Full wwPDB EM Validation Report (i)

Aug 5, 2026 – 07:21 AM EDT

PDB ID	:	7KC0 / pdb_00007kc0
EMDB ID	:	EMD-22803
Title	:	Structure of the Saccharomyces cerevisiae replicative polymerase delta in complex with a primer/template and the PCNA clamp
Authors	:	Zheng, F.; Georgescu, R.; Li, H.; O'Donnell, M.E.
Deposited on	:	2020-10-04
Resolution	:	3.20 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 (i) 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 (i)) were used in the production of this report:

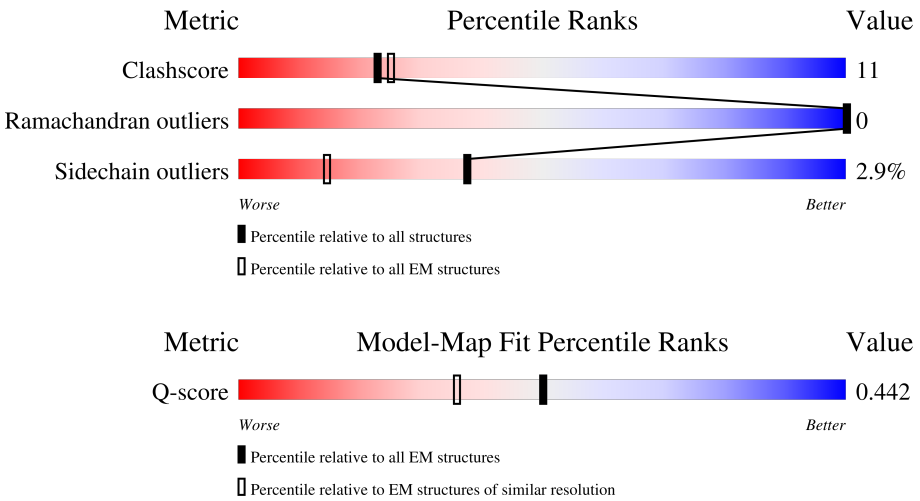
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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 <=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	P	25	52% 32% 16%
2	T	38	39% 26% 34%
3	E	258	43% 62% 33% • •
3	F	258	9% 67% 29% • •

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Mol	Chain	Length	Quality of chain
3	G	258	42% 65% 30%
4	A	1097	72% 19% 8%
5	B	487	66% 28% 5%
6	C	350	23% 8% 69%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 19553 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 DNA chain called DNA (5'-D(P*AP*TP*GP*AP*CP*CP*AP*TP*GP*AP*TP*TP*AP*CP*GP*AP*AP*TP*TP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	P	21	430	206	79	124	21	0	0

- Molecule 2 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	T	25	512	246	90	151	25	0	0

- Molecule 3 is a protein called Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	F	254	1995	1277	314	394	10	0	0
3	E	253	1987	1270	314	396	7	0	0
3	G	251	1971	1261	312	392	6	0	0

- Molecule 4 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	1004	8009	5103	1373	1492	41	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	MET	ILE	conflict	UNP A0A6A5Q0V0
A	321	SER	ASP	conflict	UNP A0A6A5Q0V0
A	323	SER	GLU	conflict	UNP A0A6A5Q0V0
A	367	PRO	HIS	conflict	UNP A0A6A5Q0V0

- Molecule 5 is a protein called POL31 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	463	3705	2366	610	709	20	0	0

- Molecule 6 is a protein called POL32 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	109	905	597	138	163	7	0	0

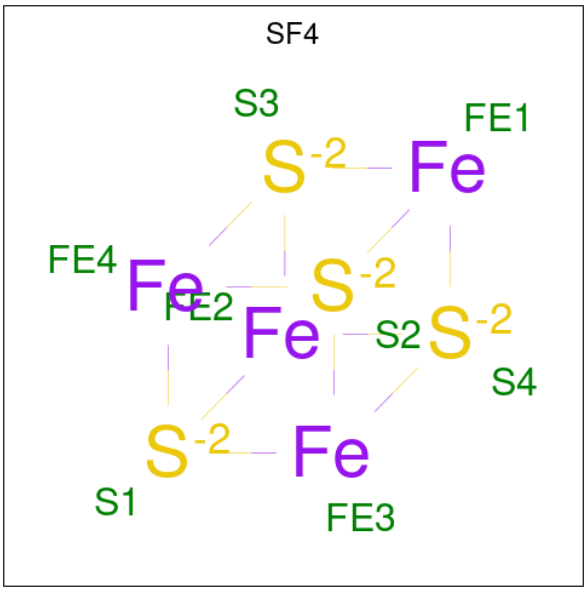
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	initiating methionine	UNP A0A6A5PT00
C	2	ASP	-	expression tag	UNP A0A6A5PT00
C	3	GLN	-	expression tag	UNP A0A6A5PT00
C	4	LYS	-	expression tag	UNP A0A6A5PT00
C	5	ALA	-	expression tag	UNP A0A6A5PT00
C	6	SER	-	expression tag	UNP A0A6A5PT00
C	7	TYR	-	expression tag	UNP A0A6A5PT00
C	223	THR	ALA	conflict	UNP A0A6A5PT00
C	228	GLY	GLU	conflict	UNP A0A6A5PT00
C	274	SER	PRO	conflict	UNP A0A6A5PT00

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

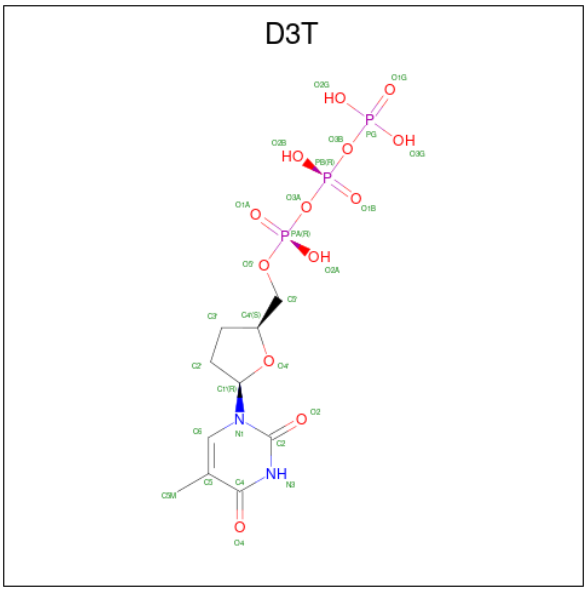
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
7	P	1	1	1	0
7	A	1	1	1	0

- Molecule 8 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 9 is 2',3'-DIDEOXY-THYMIDINE-5'-TRIPHOSPHATE (CCD ID: D3T) (formula: $C_{10}H_{17}N_2O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
9	A	1	28	10	2	13	3	0

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

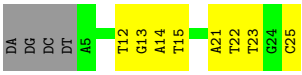
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
10	A	1	1	1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

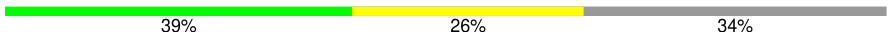
• Molecule 1: DNA (5'-D(P*AP*TP*GP*AP*CP*CP*AP*TP*GP*AP*TP*TP*AP*CP*GP*AP*AP*TP*TP*GP*C)-3')

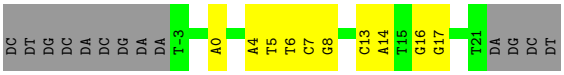
Chain P:



• Molecule 2: DNA (25-MER)

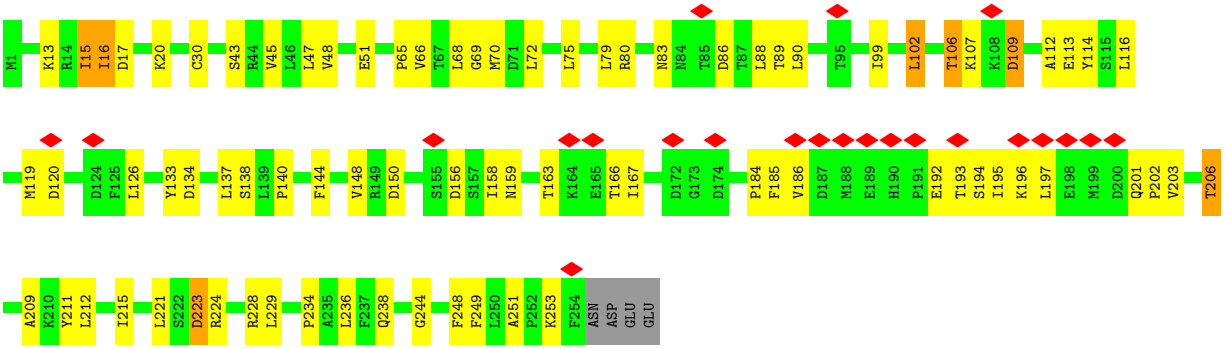
Chain T:





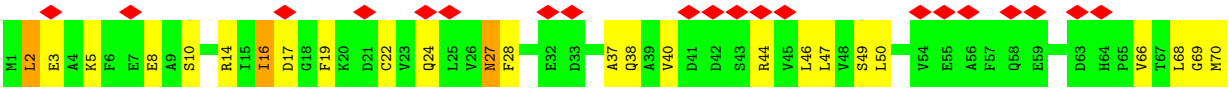
• Molecule 3: Proliferating cell nuclear antigen

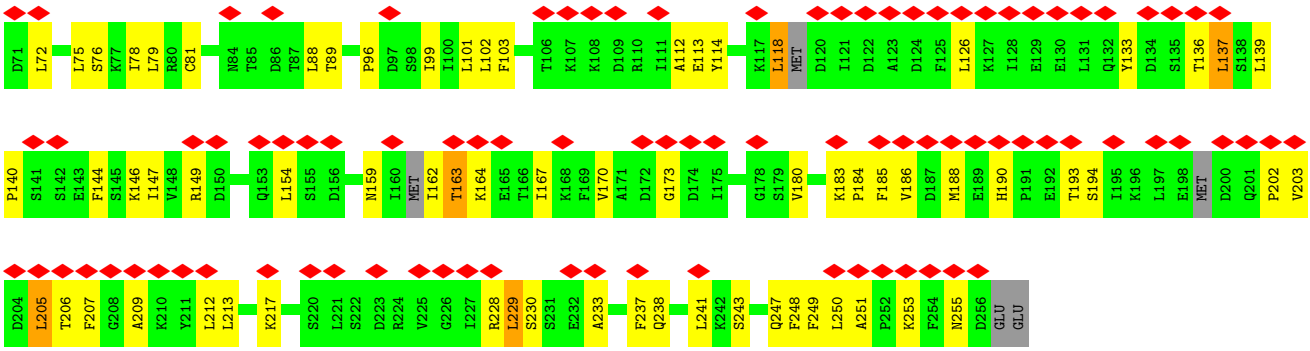
Chain F:



• Molecule 3: Proliferating cell nuclear antigen

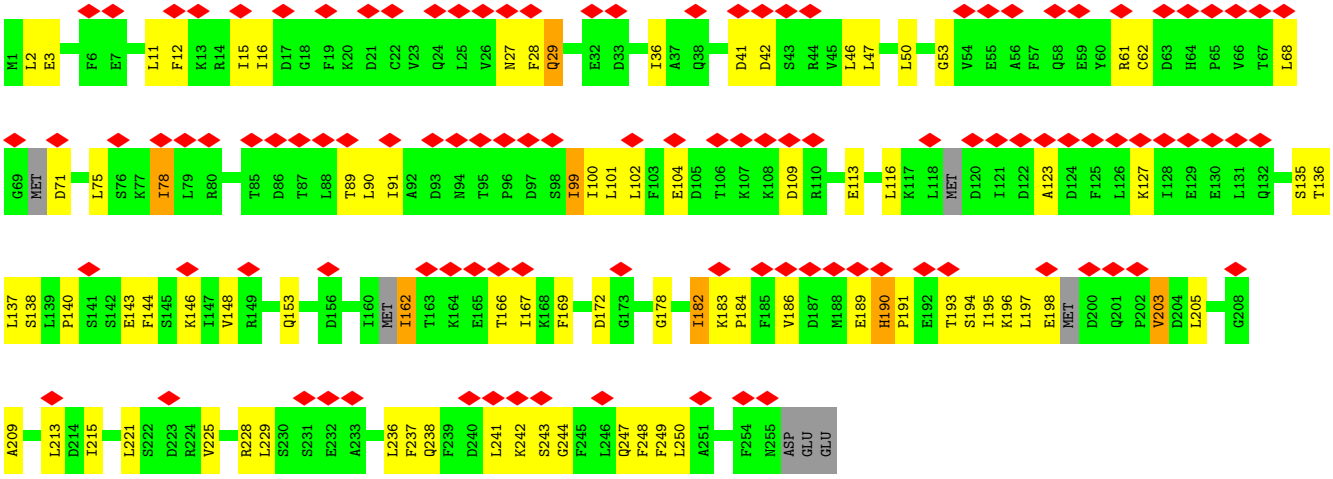
Chain E:





