10	E	309/684 (45%)	277 (90%)	32 (10%)	0	100	100
10	G	81/684 (12%)	79 (98%)	2 (2%)	0	100	100
All	All	2452/5123 (48%)	2344 (96%)	105 (4%)	3 (0%)	49	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	A	103	LYS
8	A	405	GLU
8	A	104	PHE

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	D	208/359 (58%)	206 (99%)	2 (1%)	68	89
1	F	177/359 (49%)	176 (99%)	1 (1%)	78	93
2	O	85/108 (79%)	85 (100%)	0	100	100
2	S	84/108 (78%)	84 (100%)	0	100	100
3	P	66/78 (85%)	65 (98%)	1 (2%)	57	84
3	T	66/78 (85%)	66 (100%)	0	100	100
4	Q	84/101 (83%)	84 (100%)	0	100	100
4	U	84/101 (83%)	84 (100%)	0	100	100
5	R	80/102 (78%)	80 (100%)	0	100	100
5	V	78/102 (76%)	78 (100%)	0	100	100
8	A	326/367 (89%)	324 (99%)	2 (1%)	78	93
9	B	501/1399 (36%)	498 (99%)	3 (1%)	78	93
10	E	301/653 (46%)	298 (99%)	3 (1%)	68	89
10	G	83/653 (13%)	83 (100%)	0	100	100
All	All	2223/4568 (49%)	2211 (100%)	12 (0%)	78	93

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	347	MET
1	D	358	GLN
1	F	305	GLN
3	P	96	THR
8	A	214	PHE
8	A	325	GLU
9	B	770	ARG
9	B	785	HIS
9	B	812	GLU
10	E	540	THR
10	E	549	TYR
10	E	559	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	82	GLN
1	D	389	ASN
1	F	259	ASN
1	F	350	GLN
4	Q	104	GLN
5	R	92	GLN
5	V	64	ASN
5	V	81	ASN
8	A	31	ASN
8	A	72	GLN
8	A	144	ASN
8	A	209	HIS
8	A	375	ASN
9	B	722	ASN
9	B	836	ASN
9	B	848	ASN
9	B	1289	GLN
10	E	65	ASN
10	E	294	ASN
10	E	325	ASN
10	E	342	ASN
10	E	347	ASN
10	G	331	ASN
10	G	332	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	$\# Z > 2$
2	M3L	S	36	2	10,11,12	0.53	0	9,14,16	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	M3L	O	36	2	10,11,12	0.53	0	9,14,16	0.50	0

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
2	M3L	S	36	2	-	0/9/10/12	-
2	M3L	O	36	2	-	0/9/10/12	-

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.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

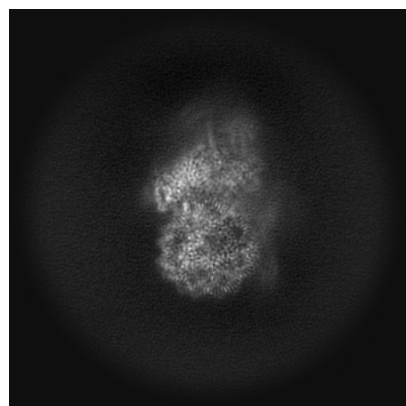
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37125. These allow visual inspection of the internal detail of the map and identification of artifacts.

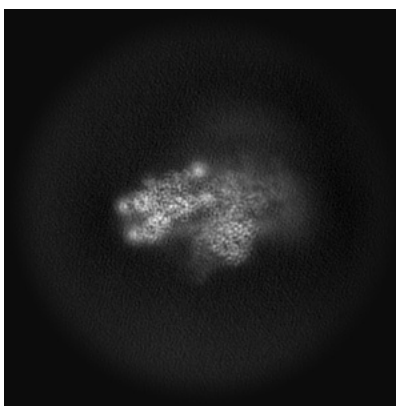
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

