



Full wwPDB EM Validation Report ⓘ

Apr 21, 2026 – 01:41 PM EDT

PDB ID : 8FS5 / pdb_00008fs5
EMDB ID : EMD-29414
Title : Structure of *S. cerevisiae* Rad24-RFC loading the 9-1-1 clamp onto a 10-nt gapped DNA in step 3 (open 9-1-1 and stably bound chamber DNA)
Authors : Zheng, F.; Georgescu, R.; Yao, Y.N.; O'Donnell, M.E.; Li, H.
Deposited on : 2023-01-09
Resolution : 2.76 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

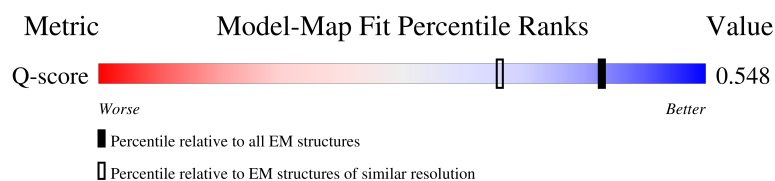
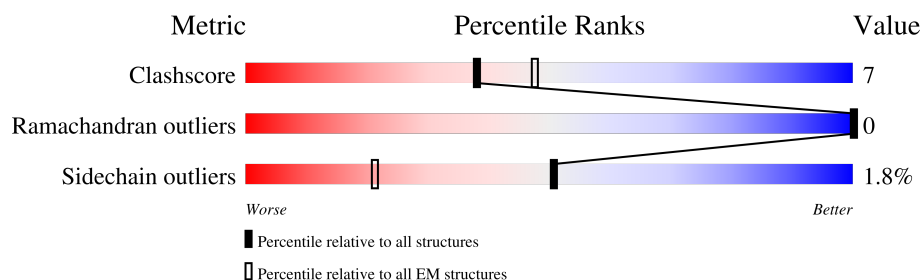
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.76 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	10642 (2.26 - 3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	545	
2	B	323	
3	C	336	
4	D	353	

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Mol	Chain	Length	Quality of chain
5	E	354	
6	F	474	
7	G	401	
8	H	612	
9	I	50	
10	J	21	
11	K	20	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 22211 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 Checkpoint protein RAD24.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	435	Total	C	N	O	S	0	0
			3559	2268	618	655	18		

- Molecule 2 is a protein called Replication factor C subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	317	Total	C	N	O	S	0	0
			2490	1570	444	463	13		

- Molecule 3 is a protein called Replication factor C subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	327	Total	C	N	O	S	0	0
			2586	1628	451	499	8		

- Molecule 4 is a protein called Replication factor C subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	330	Total	C	N	O	S	0	0
			2616	1653	452	501	10		

- Molecule 5 is a protein called Replication factor C subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	353	Total	C	N	O	S	0	0
			2787	1762	484	523	18		

- Molecule 6 is a protein called DNA damage checkpoint control protein MEC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	292	Total	C	N	O	S	0	0
			2337	1488	406	424	19		

- Molecule 7 is a protein called DNA damage checkpoint control protein RAD17.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	293	Total	C	N	O	S	0	0
			2322	1478	376	456	12		

- Molecule 8 is a protein called DDC1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	272	Total	C	N	O	S	0	0
			2193	1408	363	409	13		

- Molecule 9 is a DNA chain called Template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	32	Total	C	N	O	P	0	0
			652	313	110	197	32		

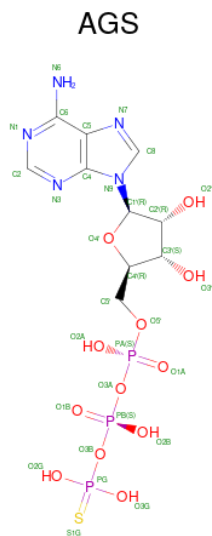
- Molecule 10 is a DNA chain called Primer strand 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	16	Total	C	N	O	P	0	0
			313	146	58	93	16		

- Molecule 11 is a DNA chain called Primer strand 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	10	Total	C	N	O	P	0	0
			201	98	34	60	9		

- Molecule 12 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).

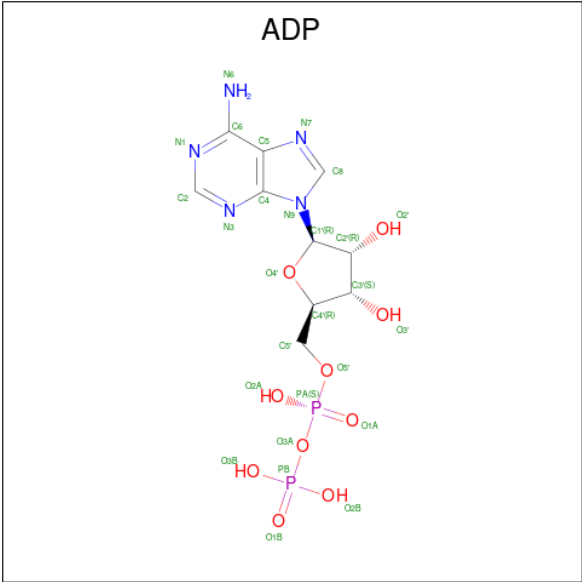


Mol	Chain	Residues	Atoms					AltConf	
12	A	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
12	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
12	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
12	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0

- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
13	A	1	Total Mg 1 1	0
13	B	1	Total Mg 1 1	0
13	C	1	Total Mg 1 1	0
13	D	1	Total Mg 1 1	0

- Molecule 14 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

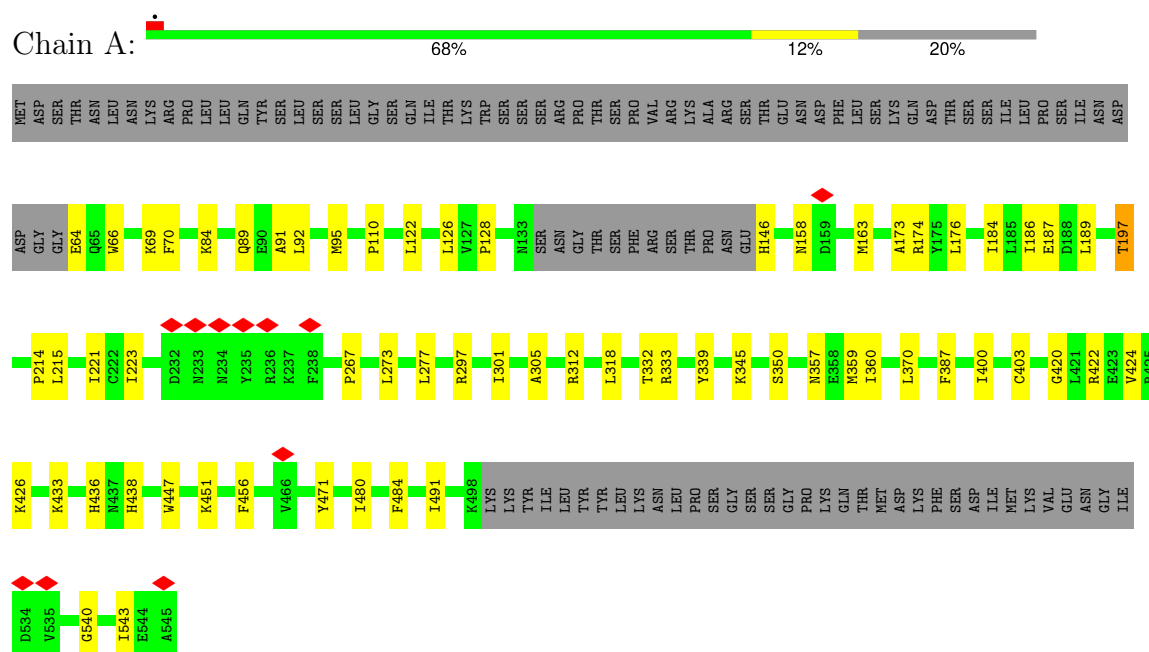


Mol	Chain	Residues	Atoms					AltConf
14	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

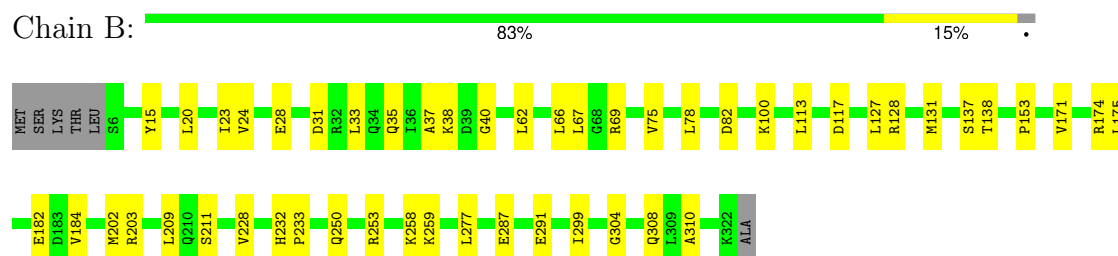
3 Residue-property plots

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.

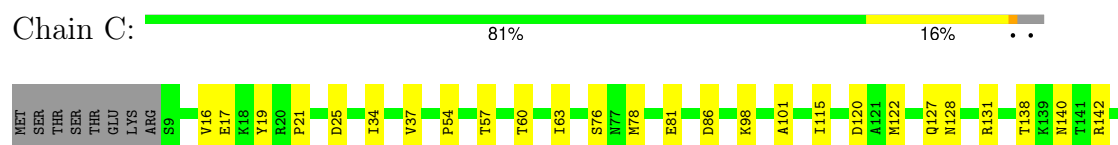
• Molecule 1: Checkpoint protein RAD24



• Molecule 2: Replication factor C subunit 4



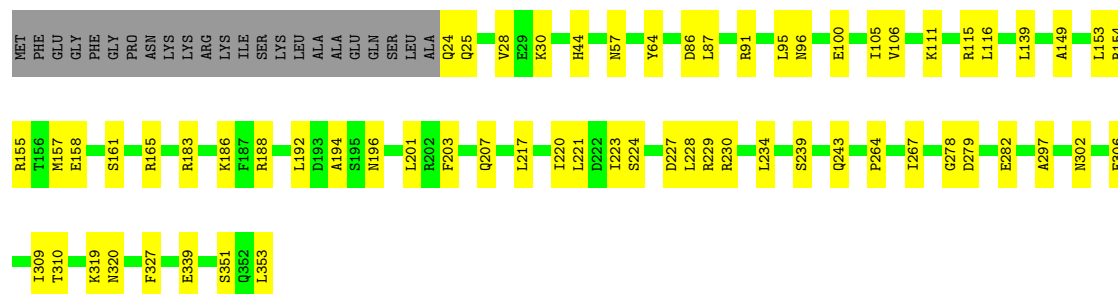
• Molecule 3: Replication factor C subunit 3





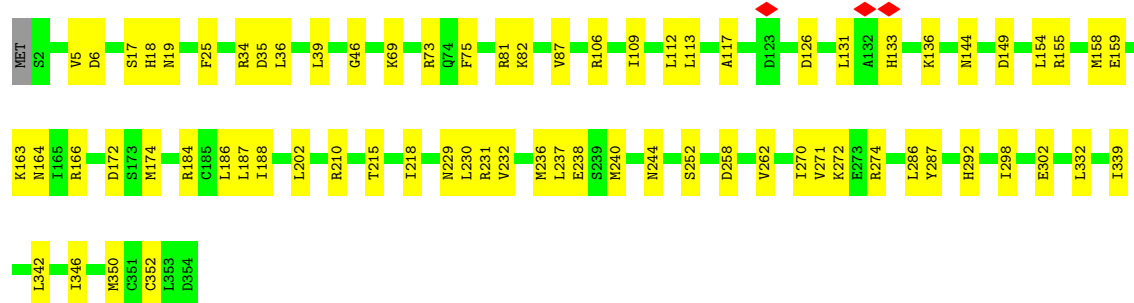
• Molecule 4: Replication factor C subunit 2

Chain D: 75% 18% 7%



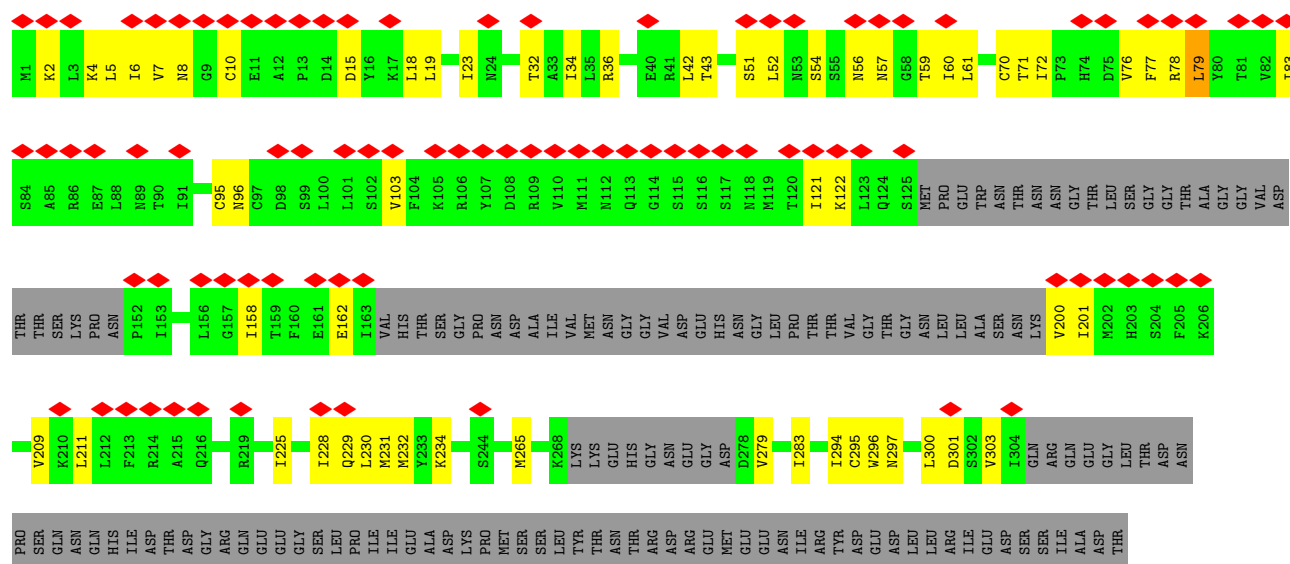
• Molecule 5: Replication factor C subunit 5

