



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:32 PM UTC

PDB ID : 7CRQ / pdb_00007crq
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

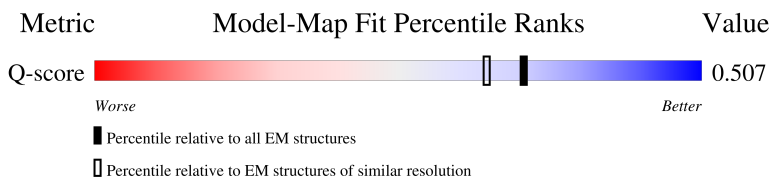
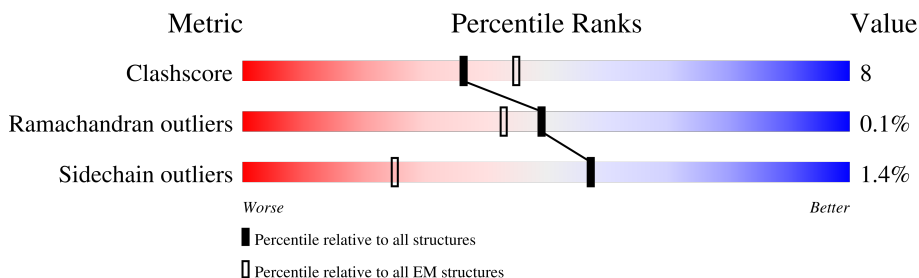
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 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.



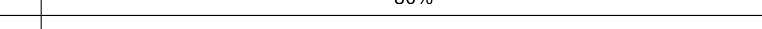
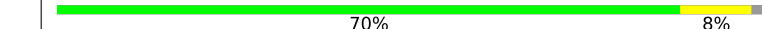
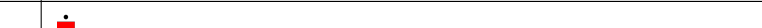
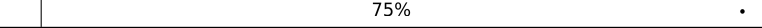
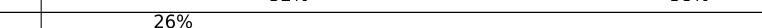
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14486 (2.65 - 3.65)

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

Mol	Chain	Length	Quality of chain
1	E	135	
1	M	135	
2	B	102	
2	F	102	

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Mol	Chain	Length	Quality of chain
3	C	129	 78%6%16%
3	G	129	 80%5%15%
4	D	122	 70%8%22%
4	H	122	 75%20%5%
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

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
1	M	103	Total	C	N	O	S	0	0
			833	528	159	145	1		
1	E	100	Total	C	N	O	S	0	0
			818	520	156	141	1		

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
2	B	82	Total	C	N	O	S	0	0
			653	413	127	112	1		
2	F	86	Total	C	N	O	S	0	0
			672	424	130	117	1		

- Molecule 3 is a protein called Histone H2A.

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

- Molecule 4 is a protein called Histone H2B.

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

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

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

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

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

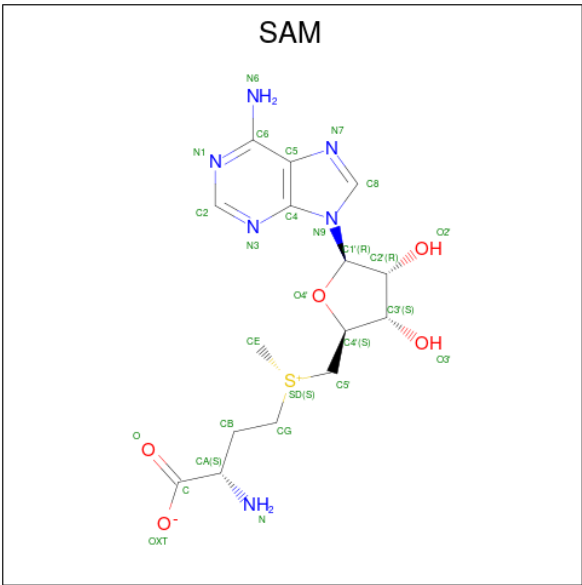
- Molecule 7 is a protein called Histone-lysine N-methyltransferase NSD3.

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

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 (CCD ID: SAM) (formula: C₁₅H₂₂N₆O₅S) (labeled as "Ligand of Interest" by depositor).



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

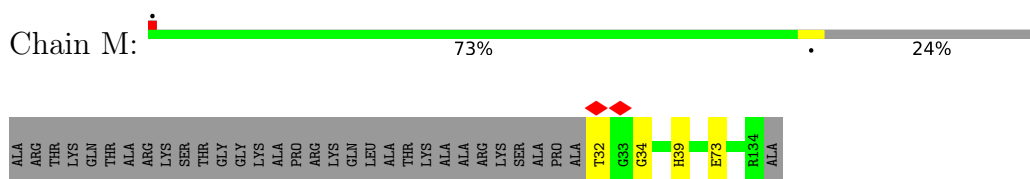
- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

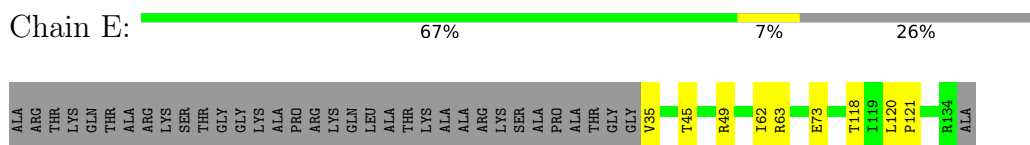
3 Residue-property plots [i](#)

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.

