



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 11:10 PM UTC

PDB ID : 8PJJ / pdb_00008pjj
EMDB ID : EMD-17711
Title : Cryo-EM structure of MLE in complex with SL7UUC RNA and ADP
Authors : Jagtap, P.K.A.; Hennig, J.
Deposited on : 2023-06-23
Resolution : 4.24 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

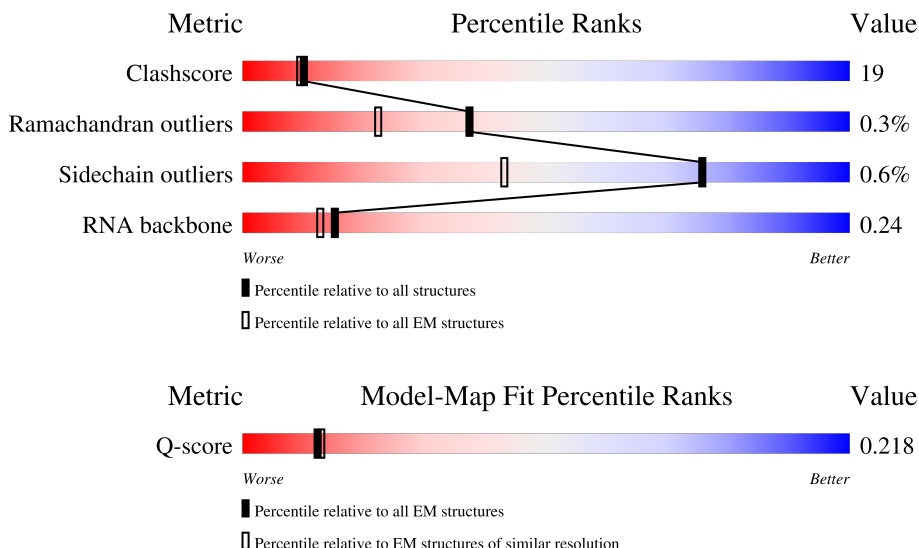
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.24 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	4688 (3.74 - 4.74)

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

Mol	Chain	Length	Quality of chain
1	A	1158	
2	B	60	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8348 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.

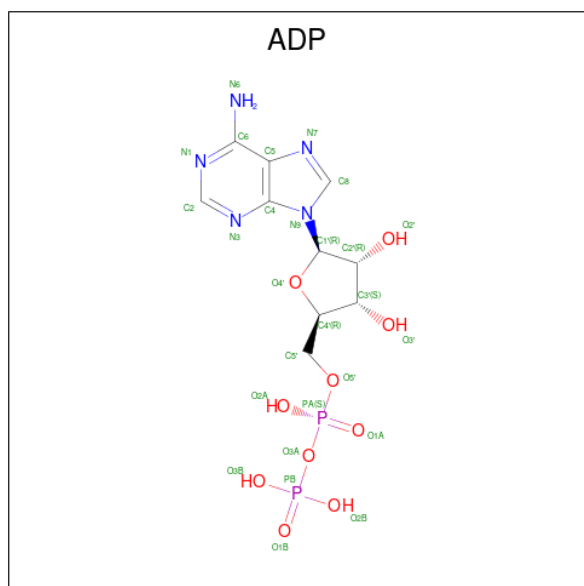
- Molecule 1 is a protein called Dosage compensation regulator.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	946	7474	4748	1288	1391	47	2	0

- Molecule 2 is a RNA chain called SL7UUC RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	40	847	379	145	283	40	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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



G1	U1	U2	G3	U4	A5	A6	A7	U8	U9	G10	U11	U12	G13	U14	U15	G16	G17	G18	A19	U20	U21	U22	U23	U24	U25	U26	U27	U28	U29	A30	G31	U32	U33	U34	U35	U36	U37	U38	U39	U40	A41	C42	G43	C44	C45	C46	U47	U48	U49	U50	U51	U52	U53	U54	U55	U56	U57	U58	U59	U60	U61	U62	U63	U64	U65	U66	U67	U68	U69	U70	U71	U72	U73	U74	U75	U76	U77	U78	U79	U80	U81	U82	U83	U84	U85	U86	U87	U88	U89	U90	U91	U92	U93	U94	U95	U96	U97	U98	U99	U100	U101	U102	U103	U104	U105	U106	U107	U108	U109	U110	U111	U112	U113	U114	U115	U116	U117	U118	U119	U120	U121	U122	U123	U124	U125	U126	U127	U128	U129	U130	U131	U132	U133	U134	U135	U136	U137	U138	U139	U140	U141	U142	U143	U144	U145	U146	U147	U148	U149	U150	U151	U152	U153	U154	U155	U156	U157	U158	U159	U160	U161	U162	U163	U164	U165	U166	U167	U168	U169	U170	U171	U172	U173	U174	U175	U176	U177	U178	U179	U180	U181	U182	U183	U184	U185	U186	U187	U188	U189	U190	U191	U192	U193	U194	U195	U196	U197	U198	U199	U200	U201	U202	U203	U204	U205	U206	U207	U208	U209	U210	U211	U212	U213	U214	U215	U216	U217	U218	U219	U220	U221	U222	U223	U224	U225	U226	U227	U228	U229	U230	U231	U232	U233	U234	U235	U236	U237	U238	U239	U240	U241	U242	U243	U244	U245	U246	U247	U248	U249	U250	U251	U252	U253	U254	U255	U256	U257	U258	U259	U260	U261	U262	U263	U264	U265	U266	U267	U268	U269	U270	U271	U272	U273	U274	U275	U276	U277	U278	U279	U280	U281	U282	U283	U284	U285	U286	U287	U288	U289	U290	U291	U292	U293	U294	U295	U296	U297	U298	U299	U300	U301	U302	U303	U304	U305	U306	U307	U308	U309	U310	U311	U312	U313	U314	U315	U316	U317	U318	U319	U320	U321	U322	U323	U324	U325	U326	U327	U328	U329	U330	U331	U332	U333	U334	U335	U336	U337	U338	U339	U340	U341	U342	U343	U344	U345	U346	U347	U348	U349	U350	U351	U352	U353	U354	U355	U356	U357	U358	U359	U360	U361	U362	U363	U364	U365	U366	U367	U368	U369	U370	U371	U372	U373	U374	U375	U376	U377	U378	U379	U380	U381	U382	U383	U384	U385	U386	U387	U388	U389	U390	U391	U392	U393	U394	U395	U396	U397	U398	U399	U400	U401	U402	U403	U404	U405	U406	U407	U408	U409	U410	U411	U412	U413	U414	U415	U416	U417	U418	U419	U420	U421	U422	U423	U424	U425	U426	U427	U428	U429	U430	U431	U432	U433	U434	U435	U436	U437	U438	U439	U440	U441	U442	U443	U444	U445	U446	U447	U448	U449	U450	U451	U452	U453	U454	U455	U456	U457	U458	U459	U460	U461	U462	U463	U464	U465	U466	U467	U4
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61690	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 ($e^-/\text{\AA}^2$)	52.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.250	Depositor
Minimum map value	-0.073	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.029	Depositor
Map size (Å)	238.592, 238.592, 238.592	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.932, 0.932, 0.932	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.15	0/7623	0.41	0/10328
2	B	0.13	0/944	0.31	0/1465
All	All	0.15	0/8567	0.40	0/11793

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7474	0	7550	294	0
2	B	847	0	429	21	0
3	A	27	0	12	1	0
All	All	8348	0	7991	310	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 19.

