Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 11:07 PM JST

PDB ID	:	7CRQ
EMDB ID	:	EMD-30456
Title	:	NSD3 bearing E1181K/T1232A dual mutation in complex with 187-bp NCP (2:1 binding mode)
Authors	:	Li, W.; Tian, W.; Yuan, G.; Deng, P.; Gozani, O.; Patel, D.; Wang, Z.
Deposited on	:	2020-08-14
Resolution	:	3.15 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 (1)) were used in the production of this report:

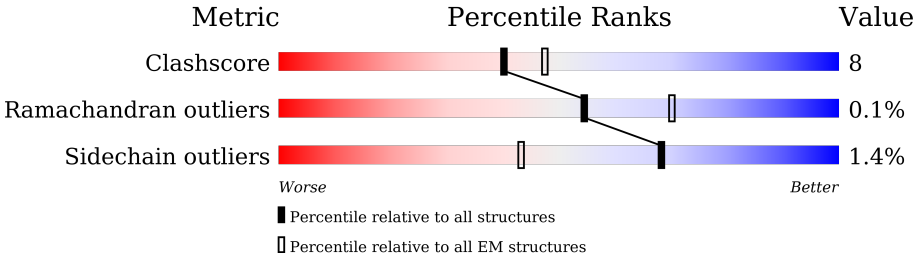
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.15 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

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	E	135	67% 7% 26%
1	M	135	73% • 24%
2	B	102	75% 6% 20%
2	F	102	5% 82% • 16%
3	C	129	80% 5% 16%
3	G	129	81% 5% 15%
4	D	122	70% 8% 22%
4	H	122	74% 6% 20%

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Mol	Chain	Length	Quality of chain
5	A	187	26% 52% 38% 10%
6	K	187	26% 60% 30% 10%
7	I	758	5% 21% 8% 71%
7	L	758	6% 20% 9% 71%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 16633 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 Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	M	103	833	528	159	145	1	0	0
1	E	100	818	520	156	141	1	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	36	NLE	LYS	engineered mutation	UNP Q92133
M	90	NLE	MET	engineered mutation	UNP Q92133
M	120	NLE	MET	engineered mutation	UNP Q92133
E	36	NLE	LYS	engineered mutation	UNP Q92133
E	90	NLE	MET	engineered mutation	UNP Q92133
E	120	NLE	MET	engineered mutation	UNP Q92133

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	82	653	413	127	112	1	0	0
2	F	86	672	424	130	117	1	0	0

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	109	837	526	165	146	0	0
3	G	110	850	535	168	147	0	0

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	95	746	469	136	139	2	0	0
4	H	97	766	481	142	141	2	0	0

- Molecule 5 is a DNA chain called DNA (168-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	A	168	3420	1623	618	1011	168	0	0

- Molecule 6 is a DNA chain called DNA (168-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	K	168	3468	1638	657	1005	168	0	0

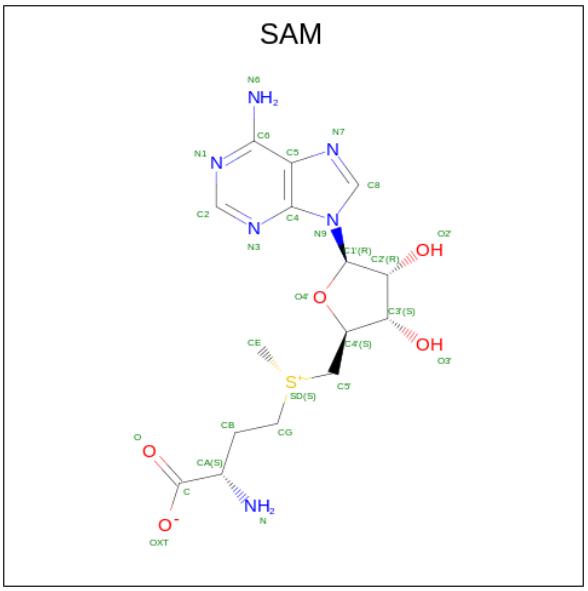
- Molecule 7 is a protein called Histone-lysine N-methyltransferase NSD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I	222	1755	1084	326	325	20	0	0
7	L	222	1755	1084	326	325	20	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1181	LYS	GLU	engineered mutation	UNP Q9BZ95
I	1232	ALA	THR	engineered mutation	UNP Q9BZ95
L	1181	LYS	GLU	engineered mutation	UNP Q9BZ95
L	1232	ALA	THR	engineered mutation	UNP Q9BZ95

- Molecule 8 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
8	I	1	27	15	6	5	1	0
8	L	1	27	15	6	5	1	0

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

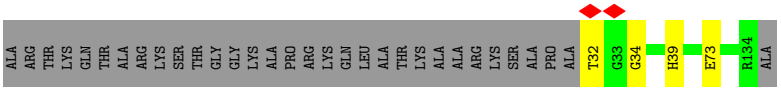
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
9	I	3	3	3	0
9	L	3	3	3	0

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: Histone H3

Chain M:

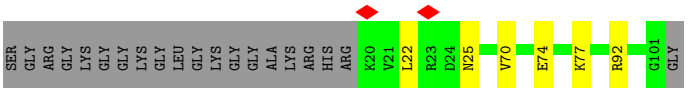


- Molecule 1: Histone H3

Chain E:

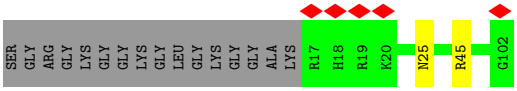
- Molecule 2: Histone H4

Chain B:



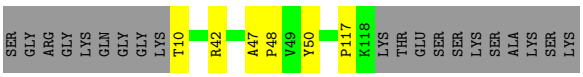
- Molecule 2: Histone H4

Chain F:



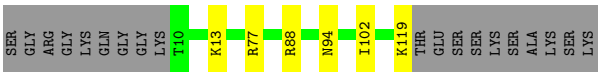
- Molecule 3: Histone H2A

Chain C:



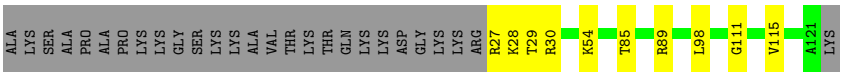
- Molecule 3: Histone H2A

Chain G:



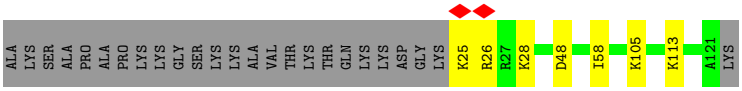
• Molecule 4: Histone H2B

Chain D:



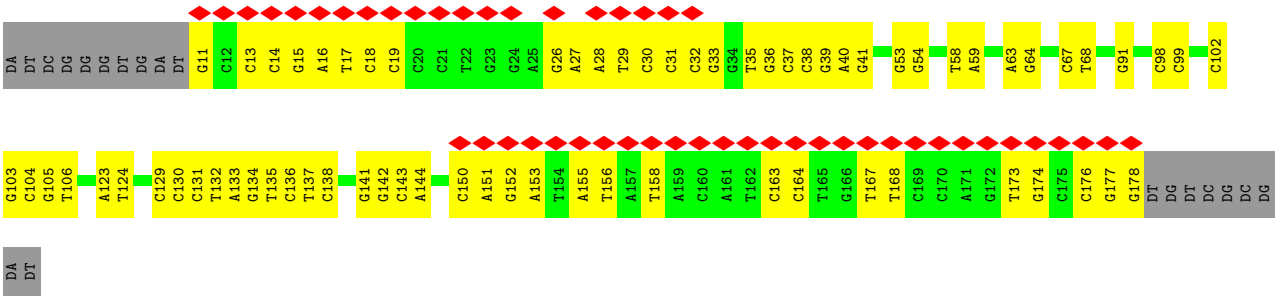
• Molecule 4: Histone H2B

Chain H:



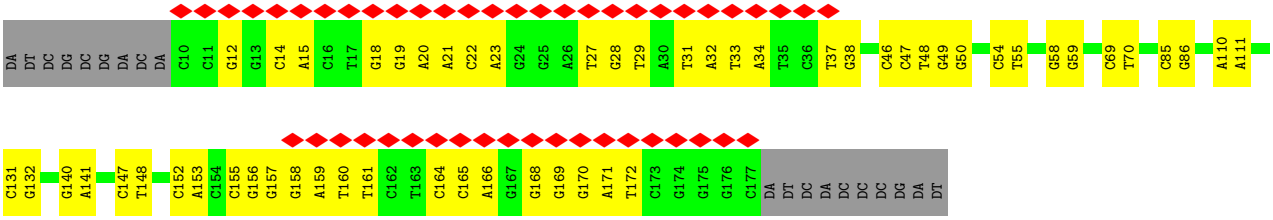
• Molecule 5: DNA (168-MER)

Chain A:



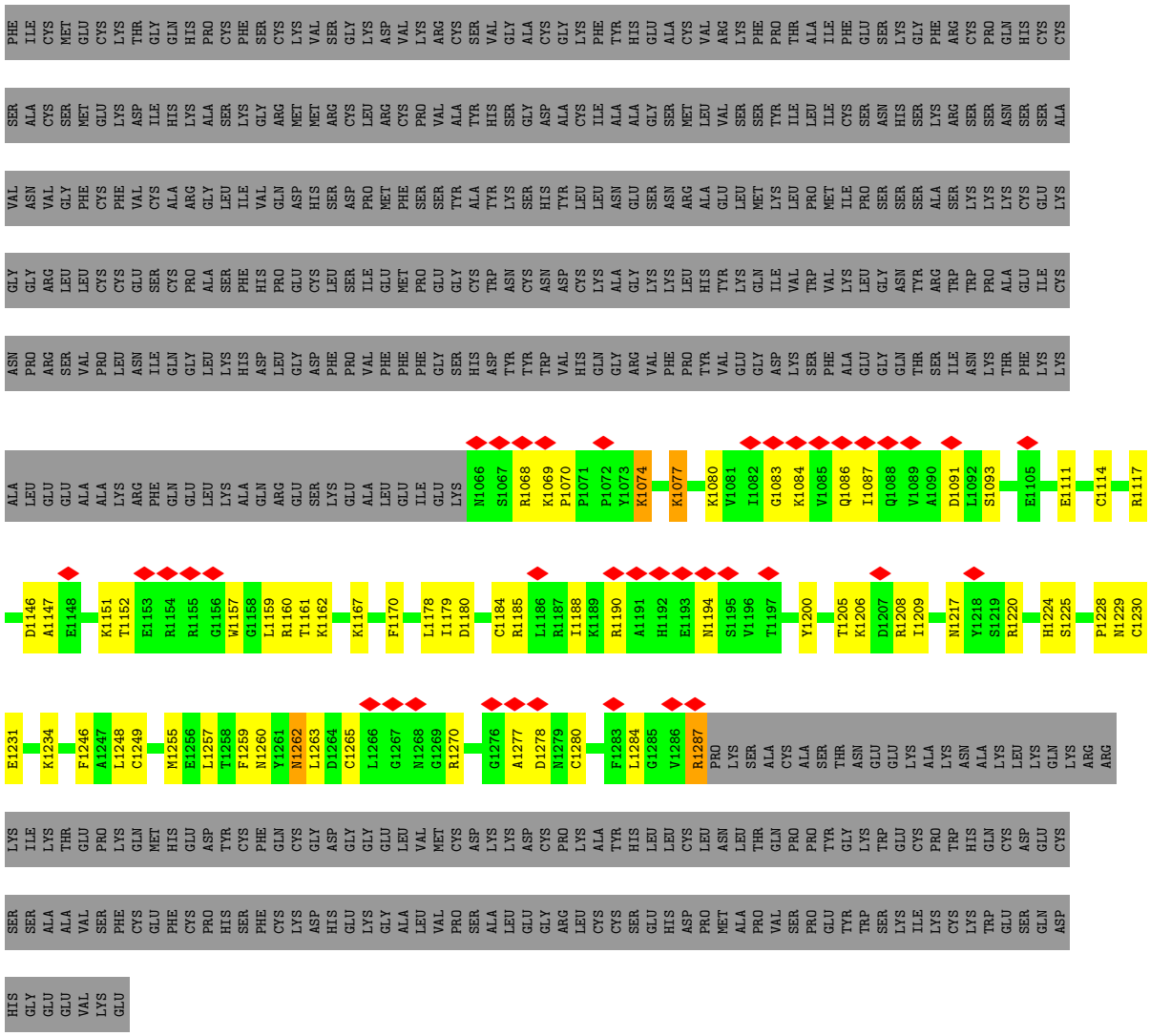
• Molecule 6: DNA (168-MER)

Chain K:



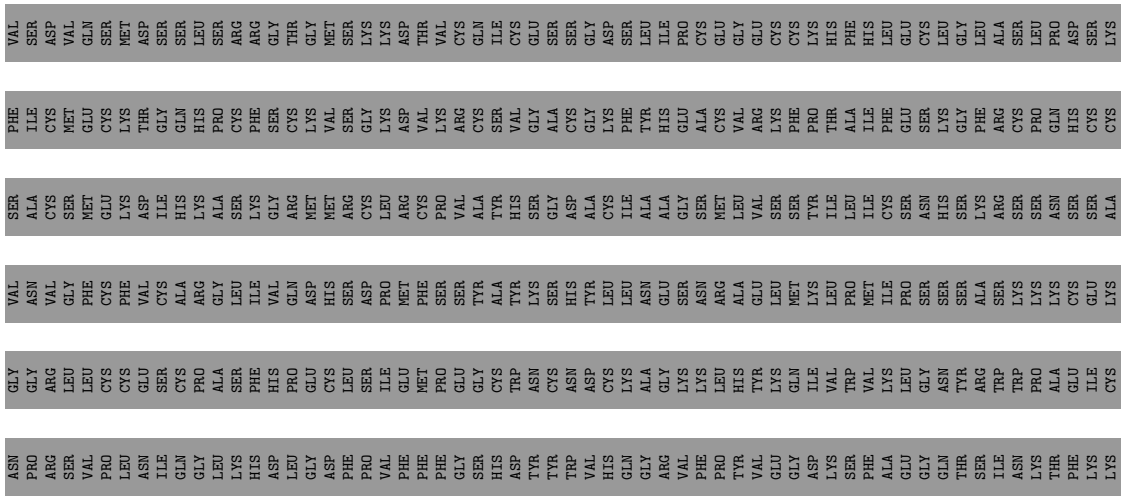
• Molecule 7: Histone-lysine N-methyltransferase NSD3

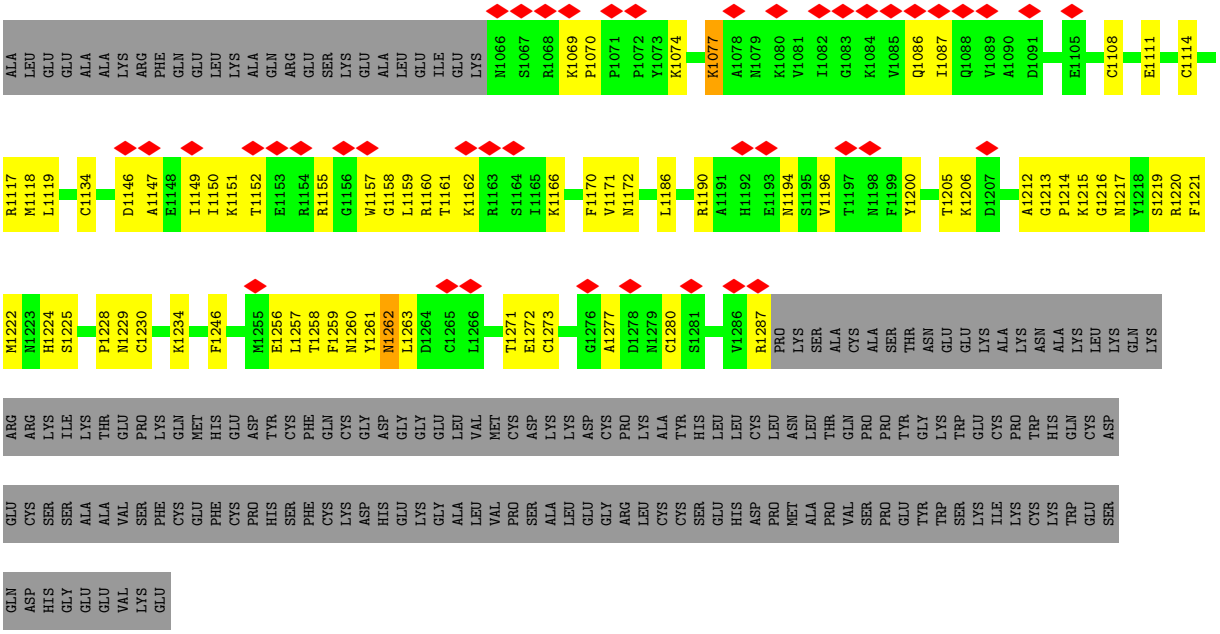
Chain I:



• Molecule 7: Histone-lysine N-methyltransferase NSD3

Chain L:




ALA LEU GLU GLU ALA ALA LYS ARG PHE GLN GLU LEU LYS ALA GLN ARG GLU SER LYS GLU ALA LEU GLU ILE GLU LYS
N1066 S1067 R1068 K1069 P1070 P1071 P1072 Y1073 K1074 K1077 A1078 N1079 K1080 V1081 I1082 G1083 K1084 V1085 Q1086 I1087 Q1088 V1089 A1090 D1091 E1105 C1108 E1111 C1114
R1117 M1118 L1119 C1134 D1146 A1147 E1148 I1149 I1150 K1151 T1152 E1153 R1154 R1155 G1156 W1157 G1158 L1159 R1160 T1161 K1162 R1163 S1164 I1165 K1166 F1170 V1171 N1172 L1186 R1190 A1191 H1192 E1193 N1194 S1195 V1196 T1197 N1198 F1199 Y1200 T1205 K1206 D1207 A1212 G1213 P1214 K1215 G1216 N1217 Y1218 S1219 R1220 F1221
M1222 N1223 H1224 S1225 P1228 N1229 C1230 K1234 F1246 M1255 E1256 L1257 T1258 F1259 N1260 Y1261 N1262 L1263 D1264 C1265 L1266 T1271 E1272 C1273 G1276 A1277 D1278 N1279 C1280 S1281 V1286 R1287 PRO LYS SER ALA CYS ALA SER THR ASN GLU GLU LYS ALA LYS ASN ALA LYS LEU LYS GLN LYS
ARG ARG LYS ILE LYS THR GLU PRO LYS GLN MET HIS GLU ASP TYR CYS PHE GLN CYS GLY ASP GLY GLY GLU LEU VAL MET CYS ASP LYS LYS ASP CYS PRO LYS ALA TYR HIS LEU LEU CYS LEU ASN LEU THR GLN PRO PRO TYR GLY LYS TRP GLU CYS PRO TRP HIS GLN CYS ASP
GLU CYS SER SER ALA ALA VAL SER PHE CYS GLU PHE CYS PRO HIS SER PHE CYS LYS ASP HIS GLU LYS GLY ALA LEU VAL PRO SER ALA LEU GLU GLY ARG LEU CYS CYS SER GLU HIS ASP PRO MET ALA PRO VAL SER PRO GLU TYR TRP SER LYS ILE LYS CYS LYS TRP GLU SER
GLN ASP HIS GLY GLU GLU VAL LYS GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	281815	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.220	Depositor
Minimum map value	-0.127	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0184	Depositor
Map size (Å)	233.28001, 233.28001, 233.28001	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: NLE, SAM, 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	E	0.37	0/803	0.47	0/1073
1	M	0.37	0/818	0.48	0/1093
2	B	0.41	0/660	0.50	0/885
2	F	0.40	0/680	0.49	0/912
3	C	0.32	0/847	0.46	0/1144
3	G	0.34	0/860	0.49	0/1159
4	D	0.35	0/757	0.47	0/1018
4	H	0.37	0/777	0.49	0/1043
5	A	0.64	0/3830	0.94	0/5903
6	K	0.64	0/3896	0.90	0/6017
7	I	0.26	0/1789	0.51	0/2410
7	L	0.26	0/1789	0.48	0/2410
All	All	0.49	0/17506	0.72	0/25067