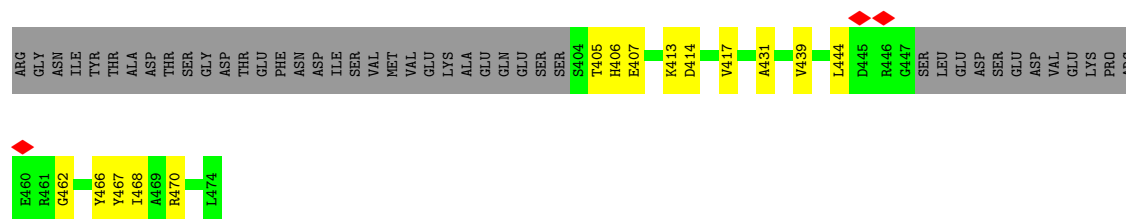
Chain E: 79% 20%



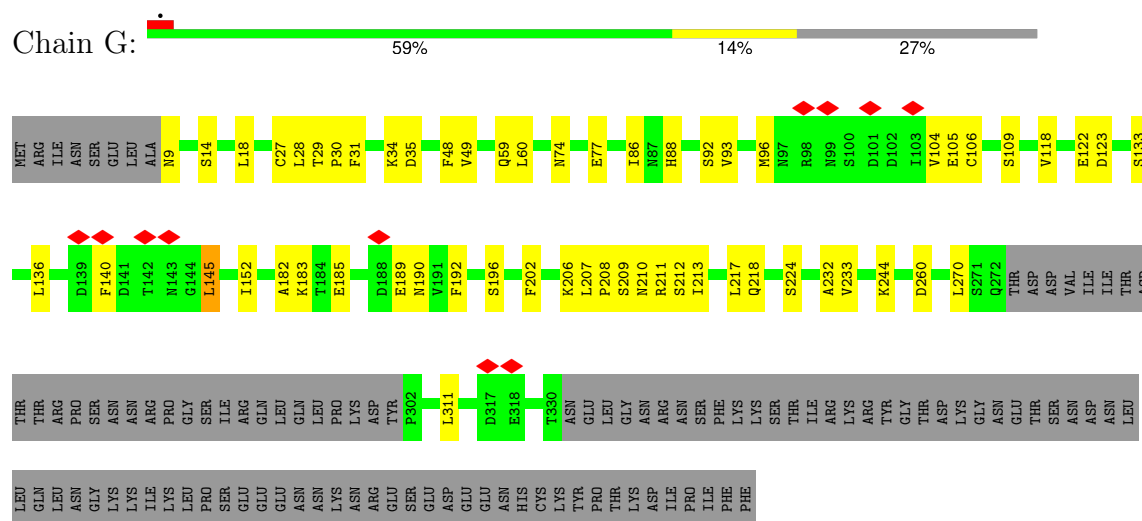
• Molecule 6: DNA damage checkpoint control protein MEC3

Chain F: 20% 46% 15% 38%

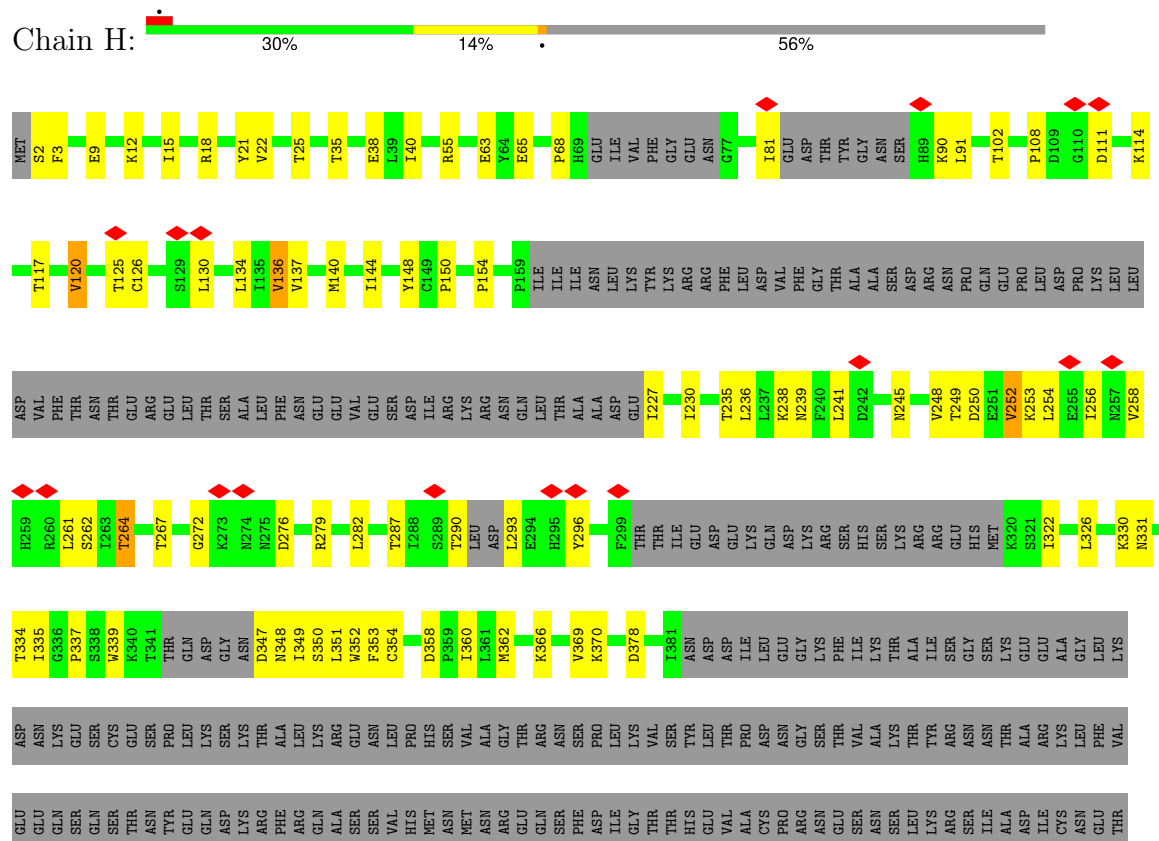




• Molecule 7: DNA damage checkpoint control protein RAD17



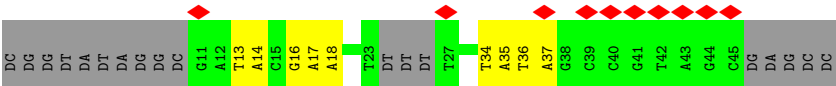
• Molecule 8: DDC1 isoform 1



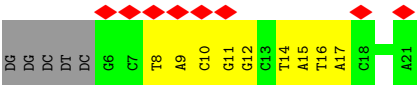
GLU ASP
THR PRO
GLN GLN
SER THR
PHE PHE
ALA LYS
ARG ARG
ALA ASP
THR THR
THR VAL
THR THR
TTP GLY
LYS LYS
ALA PRO
LEU LEU
PRO PRO
ALA ALA
ASP ASP
GLU VAL
SER SER
CYS SER
ASN ASN
ILE ASP
ASP ARG
LYS LYS
MET MET
LYS LYS
GLY GLY
LEU LEU
ASN ASN
GLN GLN
ASP THR
THR SER

ASN
HIS
LYS
LYS
ASP
ASN
LYS
GLU
MET
GLU
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ASP

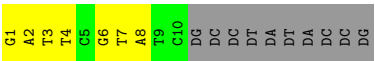
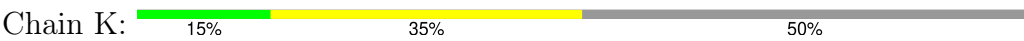
● Molecule 9: Template strand



● Molecule 10: Primer strand 1



● Molecule 11: Primer strand 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	400932	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.801	Depositor
Minimum map value	-1.418	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.17	Depositor
Map size ($\text{\AA}$)	347.76, 347.76, 347.76	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.828, 0.828, 0.828	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, AGS

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.22	0/3635	0.50	0/4901
2	B	0.18	0/2525	0.44	0/3404
3	C	0.19	0/2626	0.45	0/3552
4	D	0.12	0/2661	0.41	0/3600
5	E	0.19	0/2827	0.46	0/3819
6	F	0.25	0/2377	0.47	0/3204
7	G	0.21	0/2358	0.44	0/3176
8	H	0.16	0/2234	0.39	0/3020
9	I	0.17	0/727	0.40	0/1117
10	J	0.14	0/350	0.33	0/539
11	K	0.15	0/224	0.40	0/344
All	All	0.19	0/22544	0.44	0/30676

