



## Full wwPDB EM Validation Report ⓘ

Jun 9, 2024 – 06:59 AM EDT

PDB ID : 8EXY  
EMDB ID : EMD-28665  
Title : M. tuberculosis RNAP paused complex with B. subtilis NusG and GMPCPP  
Authors : Vishwakarma, R.K.; Murakami, K.S.  
Deposited on : 2022-10-26  
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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

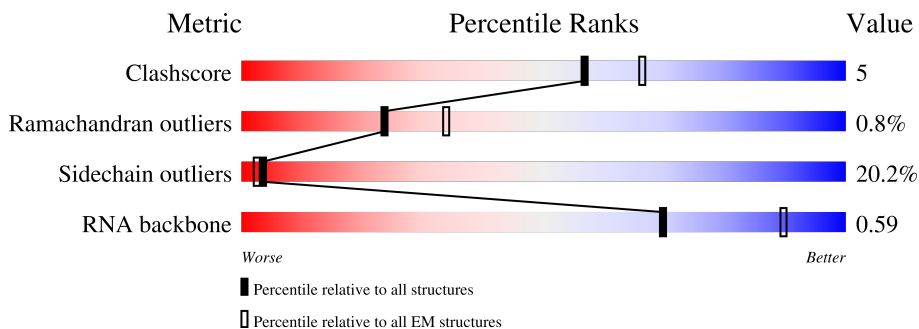
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 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	347	
1	B	347	
2	C	1178	
3	D	1316	
4	E	110	
5	G	177	
6	T	40	

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Mol	Chain	Length	Quality of chain
7	N	40	<div><div></div><div>8%</div><div>52%</div><div>42%</div><div>5%</div></div>
8	R	30	<div><div></div><div>23%</div><div>60%</div><div>33%</div><div></div><div></div></div>

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 25711 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	226	Total	C	N	O	S	0	0
			1724	1085	297	339	3		
1	B	237	Total	C	N	O	S	0	0
			1765	1115	301	346	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1104	Total	C	N	O	S	0	0
			8540	5346	1501	1654	39		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1273	Total	C	N	O	S	0	0
			9953	6229	1811	1872	41		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	83	Total	C	N	O	0	0
			649	414	108	127		

- Molecule 5 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	110	Total	C	N	O	S	1	0
			878	563	147	165	3		

- Molecule 6 is a DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	38	Total	C	N	O	P	0	0
			772	365	142	227	38		

- Molecule 7 is a DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	38	Total	C	N	O	P	0	0
			770	366	132	234	38		

- Molecule 8 is a RNA chain called RNA (29-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	29	Total	C	N	O	P	0	0
			625	278	116	202	29		

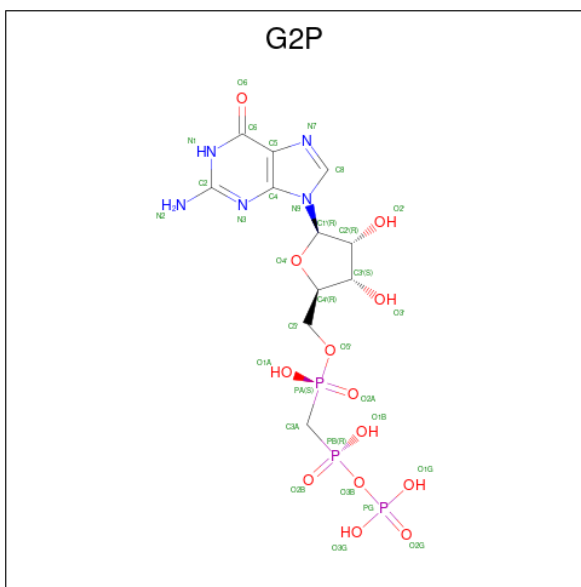
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
9	D	1	Total	Mg	0
			1	1	

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
10	D	2	Total	Zn	0
			2	2	

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: G2P) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

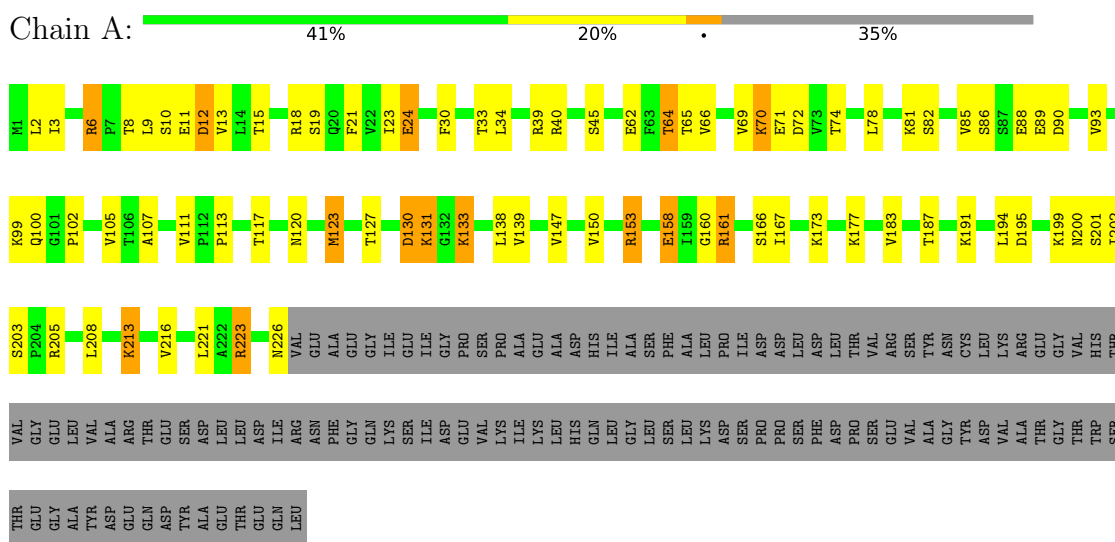


Mol	Chain	Residues	Atoms					AltConf
11	D	1	Total	C	N	O	P	0
			32	11	5	13	3	

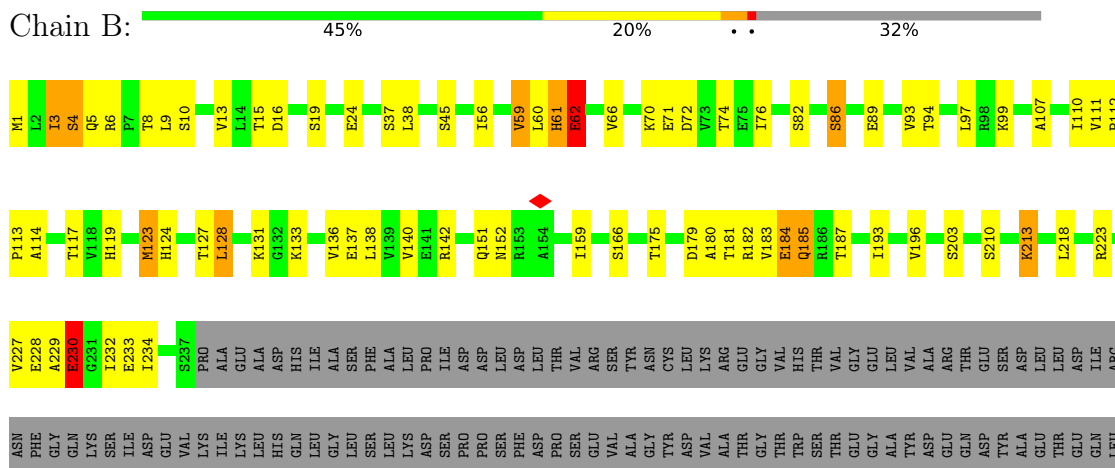
### 3 Residue-property plots

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

#### • Molecule 1: DNA-directed RNA polymerase subunit alpha

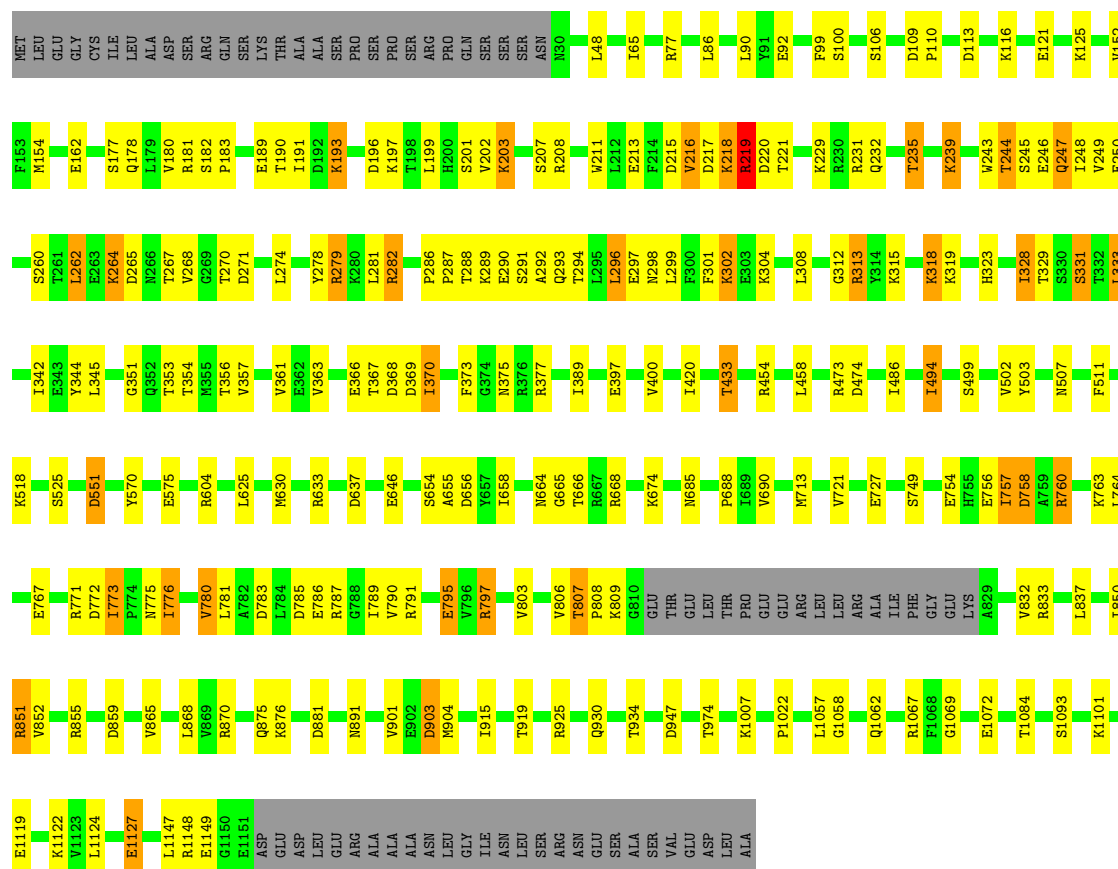


#### • Molecule 1: DNA-directed RNA polymerase subunit alpha

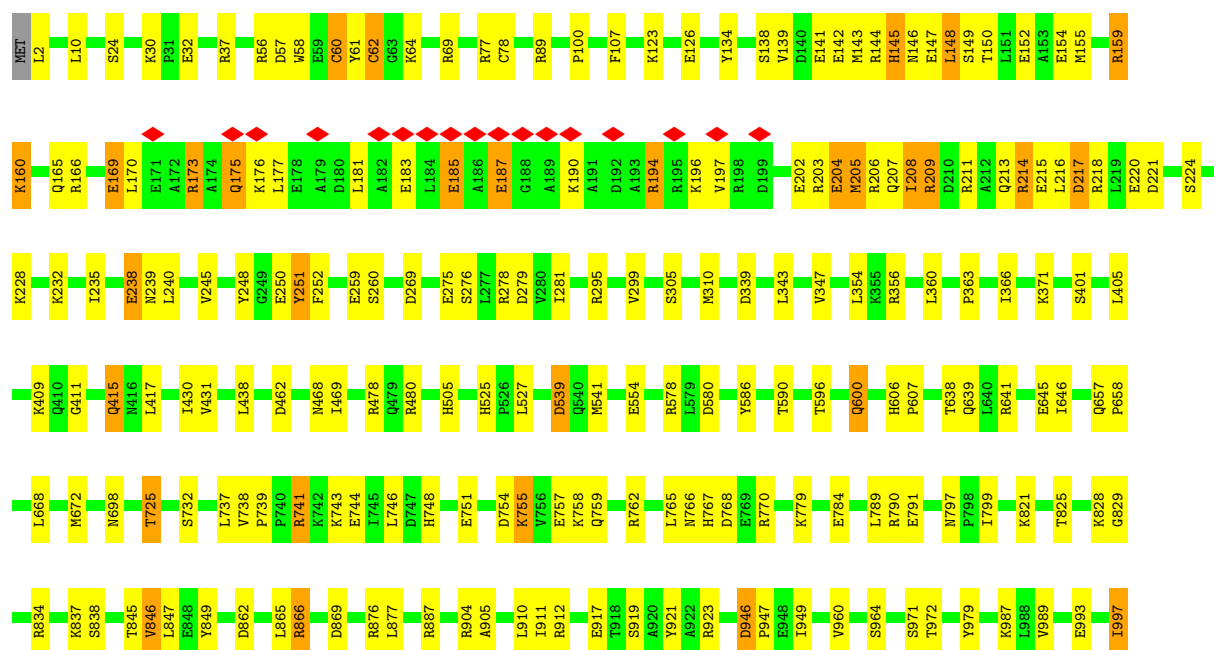
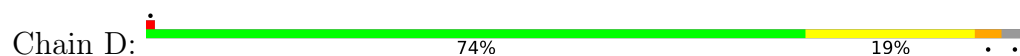