All (310) 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:A:173:ARG:H	1:A:249:SER:HB3	1.44	0.81
1:A:621:GLN:HB2	1:A:624:ARG:HB2	1.64	0.79
1:A:226:SER:HA	1:A:229:LYS:HB2	1.66	0.78
1:A:198:ARG:NH1	2:B:29:U:O2	2.17	0.78
1:A:413:LYS:HG3	1:A:538:MET:HE3	1.66	0.78
1:A:412:GLY:HA2	3:A:1201:ADP:H4'	1.67	0.75
1:A:759:LYS:HB3	1:A:791:ASP:HA	1.68	0.75
1:A:198:ARG:HE	2:B:30:A:H1'	1.52	0.74
1:A:386:ILE:HD13	1:A:559:VAL:HG11	1.72	0.71
1:A:1075:ILE:O	1:A:1112:LYS:NZ	2.23	0.71
1:A:512:ARG:NH2	1:A:826:GLU:OE2	2.25	0.69
1:A:1001:LEU:HD21	1:A:1069:VAL:HA	1.74	0.69
1:A:726:ILE:HG22	1:A:728:ASP:H	1.58	0.68
1:A:329:ALA:H	1:A:499:ARG:HA	1.59	0.68
2:B:11:U:H3'	2:B:12:U:H5''	1.75	0.67
1:A:332:GLN:O	1:A:479:TYR:OH	2.12	0.67
1:A:740:MET:HG3	1:A:755:VAL:HG23	1.78	0.66
1:A:326:ILE:HD12	1:A:497:GLY:HA2	1.78	0.66
1:A:931:MET:HA	1:A:934:ARG:HG2	1.77	0.66
1:A:670:MET:HE3	1:A:715:LEU:HD23	1.78	0.65
1:A:612:ASN:ND2	1:A:632:GLU:OE1	2.30	0.64
1:A:549:LYS:HA	1:A:553:ILE:HD13	1.80	0.64
1:A:1053:GLY:N	1:A:1064:LYS:O	2.25	0.64
1:A:416:GLN:NE2	1:A:456:GLU:OE1	2.31	0.64
1:A:438:VAL:HG22	1:A:505:ILE:HB	1.79	0.63
1:A:857:ARG:HG2	1:A:861:ARG:HH12	1.63	0.63
1:A:1112:LYS:HD3	1:A:1115:LEU:HD21	1.79	0.63
1:A:1019:ARG:NH1	1:A:1039:SER:O	2.30	0.63
1:A:260:LEU:HD12	1:A:261:LYS:HG2	1.81	0.63
1:A:223:ASN:N	1:A:226:SER:OG	2.32	0.63
1:A:809:ILE:HG13	1:A:814:LEU:HD12	1.80	0.63
1:A:934:ARG:O	1:A:938:ARG:NH1	2.32	0.63
1:A:490:LEU:HD23	1:A:519:LEU:HD11	1.79	0.62
1:A:1074:VAL:HG12	1:A:1075:ILE:HG13	1.80	0.62
1:A:658:VAL:HG12	1:A:733:ILE:HB	1.80	0.62
1:A:947:CYS:HB2	1:A:954:MET:HE1	1.82	0.61
1:A:267:LEU:HD12	1:A:271:LEU:HG	1.80	0.61
1:A:748:ASN:O	1:A:1055:LYS:NZ	2.26	0.61
1:A:518:PHE:HZ	1:A:809:ILE:HB	1.64	0.61
1:A:907:LEU:HD12	1:A:1036:VAL:HA	1.81	0.61
2:B:38:U:H2'	2:B:39:U:H5''	1.81	0.61
1:A:328:TRP:HH2	1:A:532:ASP:HB3	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:VAL:HG23	1:A:715:LEU:HD13	1.84	0.60
2:B:8:A:H2'	2:B:9:U:C6	2.36	0.60
1:A:1070[B]:SER:OG	1:A:1073:GLN:OE1	2.19	0.60
1:A:225:LYS:O	1:A:229:LYS:N	2.28	0.60
1:A:492:ARG:HH12	1:A:863:PRO:HB3	1.67	0.60
1:A:1073:GLN:O	1:A:1076:LEU:N	2.35	0.60
1:A:425:TYR:OH	1:A:503:HIS:NE2	2.33	0.60
1:A:918:LYS:NZ	1:A:987:ASP:O	2.35	0.59
1:A:223:ASN:OD1	1:A:226:SER:N	2.33	0.59
1:A:694:ILE:HD12	1:A:698:GLU:HB3	1.85	0.59
1:A:686:GLN:HG2	1:A:710:VAL:HG12	1.83	0.59
1:A:691:HIS:O	1:A:699:GLN:NE2	2.36	0.59
1:A:437:TYR:HE1	1:A:483:LEU:HD23	1.68	0.58
1:A:880:CYS:SG	1:A:1000:SER:OG	2.61	0.58
1:A:686:GLN:HG3	1:A:706:VAL:HG21	1.83	0.58
1:A:681:ASP:O	1:A:685:TYR:N	2.29	0.58
1:A:367:ARG:O	1:A:375:ARG:NH1	2.31	0.58
1:A:915:SER:HB3	1:A:1036:VAL:HG21	1.84	0.57
1:A:1002:ALA:HB1	1:A:1077:PHE:HE2	1.70	0.57
1:A:524:ARG:HH22	1:A:823:LYS:HB2	1.68	0.57
1:A:381:ARG:NE	1:A:416:GLN:OE1	2.36	0.57
1:A:397:ILE:HA	1:A:403:VAL:HG21	1.85	0.57
1:A:871:MET:SD	1:A:1007:GLY:HA2	2.45	0.57
1:A:1128:ASP:HB2	1:A:1131:ARG:HG3	1.87	0.57
1:A:886:ILE:HG12	1:A:964:LYS:HD3	1.87	0.56
1:A:990:ILE:HG13	1:A:992:GLY:H	1.70	0.56
2:B:1:G:N7	2:B:46:C:O2'	2.37	0.56
1:A:1073:GLN:O	1:A:1075:ILE:N	2.38	0.56
1:A:1015:HIS:HA	1:A:1021:VAL:HG12	1.87	0.56
1:A:1027:LYS:HE3	1:A:1060:ALA:HB3	1.87	0.56
1:A:404:ILE:HG12	1:A:537:LEU:HB2	1.87	0.56
1:A:437:TYR:HE2	1:A:490:LEU:HD22	1.71	0.55
1:A:375:ARG:O	1:A:378:LEU:HG	2.06	0.55
1:A:1092:VAL:HB	1:A:1096:LEU:HB3	1.88	0.55
1:A:498:LEU:HD12	1:A:501:VAL:HG11	1.89	0.55
1:A:367:ARG:HG2	1:A:375:ARG:HH22	1.72	0.54
1:A:406:ARG:NH1	1:A:542:ILE:O	2.40	0.54
1:A:264:PRO:C	1:A:1100:ILE:HD11	2.33	0.54
1:A:947:CYS:HB3	1:A:952:LEU:HB2	1.90	0.54
2:B:34:A:O2'	2:B:35:C:OP1	2.24	0.54
1:A:645:MET:HA	1:A:648:LYS:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1032:HIS:O	1:A:1035:SER:OG	2.23	0.54
1:A:810:LYS:HB3	1:A:852:LEU:HD21	1.89	0.54
1:A:581:VAL:H	1:A:582:PRO:HD3	1.73	0.54
1:A:708:GLU:OE1	1:A:712:LYS:NZ	2.41	0.54
1:A:915:SER:HB2	1:A:919:CYS:HA	1.90	0.54
1:A:526:MET:HA	1:A:526:MET:HE2	1.90	0.54
1:A:843:MET:SD	1:A:867:ARG:NH1	2.80	0.54
1:A:271:LEU:HA	1:A:274:LYS:HZ3	1.72	0.53
1:A:343:ILE:HD11	1:A:348:LEU:HB3	1.89	0.53
1:A:510:HIS:CE1	1:A:540:ALA:H	2.25	0.53
1:A:821:LEU:HB2	1:A:828:PRO:HD2	1.90	0.53
1:A:371:ASP:O	1:A:375:ARG:NH1	2.42	0.53
1:A:386:ILE:HG13	1:A:413:LYS:HB3	1.91	0.53
1:A:961:TRP:CD1	1:A:964:LYS:HZ1	2.27	0.53
1:A:1013:CYS:HB3	1:A:1052:PHE:HE2	1.74	0.53
1:A:507:ASP:CG	1:A:508:GLU:H	2.16	0.53
1:A:367:ARG:NH2	1:A:459:GLU:OE2	2.42	0.53
1:A:571:LEU:HD23	1:A:782:SER:HA	1.90	0.53
1:A:907:LEU:HB3	1:A:911:GLN:HB2	1.91	0.52
1:A:819:HIS:O	1:A:823:LYS:HG2	2.10	0.52
1:A:167:ILE:HG12	1:A:233:LEU:HB2	1.91	0.52
2:B:30:A:H2'	2:B:31:G:H8	1.75	0.51
1:A:513:ASP:OD1	1:A:513:ASP:N	2.44	0.51
1:A:1013:CYS:HB3	1:A:1052:PHE:CE2	2.45	0.51
2:B:4:U:O4	2:B:41:A:N6	2.44	0.51
1:A:629:MET:O	1:A:630:LEU:HG	2.10	0.51
1:A:169:ASN:HB2	1:A:248:PHE:HA	1.92	0.51
1:A:930:GLN:OE1	1:A:934:ARG:NH1	2.44	0.51
1:A:515:ASN:OD1	1:A:516:SER:N	2.43	0.51
1:A:940:GLU:HA	1:A:943:GLU:HB3	1.92	0.50
1:A:739:ARG:NH1	1:A:752:TYR:O	2.45	0.50
1:A:1133:GLU:CD	1:A:1135:PRO:HD2	2.36	0.50
1:A:759:LYS:O	1:A:762:LEU:N	2.45	0.50
1:A:802:LEU:HD13	1:A:832:ALA:HB1	1.93	0.50
1:A:739:ARG:O	1:A:740:MET:HE2	2.11	0.50
1:A:859:LEU:HD13	1:A:866:PRO:HB3	1.94	0.50
1:A:956:THR:O	1:A:960:ILE:HG12	2.11	0.49
1:A:986:VAL:HG11	1:A:997:LEU:HD22	1.94	0.49
1:A:463:ASP:OD1	1:A:464:THR:N	2.43	0.49
1:A:1037:ASN:HB3	1:A:1045:PHE:CZ	2.47	0.49
1:A:403:VAL:HG13	1:A:557:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:LEU:HD21	1:A:457:ARG:HH22	1.76	0.49
1:A:194:PRO:HD2	1:A:197:ALA:HB3	1.94	0.49
1:A:464:THR:O	1:A:482:ILE:N	2.39	0.49
1:A:868:LEU:O	1:A:872:MET:HG2	2.12	0.49
1:A:905:ARG:HA	1:A:1033:LYS:HD3	1.94	0.49
1:A:953:GLN:HG3	1:A:956:THR:HB	1.94	0.49
1:A:977:PRO:HD2	1:A:1129:ILE:HG22	1.93	0.49
1:A:256:LYS:HB2	1:A:1022:LEU:HD21	1.95	0.49
2:B:9:U:H3'	2:B:10:G:O4'	2.13	0.49
1:A:404:ILE:HB	1:A:556:VAL:HG22	1.94	0.49
1:A:575:ILE:HG13	1:A:580:PHE:H	1.78	0.49
1:A:832:ALA:O	1:A:835:GLU:HG3	2.13	0.49
1:A:887:MET:HE2	1:A:1004:LEU:HD13	1.94	0.49
2:B:13:G:H2'	2:B:14:C:O4'	2.12	0.49
1:A:278:VAL:HG22	1:A:1138:GLN:OE1	2.13	0.48
1:A:374:TYR:HE2	1:A:457:ARG:HD3	1.77	0.48
1:A:784:ALA:O	1:A:788:ALA:HB2	2.13	0.48
1:A:810:LYS:HB3	1:A:852:LEU:HD11	1.94	0.48
1:A:1076:LEU:HD12	1:A:1111:LEU:HD11	1.95	0.48
1:A:575:ILE:O	1:A:620:SER:OG	2.26	0.48
1:A:282:LEU:HD23	1:A:284:LEU:HD11	1.95	0.48
1:A:722:THR:O	1:A:724:ILE:N	2.46	0.48
2:B:41:A:H2'	2:B:42:C:C6	2.49	0.48
1:A:174:LEU:HD11	1:A:206:ILE:HG12	1.95	0.48
1:A:884:MET:HA	1:A:887:MET:HG3	1.94	0.48
1:A:278:VAL:HG21	1:A:1142:VAL:HG11	1.94	0.48
1:A:581:VAL:H	1:A:582:PRO:CD	2.27	0.48
1:A:764:GLN:HE22	1:A:768:ARG:HD3	1.78	0.48
1:A:1009:TYR:HE2	1:A:1080:ARG:HH11	1.61	0.48
1:A:1012:ILE:HG22	1:A:1051:VAL:HG12	1.96	0.48
1:A:373:GLU:O	1:A:376:GLN:HG2	2.13	0.48
1:A:374:TYR:OH	1:A:419:GLN:NE2	2.47	0.48