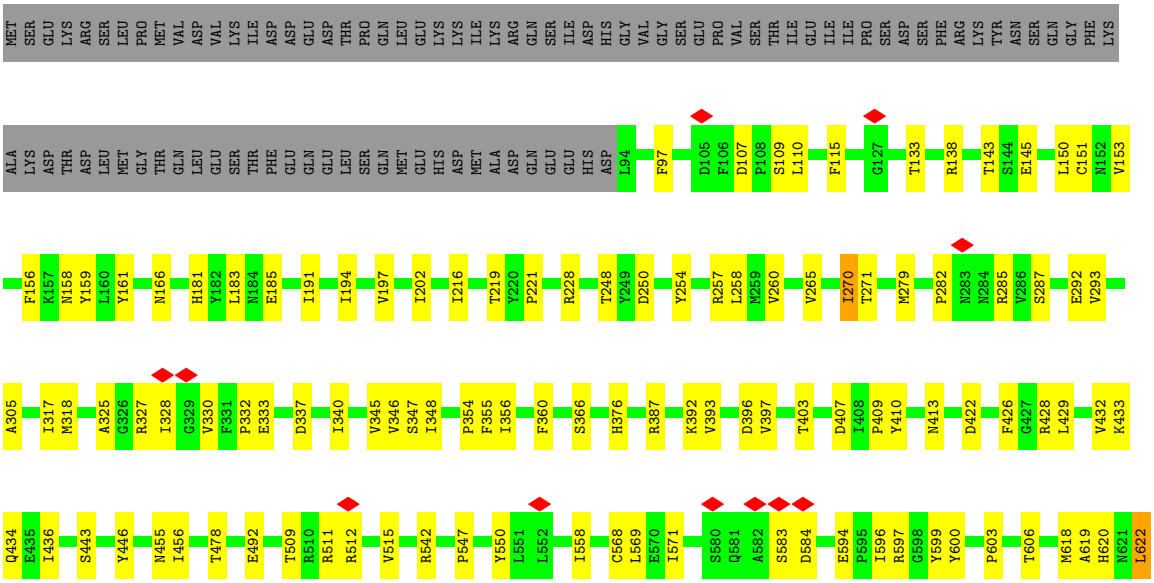
- Molecule 3: Proliferating cell nuclear antigen

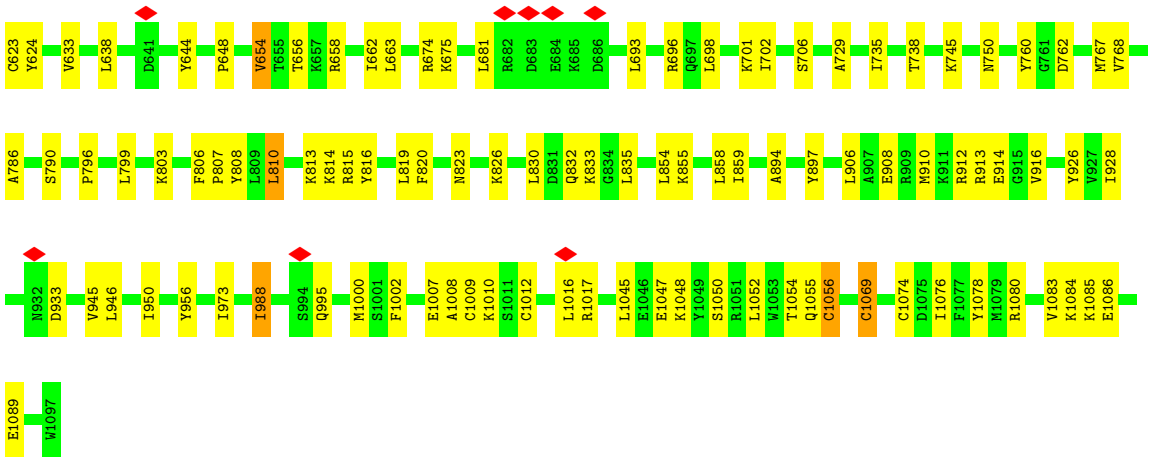
Chain G:



- Molecule 4: DNA polymerase

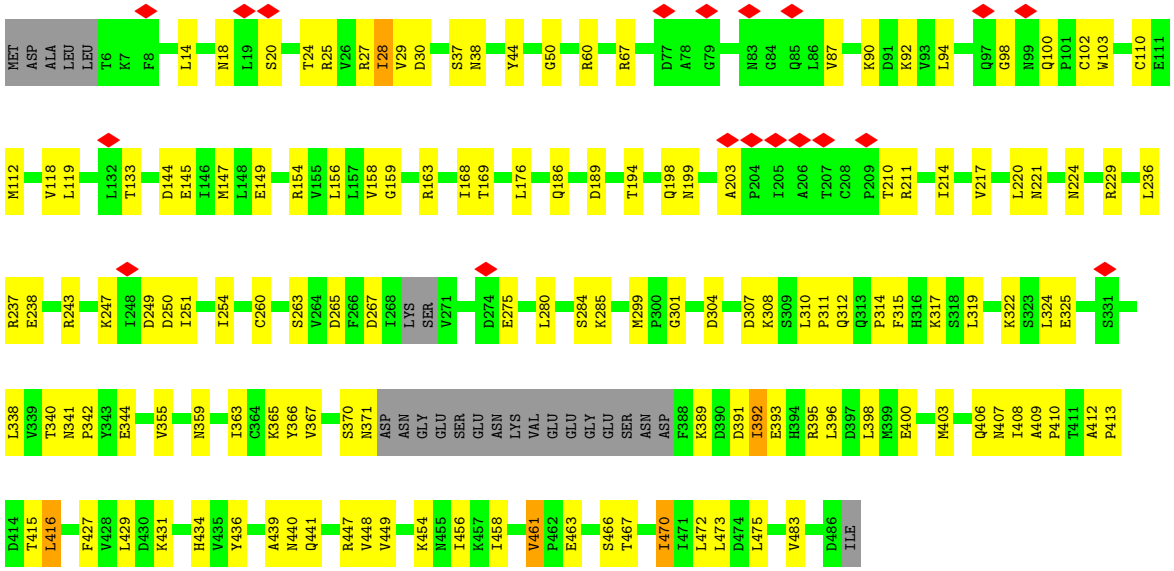
Chain A:





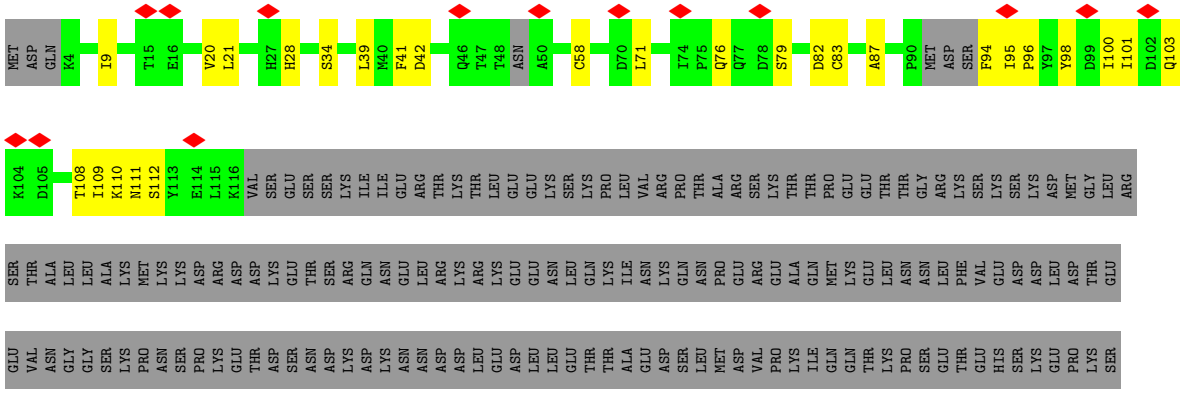
• Molecule 5: POL31 isoform 1

Chain B:



• Molecule 6: POL32 isoform 1

Chain C:



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

PHE LYS ARG LYS ALA LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	133468	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 ($e^-/Å^2$)	68	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.968	Depositor
Minimum map value	-0.448	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	346.91998, 346.91998, 346.91998	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.826, 0.826, 0.826	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: MG, SF4, D3T, 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	P	0.22	0/482	0.48	0/741
2	T	0.20	0/573	0.37	0/882
3	E	0.28	0/2014	0.48	1/2714 (0.0%)
3	F	0.12	0/2025	0.30	0/2731
3	G	0.29	0/1997	0.46	0/2690
4	A	0.21	0/8171	0.37	0/11056
5	B	0.19	0/3785	0.38	0/5135
6	C	0.15	0/926	0.34	0/1249
All	All	0.21	0/19973	0.39	1/27198 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	184	PRO	N-CA-C	5.09	120.75	113.47

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	P	430	0	236	6	0
2	T	512	0	285	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1987	0	1999	61	0
3	F	1995	0	2019	54	0
3	G	1971	0	1985	76	0
4	A	8009	0	8067	136	0
5	B	3705	0	3679	97	0
6	C	905	0	910	20	0
7	A	1	0	0	0	0
7	P	1	0	0	0	0
8	A	8	0	0	1	0
9	A	28	0	13	4	0
10	A	1	0	0	0	0
All	All	19553	0	19193	434	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 11.