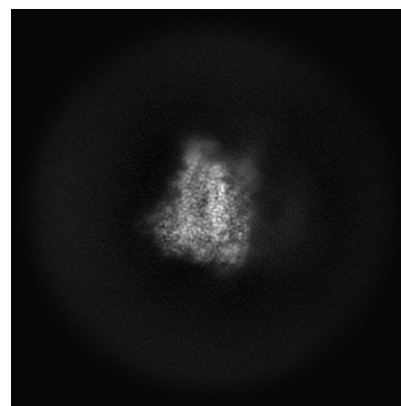
6.1.1 Primary map



X

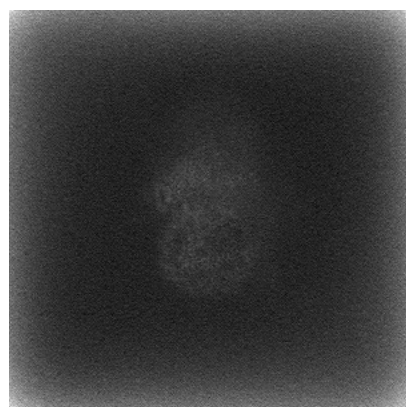


Y

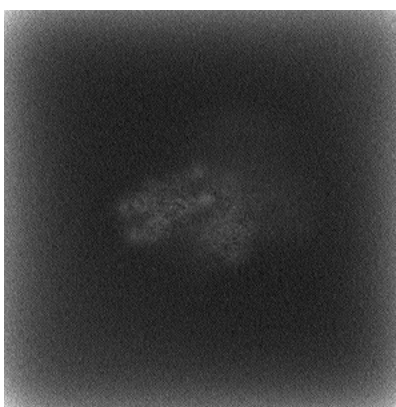


Z

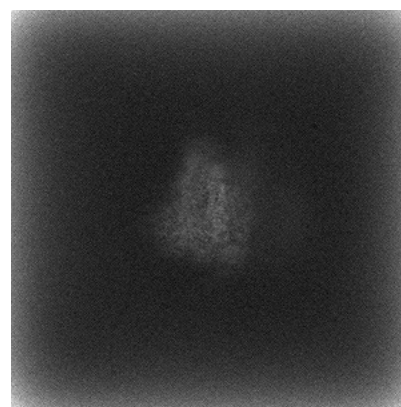
6.1.2 Raw map



X



Y

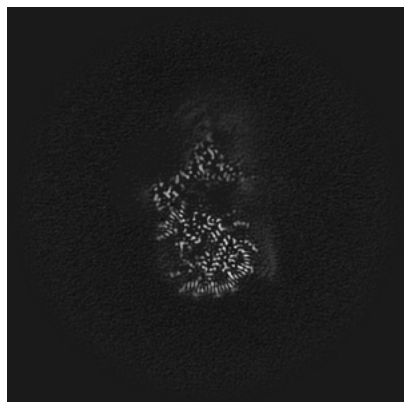


Z

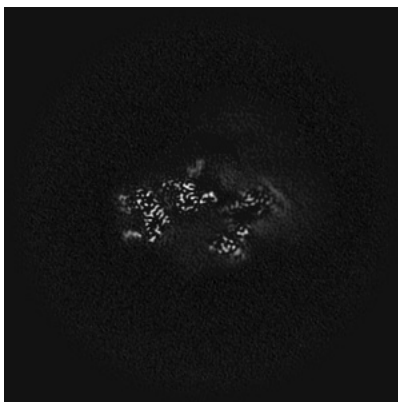
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 270

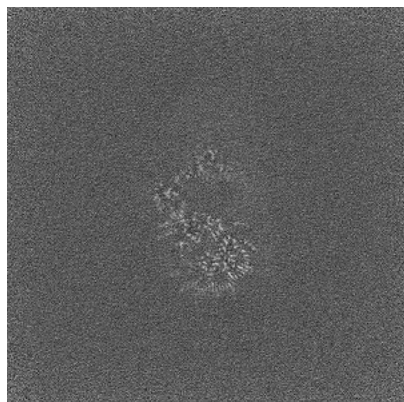


Y Index: 270

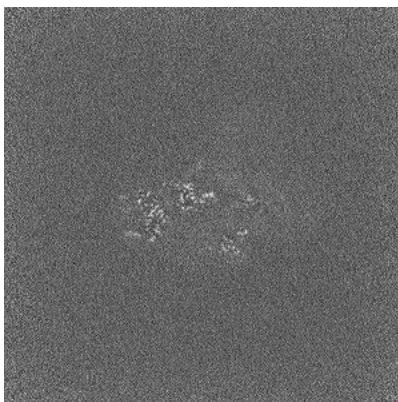


Z Index: 270

6.2.2 Raw map



X Index: 270



Y Index: 270

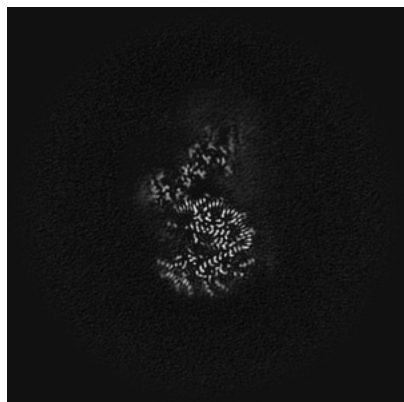


Z Index: 270

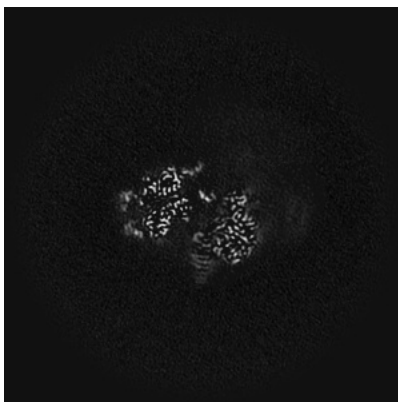
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

