



## Full wwPDB EM Validation Report ⓘ

Nov 5, 2022 – 01:44 PM EDT

PDB ID : 5VZL  
EMDB ID : EMD-8749  
Title : cryo-EM structure of the Cas9-sgRNA-AcrIIA4 anti-CRISPR complex  
Authors : Jiang, F.; Liu, J.J.; Nogales, E.; Doudna, J.A.  
Deposited on : 2017-05-29  
Resolution : 3.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
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) : 2.31.2

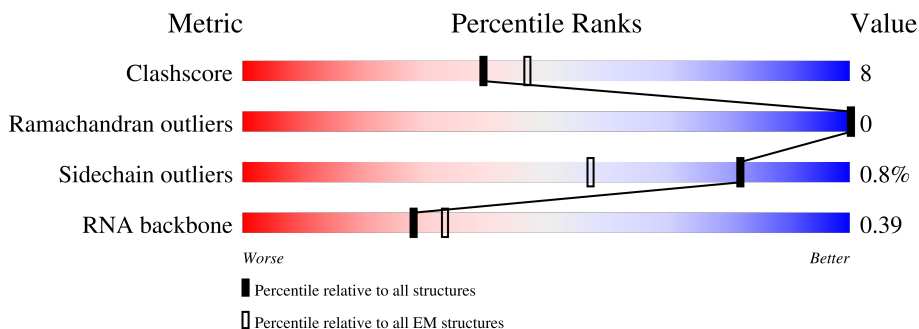
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	B	118	<div> <div>92%</div> <div>44%</div> <div>40%</div> <div>13%</div> <div>..</div> </div>
2	A	1369	<div> <div>91%</div> <div>80%</div> <div>20%</div> </div>
3	C	87	<div> <div>92%</div> <div>71%</div> <div>28%</div> <div>.</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13915 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 RNA chain called single guide RNA (116-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	116	Total	C	N	O	P	0	0
			2494	1112	455	809	118		

- Molecule 2 is a protein called CRISPR-associated endonuclease Cas9.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1364	Total	C	N	O	S	0	0
			10711	6813	1851	2024	23		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP A0A0C6FZC2

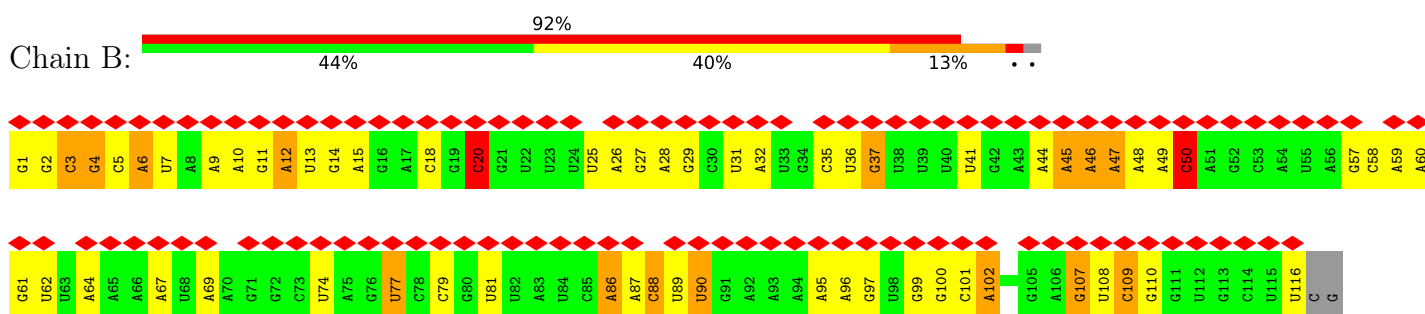
- Molecule 3 is a protein called phage anti-CRISPR AcrIIA4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	87	Total	C	N	O	S	0	0
			710	439	114	155	2		