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3559	0	3561	41	0
2	B	2490	0	2582	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2586	0	2614	37	0
4	D	2616	0	2647	45	0
5	E	2787	0	2901	51	0
6	F	2337	0	2380	43	0
7	G	2322	0	2316	32	0
8	H	2193	0	2201	53	0
9	I	652	0	366	7	0
10	J	313	0	168	5	0
11	K	201	0	116	6	0
12	A	31	0	12	1	0
12	B	31	0	12	4	0
12	C	31	0	12	3	0
12	D	31	0	12	3	0
13	A	1	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	D	1	0	0	0	0
14	E	27	0	12	3	0
All	All	22211	0	21912	326	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 (326) 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)
6:F:95:CYS:HB3	6:F:209:VAL:HG23	1.71	0.72
12:C:401:AGS:S1G	4:D:183:ARG:NH2	2.64	0.71
1:A:480:ILE:HA	1:A:484:PHE:HB2	1.74	0.70
2:B:40:GLY:HA2	2:B:66:LEU:HD11	1.74	0.69
2:B:171:VAL:HA	2:B:202:MET:HE1	1.76	0.68
1:A:163:MET:HE3	9:I:34:DT:H5'	1.75	0.68
3:C:101:ALA:O	3:C:140:ASN:ND2	2.27	0.67
5:E:136:LYS:HZ1	6:F:60:ILE:HG23	1.58	0.67
6:F:70:CYS:SG	6:F:71:THR:N	2.67	0.67
8:H:250:ASP:OD2	8:H:279:ARG:NH2	2.28	0.66
8:H:55:ARG:HB2	8:H:370:LYS:HB2	1.77	0.66
7:G:152:ILE:HB	7:G:224:SER:HB3	1.79	0.65
1:A:163:MET:HG2	1:A:197:THR:HB	1.79	0.65
6:F:431:ALA:HB3	6:F:439:VAL:HB	1.79	0.65
5:E:109:ILE:HD12	5:E:113:LEU:HD12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:174:MET:HE1	5:E:187:LEU:HD13	1.79	0.65
6:F:18:LEU:HD21	6:F:462:GLY:HA3	1.79	0.65
8:H:126:CYS:HB2	8:H:130:LEU:HD12	1.80	0.64
4:D:309:ILE:O	4:D:319:LYS:NZ	2.30	0.64
1:A:158:ASN:HD21	8:H:102:THR:HG21	1.63	0.63
8:H:117:THR:HB	8:H:137:VAL:HB	1.80	0.63
5:E:17:SER:H	14:E:500:ADP:HN62	1.47	0.63
3:C:206:ARG:NH2	12:C:401:AGS:S1G	2.71	0.62
8:H:111:ASP:HB3	8:H:140:MET:HE3	1.81	0.62
2:B:24:VAL:O	12:B:401:AGS:N6	2.33	0.62
1:A:174:ARG:NH2	8:H:378:ASP:OD2	2.31	0.62
2:B:203:ARG:NH2	12:B:401:AGS:S1G	2.71	0.62
2:B:308:GLN:NE2	3:C:307:GLU:OE2	2.30	0.61
6:F:42:LEU:HB3	6:F:72:ILE:HB	1.83	0.61
4:D:24:GLN:HG2	4:D:25:GLN:HG2	1.83	0.61
5:E:126:ASP:OD2	5:E:133:HIS:NE2	2.34	0.61
8:H:227:ILE:HG22	8:H:354:CYS:HB2	1.83	0.61
4:D:100:GLU:OE2	4:D:100:GLU:N	2.29	0.60
8:H:68:PRO:HB2	8:H:90:LYS:HD2	1.83	0.60
8:H:108:PRO:HG2	8:H:140:MET:HE1	1.82	0.60
2:B:253:ARG:NH1	3:C:286:GLU:OE1	2.35	0.60
5:E:231:ARG:HB2	14:E:500:ADP:H5'1	1.84	0.60
5:E:144:ASN:ND2	5:E:172:ASP:O	2.35	0.59
6:F:8:ASN:ND2	6:F:10:CYS:SG	2.72	0.59
1:A:387:PHE:O	1:A:438:HIS:ND1	2.34	0.59
11:K:6:DG:H2"	11:K:7:DT:H5"	1.85	0.59
5:E:117:ALA:O	5:E:164:ASN:ND2	2.36	0.59
8:H:134:LEU:HB3	8:H:150:PRO:HG2	1.84	0.59
8:H:245:ASN:HB3	8:H:248:VAL:HG22	1.85	0.59
5:E:75:PHE:HZ	5:E:112:LEU:HD12	1.68	0.58
5:E:202:LEU:HD22	5:E:237:LEU:HD22	1.84	0.58
1:A:189:LEU:HD11	1:A:223:ILE:HG12	1.85	0.58
5:E:258:ASP:N	5:E:258:ASP:OD1	2.35	0.58
8:H:9:GLU:HB2	8:H:12:LYS:HB2	1.85	0.58
3:C:76:SER:HB2	7:G:140:PHE:HA	1.84	0.58
1:A:357:ASN:OD1	1:A:422:ARG:NH2	2.34	0.58
5:E:270:ILE:HG23	5:E:350:MET:HG2	1.86	0.57
2:B:127:LEU:O	2:B:131:MET:HG3	2.05	0.57
6:F:230:LEU:HD21	6:F:431:ALA:HB1	1.87	0.57
8:H:81:ILE:HD13	8:H:91:LEU:HD12	1.87	0.57
5:E:232:VAL:HG12	5:E:236:MET:HE2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:40:ILE:HG12	8:H:55:ARG:HG2	1.86	0.57
8:H:290:THR:HA	8:H:293:LEU:HB2	1.85	0.57
2:B:67:LEU:HD12	2:B:75:VAL:HG23	1.87	0.57
2:B:250:GLN:OE1	2:B:253:ARG:NH2	2.38	0.56
3:C:267:ARG:NH1	3:C:316:ASP:OD2	2.38	0.56
6:F:78:ARG:HG2	6:F:79:LEU:HD23	1.86	0.56
7:G:93:VAL:HA	7:G:96:MET:HG3	1.86	0.56
8:H:235:THR:HA	8:H:238:LYS:HB2	1.88	0.56
4:D:25:GLN:HG3	4:D:30:LYS:HB2	1.87	0.56
4:D:279:ASP:HB3	4:D:282:GLU:HG2	1.86	0.56
7:G:208:PRO:HD2	7:G:213:ILE:HG21	1.87	0.56
7:G:209:SER:O	7:G:211:ARG:NH1	2.39	0.55
2:B:259:LYS:O	3:C:165:ARG:NE	2.38	0.55
7:G:29:THR:N	7:G:30:PRO:HD2	2.20	0.55
12:D:401:AGS:S1G	5:E:155:ARG:NH2	2.79	0.55
3:C:86:ASP:OD1	4:D:111:LYS:NZ	2.39	0.55
10:J:8:DT:H2"	10:J:9:DA:C8	2.42	0.55
1:A:297:ARG:O	1:A:301:ILE:HD12	2.07	0.55
3:C:213:GLN:NE2	4:D:57:ASN:O	2.40	0.55
8:H:347:ASP:OD1	8:H:347:ASP:N	2.38	0.55
4:D:161:SER:O	4:D:165:ARG:NH1	2.40	0.54
2:B:15:TYR:O	2:B:174:ARG:NH2	2.38	0.54
4:D:87:LEU:HG	4:D:91:ARG:HG3	1.88	0.54
4:D:115:ARG:NH1	7:G:136:LEU:O	2.40	0.54
5:E:73:ARG:HH21	6:F:61:LEU:HD22	1.72	0.54
2:B:33:LEU:HD22	2:B:62:LEU:HD22	1.90	0.54
4:D:229:ARG:NH1	5:E:159:GLU:OE2	2.41	0.54
1:A:89:GLN:HG2	1:A:122:LEU:HD21	1.90	0.54
1:A:128:PRO:HD3	1:A:146:HIS:HA	1.89	0.54
6:F:15:ASP:HB2	6:F:76:VAL:HG13	1.90	0.54
8:H:261:LEU:HD13	8:H:293:LEU:HD11	1.91	0.53
2:B:31:ASP:O	2:B:35:GLN:HG3	2.08	0.53
6:F:414:ASP:HB3	6:F:468:ILE:HD13	1.90	0.53
4:D:116:LEU:HD21	7:G:133:SER:HB2	1.90	0.53
1:A:92:LEU:HD12	1:A:122:LEU:HD13	1.90	0.53
4:D:153:LEU:O	4:D:157:MET:HG3	2.09	0.52
4:D:192:LEU:HD12	4:D:228:LEU:HB2	1.91	0.52
8:H:38:GLU:OE1	8:H:55:ARG:NE	2.42	0.52
9:I:36:DT:H2"	9:I:37:DA:C8	2.45	0.52
7:G:27:CYS:HB2	7:G:60:LEU:HD21	1.91	0.52
8:H:331:ASN:O	8:H:335:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:TYR:OH	2:B:182:GLU:OE1	2.23	0.52
7:G:185:GLU:HB2	7:G:189:GLU:HB3	1.92	0.52
2:B:37:ALA:HA	2:B:66:LEU:HD13	1.90	0.52
5:E:244:ASN:OD1	5:E:252:SER:OG	2.25	0.52
6:F:51:SER:HB2	6:F:54:SER:HB3	1.90	0.52
4:D:217:LEU:HD23	4:D:220:ILE:HD12	1.91	0.52
1:A:66:TRP:HA	1:A:69:LYS:HG2	1.92	0.51
1:A:173:ALA:HB1	1:A:184:ILE:HG12	1.92	0.51
7:G:190:ASN:HB3	7:G:217:LEU:HD23	1.92	0.51
7:G:18:LEU:HD11	7:G:106:CYS:H	1.76	0.51
7:G:9:ASN:OD1	7:G:109:SER:OG	2.29	0.51
4:D:306:GLU:O	4:D:310:THR:OG1	2.26	0.51
4:D:223:ILE:HG22	4:D:230:ARG:HH22	1.76	0.51
5:E:232:VAL:O	5:E:236:MET:HG3	2.10	0.51
3:C:54:PRO:HD2	3:C:57:THR:HG21	1.92	0.51
12:D:401:AGS:O3G	5:E:184:ARG:NH2	2.41	0.51
3:C:81:GLU:HG2	3:C:115:ILE:HB	1.93	0.51
4:D:100:GLU:HG2	4:D:105:ILE:HG13	1.92	0.50
5:E:5:VAL:HG23	5:E:6:ASP:OD1	2.10	0.50
7:G:74:ASN:ND2	7:G:77:GLU:O	2.45	0.50
1:A:339:TYR:HA	1:A:370:LEU:HD21	1.94	0.50
7:G:109:SER:HB3	7:G:118:VAL:HB	1.92	0.50
7:G:49:VAL:HG22	7:G:59:GLN:HG3	1.91	0.50
4:D:278:GLY:HA2	4:D:351:SER:HB2	1.93	0.50
7:G:260:ASP:OD1	7:G:260:ASP:N	2.45	0.50
8:H:3:PHE:HD2	8:H:120:VAL:HG12	1.77	0.50
6:F:2:LYS:HB3	6:F:83:ILE:HB	1.93	0.50
6:F:295:CYS:SG	6:F:296:TRP:N	2.85	0.50
7:G:31:PHE:CE1	7:G:244:LYS:HB3	2.47	0.50
1:A:332:THR:OG1	1:A:333:ARG:N	2.43	0.50
1:A:543:ILE:HG12	5:E:292:HIS:CD2	2.48	0.49
2:B:128:ARG:HD2	2:B:153:PRO:HB2	1.93	0.49
8:H:254:LEU:HB3	8:H:322:ILE:HG22	1.94	0.49
8:H:350:SER:HB3	8:H:352:TRP:HE1	1.76	0.49
5:E:286:LEU:HD13	5:E:342:LEU:HB3	1.94	0.49
8:H:15:ILE:HB	8:H:339:TRP:HB2	1.94	0.49
8:H:262:SER:HB2	8:H:287:THR:HG23	1.94	0.49
1:A:312:ARG:NH2	12:A:601:AGS:S1G	2.85	0.49
3:C:206:ARG:HD2	4:D:183:ARG:HA	1.93	0.49
3:C:256:TRP:NE1	4:D:320:ASN:OD1	2.31	0.49
3:C:292:ASN:ND2	3:C:333:ASN:HB3	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:35:ASP:H	7:G:86:ILE:HG22	1.78	0.49
5:E:106:ARG:HD3	5:E:149:ASP:HB3	1.95	0.49
6:F:34:ILE:HD11	6:F:51:SER:HA	1.94	0.49
4:D:201:LEU:HG	4:D:217:LEU:HD22	1.95	0.49
5:E:164:ASN:N	5:E:164:ASN:OD1	2.45	0.49
6:F:5:LEU:HD11	6:F:121:ILE:HD12	1.93	0.49
8:H:241:LEU:HD12	8:H:330:LYS:HG2	1.95	0.49
5:E:34:ARG:O	5:E:166:ARG:NH2	2.46	0.48
6:F:228:ILE:HG23	6:F:229:GLN:HG3	1.94	0.48
4:D:154:ARG:HE	4:D:183:ARG:NH2	2.11	0.48
8:H:267:THR:HG22	8:H:282:LEU:H	1.77	0.48
1:A:359:MET:HE2	1:A:360:ILE:HG13	1.94	0.48
3:C:235:CYS:SG	3:C:236:CYS:N	2.86	0.48
5:E:35:ASP:OD1	5:E:35:ASP:N	2.33	0.48
1:A:84:LYS:NZ	9:I:18:DA:OP1	2.40	0.48
4:D:86:ASP:OD1	4:D:86:ASP:N	2.41	0.48
8:H:136:VAL:HG13	8:H:148:TYR:HB2	1.96	0.48
1:A:273:LEU:HD23	1:A:305:ALA:HA	1.95	0.48
2:B:117:ASP:OD1	2:B:117:ASP:N	2.35	0.48
6:F:18:LEU:HD22	6:F:444:LEU:HD23	1.96	0.48
6:F:51:SER:CB	6:F:54:SER:HB3	2.43	0.48
6:F:36:ARG:HB3	6:F:43:THR:HB	1.96	0.48
2:B:310:ALA:HB1	3:C:300:LEU:HD13	1.96	0.47
4:D:203:PHE:O	4:D:207:GLN:HG2	2.14	0.47
2:B:175:LEU:HD22	2:B:209:LEU:HD22	1.96	0.47
8:H:349:ILE:HD11	8:H:362:MET:HG2	1.96	0.47
11:K:7:DT:H2''	11:K:8:DA:C8	2.49	0.47
4:D:297:ALA:HB2	4:D:339:GLU:HB3	1.97	0.47
3:C:21:PRO:HD3	12:C:401:AGS:H2'	1.95	0.47
4:D:264:PRO:HD2	4:D:267:ILE:HD12	1.97	0.47
5:E:36:LEU:HD11	5:E:39:LEU:HD11	1.97	0.47
6:F:265:MET:HG3	6:F:407:GLU:HG2	1.95	0.47
1:A:543:ILE:HG22	5:E:262:VAL:HG21	1.96	0.47
5:E:34:ARG:NH1	5:E:131:LEU:HB3	2.30	0.47
11:K:1:DG:H2''	11:K:2:DA:H8	1.79	0.47
3:C:78:MET:HE2	3:C:78:MET:HA	1.96	0.46
4:D:95:LEU:HB2	4:D:139:LEU:HD23	1.97	0.46
8:H:248:VAL:HG23	8:H:249:THR:HG23	1.97	0.46
4:D:28:VAL:O	12:D:401:AGS:O3'	2.30	0.46
10:J:11:DG:H2''	10:J:12:DG:C8	2.51	0.46
2:B:78:LEU:HB2	2:B:113:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:LYS:HE3	2:B:100:LYS:HB3	1.85	0.46
3:C:156:ALA:O	3:C:160:ARG:HG2	2.15	0.46
6:F:103:VAL:HG11	6:F:158:ILE:HG21	1.98	0.46
5:E:229:ASN:HB3	5:E:232:VAL:HB	1.97	0.46
2:B:232:HIS:ND1	2:B:233:PRO:HD3	2.31	0.46
4:D:239:SER:O	4:D:243:GLN:HG2	2.16	0.46
6:F:19:LEU:O	6:F:23:ILE:HG12	2.16	0.46
1:A:89:GLN:HG2	1:A:122:LEU:HD11	1.98	0.45
6:F:413:LYS:O	6:F:417:VAL:HG22	2.16	0.45
10:J:14:DT:H2"	10:J:15:DA:C8	2.51	0.45
1:A:214:PRO:HG2	1:A:215:LEU:HD23	1.98	0.45
1:A:350:SER:HA	11:K:1:DG:H5"	1.98	0.45
8:H:258:VAL:HG23	8:H:296:TYR:HE2	1.81	0.45
10:J:16:DT:H2"	10:J:17:DA:C8	2.52	0.45
3:C:292:ASN:HD22	3:C:333:ASN:HB3	1.81	0.45
2:B:69:ARG:H	2:B:69:ARG:HD2	1.82	0.45
4:D:154:ARG:HB3	4:D:183:ARG:CZ	2.47	0.45
4:D:229:ARG:HD2	5:E:184:ARG:HA	1.98	0.45
7:G:145:LEU:HD21	7:G:311:LEU:HG	1.99	0.45
8:H:252:VAL:HB	8:H:326:LEU:HD13	1.97	0.45
3:C:140:ASN:OD1	3:C:140:ASN:N	2.49	0.45
8:H:253:LYS:HB3	8:H:264:THR:HG23	1.97	0.45
4:D:106:VAL:HG21	4:D:149:ALA:HB1	1.99	0.45
5:E:113:LEU:HD13	5:E:154:LEU:HD21	1.98	0.45
1:A:447:TRP:O	1:A:451:LYS:HG3	2.17	0.45
3:C:63:ILE:HG21	3:C:146:LEU:HD11	1.99	0.44
4:D:196:ASN:N	4:D:196:ASN:OD1	2.50	0.44
4:D:224:SER:OG	4:D:227:ASP:O	2.32	0.44
5:E:272:LYS:HB3	5:E:272:LYS:HE3	1.77	0.44
4:D:44:HIS:NE2	4:D:188:ARG:O	2.34	0.44
7:G:182:ALA:HB3	7:G:233:VAL:HG22	1.98	0.44
5:E:346:ILE:O	5:E:350:MET:HG3	2.17	0.44
8:H:261:LEU:HB3	8:H:293:LEU:HD21	1.98	0.44
8:H:330:LYS:O	8:H:334:THR:HG22	2.16	0.44
1:A:110:PRO:HG2	1:A:267:PRO:HG3	2.00	0.44
3:C:60:THR:HA	3:C:63:ILE:HG22	2.00	0.44
8:H:353:PHE:HB3	8:H:360:ILE:HG13	2.00	0.44
7:G:9:ASN:N	7:G:9:ASN:HD22	2.14	0.44
4:D:194:ALA:HA	4:D:221:LEU:HD13	1.98	0.44
7:G:183:LYS:HB2	7:G:232:ALA:HB2	1.98	0.44
8:H:18:ARG:HG3	8:H:335:ILE:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:16:DG:H2''	9:I:17:DA:C8	2.52	0.44
2:B:82:ASP:OD1	3:C:98:LYS:NZ	2.51	0.44
6:F:57:ASN:HA	6:F:60:ILE:HD13	2.00	0.44
6:F:232:MET:N	6:F:232:MET:SD	2.91	0.44
6:F:234:LYS:HB3	6:F:301:ASP:HB2	2.00	0.44
10:J:10:DC:H2''	10:J:11:DG:C8	2.53	0.44
1:A:345:LYS:HG2	11:K:1:DG:H5'	2.00	0.43
5:E:215:THR:O	5:E:218:ILE:HD12	2.17	0.43
6:F:4:LYS:HG3	6:F:122:LYS:HG2	2.00	0.43
6:F:225:ILE:HG21	6:F:439:VAL:HG21	1.99	0.43
8:H:238:LYS:HD2	8:H:337:PRO:HG3	2.00	0.43
5:E:81:ARG:NH1	5:E:82:LYS:O	2.51	0.43
7:G:34:LYS:HB3	7:G:34:LYS:HE2	1.82	0.43
2:B:202:MET:HG2	12:B:401:AGS:C4	2.47	0.43
3:C:34:ILE:HA	3:C:37:VAL:HG22	2.00	0.43
3:C:212:LEU:HD23	3:C:212:LEU:HA	1.92	0.43
6:F:32:THR:HA	6:F:96:ASN:HA	1.99	0.43
6:F:162:GLU:HG3	6:F:201:ILE:HB	2.00	0.43
8:H:114:LYS:HB3	8:H:114:LYS:HE3	1.88	0.43
3:C:128:ASN:HA	3:C:131:ARG:HD3	2.01	0.43
8:H:21:TYR:O	8:H:25:THR:HG23	2.17	0.43
12:B:401:AGS:O1B	12:B:401:AGS:O2G	2.36	0.43
5:E:69:LYS:NZ	6:F:56:ASN:O	2.48	0.43
9:I:13:DT:H2''	9:I:14:DA:C8	2.53	0.43
5:E:271:VAL:O	5:E:274:ARG:NH1	2.51	0.43
3:C:276:ASP:OD1	3:C:277:LEU:N	2.52	0.43
4:D:302:ASN:O	4:D:306:GLU:HG3	2.19	0.43
8:H:348:ASN:OD1	8:H:348:ASN:N	2.51	0.43
5:E:5:VAL:O	14:E:500:ADP:O3'	2.30	0.43
7:G:210:ASN:OD1	7:G:212:SER:OG	2.20	0.43
1:A:491:ILE:HD12	5:E:238:GLU:HG2	2.00	0.42
8:H:22:VAL:HG22	8:H:331:ASN:HB3	2.00	0.42
8:H:272:GLY:N	8:H:276:ASP:O	2.39	0.42
1:A:66:TRP:O	1:A:70:PHE:HB2	2.19	0.42
1:A:186:ILE:HD12	1:A:221:ILE:HG12	2.00	0.42
8:H:366:LYS:HB2	8:H:369:VAL:HB	2.02	0.42
2:B:299:ILE:HD13	2:B:304:GLY:HA2	2.00	0.42
5:E:39:LEU:HD22	5:E:188:ILE:HD11	2.01	0.42
6:F:7:VAL:HG22	6:F:77:PHE:HD1	1.84	0.42
3:C:122:MET:HB3	3:C:127:GLN:HE21	1.83	0.42
1:A:403:CYS:SG	1:A:420:GLY:HA2	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:LYS:HD3	8:H:154:PRO:HD2	2.02	0.42
6:F:283:ILE:O	6:F:294:ILE:N	2.47	0.42
8:H:230:ILE:HB	8:H:351:LEU:HB2	2.01	0.42
1:A:95:MET:HE3	1:A:95:MET:HB3	1.91	0.42
2:B:287:GLU:O	2:B:291:GLU:HG2	2.20	0.42
3:C:322:ALA:HB2	4:D:327:PHE:HB2	2.01	0.42
5:E:87:VAL:HG21	5:E:112:LEU:HD11	2.02	0.42
6:F:234:LYS:HB2	6:F:303:VAL:HG13	2.02	0.42
7:G:208:PRO:HD3	8:H:144:ILE:HG12	2.01	0.42
1:A:69:LYS:HG3	1:A:70:PHE:CD2	2.54	0.42
1:A:176:LEU:HD12	1:A:184:ILE:HD11	2.02	0.42
1:A:400:ILE:HG23	1:A:424:VAL:HG22	2.02	0.42
6:F:279:VAL:HG23	6:F:300:LEU:HD23	2.02	0.42
6:F:417:VAL:HG21	6:F:466:TYR:HE2	1.84	0.42
5:E:25:PHE:HZ	5:E:186:LEU:HD21	1.85	0.42
7:G:206:LYS:HE3	7:G:206:LYS:HB3	1.87	0.42
3:C:275:ILE:HD12	3:C:275:ILE:HA	1.92	0.41
4:D:155:ARG:NH1	4:D:158:GLU:OE1	2.54	0.41
5:E:298:ILE:O	5:E:302:GLU:HG2	2.20	0.41
8:H:22:VAL:HG11	8:H:335:ILE:HD11	2.01	0.41
8:H:236:LEU:HA	8:H:239:ASN:HD21	1.85	0.41
1:A:277:LEU:HD22	1:A:318:LEU:HD22	2.02	0.41
2:B:28:GLU:H	2:B:28:GLU:HG3	1.71	0.41
1:A:91:ALA:O	1:A:95:MET:HG3	2.20	0.41
4:D:220:ILE:HG23	4:D:234:LEU:HD23	2.02	0.41
5:E:46:GLY:HA3	5:E:229:ASN:OD1	2.21	0.41
9:I:34:DT:H2"	9:I:35:DA:C8	2.56	0.41
2:B:20:LEU:HD23	2:B:23:ILE:HD12	2.02	0.41
1:A:456:PHE:CD2	1:A:540:GLY:HA3	2.56	0.41
2:B:232:HIS:CG	2:B:233:PRO:HD3	2.55	0.41
3:C:54:PRO:HG2	3:C:168:PRO:HG3	2.03	0.41
2:B:277:LEU:HA	2:B:277:LEU:HD12	1.84	0.41
3:C:248:LEU:HD13	3:C:281:ILE:HG23	2.03	0.41
4:D:64:TYR:HE1	4:D:186:LYS:HB3	1.86	0.41
5:E:136:LYS:NZ	6:F:60:ILE:HG23	2.34	0.41
5:E:287:TYR:CZ	5:E:339:ILE:HG12	2.55	0.41
6:F:6:ILE:HD12	6:F:79:LEU:HD21	2.02	0.41
6:F:231:MET:HE3	6:F:406:HIS:HE1	1.85	0.41
9:I:16:DG:H2"	9:I:17:DA:H8	1.85	0.41
1:A:426:LYS:HB3	1:A:426:LYS:HE3	1.84	0.41
3:C:16:VAL:HG23	3:C:17:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:19:TYR:HB3	3:C:177:ARG:HH21	1.86	0.41
5:E:236:MET:O	5:E:240:MET:HG3	2.19	0.41
7:G:28:LEU:HD11	7:G:48:PHE:HB2	2.03	0.41
3:C:215:CYS:SG	3:C:232:ILE:HG12	2.60	0.40
5:E:154:LEU:O	5:E:158:MET:HG2	2.20	0.40
5:E:210:ARG:HD3	5:E:210:ARG:HA	1.94	0.40
8:H:256:ILE:HD13	8:H:261:LEU:HD12	2.02	0.40
4:D:96:ASN:OD1	4:D:96:ASN:N	2.53	0.40
7:G:14:SER:OG	7:G:105:GLU:OE2	2.37	0.40
5:E:163:LYS:HE2	5:E:163:LYS:HB2	1.83	0.40
6:F:211:LEU:HD23	6:F:211:LEU:HA	1.95	0.40
6:F:466:TYR:HD1	6:F:467:TYR:N	2.19	0.40
7:G:104:VAL:HG22	7:G:123:ASP:OD1	2.21	0.40
11:K:3:DT:H2'	11:K:4:DT:H71	2.03	0.40
3:C:138:THR:O	3:C:142:ARG:NH1	2.55	0.40
4:D:353:LEU:HD12	4:D:353:LEU:HA	1.94	0.40
7:G:88:HIS:O	7:G:92:SER:OG	2.27	0.40
8:H:358:ASP:OD1	8:H:358:ASP:N	2.54	0.40
8:H:362:MET:HE3	8:H:362:MET:HB2	2.01	0.40
1:A:433:LYS:H	1:A:436:HIS:CE1	2.40	0.40
2:B:35:GLN:HA	2:B:38:LYS:HG2	2.02	0.40
2:B:66:LEU:HD12	2:B:66:LEU:HA	1.96	0.40
2:B:253:ARG:O	2:B:258:LYS:HG2	2.21	0.40
7:G:192:PHE:HD2	7:G:207:LEU:HD23	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	429/545 (79%)	411 (96%)	18 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	315/323 (98%)	307 (98%)	8 (2%)	0	100	100
3	C	325/336 (97%)	321 (99%)	4 (1%)	0	100	100
4	D	328/353 (93%)	323 (98%)	5 (2%)	0	100	100
5	E	351/354 (99%)	334 (95%)	17 (5%)	0	100	100
6	F	280/474 (59%)	265 (95%)	15 (5%)	0	100	100
7	G	289/401 (72%)	271 (94%)	18 (6%)	0	100	100
8	H	258/612 (42%)	250 (97%)	8 (3%)	0	100	100
All	All	2575/3398 (76%)	2482 (96%)	93 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	402/504 (80%)	397 (99%)	5 (1%)	63	78
2	B	278/283 (98%)	273 (98%)	5 (2%)	51	71
3	C	284/293 (97%)	278 (98%)	6 (2%)	47	67
4	D	294/312 (94%)	294 (100%)	0	100	100
5	E	323/324 (100%)	318 (98%)	5 (2%)	57	74
6	F	267/424 (63%)	260 (97%)	7 (3%)	40	63
7	G	267/369 (72%)	261 (98%)	6 (2%)	45	67
8	H	255/560 (46%)	246 (96%)	9 (4%)	32	56
All	All	2370/3069 (77%)	2327 (98%)	43 (2%)	51	71