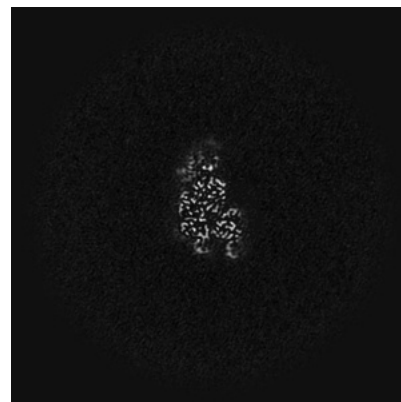
6.3.1 Primary map



X Index: 281

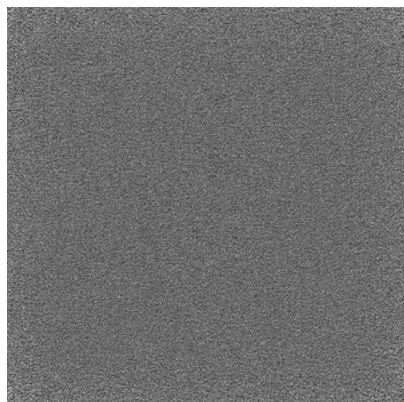


Y Index: 243

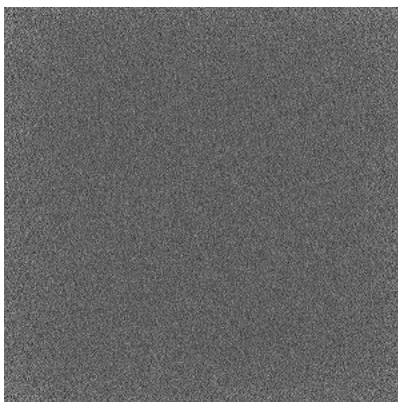


Z Index: 204

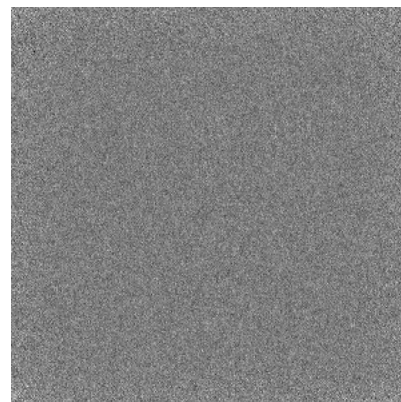
6.3.2 Raw map



X Index: 0



Y Index: 0

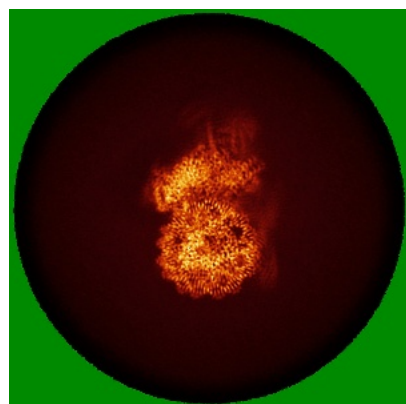


Z Index: 0

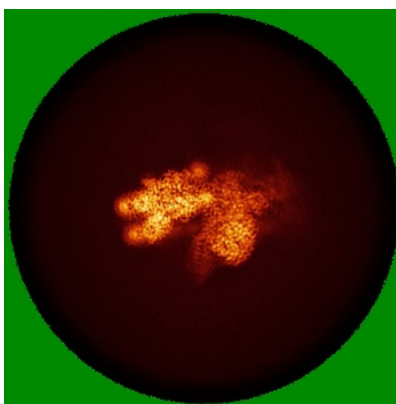
The images above show the largest variance slices of the map in three orthogonal directions.

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

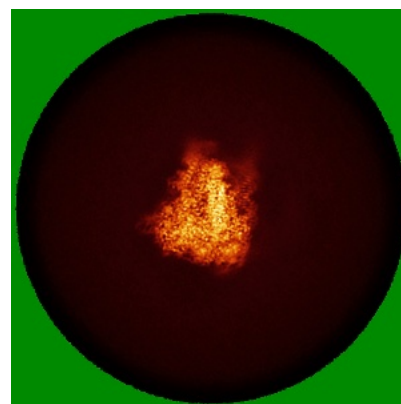
6.4.1 Primary map



X

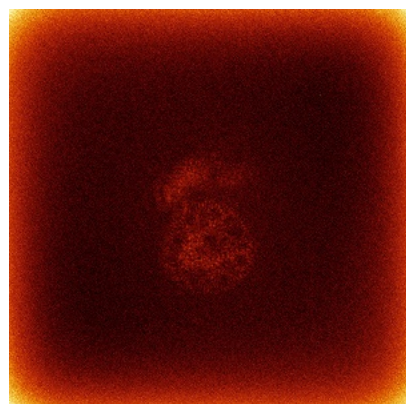


Y

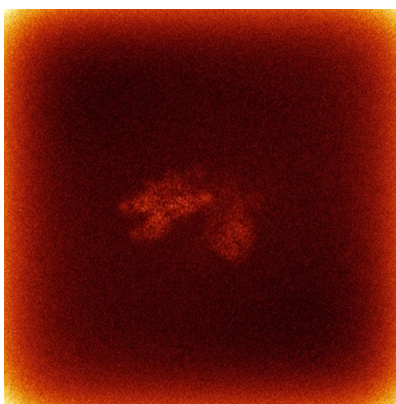


Z

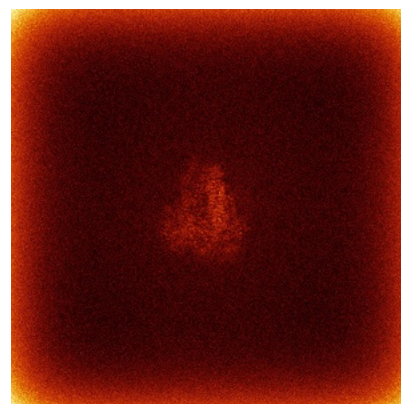
6.4.2 Raw map



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](#)

This section was not generated.