1:A:873:VAL:HG11	1:A:1119:ILE:HG23	1.96	0.48
1:A:368:ARG:HA	1:A:375:ARG:CZ	2.44	0.48
1:A:386:ILE:HD11	1:A:411:CYS:HB3	1.96	0.47
1:A:1041:LEU:HD23	1:A:1041:LEU:H	1.78	0.47
1:A:370:ASN:OD1	1:A:371:ASP:N	2.47	0.47
1:A:265:VAL:HG13	1:A:266:LYS:N	2.30	0.47
1:A:655:ALA:HB3	1:A:729:ILE:HA	1.95	0.47
1:A:574:ILE:HA	1:A:577:MET:SD	2.54	0.47
1:A:604:LYS:HB2	1:A:605:ASP:H	1.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ALA:HB2	1:A:235:LEU:HB2	1.95	0.47
1:A:258:GLU:O	1:A:260:LEU:N	2.48	0.47
1:A:923:VAL:HG12	1:A:997:LEU:HD11	1.96	0.47
1:A:196:HIS:HA	1:A:198:ARG:HH11	1.78	0.47
1:A:256:LYS:HE3	1:A:1022:LEU:HD21	1.96	0.47
1:A:384:LEU:HG	1:A:385:PRO:HD2	1.97	0.47
1:A:572:GLU:O	1:A:575:ILE:HG22	2.15	0.47
1:A:581:VAL:HG11	1:A:626:ALA:HB2	1.97	0.47
1:A:743:PHE:HD1	1:A:750:THR:HG22	1.80	0.47
1:A:882:ASP:OD2	1:A:883:LEU:N	2.48	0.47
1:A:407:GLY:O	1:A:540:ALA:HA	2.14	0.47
1:A:686:GLN:N	1:A:711:THR:O	2.48	0.47
1:A:871:MET:HE2	1:A:1006:LEU:HG	1.96	0.47
1:A:375:ARG:O	1:A:379:GLU:OE1	2.33	0.47
1:A:744:THR:OG1	1:A:747:ASN:OD1	2.21	0.47
1:A:548:SER:OG	1:A:554:CYS:O	2.23	0.46
1:A:884:MET:SD	1:A:1003:LEU:HD22	2.56	0.46
1:A:1019:ARG:HA	1:A:1031:LEU:HD13	1.97	0.46
1:A:375:ARG:HE	1:A:378:LEU:HD21	1.80	0.46
1:A:570:PHE:O	1:A:574:ILE:HG12	2.15	0.46
1:A:1005:CYS:SG	1:A:1073:GLN:HG3	2.55	0.46
1:A:198:ARG:HE	2:B:30:A:C1'	2.24	0.46
1:A:1000:SER:O	1:A:1004:LEU:HD23	2.14	0.46
1:A:328:TRP:CH2	1:A:532:ASP:HB3	2.47	0.46
1:A:637:PHE:HA	1:A:640:LEU:HG	1.97	0.46
1:A:875:GLY:HA3	1:A:884:MET:HG3	1.97	0.46
1:A:1006:LEU:HB2	1:A:1077:PHE:CG	2.51	0.46
1:A:1008:LEU:HD23	1:A:1053:GLY:HA2	1.98	0.46
1:A:1103:GLU:HG2	1:A:1104:LEU:HD12	1.98	0.46
1:A:187:TYR:HB3	1:A:202:ALA:HB1	1.98	0.46
1:A:229:LYS:NZ	2:B:8:A:OP2	2.42	0.46
1:A:1135:PRO:HA	1:A:1138:GLN:HE21	1.79	0.46
1:A:271:LEU:O	1:A:275:ILE:HG12	2.15	0.46
1:A:835:GLU:HA	1:A:838:VAL:HG22	1.98	0.46
1:A:1103:GLU:O	1:A:1107:LYS:HG2	2.16	0.46
1:A:1024:THR:HG22	1:A:1025:GLU:HG2	1.98	0.45
2:B:16:A:H2'	2:B:17:G:C8	2.52	0.45
1:A:690:CYS:HB3	1:A:716:SER:HB2	1.98	0.45
1:A:1105:ALA:HA	1:A:1108:ILE:HG22	1.98	0.45
1:A:378:LEU:HA	1:A:381:ARG:HH11	1.81	0.45
1:A:805:MET:HE2	1:A:805:MET:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:843:MET:HE3	1:A:845:CYS:SG	2.56	0.45
1:A:217:ALA:HB1	1:A:231:CYS:HB3	1.98	0.45
1:A:963:ALA:O	1:A:967:LEU:HD23	2.16	0.45
1:A:688:LEU:HB3	1:A:702:VAL:HG22	1.99	0.45
1:A:811:LEU:HD12	1:A:857:ARG:HA	1.98	0.45
2:B:4:U:H5	2:B:5:A:H62	1.65	0.45
2:B:16:A:O5'	2:B:16:A:H8	2.00	0.45
1:A:178:LYS:HD2	1:A:206:ILE:HG13	1.99	0.44
1:A:933:ARG:HE	1:A:961:TRP:HE1	1.64	0.44
1:A:324:SER:OG	1:A:325:VAL:N	2.50	0.44
1:A:442:ARG:HB3	1:A:445:SER:OG	2.17	0.44
1:A:422:LEU:HD22	1:A:482:ILE:HD11	1.99	0.44
1:A:1009:TYR:CZ	1:A:1079:SER:HA	2.52	0.44
1:A:1059:ARG:HG3	1:A:1061:VAL:HG13	1.98	0.44
1:A:660:LEU:HD21	1:A:665:LEU:CB	2.47	0.44
1:A:799:ARG:O	1:A:799:ARG:HG2	2.18	0.44
1:A:1075:ILE:HG21	1:A:1082:ILE:HD12	1.99	0.44
2:B:42:C:H2'	2:B:43:G:C8	2.52	0.44
1:A:195:GLU:O	1:A:198:ARG:NH1	2.50	0.44
1:A:465:VAL:HA	1:A:482:ILE:HB	1.99	0.44
1:A:872:MET:HE3	1:A:888:ALA:HB2	2.00	0.44
2:B:40:U:H2'	2:B:41:A:O4'	2.18	0.44
1:A:196:HIS:HA	1:A:198:ARG:NH1	2.33	0.44
1:A:1024:THR:HG23	1:A:1095:TRP:CD1	2.53	0.44
1:A:265:VAL:HG13	1:A:266:LYS:H	1.82	0.44
1:A:1019:ARG:O	1:A:1030:LEU:HA	2.18	0.43
1:A:697:ASP:OD1	1:A:698:GLU:N	2.51	0.43
1:A:927:VAL:O	1:A:931:MET:HE3	2.19	0.43
1:A:932:TRP:CD2	1:A:957:MET:HE1	2.53	0.43
1:A:378:LEU:HA	1:A:381:ARG:HD3	1.99	0.43
1:A:581:VAL:HG21	1:A:622:LYS:HA	2.00	0.43
1:A:393:ILE:HD13	1:A:557:LEU:HD22	2.01	0.43
1:A:662:GLY:O	1:A:666:ILE:HG12	2.19	0.43
1:A:1134:GLU:HB3	1:A:1135:PRO:HD3	2.00	0.43
1:A:387:ALA:HA	1:A:390:ARG:HG3	2.00	0.43
1:A:660:LEU:HG	1:A:661:PRO:HD2	2.00	0.43
1:A:884:MET:SD	1:A:1003:LEU:HD13	2.58	0.43
1:A:334:ASN:HD21	1:A:344:ASP:HA	1.82	0.43
1:A:841:ARG:HD3	1:A:846:LEU:HB3	2.00	0.43
1:A:503:HIS:CE1	1:A:534:HIS:HB2	2.54	0.43
1:A:229:LYS:HG2	2:B:8:A:OP1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1111:LEU:HD12	1:A:1115:LEU:HD23	1.99	0.43
1:A:325:VAL:HB	1:A:526:MET:HE1	2.00	0.43
1:A:436:ILE:HD11	1:A:505:ILE:HD11	2.01	0.43
1:A:198:ARG:H	1:A:198:ARG:HD3	1.84	0.43
1:A:374:TYR:HE2	1:A:457:ARG:HA	1.84	0.43
1:A:505:ILE:HA	1:A:536:ILE:HB	2.00	0.43
1:A:882:ASP:OD2	1:A:984:HIS:ND1	2.51	0.43
1:A:166:THR:HB	1:A:169:ASN:ND2	2.34	0.42
1:A:636:SER:HA	1:A:672:PHE:HZ	1.84	0.42
1:A:686:GLN:HG2	1:A:710:VAL:CG1	2.49	0.42
1:A:487:VAL:HG13	1:A:519:LEU:HD12	2.01	0.42
1:A:467:TYR:O	1:A:474:VAL:HG22	2.19	0.42
1:A:166:THR:HB	1:A:169:ASN:HD21	1.84	0.42
1:A:371:ASP:O	1:A:375:ARG:HG2	2.19	0.42
1:A:543:ASP:OD1	1:A:543:ASP:N	2.49	0.42
1:A:579:ASP:C	1:A:630:LEU:HD11	2.44	0.42
1:A:604:LYS:HB3	1:A:604:LYS:HE3	1.63	0.42
1:A:657:LEU:HD11	1:A:732:VAL:HG12	2.01	0.42
1:A:919:CYS:HB3	1:A:1068:MET:HE1	2.01	0.42
1:A:419:GLN:HG3	1:A:457:ARG:HH21	1.83	0.42
1:A:638:GLU:HG2	1:A:639:LEU:N	2.34	0.42
1:A:453:VAL:HG11	1:A:465:VAL:HG21	2.01	0.42
1:A:215:VAL:HG21	1:A:239:LEU:HD12	2.02	0.42
1:A:735:ILE:HG22	1:A:735:ILE:O	2.20	0.42
1:A:170:ALA:HB3	1:A:236:VAL:HG13	2.02	0.42
1:A:477:ARG:NH2	1:A:480:GLY:O	2.53	0.41
1:A:611:TYR:HD2	1:A:785:ARG:HG2	1.85	0.41
1:A:668:ALA:O	1:A:671:LYS:HG2	2.20	0.41
1:A:744:THR:HB	1:A:746:HIS:CE1	2.54	0.41
1:A:749:LEU:HD13	1:A:1055:LYS:HE2	2.02	0.41
1:A:897:VAL:HG22	1:A:1034:THR:HG22	2.02	0.41
1:A:1085:ALA:HB2	1:A:1091:ARG:HG2	2.02	0.41
1:A:266:LYS:HD3	1:A:1156:LEU:HB3	2.02	0.41
1:A:523:LEU:HA	1:A:526:MET:HB2	2.01	0.41
1:A:1112:LYS:HB2	1:A:1113:PRO:HD3	2.03	0.41
2:B:12:U:C2	2:B:13:G:C8	3.08	0.41
1:A:581:VAL:CG1	1:A:626:ALA:HB2	2.50	0.41
1:A:338:TRP:CH2	1:A:481:ALA:HB3	2.56	0.41
1:A:400:ASN:O	1:A:534:HIS:ND1	2.47	0.41
1:A:477:ARG:NE	1:A:479:TYR:O	2.53	0.41
1:A:675:ASN:OD1	1:A:676:THR:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1079:SER:OG	1:A:1081:LYS:O	2.38	0.41
1:A:365:ARG:HE	1:A:369:GLN:HG3	1.85	0.41
1:A:582:PRO:HG3	1:A:626:ALA:HA	2.03	0.41
1:A:661:PRO:O	1:A:739:ARG:HG2	2.20	0.41
1:A:413:LYS:O	1:A:417:ILE:HG12	2.21	0.41
1:A:759:LYS:NZ	1:A:786:PHE:O	2.39	0.41
1:A:722:THR:C	1:A:723:SER:HG	2.29	0.41
1:A:965:GLN:O	1:A:968:LEU:HG	2.21	0.41
1:A:1012:ILE:HG13	1:A:1095:TRP:HZ2	1.86	0.41
1:A:726:ILE:HB	1:A:729:ILE:HG23	2.02	0.41
1:A:759:LYS:HE3	1:A:759:LYS:HB2	1.96	0.41
1:A:1015:HIS:NE2	1:A:1018:LYS:O	2.51	0.41
1:A:486:THR:HG23	1:A:489:VAL:H	1.86	0.40
1:A:574:ILE:O	1:A:579:ASP:N	2.53	0.40
1:A:575:ILE:HD11	1:A:622:LYS:HA	2.03	0.40
1:A:945:ARG:HH11	1:A:946:PHE:HD1	1.69	0.40
1:A:1091:ARG:HH12	1:A:1097:ASN:HB2	1.86	0.40
1:A:636:SER:HA	1:A:672:PHE:CZ	2.56	0.40
1:A:880:CYS:O	1:A:884:MET:HG2	2.21	0.40
1:A:567:GLN:HE22	1:A:776:PHE:HA	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	942/1158 (81%)	848 (90%)	91 (10%)	3 (0%)	36 71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1074	VAL