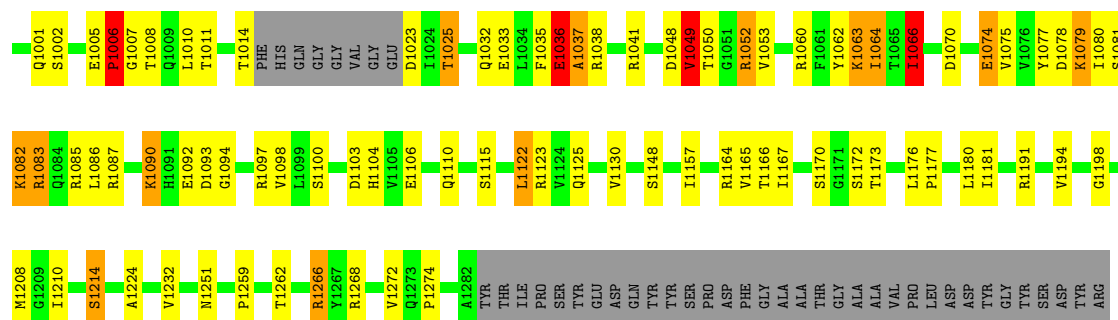
#### • Molecule 2: DNA-directed RNA polymerase subunit beta





• Molecule 3: DNA-directed RNA polymerase subunit beta'

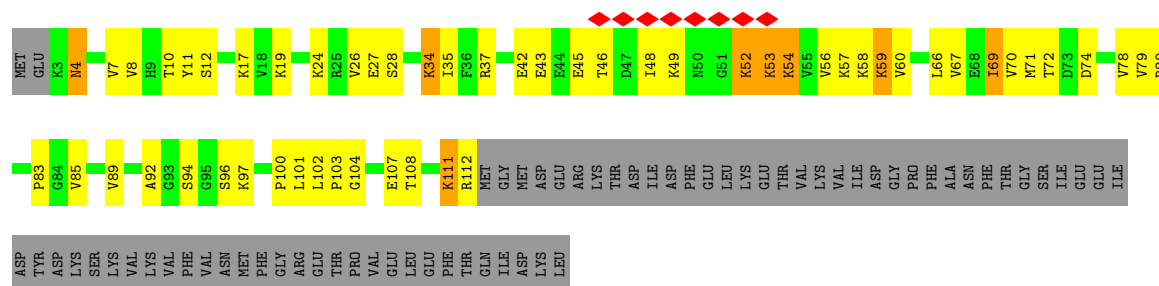
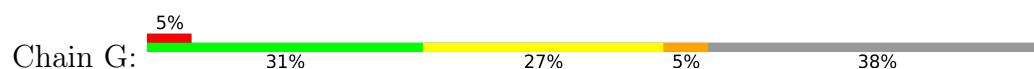




- Molecule 4: DNA-directed RNA polymerase subunit omega



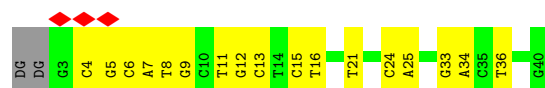
- Molecule 5: Transcription termination/antitermination protein NusG



- Molecule 6: DNA (38-MER)



- Molecule 7: DNA (38-MER)



- Molecule 8: RNA (29-MER)





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	107121	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.814	Depositor
Minimum map value	-0.455	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.064	Depositor
Recommended contour level	0.27	Depositor
Map size (Å)	348.0, 348.0, 348.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	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, ZN, G2P

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	0.27	0/1750	0.56	0/2380
1	B	0.26	0/1792	0.53	0/2442
2	C	0.27	0/8696	0.51	0/11790
3	D	0.27	0/10119	0.53	1/13679 (0.0%)
4	E	0.27	0/662	0.48	0/901
5	G	0.25	0/896	0.44	0/1209
6	T	0.53	0/864	0.86	0/1329
7	N	0.50	0/859	0.93	0/1322
8	R	0.23	0/699	0.75	0/1089
All	All	0.29	0/26337	0.57	1/36141 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1006	PRO	CA-N-CD	-5.39	103.95	111.50

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	1724	0	1768	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1765	0	1794	15	0
2	C	8540	0	8469	79	0
3	D	9953	0	10020	115	0
4	E	649	0	645	4	0
5	G	878	0	896	14	0
6	T	772	0	425	12	0
7	N	770	0	429	14	0
8	R	625	0	314	5	0
9	D	1	0	0	0	0
10	D	2	0	0	0	0
11	D	32	0	13	1	0
All	All	25711	0	24773	256	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 5.