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	818	0	859	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	833	0	872	4	0
2	B	653	0	695	5	0
2	F	672	0	698	2	0
3	C	837	0	891	8	0
3	G	850	0	915	5	0
4	D	746	0	773	8	0
4	H	766	0	799	5	0
5	A	3420	0	1885	57	0
6	K	3468	0	1882	42	0
7	I	1755	0	1720	50	0
7	L	1755	0	1718	56	0
8	I	27	0	22	2	0
8	L	27	0	22	4	0
9	I	3	0	0	0	0
9	L	3	0	0	0	0
All	All	16633	0	13751	229	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (229) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:165:DC:OP1	7:I:1074:LYS:NZ	1.61	1.34
3:C:117:PRO:HD2	7:L:1118:MET:SD	2.10	0.90
7:I:1077:LYS:HE2	7:I:1077:LYS:H	1.38	0.88
3:C:117:PRO:CG	7:L:1118:MET:SD	2.65	0.83
3:C:117:PRO:CD	7:L:1118:MET:SD	2.68	0.81
5:A:151:DA:H2'	5:A:152:DG:H4'	1.62	0.79
8:L:1504:SAM:SD	8:L:1504:SAM:N	2.57	0.76
7:I:1147:ALA:H	7:I:1162:LYS:HE3	1.49	0.75
3:C:10:THR:OG1	5:A:138:DC:H4'	1.88	0.74
3:C:117:PRO:HG2	7:L:1118:MET:SD	2.27	0.73
7:L:1077:LYS:H	7:L:1077:LYS:HD2	1.55	0.72
7:I:1277:ALA:HB3	7:I:1280:CYS:HB3	1.74	0.69
7:L:1077:LYS:H	7:L:1077:LYS:CD	2.06	0.68
5:A:136:DC:H2"	5:A:137:DT:H5"	1.74	0.68
6:K:37:DT:H4'	6:K:38:DG:H5'	1.75	0.68
7:I:1068:ARG:HG2	7:I:1069:LYS:H	1.58	0.68
7:I:1262:ASN:ND2	7:I:1262:ASN:H	1.91	0.67
7:I:1114:CYS:HB3	7:I:1117:ARG:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:1229:ASN:HD21	7:L:1257:LEU:HA	1.59	0.67
5:A:33:DG:H1	6:K:155:DC:H42	1.41	0.66
7:I:1111:GLU:OE1	7:I:1111:GLU:HA	1.94	0.66
5:A:153:DA:H8	5:A:153:DA:H5"	1.61	0.66
5:A:38:DC:H2"	5:A:39:DG:C8	2.31	0.65
7:I:1167:LYS:HE3	7:I:1249:CYS:HA	1.78	0.65
7:L:1111:GLU:OE1	7:L:1111:GLU:HA	1.98	0.64
1:M:39:HIS:ND1	7:I:1231:GLU:OE2	2.30	0.64
4:H:26:ARG:O	4:H:26:ARG:NH2	2.31	0.64
6:K:18:DG:H2"	6:K:19:DG:N7	2.14	0.64
5:A:39:DG:H2"	5:A:40:DA:C8	2.34	0.62
7:L:1212:ALA:O	7:L:1220:ARG:NE	2.32	0.62
5:A:176:DC:H42	6:K:12:DG:H1	1.46	0.62
7:L:1150:ILE:HG22	7:L:1151:LYS:H	1.64	0.62
5:A:40:DA:H2"	5:A:41:DG:H5"	1.80	0.62
7:L:1077:LYS:HD2	7:L:1077:LYS:N	2.15	0.62
6:K:165:DC:P	7:I:1074:LYS:HZ1	2.17	0.61
6:K:168:DG:H2'	6:K:169:DG:C8	2.35	0.61
7:I:1152:THR:HA	7:I:1160:ARG:HH22	1.65	0.60
7:L:1213:GLY:O	7:L:1220:ARG:NH1	2.34	0.60
5:A:18:DC:H2"	5:A:19:DC:C5	2.37	0.60
1:M:73:GLU:OE1	2:B:25:ASN:ND2	2.31	0.59
7:L:1114:CYS:HB3	7:L:1117:ARG:HB3	1.84	0.59
4:D:29:THR:HG23	4:D:30:ARG:H	1.67	0.59
1:E:45:THR:O	1:E:49:ARG:HG3	2.02	0.58
7:L:1277:ALA:HB3	7:L:1280:CYS:SG	2.43	0.58
3:G:13:LYS:NZ	6:K:140:DG:OP1	2.37	0.58
6:K:27:DT:H2"	6:K:28:DG:N7	2.19	0.58
6:K:48:DT:H2"	6:K:49:DG:C8	2.38	0.58
7:L:1222:MET:HE2	7:L:1258:THR:HG23	1.86	0.57
6:K:110:DA:H2"	6:K:111:DA:C8	2.39	0.57
6:K:170:DG:H2"	6:K:171:DA:N7	2.19	0.57
7:L:1070:PRO:HD3	7:L:1157:TRP:NE1	2.19	0.57
1:M:32:THR:OG1	7:I:1270:ARG:NH1	2.39	0.56
5:A:135:DT:H2"	5:A:136:DC:H5"	1.88	0.55
1:E:73:GLU:OE1	2:F:25:ASN:ND2	2.32	0.55
3:C:42:ARG:HB2	4:D:85:THR:HG22	1.88	0.55
5:A:155:DA:H2"	5:A:156:DT:H5"	1.88	0.54
7:L:1146:ASP:OD2	7:L:1161:THR:OG1	2.25	0.54
6:K:37:DT:H1'	6:K:38:DG:C8	2.43	0.54
6:K:28:DG:H2"	6:K:29:DT:C5	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:27:DA:H2"	5:A:28:DA:N7	2.23	0.53
7:L:1217:ASN:OD1	7:L:1219:SER:OG	2.21	0.53
5:A:143:DC:H2"	5:A:144:DA:C8	2.43	0.53
6:K:165:DC:H2"	6:K:166:DA:C8	2.43	0.53
7:L:1262:ASN:O	7:L:1262:ASN:ND2	2.40	0.53
5:A:141:DG:H2"	5:A:142:DG:C8	2.44	0.53
6:K:159:DA:H1'	6:K:160:DT:C5	2.44	0.53
7:I:1205:THR:HB	7:I:1208:ARG:HB2	1.90	0.53
3:G:88:ARG:NH1	3:G:94:ASN:OD1	2.42	0.52
7:I:1077:LYS:H	7:I:1077:LYS:CE	2.18	0.52
5:A:14:DC:H2"	5:A:15:DG:C8	2.44	0.52
7:I:1091:ASP:OD1	7:I:1093:SER:OG	2.23	0.52
5:A:67:DC:H2"	5:A:68:DT:H71	1.90	0.52
5:A:91:DG:H8	5:A:91:DG:H5"	1.75	0.52
5:A:130:DC:H2"	5:A:131:DC:C5	2.45	0.52
2:B:77:LYS:HE2	4:D:89:ARG:HH12	1.74	0.52
7:L:1230:CYS:HB2	7:L:1259:PHE:HB3	1.91	0.51
1:E:49:ARG:HG2	7:L:1119:LEU:HD13	1.92	0.51
5:A:105:DG:H2"	5:A:106:DT:H5"	1.92	0.51
5:A:13:DC:H2"	5:A:14:DC:H5	1.76	0.51
5:A:163:DC:C4	5:A:164:DC:N4	2.79	0.51
7:I:1077:LYS:HE2	7:I:1077:LYS:N	2.18	0.51
5:A:150:DC:H2'	5:A:151:DA:N7	2.25	0.51
7:I:1083:GLY:C	7:I:1084:LYS:HD3	2.32	0.51
5:A:167:DT:H2"	5:A:168:DT:C5	2.46	0.50
7:L:1260:ASN:OD1	7:L:1261:TYR:N	2.44	0.50
7:I:1151:LYS:O	7:I:1160:ARG:NH2	2.45	0.50
6:K:171:DA:H1'	6:K:172:DT:H5'	1.93	0.50
7:I:1147:ALA:HB2	7:I:1161:THR:HA	1.92	0.50
7:L:1152:THR:HA	7:L:1160:ARG:HH12	1.76	0.50
5:A:27:DA:H2"	5:A:28:DA:C8	2.47	0.50
7:L:1158:GLY:O	7:L:1159:LEU:HD23	2.12	0.50
7:L:1186:LEU:O	7:L:1190:ARG:HG3	2.11	0.50
1:M:34:GLY:HA2	7:I:1265:CYS:HB3	1.94	0.49
5:A:28:DA:H1'	5:A:29:DT:H5'	1.92	0.49
7:L:1108:CYS:HB2	7:L:1134:CYS:HB2	1.93	0.49
3:G:77:ARG:NH1	5:A:40:DA:O5'	2.45	0.49
6:K:160:DT:H2"	6:K:161:DT:C5	2.47	0.49
6:K:20:DA:H2"	6:K:21:DA:C8	2.48	0.49
7:I:1228:PRO:HG3	7:I:1260:ASN:HB2	1.94	0.49
7:L:1152:THR:HG22	7:L:1155:ARG:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:11:DG:N3	5:A:11:DG:H2'	2.28	0.48
7:I:1229:ASN:HD21	7:I:1257:LEU:HA	1.76	0.48
6:K:158:DG:H2"	6:K:159:DA:H5'	1.94	0.48
1:E:118:THR:HG23	5:A:91:DG:OP1	2.14	0.48
6:K:157:DG:H2"	6:K:158:DG:N7	2.27	0.48
7:L:1147:ALA:HB2	7:L:1161:THR:HA	1.95	0.48
5:A:29:DT:H1'	5:A:30:DC:H5	1.78	0.48
6:K:58:DG:H2"	6:K:59:DG:N7	2.29	0.48
6:K:14:DC:H2"	6:K:15:DA:C8	2.49	0.48
7:L:1214:PRO:HB2	7:L:1215:LYS:HD2	1.96	0.48
3:C:50:TYR:HD2	4:D:115:VAL:HG21	1.79	0.48
7:L:1271:THR:OG1	7:L:1272:GLU:N	2.47	0.48
5:A:63:DA:H2"	5:A:64:DG:H5"	1.95	0.47
7:I:1151:LYS:HG3	7:I:1152:THR:N	2.29	0.47
6:K:131:DC:H2"	6:K:132:DG:C8	2.50	0.47
5:A:153:DA:H5"	5:A:153:DA:C8	2.45	0.47