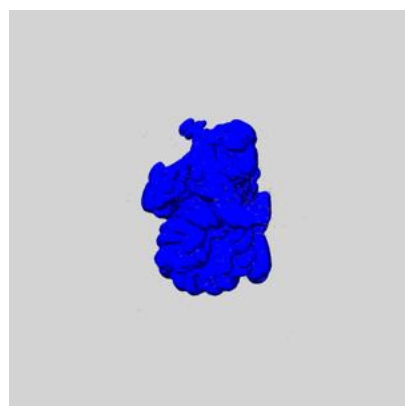
6.6 Mask visualisation [i](#)

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

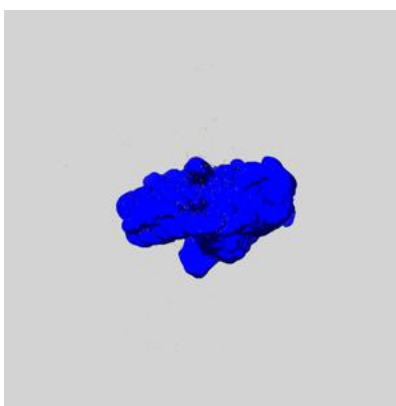
A mask typically either:

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

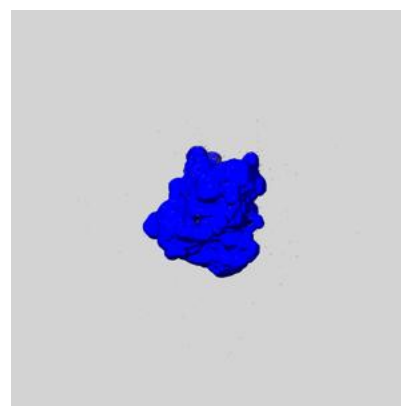
6.6.1 emd_37125_msk_1.map [i](#)