All (256) 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)
1:B:3:ILE:HG13	1:B:234:ILE:HA	1.66	0.76
2:C:776:ILE:HD11	2:C:781:LEU:HG	1.68	0.75
2:C:218:LYS:HD2	2:C:219:ARG:HE	1.53	0.72
3:D:917:GLU:HA	3:D:921:TYR:HD2	1.55	0.72
3:D:1251:ASN:HD22	3:D:1259:PRO:HD3	1.54	0.71
3:D:185:GLU:HA	3:D:194:ARG:HG2	1.72	0.71
3:D:1194:VAL:HA	3:D:1198:GLY:HA2	1.74	0.70
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.73	0.69
3:D:159:ARG:HH22	3:D:220:GLU:HB2	1.59	0.68
3:D:123:LYS:NZ	7:N:36:DT:OP2	2.29	0.65
3:D:1053:VAL:HA	3:D:1066:ILE:HA	1.79	0.65
3:D:275:GLU:OE2	3:D:278:ARG:NH2	2.29	0.64
3:D:1053:VAL:HG12	3:D:1066:ILE:HG12	1.78	0.64
7:N:15:DC:H2''	7:N:16:DT:H5'	1.80	0.64
2:C:1058:GLY:O	2:C:1062:GLN:NE2	2.31	0.64
3:D:181:LEU:HA	3:D:194:ARG:HH21	1.62	0.64
3:D:238:GLU:HG3	5:G:92:ALA:HB1	1.80	0.64
3:D:1122:LEU:HG	3:D:1130:VAL:HG21	1.79	0.63
1:A:153:ARG:HG3	2:C:795:GLU:HB3	1.80	0.63
3:D:62:CYS:HB3	3:D:78:CYS:SG	2.37	0.63
3:D:1167:ILE:HD11	3:D:1181:ILE:HD11	1.81	0.63
3:D:739:PRO:HG3	3:D:789:LEU:HD13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:SER:HB3	1:B:119:HIS:HE1	1.64	0.62
3:D:877:LEU:HD22	3:D:1157:ILE:HD13	1.82	0.62
2:C:1122:LYS:NZ	2:C:1149:GLU:OE2	2.33	0.61
3:D:1086:LEU:HB2	3:D:1098:VAL:HB	1.82	0.61
2:C:486:ILE:HD11	3:D:849:TYR:HE2	1.66	0.61
5:G:53:LYS:HZ2	5:G:54:LYS:H	1.47	0.61
3:D:751:GLU:OE1	3:D:755:LYS:NZ	2.35	0.60
3:D:1274:PRO:HG3	4:E:79:VAL:HG21	1.84	0.60
2:C:1119:GLU:OE2	3:D:89:ARG:NH2	2.33	0.59
3:D:866:ARG:HG2	3:D:1025:THR:HB	1.85	0.58
3:D:641:ARG:HA	3:D:657:GLN:HG3	1.86	0.58
2:C:807:THR:HG23	2:C:833:ARG:HB2	1.86	0.58
1:A:102:PRO:HG3	1:A:130:ASP:HB3	1.85	0.58
3:D:1007:GLY:O	3:D:1011:THR:HG23	2.03	0.58
1:A:40:ARG:NH1	2:C:903:ASP:OD1	2.35	0.57
2:C:369:ASP:O	2:C:375:ASN:ND2	2.35	0.57
3:D:214:ARG:HH21	3:D:215:GLU:HB2	1.69	0.57
6:T:26:DG:H1	7:N:16:DT:H3	1.52	0.57
2:C:551:ASP:OD1	2:C:551:ASP:N	2.30	0.57
3:D:1063:LYS:HG3	3:D:1078:ASP:HA	1.87	0.57
8:R:20:C:O2	8:R:21:A:N6	2.38	0.57
2:C:654:SER:OG	2:C:655:ALA:N	2.39	0.56
3:D:1060:ARG:HG2	3:D:1083:ARG:HH22	1.70	0.56
2:C:278:TYR:HD2	2:C:287:PRO:HA	1.71	0.56
2:C:86:LEU:HD21	2:C:389:ILE:HD13	1.88	0.56
1:A:69:VAL:HG12	1:A:71:GLU:H	1.70	0.55
3:D:1092:GLU:HG3	3:D:1104:HIS:HB3	1.88	0.55
3:D:1166:THR:HG22	3:D:1180:LEU:HD23	1.88	0.55
3:D:64:LYS:HB2	3:D:77:ARG:HH21	1.71	0.55
3:D:204:GLU:O	3:D:208:ILE:HG13	2.07	0.55
3:D:638:THR:HG22	3:D:639:GLN:HG2	1.88	0.55
3:D:203:ARG:HG3	3:D:206:ARG:HH21	1.73	0.54
3:D:147:GLU:HA	3:D:150:THR:HB	1.90	0.54
6:T:30:DA:H61	7:N:11:DT:H3	1.55	0.54
2:C:433:THR:O	2:C:433:THR:OG1	2.24	0.54
3:D:1210:ILE:O	3:D:1214:SER:OG	2.25	0.54
6:T:4:DC:H2"	6:T:5:DA:C8	2.43	0.54
1:B:86:SER:HB3	1:B:119:HIS:CE1	2.43	0.53
2:C:727:GLU:H	3:D:725:THR:HG21	1.74	0.53
3:D:946:ASP:OD1	3:D:947:PRO:HD3	2.08	0.53
2:C:308:LEU:O	2:C:331:SER:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:430:ILE:HG21	3:D:541:MET:HG3	1.90	0.53
2:C:757:ILE:HD13	2:C:837:LEU:HB2	1.91	0.52
2:C:178:GLN:NE2	2:C:458:LEU:O	2.43	0.52
6:T:15:DT:H2'	6:T:16:DA:C8	2.45	0.52
2:C:235:THR:HG21	2:C:262:LEU:HA	1.91	0.51
3:D:904:ARG:HG3	3:D:910:LEU:HD23	1.93	0.51
3:D:1035:PHE:C	3:D:1037:ALA:H	2.13	0.51
2:C:243:TRP:HE3	2:C:248:ILE:HG12	1.76	0.51
3:D:845:THR:HG22	3:D:846:VAL:H	1.75	0.51
3:D:1062:TYR:N	3:D:1080:ILE:O	2.43	0.51
5:G:103:PRO:O	5:G:107:GLU:HG2	2.11	0.51
3:D:1005:GLU:HB3	3:D:1006:PRO:HD2	1.92	0.51
7:N:4:DC:H2''	7:N:5:DG:C8	2.46	0.51
1:A:223:ARG:HH12	1:B:213:LYS:HG3	1.76	0.50
6:T:36:DC:H2''	6:T:37:DG:C8	2.47	0.50
3:D:1090:LYS:HE2	3:D:1094:GLY:HA2	1.92	0.50
1:A:70:LYS:O	1:A:70:LYS:HG2	2.11	0.50
4:E:67:TYR:HD1	4:E:76:LEU:HD11	1.77	0.49
5:G:104:GLY:O	5:G:108:THR:HG23	2.12	0.49
6:T:26:DG:H22	7:N:16:DT:H3	1.59	0.49
6:T:32:DC:H2''	6:T:33:DA:C8	2.48	0.49
2:C:154:MET:HA	2:C:420:ILE:HD12	1.95	0.49
2:C:183:PRO:O	2:C:312:GLY:HA2	2.12	0.49
3:D:657:GLN:N	3:D:658:PRO:HD2	2.27	0.49
4:E:40:ILE:HG12	4:E:44:LEU:HD13	1.95	0.49
2:C:282:ARG:HH22	7:N:21:DT:H5'	1.77	0.48
2:C:925:ARG:NH1	11:D:2004:G2P:O2G	2.46	0.48
3:D:645:GLU:HG2	3:D:646:ILE:N	2.28	0.48
2:C:278:TYR:O	2:C:282:ARG:HB2	2.13	0.48
2:C:760:ARG:HE	2:C:760:ARG:HB3	1.39	0.48
1:B:56:ILE:HG23	1:B:59:VAL:HG21	1.96	0.48
3:D:37:ARG:NH2	7:N:13:DC:OP2	2.42	0.48
3:D:141:GLU:O	3:D:145:HIS:HB3	2.13	0.48
6:T:34:DT:H2''	6:T:35:DG:C8	2.48	0.48
7:N:6:DC:H2''	7:N:7:DA:C8	2.49	0.48
7:N:24:DC:H1'	7:N:25:DA:C8	2.48	0.48
6:T:15:DT:H2'	6:T:16:DA:H8	1.78	0.48
3:D:1062:TYR:CE2	3:D:1082:LYS:HA	2.48	0.48
2:C:278:TYR:HB2	2:C:292:ALA:HB2	1.96	0.48
3:D:1005:GLU:HB3	3:D:1006:PRO:CD	2.44	0.48
7:N:15:DC:H2'	7:N:16:DT:H71	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:160:LYS:HA	3:D:160:LYS:HD2	1.41	0.47
2:C:809:LYS:HG3	2:C:833:ARG:HH22	1.79	0.47
3:D:979:TYR:HD2	3:D:989:VAL:HG21	1.78	0.47
3:D:1052:ARG:HA	3:D:1104:HIS:HA	1.96	0.47
3:D:295:ARG:O	3:D:299:VAL:HG23	2.15	0.47
2:C:370:ILE:H	2:C:370:ILE:HG13	1.50	0.47
3:D:177:LEU:O	3:D:181:LEU:HG	2.15	0.47
1:A:158:GLU:CD	1:A:160:GLY:H	2.19	0.47
3:D:1002:SER:O	3:D:1006:PRO:HD2	2.14	0.47
2:C:930:GLN:O	2:C:934:THR:HG23	2.15	0.46
3:D:1170:SER:O	3:D:1173:THR:OG1	2.25	0.46
6:T:22:DC:H2''	6:T:23:DC:H5'	1.96	0.46
3:D:409:LYS:NZ	6:T:14:DC:OP1	2.46	0.46
3:D:525:HIS:HD2	3:D:527:LEU:HB2	1.79	0.46
3:D:1053:VAL:HG22	3:D:1103:ASP:H	1.79	0.46
3:D:905:ALA:HB2	3:D:911:ILE:HD11	1.97	0.46
2:C:756:GLU:HB3	2:C:870:ARG:HG2	1.97	0.46
3:D:150:THR:O	3:D:154:GLU:HG2	2.16	0.46
3:D:169:GLU:OE2	3:D:209:ARG:NH2	2.47	0.46
1:B:233:GLU:H	1:B:233:GLU:HG2	1.57	0.46
3:D:1224:ALA:HA	3:D:1232:VAL:HG21	1.96	0.46
5:G:111:LYS:HA	5:G:111:LYS:HD3	1.60	0.46
2:C:1147:LEU:HD12	3:D:2:LEU:HD13	1.97	0.46
3:D:866:ARG:HA	3:D:866:ARG:HD3	1.75	0.46
5:G:26:VAL:HG22	5:G:35:ILE:HD13	1.98	0.46
5:G:74:ASP:O	5:G:78:VAL:HG12	2.16	0.46
2:C:757:ILE:HG13	2:C:758:ASP:H	1.81	0.46
3:D:1063:LYS:HB2	3:D:1063:LYS:HE2	1.66	0.46
1:A:64:THR:HG23	1:A:65:THR:N	2.31	0.45
3:D:755:LYS:HA	3:D:755:LYS:HD3	1.52	0.45
2:C:298:ASN:HA	2:C:302:LYS:HG2	1.98	0.45
2:C:1007:LYS:HB3	2:C:1022:PRO:HB2	1.98	0.45
3:D:194:ARG:HA	3:D:197:VAL:HG22	1.98	0.45
3:D:214:ARG:HA	3:D:217:ASP:OD2	2.16	0.45
3:D:1164:ARG:HD2	3:D:1208:MET:SD	2.56	0.45
7:N:8:DT:H2''	7:N:9:DG:C8	2.51	0.45
2:C:216:VAL:HG22	2:C:345:LEU:HD21	1.99	0.45
2:C:333:LEU:HD23	2:C:333:LEU:HA	1.87	0.45
2:C:633:ARG:NH2	2:C:637:ASP:OD2	2.39	0.45
3:D:209:ARG:HA	3:D:209:ARG:HD3	1.55	0.45
2:C:721:VAL:HG13	2:C:915:ILE:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1084:THR:OG1	3:D:554:GLU:OE1	2.34	0.45
5:G:53:LYS:HD2	5:G:53:LYS:HA	1.54	0.45
1:A:11:GLU:HG2	1:A:12:ASP:N	2.32	0.45
2:C:674:LYS:HA	2:C:674:LYS:HD2	1.81	0.45
3:D:343:LEU:O	3:D:347:VAL:HG23	2.17	0.44
8:R:17:C:H2'	8:R:18:G:H8	1.81	0.44
1:B:182:ARG:NH1	1:B:184:GLU:O	2.48	0.44
3:D:194:ARG:HA	3:D:194:ARG:HD2	1.64	0.44
2:C:279:ARG:HA	2:C:287:PRO:HG3	1.99	0.44
2:C:328:ILE:H	2:C:328:ILE:HG12	1.67	0.44
3:D:173:ARG:HE	3:D:173:ARG:HB3	1.57	0.44
1:B:107:ALA:HB2	1:B:123:MET:HG2	1.99	0.44
2:C:664:ASN:OD1	2:C:665:GLY:N	2.51	0.44
1:B:61:HIS:HB2	1:B:62:GLU:H	1.60	0.44
3:D:554:GLU:HG3	4:E:54:VAL:HG11	1.98	0.44
3:D:979:TYR:CD2	3:D:989:VAL:HG21	2.52	0.44
2:C:239:LYS:HE2	2:C:239:LYS:HB2	1.61	0.44
3:D:997:ILE:O	3:D:1001:GLN:HG3	2.17	0.44
5:G:59:LYS:H	5:G:59:LYS:HG2	1.36	0.44
2:C:90:LEU:HD12	2:C:110:PRO:HG3	2.00	0.44
1:A:6:ARG:HE	1:A:6:ARG:HB2	1.60	0.44
1:A:24:GLU:HG2	1:A:191:LYS:HD2	1.99	0.44
2:C:121:GLU:O	2:C:125:LYS:HG2	2.18	0.44
3:D:363:PRO:HG2	3:D:366:ILE:HD12	1.98	0.44
2:C:1127:GLU:OE2	3:D:405:LEU:HD12	2.17	0.43
3:D:100:PRO:HD2	3:D:259:GLU:HG3	2.00	0.43
5:G:69:ILE:HD12	5:G:79:VAL:HG21	2.00	0.43
7:N:33:DG:H2''	7:N:34:DA:C8	2.52	0.43
1:A:133:LYS:HE2	1:A:133:LYS:HB2	1.89	0.43
2:C:282:ARG:HA	2:C:282:ARG:HD3	1.77	0.43
2:C:604:ARG:HA	2:C:604:ARG:HD2	1.71	0.43
3:D:278:ARG:HA	3:D:281:ILE:HG22	1.98	0.43
3:D:1077:TYR:HB3	3:D:1080:ILE:HD11	2.00	0.43
2:C:1101:LYS:HB2	2:C:1101:LYS:HE2	1.78	0.43
1:A:213:LYS:HB3	1:A:213:LYS:HE2	1.42	0.43
2:C:313:ARG:HA	2:C:313:ARG:HD2	1.49	0.43
3:D:57:ASP:HB3	3:D:58:TRP:CD1	2.53	0.43
3:D:668:LEU:O	3:D:672:MET:HG3	2.18	0.43
3:D:60:CYS:SG	3:D:61:TYR:N	2.92	0.43
3:D:469:ILE:HD13	3:D:469:ILE:HA	1.85	0.43
1:B:112:PRO:HA	1:B:113:PRO:HD3	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:299:LEU:HD23	2:C:299:LEU:HA	1.82	0.43
2:C:318:LYS:HB2	2:C:318:LYS:HE3	1.93	0.43
5:G:52:LYS:HE3	5:G:52:LYS:HB2	1.30	0.43
1:A:139:VAL:HG21	1:A:161:ARG:HH12	1.83	0.42
2:C:244:THR:HG22	2:C:247:GLN:HG3	2.00	0.42
3:D:354:LEU:HD21	3:D:371:LYS:HG2	2.01	0.42
3:D:1266:ARG:H	3:D:1266:ARG:HG3	1.67	0.42
8:R:8:C:H2'	8:R:9:U:O4'	2.19	0.42
1:B:213:LYS:HB3	1:B:213:LYS:HE3	1.43	0.42
3:D:949:ILE:HD13	3:D:949:ILE:HA	1.82	0.42
5:G:54:LYS:HB2	5:G:54:LYS:HE2	1.33	0.42
1:A:11:GLU:HG3	1:A:21:PHE:CE2	2.54	0.42
1:A:107:ALA:HB2	1:A:123:MET:HG2	2.02	0.42
3:D:1083:ARG:H	3:D:1083:ARG:HG2	1.60	0.42
5:G:4:ASN:HB2	5:G:100:PRO:HB3	2.01	0.42
1:B:185:GLN:H	1:B:185:GLN:HG3	1.55	0.42
3:D:134:TYR:HB2	3:D:235:ILE:HG23	2.01	0.42
2:C:397:GLU:HA	2:C:400:VAL:HG12	2.01	0.42
2:C:851:ARG:HA	2:C:851:ARG:HD2	1.78	0.42
3:D:1052:ARG:HE	3:D:1104:HIS:HB2	1.84	0.42
2:C:1124:LEU:HD22	3:D:417:LEU:HD11	2.01	0.42
3:D:187:GLU:H	3:D:187:GLU:HG2	1.50	0.42
8:R:4:G:H2'	8:R:5:A:H8	1.83	0.42
2:C:518:LYS:O	2:C:525:SER:OG	2.24	0.42
3:D:539:ASP:OD1	3:D:539:ASP:N	2.52	0.42
1:A:153:ARG:HB2	2:C:797:ARG:HH12	1.85	0.42
2:C:773:ILE:HB	2:C:776:ILE:HG12	2.02	0.42
1:B:179:ASP:HB3	1:B:180:ALA:H	1.70	0.41
2:C:193:LYS:HE2	2:C:193:LYS:HB3	1.48	0.41
3:D:30:LYS:HB3	3:D:32:GLU:HG3	2.02	0.41
2:C:279:ARG:CZ	2:C:287:PRO:HG2	2.51	0.41
2:C:473:ARG:HD3	2:C:494:ILE:O	2.20	0.41
2:C:502:VAL:HG23	2:C:503:TYR:CD2	2.56	0.41
2:C:507:ASN:HB2	2:C:511:PHE:O	2.21	0.41
3:D:175:GLN:HG2	3:D:176:LYS:N	2.35	0.41
3:D:600:GLN:HE21	3:D:600:GLN:HB3	1.53	0.41
3:D:1064:ILE:HG23	3:D:1077:TYR:HB2	2.03	0.41
3:D:1079:LYS:HA	3:D:1079:LYS:HD2	1.70	0.41
2:C:296:LEU:HD22	2:C:296:LEU:HA	1.81	0.41
2:C:809:LYS:HE2	2:C:833:ARG:HH12	1.85	0.41
3:D:1074:GLU:H	3:D:1074:GLU:HG2	1.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:17:C:H2'	8:R:18:G:C8	2.56	0.41
1:B:128:LEU:HD13	1:B:128:LEU:HA	1.87	0.41
1:B:229:ALA:O	1:B:230:GLU:HB3	2.20	0.41
3:D:411:GLY:O	3:D:415:GLN:HB2	2.21	0.41
3:D:876:ARG:NH1	3:D:1036:GLU:HG3	2.36	0.41
7:N:12:DG:H1'	7:N:13:DC:H5'	2.02	0.41
2:C:278:TYR:CZ	2:C:282:ARG:HG3	2.55	0.41
2:C:286:PRO:HA	2:C:287:PRO:HD3	1.96	0.41
3:D:147:GLU:HG3	3:D:251:TYR:OH	2.20	0.41
2:C:1057:LEU:HD23	2:C:1057:LEU:HA	1.89	0.41
3:D:430:ILE:CG2	3:D:541:MET:HG3	2.50	0.41
3:D:751:GLU:HA	3:D:754:ASP:OD2	2.21	0.41
1:A:161:ARG:HE	1:A:161:ARG:HB2	1.77	0.41
2:C:630:MET:O	2:C:630:MET:HG3	2.21	0.41
2:C:781:LEU:HD23	2:C:781:LEU:HA	1.80	0.41
2:C:797:ARG:H	2:C:797:ARG:HG2	1.74	0.41
3:D:586:TYR:O	3:D:590:THR:OG1	2.30	0.41
5:G:34:LYS:HG3	5:G:70:VAL:HB	2.03	0.41
3:D:69:ARG:HE	3:D:69:ARG:HB2	1.68	0.41
6:T:37:DG:H2''	6:T:38:DC:C6	2.55	0.41
2:C:202:VAL:HG12	2:C:203:LYS:H	1.85	0.40
2:C:656:ASP:OD1	2:C:656:ASP:N	2.54	0.40
2:C:1069:GLY:N	2:C:1072:GLU:OE1	2.41	0.40
3:D:741:ARG:H	3:D:741:ARG:HG3	1.82	0.40
3:D:1062:TYR:CE1	3:D:1082:LYS:HD2	2.56	0.40
1:A:131:LYS:HE3	1:A:131:LYS:HB3	1.57	0.40
3:D:1049:VAL:HB	3:D:1050:THR:H	1.73	0.40
3:D:146:ASN:C	3:D:148:LEU:N	2.75	0.40
3:D:205:MET:HE2	3:D:205:MET:HB3	1.84	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	224/347 (65%)	186 (83%)	36 (16%)	2 (1%)	17	56
1	B	235/347 (68%)	186 (79%)	44 (19%)	5 (2%)	7	37
2	C	1100/1178 (93%)	1003 (91%)	90 (8%)	7 (1%)	25	64
3	D	1269/1316 (96%)	1172 (92%)	90 (7%)	7 (1%)	25	64
4	E	81/110 (74%)	81 (100%)	0	0	100	100
5	G	109/177 (62%)	83 (76%)	24 (22%)	2 (2%)	8	41
All	All	3018/3475 (87%)	2711 (90%)	284 (9%)	23 (1%)	24	58