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Mol	Chain	Res	Type
1	A	581	VAL
1	A	954	MET

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	832/1010 (82%)	826 (99%)	6 (1%)	76 78

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	602	GLU
1	A	603	ASP
1	A	604	LYS
1	A	605	ASP
1	A	771[A]	ARG
1	A	771[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	ASN
1	A	419	GLN
1	A	686	GLN
1	A	958	ASN
1	A	1037	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	38/60 (63%)	19 (50%)	1 (2%)

All (19) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	U
2	B	3	G
2	B	4	U
2	B	5	A
2	B	6	A
2	B	7	A
2	B	8	A
2	B	9	U
2	B	10	G
2	B	12	U
2	B	19	A
2	B	35	C
2	B	38	U
2	B	39	U
2	B	42	C
2	B	43	G
2	B	44	C
2	B	45	C
2	B	46	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	34	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
3	ADP	A	1201	-	28,29,29	1.41	4 (14%)	43,45,45	1.81	10 (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
3	ADP	A	1201	-	-	7/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1201	ADP	C5-C4	4.65	1.47	1.39
3	A	1201	ADP	C5-C6	2.75	1.48	1.41
3	A	1201	ADP	C8-N7	2.41	1.36	1.31
3	A	1201	ADP	C5-N7	-2.27	1.34	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1201	ADP	C5-C4-N3	-5.66	118.92	126.72
3	A	1201	ADP	N3-C4-N9	4.49	134.80	127.17
3	A	1201	ADP	C2-N3-C4	3.67	120.79	111.83
3	A	1201	ADP	C4-C5-N7	-3.43	106.66	110.58
3	A	1201	ADP	N3-C2-N1	-3.28	123.62	128.58
3	A	1201	ADP	C4-N9-C8	2.75	108.62	105.74
3	A	1201	ADP	C5-N7-C8	2.56	107.47	103.45
3	A	1201	ADP	C6-C5-N7	2.13	136.20	132.09
3	A	1201	ADP	C3'-C2'-C1'	2.12	105.48	101.46
3	A	1201	ADP	N9-C8-N7	-2.09	110.97	113.94

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1201	ADP	C5'-O5'-PA-O2A
3	A	1201	ADP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

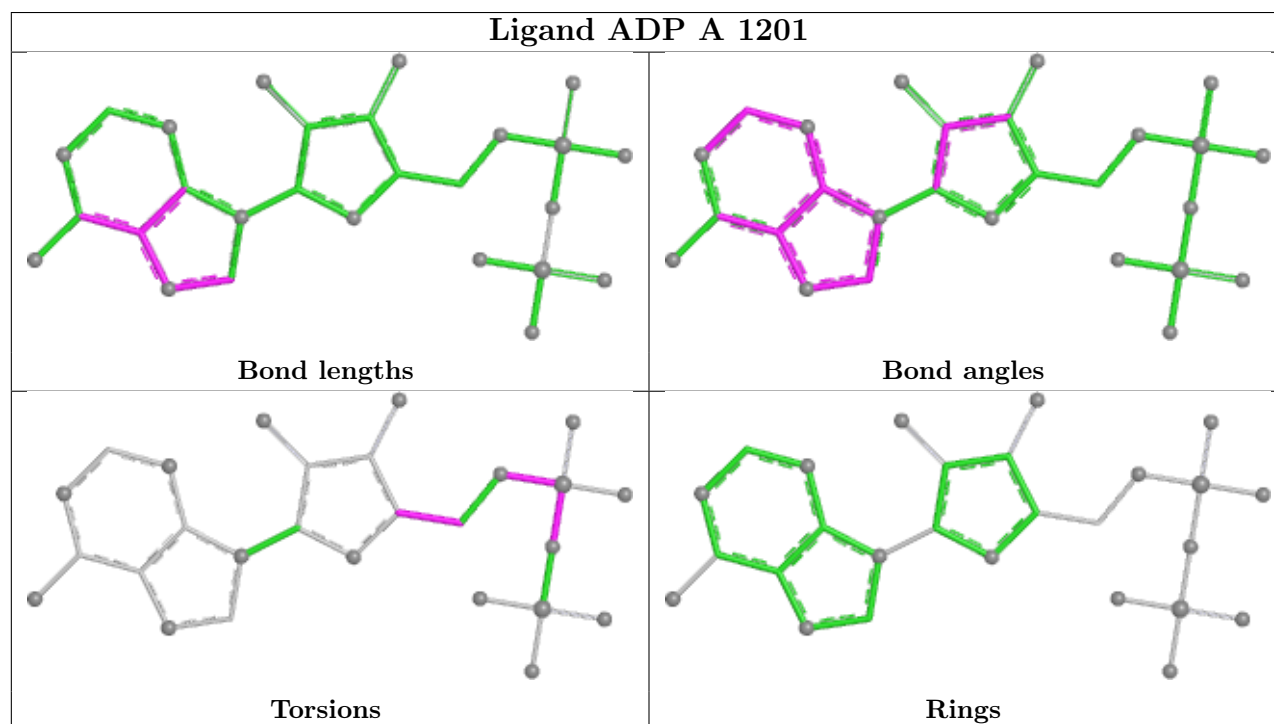
Mol	Chain	Res	Type	Atoms
3	A	1201	ADP	O4'-C4'-C5'-O5'
3	A	1201	ADP	C3'-C4'-C5'-O5'
3	A	1201	ADP	PB-O3A-PA-O2A
3	A	1201	ADP	C5'-O5'-PA-O1A
3	A	1201	ADP	PB-O3A-PA-O1A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1201	ADP	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.

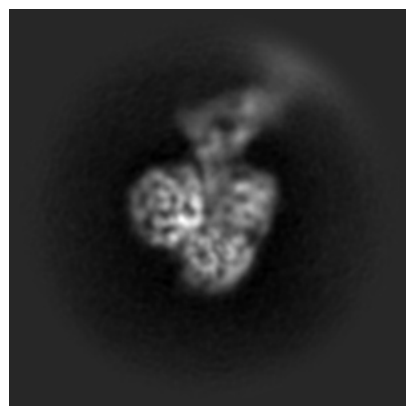
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17711. These allow visual inspection of the internal detail of the map and identification of artifacts.