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	GLU
1	A	126	LEU

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Mol	Chain	Res	Type
1	A	187	GLU
1	A	197	THR
1	A	471	TYR
2	B	137	SER
2	B	138	THR
2	B	184	VAL
2	B	211	SER
2	B	228	VAL
3	C	25	ASP
3	C	120	ASP
3	C	186	LYS
3	C	235	CYS
3	C	250	SER
3	C	256	TRP
5	E	18	HIS
5	E	19	ASN
5	E	230	LEU
5	E	332	LEU
5	E	352	CYS
6	F	52	LEU
6	F	59	THR
6	F	79	LEU
6	F	200	VAL
6	F	297	ASN
6	F	405	THR
6	F	470	ARG
7	G	122	GLU
7	G	145	LEU
7	G	196	SER
7	G	202	PHE
7	G	218	GLN
7	G	270	LEU
8	H	2	SER
8	H	35	THR
8	H	63	GLU
8	H	65	GLU
8	H	120	VAL
8	H	125	THR
8	H	136	VAL
8	H	252	VAL
8	H	264	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	132	GLN
1	A	207	GLN
1	A	234	ASN
1	A	411	ASN
1	A	475	HIS
1	A	495	GLN
2	B	102	HIS
2	B	204	GLN
3	C	105	GLN
3	C	221	ASN
4	D	42	GLN
4	D	171	ASN
4	D	255	GLN
4	D	334	ASN
4	D	338	ASN
5	E	14	ASN
5	E	336	ASN
7	G	52	ASN
7	G	164	HIS
8	H	14	ASN
8	H	27	GLN
8	H	45	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
12	AGS	C	401	13	32,33,33	0.46	1 (3%)	45,52,52	0.65	1 (2%)
12	AGS	D	401	13	32,33,33	0.46	1 (3%)	45,52,52	0.66	1 (2%)
14	ADP	E	500	-	28,29,29	1.42	4 (14%)	43,45,45	1.84	10 (23%)
12	AGS	A	601	13	32,33,33	0.52	1 (3%)	45,52,52	0.67	1 (2%)
12	AGS	B	401	13	32,33,33	0.46	1 (3%)	45,52,52	0.65	1 (2%)

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
12	AGS	C	401	13	-	1/21/38/38	0/3/3/3
12	AGS	D	401	13	-	2/21/38/38	0/3/3/3
14	ADP	E	500	-	-	5/16/32/32	0/3/3/3
12	AGS	A	601	13	-	6/21/38/38	0/3/3/3
12	AGS	B	401	13	-	7/21/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	E	500	ADP	C5-C4	4.69	1.47	1.39
14	E	500	ADP	C5-C6	2.76	1.48	1.41
14	E	500	ADP	C8-N7	2.36	1.36	1.31
14	E	500	ADP	C5-N7	-2.25	1.35	1.39
12	A	601	AGS	PG-S1G	2.14	1.95	1.90
12	B	401	AGS	PG-S1G	2.13	1.95	1.90
12	D	401	AGS	PG-S1G	2.09	1.95	1.90
12	C	401	AGS	PG-S1G	2.08	1.95	1.90

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	E	500	ADP	C5-C4-N3	-5.79	118.75	126.72
14	E	500	ADP	N3-C4-N9	4.57	134.95	127.17
14	E	500	ADP	C2-N3-C4	3.70	120.87	111.83
12	A	601	AGS	PB-O3B-PG	-3.63	119.90	133.17
12	D	401	AGS	PB-O3B-PG	-3.53	120.23	133.17
14	E	500	ADP	C4-C5-N7	-3.50	106.58	110.58
12	C	401	AGS	PB-O3B-PG	-3.49	120.39	133.17
12	B	401	AGS	PB-O3B-PG	-3.49	120.41	133.17
14	E	500	ADP	N3-C2-N1	-3.25	123.66	128.58
14	E	500	ADP	C4-N9-C8	2.66	108.53	105.74
14	E	500	ADP	C5-N7-C8	2.60	107.53	103.45
14	E	500	ADP	C6-C5-N7	2.14	136.21	132.09
14	E	500	ADP	C3'-C2'-C1'	2.12	105.48	101.46
14	E	500	ADP	N9-C8-N7	-2.03	111.05	113.94

There are no chirality outliers.

All (21) torsion outliers are listed below:

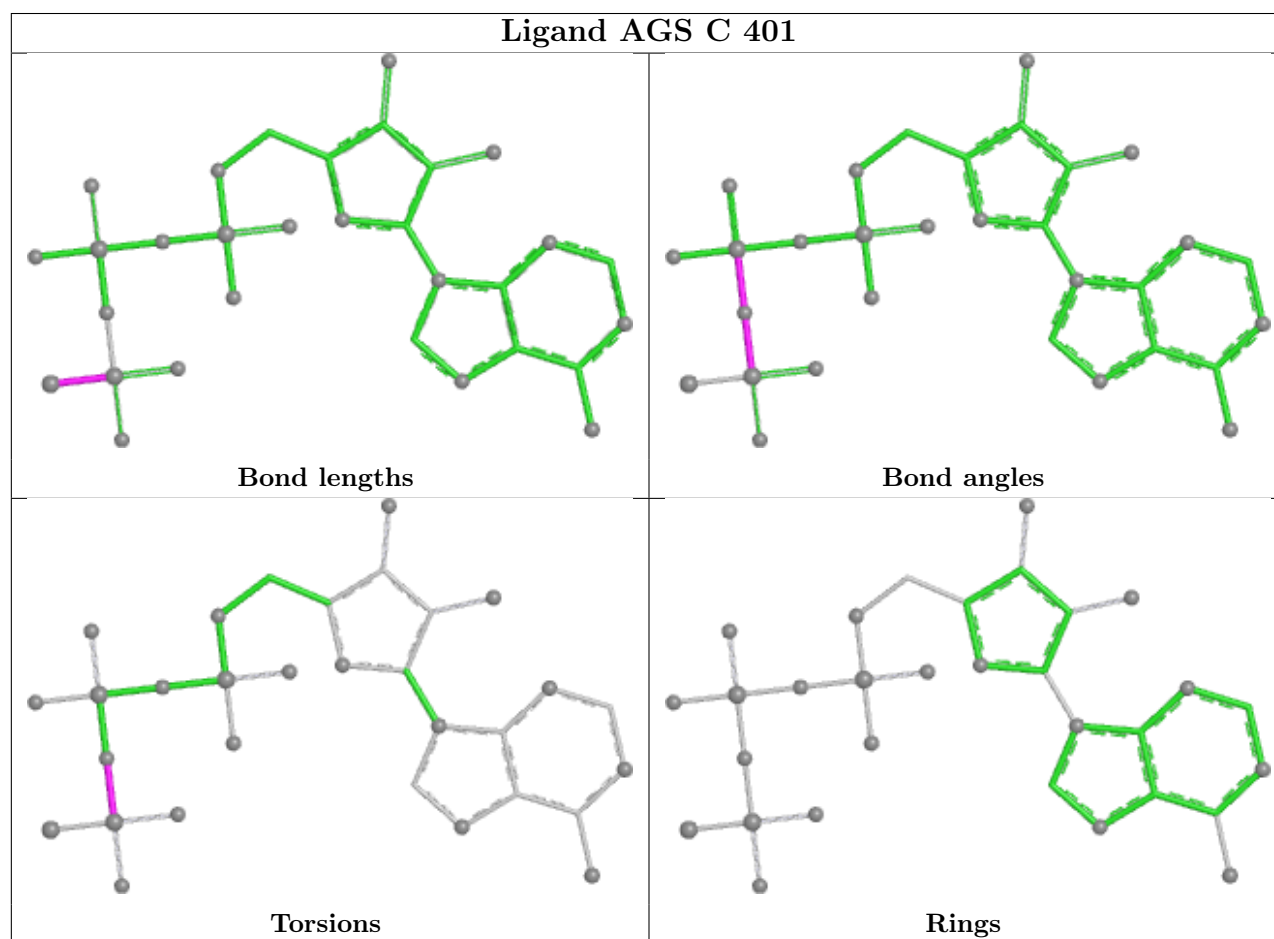
Mol	Chain	Res	Type	Atoms
12	A	601	AGS	C5'-O5'-PA-O3A
12	B	401	AGS	PB-O3B-PG-O2G
12	B	401	AGS	PB-O3B-PG-O3G
12	B	401	AGS	C5'-O5'-PA-O1A
12	B	401	AGS	C5'-O5'-PA-O3A
12	B	401	AGS	O4'-C4'-C5'-O5'
12	C	401	AGS	PB-O3B-PG-O2G
14	E	500	ADP	C5'-O5'-PA-O1A
14	E	500	ADP	C5'-O5'-PA-O2A
14	E	500	ADP	C5'-O5'-PA-O3A
12	B	401	AGS	C3'-C4'-C5'-O5'
14	E	500	ADP	O4'-C4'-C5'-O5'
14	E	500	ADP	C3'-C4'-C5'-O5'
12	A	601	AGS	C5'-O5'-PA-O1A
12	B	401	AGS	C5'-O5'-PA-O2A
12	A	601	AGS	PG-O3B-PB-O2B
12	D	401	AGS	PG-O3B-PB-O1B
12	A	601	AGS	O4'-C4'-C5'-O5'
12	A	601	AGS	PB-O3A-PA-O1A
12	A	601	AGS	PB-O3A-PA-O2A
12	D	401	AGS	PB-O3A-PA-O2A