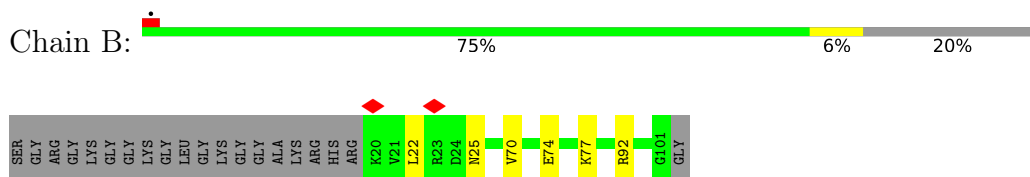
- Molecule 1: Histone H3



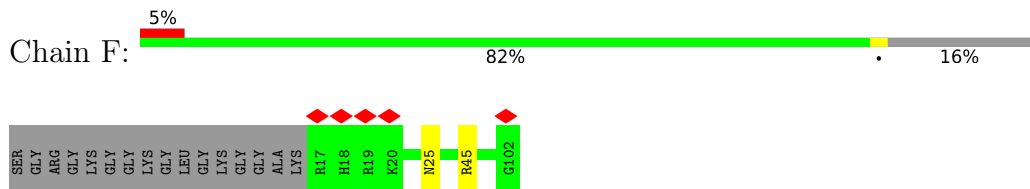
- Molecule 1: Histone H3



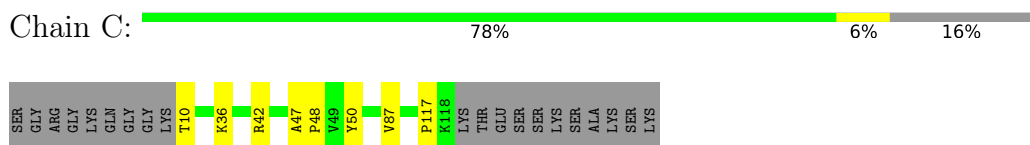
- Molecule 2: Histone H4



- Molecule 2: Histone H4



- Molecule 3: Histone H2A



- Molecule 3: Histone H2A

SER	GLY	ARG	GLY	LYS	GLN	GLY	GLY	T10	K13	V54	R77	R88	N94	T102	K119	THR	GLU	SER	SER	LYS	SER	ALA	LYS	SER	LYS
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ALA	LYS	ALA	PRO	ALA	PRO	LYS	GLY	SER	LYS	LYS	VAL	THR	LYS	THR	GLN	LYS	LYS	ASP	GLY	LYS	LYS	ARG	R27	K28	T29	R30	K54	T85	R89	L98	G111	V115	A121	LYS
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PRO
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PRO
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LYS
LYS
ALA
ALA
VAL
THR
LYS
THR
GLN
LYS
LYS
ASP
GLY
LYS
K25
R26
D48
I58
K105
K113
A121
LYS

DA	DT	DC	DG	DG	DG	DT	DT	DT	DT	G11	G12	C13	C14	G15	A16	T17	C18	C19	C20	C21	T22	G23	G24	A25	G26	A27	A28	T29	C30	C31	C32	G33	G34	T35	G36	C37	C38	G39	A40	G41	G53	G54	T58	A59	A63	G64	C67	T68	G91	C98	C99	C102		
G103	G104	G105	T106	A123	T124	C129	C130	C131	T132	A133	G134	T135	C136	T137	C138	G141	G142	C143	A144	C150	A151	G152	A153	T154	A155	T156	A157	T158	A159	C160	A161	T162	C163	C164	T165	G166	T167	T168	C169	C170	A171	G172	T173	G174	C175	C176	G177	G178	DT	DG	DT	DC	DG	DC

[illegible]

VAL	SER	ASP	VAL	GLN	SER	MET	ASP	SER	SER	LEU	SER	ARG	ARG	GLY	THR	GLY	MET	SER	LYS	ASP	ASP	THR	VAL	VAL	CYS	GLN	GLU	SER	SER	ASP	SER	LEU	ILE	PRO	CYS	GLU	GLY	GLU	CYS	CYS	LYS	HIS	PHE	HIS	LEU	GLU	CYS	LEU	GLY	LEU	ALA	SER	LEU	PRO	ASP	SER
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ALA	LEU	GLU	GLU	ALA	ALA	LYS	ARG	PHE	GLN	LEU	LYS	ALA	GLN	ARG	GLU	SER	LYS	GLU	ALA	LEU	ILE	GLU	LYS	M1066	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	M1229	C1230	K1234	F1246	M1255	E1256	L1257	T1258	F1259	M1260	Y1261	M1262	L1263	D1264	C1265	L1266	T1271	E1272	C1273	G1276	A1277	D1278	M1279	C1280	S1281	V1286	R1287	PRO	LYS	SER	ALA	CYS	ALA	SER	SER	THR	ASN	GLU	GLU	LYS	ALA	LYS	ASN	ALA	LYS	LEU	GLN	LYS		
ARG	ARG	LYS	ILE	THR	GLU	PRO	LYS	GLN	MET	HIS	GLU	CYS	ASP	TYR	CYS	PHE	GLN	CYS	GLY	ASP	GLY	GLU	LEU	VAL	MET	CYS	ASP	LYS	LYS	ASP	CYS	PRO	LEU	LEU	ASN	LEU	THR	GLN	PRO	PRO	GLU	TYR	GLY	LYS	TRP	CYS	PRO	LYS	TRP	HIS	GLN	CYS	GLU	SER
GLU	CYS	SER	SER	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	GLY	ARG	LEU	CYS	CYS	SER	GLU	VAL	PRO	PRO	GLU	TYR	TRP	LYS	ILE	LYS	CYS	PRO	LYS	TRP	GLU	SER			
GLN	ASP	HIS	GLY	GLU	VAL	LYS	GLU																																															

4 Experimental information

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 ($e^-/\text{\AA}^2$)	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: SAM, NLE, 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	0.31	0/803	0.46	0/1073
1	M	0.31	0/818	0.44	0/1093
2	B	0.32	0/660	0.48	0/885
2	F	0.31	0/680	0.46	0/912
3	C	0.27	0/847	0.44	0/1144
3	G	0.29	0/860	0.54	1/1159 (0.1%)
4	D	0.27	0/757	0.41	0/1018
4	H	0.29	0/777	0.42	0/1043
5	A	0.25	0/3830	0.44	0/5903
6	K	0.24	0/3896	0.38	0/6017
7	I	0.20	0/1789	0.54	1/2410 (0.0%)
7	L	0.19	0/1789	0.50	1/2410 (0.0%)
All	All	0.26	0/17506	0.45	3/25067 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	1181	LYS	N-CA-C	5.39	116.84	110.97
7	L	1234	LYS	N-CA-C	5.05	117.84	109.46
3	G	54	VAL	N-CA-C	-5.02	107.50	111.81