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	1037	ALA
1	B	4	SER
3	D	1066	ILE
5	G	11	TYR
1	B	62	GLU
2	C	264	LYS
2	C	297	GLU
3	D	1036	GLU
1	A	113	PRO
1	A	199	LYS
1	B	114	ALA
2	C	219	ARG
3	D	607	PRO
1	B	184	GLU
2	C	373	PHE
2	C	808	PRO
3	D	829	GLY
1	B	230	GLU
3	D	251	TYR
5	G	83	PRO
2	C	780	VAL
3	D	1049	VAL
2	C	351	GLY

### 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	195/297 (66%)	126 (65%)	69 (35%)	0	0
1	B	195/297 (66%)	128 (66%)	67 (34%)	0	0
2	C	929/998 (93%)	775 (83%)	154 (17%)	2	10
3	D	1054/1095 (96%)	879 (83%)	175 (17%)	2	10
4	E	69/90 (77%)	62 (90%)	7 (10%)	7	29
5	G	98/159 (62%)	57 (58%)	41 (42%)	0	0
All	All	2540/2936 (86%)	2027 (80%)	513 (20%)	3	6

All (513) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	3	ILE
1	A	6	ARG
1	A	8	THR
1	A	9	LEU
1	A	10	SER
1	A	12	ASP
1	A	13	VAL
1	A	15	THR
1	A	18	ARG
1	A	19	SER
1	A	23	ILE
1	A	24	GLU
1	A	30	PHE
1	A	33	THR
1	A	34	LEU
1	A	39	ARG
1	A	45	SER
1	A	62	GLU
1	A	64	THR
1	A	66	VAL
1	A	70	LYS
1	A	72	ASP
1	A	74	THR
1	A	78	LEU
1	A	81	LYS
1	A	82	SER

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Mol	Chain	Res	Type
1	A	85	VAL
1	A	86	SER
1	A	88	GLU
1	A	89	GLU
1	A	90	ASP
1	A	93	VAL
1	A	99	LYS
1	A	100	GLN
1	A	105	VAL
1	A	111	VAL
1	A	117	THR
1	A	120	ASN
1	A	123	MET
1	A	127	THR
1	A	130	ASP
1	A	131	LYS
1	A	133	LYS
1	A	138	LEU
1	A	147	VAL
1	A	150	VAL
1	A	153	ARG
1	A	158	GLU
1	A	161	ARG
1	A	166	SER
1	A	167	ILE
1	A	173	LYS
1	A	177	LYS
1	A	183	VAL
1	A	187	THR
1	A	194	LEU
1	A	195	ASP
1	A	200	ASN
1	A	201	SER
1	A	202	ILE
1	A	203	SER
1	A	205	ARG
1	A	208	LEU
1	A	213	LYS
1	A	216	VAL
1	A	221	LEU
1	A	223	ARG
1	A	226	ASN

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Mol	Chain	Res	Type
1	B	1	MET
1	B	3	ILE
1	B	4	SER
1	B	5	GLN
1	B	6	ARG
1	B	8	THR
1	B	9	LEU
1	B	10	SER
1	B	13	VAL
1	B	15	THR
1	B	16	ASP
1	B	19	SER
1	B	24	GLU
1	B	37	SER
1	B	38	LEU
1	B	45	SER
1	B	59	VAL
1	B	60	LEU
1	B	61	HIS
1	B	62	GLU
1	B	66	VAL
1	B	70	LYS
1	B	71	GLU
1	B	72	ASP
1	B	74	THR
1	B	76	ILE
1	B	82	SER
1	B	86	SER
1	B	89	GLU
1	B	93	VAL
1	B	94	THR
1	B	97	LEU
1	B	99	LYS
1	B	110	ILE
1	B	111	VAL
1	B	117	THR
1	B	123	MET
1	B	124	HIS
1	B	127	THR
1	B	128	LEU
1	B	131	LYS
1	B	133	LYS

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Mol	Chain	Res	Type
1	B	136	VAL
1	B	137	GLU
1	B	138	LEU
1	B	140	VAL
1	B	142	ARG
1	B	151	GLN
1	B	152	ASN
1	B	159	ILE
1	B	166	SER
1	B	175	THR
1	B	181	THR
1	B	183	VAL
1	B	185	GLN
1	B	187	THR
1	B	193	ILE
1	B	196	VAL
1	B	203	SER
1	B	210	SER
1	B	213	LYS
1	B	218	LEU
1	B	223	ARG
1	B	227	VAL
1	B	228	GLU
1	B	230	GLU
1	B	232	ILE
2	C	48	LEU
2	C	65	ILE
2	C	77	ARG
2	C	92	GLU
2	C	99	PHE
2	C	100	SER
2	C	106	SER
2	C	109	ASP
2	C	113	ASP
2	C	116	LYS
2	C	152	VAL
2	C	162	GLU
2	C	177	SER
2	C	180	VAL
2	C	181	ARG
2	C	182	SER
2	C	189	GLU

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Mol	Chain	Res	Type
2	C	190	THR
2	C	191	ILE
2	C	193	LYS
2	C	196	ASP
2	C	197	LYS
2	C	199	LEU
2	C	201	SER
2	C	203	LYS
2	C	207	SER
2	C	208	ARG
2	C	211	TRP
2	C	213	GLU
2	C	215	ASP
2	C	216	VAL
2	C	217	ASP
2	C	218	LYS
2	C	219	ARG
2	C	220	ASP
2	C	221	THR
2	C	229	LYS
2	C	231	ARG
2	C	232	GLN
2	C	235	THR
2	C	239	LYS
2	C	244	THR
2	C	245	SER
2	C	246	GLU
2	C	247	GLN
2	C	249	VAL
2	C	250	GLU
2	C	260	SER
2	C	262	LEU
2	C	264	LYS
2	C	265	ASP
2	C	267	THR
2	C	268	VAL
2	C	270	THR
2	C	271	ASP
2	C	274	LEU
2	C	279	ARG
2	C	281	LEU
2	C	282	ARG

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Mol	Chain	Res	Type
2	C	288	THR
2	C	289	LYS
2	C	290	GLU
2	C	291	SER
2	C	293	GLN
2	C	294	THR
2	C	296	LEU
2	C	301	PHE
2	C	302	LYS
2	C	304	LYS
2	C	313	ARG
2	C	315	LYS
2	C	318	LYS
2	C	319	LYS
2	C	323	HIS
2	C	328	ILE
2	C	329	THR
2	C	331	SER
2	C	333	LEU
2	C	342	ILE
2	C	344	TYR
2	C	353	THR
2	C	354	THR
2	C	356	THR
2	C	357	VAL
2	C	361	VAL
2	C	363	VAL
2	C	366	GLU
2	C	367	THR
2	C	368	ASP
2	C	370	ILE
2	C	377	ARG
2	C	433	THR
2	C	454	ARG
2	C	474	ASP
2	C	494	ILE
2	C	499	SER
2	C	551	ASP
2	C	570	TYR
2	C	575	GLU
2	C	625	LEU
2	C	646	GLU

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Mol	Chain	Res	Type
2	C	666	THR
2	C	668	ARG
2	C	685	ASN
2	C	690	VAL
2	C	713	MET
2	C	749	SER
2	C	754	GLU
2	C	757	ILE
2	C	758	ASP
2	C	760	ARG
2	C	763	LYS
2	C	764	LEU
2	C	767	GLU
2	C	771	ARG
2	C	772	ASP
2	C	773	ILE
2	C	775	ASN
2	C	776	ILE
2	C	780	VAL
2	C	783	ASP
2	C	785	ASP
2	C	786	GLU
2	C	787	ARG
2	C	789	ILE
2	C	790	VAL
2	C	791	ARG
2	C	795	GLU
2	C	797	ARG
2	C	803	VAL
2	C	806	VAL
2	C	807	THR
2	C	832	VAL
2	C	850	ILE
2	C	851	ARG
2	C	852	VAL
2	C	855	ARG
2	C	859	ASP
2	C	865	VAL
2	C	868	LEU
2	C	875	GLN
2	C	876	LYS
2	C	881	ASP

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Mol	Chain	Res	Type
2	C	891	ASN
2	C	901	VAL
2	C	903	ASP
2	C	904	MET
2	C	919	THR
2	C	947	ASP
2	C	974	THR
2	C	1067	ARG
2	C	1093	SER
2	C	1127	GLU
2	C	1148	ARG
3	D	10	LEU
3	D	24	SER
3	D	56	ARG
3	D	60	CYS
3	D	62	CYS
3	D	107	PHE
3	D	126	GLU
3	D	138	SER
3	D	139	VAL
3	D	142	GLU
3	D	143	MET
3	D	144	ARG
3	D	145	HIS
3	D	148	LEU
3	D	149	SER
3	D	152	GLU
3	D	155	MET
3	D	159	ARG
3	D	160	LYS
3	D	165	GLN
3	D	166	ARG
3	D	169	GLU
3	D	170	LEU
3	D	173	ARG
3	D	175	GLN
3	D	183	GLU
3	D	185	GLU
3	D	187	GLU
3	D	190	LYS
3	D	194	ARG
3	D	196	LYS

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Mol	Chain	Res	Type
3	D	202	GLU
3	D	204	GLU
3	D	205	MET
3	D	207	GLN
3	D	208	ILE
3	D	209	ARG
3	D	211	ARG
3	D	213	GLN
3	D	214	ARG
3	D	216	LEU
3	D	217	ASP
3	D	218	ARG
3	D	221	ASP
3	D	224	SER
3	D	228	LYS
3	D	232	LYS
3	D	238	GLU
3	D	239	ASN
3	D	240	LEU
3	D	245	VAL
3	D	248	TYR
3	D	250	GLU
3	D	252	PHE
3	D	260	SER
3	D	269	ASP
3	D	276	SER
3	D	279	ASP
3	D	305	SER
3	D	310	MET
3	D	339	ASP
3	D	356	ARG
3	D	360	LEU
3	D	401	SER
3	D	415	GLN
3	D	431	VAL
3	D	438	LEU
3	D	462	ASP
3	D	468	ASN
3	D	478	ARG
3	D	480	ARG
3	D	505	HIS
3	D	539	ASP