All (434) 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)
3:G:137:LEU:HD22	3:G:167:ILE:CD1	1.95	0.96
3:G:137:LEU:HD22	3:G:167:ILE:HD13	1.61	0.83
3:G:3:GLU:HB3	3:G:61:ARG:HD3	1.63	0.81
4:A:1056:CYS:SG	4:A:1080:ARG:NH2	2.54	0.81
3:G:137:LEU:HD22	3:G:167:ILE:HD11	1.61	0.80
3:E:68:LEU:HB3	3:E:118:LEU:HD13	1.63	0.80
3:F:51:GLU:O	3:F:244:GLY:HA3	1.81	0.79
3:G:184:PRO:HA	3:G:195:ILE:HB	1.63	0.79
3:G:136:THR:HG22	3:G:228:ARG:HG2	1.65	0.78
3:G:162:ILE:N	3:G:162:ILE:HD12	2.01	0.75
4:A:1050:SER:O	4:A:1054:THR:HG23	1.87	0.74
4:A:806:PHE:HB3	4:A:807:PRO:HD3	1.69	0.74
3:G:162:ILE:HD12	3:G:203:VAL:HG13	1.69	0.74
3:F:70:MET:HE1	3:F:99:ILE:HG21	1.71	0.73
4:A:387:ARG:HG2	4:A:426:PHE:HB3	1.70	0.72
4:A:760:TYR:HB2	4:A:810:LEU:HD11	1.73	0.71
5:B:324:LEU:H	5:B:324:LEU:HD22	1.54	0.70
4:A:600:TYR:HB2	4:A:808:TYR:HB3	1.71	0.69
6:C:21:LEU:HD13	6:C:87:ALA:HB2	1.74	0.69
3:F:184:PRO:HG3	3:F:197:LEU:HD13	1.75	0.69
4:A:807:PRO:HB2	4:A:858:LEU:HD22	1.76	0.68
3:G:167:ILE:HD12	3:G:182:ILE:HG21	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:101:ILE:HG13	6:C:103:GLN:H	1.57	0.68
3:G:47:LEU:HB3	3:G:249:PHE:HB2	1.76	0.68
6:C:76:GLN:HB3	6:C:79:SER:HB3	1.75	0.67
4:A:250:ASP:OD2	4:A:257:ARG:NH2	2.28	0.67
5:B:199:ASN:O	5:B:434:HIS:NE2	2.28	0.66
5:B:60:ARG:NH2	5:B:409:ALA:O	2.28	0.66
5:B:211:ARG:NH1	5:B:475:LEU:O	2.28	0.66
4:A:623:CYS:SG	4:A:624:TYR:N	2.68	0.66
3:E:237:PHE:HB2	3:E:248:PHE:HB2	1.77	0.66
3:G:169:PHE:HD1	3:G:182:ILE:CD1	2.10	0.65
3:G:203:VAL:HG21	3:G:229:LEU:HB3	1.79	0.65
5:B:168:ILE:HG21	5:B:363:ILE:HD12	1.78	0.64
5:B:133:THR:O	5:B:365:LYS:NZ	2.31	0.64
3:E:183:LYS:HB2	3:G:109:ASP:HB2	1.80	0.64
5:B:395:ARG:NH1	5:B:441:GLN:OE1	2.31	0.63
5:B:29:VAL:HG22	6:C:112:SER:HB3	1.81	0.63
4:A:633:VAL:HG23	4:A:638:LEU:HB2	1.81	0.63
3:F:86:ASP:OD1	3:F:86:ASP:N	2.32	0.63
5:B:314:PRO:HD3	5:B:340:THR:HG22	1.80	0.63
4:A:492:GLU:HG3	4:A:1069:CYS:HB2	1.81	0.62
4:A:606:THR:HG21	4:A:803:LYS:HE3	1.79	0.62
3:G:228:ARG:HB2	3:G:236:LEU:HB3	1.81	0.62
4:A:327:ARG:NH2	4:A:333:GLU:OE2	2.32	0.62
3:F:13:LYS:NZ	3:F:79:LEU:O	2.33	0.62
4:A:409:PRO:O	4:A:413:ASN:ND2	2.33	0.62
6:C:95:ILE:HD12	6:C:96:PRO:HD2	1.81	0.62
3:E:99:ILE:N	3:E:118:LEU:HD21	2.15	0.62
3:G:186:VAL:HG12	3:G:186:VAL:O	2.00	0.61
3:F:223:ASP:OD1	3:F:223:ASP:N	2.30	0.61
3:F:194:SER:O	3:F:224:ARG:NH2	2.31	0.61
4:A:1084:LYS:HD2	5:B:50:GLY:HA2	1.82	0.61
5:B:311:PRO:HD3	5:B:427:PHE:HZ	1.66	0.60
4:A:745:LYS:O	4:A:750:ASN:ND2	2.34	0.60
3:E:38:GLN:HG2	3:E:49:SER:HA	1.82	0.60
5:B:110:CYS:H	5:B:169:THR:HB	1.66	0.60
5:B:403:MET:HG3	5:B:456:ILE:HD11	1.82	0.60
3:E:99:ILE:H	3:E:118:LEU:HD21	1.66	0.60
3:G:91:ILE:HB	3:G:100:ILE:HB	1.84	0.60
4:A:1080:ARG:NH2	8:A:1101:SF4:S4	2.75	0.59
5:B:194:THR:O	5:B:406:GLN:NE2	2.35	0.59
3:F:16:ILE:HG23	3:F:72:LEU:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:347:SER:OG	4:A:348:ILE:N	2.35	0.59
4:A:1047:GLU:HB2	5:B:308:LYS:HD2	1.85	0.59
4:A:97:PHE:HD2	4:A:392:LYS:HE3	1.67	0.59
3:G:90:LEU:HG	3:G:99:ILE:HD11	1.84	0.59
3:E:5:LYS:NZ	3:E:89:THR:OG1	2.29	0.59
2:T:4:DA:H5"	4:A:813:LYS:HD3	1.85	0.59
3:G:237:PHE:O	3:G:248:PHE:N	2.34	0.59
4:A:648:PRO:HB2	4:A:729:ALA:HB1	1.85	0.58
5:B:391:ASP:OD1	5:B:391:ASP:N	2.35	0.58
3:G:189:GLU:OE1	3:G:189:GLU:N	2.29	0.58
4:A:908:GLU:OE1	4:A:912:ARG:NH1	2.31	0.58
3:F:120:ASP:OD1	3:F:120:ASP:N	2.36	0.58
3:E:47:LEU:HB2	3:E:249:PHE:HB2	1.85	0.58
3:E:185:PHE:O	3:G:109:ASP:OD2	2.21	0.58
6:C:110:LYS:NZ	6:C:111:ASN:O	2.34	0.58
3:E:136:THR:HB	3:E:228:ARG:HH11	1.68	0.58
3:E:203:VAL:HG11	3:E:229:LEU:HB3	1.86	0.58
3:G:162:ILE:HG21	3:G:197:LEU:HD21	1.85	0.58
5:B:359:ASN:HA	5:B:416:LEU:HD22	1.85	0.58
4:A:790:SER:OG	4:A:799:LEU:N	2.30	0.57
3:G:238:GLN:HA	3:G:247:GLN:HA	1.86	0.57
3:F:163:THR:HG22	3:F:202:PRO:HB3	1.85	0.57
4:A:183:LEU:HB3	4:A:191:ILE:HD13	1.85	0.57
4:A:1045:LEU:HD11	4:A:1086:GLU:HG2	1.87	0.57
3:E:103:PHE:HB2	3:E:112:ALA:HB3	1.86	0.57
5:B:439:ALA:HA	5:B:461:VAL:HG13	1.85	0.57
4:A:107:ASP:OD1	4:A:107:ASP:N	2.38	0.56
3:G:237:PHE:HB2	3:G:248:PHE:HB2	1.86	0.56
5:B:341:ASN:HB3	5:B:342:PRO:HD3	1.86	0.56
3:G:78:ILE:HG21	3:G:101:LEU:HD13	1.86	0.56
3:G:169:PHE:HD1	3:G:182:ILE:HD13	1.68	0.56
5:B:260:CYS:HA	5:B:299:MET:HB2	1.87	0.56
4:A:346:VAL:HG11	4:A:393:VAL:HG11	1.87	0.56
3:E:78:ILE:HG21	3:E:101:LEU:HD13	1.88	0.56
4:A:906:LEU:HD22	4:A:926:TYR:HB3	1.88	0.56
4:A:762:ASP:OD1	4:A:814:LYS:NZ	2.37	0.56
3:G:169:PHE:CD1	3:G:182:ILE:HD13	2.41	0.56
3:F:185:PHE:H	3:F:195:ILE:HB	1.71	0.55
4:A:786:ALA:HA	4:A:799:LEU:HD23	1.87	0.55
5:B:324:LEU:HD22	5:B:324:LEU:N	2.21	0.55
3:F:80:ARG:NH1	3:G:153:GLN:OE1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:280:LEU:HD22	5:B:319:LEU:HB3	1.89	0.55
3:G:78:ILE:HD12	3:G:116:LEU:HB2	1.88	0.55
5:B:400:GLU:HG3	5:B:449:VAL:HG11	1.88	0.55
3:E:27:ASN:N	3:E:27:ASN:HD22	2.04	0.55
3:E:19:PHE:HZ	3:E:50:LEU:HB2	1.71	0.55
4:A:202:ILE:HD11	4:A:662:ILE:HD11	1.88	0.55
4:A:360:PHE:HD2	4:A:376:HIS:HE2	1.53	0.55
4:A:597:ARG:H	4:A:597:ARG:HD2	1.72	0.55
4:A:945:VAL:HG22	4:A:950:ILE:HD11	1.88	0.55
3:E:164:LYS:HE3	3:E:202:PRO:HG3	1.88	0.55
2:T:4:DA:O3'	4:A:813:LYS:HD2	2.06	0.54
4:A:396:ASP:OD1	4:A:428:ARG:NH1	2.40	0.54
5:B:393:GLU:OE2	5:B:447:ARG:NH2	2.36	0.54
4:A:995:GLN:HB3	4:A:1000:MET:HE2	1.88	0.54
4:A:433:LYS:O	4:A:455:ASN:ND2	2.32	0.54
3:E:162:ILE:N	3:E:203:VAL:O	2.41	0.54
1:P:14:DA:H2'	1:P:15:DT:H71	1.89	0.54
3:F:236:LEU:HD21	3:F:238:GLN:HB2	1.90	0.54
3:E:38:GLN:HB2	3:E:126:LEU:HD22	1.90	0.54
3:G:228:ARG:HD2	3:G:236:LEU:HD22	1.89	0.54
3:G:137:LEU:CD2	3:G:167:ILE:HD13	2.37	0.54
3:G:205:LEU:HD22	3:G:229:LEU:HD22	1.90	0.54
3:G:169:PHE:CD1	3:G:182:ILE:CD1	2.91	0.53
4:A:606:THR:HB	4:A:803:LYS:HG3	1.90	0.53
5:B:247:LYS:HG3	5:B:251:ILE:HG22	1.90	0.53
5:B:250:ASP:OD1	5:B:250:ASP:N	2.41	0.53
4:A:318:MET:HG3	4:A:346:VAL:HG22	1.91	0.53
5:B:144:ASP:OD1	5:B:144:ASP:N	2.36	0.53
3:E:27:ASN:HA	3:E:69:GLY:HA2	1.90	0.53
3:G:89:THR:HB	3:G:102:LEU:HB3	1.90	0.53
5:B:344:GLU:OE2	5:B:431:LYS:NZ	2.42	0.53
3:F:17:ASP:HA	3:F:20:LYS:HG2	1.91	0.53
4:A:618:MET:HE3	4:A:796:PRO:HB3	1.90	0.53
1:P:22:DT:H2'	1:P:23:DT:H71	1.91	0.53
3:F:13:LYS:HA	3:F:79:LEU:HD13	1.90	0.53
4:A:282:PRO:HA	4:A:285:ARG:HD3	1.91	0.53
4:A:434:GLN:HG2	4:A:456:ILE:HG12	1.91	0.53
5:B:27:ARG:HG3	6:C:109:ILE:HD11	1.90	0.53
3:E:102:LEU:HD13	3:E:113:GLU:HG2	1.90	0.53
3:F:140:PRO:HG3	3:F:193:THR:HA	1.90	0.52
4:A:807:PRO:HD2	4:A:819:LEU:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:815:ARG:HA	4:A:833:LYS:O	2.09	0.52
3:G:53:GLY:N	3:G:243:SER:O	2.40	0.52
3:G:138:SER:HB3	3:G:196:LYS:HB2	1.91	0.52
3:G:215:ILE:HD12	3:G:250:LEU:HD12	1.92	0.52
3:F:137:LEU:HD11	3:F:195:ILE:HG23	1.92	0.52
5:B:301:GLY:H	5:B:304:ASP:HB2	1.74	0.52
3:F:89:THR:HB	3:F:102:LEU:HG	1.91	0.52
4:A:933:ASP:OD1	4:A:933:ASP:N	2.40	0.52
5:B:363:ILE:HD11	5:B:410:PRO:HG2	1.92	0.52
3:G:28:PHE:HB2	3:G:68:LEU:HB2	1.91	0.52
3:F:114:TYR:HA	3:G:178:GLY:HA2	1.91	0.52
4:A:1009:CYS:HA	4:A:1017:ARG:HD2	1.91	0.52
5:B:221:ASN:HB2	5:B:265:ASP:HB2	1.89	0.52
3:G:46:LEU:HD11	3:G:215:ILE:HD11	1.91	0.52
3:G:102:LEU:HG	3:G:104:GLU:HG3	1.91	0.52
4:A:702:ILE:O	4:A:706:SER:N	2.43	0.52
5:B:247:LYS:HG2	5:B:249:ASP:H	1.76	0.51
3:F:148:VAL:HG11	3:F:212:LEU:HB3	1.92	0.51
3:F:159:ASN:HA	3:F:206:THR:HA	1.92	0.51
3:F:206:THR:OG1	3:F:253:LYS:NZ	2.38	0.51
4:A:1085:LYS:O	4:A:1089:GLU:HG2	2.11	0.51
4:A:599:TYR:CD1	4:A:973:ILE:HD11	2.45	0.51
5:B:267:ASP:OD1	5:B:267:ASP:N	2.42	0.51
3:E:112:ALA:HB1	3:E:114:TYR:HE1	1.74	0.51
4:A:228:ARG:HG3	4:A:248:THR:HG21	1.91	0.51
3:E:118:LEU:HD23	3:E:118:LEU:N	2.26	0.51
3:E:76:SER:HA	3:E:79:LEU:HD12	1.92	0.51
4:A:150:LEU:HD22	4:A:287:SER:HB3	1.92	0.51
5:B:37:SER:OG	5:B:38:ASN:N	2.44	0.51
3:E:147:ILE:HD12	3:E:180:VAL:HG11	1.93	0.51
3:E:230:SER:HB3	3:E:233:ALA:HB3	1.93	0.51
4:A:832:GLN:HG2	4:A:835:LEU:HD12	1.94	0.50
3:G:162:ILE:HD12	3:G:203:VAL:CG1	2.41	0.50
4:A:279:MET:HG2	4:A:293:VAL:HG12	1.94	0.50
3:E:238:GLN:HA	3:E:247:GLN:HA	1.92	0.50
3:G:140:PRO:HB2	3:G:143:GLU:HG3	1.93	0.50
3:E:139:LEU:HD11	3:E:144:PHE:HB2	1.94	0.50
4:A:260:VAL:HG12	4:A:569:LEU:HD13	1.94	0.50
3:E:22:CYS:O	3:E:24:GLN:NE2	2.44	0.50
5:B:25:ARG:O	6:C:109:ILE:HG13	2.11	0.50
3:F:30:CYS:HB2	3:F:66:VAL:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:83:ASN:OD1	3:G:146:LYS:NZ	2.45	0.50
4:A:1052:LEU:HD22	4:A:1076:ILE:HG23	1.93	0.50
4:A:355:PHE:HD1	4:A:356:ILE:HG23	1.77	0.50
6:C:82:ASP:OD1	6:C:83:CYS:N	2.44	0.50
3:G:162:ILE:CD1	3:G:203:VAL:CG1	2.90	0.50
5:B:44:TYR:OH	5:B:307:ASP:OD1	2.25	0.49
3:G:41:ASP:HB2	3:G:46:LEU:HB3	1.94	0.49
4:A:285:ARG:HG2	4:A:292:GLU:HB3	1.94	0.49
4:A:429:LEU:HB2	4:A:432:VAL:HG22	1.94	0.49
5:B:189:ASP:OD1	5:B:189:ASP:N	2.46	0.49
5:B:220:LEU:HB2	5:B:263:SER:HA	1.94	0.49
5:B:203:ALA:O	5:B:211:ARG:NH2	2.46	0.49
5:B:317:LYS:HB2	5:B:325:GLU:OE1	2.13	0.49
3:G:189:GLU:H	3:G:189:GLU:CD	2.17	0.49
5:B:370:SER:OG	5:B:371:ASN:N	2.45	0.49
5:B:237:ARG:HE	6:C:98:TYR:HE1	1.60	0.49
3:E:163:THR:HG22	3:E:164:LYS:H	1.77	0.49
4:A:138:ARG:HB3	4:A:150:LEU:HD11	1.94	0.49
4:A:674:ARG:NH1	9:A:1102:D3T:O3G	2.46	0.49
3:F:48:VAL:HG12	3:F:248:PHE:CD2	2.48	0.49
3:F:75:LEU:HD13	3:F:116:LEU:HD22	1.94	0.49
3:F:192:GLU:O	3:F:224:ARG:NH1	2.45	0.49
4:A:181:HIS:O	4:A:185:GLU:HG2	2.12	0.49
3:E:237:PHE:HE1	3:E:250:LEU:HB3	1.78	0.48
4:A:143:THR:HG23	4:A:145:GLU:H	1.78	0.48
3:E:16:ILE:HD12	3:E:79:LEU:HD11	1.94	0.48
3:E:188:MET:HG3	3:E:190:HIS:CD2	2.48	0.48
4:A:115:PHE:HA	4:A:143:THR:HA	1.95	0.48
4:A:568:CYS:HA	4:A:571:ILE:HG22	1.94	0.48
4:A:599:TYR:CG	4:A:973:ILE:HD11	2.48	0.48
3:E:2:LEU:HD12	3:E:2:LEU:C	2.37	0.48
4:A:153:VAL:HG11	4:A:258:LEU:HD21	1.95	0.48
4:A:328:ILE:HD12	4:A:328:ILE:H	1.78	0.48
4:A:910:MET:HG2	4:A:913:ARG:HH11	1.78	0.48
3:G:144:PHE:O	3:G:148:VAL:HG23	2.13	0.48
4:A:151:CYS:HA	4:A:293:VAL:HG23	1.96	0.48
4:A:583:SER:OG	4:A:584:ASP:N	2.47	0.48
1:P:12:DT:H2"	1:P:13:DG:C8	2.47	0.48
3:F:186:VAL:HB	3:F:196:LYS:HD3	1.95	0.48