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
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	51	0
7	L	1755	0	1718	58	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	232	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 (232) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
7:L:1111:GLU:OE1	7:L:1111:GLU:HA	1.98	0.63
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
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
7:L:1222:MET:HE2	7:L:1258:THR:HG23	1.88	0.56
5:A:135:DT:H2''	5:A:136:DC:H5''	1.88	0.55
7:I:1083:GLY:C	7:I:1084:LYS:HD3	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
7:I:1222:MET:HE2	7:I:1258:THR:HA	1.92	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1161:THR:C	7:L:1162:LYS:HD3	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
7:L:1222:MET:HE3	7:L:1223:ASN:H	1.82	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:1222:MET:HE3	7:L:1223:ASN:N	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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 ⓘ

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	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%)	24	55
7	L	220/758 (29%)	187 (85%)	33 (15%)	0	100	100
All	All	1200/2492 (48%)	1094 (91%)	105 (9%)	1 (0%)	49	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	I	1146	ASP

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	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%)	83 (98%)	2 (2%)	43	66
3	G	87/101 (86%)	86 (99%)	1 (1%)	65	75
4	D	81/102 (79%)	81 (100%)	0	100	100
4	H	83/102 (81%)	83 (100%)	0	100	100
7	I	194/663 (29%)	188 (97%)	6 (3%)	35	61
7	L	194/663 (29%)	189 (97%)	5 (3%)	40	64
All	All	1027/2102 (49%)	1013 (99%)	14 (1%)	57	73

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

Mol	Chain	Res	Type
3	C	36	LYS
3	C	87	VAL
3	G	119	LYS
7	I	1074	LYS
7	I	1077	LYS
7	I	1087	ILE
7	I	1111	GLU
7	I	1262	ASN
7	I	1287	ARG
7	L	1074	LYS
7	L	1077	LYS

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Mol	Chain	Res	Type
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 (18) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	73	ASN
3	C	82	HIS
3	C	84	GLN
3	C	112	GLN
4	D	81	ASN
1	E	113	HIS
1	E	125	GLN
3	G	38	ASN
4	H	46	HIS
7	I	1066	ASN
7	I	1099	ASN
7	I	1124	HIS
7	I	1192	HIS
7	I	1224	HIS
7	I	1233	GLN
7	I	1238	ASN
7	I	1262	ASN
7	L	1198	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	E	120	1	6,7,8	0.67	0	2,7,9	0.47	0
1	NLE	M	120	1	6,7,8	0.66	0	2,7,9	0.49	0
1	NLE	M	36	1	6,7,8	0.47	0	2,7,9	0.42	0
1	NLE	E	36	1	6,7,8	0.72	0	2,7,9	0.45	0
1	NLE	E	90	1	6,7,8	0.72	0	2,7,9	0.47	0
1	NLE	M	90	1	6,7,8	0.64	0	2,7,9	0.43	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	E	120	1	-	2/5/6/8	-
1	NLE	M	120	1	-	3/5/6/8	-
1	NLE	M	36	1	-	0/5/6/8	-
1	NLE	E	36	1	-	3/5/6/8	-
1	NLE	E	90	1	-	2/5/6/8	-
1	NLE	M	90	1	-	2/5/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) 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	E	90	NLE	CE-CD-CG-CB
1	M	90	NLE	CE-CD-CG-CB
1	E	36	NLE	CE-CD-CG-CB
1	M	120	NLE	CA-CB-CG-CD
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	M	90	NLE	C-CA-CB-CG
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 oligosaccharides 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	L	1504	-	27,29,29	1.11	4 (14%)	34,42,42	1.97	10 (29%)
8	SAM	I	1501	-	27,29,29	1.11	4 (14%)	34,42,42	1.99	8 (23%)

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	L	1504	-	-	3/17/33/33	0/3/3/3
8	SAM	I	1501	-	-	7/17/33/33	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	1504	SAM	C2-N1	2.62	1.38	1.33
8	I	1501	SAM	C2-N1	2.62	1.38	1.33
8	L	1504	SAM	C2-N3	2.56	1.38	1.33
8	I	1501	SAM	C2-N3	2.51	1.38	1.33
8	I	1501	SAM	OXT-C	-2.26	1.23	1.30

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	1504	SAM	OXT-C	-2.25	1.23	1.30
8	L	1504	SAM	C5-N7	-2.02	1.35	1.39
8	I	1501	SAM	C5-N7	-2.00	1.35	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1501	SAM	N3-C2-N1	-5.47	120.30	128.58
8	L	1504	SAM	N3-C2-N1	-5.42	120.38	128.58
8	L	1504	SAM	C5-C4-N3	-4.60	120.38	126.72
8	I	1501	SAM	C5-C4-N3	-4.54	120.46	126.72
8	I	1501	SAM	N9-C8-N7	-3.86	108.46	113.94
8	L	1504	SAM	N9-C8-N7	-3.54	108.92	113.94
8	I	1501	SAM	C5-N7-C8	3.40	108.79	103.45
8	I	1501	SAM	C2-N3-C4	3.39	120.11	111.83
8	L	1504	SAM	C2-N3-C4	3.36	120.04	111.83
8	L	1504	SAM	N3-C4-N9	3.15	132.53	127.17
8	L	1504	SAM	C5-N7-C8	3.15	108.39	103.45
8	I	1501	SAM	N3-C4-N9	3.08	132.40	127.17
8	I	1501	SAM	OXT-C-O	-2.83	117.65	124.08
8	L	1504	SAM	OXT-C-O	-2.46	118.51	124.08
8	I	1501	SAM	C4-C5-N7	-2.35	107.90	110.58
8	L	1504	SAM	C4-C5-N7	-2.11	108.17	110.58
8	L	1504	SAM	C3'-C2'-C1'	2.04	105.32	101.46
8	L	1504	SAM	C6-C5-C4	2.03	119.95	117.18

There are no chirality outliers.