X



Y

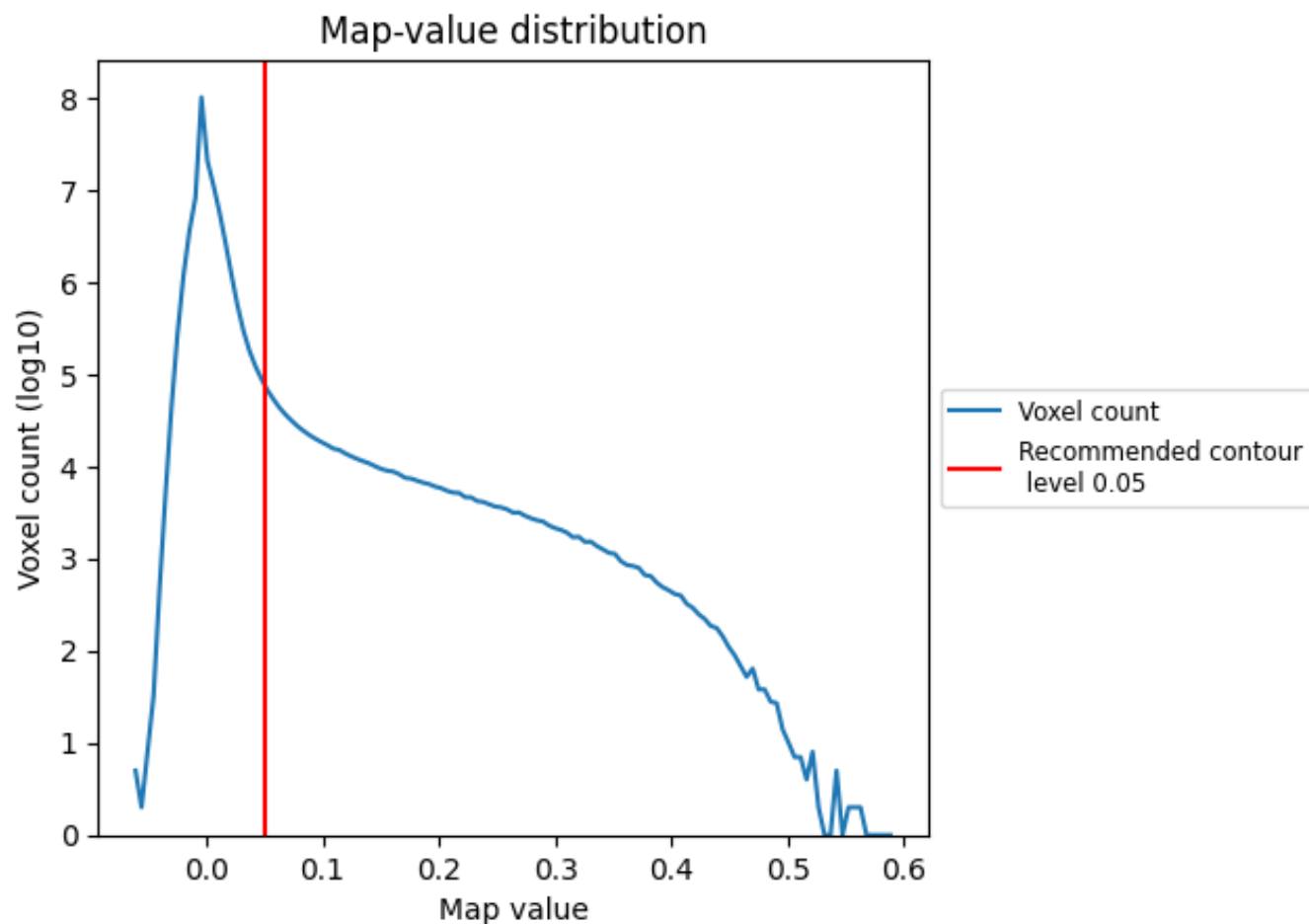


Z

7 Map analysis [i](#)

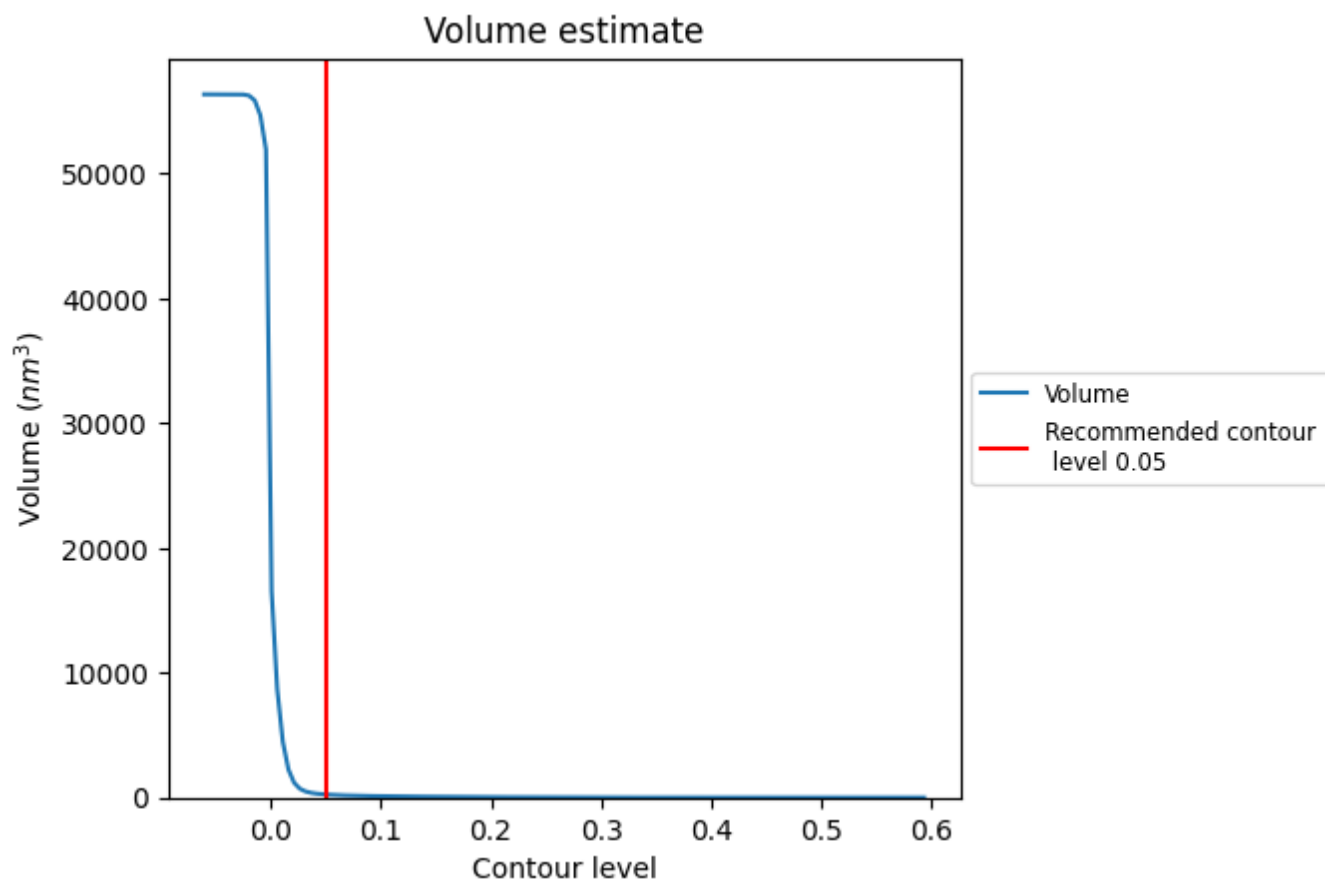
This section contains the results of statistical analysis of the map.

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.