4:A:638:LEU:HD22	4:A:658:ARG:HE	1.79	0.48
4:A:159:TYR:CZ	4:A:257:ARG:HD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:367:VAL:HG11	5:B:389:LYS:HD2	1.94	0.48
3:G:11:LEU:O	3:G:15:ILE:HG12	2.14	0.48
4:A:403:THR:HA	4:A:407:ASP:HB2	1.96	0.48
5:B:25:ARG:HD3	5:B:247:LYS:HD2	1.95	0.48
3:E:241:LEU:HD23	3:E:243:SER:H	1.79	0.48
3:F:43:SER:OG	3:F:45:VAL:HG12	2.14	0.48
3:F:134:ASP:HB3	3:F:201:GLN:HB2	1.96	0.48
4:A:194:ILE:HG12	4:A:216:ILE:HG12	1.95	0.48
4:A:735:ILE:HA	4:A:738:THR:HG22	1.96	0.48
5:B:214:ILE:HD11	5:B:473:LEU:HD23	1.96	0.48
3:G:27:ASN:HD22	3:G:123:ALA:HB2	1.79	0.48
3:F:106:THR:HG23	3:F:107:LYS:H	1.80	0.47
4:A:347:SER:HB2	4:A:354:PRO:HB3	1.95	0.47
3:G:2:LEU:HA	3:G:62:CYS:HA	1.95	0.47
2:T:5:DT:H2'	2:T:6:DT:H71	1.95	0.47
5:B:27:ARG:HG2	5:B:28:ILE:H	1.79	0.47
5:B:112:MET:HG3	5:B:144:ASP:HB3	1.95	0.47
5:B:359:ASN:O	5:B:363:ILE:HG12	2.14	0.47
3:G:127:LYS:O	3:G:127:LYS:HG3	2.14	0.47
3:F:236:LEU:HD12	3:F:249:PHE:CE1	2.49	0.47
5:B:285:LYS:HG2	6:C:100:ILE:HD11	1.95	0.47
3:G:15:ILE:HD13	3:G:221:LEU:HD22	1.96	0.47
3:G:162:ILE:N	3:G:203:VAL:O	2.47	0.47
4:A:855:LYS:HG3	4:A:859:ILE:HD12	1.97	0.47
4:A:946:LEU:HD13	4:A:1078:TYR:HD1	1.79	0.47
3:G:169:PHE:HD1	3:G:182:ILE:HD11	1.80	0.47
1:P:21:DA:OP1	4:A:897:TYR:OH	2.25	0.47
4:A:158:ASN:HB2	4:A:221:PRO:HB3	1.97	0.47
4:A:443:SER:HB3	4:A:446:TYR:HB2	1.96	0.47
4:A:1009:CYS:SG	4:A:1010:LYS:N	2.88	0.47
3:G:162:ILE:CG1	3:G:167:ILE:HG12	2.44	0.47
4:A:325:ALA:HB2	4:A:340:ILE:HD13	1.97	0.47
3:G:140:PRO:HG3	3:G:193:THR:HA	1.97	0.47
4:A:332:PRO:HA	4:A:337:ASP:OD2	2.15	0.47
6:C:21:LEU:HD21	6:C:95:ILE:HG21	1.96	0.46
4:A:270:ILE:HG22	4:A:271:THR:H	1.79	0.46
5:B:14:LEU:HD13	6:C:41:PHE:HB2	1.97	0.46
3:F:144:PHE:O	3:F:148:VAL:HG23	2.15	0.46
4:A:159:TYR:OH	4:A:257:ARG:NH1	2.48	0.46
4:A:674:ARG:NE	4:A:701:LYS:HB3	2.30	0.46
5:B:436:TYR:HB3	5:B:458:ILE:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:10:SER:O	3:E:14:ARG:HG3	2.14	0.46
3:E:68:LEU:HD21	3:E:96:PRO:HG2	1.98	0.46
4:A:337:ASP:O	4:A:410:TYR:OH	2.23	0.46
4:A:803:LYS:HD3	4:A:820:PHE:CE2	2.50	0.46
3:G:241:LEU:HB2	3:G:244:GLY:C	2.40	0.46
3:F:15:ILE:HA	3:F:221:LEU:HD11	1.97	0.46
4:A:318:MET:HA	4:A:346:VAL:HA	1.97	0.46
3:F:65:PRO:HG3	4:A:1016:LEU:HD22	1.97	0.46
4:A:547:PRO:HD2	4:A:550:TYR:CD2	2.50	0.46
3:E:8:GLU:OE2	3:E:14:ARG:NH2	2.48	0.46
4:A:928:ILE:HG13	4:A:956:TYR:CE2	2.52	0.45
4:A:433:LYS:HE2	4:A:433:LYS:HB3	1.77	0.45
4:A:603:PRO:HG3	4:A:806:PHE:CD1	2.50	0.45
3:E:159:ASN:HB3	3:E:170:VAL:HG13	1.99	0.45
5:B:103:TRP:HB3	5:B:176:LEU:HD13	1.99	0.45
5:B:147:MET:HB3	5:B:154:ARG:HG3	1.97	0.45
3:G:71:ASP:O	3:G:75:LEU:HG	2.16	0.45
1:P:25:DC:H2'	9:A:1102:D3T:O4'	2.16	0.45
5:B:25:ARG:HH22	5:B:249:ASP:HB2	1.81	0.45
5:B:87:VAL:HG22	5:B:103:TRP:HD1	1.82	0.45
5:B:412:ALA:HB3	5:B:413:PRO:HD3	1.98	0.45
3:G:186:VAL:HG22	3:G:194:SER:HB3	1.98	0.45
4:A:512:ARG:O	4:A:515:VAL:HG12	2.16	0.45
2:T:13:DC:H2"	2:T:14:DA:C8	2.52	0.45
5:B:24:THR:HB	6:C:110:LYS:HB3	1.99	0.45
5:B:408:ILE:HG23	5:B:429:LEU:HD21	1.98	0.45
3:F:211:TYR:O	3:F:215:ILE:HG12	2.17	0.45
3:F:45:VAL:HG23	3:F:251:ALA:HB3	1.99	0.45
3:F:88:LEU:HA	3:F:102:LEU:O	2.18	0.45
3:E:183:LYS:HD2	3:G:109:ASP:HA	1.99	0.45
3:E:186:VAL:HG21	3:E:194:SER:HA	1.99	0.45
3:E:209:ALA:O	3:E:213:LEU:HG	2.16	0.44
4:A:1074:CYS:SG	5:B:119:LEU:HD11	2.57	0.44
5:B:393:GLU:HG2	5:B:396:LEU:HD12	2.00	0.44
5:B:92:LYS:HE2	5:B:94:LEU:HB3	1.99	0.44
3:E:75:LEU:HG	3:E:79:LEU:HD11	1.99	0.44
4:A:509:THR:O	4:A:512:ARG:HG2	2.16	0.44
5:B:158:VAL:O	5:B:186:GLN:HA	2.18	0.44
5:B:342:PRO:HB3	5:B:355:VAL:HG12	2.00	0.44
5:B:407:ASN:HD21	5:B:410:PRO:HA	1.83	0.44
4:A:345:VAL:HG12	4:A:345:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:644:TYR:HA	4:A:654:VAL:HA	1.99	0.44
3:G:102:LEU:HD13	3:G:113:GLU:HB3	1.99	0.44
3:F:203:VAL:HG11	3:F:229:LEU:HB3	1.99	0.44
4:A:156:PHE:HB3	4:A:254:TYR:OH	2.18	0.44
3:E:205:LEU:HD13	3:E:207:PHE:CE1	2.52	0.44
3:G:12:PHE:O	3:G:16:ILE:HG22	2.18	0.44
5:B:145:GLU:HG2	5:B:156:LEU:HD11	1.99	0.43
3:F:68:LEU:HD13	3:F:99:ILE:HD12	2.00	0.43
3:F:102:LEU:HB3	3:F:113:GLU:OE2	2.18	0.43
4:A:681:LEU:HA	4:A:693:LEU:HD13	1.99	0.43
5:B:18:ASN:HB3	6:C:34:SER:HB3	1.99	0.43
5:B:315:PHE:HB2	5:B:338:LEU:HD22	2.00	0.43
6:C:94:PHE:HD2	6:C:95:ILE:HG22	1.82	0.43
3:E:140:PRO:HG3	3:E:193:THR:HA	1.99	0.43
3:G:209:ALA:O	3:G:213:LEU:HG	2.18	0.43
4:A:619:ALA:HA	4:A:796:PRO:HG2	1.99	0.43
5:B:92:LYS:O	5:B:94:LEU:N	2.51	0.43
4:A:674:ARG:NH2	9:A:1102:D3T:O1G	2.44	0.43
3:F:137:LEU:HD12	3:F:138:SER:H	1.83	0.43
6:C:9:ILE:HD13	6:C:28:HIS:HB3	2.01	0.43
3:G:189:GLU:N	3:G:189:GLU:CD	2.76	0.43
2:T:4:DA:C8	2:T:5:DT:H72	2.54	0.43
5:B:30:ASP:OD1	5:B:30:ASP:N	2.52	0.43
5:B:67:ARG:NH1	5:B:406:GLN:OE1	2.51	0.43
3:E:46:LEU:HD11	3:E:248:PHE:HB3	2.00	0.43
3:E:207:PHE:HB3	3:E:250:LEU:HD21	2.00	0.43
4:A:693:LEU:HD23	4:A:696:ARG:HD3	2.01	0.43
4:A:830:LEU:HD11	4:A:854:LEU:HB3	2.01	0.43
5:B:392:ILE:HG23	5:B:393:GLU:H	1.84	0.43
3:E:146:LYS:HA	3:E:149:ARG:HE	1.84	0.43
5:B:284:SER:HB3	5:B:324:LEU:CD2	2.49	0.42
5:B:310:LEU:HD22	5:B:416:LEU:HD11	2.01	0.42
3:E:40:VAL:HB	3:E:44:ARG:HH11	1.84	0.42
5:B:254:ILE:HD12	5:B:472:LEU:HD22	2.01	0.42
3:F:102:LEU:HA	3:F:112:ALA:O	2.19	0.42
3:F:228:ARG:HD2	3:F:236:LEU:HD22	2.00	0.42
4:A:305:ALA:HB1	4:A:542:ARG:HD3	2.02	0.42
5:B:466:SER:OG	5:B:467:THR:N	2.52	0.42
4:A:366:SER:HB2	4:A:511:ARG:HD2	2.02	0.42
5:B:440:ASN:HA	5:B:463:GLU:HG3	2.01	0.42
6:C:71:LEU:HD13	6:C:71:LEU:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:206:THR:HB	3:E:255:ASN:HD21	1.85	0.42
3:F:150:ASP:OD1	3:E:81:CYS:HB3	2.19	0.42
4:A:109:SER:OG	4:A:110:LEU:N	2.52	0.42
5:B:149:GLU:OE1	5:B:154:ARG:NE	2.46	0.42
5:B:301:GLY:N	5:B:304:ASP:OD2	2.52	0.42
2:T:0:DA:N1	9:A:1102:D3T:N3	2.58	0.42
4:A:327:ARG:CZ	4:A:330:VAL:HG21	2.49	0.42
5:B:470:ILE:HG12	5:B:483:VAL:HB	2.00	0.42
2:T:16:DG:H2"	2:T:17:DG:C8	2.54	0.42
4:A:166:ASN:OD1	4:A:166:ASN:N	2.44	0.42
4:A:1007:GLU:O	4:A:1017:ARG:NH2	2.53	0.42
5:B:159:GLY:O	5:B:163:ARG:NH1	2.53	0.42
5:B:236:LEU:HD13	5:B:470:ILE:HG21	2.02	0.42
3:E:2:LEU:HD12	3:E:3:GLU:N	2.34	0.42
3:E:139:LEU:HD21	3:E:144:PHE:HB2	2.02	0.42
3:E:154:LEU:O	3:E:173:GLY:HA3	2.20	0.42
3:G:135:SER:CB	3:G:162:ILE:HD13	2.49	0.42
4:A:596:ILE:HG22	4:A:600:TYR:OH	2.19	0.42
4:A:623:CYS:HA	4:A:663:LEU:HD12	2.02	0.42
3:G:136:THR:OG1	3:G:198:GLU:HB3	2.20	0.42
5:B:310:LEU:O	5:B:312:GLN:N	2.51	0.42
6:C:58:CYS:HA	6:C:83:CYS:HA	2.01	0.41
3:G:162:ILE:HG23	3:G:167:ILE:N	2.35	0.41
3:G:190:HIS:CD2	3:G:190:HIS:H	2.37	0.41
3:G:191:PRO:HA	3:G:194:SER:OG	2.19	0.41
3:F:133:TYR:CG	3:F:228:ARG:HB3	2.54	0.41
3:F:234:PRO:HD3	4:A:1002:PHE:CE2	2.55	0.41
4:A:988:ILE:HD13	4:A:988:ILE:HA	1.93	0.41
4:A:1008:ALA:O	4:A:1017:ARG:NH2	2.50	0.41
5:B:238:GLU:OE1	5:B:243:ARG:NH2	2.49	0.41
5:B:304:ASP:HB3	5:B:315:PHE:CZ	2.55	0.41
3:G:90:LEU:HD12	3:G:90:LEU:HA	1.92	0.41
3:F:47:LEU:HB3	3:F:249:PHE:HB2	2.01	0.41
3:F:156:ASP:OD1	3:F:156:ASP:N	2.51	0.41
4:A:337:ASP:N	4:A:337:ASP:OD1	2.53	0.41
5:B:98:GLY:HA3	5:B:100:GLN:NE2	2.35	0.41
3:F:107:LYS:NZ	3:F:109:ASP:OD2	2.34	0.41
3:F:195:ILE:O	3:F:196:LYS:HD2	2.20	0.41
4:A:1048:LYS:HD3	4:A:1083:VAL:HG21	2.02	0.41
5:B:90:LYS:HG3	5:B:102:CYS:SG	2.60	0.41
5:B:198:GLN:HB3	5:B:454:LYS:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:221:ASN:O	5:B:229:ARG:NH1	2.53	0.41
3:G:29:GLN:HB2	3:G:36:ILE:HG23	2.02	0.41
4:A:355:PHE:CD1	4:A:356:ILE:HG23	2.56	0.41
4:A:675:LYS:HE3	4:A:675:LYS:HB3	1.85	0.41
3:G:190:HIS:HA	3:G:191:PRO:HD3	1.93	0.41
4:A:161:TYR:HE1	4:A:197:VAL:HG21	1.86	0.41
4:A:674:ARG:HH21	4:A:701:LYS:HD2	1.84	0.41
5:B:324:LEU:H	5:B:324:LEU:CD2	2.27	0.41
3:E:28:PHE:HA	3:E:37:ALA:HB2	2.02	0.41
3:E:251:ALA:O	3:E:253:LYS:NZ	2.48	0.41
3:G:41:ASP:OD2	3:G:42:ASP:N	2.54	0.41
5:B:20:SER:O	5:B:20:SER:OG	2.30	0.41
5:B:224:ASN:CG	5:B:275:GLU:HG3	2.46	0.41
3:E:14:ARG:HA	3:E:17:ASP:OD2	2.20	0.41
3:G:242:LYS:HA	3:G:242:LYS:HD2	1.79	0.41
1:P:12:DT:H2"	1:P:13:DG:H8	1.86	0.41
3:F:69:GLY:O	3:F:119:MET:HG2	2.21	0.41
3:F:72:LEU:HD13	3:F:72:LEU:HA	1.93	0.41
4:A:594:GLU:OE2	4:A:594:GLU:HA	2.21	0.41
4:A:620:HIS:HB2	4:A:622:LEU:HD13	2.03	0.41
4:A:767:MET:HE1	4:A:816:TYR:CZ	2.56	0.41
4:A:1055:GLN:HB2	5:B:118:VAL:HG12	2.02	0.41
5:B:366:TYR:OH	5:B:415:THR:OG1	2.27	0.41
3:E:16:ILE:HG23	3:E:72:LEU:HD22	2.02	0.41
3:E:137:LEU:HD13	3:E:167:ILE:HD13	2.01	0.41
3:G:36:ILE:HD12	3:G:50:LEU:O	2.21	0.41
3:G:183:LYS:HE3	3:G:183:LYS:HB3	1.80	0.41
2:T:7:DC:H2"	2:T:8:DG:C8	2.56	0.41
4:A:156:PHE:HD1	4:A:254:TYR:HE1	1.69	0.40
4:A:894:ALA:HB3	4:A:897:TYR:CZ	2.56	0.40
4:A:914:GLU:OE1	4:A:916:VAL:N	2.51	0.40
3:E:133:TYR:HD2	3:E:230:SER:HB2	1.87	0.40
3:E:209:ALA:HA	3:E:212:LEU:HD12	2.04	0.40
3:E:213:LEU:O	3:E:217:LYS:HG3	2.21	0.40
3:F:158:ILE:HG12	3:F:209:ALA:HB2	2.03	0.40
4:A:760:TYR:CB	4:A:810:LEU:HD11	2.47	0.40
4:A:823:ASN:OD1	4:A:826:LYS:N	2.55	0.40
5:B:221:ASN:OD1	5:B:229:ARG:NH1	2.55	0.40
5:B:301:GLY:O	5:B:312:GLN:NE2	2.44	0.40
4:A:1045:LEU:HD23	4:A:1045:LEU:HA	1.91	0.40
4:A:133:THR:OG1	4:A:219:THR:O	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:322:LYS:HE3	5:B:322:LYS:HA	2.02	0.40
6:C:39:LEU:HA	6:C:42:ASP:OD2	2.22	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	
3	E	245/258 (95%)	240 (98%)	5 (2%)	0	100	100
3	F	252/258 (98%)	239 (95%)	13 (5%)	0	100	100
3	G	241/258 (93%)	230 (95%)	11 (5%)	0	100	100
4	A	1002/1097 (91%)	946 (94%)	56 (6%)	0	100	100
5	B	457/487 (94%)	417 (91%)	40 (9%)	0	100	100
6	C	103/350 (29%)	89 (86%)	14 (14%)	0	100	100
All	All	2300/2708 (85%)	2161 (94%)	139 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	228/233 (98%)	217 (95%)	11 (5%)	23	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	229/233 (98%)	218 (95%)	11 (5%)	23	56
3	G	226/233 (97%)	216 (96%)	10 (4%)	25	59
4	A	892/980 (91%)	874 (98%)	18 (2%)	48	72
5	B	424/445 (95%)	415 (98%)	9 (2%)	47	71
6	C	104/331 (31%)	102 (98%)	2 (2%)	50	73
All	All	2103/2455 (86%)	2042 (97%)	61 (3%)	38	67