1:E:35:VAL:O	1:E:35:VAL:HG13	2.14	0.47
6:K:147:DC:H2"	6:K:148:DT:O4'	2.15	0.47
7:I:1159:LEU:HD12	7:I:1160:ARG:H	1.80	0.47
7:I:1229:ASN:O	7:I:1248:LEU:N	2.38	0.47
7:I:1084:LYS:HD3	7:I:1084:LYS:N	2.29	0.47
7:I:1179:ILE:HG23	7:I:1209:ILE:HB	1.96	0.47
2:B:70:VAL:O	2:B:74:GLU:HG3	2.15	0.46
7:L:1224:HIS:HB2	7:L:1261:TYR:CZ	2.50	0.46
6:K:22:DC:H2"	6:K:23:DA:C8	2.50	0.46
5:A:37:DC:H6	5:A:37:DC:H5'	1.79	0.46
7:I:1147:ALA:CB	7:I:1161:THR:HA	2.44	0.46
7:I:1277:ALA:N	7:I:1280:CYS:SG	2.88	0.46
6:K:140:DG:H2"	6:K:141:DA:N7	2.31	0.46
7:L:1069:LYS:HG3	7:L:1070:PRO:HD2	1.98	0.46
7:L:1171:VAL:HG12	7:L:1172:ASN:H	1.80	0.46
7:L:1273:CYS:HA	8:L:1504:SAM:N1	2.31	0.46
7:L:1150:ILE:HD12	7:L:1160:ARG:H	1.81	0.46
7:I:1263:LEU:HD21	7:I:1284:LEU:HB3	1.98	0.46
8:L:1504:SAM:H5'1	8:L:1504:SAM:H8	1.97	0.46
7:I:1190:ARG:HH11	7:I:1194:ASN:HD21	1.64	0.45
7:L:1200:TYR:HD2	7:L:1213:GLY:HA2	1.81	0.45
7:L:1149:ILE:HD11	7:L:1157:TRP:CD1	2.51	0.45
7:L:1205:THR:HG22	7:L:1206:LYS:N	2.32	0.45
4:D:111:GLY:O	4:D:115:VAL:HG23	2.16	0.45
5:A:35:DT:H2"	5:A:36:DG:C8	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:54:DC:H2'	6:K:55:DT:C6	2.51	0.45
7:L:1150:ILE:HG22	7:L:1151:LYS:N	2.30	0.45
5:A:151:DA:C2'	5:A:152:DG:H4'	2.39	0.45
5:A:133:DA:H2"	5:A:134:DG:H5'	1.99	0.45
5:A:177:DG:H2"	5:A:178:DG:C8	2.51	0.45
6:K:46:DC:H2"	6:K:47:DC:C5	2.51	0.45
7:I:1190:ARG:HG2	7:I:1194:ASN:HD21	1.81	0.45
7:I:1230:CYS:HB2	7:I:1259:PHE:HB3	1.98	0.45
5:A:26:DG:H1'	5:A:27:DA:H5'	1.98	0.45
6:K:164:DC:H2"	6:K:165:DC:C5	2.52	0.45
7:L:1170:PHE:HA	7:L:1246:PHE:HA	1.99	0.45
7:L:1200:TYR:OH	8:L:1504:SAM:HA	2.17	0.45
4:H:48:ASP:OD1	4:H:48:ASP:N	2.50	0.45
7:I:1262:ASN:ND2	7:I:1262:ASN:N	2.61	0.45
7:L:1194:ASN:OD1	7:L:1196:VAL:HG23	2.17	0.45
5:A:129:DC:H2"	5:A:130:DC:C5	2.52	0.45
6:K:155:DC:H2"	6:K:156:DG:H5"	1.98	0.45
1:E:118:THR:HG22	2:F:45:ARG:HB3	1.98	0.44
7:L:1262:ASN:ND2	7:L:1262:ASN:H	2.15	0.44
4:D:54:LYS:HB3	4:D:54:LYS:HE3	1.73	0.44
6:K:69:DC:H2"	6:K:70:DT:H72	2.00	0.44
6:K:168:DG:H2'	6:K:169:DG:H8	1.78	0.44
7:L:1228:PRO:HG3	7:L:1260:ASN:HB2	1.98	0.44
7:L:1166:LYS:HD2	7:L:1166:LYS:HA	1.75	0.44
5:A:91:DG:H5"	5:A:91:DG:C8	2.52	0.44
5:A:102:DC:H2"	5:A:103:DG:C8	2.53	0.44
7:I:1080:LYS:O	7:I:1178:LEU:HD23	2.17	0.44
7:I:1200:TYR:OH	8:I:1501:SAM:HG1	2.16	0.44
5:A:104:DC:H2"	5:A:105:DG:H5"	2.00	0.44
6:K:152:DC:H2"	6:K:153:DA:C8	2.53	0.44
4:H:113:LYS:HB3	4:H:113:LYS:HE2	1.65	0.44
5:A:98:DC:H2"	5:A:99:DC:C5	2.53	0.44
5:A:158:DT:H6	5:A:158:DT:H2'	1.69	0.44
7:I:1206:LYS:HD2	7:I:1206:LYS:HA	1.76	0.44
5:A:163:DC:C2	5:A:164:DC:C4	3.06	0.43
5:A:28:DA:H4'	5:A:29:DT:OP1	2.18	0.43
6:K:33:DT:H2"	6:K:34:DA:C8	2.53	0.43
7:I:1086:GLN:N	7:I:1086:GLN:OE1	2.51	0.43
7:I:1161:THR:HG22	7:I:1255:MET:O	2.18	0.43
7:I:1185:ARG:O	7:I:1188:ILE:HG22	2.18	0.43
7:I:1147:ALA:HB1	7:I:1160:ARG:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:1171:VAL:HG12	7:L:1172:ASN:N	2.33	0.43
2:B:22:LEU:HB3	2:B:25:ASN:HD21	1.83	0.43
4:D:27:ARG:HG3	4:D:28:LYS:NZ	2.34	0.43
7:I:1152:THR:CA	7:I:1160:ARG:HH22	2.31	0.43
2:B:92:ARG:HH21	4:D:98:LEU:HD22	1.84	0.43
4:H:105:LYS:HB3	4:H:105:LYS:HE2	1.82	0.43
8:I:1501:SAM:H5'2	8:I:1501:SAM:HB2	1.66	0.43
6:K:31:DT:H2"	6:K:32:DA:C8	2.54	0.42
7:I:1170:PHE:HB3	7:I:1246:PHE:CD2	2.54	0.42
1:E:120:NLE:HB2	1:E:121:PRO:HD2	2.01	0.42
5:A:28:DA:C1'	5:A:29:DT:H5'	2.48	0.42
7:L:1287:ARG:O	7:L:1287:ARG:HG3	2.18	0.42
6:K:49:DG:H2"	6:K:50:DG:C8	2.54	0.42
5:A:58:DT:H2"	5:A:59:DA:C8	2.53	0.42
5:A:67:DC:H2"	5:A:68:DT:C7	2.50	0.42
6:K:159:DA:H1'	6:K:160:DT:C6	2.55	0.42
7:I:1224:HIS:CG	7:I:1225:SER:N	2.88	0.42
5:A:163:DC:N3	5:A:164:DC:N4	2.68	0.42
7:I:1287:ARG:HD3	7:I:1287:ARG:HA	1.76	0.42
7:L:1224:HIS:CG	7:L:1225:SER:N	2.88	0.42
3:G:13:LYS:HD2	3:G:13:LYS:HA	1.85	0.42
7:I:1180:ASP:O	7:I:1184:CYS:HB2	2.19	0.42
5:A:173:DT:H2"	5:A:174:DG:C8	2.55	0.42
5:A:17:DT:H2"	5:A:18:DC:C6	2.55	0.41
5:A:16:DA:H2'	5:A:17:DT:H71	2.01	0.41
6:K:156:DG:H2"	6:K:157:DG:H5'	2.02	0.41
3:G:102:ILE:HG23	4:H:58:ILE:HD13	2.02	0.41
5:A:31:DC:H2"	5:A:32:DC:C6	2.55	0.41
7:I:1217:ASN:O	7:I:1220:ARG:HG2	2.20	0.41
7:L:1151:LYS:HB3	7:L:1151:LYS:HE3	1.70	0.41
7:L:1070:PRO:HG3	7:L:1221:PHE:HE2	1.84	0.41
5:A:132:DT:H2"	5:A:133:DA:C8	2.56	0.41
7:I:1070:PRO:HD3	7:I:1157:TRP:CD1	2.55	0.41
7:L:1086:GLN:N	7:L:1086:GLN:OE1	2.54	0.41
7:I:1278:ASP:OD1	7:I:1278:ASP:N	2.53	0.41
7:L:1263:LEU:HD23	7:L:1263:LEU:HA	1.86	0.41
5:A:53:DG:H2"	5:A:54:DG:H5"	2.01	0.41
7:L:1161:THR:C	7:L:1162:LYS:HD3	2.40	0.41
6:K:170:DG:H2"	6:K:171:DA:C8	2.55	0.41
7:L:1216:GLY:HA3	7:L:1220:ARG:HD2	2.03	0.41
6:K:21:DA:H2"	6:K:22:DC:C5	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:85:DC:H2"	6:K:86:DG:C8	2.55	0.41
5:A:123:DA:H2"	5:A:124:DT:H71	2.03	0.40
3:C:47:ALA:HB3	3:C:48:PRO:HD3	2.02	0.40
1:E:62:ILE:HG22	1:E:63:ARG:N	2.37	0.40
7:L:1205:THR:HG22	7:L:1206:LYS:H	1.86	0.40
7:L:1159:LEU:O	7:L:1256:GLU:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	95/135 (70%)	90 (95%)	5 (5%)	0	100	100
1	M	98/135 (73%)	94 (96%)	4 (4%)	0	100	100
2	B	80/102 (78%)	77 (96%)	3 (4%)	0	100	100
2	F	84/102 (82%)	78 (93%)	6 (7%)	0	100	100
3	C	107/129 (83%)	101 (94%)	6 (6%)	0	100	100
3	G	108/129 (84%)	98 (91%)	10 (9%)	0	100	100
4	D	93/122 (76%)	89 (96%)	4 (4%)	0	100	100
4	H	95/122 (78%)	93 (98%)	2 (2%)	0	100	100
7	I	220/758 (29%)	187 (85%)	32 (14%)	1 (0%)	29	65
7	L	220/758 (29%)	187 (85%)	33 (15%)	0	100	100
All	All	1200/2492 (48%)	1094 (91%)	105 (9%)	1 (0%)	54	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	I	1146	ASP