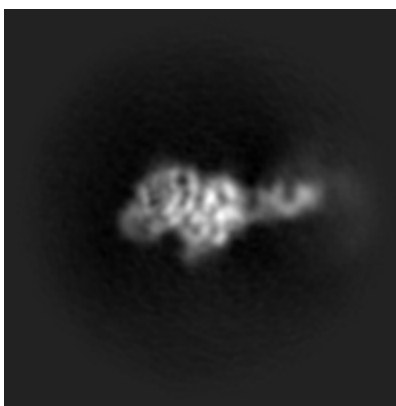
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

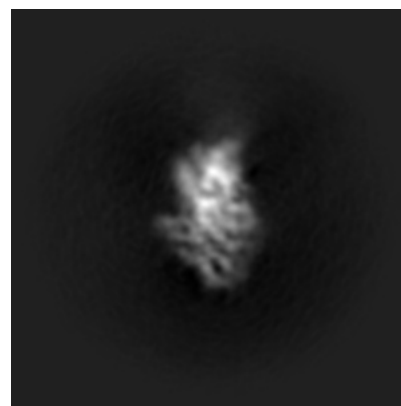
6.1.1 Primary map



X

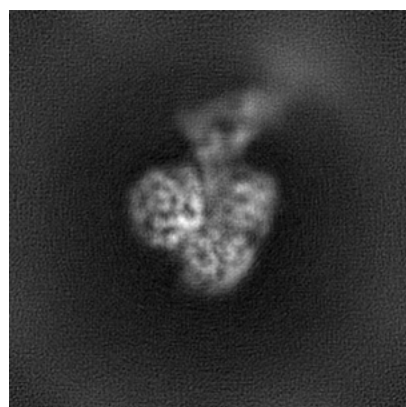


Y

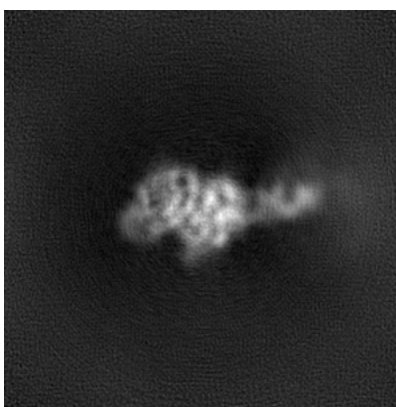


Z

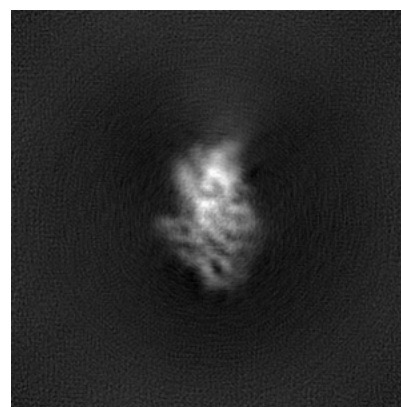
6.1.2 Raw map



X



Y

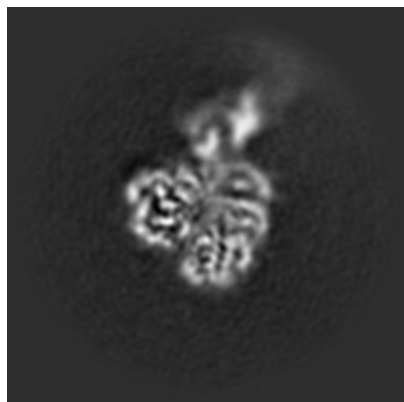


Z

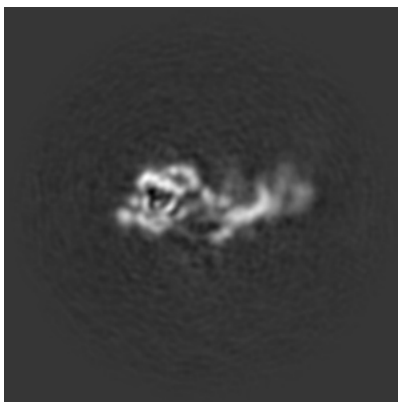
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

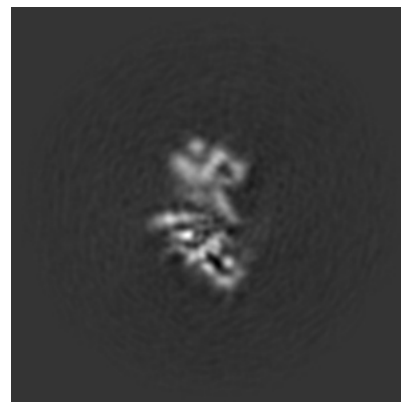
6.2.1 Primary map



X Index: 128

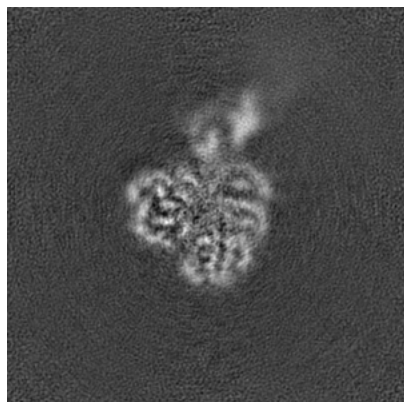


Y Index: 128

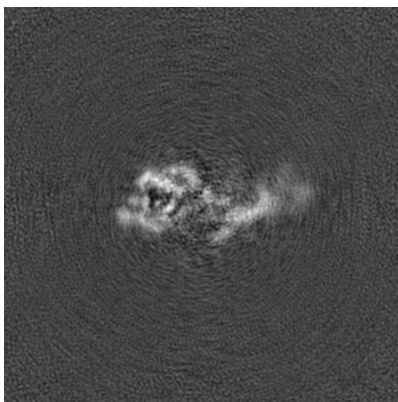


Z Index: 128

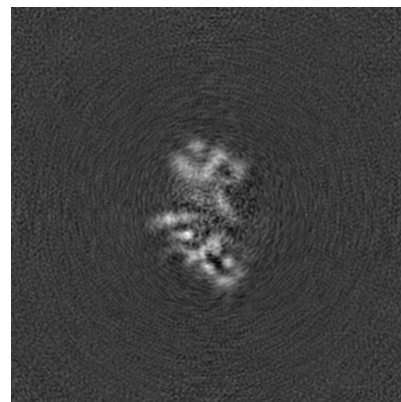
6.2.2 Raw map



X Index: 128



Y Index: 128

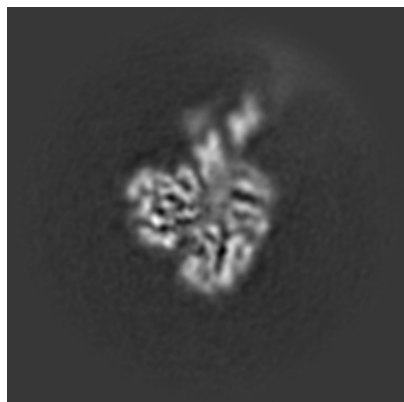


Z Index: 128

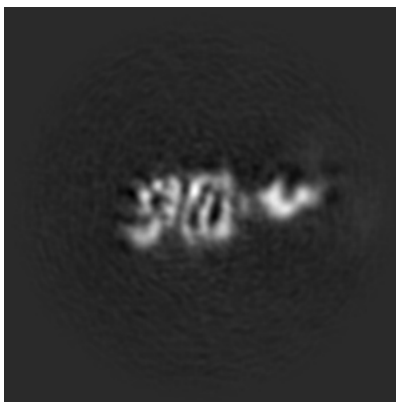
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

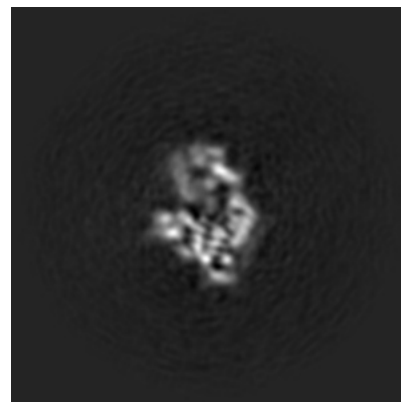
6.3.1 Primary map



X Index: 125

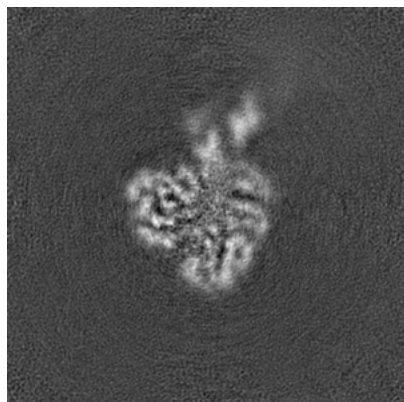


Y Index: 148

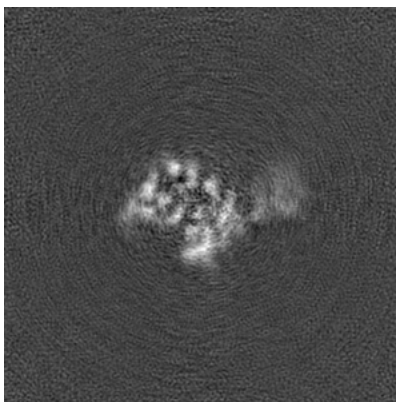


Z Index: 120

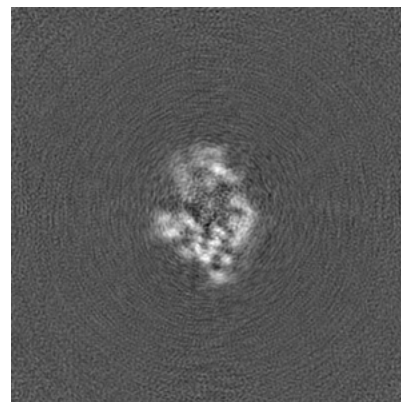
6.3.2 Raw map



X Index: 126



Y Index: 120

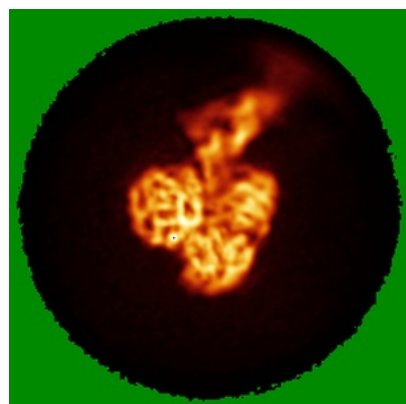


Z Index: 119

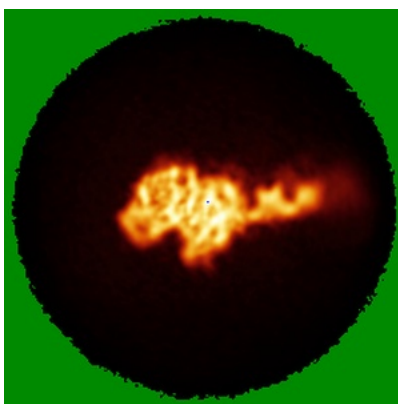
The images above show the largest variance slices of the map in three orthogonal directions.