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	15	ILE
3	F	16	ILE
3	F	90	LEU
3	F	102	LEU
3	F	106	THR
3	F	109	ASP
3	F	126	LEU
3	F	166	THR
3	F	167	ILE
3	F	206	THR
3	F	223	ASP
4	A	265	VAL
4	A	270	ILE
4	A	317	ILE
4	A	397	VAL
4	A	422	ASP
4	A	436	ILE
4	A	478	THR
4	A	558	ILE
4	A	622	LEU
4	A	654	VAL
4	A	656	THR
4	A	698	LEU
4	A	768	VAL
4	A	810	LEU
4	A	988	ILE
4	A	1012	CYS
4	A	1056	CYS
4	A	1069	CYS
5	B	28	ILE

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Mol	Chain	Res	Type
5	B	210	THR
5	B	217	VAL
5	B	392	ILE
5	B	398	LEU
5	B	416	LEU
5	B	448	VAL
5	B	461	VAL
5	B	470	ILE
6	C	20	VAL
6	C	108	THR
3	E	2	LEU
3	E	16	ILE
3	E	27	ASN
3	E	66	VAL
3	E	70	MET
3	E	88	LEU
3	E	118	LEU
3	E	137	LEU
3	E	163	THR
3	E	205	LEU
3	E	229	LEU
3	G	29	GLN
3	G	78	ILE
3	G	99	ILE
3	G	162	ILE
3	G	166	THR
3	G	172	ASP
3	G	182	ILE
3	G	190	HIS
3	G	203	VAL
3	G	225	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
3	F	58	GLN
3	F	238	GLN
4	A	177	ASN
4	A	284	ASN
4	A	358	ASN
4	A	388	ASN
4	A	453	ASN