All (10) torsion outliers are listed below:

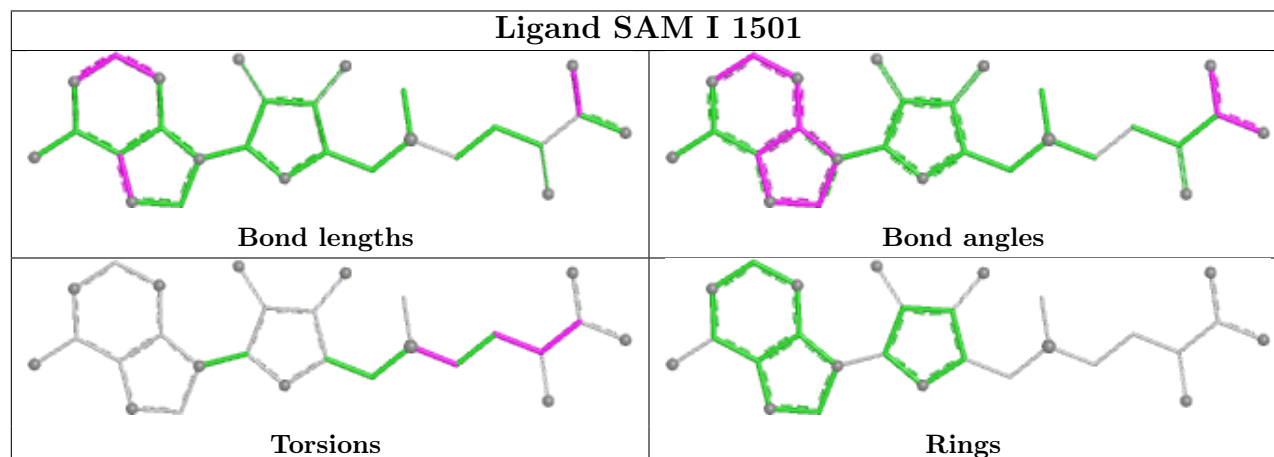
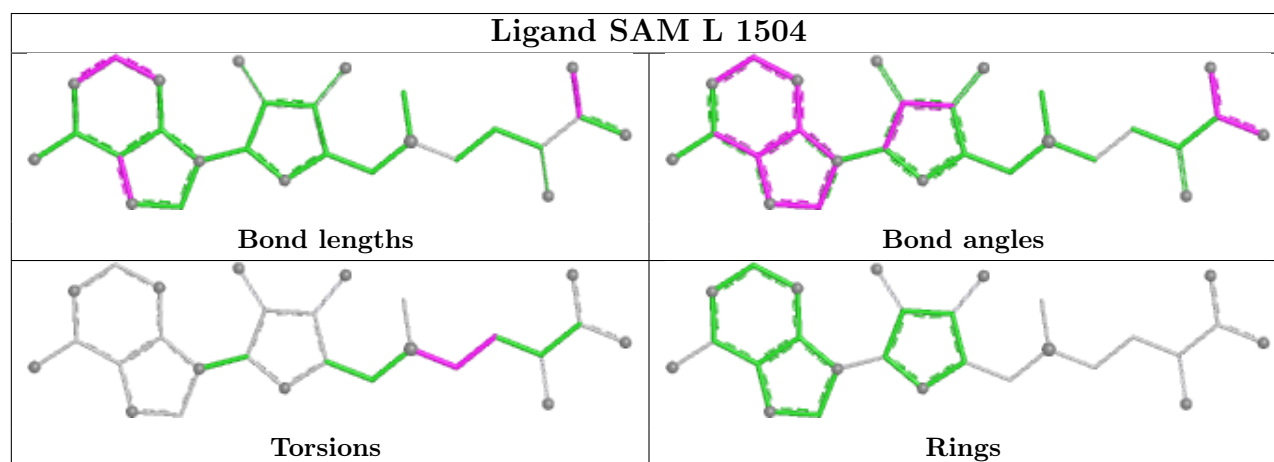
Mol	Chain	Res	Type	Atoms
8	I	1501	SAM	O-C-CA-N
8	I	1501	SAM	N-CA-CB-CG
8	L	1504	SAM	CA-CB-CG-SD
8	I	1501	SAM	OXT-C-CA-N
8	I	1501	SAM	CB-CG-SD-CE
8	I	1501	SAM	C-CA-CB-CG
8	I	1501	SAM	O-C-CA-CB
8	L	1504	SAM	CB-CG-SD-C5'
8	I	1501	SAM	OXT-C-CA-CB
8	L	1504	SAM	CB-CG-SD-CE

There are no ring outliers.

2 monomers are involved in 6 short contacts:

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

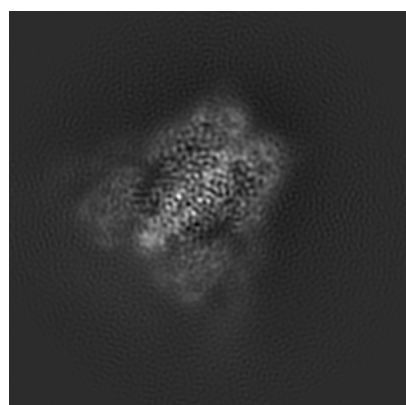
6 Map visualisation [i](#)

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

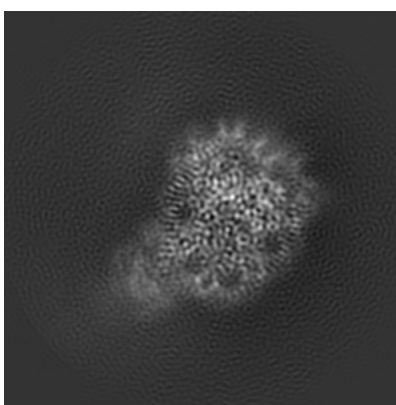
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