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

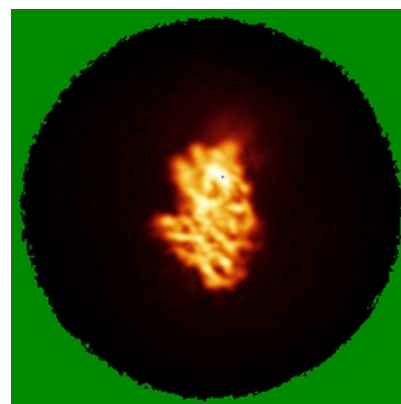
6.4.1 Primary map



X

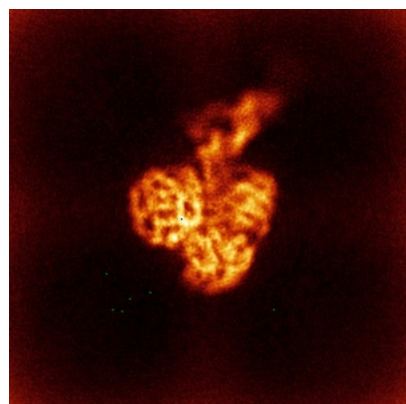


Y

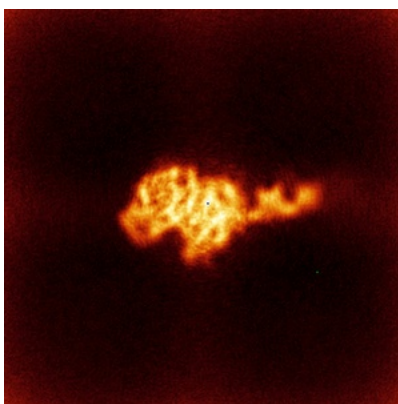


Z

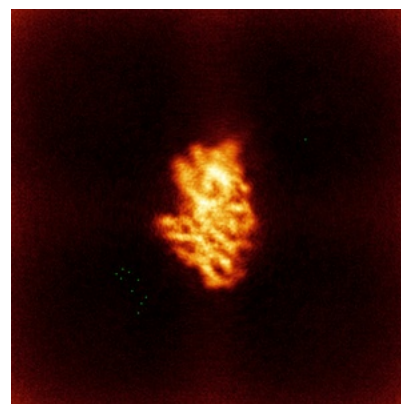
6.4.2 Raw map



X



Y

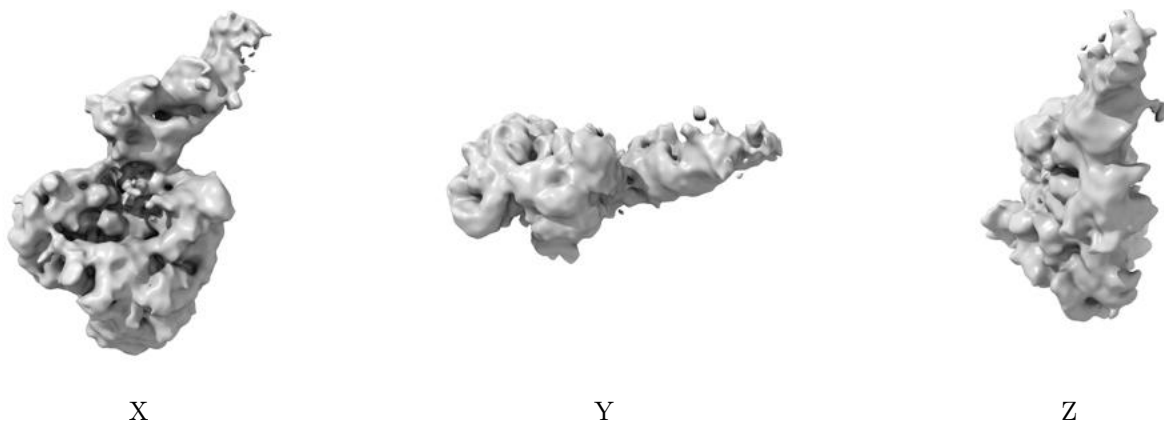


Z

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.

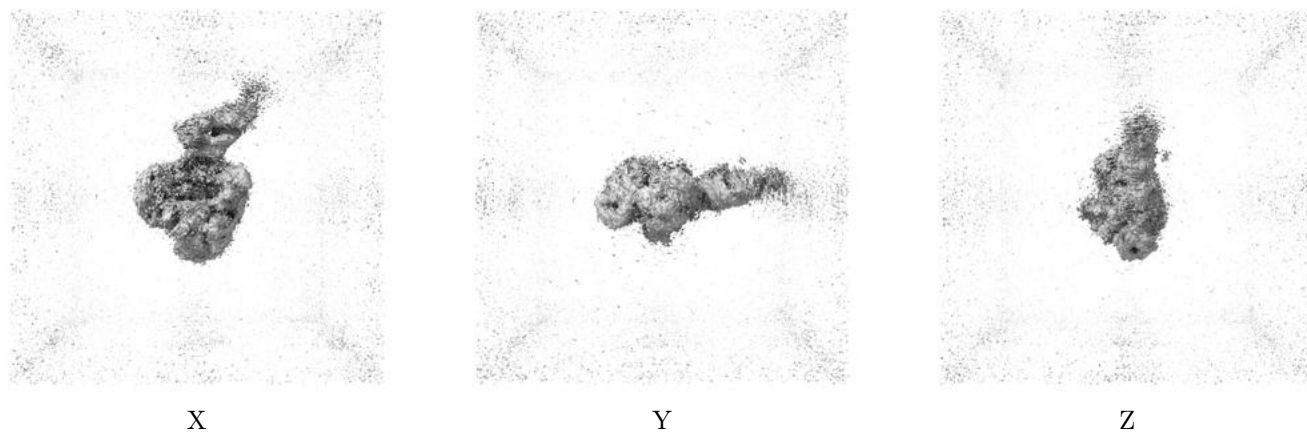
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.029. 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.

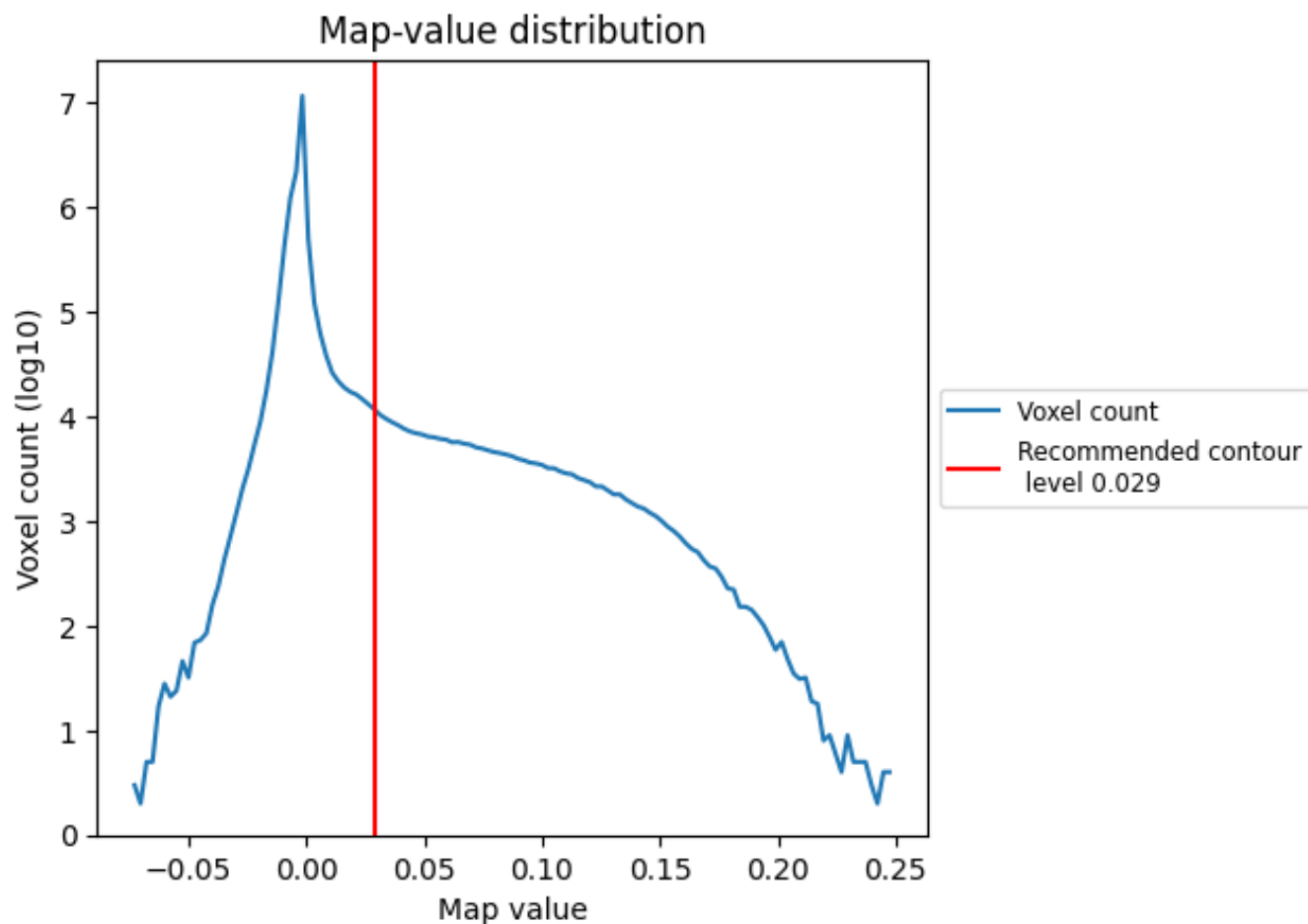
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