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	
1	E	84/107 (78%)	84 (100%)	0	100	100
1	M	85/107 (79%)	85 (100%)	0	100	100
2	B	67/78 (86%)	67 (100%)	0	100	100
2	F	67/78 (86%)	67 (100%)	0	100	100
3	C	85/101 (84%)	85 (100%)	0	100	100
3	G	87/101 (86%)	86 (99%)	1 (1%)	73	88
4	D	81/102 (79%)	81 (100%)	0	100	100
4	H	83/102 (81%)	81 (98%)	2 (2%)	49	76
7	I	194/663 (29%)	188 (97%)	6 (3%)	40	70
7	L	194/663 (29%)	189 (97%)	5 (3%)	46	74
All	All	1027/2102 (49%)	1013 (99%)	14 (1%)	68	85

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	119	LYS
4	H	25	LYS
4	H	28	LYS
7	I	1074	LYS
7	I	1077	LYS
7	I	1087	ILE
7	I	1234	LYS
7	I	1262	ASN
7	I	1287	ARG
7	L	1074	LYS
7	L	1077	LYS
7	L	1087	ILE
7	L	1234	LYS
7	L	1262	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	84	GLN
1	E	125	GLN
3	G	38	ASN
7	I	1066	ASN
7	I	1124	HIS
7	I	1192	HIS
7	I	1224	HIS
7	I	1233	GLN
7	I	1262	ASN
7	I	1279	ASN
7	L	1262	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	NLE	M	120	1	6,7,8	0.67	0	2,7,9	0.50	0
1	NLE	E	90	1	6,7,8	0.72	0	2,7,9	0.49	0
1	NLE	M	90	1	6,7,8	0.64	0	2,7,9	0.44	0
1	NLE	E	120	1	6,7,8	0.68	0	2,7,9	0.48	0
1	NLE	E	36	1	6,7,8	0.70	0	2,7,9	0.48	0
1	NLE	M	36	1	6,7,8	0.46	0	2,7,9	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	NLE	M	120	1	-	3/5/6/8	-
1	NLE	E	90	1	-	2/5/6/8	-
1	NLE	M	90	1	-	1/5/6/8	-
1	NLE	E	120	1	-	2/5/6/8	-
1	NLE	E	36	1	-	3/5/6/8	-
1	NLE	M	36	1	-	0/5/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	36	NLE	N-CA-CB-CG
1	E	36	NLE	C-CA-CB-CG
1	M	120	NLE	C-CA-CB-CG
1	M	120	NLE	CA-CB-CG-CD
1	E	90	NLE	CE-CD-CG-CB
1	M	90	NLE	CE-CD-CG-CB
1	E	36	NLE	CE-CD-CG-CB
1	E	90	NLE	CA-CB-CG-CD
1	E	120	NLE	CA-CB-CG-CD
1	M	120	NLE	CE-CD-CG-CB
1	E	120	NLE	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	120	NLE	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 6 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	$\#\|Z\| > 2$
8	SAM	I	1501	-	24,29,29	1.22	3 (12%)	23,42,42	1.58	4 (17%)
8	SAM	L	1504	-	24,29,29	1.22	3 (12%)	23,42,42	1.60	4 (17%)

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
8	SAM	I	1501	-	-	7/12/33/33	0/3/3/3
8	SAM	L	1504	-	-	3/12/33/33	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	1504	SAM	C2-N3	3.96	1.38	1.32
8	I	1501	SAM	C2-N3	3.91	1.38	1.32
8	L	1504	SAM	C2-N1	2.52	1.38	1.33
8	I	1501	SAM	C2-N1	2.51	1.38	1.33
8	I	1501	SAM	OXT-C	-2.17	1.23	1.30
8	L	1504	SAM	OXT-C	-2.16	1.23	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	I	1501	SAM	N3-C2-N1	-5.36	120.30	128.68
8	L	1504	SAM	N3-C2-N1	-5.31	120.38	128.68
8	L	1504	SAM	C3'-C2'-C1'	2.88	105.32	100.98
8	I	1501	SAM	OXT-C-O	-2.84	117.65	124.09
8	I	1501	SAM	C3'-C2'-C1'	2.55	104.82	100.98
8	L	1504	SAM	OXT-C-O	-2.46	118.51	124.09
8	I	1501	SAM	OXT-C-CA	2.14	120.68	113.38
8	L	1504	SAM	OXT-C-CA	2.06	120.39	113.38

There are no chirality outliers.

All (10) torsion outliers are listed below:

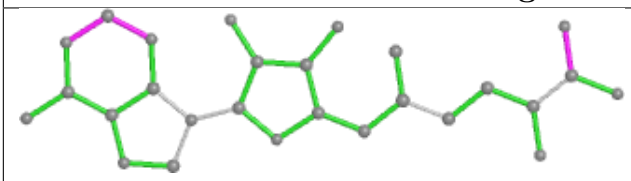
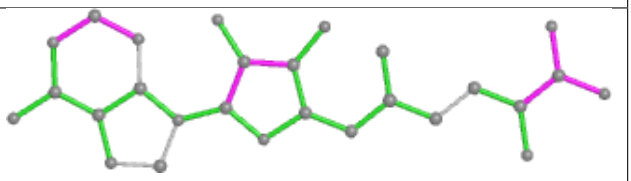
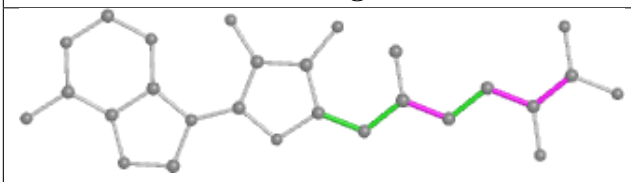
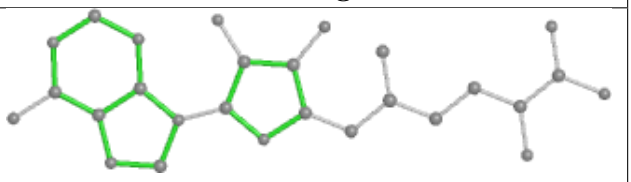
Mol	Chain	Res	Type	Atoms
8	I	1501	SAM	O-C-CA-N
8	I	1501	SAM	N-CA-CB-CG
8	L	1504	SAM	CA-CB-CG-SD
8	I	1501	SAM	OXT-C-CA-N
8	I	1501	SAM	CB-CG-SD-CE
8	I	1501	SAM	C-CA-CB-CG
8	L	1504	SAM	CB-CG-SD-C5'
8	I	1501	SAM	O-C-CA-CB
8	I	1501	SAM	OXT-C-CA-CB
8	L	1504	SAM	CB-CG-SD-CE