There are no ring outliers.

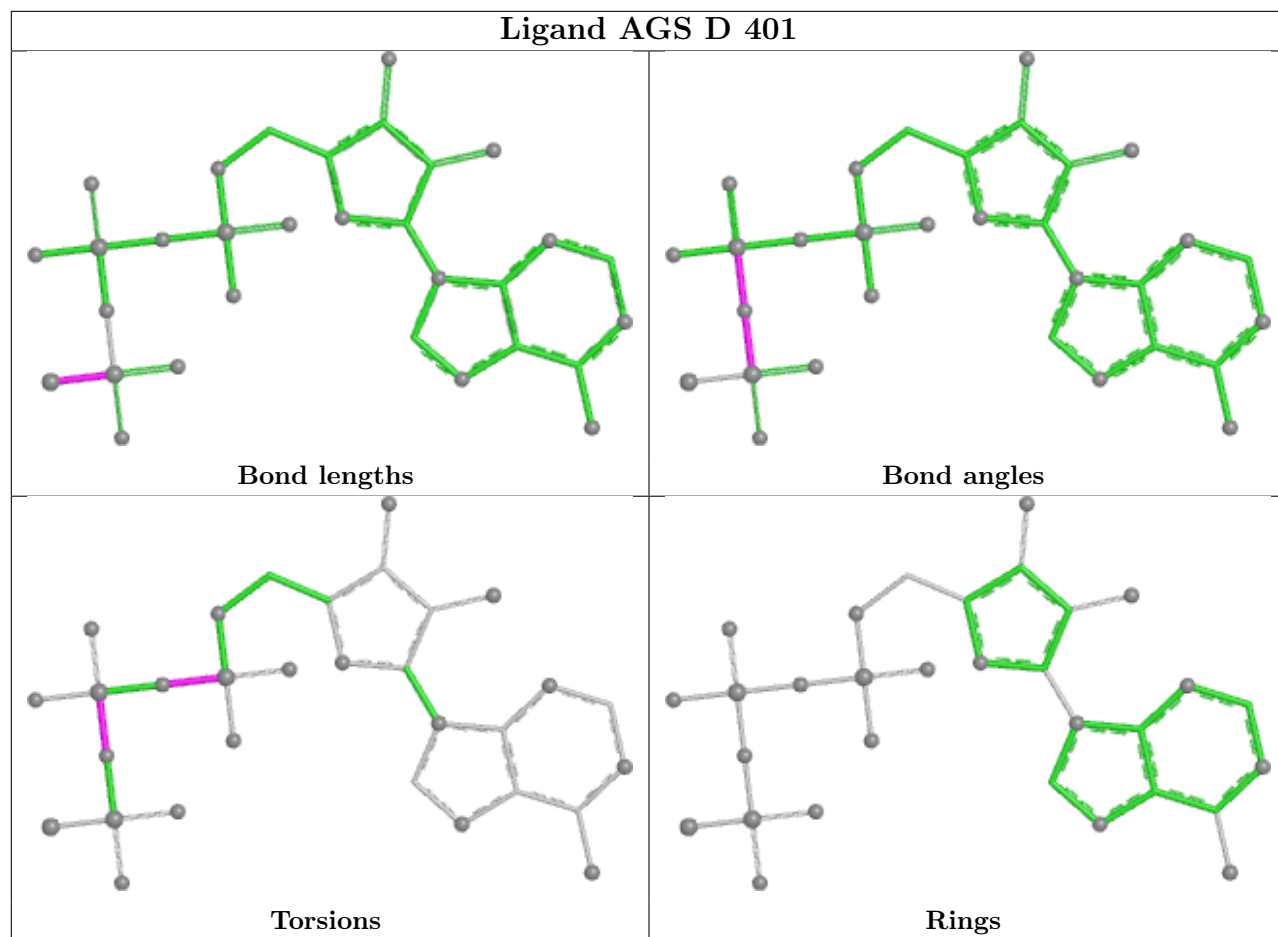
5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	401	AGS	3	0
12	D	401	AGS	3	0
14	E	500	ADP	3	0
12	A	601	AGS	1	0
12	B	401	AGS	4	0

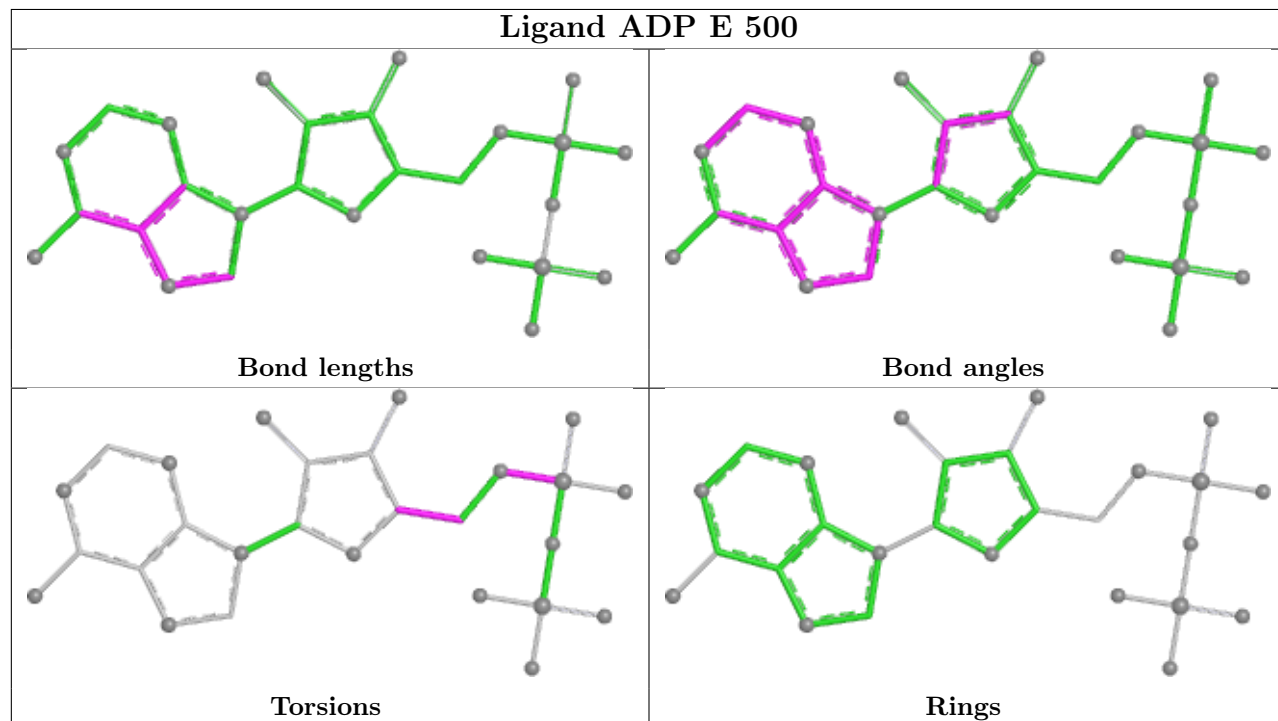
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