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Mol	Chain	Res	Type
3	D	578	ARG
3	D	580	ASP
3	D	596	THR
3	D	600	GLN
3	D	606	HIS
3	D	698	ASN
3	D	725	THR
3	D	732	SER
3	D	737	LEU
3	D	738	VAL
3	D	741	ARG
3	D	743	LYS
3	D	744	GLU
3	D	746	LEU
3	D	748	HIS
3	D	755	LYS
3	D	757	GLU
3	D	758	LYS
3	D	759	GLN
3	D	762	ARG
3	D	765	LEU
3	D	766	ASN
3	D	767	HIS
3	D	768	ASP
3	D	770	ARG
3	D	779	LYS
3	D	784	GLU
3	D	790	ARG
3	D	791	GLU
3	D	797	ASN
3	D	799	ILE
3	D	821	LYS
3	D	825	THR
3	D	828	LYS
3	D	834	ARG
3	D	837	LYS
3	D	838	SER
3	D	846	VAL
3	D	847	LEU
3	D	862	ASP
3	D	865	LEU
3	D	866	ARG

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Mol	Chain	Res	Type
3	D	869	ASP
3	D	887	ARG
3	D	912	ARG
3	D	919	SER
3	D	923	ARG
3	D	946	ASP
3	D	960	VAL
3	D	964	SER
3	D	971	SER
3	D	972	THR
3	D	987	LYS
3	D	993	GLU
3	D	997	ILE
3	D	1006	PRO
3	D	1008	THR
3	D	1010	LEU
3	D	1014	THR
3	D	1023	ASP
3	D	1025	THR
3	D	1032	GLN
3	D	1033	GLU
3	D	1036	GLU
3	D	1038	ARG
3	D	1041	ARG
3	D	1048	ASP
3	D	1049	VAL
3	D	1052	ARG
3	D	1063	LYS
3	D	1064	ILE
3	D	1066	ILE
3	D	1070	ASP
3	D	1074	GLU
3	D	1075	VAL
3	D	1079	LYS
3	D	1081	SER
3	D	1082	LYS
3	D	1083	ARG
3	D	1085	ARG
3	D	1087	ARG
3	D	1090	LYS
3	D	1093	ASP
3	D	1097	ARG

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Mol	Chain	Res	Type
3	D	1100	SER
3	D	1106	GLU
3	D	1110	GLN
3	D	1115	SER
3	D	1122	LEU
3	D	1123	ARG
3	D	1125	GLN
3	D	1148	SER
3	D	1165	VAL
3	D	1172	SER
3	D	1176	LEU
3	D	1177	PRO
3	D	1191	ARG
3	D	1214	SER
3	D	1262	THR
3	D	1266	ARG
3	D	1268	ARG
3	D	1272	VAL
4	E	33	LEU
4	E	41	ASP
4	E	56	TYR
4	E	71	LEU
4	E	76	LEU
4	E	83	VAL
4	E	87	LEU
5	G	4	ASN
5	G	7	VAL
5	G	8	VAL
5	G	10	THR
5	G	12	SER
5	G	17	LYS
5	G	19	LYS
5	G	24	LYS
5	G	27	GLU
5	G	28	SER
5	G	34	LYS
5	G	37	ARG
5	G	42	GLU
5	G	43	GLU
5	G	45	GLU
5	G	46	THR
5	G	48	ILE

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Mol	Chain	Res	Type
5	G	49	LYS
5	G	52	LYS
5	G	53	LYS
5	G	54	LYS
5	G	56	VAL
5	G	57	LYS
5	G	58	LYS
5	G	59	LYS
5	G	60	VAL
5	G	66	LEU
5	G	67	VAL
5	G	69	ILE
5	G	71	MET
5	G	72	THR
5	G	80	ARG
5	G	85	VAL
5	G	89	VAL
5	G	94	SER
5	G	96	SER
5	G	97	LYS
5	G	101	LEU
5	G	102	LEU
5	G	111	LYS
5	G	112	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	61	HIS
1	A	79	ASN
1	A	120	ASN
1	A	152	ASN
1	B	119	HIS
2	C	435	GLN
2	C	545	ASN
2	C	610	ASN
2	C	685	ASN
2	C	700	GLN
2	C	1062	GLN
2	C	1066	GLN
2	C	1077	GLN

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Mol	Chain	Res	Type
2	C	1111	ASN
2	C	1129	GLN
3	D	5	ASN
3	D	207	GLN
3	D	262	GLN
3	D	352	ASN
3	D	368	ASN
3	D	396	ASN
3	D	410	GLN
3	D	525	HIS
3	D	533	ASN
3	D	564	ASN
3	D	600	GLN
3	D	606	HIS
3	D	787	GLN
3	D	797	ASN
3	D	852	ASN
3	D	854	HIS
3	D	882	GLN
3	D	1110	GLN
3	D	1125	GLN
3	D	1131	GLN
3	D	1227	GLN
3	D	1251	ASN
3	D	1273	GLN
4	E	63	GLN
5	G	21	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	R	28/30 (93%)	4 (14%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	R	10	U
8	R	11	C
8	R	20	C
8	R	22	G

There are no RNA pucker outliers to report.

## 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	G2P	D	2004	-	27,34,34	5.25	13 (48%)	33,54,54	1.73	6 (18%)

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
11	G2P	D	2004	-	-	2/15/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	2004	G2P	O4'-C1'	14.05	1.60	1.41
11	D	2004	G2P	C2'-C1'	-12.53	1.34	1.53
11	D	2004	G2P	C4-N3	8.92	1.49	1.35
11	D	2004	G2P	C5-C6	8.09	1.55	1.41
11	D	2004	G2P	PB-O3B	7.24	1.66	1.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	2004	G2P	O4'-C4'	-6.50	1.30	1.45
11	D	2004	G2P	C2-N1	6.22	1.46	1.35
11	D	2004	G2P	C6-N1	5.30	1.42	1.33
11	D	2004	G2P	C2-N2	5.07	1.44	1.33
11	D	2004	G2P	PA-O5'	5.03	1.64	1.57
11	D	2004	G2P	O3'-C3'	-3.09	1.35	1.43
11	D	2004	G2P	C2-N3	2.56	1.46	1.34
11	D	2004	G2P	O2'-C2'	2.11	1.47	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	2004	G2P	N3-C2-N1	-5.38	120.05	127.22
11	D	2004	G2P	C2-N3-C4	4.79	120.83	115.36
11	D	2004	G2P	C3'-C2'-C1'	3.64	106.46	100.98
11	D	2004	G2P	PB-O3B-PG	-2.56	123.61	132.62
11	D	2004	G2P	C5-C6-N1	-2.42	120.13	123.43
11	D	2004	G2P	C2-N1-C6	2.20	119.43	115.93

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	D	2004	G2P	C5'-O5'-PA-O1A
11	D	2004	G2P	O4'-C4'-C5'-O5'

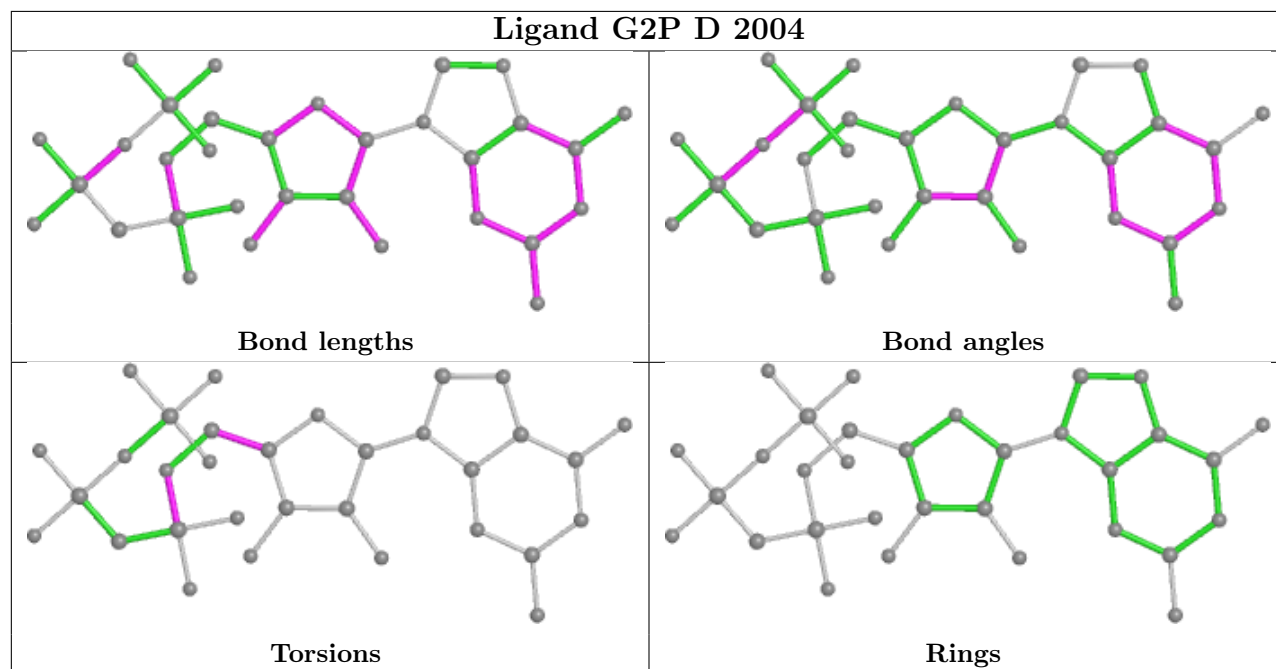
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	2004	G2P	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 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.



## 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.

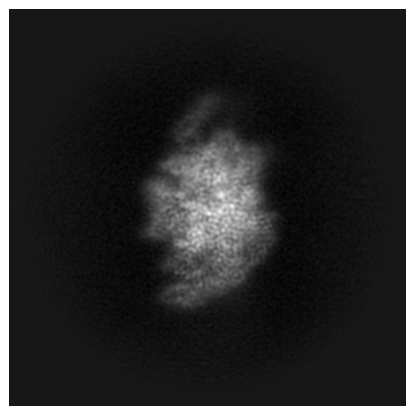
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28665. These allow visual inspection of the internal detail of the map and identification of artifacts.

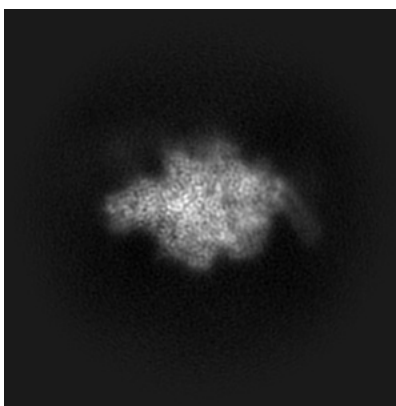
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

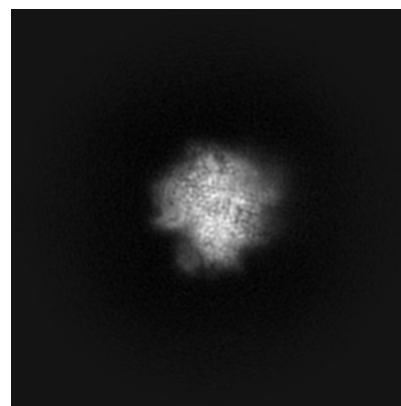
#### 6.1.1 Primary map



X

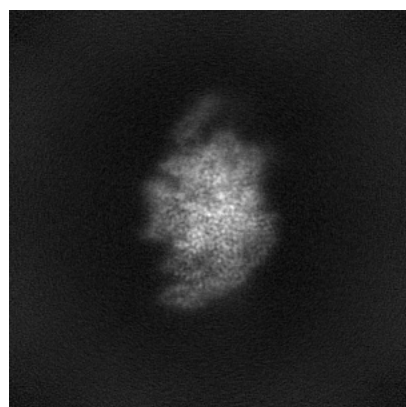


Y

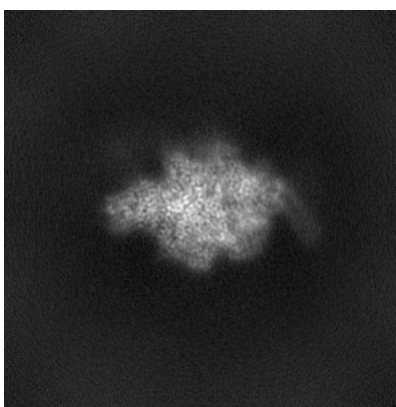


Z

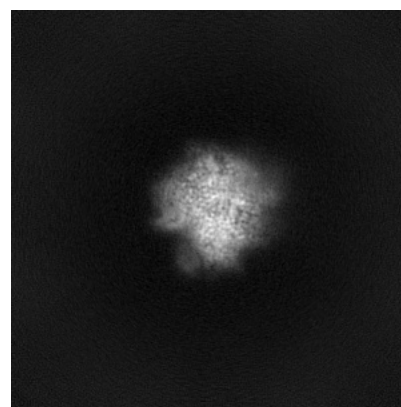
#### 6.1.2 Raw map



X



Y

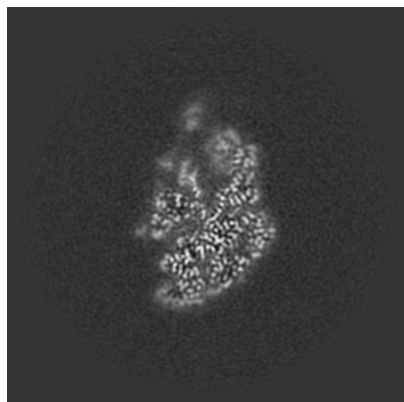


Z

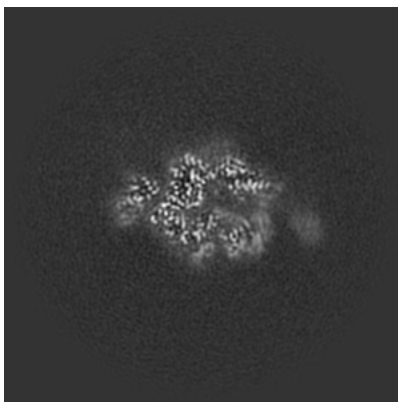
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