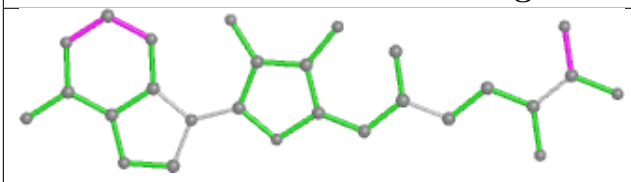
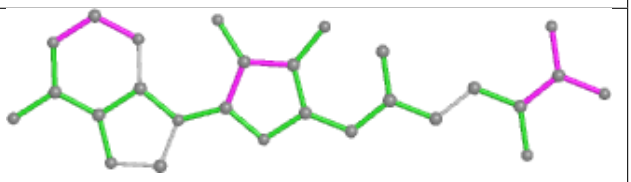
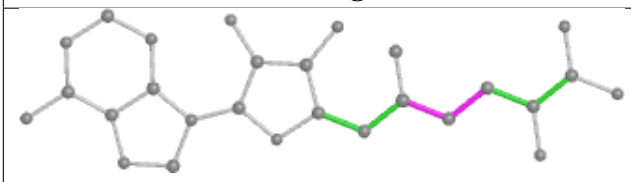
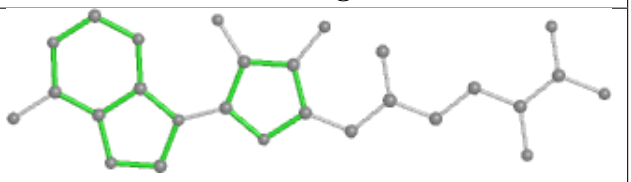
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	1501	SAM	2	0
8	L	1504	SAM	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 SAM I 1501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAM L 1504	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

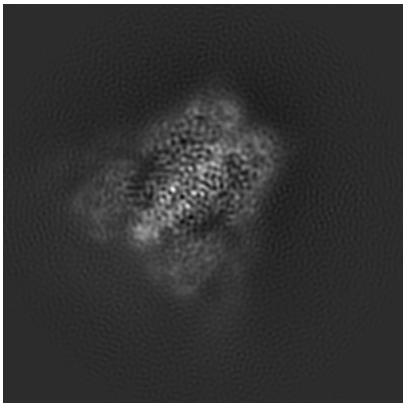
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30456. These allow visual inspection of the internal detail of the map and identification of artifacts.

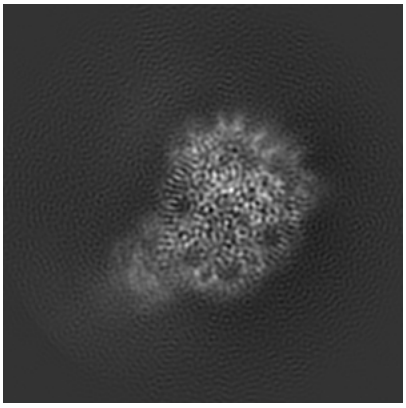
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

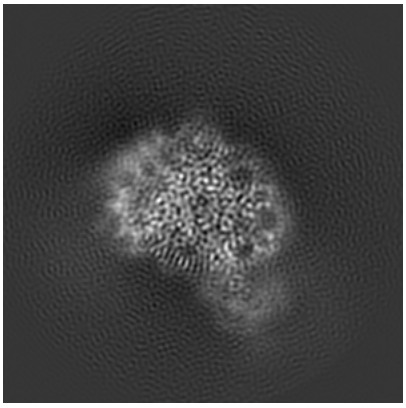
6.1.1 Primary map



X



Y

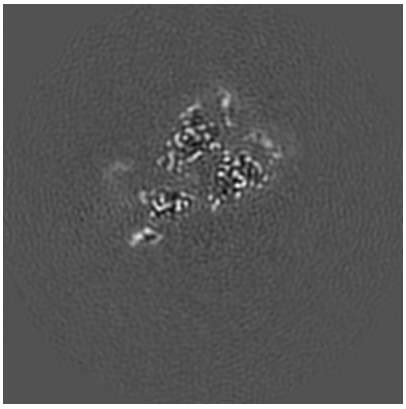


Z

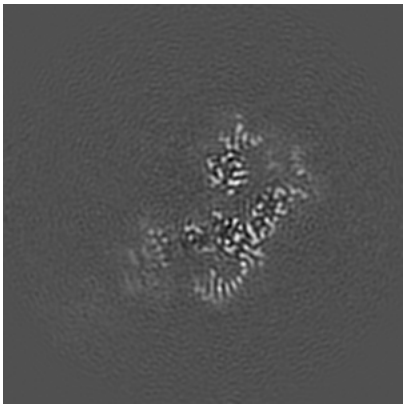
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

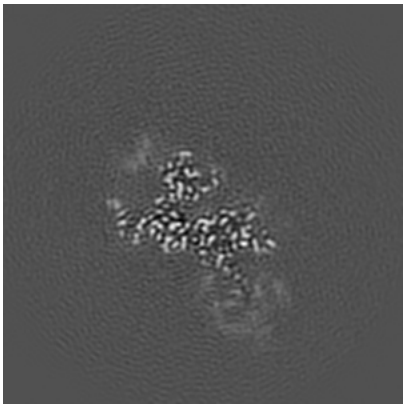
6.2.1 Primary map



X Index: 108



Y Index: 108

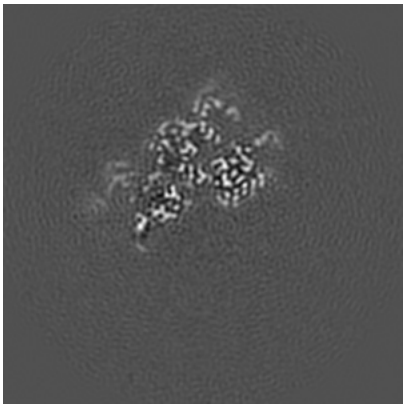


Z Index: 108

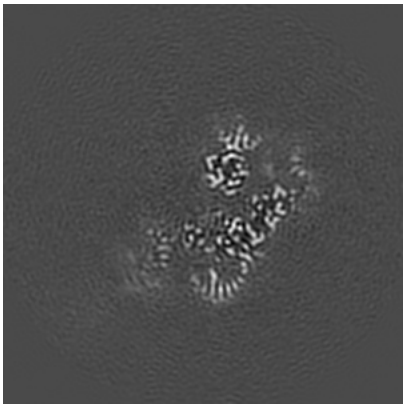
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

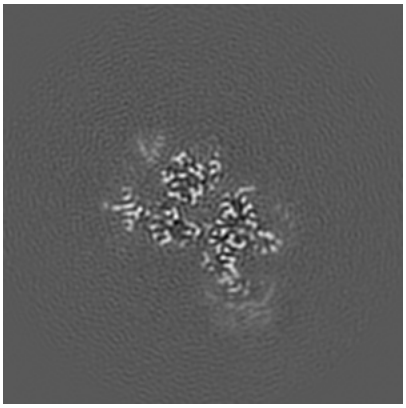
6.3.1 Primary map



X Index: 114



Y Index: 107



Z Index: 114

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0184. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

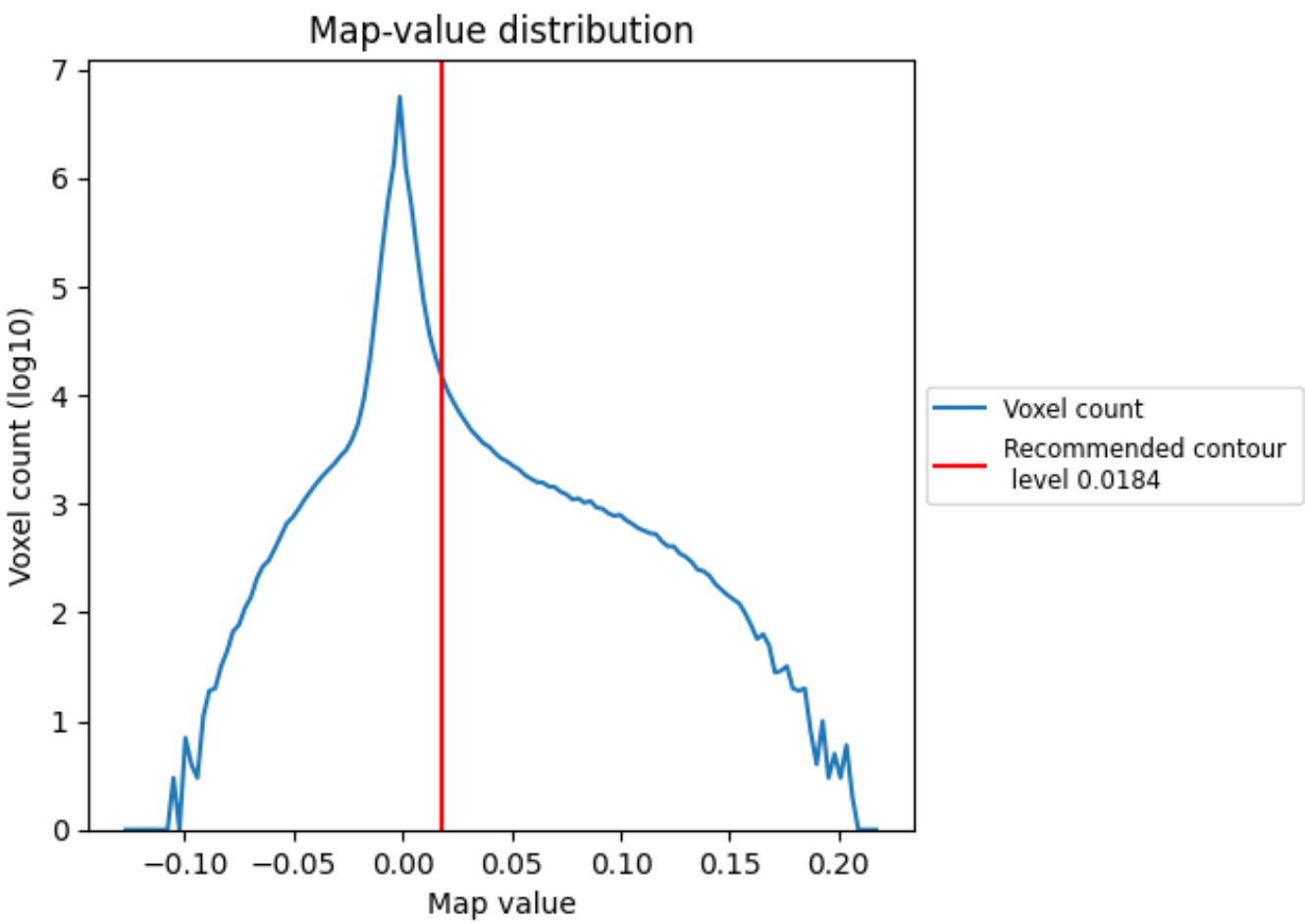
6.5 Mask visualisation (i)