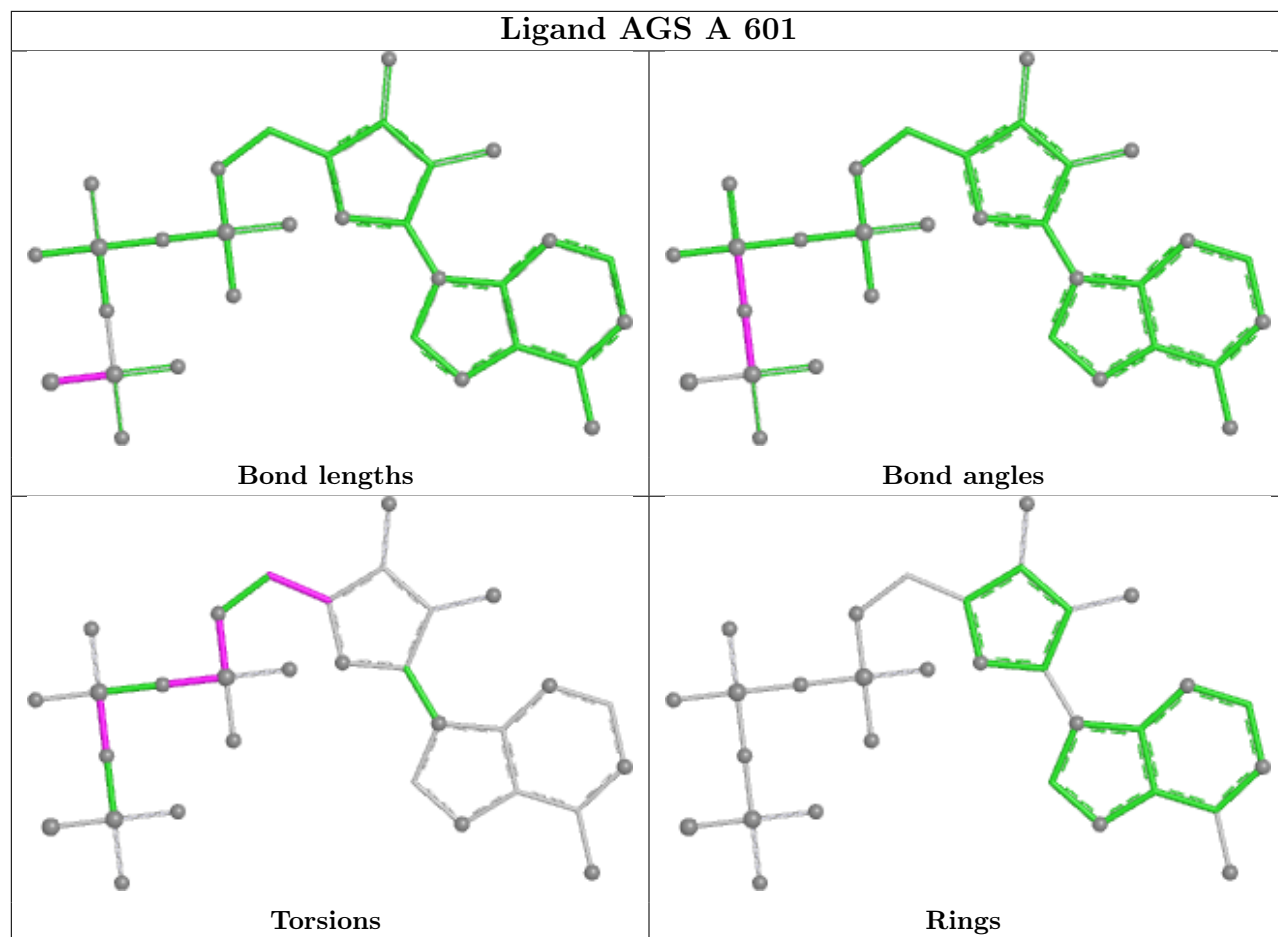


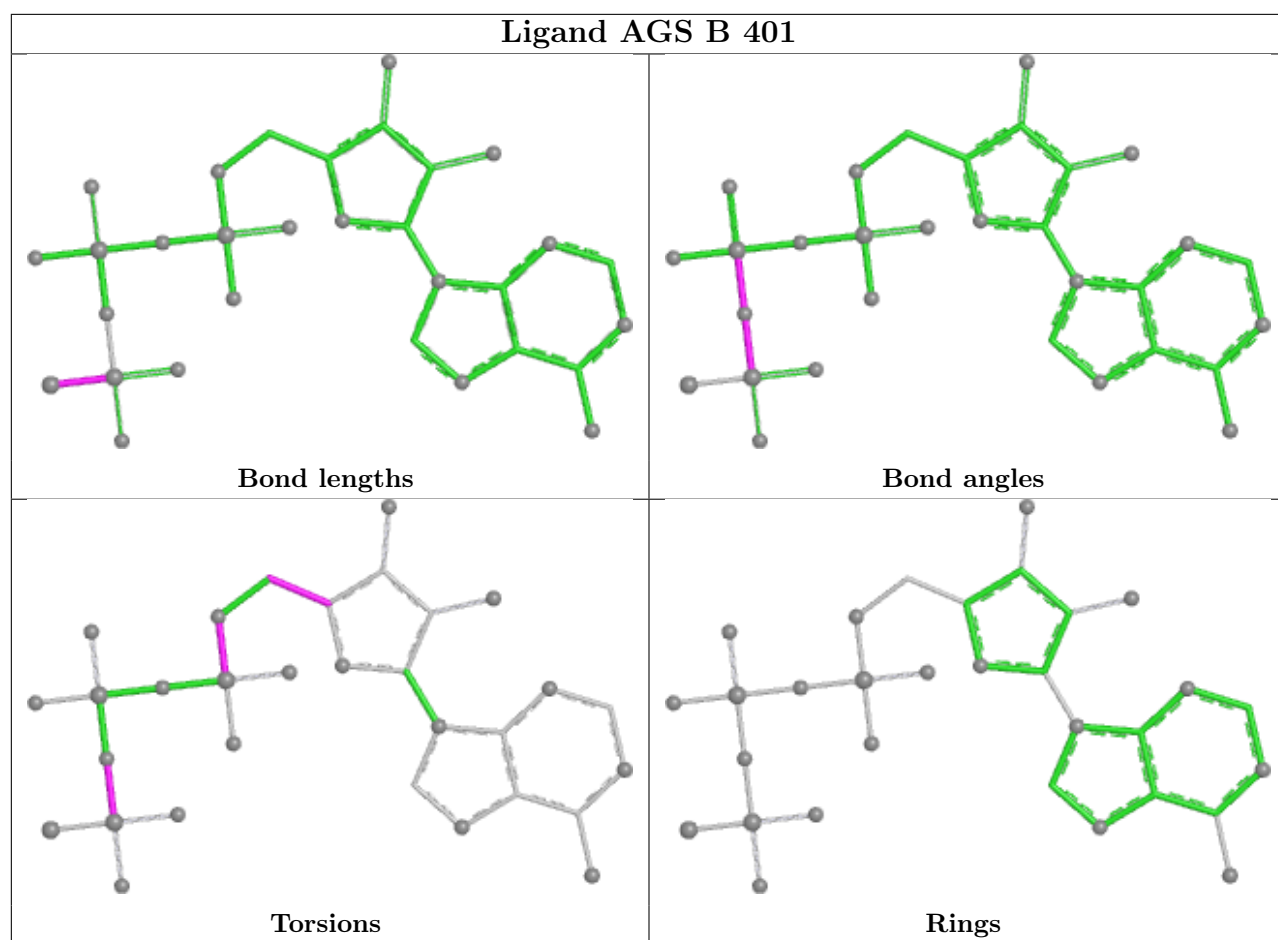
Ligand AGS D 401



Ligand ADP E 500







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

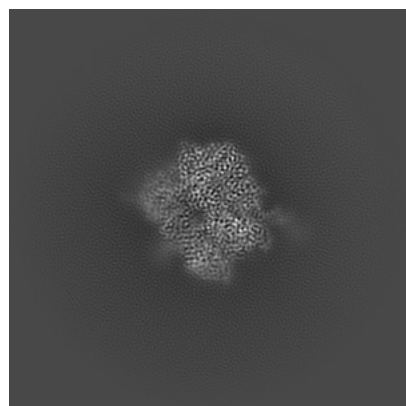
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29414. These allow visual inspection of the internal detail of the map and identification of artifacts.

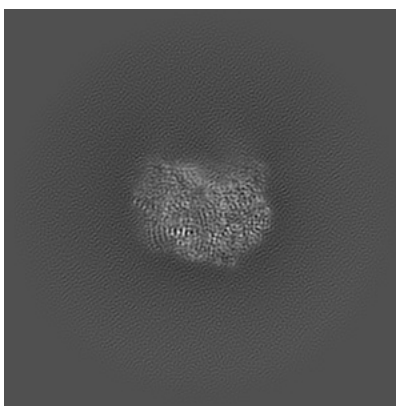
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

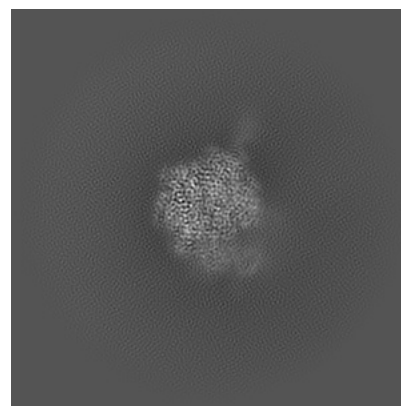
6.1.1 Primary map



X

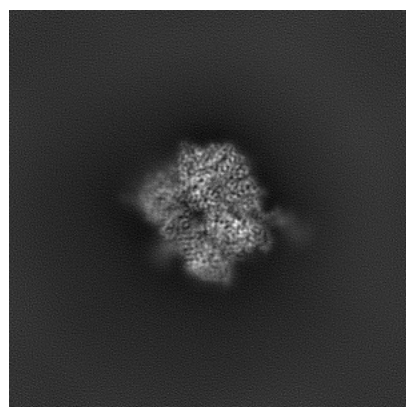


Y

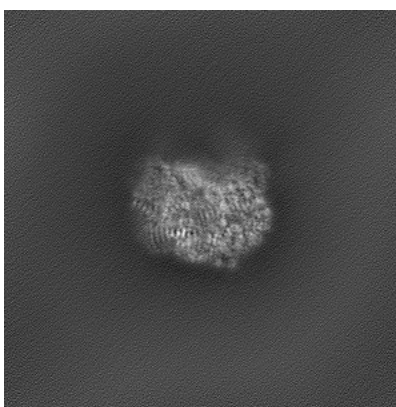


Z

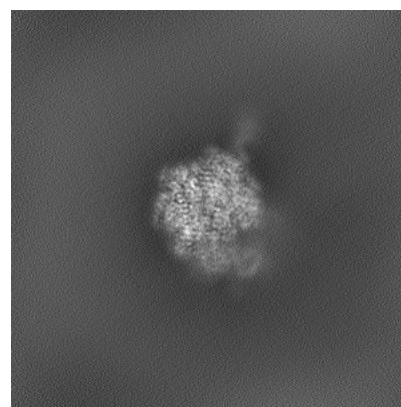
6.1.2 Raw map



X



Y

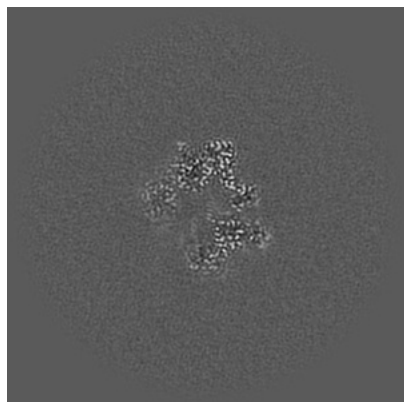


Z

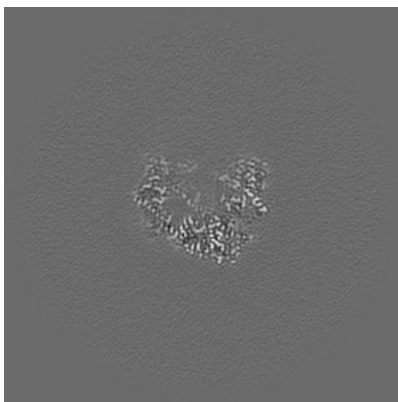
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

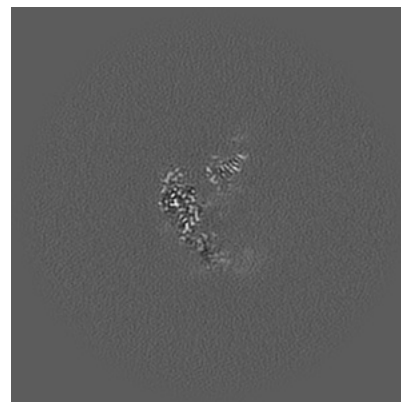
6.2.1 Primary map



X Index: 210

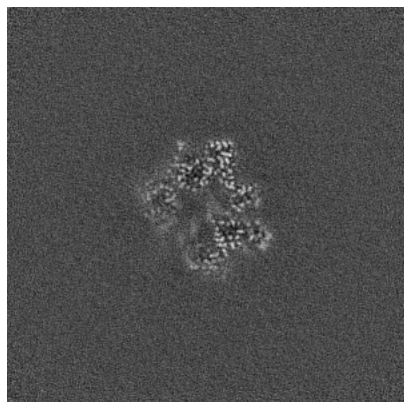


Y Index: 210

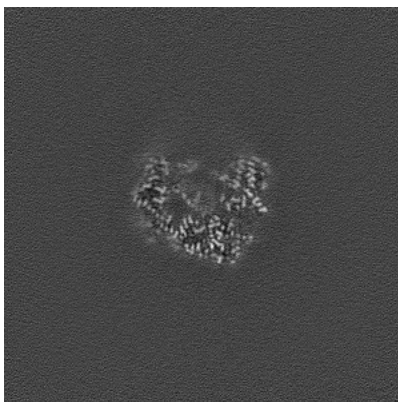


Z Index: 210

6.2.2 Raw map



X Index: 210



Y Index: 210

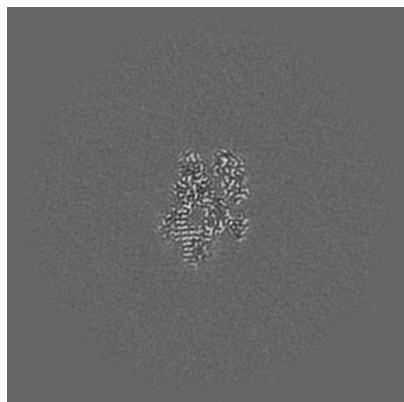


Z Index: 210

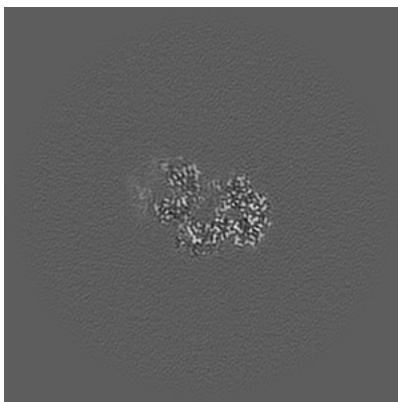
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

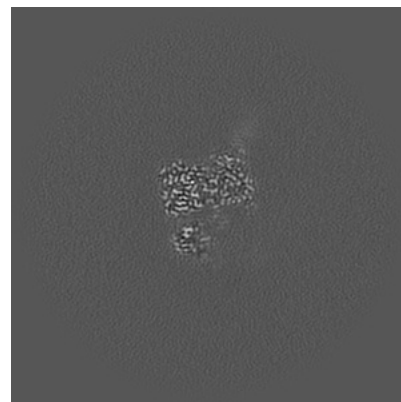
6.3.1 Primary map



X Index: 184

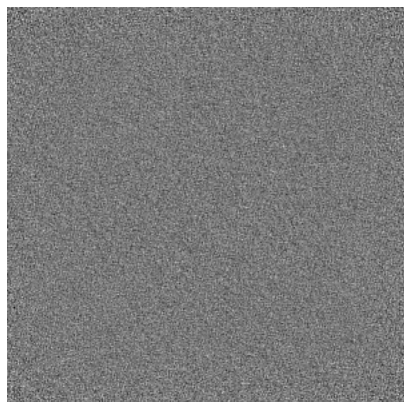


Y Index: 230

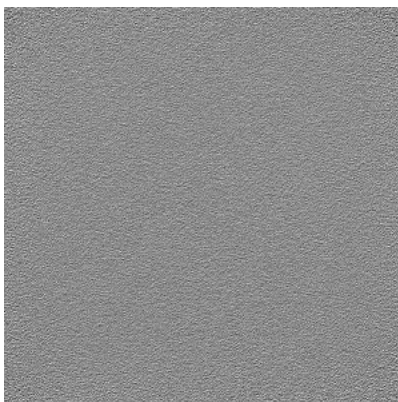


Z Index: 194

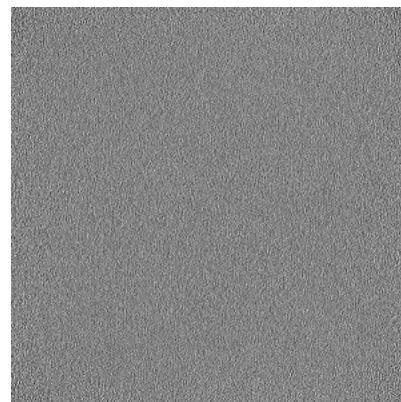
6.3.2 Raw map



X Index: 0



Y Index: 0

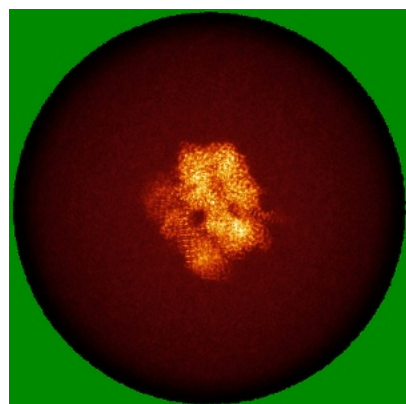


Z Index: 0

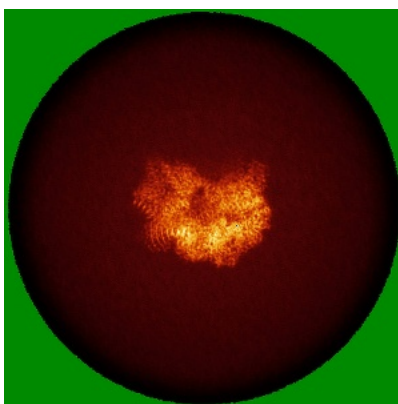
The images above show the largest variance slices of the map in three orthogonal directions.