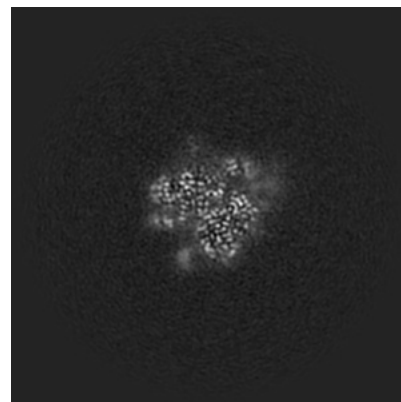
### 6.2.1 Primary map



X Index: 200

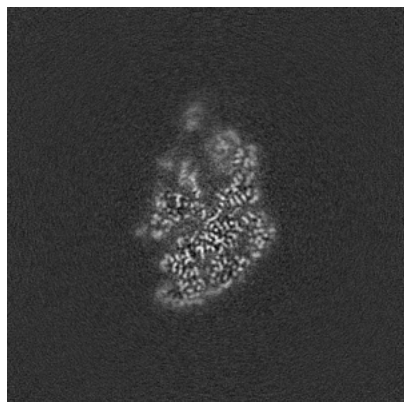


Y Index: 200

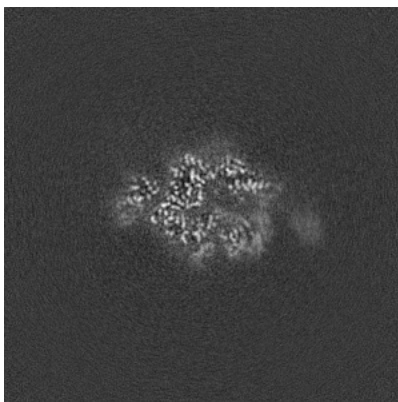


Z Index: 200

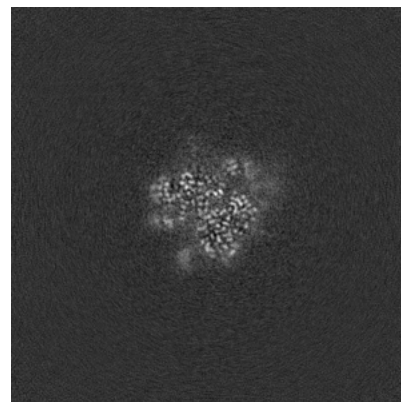
### 6.2.2 Raw map



X Index: 200



Y Index: 200

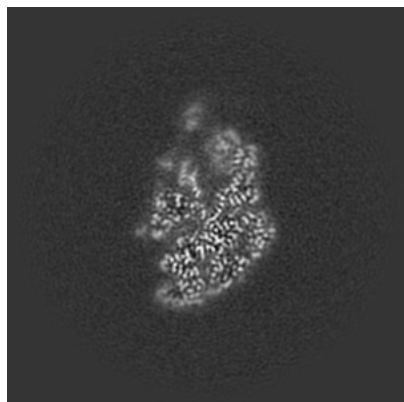


Z Index: 200

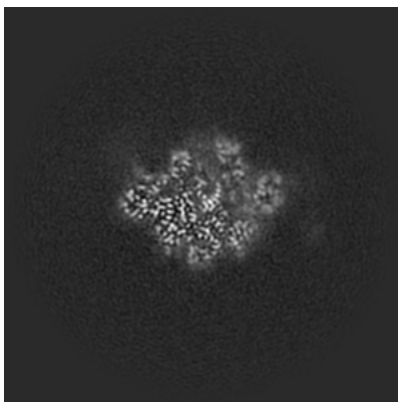
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

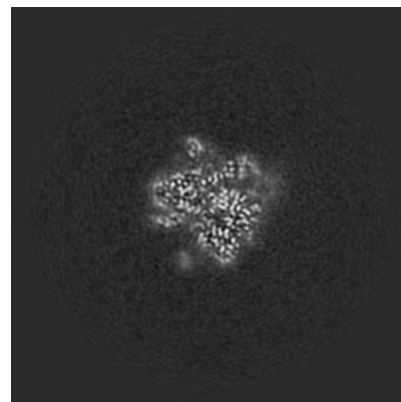
### 6.3.1 Primary map



X Index: 200

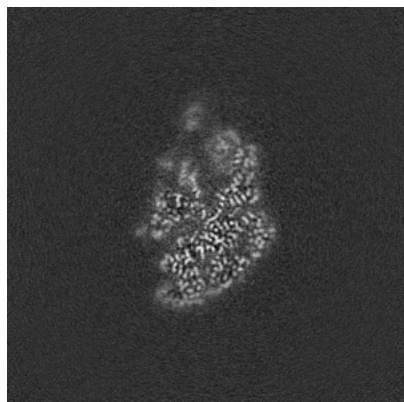


Y Index: 214

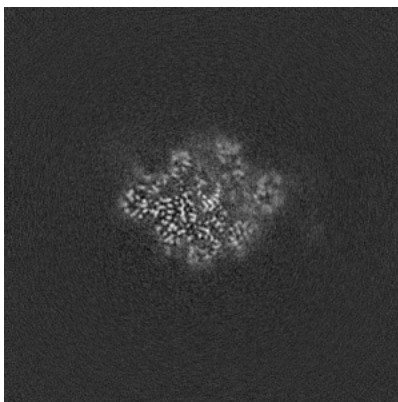


Z Index: 195

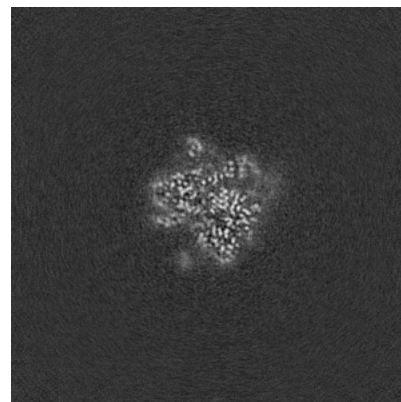
### 6.3.2 Raw map



X Index: 200



Y Index: 214

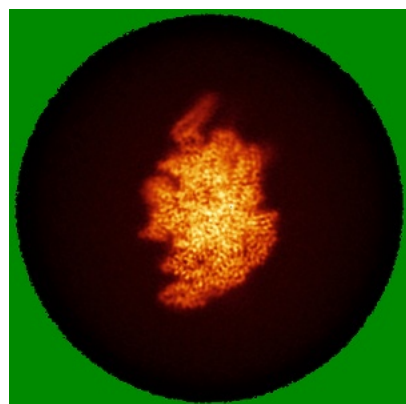


Z Index: 195

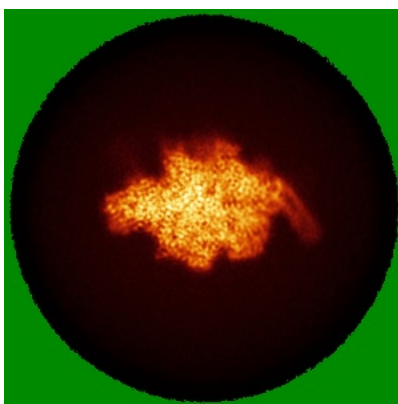
The images above show the largest variance slices of the map in three orthogonal directions.

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

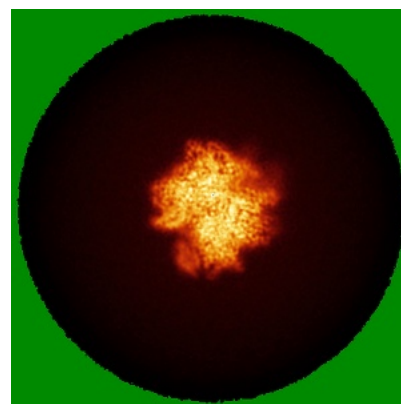
### 6.4.1 Primary map



X

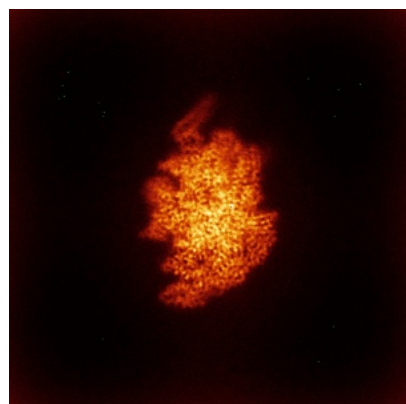


Y

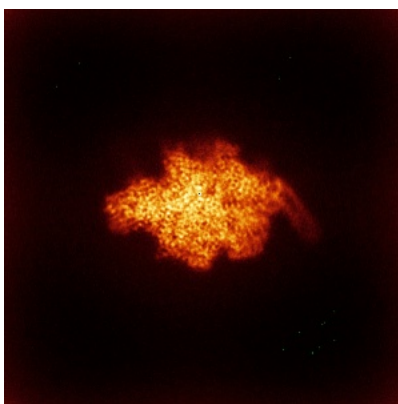


Z

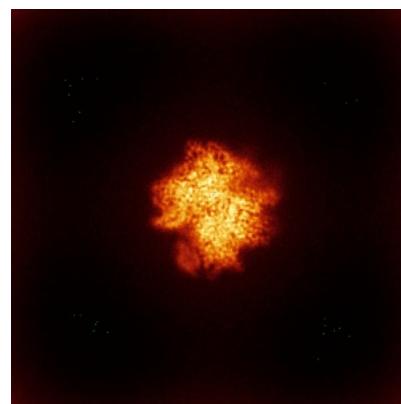
### 6.4.2 Raw map



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.

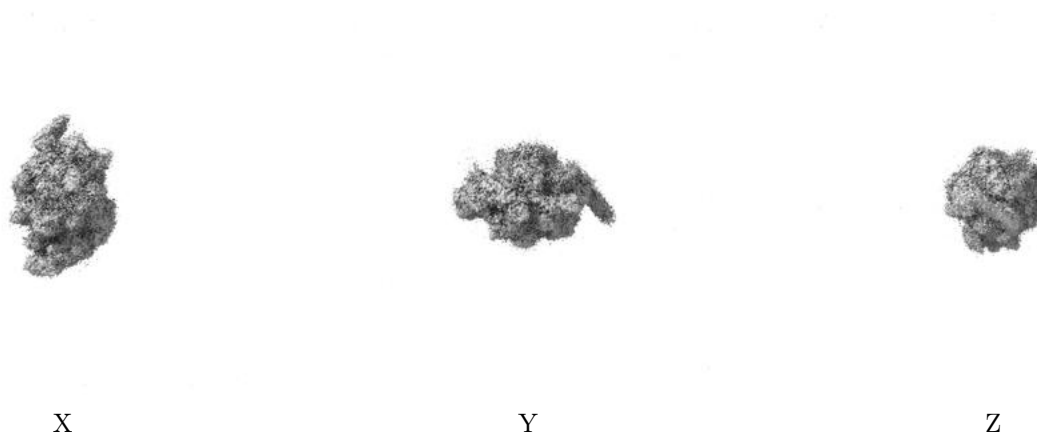
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.27. 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.