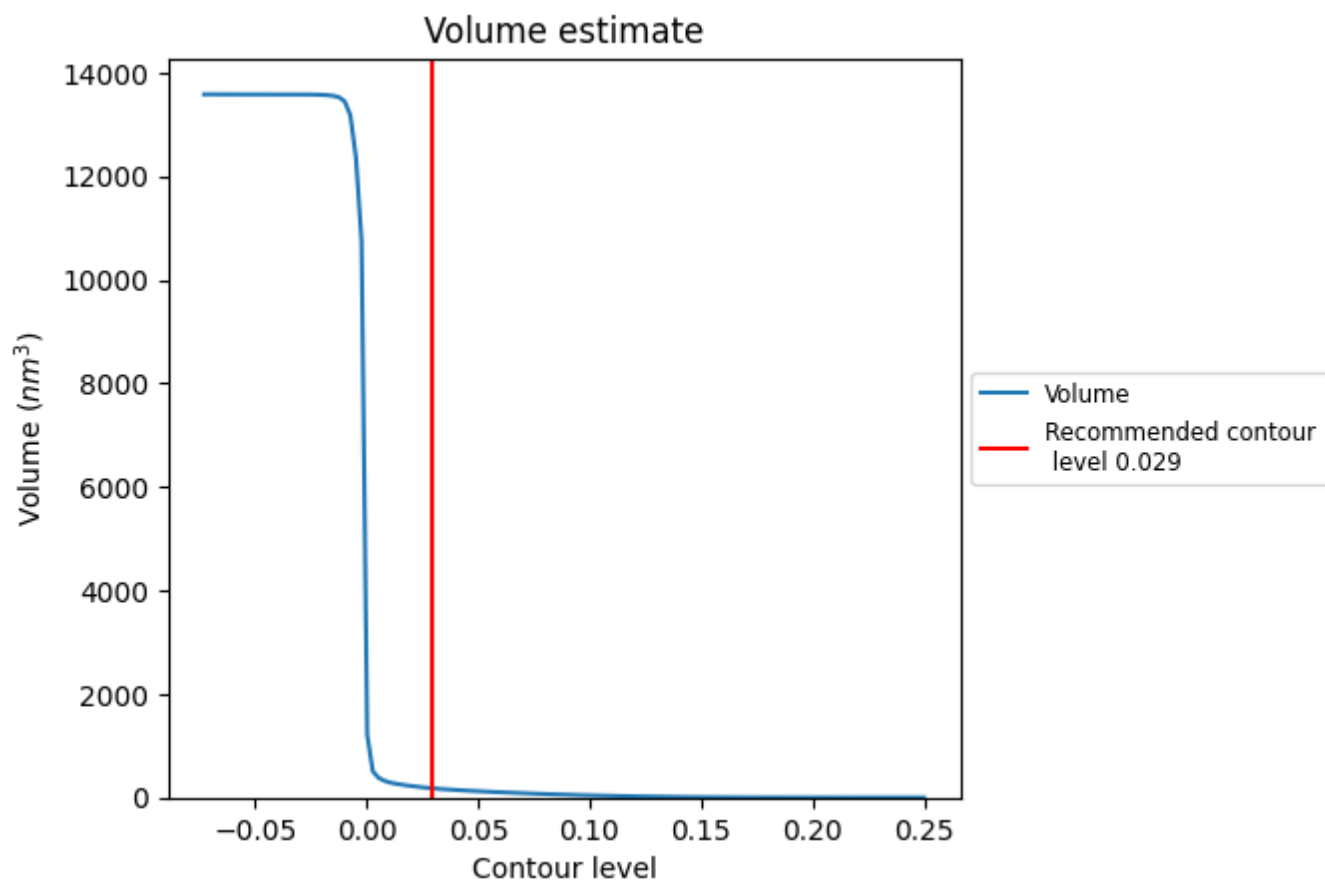
This section contains the results of statistical analysis of the map.

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.

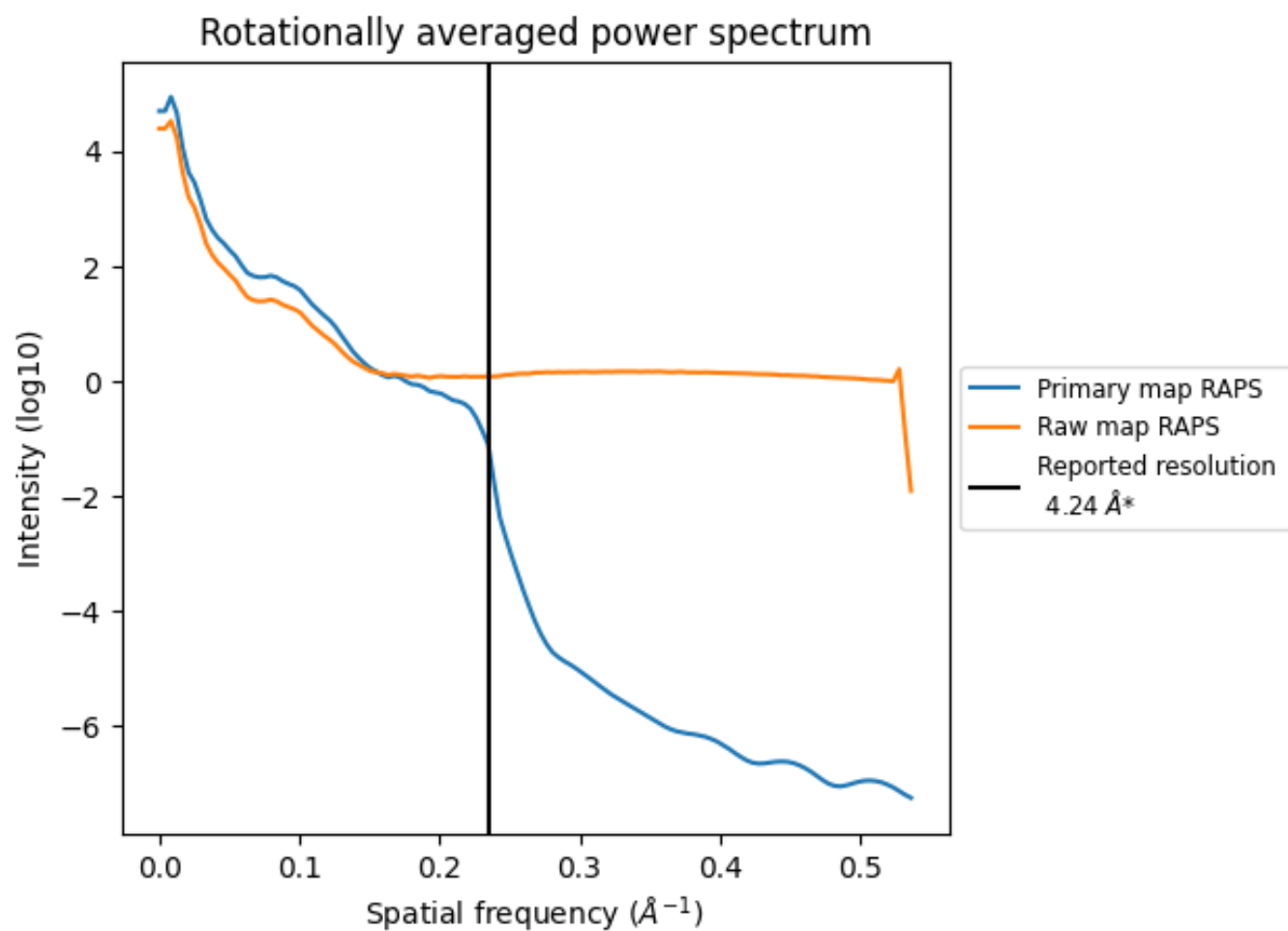
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 181 nm^3 ; this corresponds to an approximate mass of 163 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 ⓘ

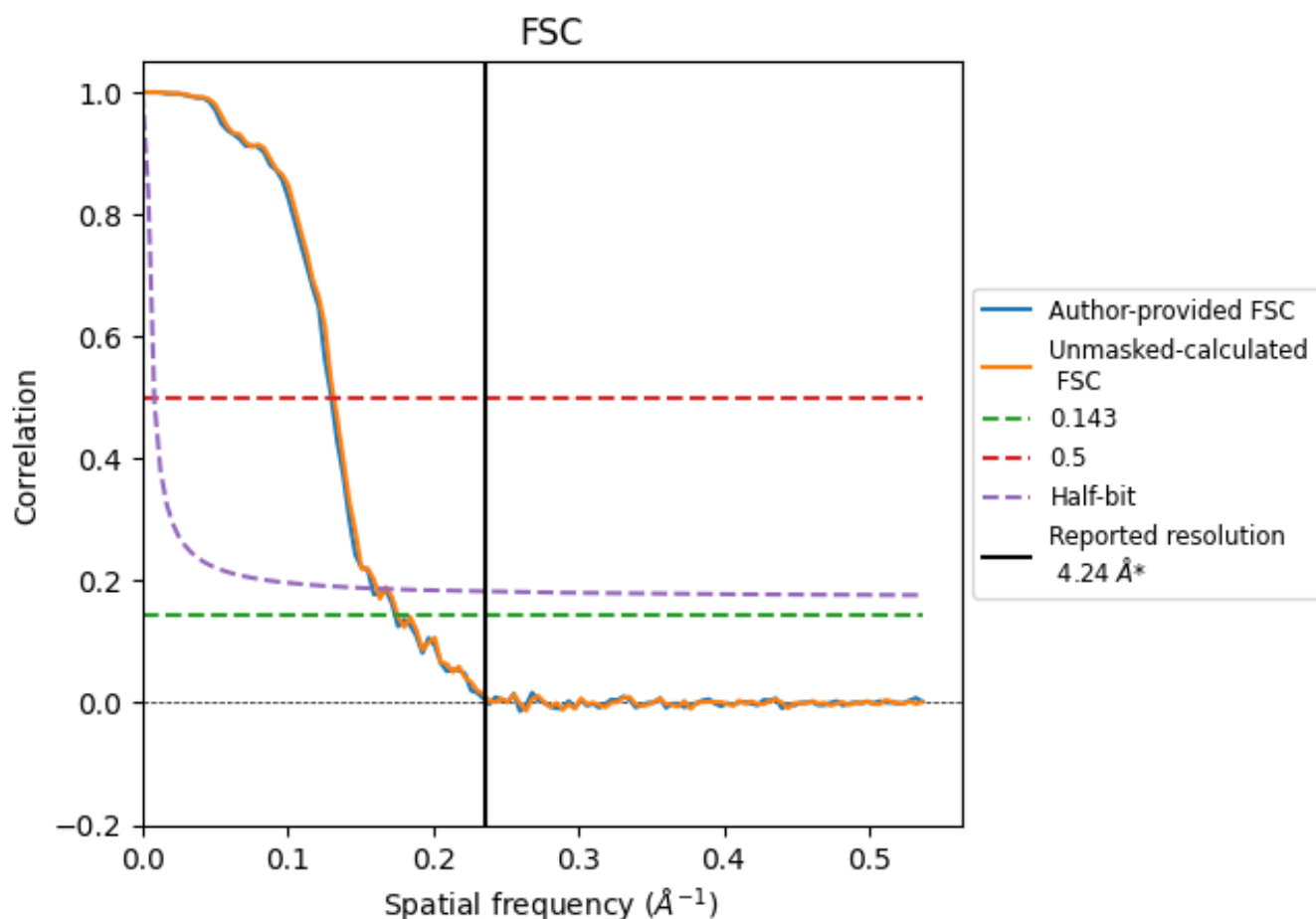


*Reported resolution corresponds to spatial frequency of 0.236 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.236 \text{ \AA}^{-1}$