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

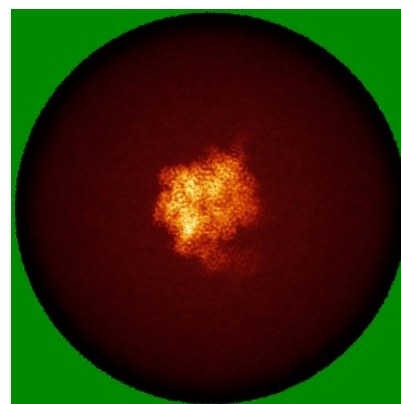
6.4.1 Primary map



X

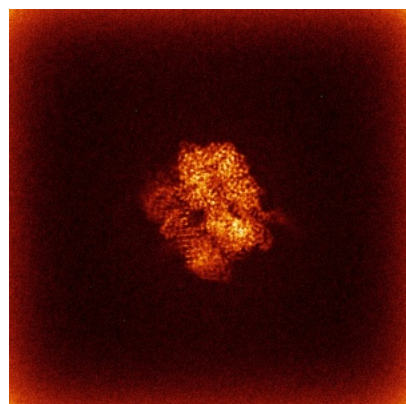


Y

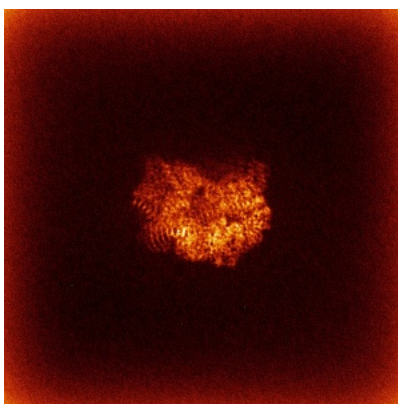


Z

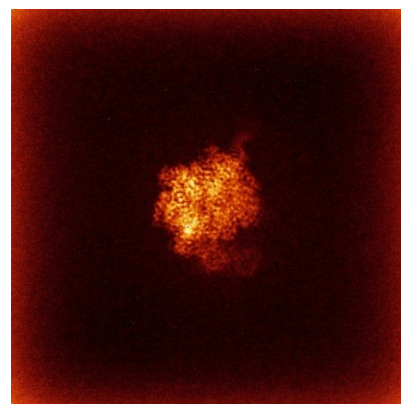
6.4.2 Raw map



X



Y

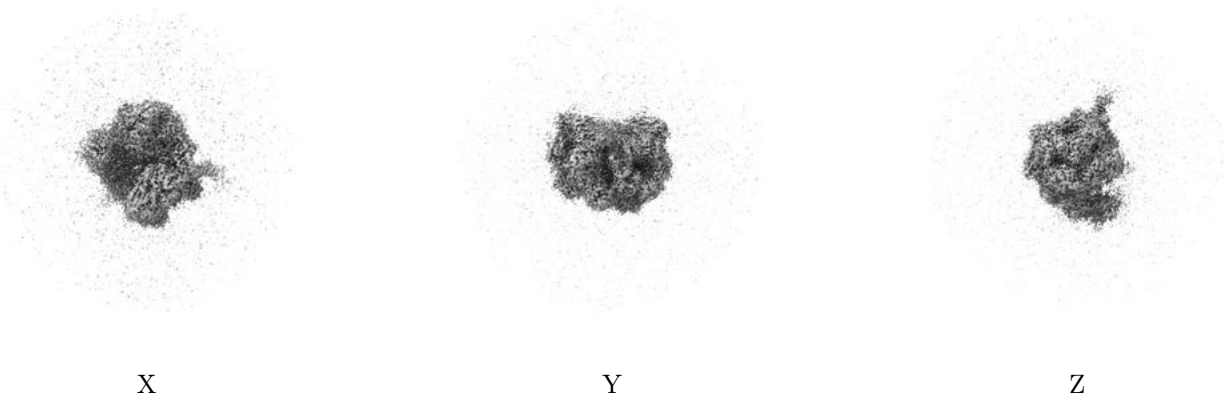


Z

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.

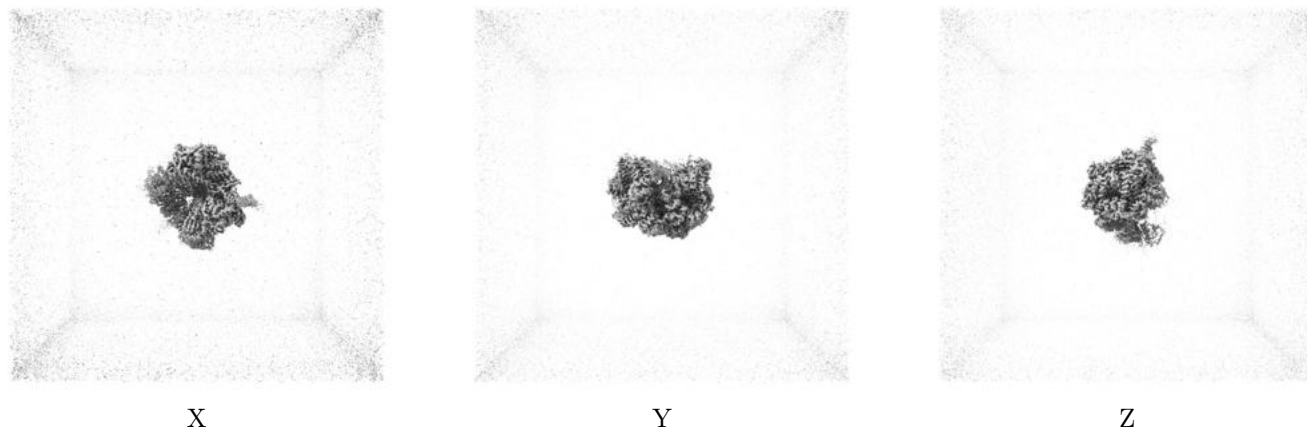
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.17. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

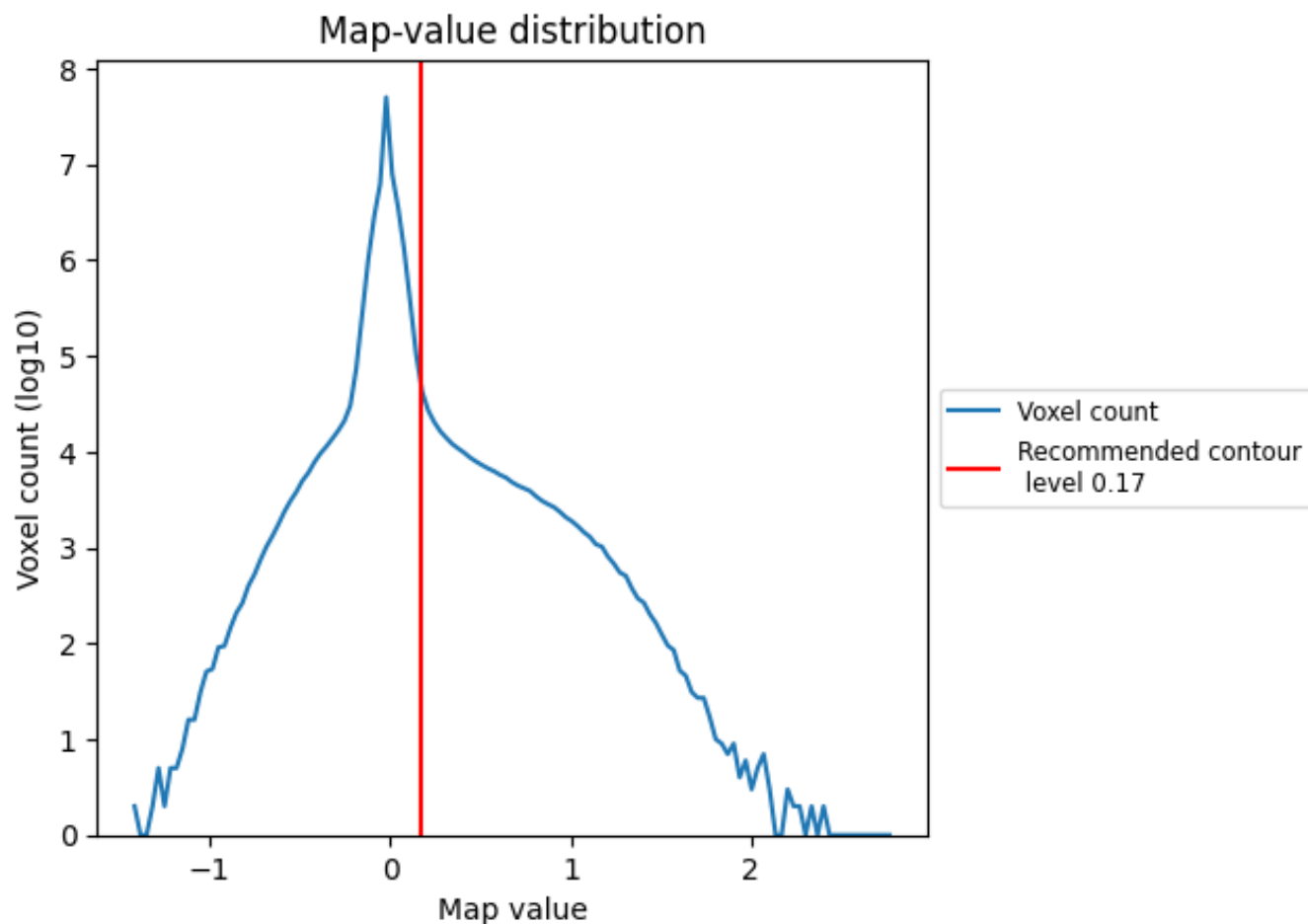
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

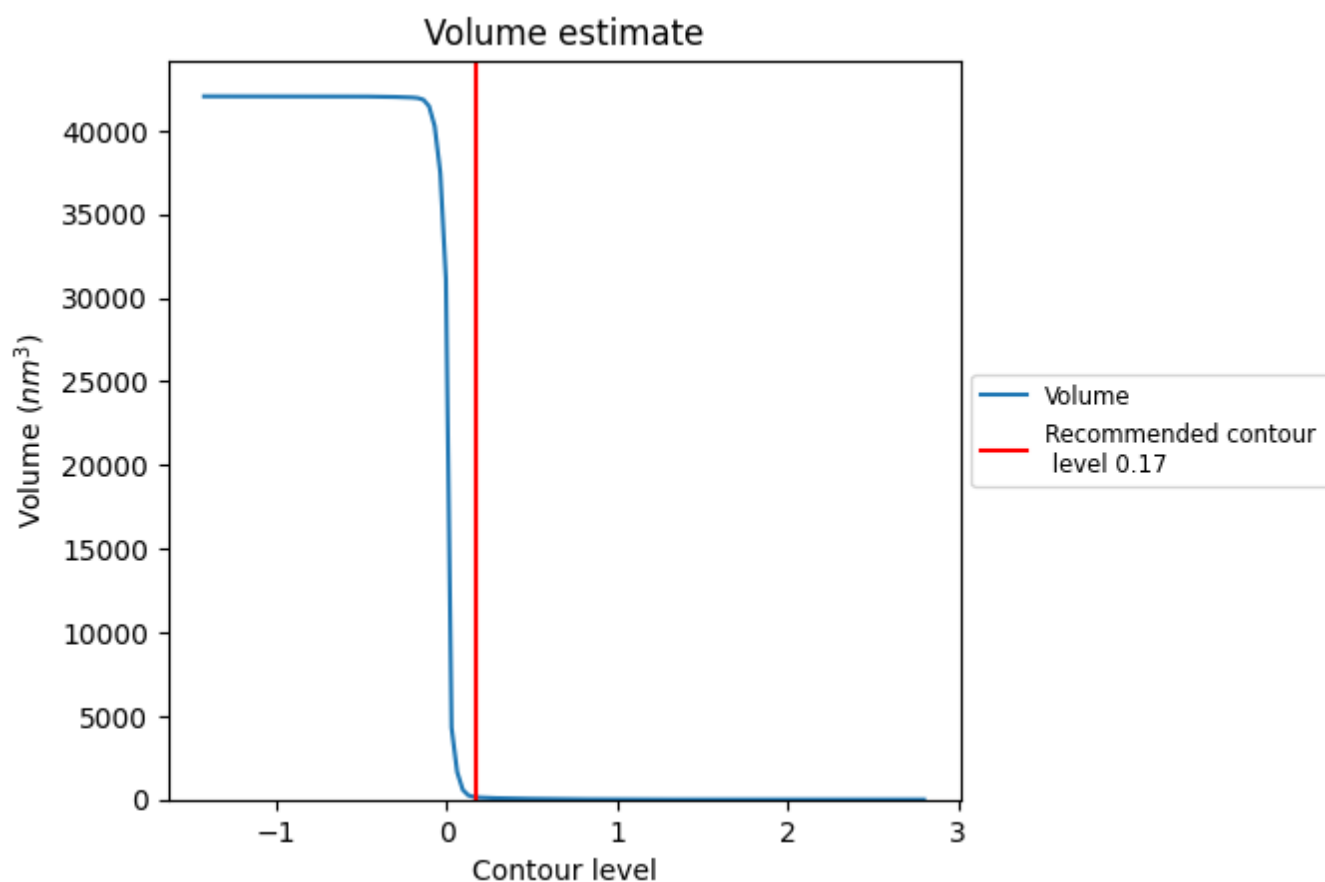
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

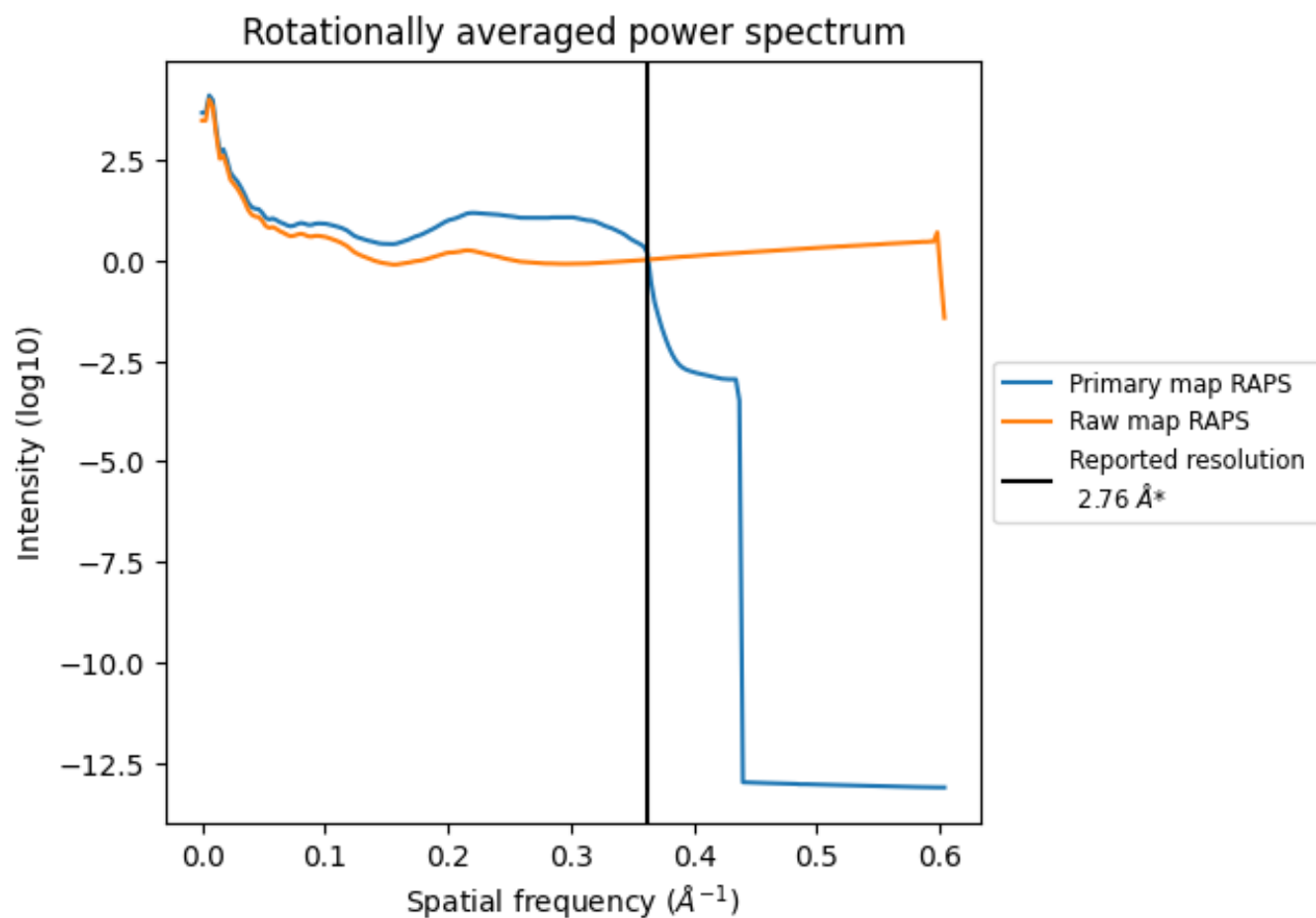
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 150 nm^3 ; this corresponds to an approximate mass of 135 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 ⓘ