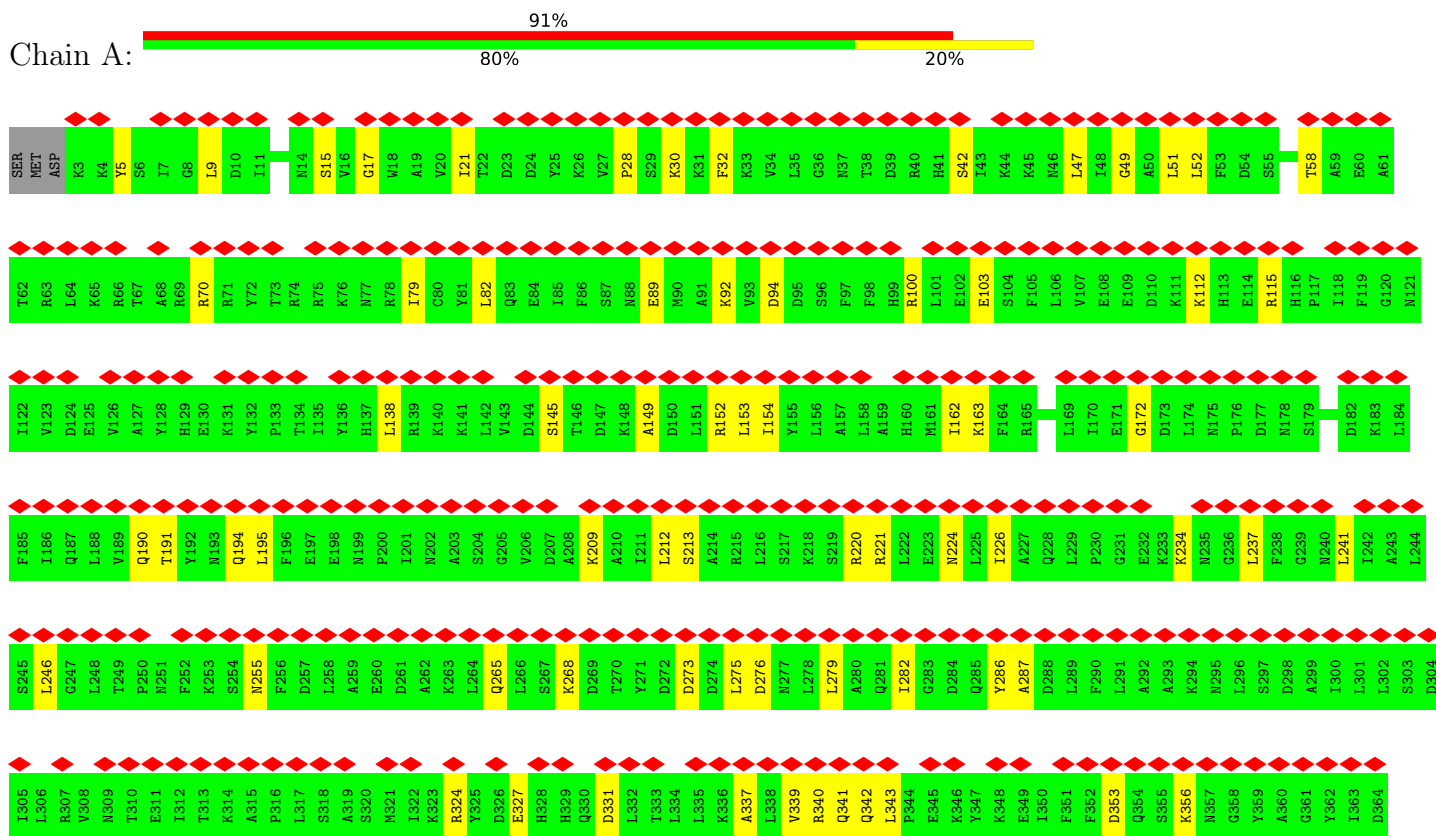
### 3 Residue-property plots

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

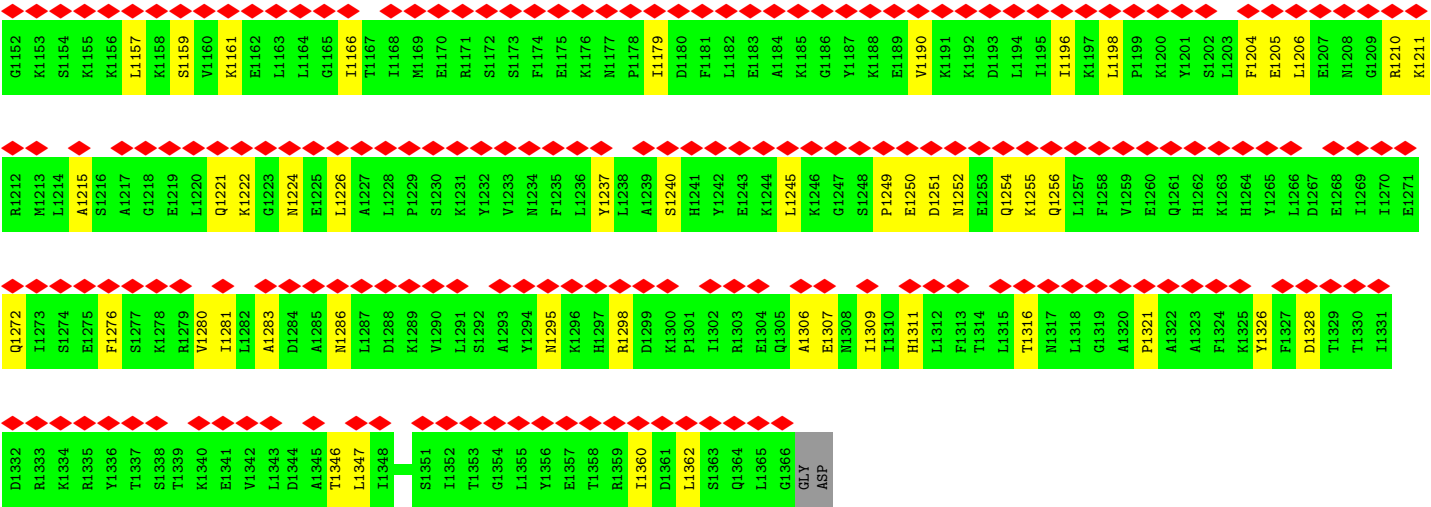
- Molecule 1: single guide RNA (116-MER)



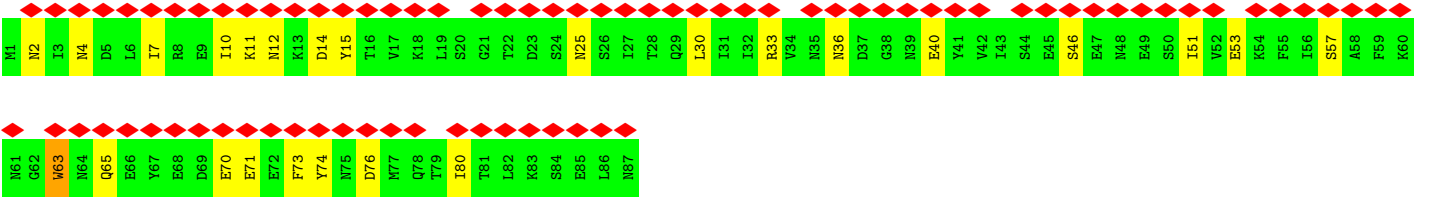
- Molecule 2: CRISPR-associated endonuclease Cas9