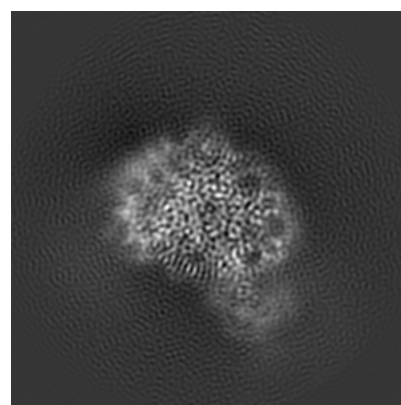
6.1.1 Primary map



X



Y

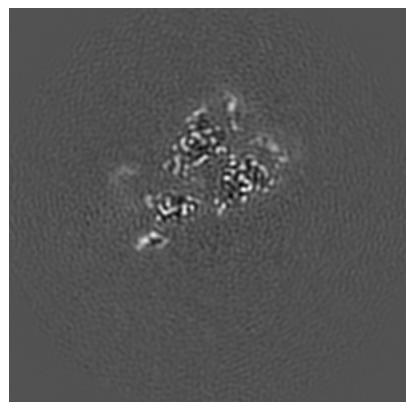


Z

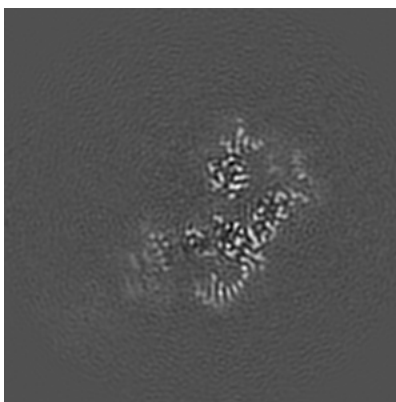
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

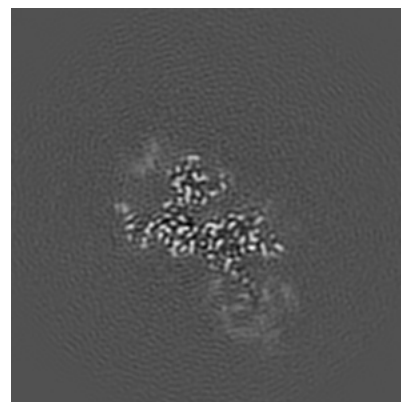
6.2.1 Primary map



X Index: 108



Y Index: 108

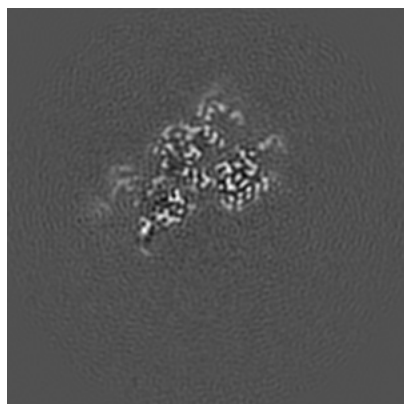


Z Index: 108

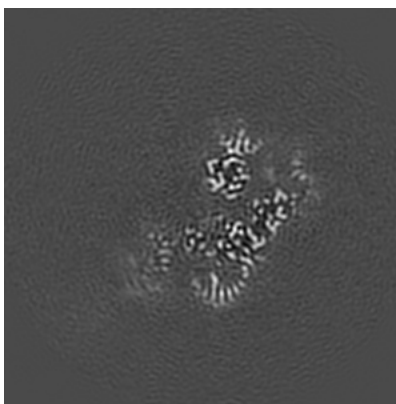
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

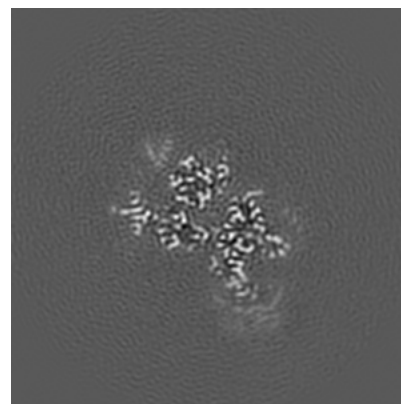
6.3.1 Primary map



X Index: 114



Y Index: 107

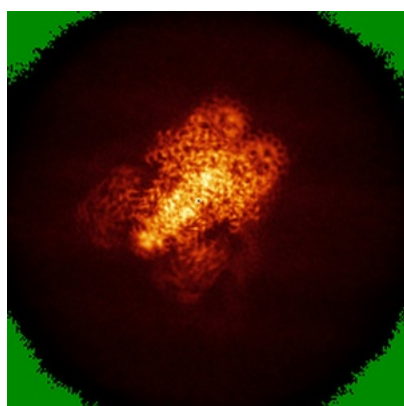


Z Index: 114

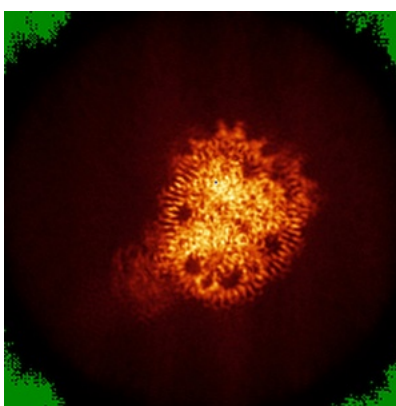
The images above show the largest variance slices of the map in three orthogonal directions.