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Mol	Chain	Res	Type
4	A	495	HIS
4	A	504	ASN
4	A	637	ASN
4	A	705	ASN
4	A	754	HIS
4	A	851	ASN
4	A	875	ASN
4	A	919	ASN
4	A	964	ASN
4	A	995	GLN
4	A	1026	ASN
5	B	15	GLN
6	C	46	GLN
6	C	63	GLN
3	E	27	ASN
3	E	190	HIS
3	E	255	ASN
3	G	24	GLN
3	G	27	ASN
3	G	58	GLN
3	G	190	HIS
3	G	247	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
9	D3T	A	1102	7	28,29,29	2.34	7 (25%)	39,45,45	2.31	13 (33%)
8	SF4	A	1101	4	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	D3T	A	1102	7	-	4/22/31/31	0/2/2/2
8	SF4	A	1101	4	-	-	0/6/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1102	D3T	PA-O3A	9.09	1.69	1.59
9	A	1102	D3T	C6-N1	3.80	1.44	1.38
9	A	1102	D3T	PB-O3B	3.48	1.63	1.59
9	A	1102	D3T	C6-C5	2.79	1.39	1.34
9	A	1102	D3T	C2-N1	2.71	1.42	1.38
9	A	1102	D3T	PB-O3A	2.59	1.62	1.59
9	A	1102	D3T	C5'-C4'	2.11	1.57	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1102	D3T	C5-C4-N3	7.07	121.47	115.32
9	A	1102	D3T	C4-N3-C2	-6.19	119.22	127.34
9	A	1102	D3T	N3-C2-N1	4.54	120.80	114.89
9	A	1102	D3T	O3G-PG-O2G	-2.91	96.87	107.80
9	A	1102	D3T	O2B-PB-O1B	-2.88	99.04	112.44
9	A	1102	D3T	O4-C4-N3	-2.87	114.72	120.11
9	A	1102	D3T	C3'-C2'-C1'	2.55	105.81	102.87
9	A	1102	D3T	O3B-PG-O1G	2.53	124.35	111.04
9	A	1102	D3T	O2-C2-N1	-2.51	119.53	122.80
9	A	1102	D3T	O2A-PA-O1A	-2.48	100.89	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1102	D3T	C5M-C5-C4	2.42	121.37	118.78
9	A	1102	D3T	C4'-O4'-C1'	2.31	111.99	109.81
9	A	1102	D3T	O2G-PG-O3B	2.26	112.22	104.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1102	D3T	O4'-C4'-C5'-O5'
9	A	1102	D3T	C3'-C4'-C5'-O5'
9	A	1102	D3T	PB-O3A-PA-O5'
9	A	1102	D3T	PA-O3A-PB-O2B

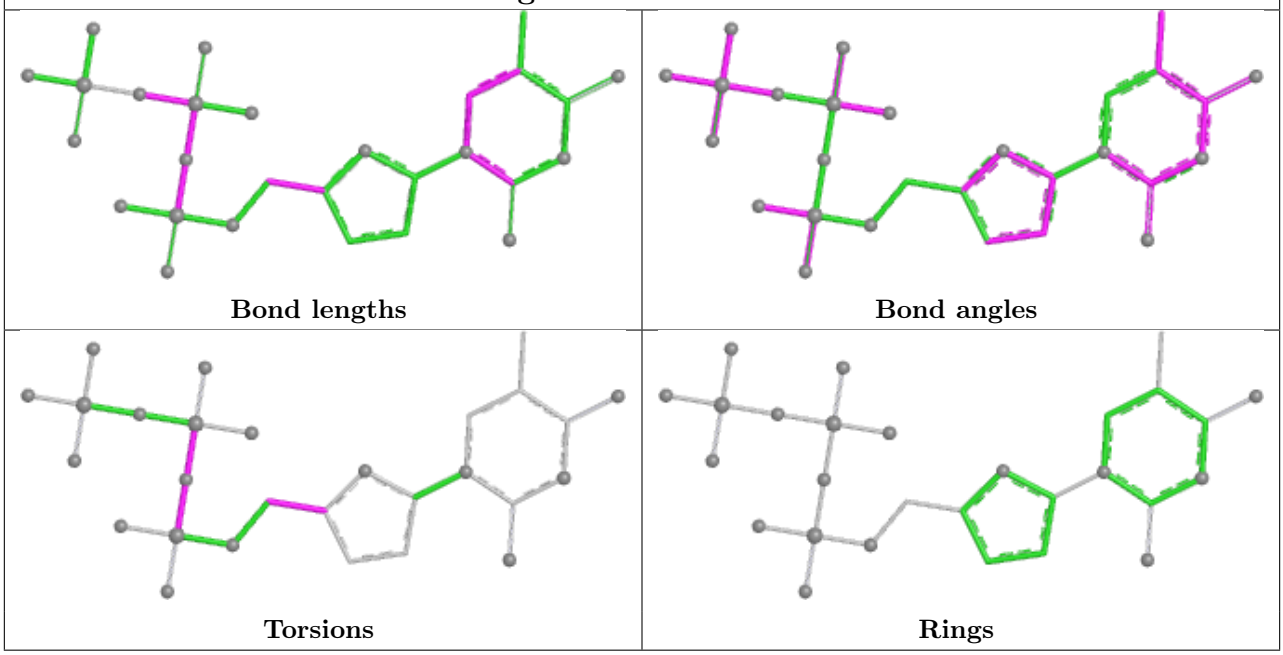
There are no ring outliers.

2 monomers are involved in 5 short contacts:

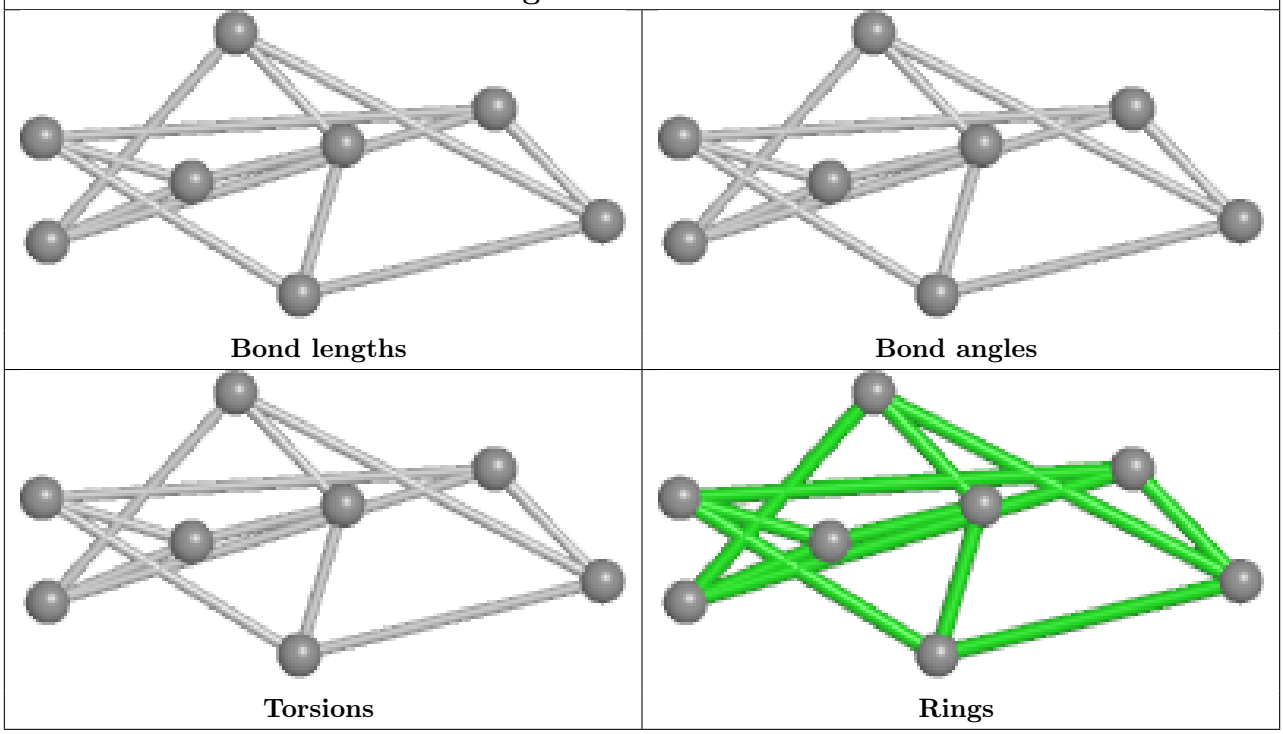
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1102	D3T	4	0
8	A	1101	SF4	1	0

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 then 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 D3T A 1102



Ligand SF4 A 1101



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.

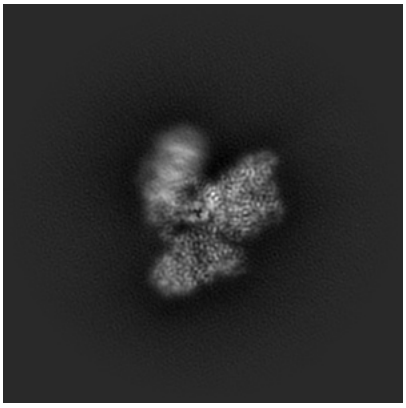
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-22803. These allow visual inspection of the internal detail of the map and identification of artifacts.

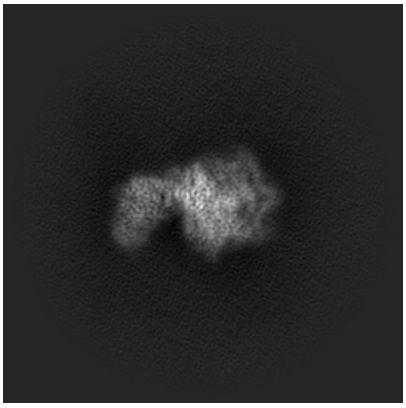
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

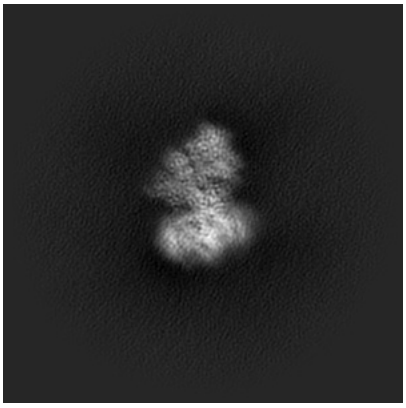
6.1.1 Primary map



X



Y

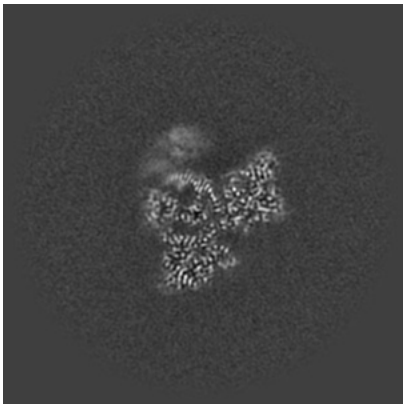


Z

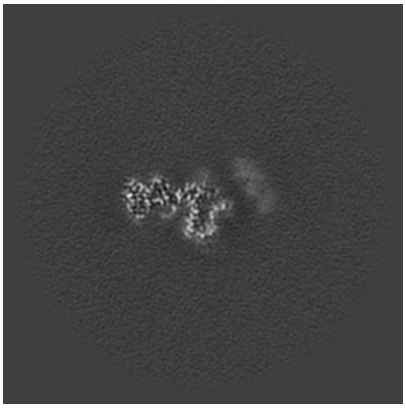
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