Q1091	V1092	N1093	I1094	V1095	K1096	K1097	T1098	E1099	V1100	Q1101	T1102	G1103	G1104	F1105	E1108	S1109	I1110	L1111	P1112	K1113	R1114	N1115	D1116	K1117	K1118	L1119	I1120	A1121	R1122	K1123	K1124	D1125	W1126	D1127	F1128	K1129	K1130	Y1131	G1132	G1133	F1134	D1135	S1136	P1137	T1138	V1139	A1140	Y1141	S1142	V1143	L1144	V1145	V1146	A1147	K1148	V1149	E1150	K1151		
K1031	A1032	T1033	A1034	K1035	Y1036	F1037	F1038	Y1039	S1040	M1041	I1042	M1043	N1044	F1045	F1046	K1047	T1048	E1049	I1050	T1051	L1052	A1053	N1054	G1055	E1056	I1057	R1058	K1059	R1060	P1061	K1124	L1062	I1063	E1064	T1065	N1066	G1067	E1068	T1069	G1070	E1071	I1072	Y1073	W1074	D1075	K1076	G1077	R1078	D1079	F1080	A1081	T1082	V1083	R1084	K1085	V1086	L1087	S1088	M1089	P1090
F970	Q971	F972	Y973	K974	N975	R976	E977	I978	N979	N980	Y981	H982		H985	D986	A987	Y988	L989	N990	A991	V992	V993	G994	T995	A996	L997	K998	K999	K1000	Y1001	P1002	K1003	L1004	E1005	S1006	E1007	F1008	Y1009	Y1010	G1011	D1012	Y1013	K1014	V1015	Y1016	D1017	Y1018	R1019	K1020	M1021	I1022	A1023	K1024	S1025	E1026	Q1027	L1028	I1029	G1030	
E910	L911	D912	K913	A914	G915	F916	I917	K918	R919	Q920	L921	V922	E923	T924	R925	Q926	I927	T928	K929	H930	V931	A932	Q933	I934	L935	D936	S937	R938	N939	N940	T941	K942	Y943	D944	E945	N946	D947	K948	L949	G950	D951	E952	K953	K954	V955	R956	T957	L958	K959	S960	K961	T962	L963	S964	D965	P966	R967	K968	D969	
D850	S851	I852	D853	N854	K855	W856	L857	T858	R859	S860	D861	K862	N863	R864	G865	K866	S867	D868	N869	W870	P871	S872	E873	E874	W875	W876	K877	K878	W879	K880	N881	Y882	Y883	R884	Q885	L886	L887	N888	A889	K890	L891	T892	Q894	R895	K896	F897	D898	K899	N899	L900	T901	K902	A903	E904	P905	G906	Q907	L908	S909	
E790	L791	G792	S793	Q794	I795	L796	K797	E798	H799	P800	V801	E802	N803	T804	Q805	L806	Q807	N808	E809	X810	L811	Y812	L813	Y814	Y815	L816	Q817	N818	G819	R820	D821	M822	Y823	N824	D825	Q826	E827	L828	D829	I830	N831	R832	L833	S834	D835	Y836	D837	N838	D839	H840	T841	W842	P843	Q844	S845	F846	L847	X848	D849	
S730	P731	A732	I733	K734	K735	G736	L737	L738	Q739	T740	V741	K742	V743	V744	D745	E746	L747	V748	K749	V750	M751	G752	G753	H754	K755	P756	E757	N758	I759	V760	I761	E762	L763	N763	A764	R765	E766	N767	Q768	T769	T770	Q771	K772	G773	Q774	K775	N776	T777	R778	E779	R780	Y781	K782	R783	I784	E785	E786	G787	L788	K789
I670	R671	D672	K673	Q674	S675	G676	K677	T678	V679	L680	D681	F682	L683	K684	S685	D686	G687	F688	A689	N690	R691	N692	F693	M694	Q695	L696	I697	K698	D699	D700	S701	L702	T703	F704	K705	E706	D707	I708	Q709	K710	A711	G712	V713	S714	G715	Q716	G717	D718	S719	L720	H721	E722	H723	I724	A725	N726	L727	A728	G729	
E610	E611	N612	E613	D614	I615	L616	E617	D618	I619	V620	L621	T622	L623	T624	L625	F626	E627	D628	R629	E630	M631	I632	E633	E634	R635	L636	S637	V638	Y639	A640	H641	L642	F643	D644	D645	K646	V647	M648	Q649	Q650	L651	K652	R653	R654	R655	T657	G658	W659	G660	R661	L662	S663	R664	K665	L666	I667	N668	G669		
D550	L551	L552	F553	K554	T555	N556	R557	K558	V559	T560	V561	K562	Q563	L564	N565	E566	D567	Y568	F569	K570	K571	I572	E573	C574	F575	D576	S577	V578	E579	I580	S581	G582	V583	E584	D585	R586	F587	N588	A589	S590	L591	G592	T593	Y594	H595	D596	L597	L598	W599	F539	I600	I601	K602	D603	E543	D605	F606	L607	D608	N609
S490	F491	I492	E493	R494	M495	T496	M497	F498	D499	K500	N501	L502	P503	N504	E505	K506	V507	L508	P509	K510	H511	S512	L513	L514	Y515	E516	Y517	F518	T519	W520	Y521	G522	N522	E523	L524	T525	K526	V527	K528	Y529	V530	T531	E532	G533	M534	R535	K536	P537	A538	F539	L540	S541	G542	E543	Q544	K545	K546	A547	I548	V549
F429	Y430	P431	F432	L433	K434	D435	M436	R437	E438	K439	I440	E441	K442	I443	L444	T445	F446	R447	I448	P449	V452	G453	P454	L455	A456	R457	G458	M459	S460	R461	F462	A463	W464	M465	T466	R467	K468	S469	E470	E471	T472	I473	T474	P475	W476	M477	F478	E479	E480	F481	V482	D483	K484	G485	A486	S487	A488	Q489		
G365		S368	Q369	E370	E371	F372	Y373	K374	F375	I376	I379	L380	E381	K382	M383	D384	G385	T386	E387	E388	L389	L390	V391	K392	L393	K394	R395	E396	D397	L398	L399	R400	K401	Q402	R403		D406	M407		I410	P411	H412	Q413	I414	H415	L416	G417	E418	L419	H420	A421	I422	L423	R424	R425	Q426	E427	A428		