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

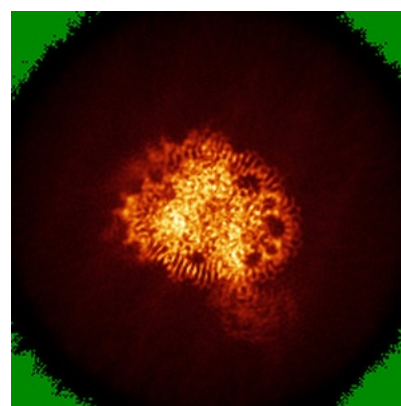
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

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

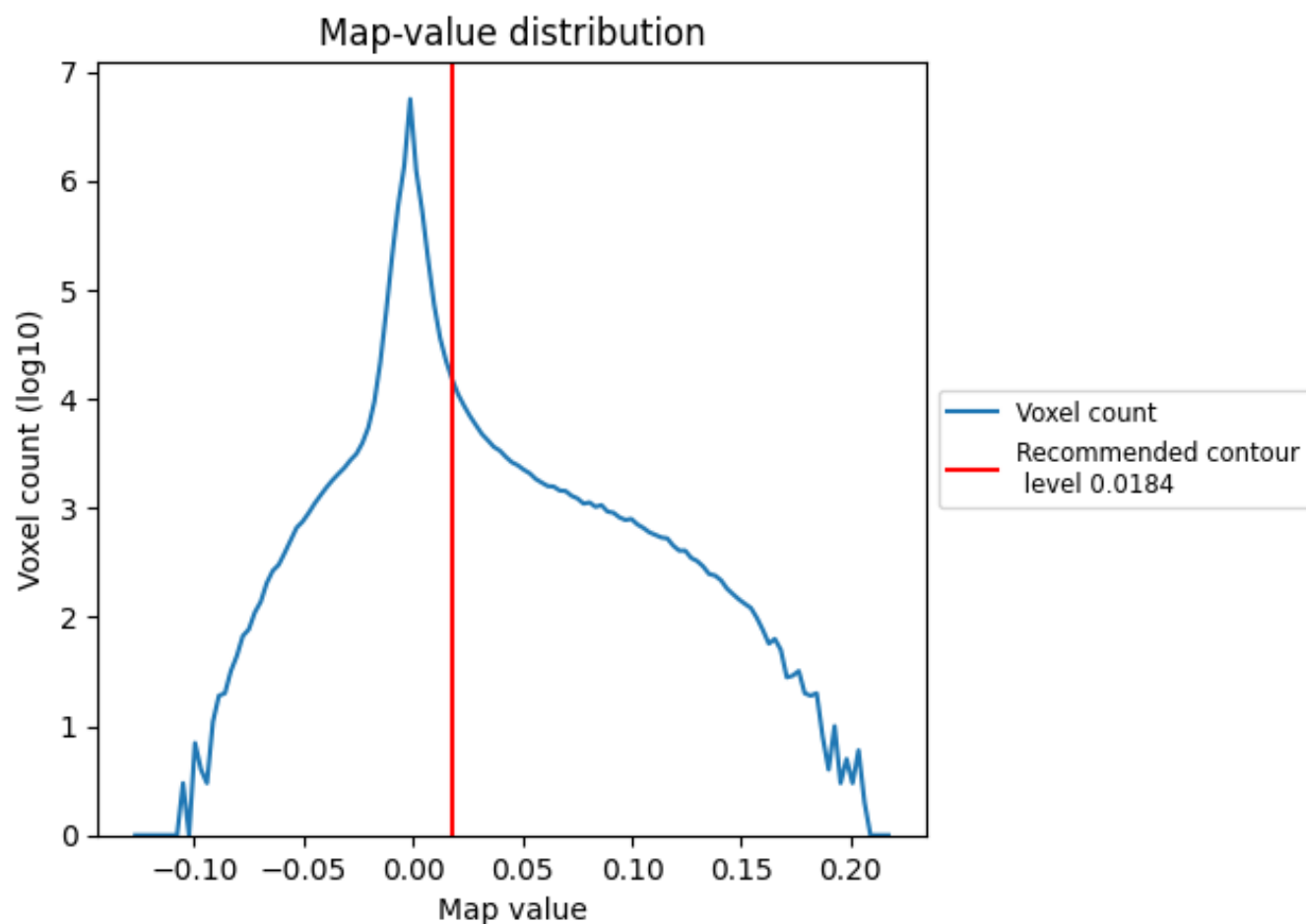
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

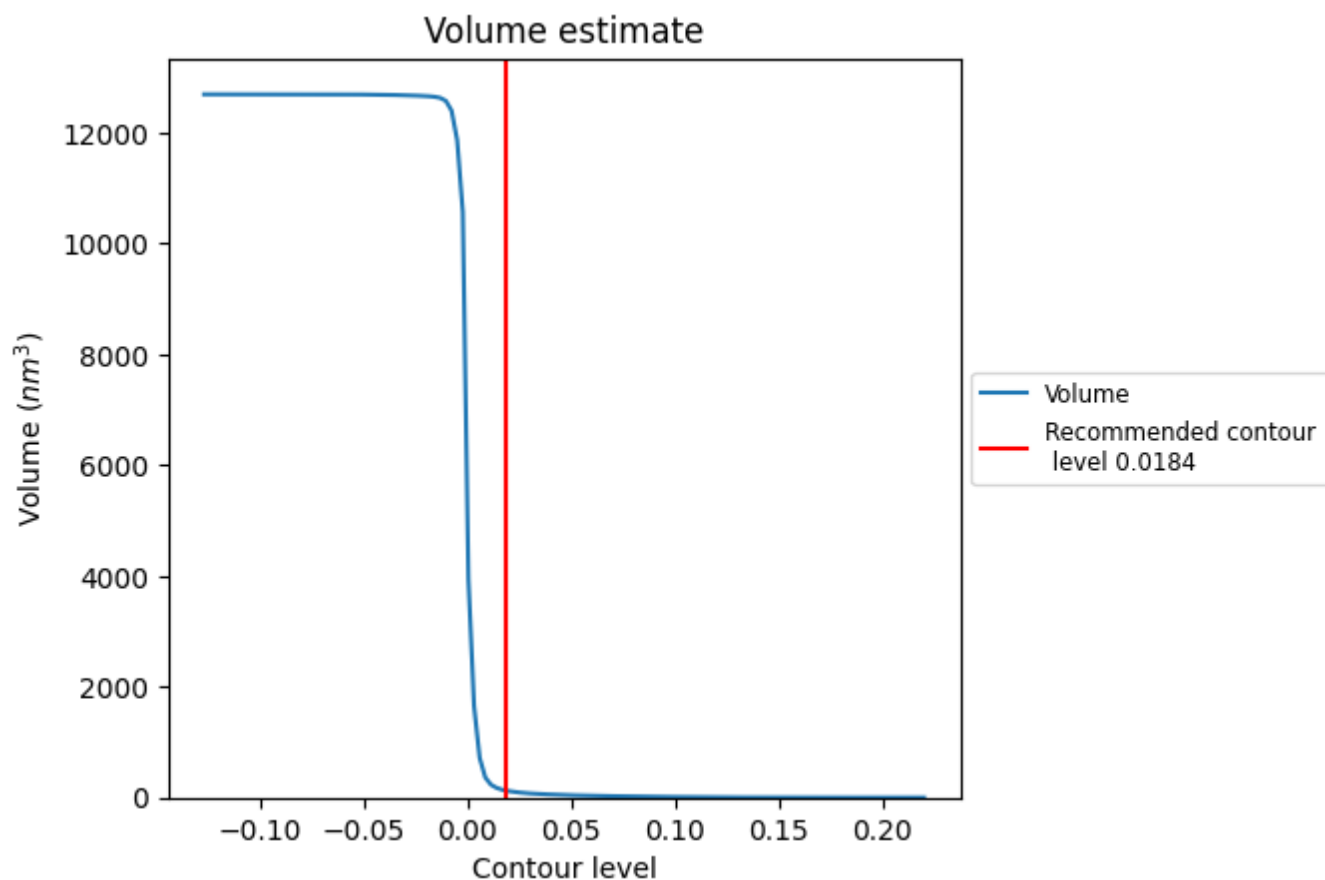
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