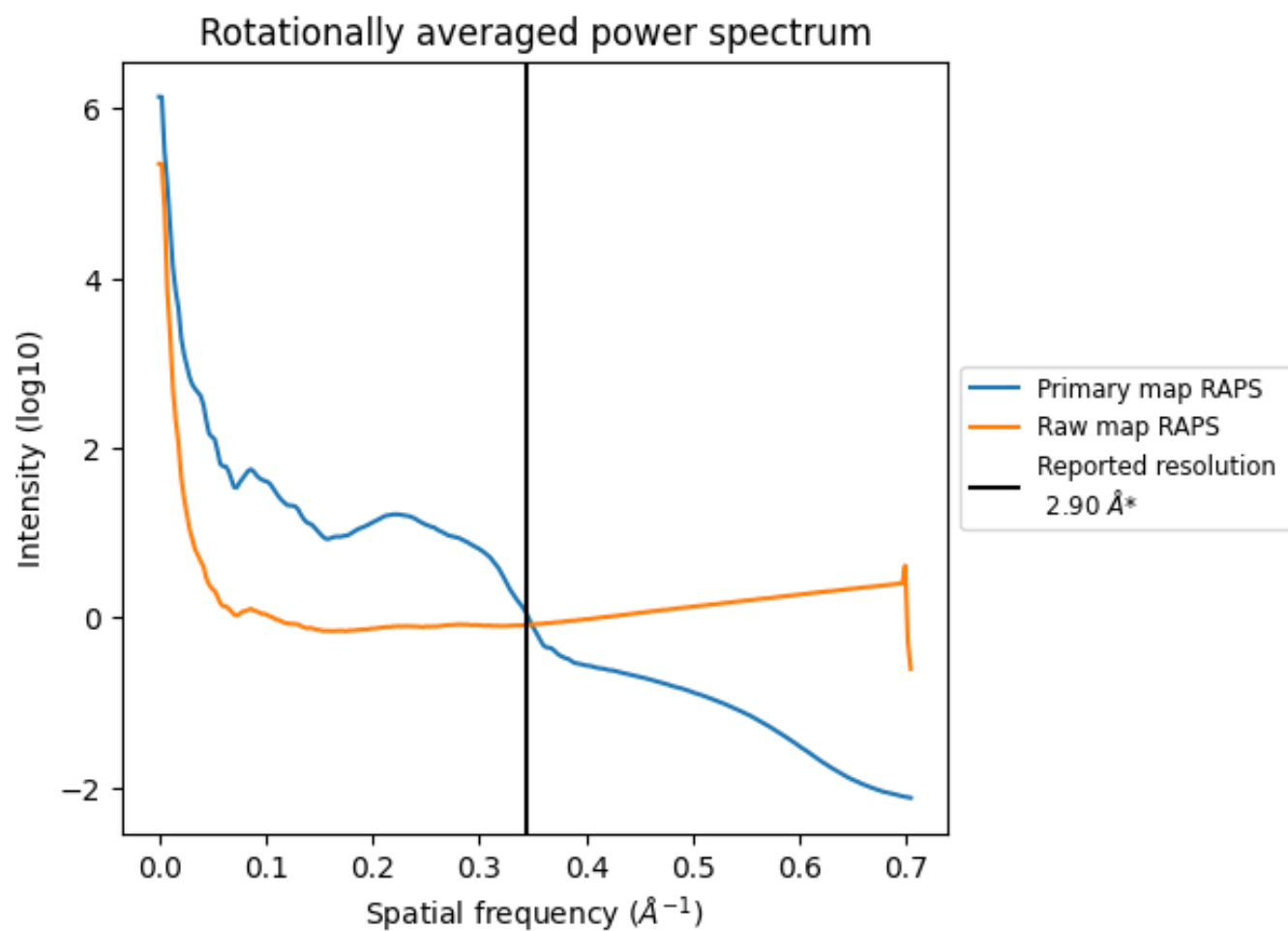
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 245 nm³; this corresponds to an approximate mass of 221 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 ⓘ