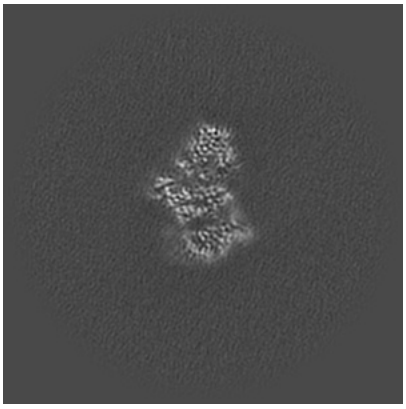
6.2.1 Primary map



X Index: 210



Y Index: 210



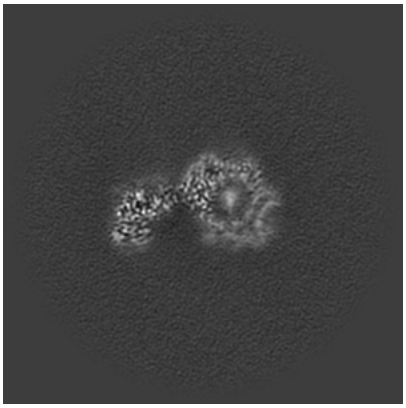
Z Index: 210

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: 218



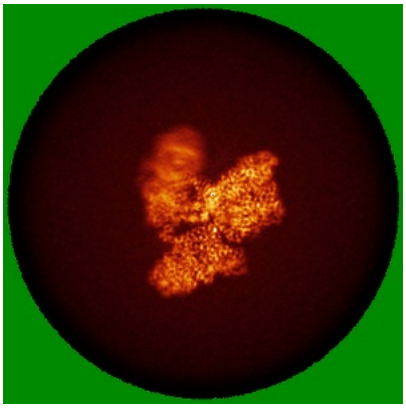
Y Index: 179

Z Index: 206

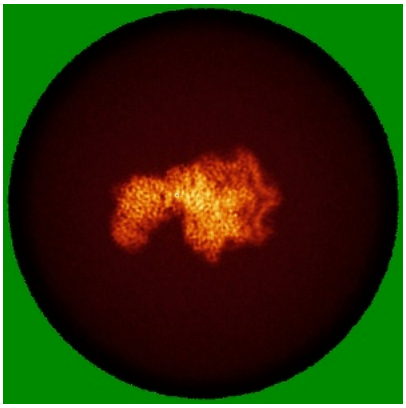
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

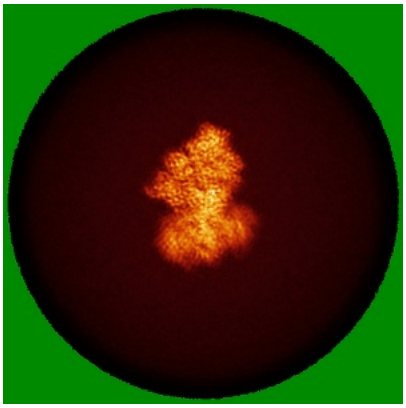
6.4.1 Primary map



X



Y

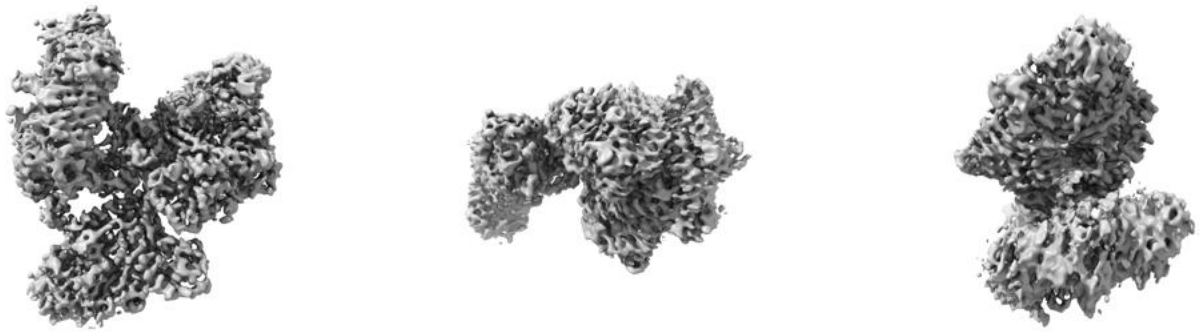


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

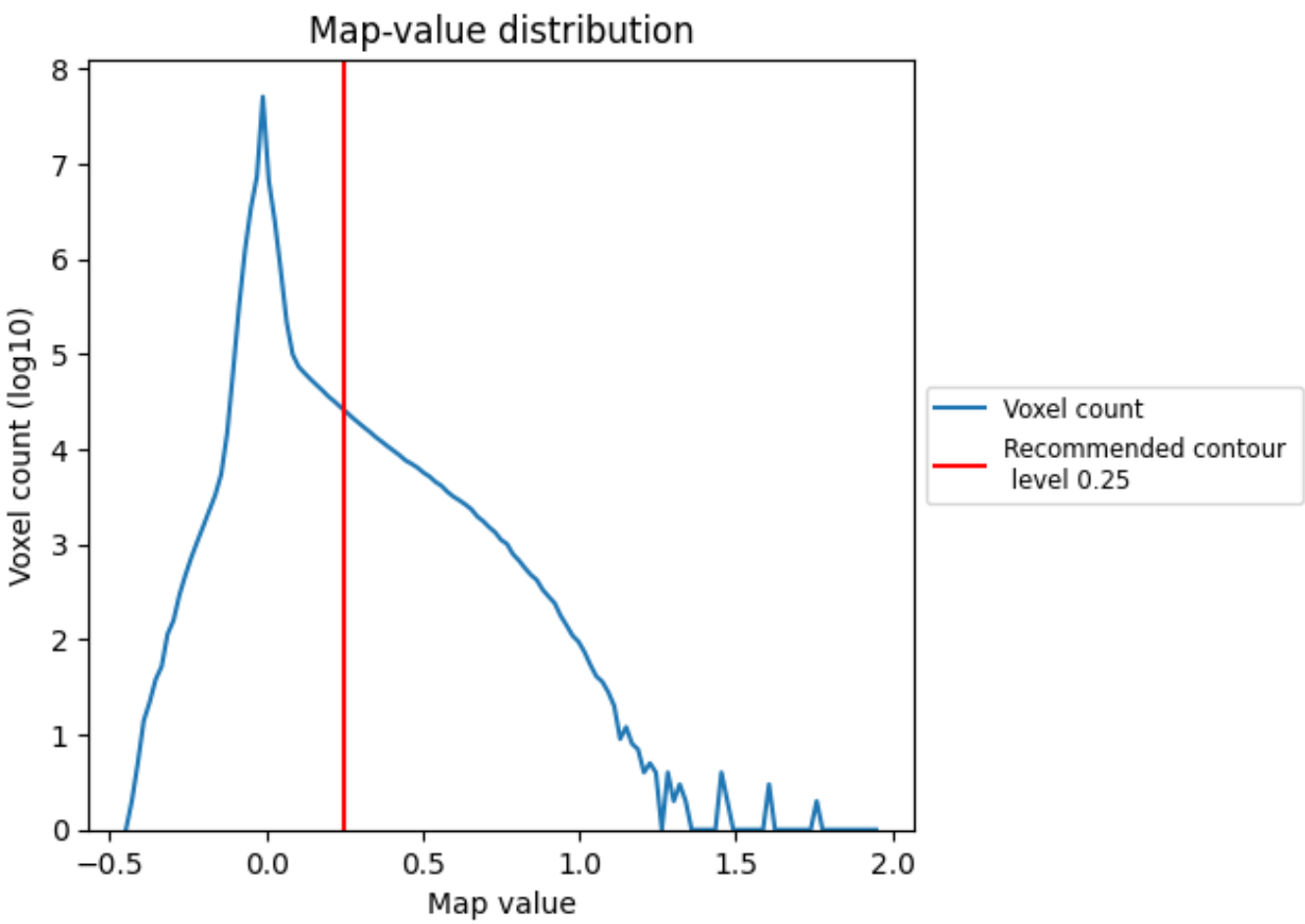
6.6 Mask visualisation (i)

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

7 Map analysis (i)

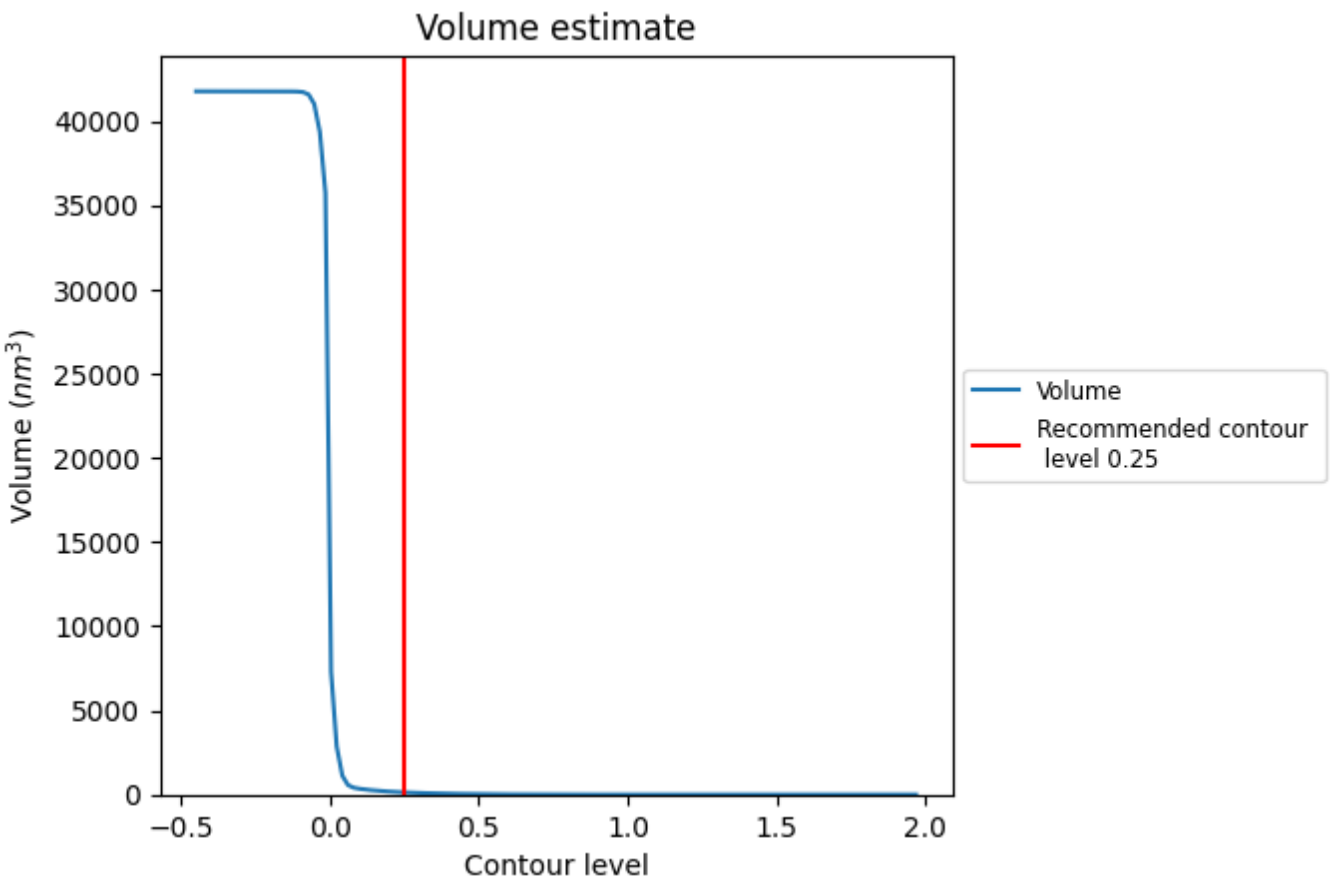
This section contains the results of statistical analysis of the map.

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.