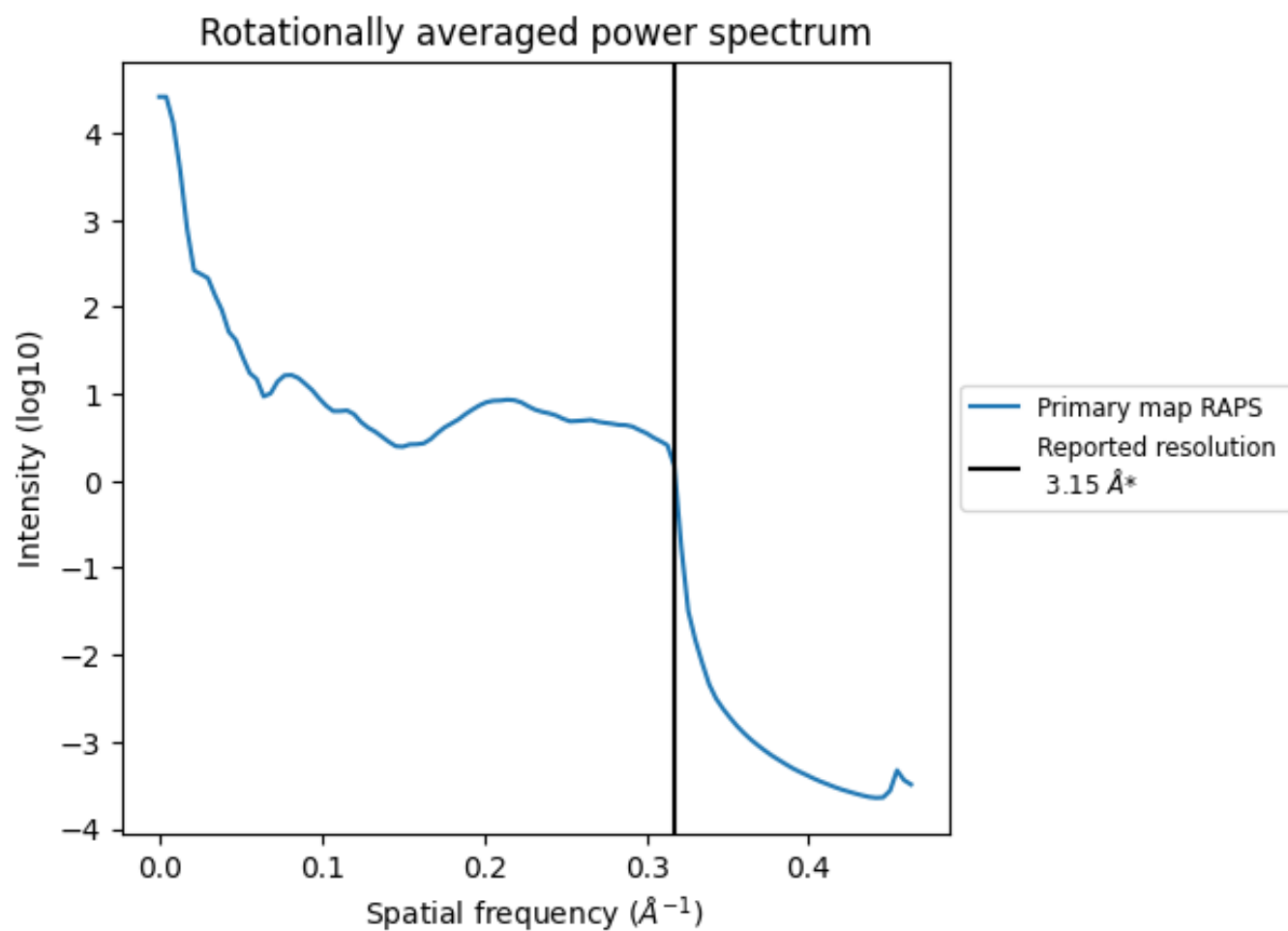
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 128 nm³; 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.317 Å⁻¹