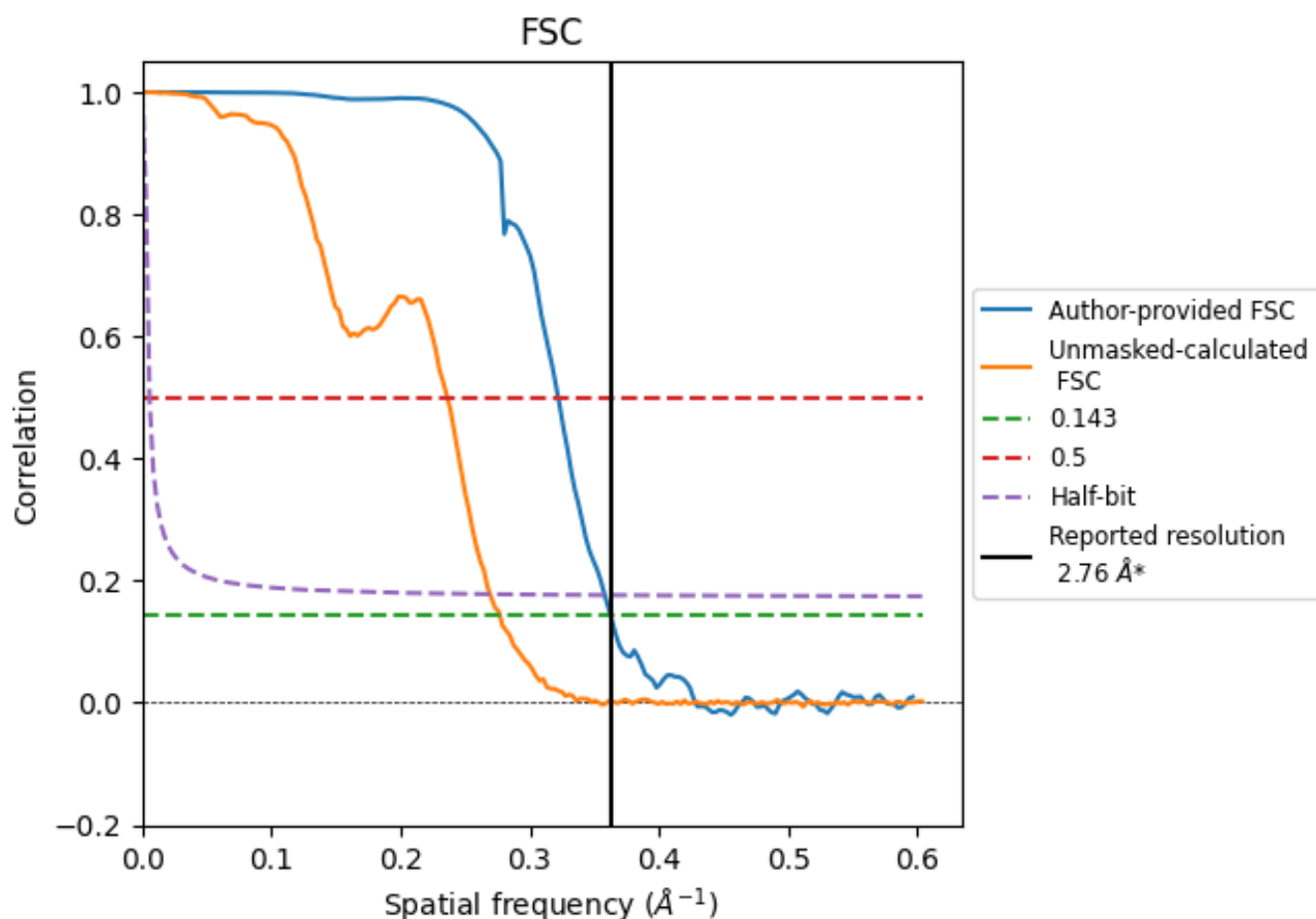


*Reported resolution corresponds to spatial frequency of 0.362 Å⁻¹

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 0.362 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

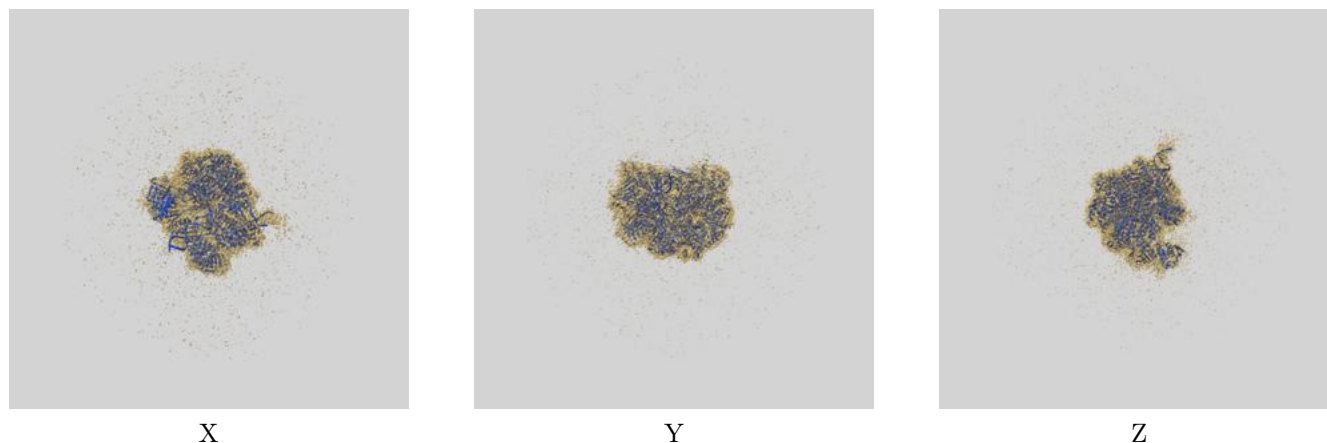
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.76	-	-
Author-provided FSC curve	2.76	3.10	2.79
Unmasked-calculated*	3.61	4.23	3.71

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.61 differs from the reported value 2.76 by more than 10 %

9 Map-model fit [i](#)

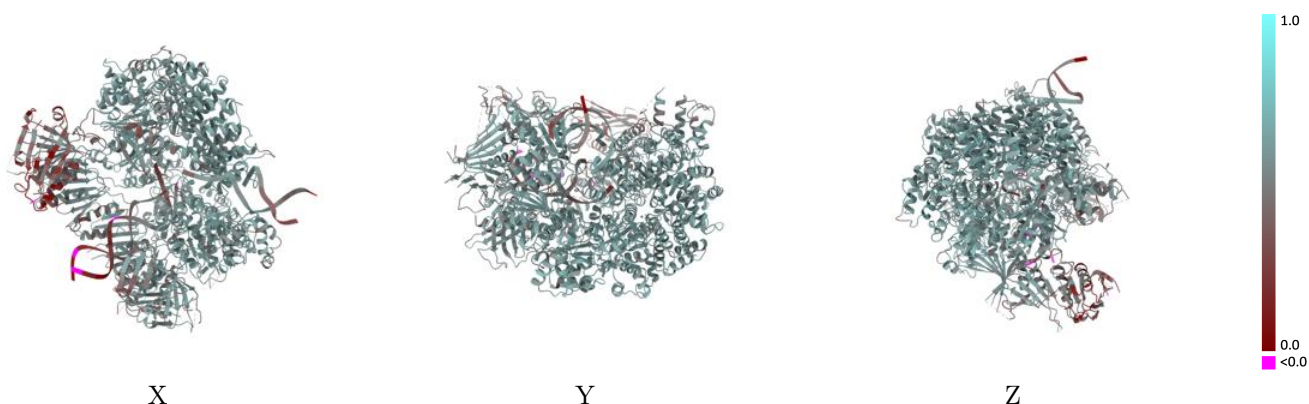
This section contains information regarding the fit between EMDB map EMD-29414 and PDB model 8FS5. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



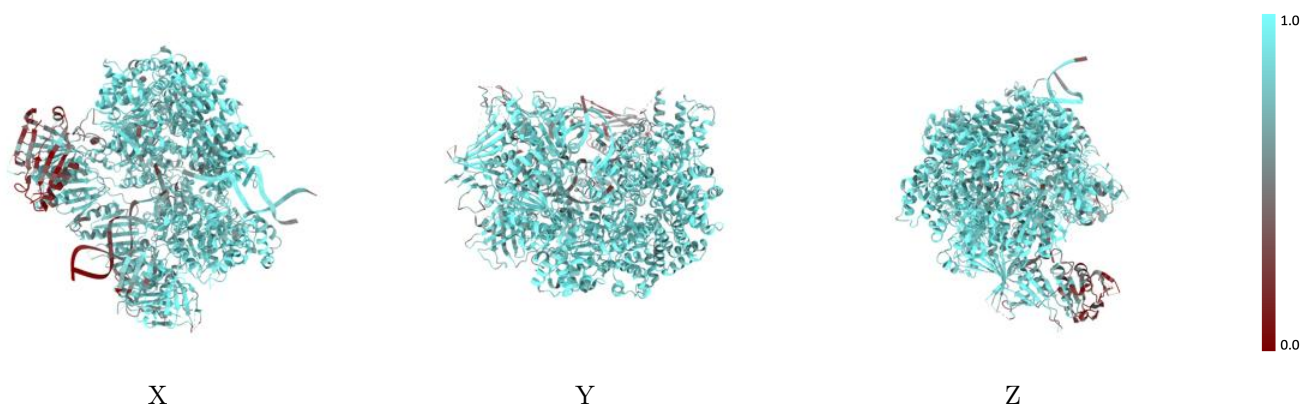
The images above show the 3D surface view of the map at the recommended contour level 0.17 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



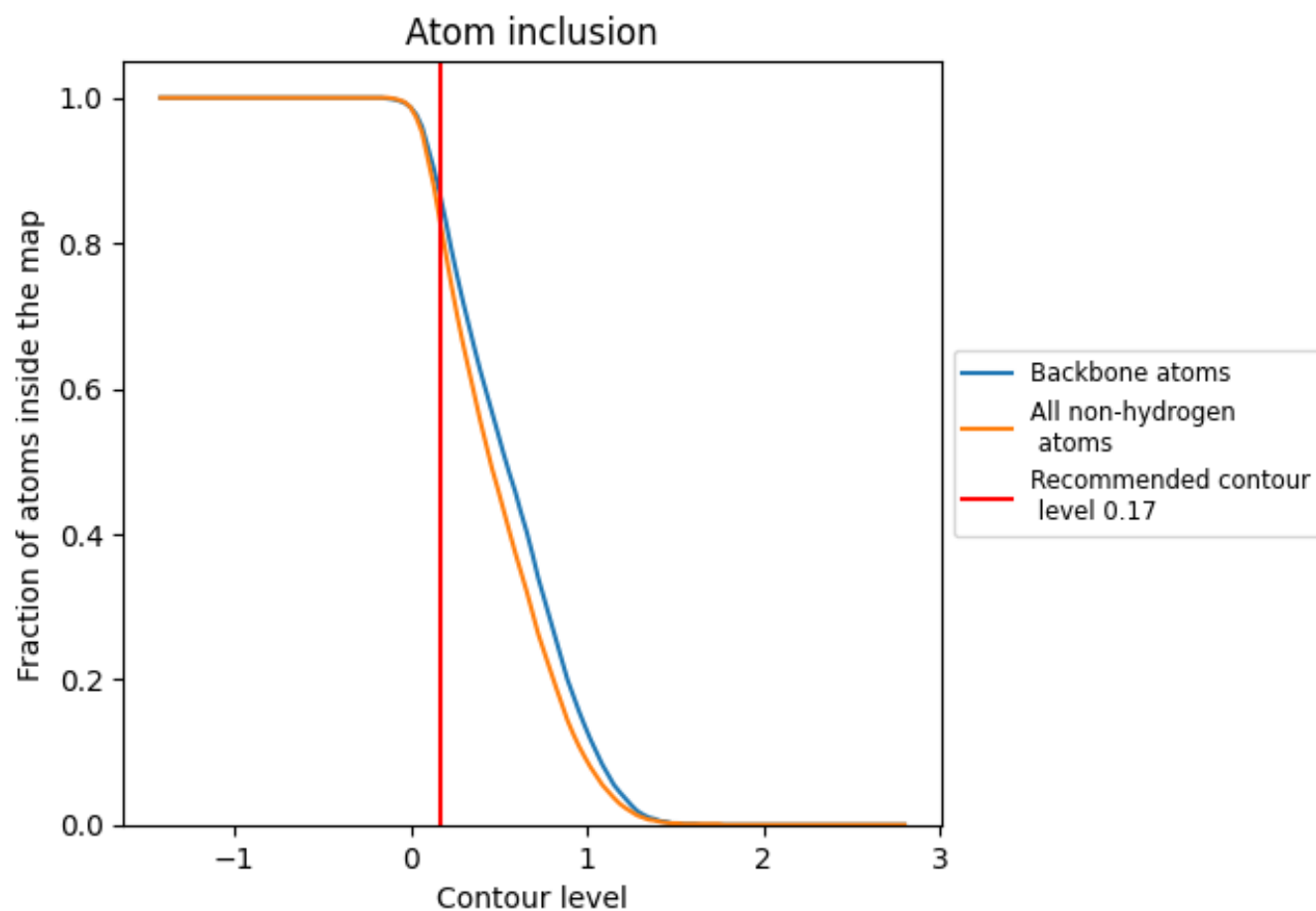
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.17).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.17) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8250	 0.5480
A	 0.8540	 0.5600
B	 0.9190	 0.5990
C	 0.9030	 0.5980
D	 0.9360	 0.6110
E	 0.8790	 0.5730
F	 0.5750	 0.4300
G	 0.8310	 0.5500
H	 0.7730	 0.5210
I	 0.5910	 0.3600
J	 0.3830	 0.3170
K	 0.8010	 0.4480