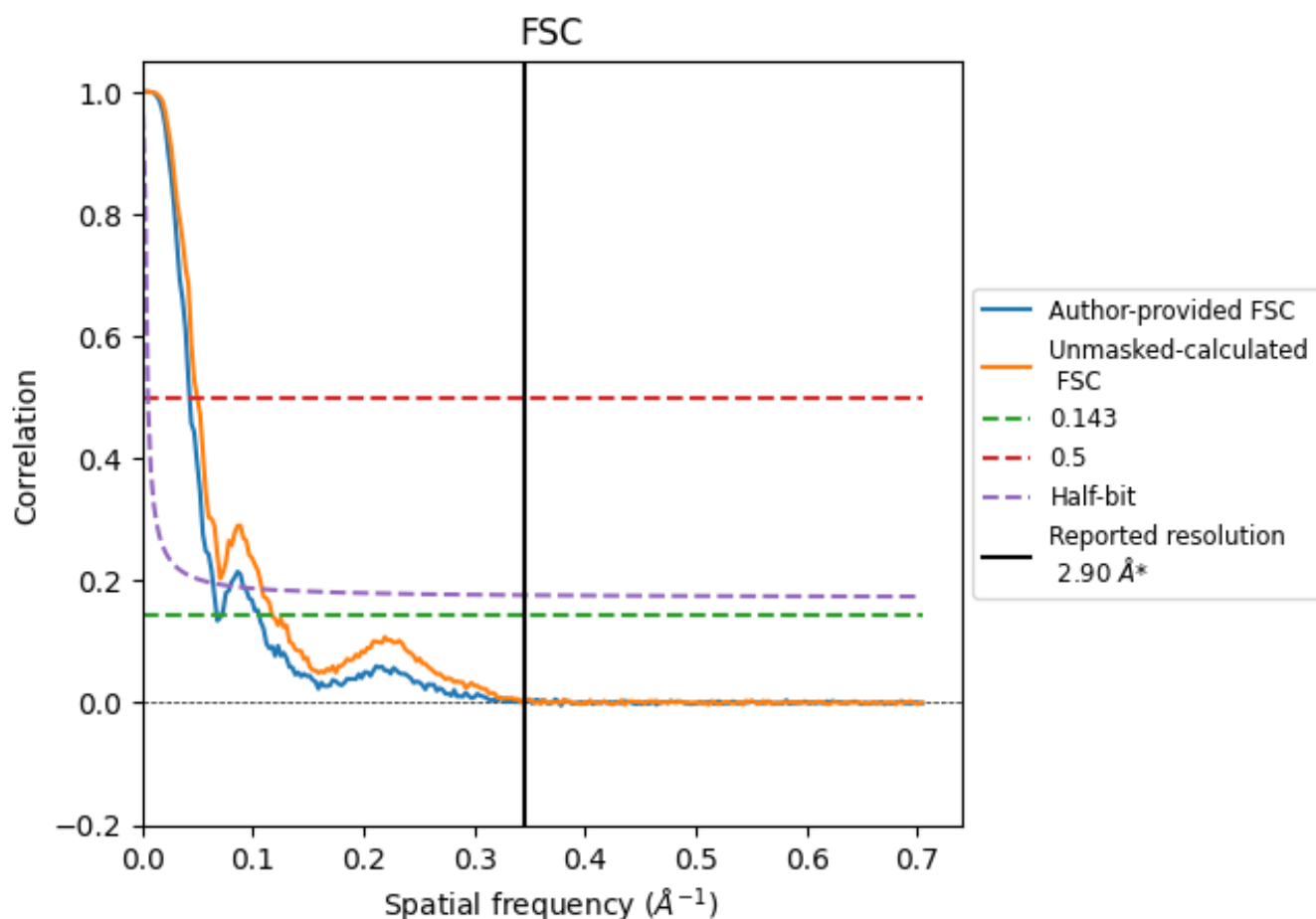


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	14.86	23.36	15.62
Unmasked-calculated*	8.53	20.20	9.24

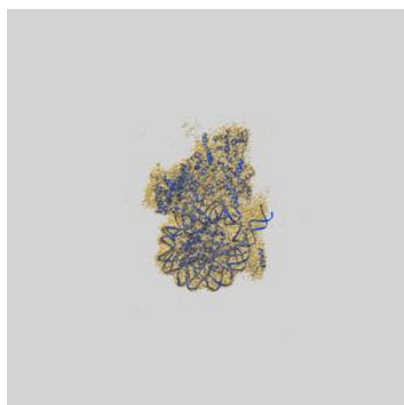
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 14.86 differs from the reported value 2.9 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.53 differs from the reported value 2.9 by more than 10 %

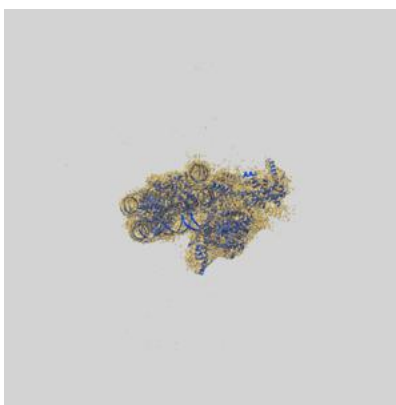
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37125 and PDB model 8KD5. Per-residue inclusion information can be found in section [3](#) on page [7](#).

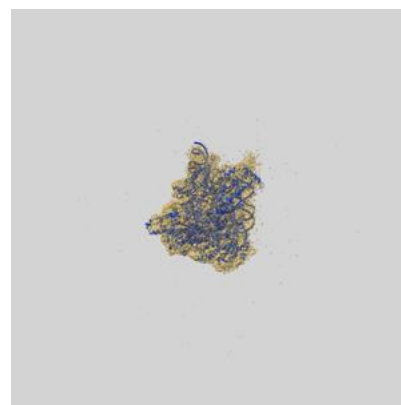
9.1 Map-model overlay [i](#)