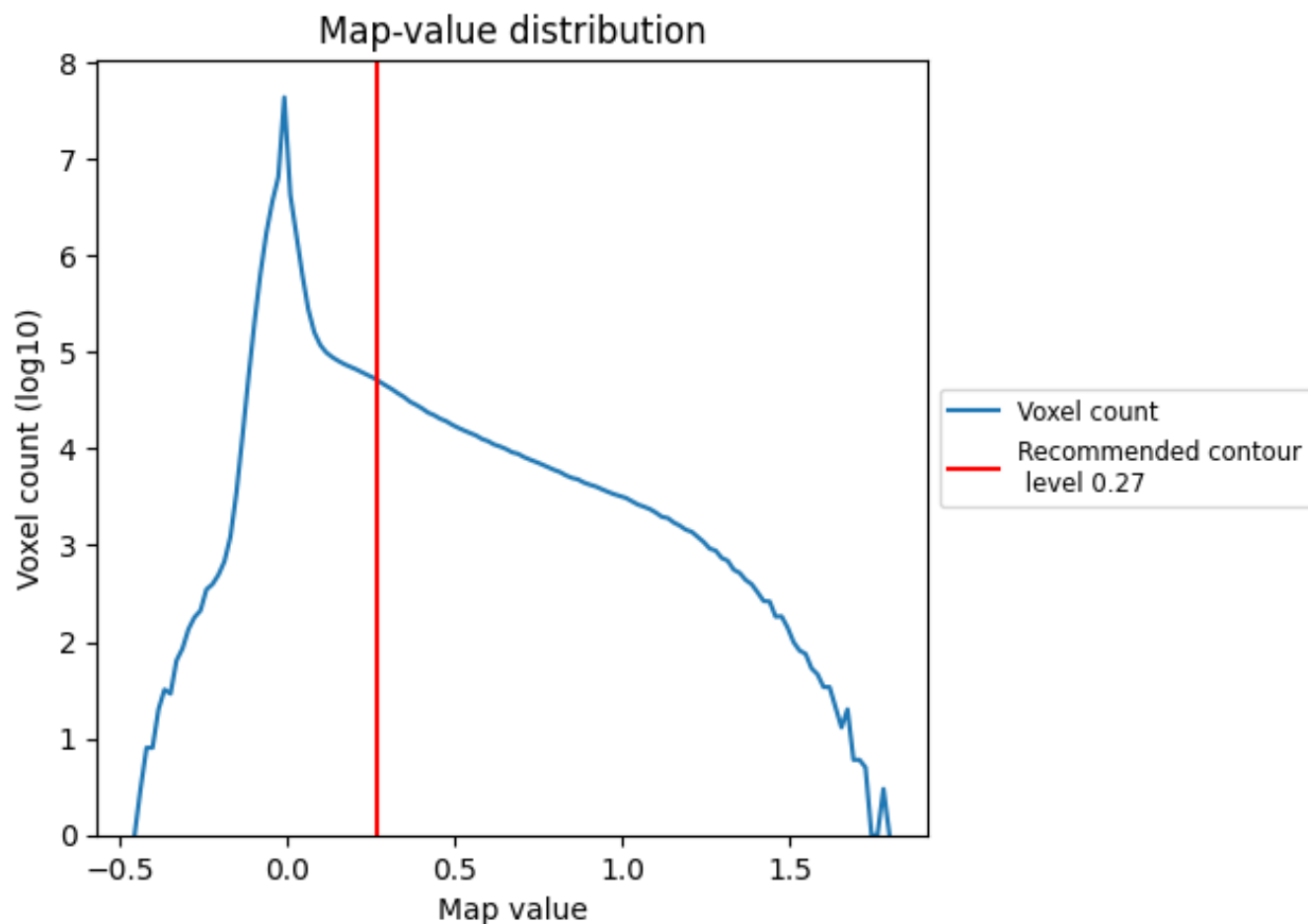
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

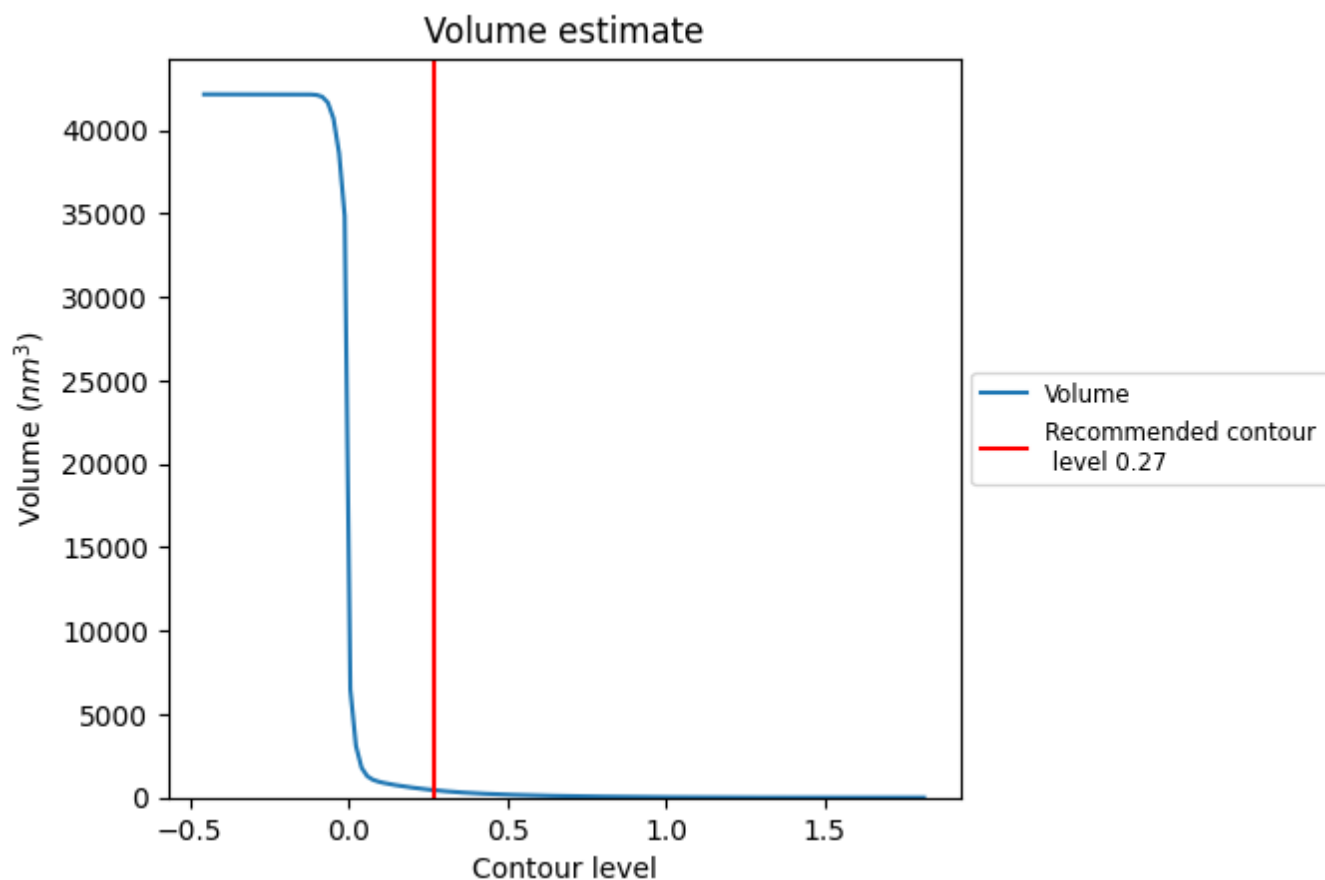
This section contains the results of statistical analysis of the map.

### 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.

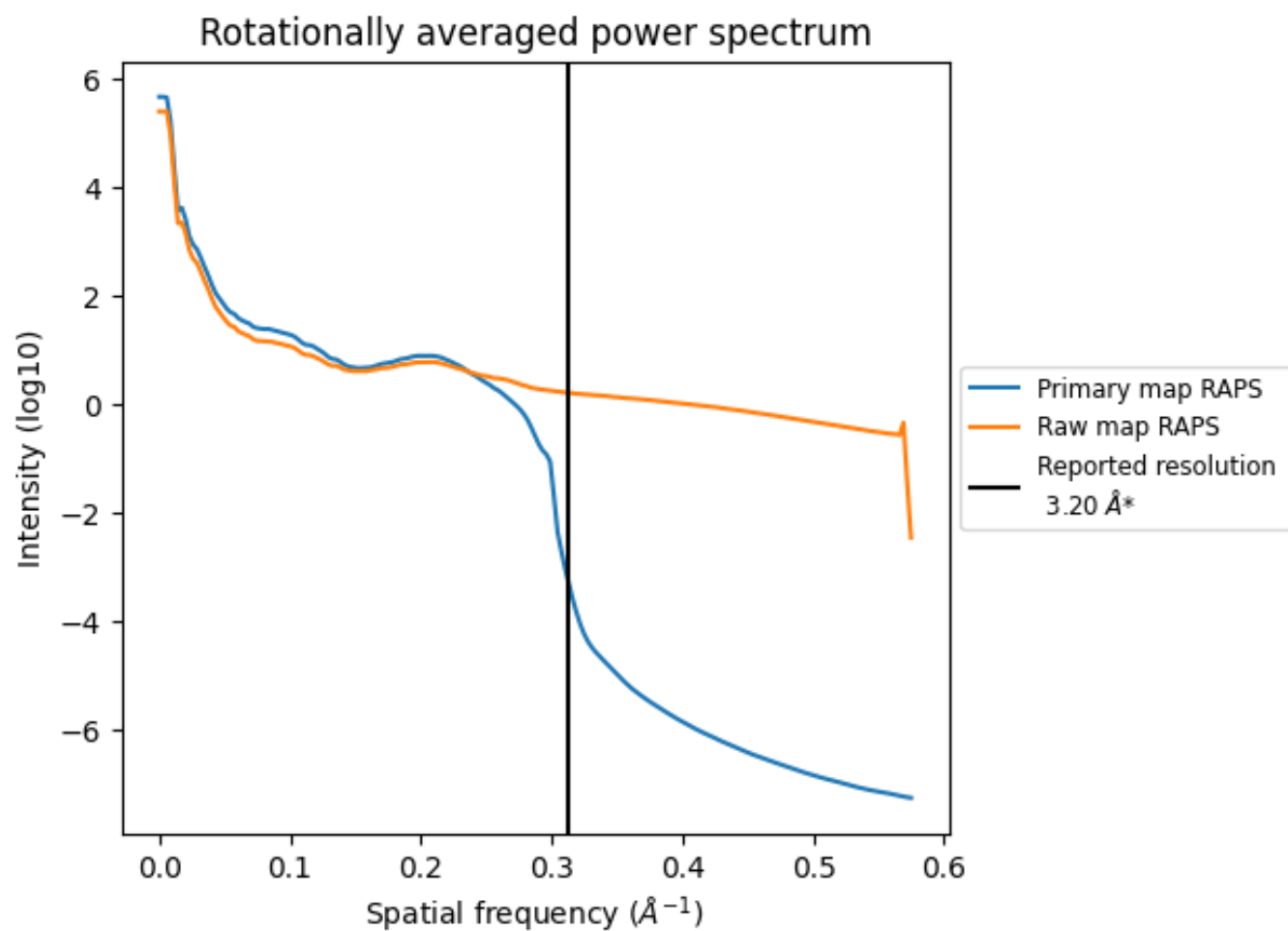
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 442 nm<sup>3</sup>; this corresponds to an approximate mass of 400 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](#)