8 Fourier-Shell correlation

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

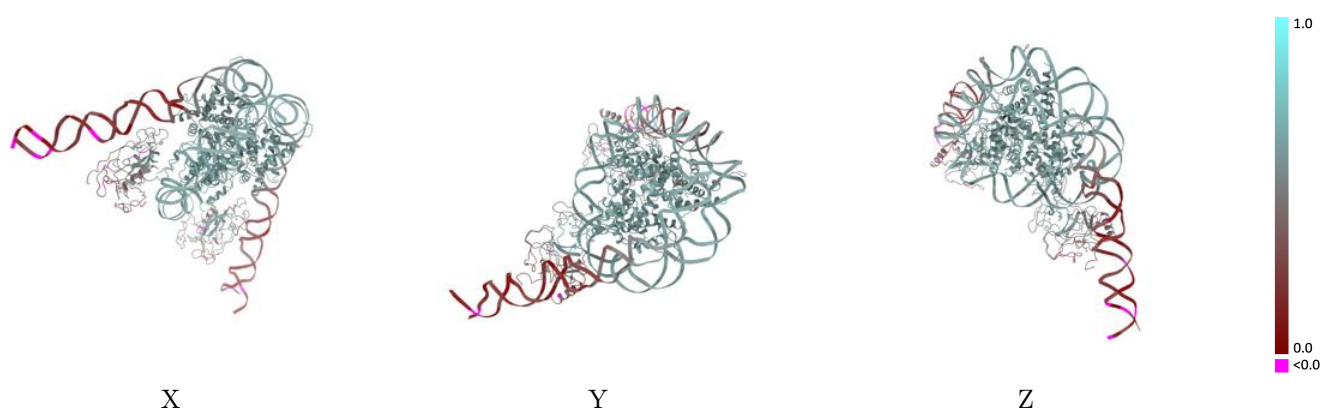
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD 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](#)

This section was not generated.

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

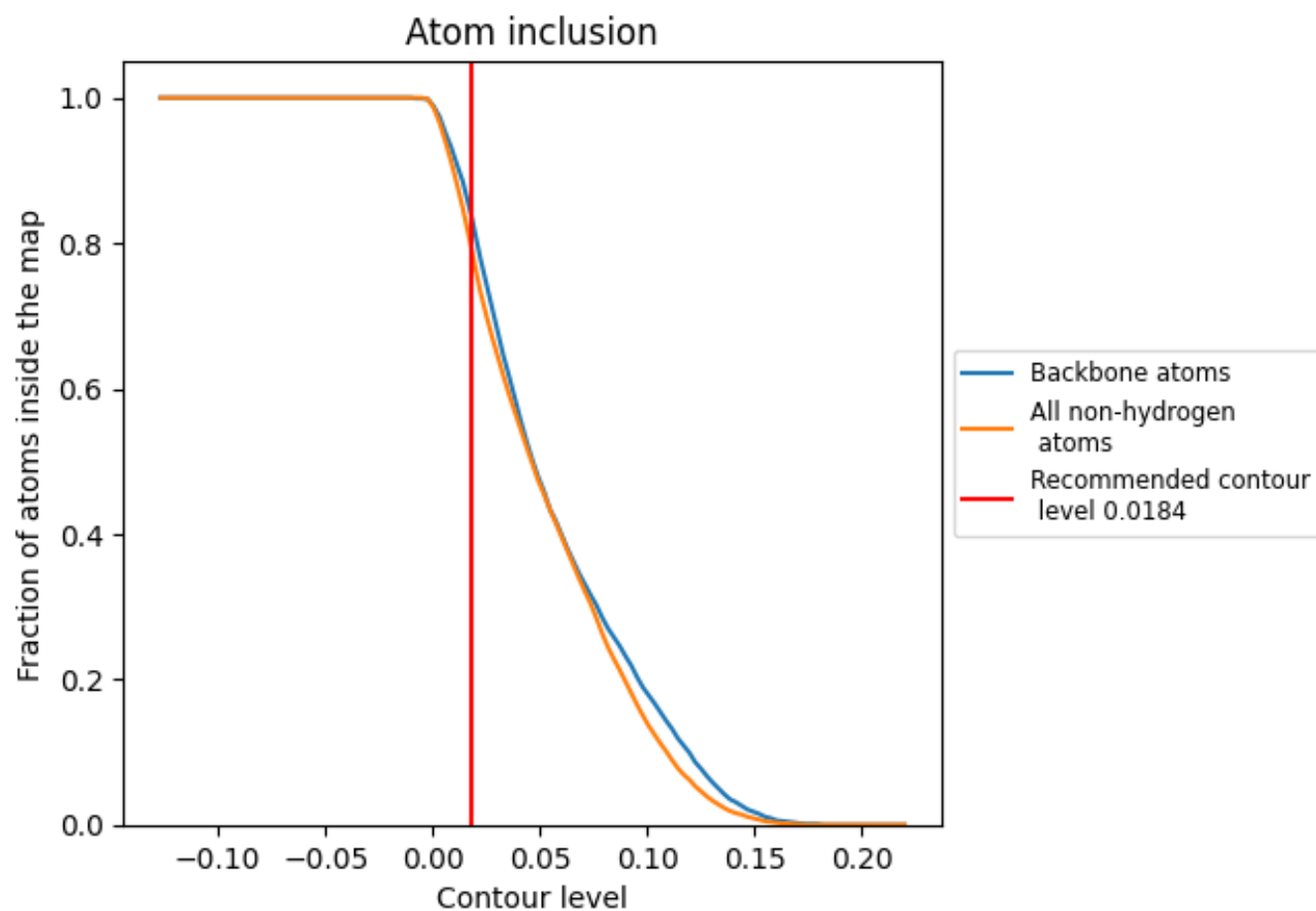


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

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 ⓘ

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	0.7890	0.5070
A	0.6980	0.4510
B	0.9590	0.6080
C	0.9670	0.5940
D	0.9530	0.5880
E	0.9680	0.6070
F	0.9410	0.6040
G	0.9610	0.6020
H	0.9410	0.5870
I	0.6970	0.4460
K	0.7040	0.4590
L	0.6560	0.4450
M	0.9520	0.6110