X



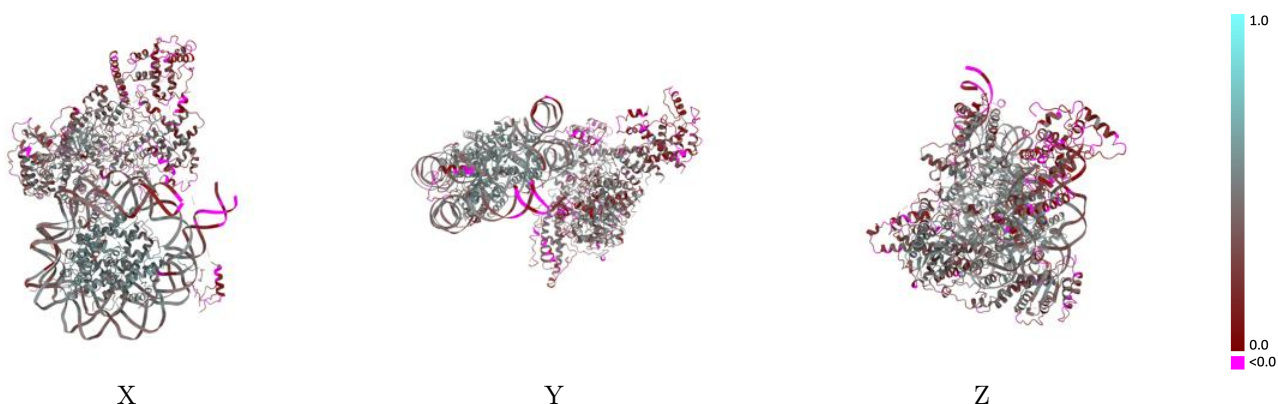
Y



Z

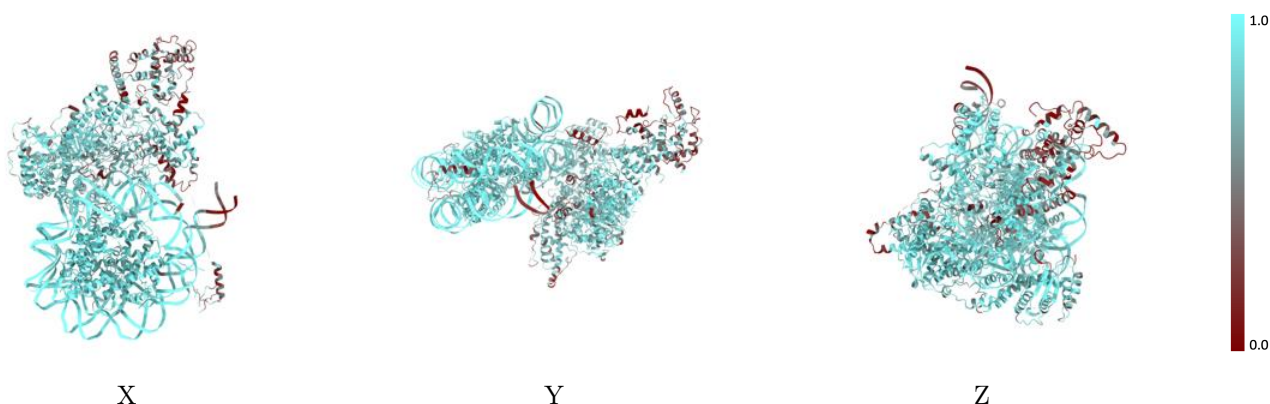
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



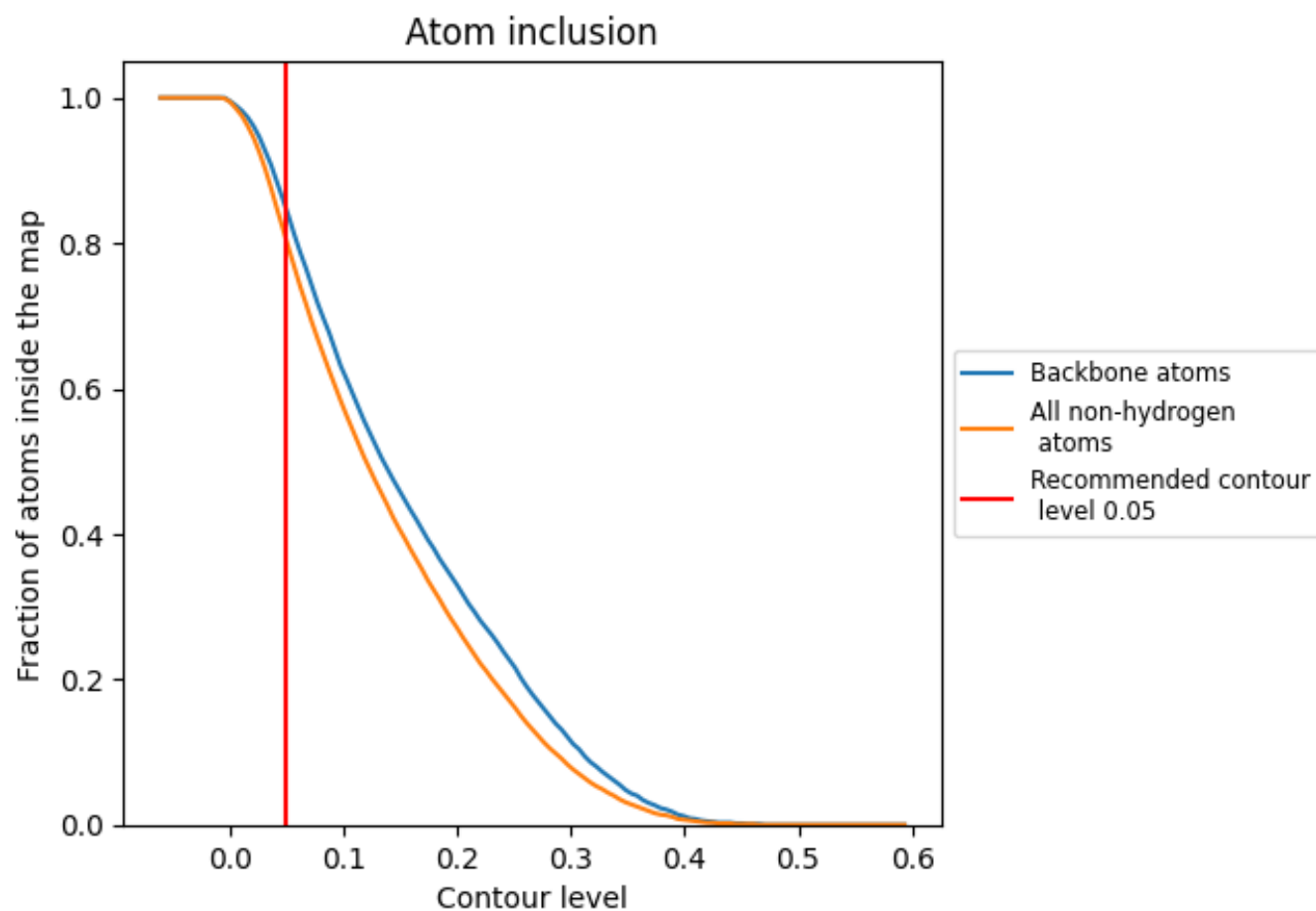
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 80% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8040	 0.3780
A	 0.8650	 0.4050
B	 0.7780	 0.3540
D	 0.7720	 0.3460
E	 0.6750	 0.2970
F	 0.4230	 0.1280
G	 0.3300	 0.1000
O	 0.9170	 0.5100
P	 0.9360	 0.5230
Q	 0.9260	 0.5190
R	 0.9370	 0.5150
S	 0.9100	 0.5030
T	 0.9230	 0.5480
U	 0.9180	 0.5070
V	 0.9240	 0.5030
X	 0.8910	 0.3880
Y	 0.8850	 0.3860