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

7 Map analysis (i)

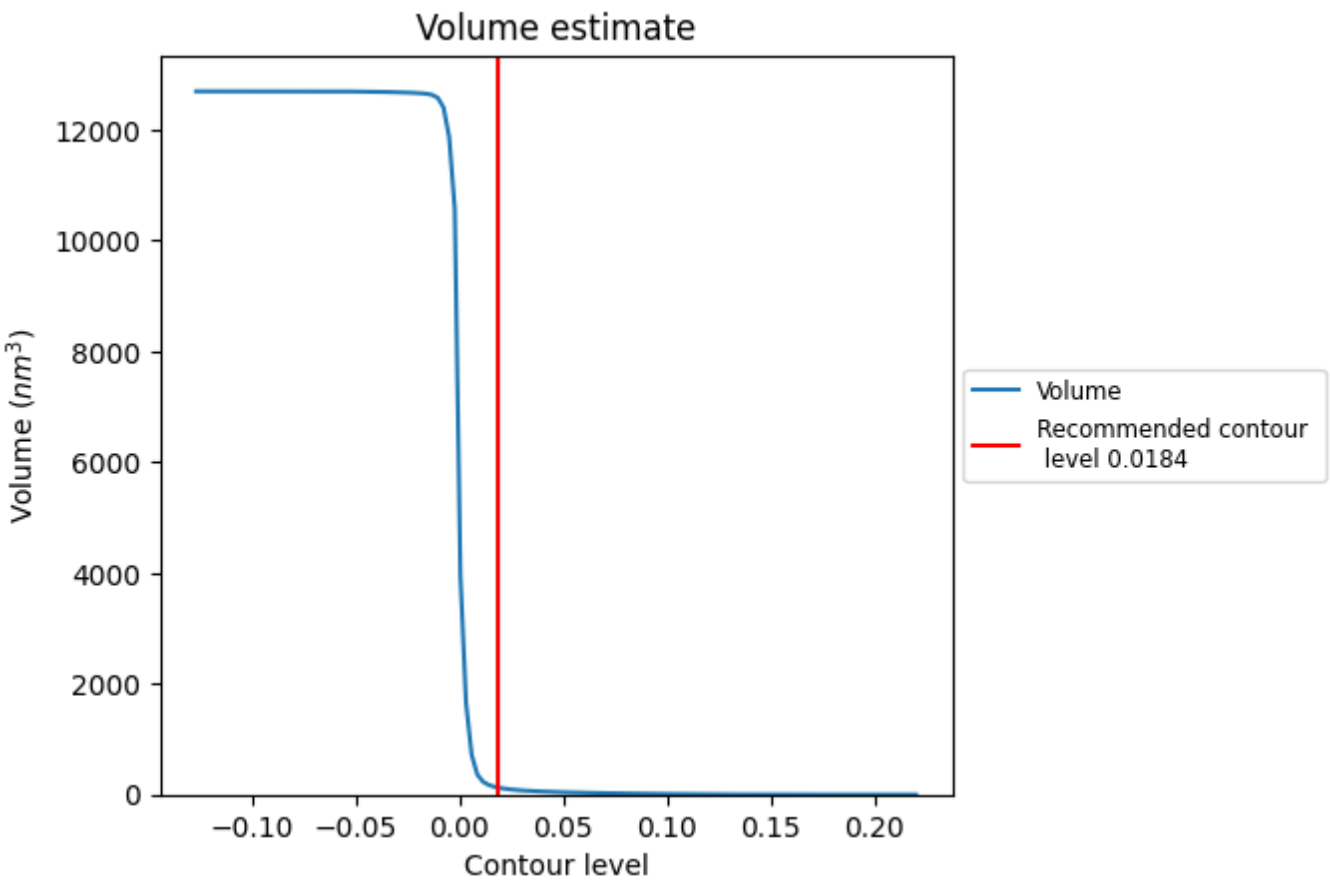
This section contains the results of statistical analysis of the map.

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.

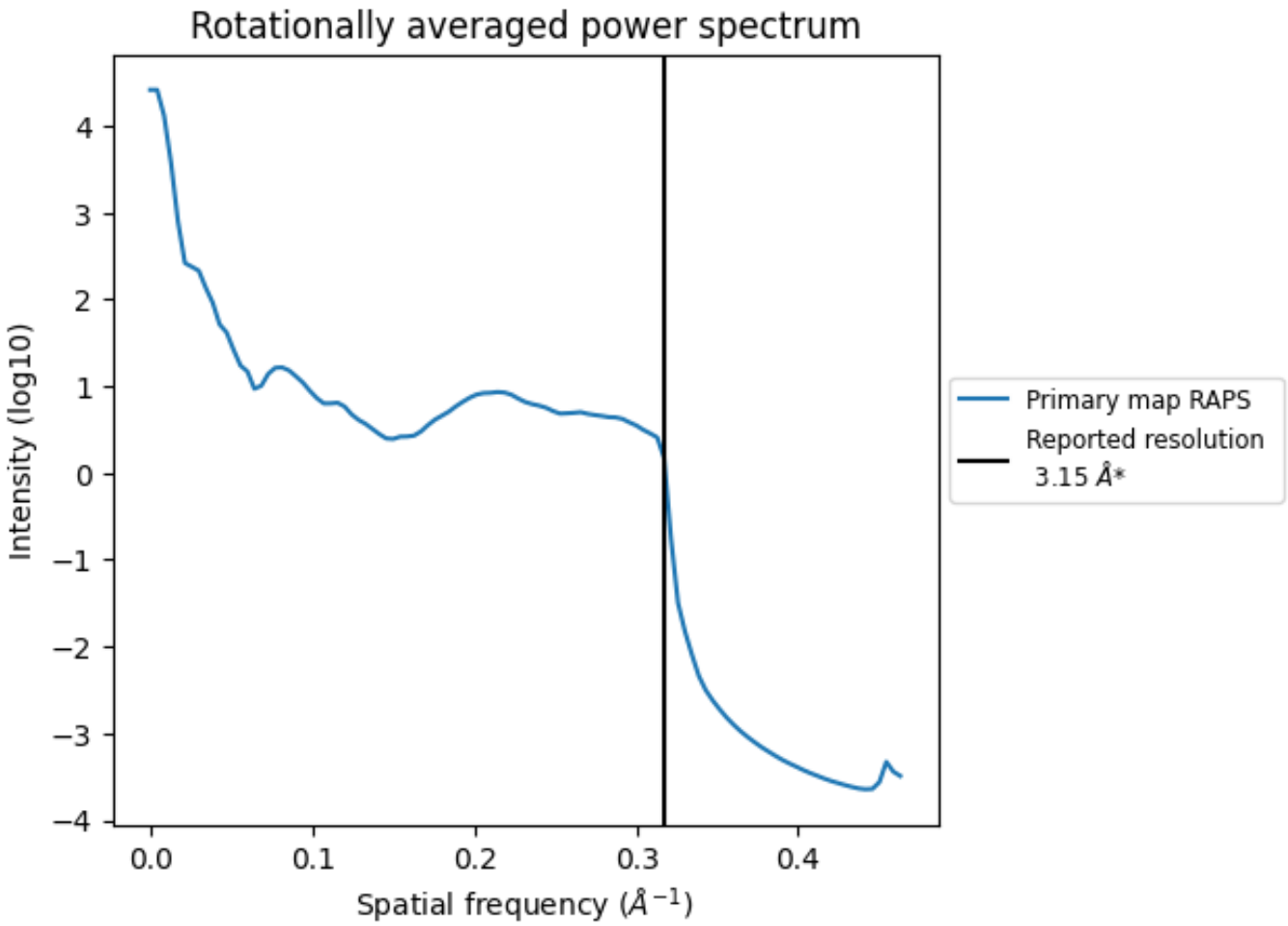
7.2 Volume estimate (i)



The volume at the recommended contour level is 128 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 0.317 Å^{-1}

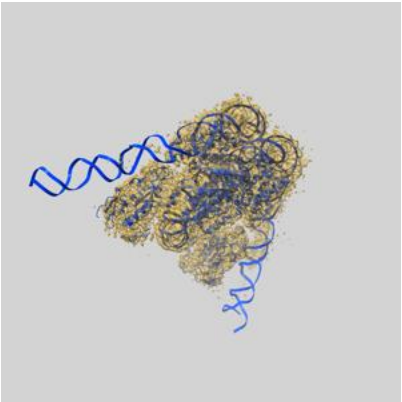
8 Fourier-Shell correlation (i)

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

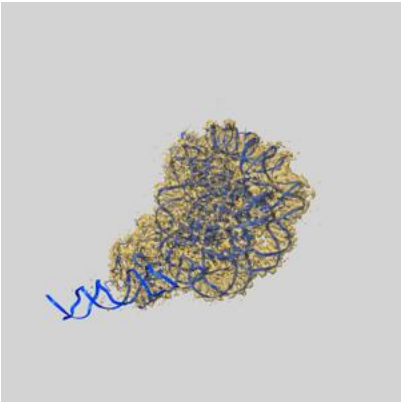
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30456 and PDB model 7CRQ. Per-residue inclusion information can be found in section 3 on page 7.