8.2 Resolution estimates

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.24	-	-
Author-provided FSC curve	5.75	7.69	6.32
Unmasked-calculated*	5.69	7.58	6.20

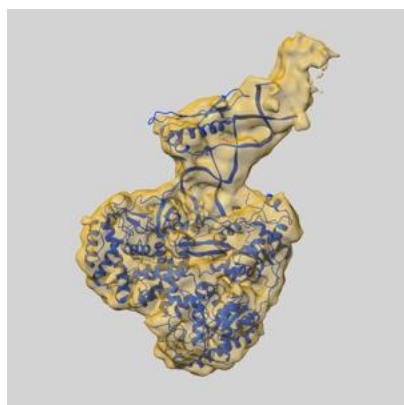
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 5.75 differs from the reported value 4.24 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.69 differs from the reported value 4.24 by more than 10 %

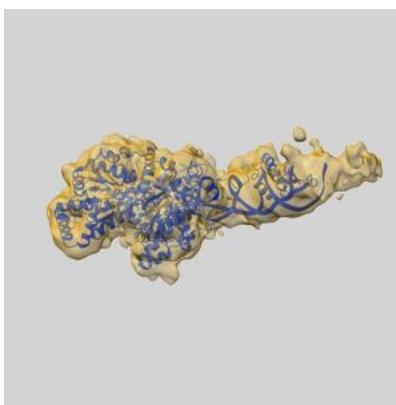
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17711 and PDB model 8PJJ. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

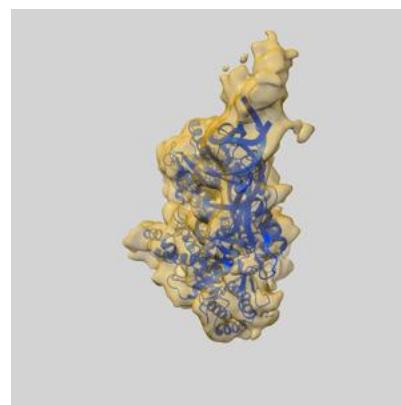
9.1 Map-model overlay [i](#)



X



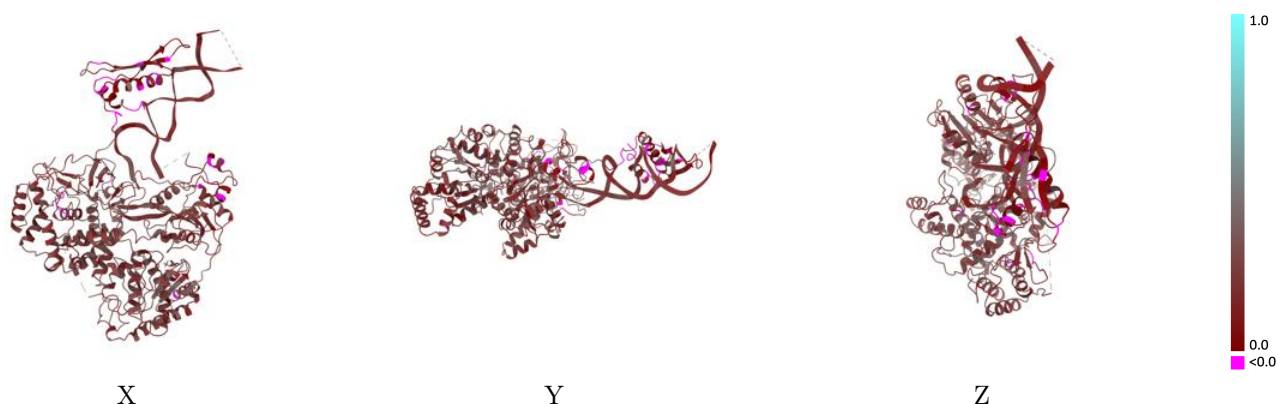
Y



Z

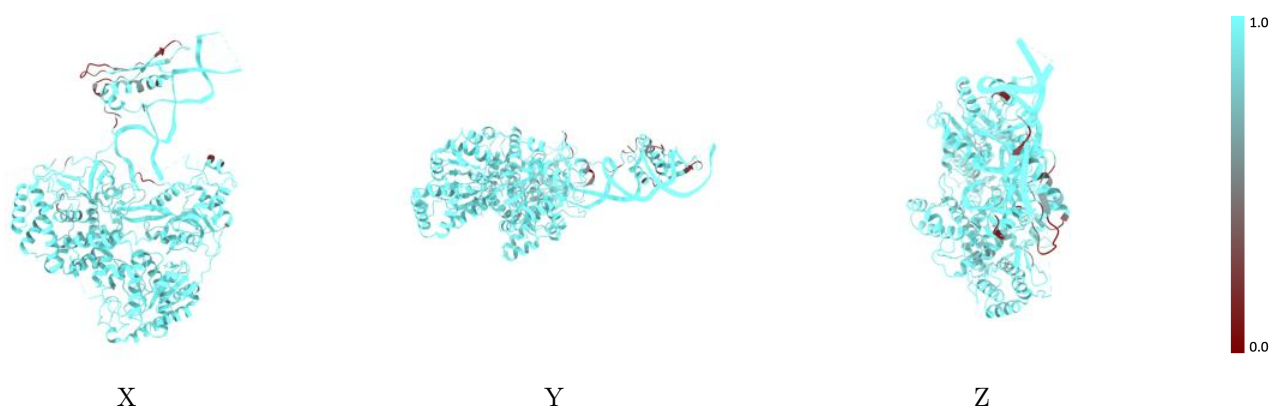
The images above show the 3D surface view of the map at the recommended contour level 0.029 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



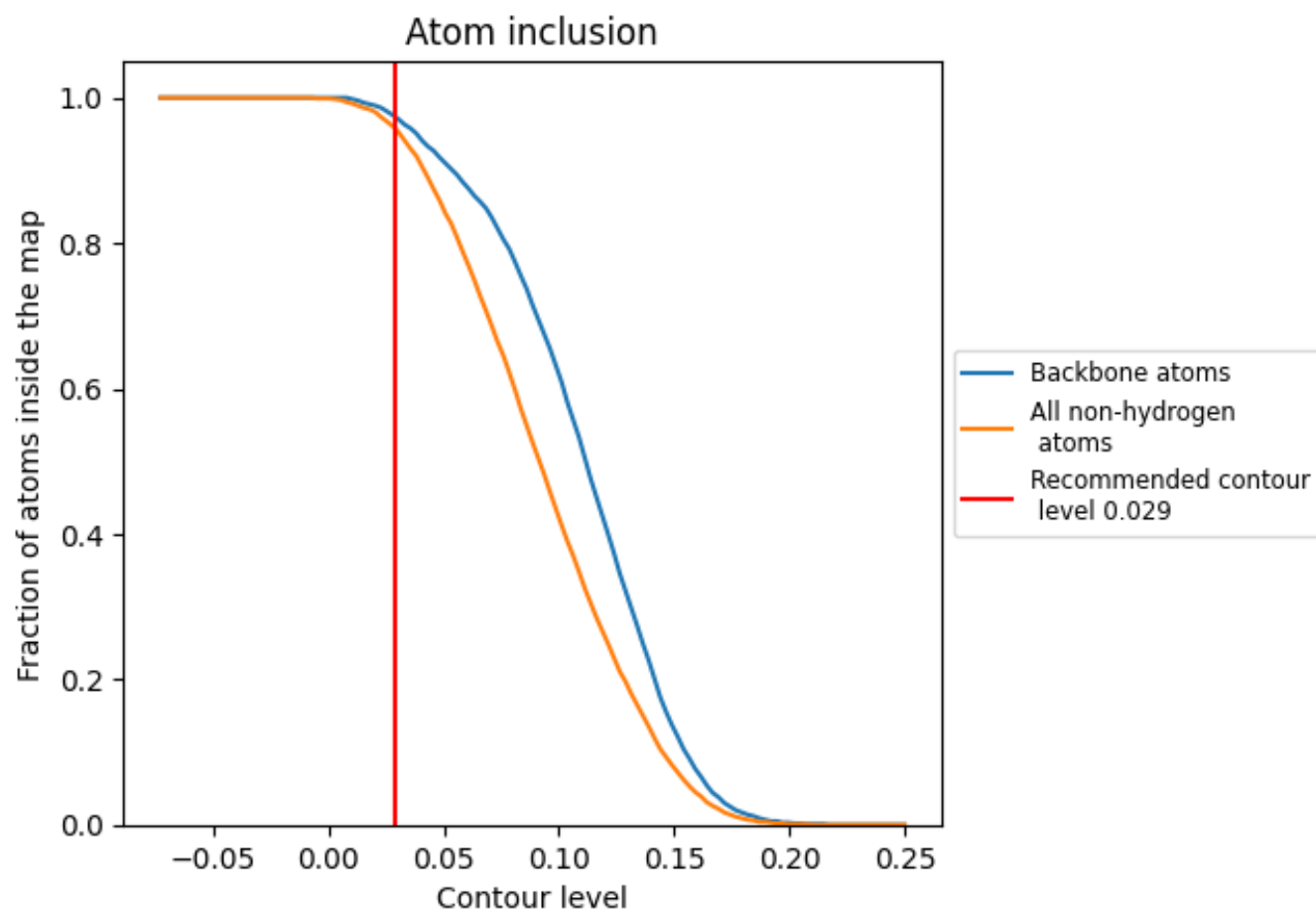
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.029).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% 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 (0.029) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9580	0.2180
A	0.9530	0.2200
B	0.9940	0.2050