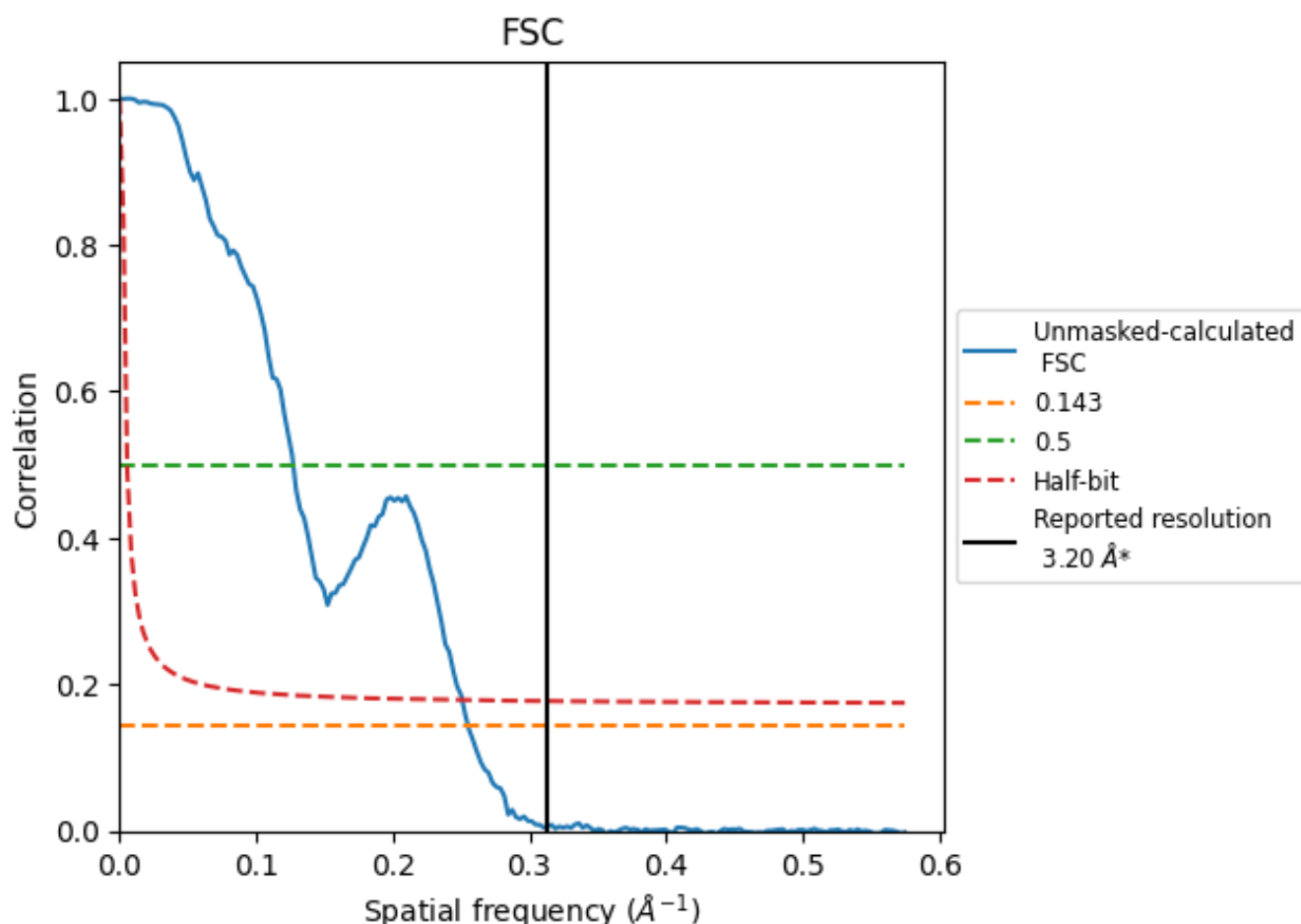


\*Reported resolution corresponds to spatial frequency of  $0.312 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.312  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

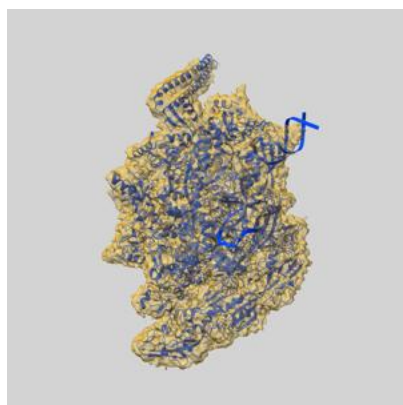
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.92	7.86	3.99

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.92 differs from the reported value 3.2 by more than 10 %

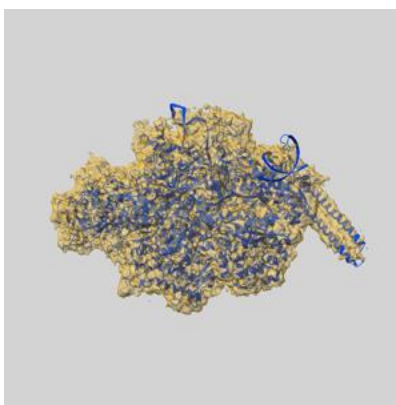
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-28665 and PDB model 8EXY. Per-residue inclusion information can be found in section 3 on page 7.

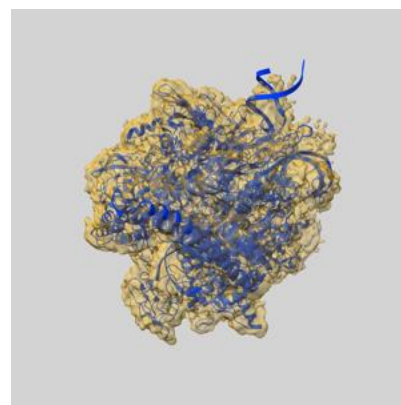
### 9.1 Map-model overlay [i](#)



X



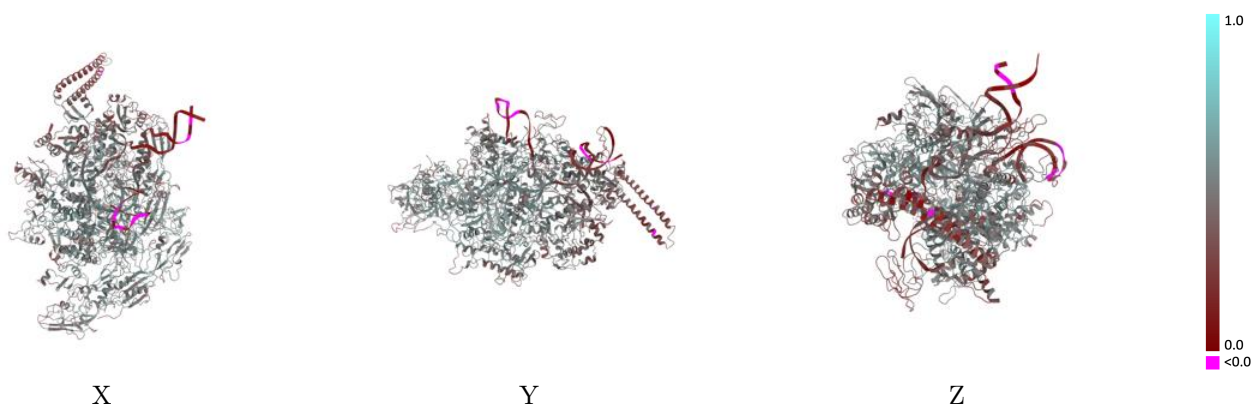
Y



Z

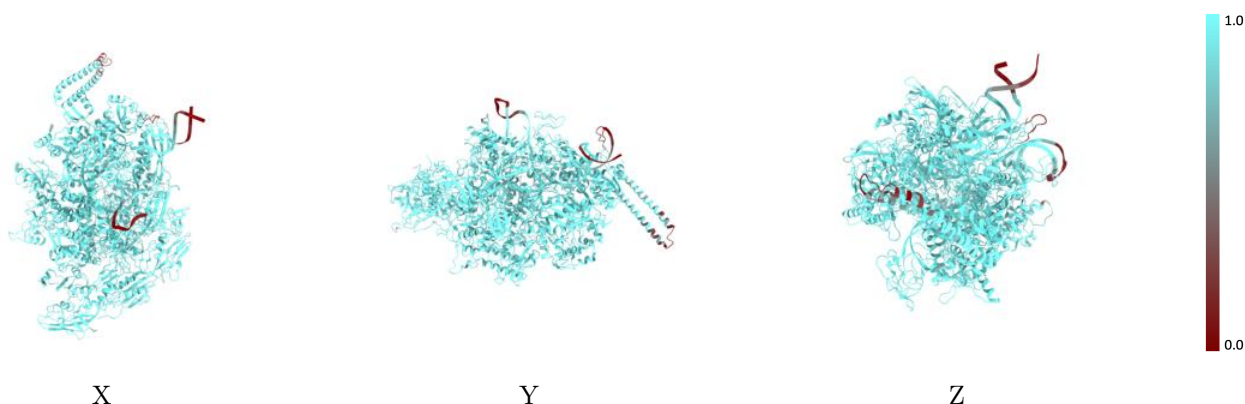
The images above show the 3D surface view of the map at the recommended contour level 0.27 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



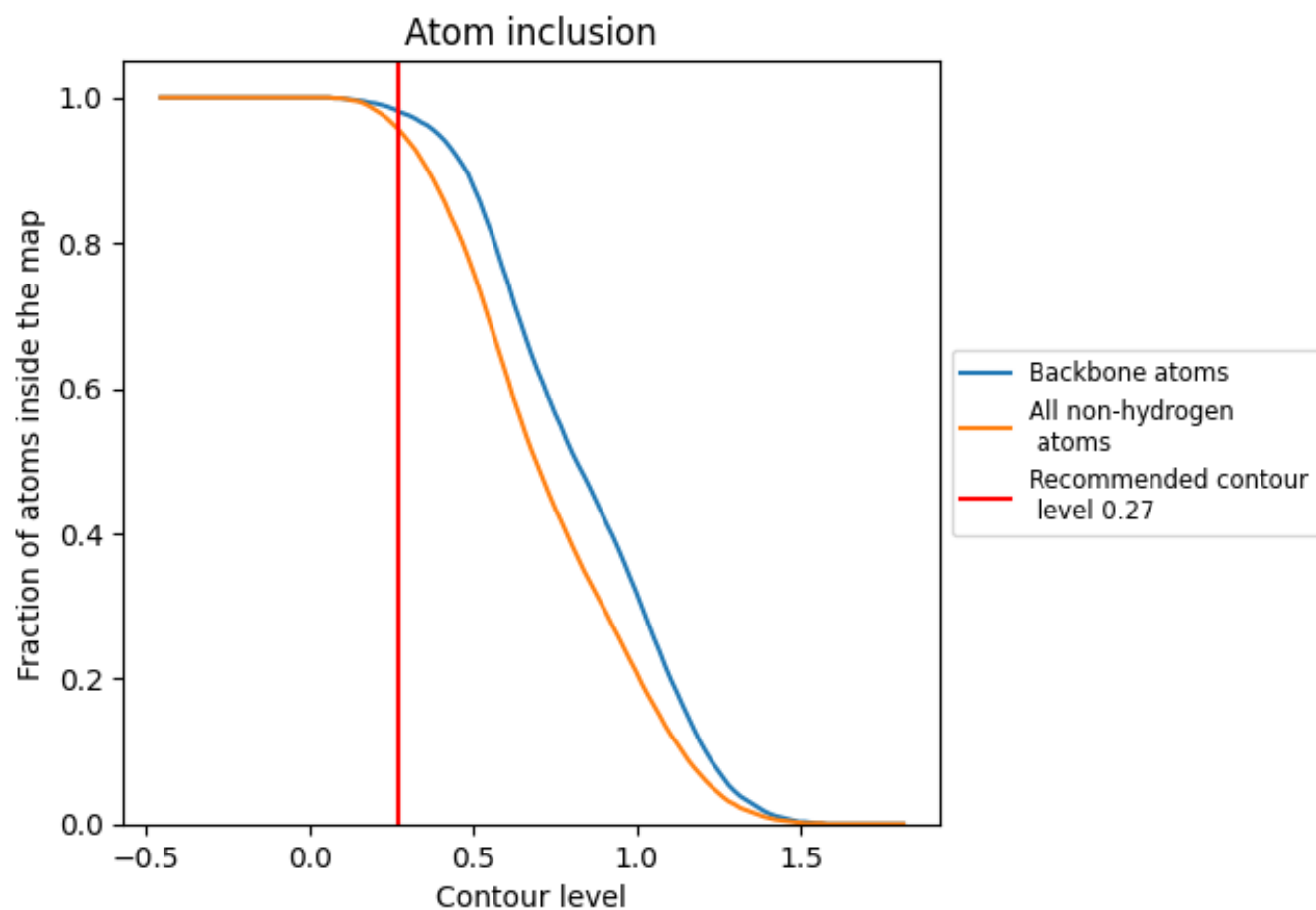
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.27).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.27) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9580	<div></div> 0.4570
A	<div></div> 0.9780	<div></div> 0.4900
B	<div></div> 0.9620	<div></div> 0.4660
C	<div></div> 0.9820	<div></div> 0.4940
D	<div></div> 0.9680	<div></div> 0.4600
E	<div></div> 0.9480	<div></div> 0.4700
G	<div></div> 0.9060	<div></div> 0.3970
N	<div></div> 0.8550	<div></div> 0.2690
R	<div></div> 0.7380	<div></div> 0.2420
T	<div></div> 0.8590	<div></div> 0.3240

1.0

0.0

<0.0