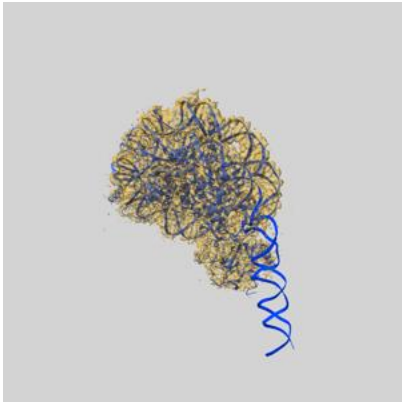
9.1 Map-model overlay (i)



X



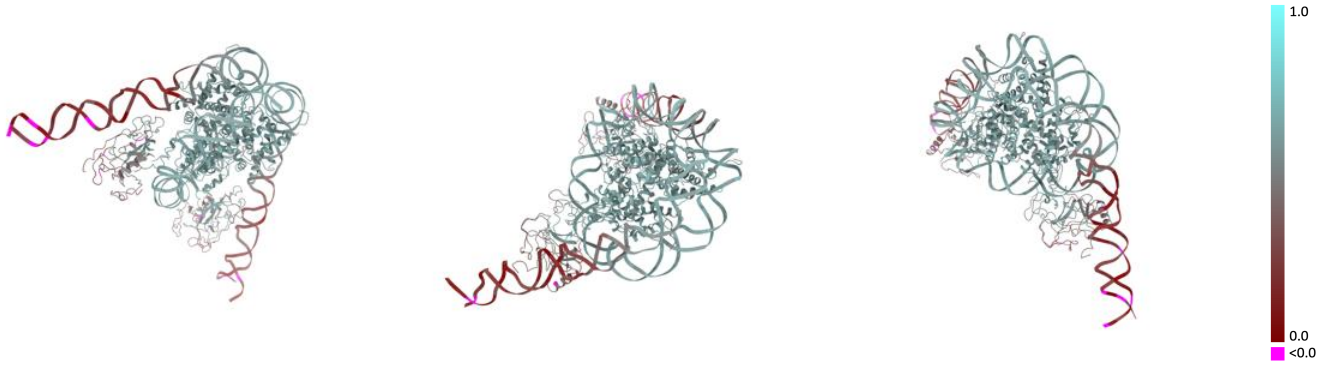
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0184 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.

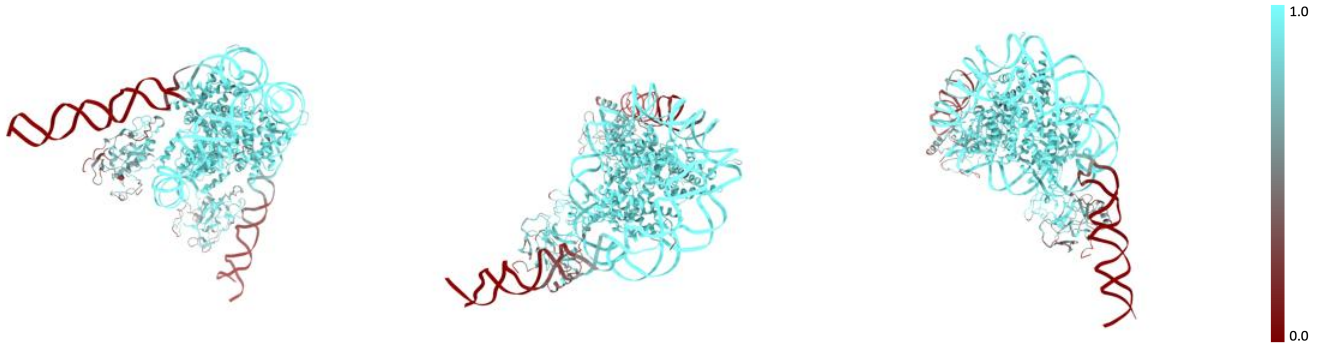
9.2 Q-score mapped to coordinate model (i)



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.

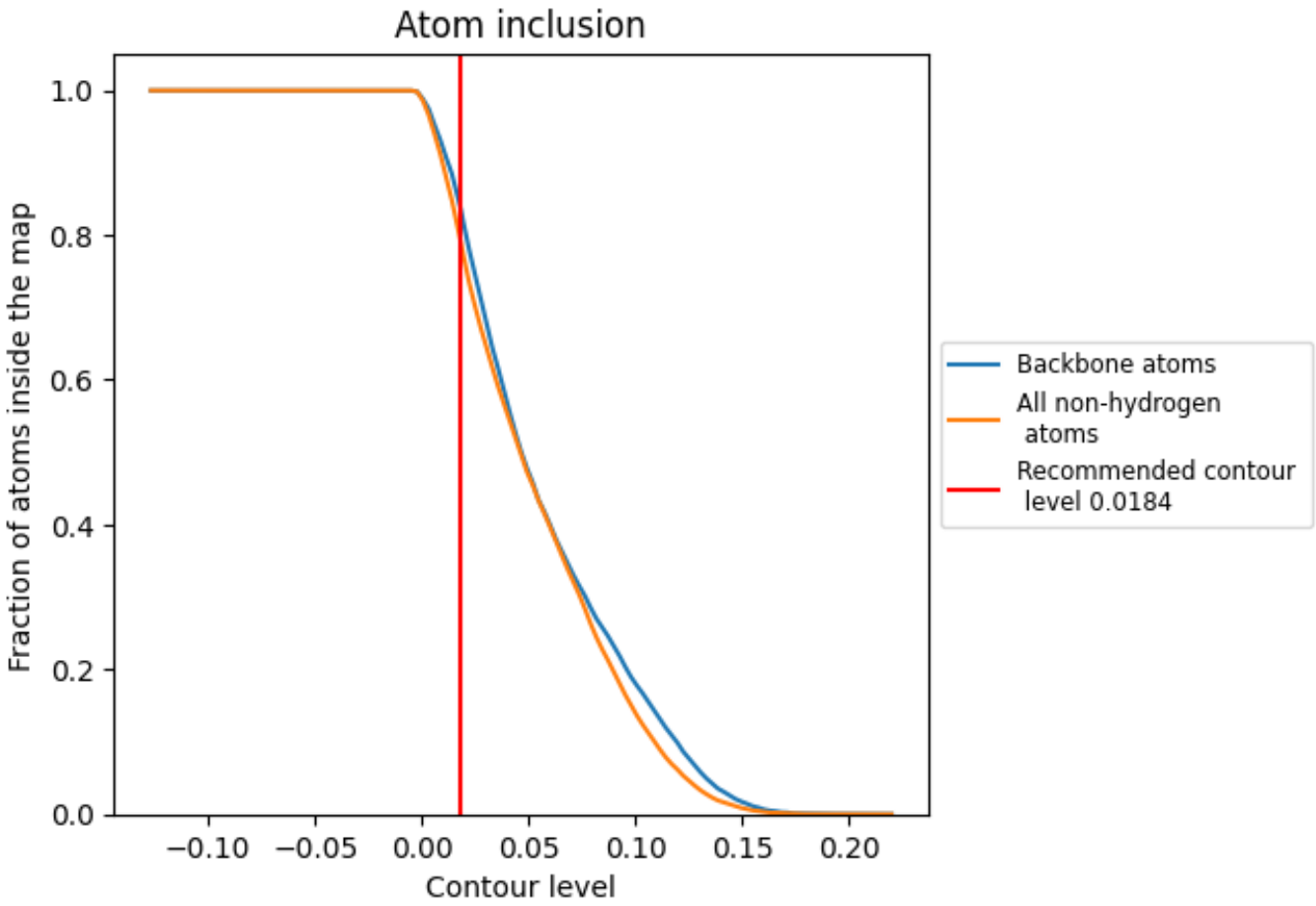
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0184).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 79% 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 (0.0184) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7888	0.5070
A	0.6982	0.4510
B	0.9585	0.6080
C	0.9667	0.5940
D	0.9532	0.5880
E	0.9683	0.6070
F	0.9414	0.6040
G	0.9611	0.6020
H	0.9409	0.5870
I	0.6969	0.4460
K	0.7039	0.4590
L	0.6556	0.4450
M	0.9515	0.6110