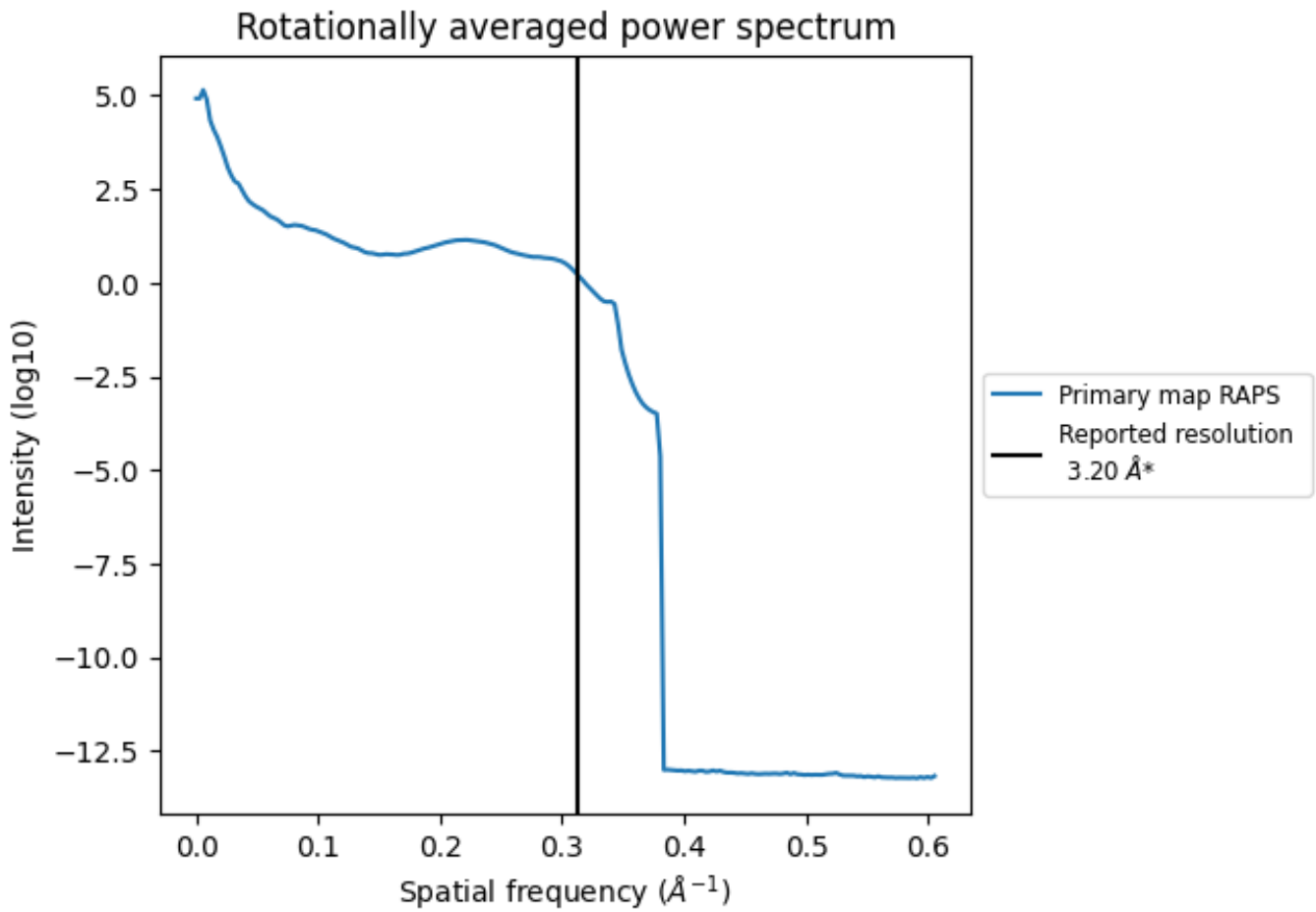
7.2 Volume estimate (i)



The volume at the recommended contour level is 129 nm^3; this corresponds to an approximate mass of 116 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 (i)



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

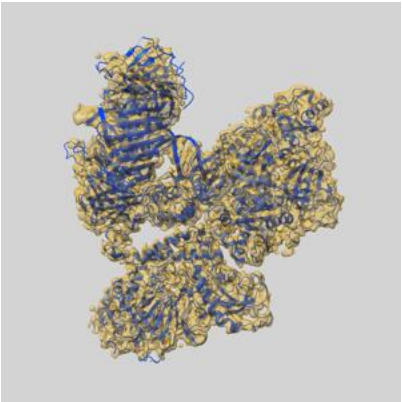
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

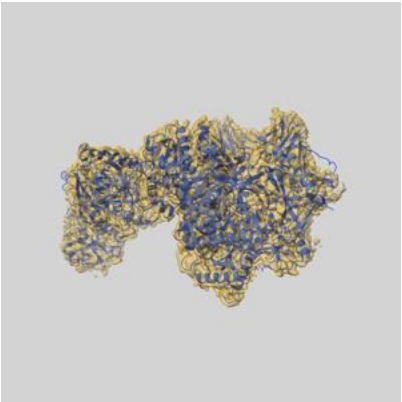
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-22803 and PDB model 7KC0. Per-residue inclusion information can be found in section 3 on page 8.

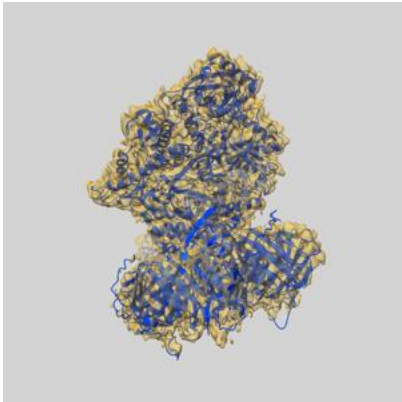
9.1 Map-model overlay (i)



X



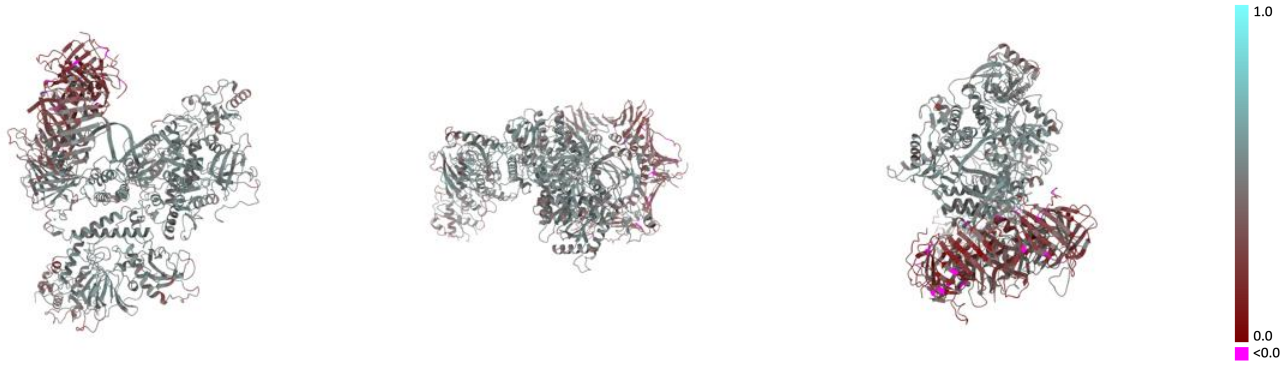
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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.

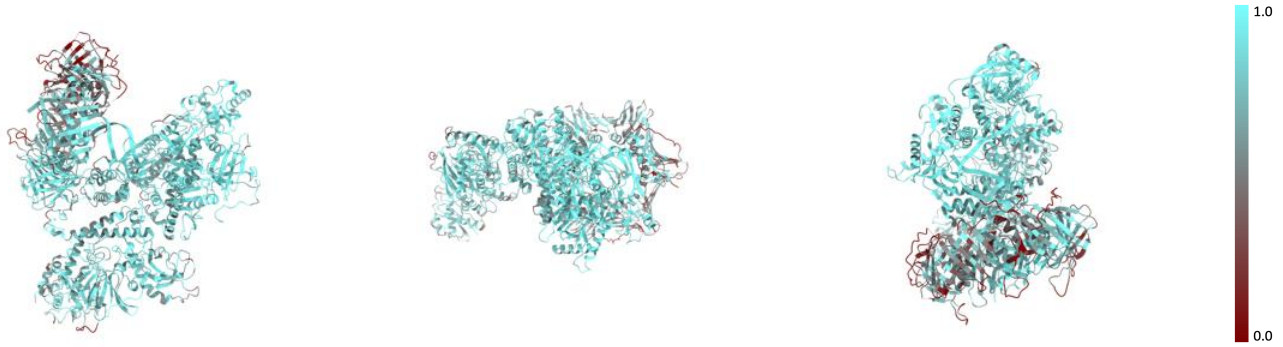
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

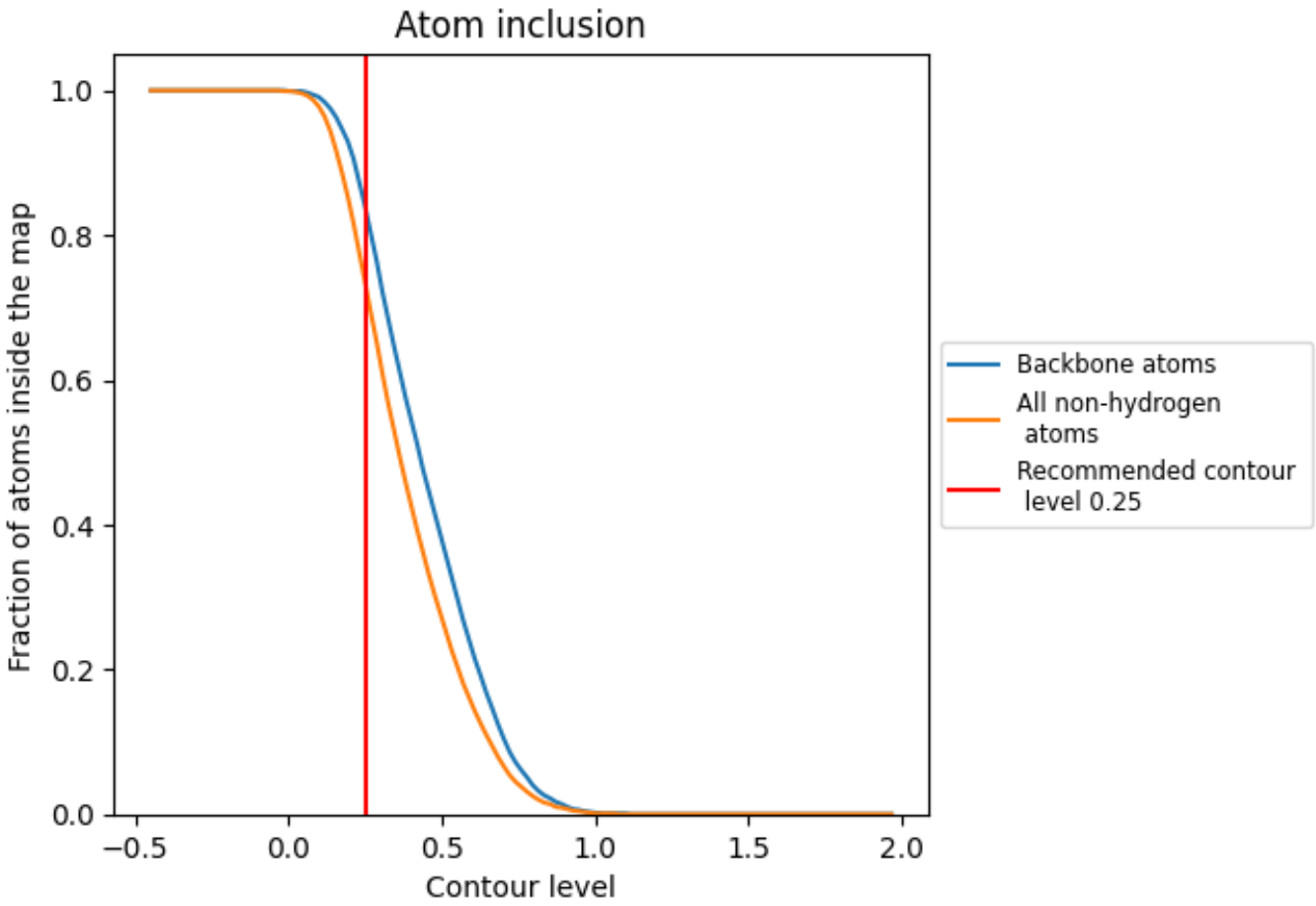
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7360	0.4420
A	0.8430	0.5080
B	0.7810	0.4880
C	0.7240	0.4130
E	0.4410	0.2520
F	0.7430	0.4530
G	0.4440	0.2730
P	0.8380	0.4210
T	0.9160	0.4780