● Molecule 3: phage anti-CRISPR AcrIIA4



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	185000	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 ( $e^-/\text{\AA}^2$ )	46	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.216	Depositor
Minimum map value	-0.136	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	273.92, 273.92, 273.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	B	0.65	0/2758	1.19	24/4297 (0.6%)
2	A	0.34	0/10903	0.54	0/14739
3	C	0.37	0/718	0.65	0/969
All	All	0.42	0/14379	0.74	24/20005 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	2
3	C	0	2
All	All	0	4

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	G	C4-N9-C1'	7.85	136.70	126.50
1	B	4	G	N3-C4-N9	7.76	130.66	126.00
1	B	4	G	N3-C4-C5	-7.58	124.81	128.60
1	B	88	C	C2-N1-C1'	7.06	126.56	118.80
1	B	20	C	N1-C2-O2	6.97	123.08	118.90
1	B	47	A	O4'-C1'-N9	-6.77	102.78	108.20
1	B	4	G	C8-N9-C1'	-6.53	118.52	127.00
1	B	47	A	P-O3'-C3'	6.28	127.23	119.70
1	B	90	U	C2-N1-C1'	6.28	125.23	117.70
1	B	20	C	N3-C2-O2	-6.06	117.66	121.90
1	B	18	C	N1-C2-O2	6.02	122.51	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	A	OP1-P-O3'	6.01	118.42	105.20
1	B	6	A	C2-N3-C4	5.74	113.47	110.60
1	B	86	A	P-O3'-C3'	5.70	126.54	119.70
1	B	77	U	N3-C2-O2	-5.53	118.33	122.20
1	B	90	U	N1-C2-O2	5.52	126.67	122.80
1	B	58	C	C2-N1-C1'	5.51	124.87	118.80
1	B	58	C	N1-C2-O2	5.48	122.19	118.90
1	B	50	C	O4'-C1'-N1	5.44	112.55	108.20
1	B	18	C	N3-C2-O2	-5.40	118.12	121.90
1	B	88	C	C6-N1-C2	-5.35	118.16	120.30
1	B	4	G	C2-N3-C4	5.19	114.49	111.90
1	B	77	U	N1-C2-O2	5.07	126.35	122.80
1	B	20	C	C2-N1-C1'	5.01	124.31	118.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	1316	THR	Peptide
2	A	1326	TYR	Peptide
3	C	46	SER	Peptide
3	C	63	TRP	Peptide

## 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	B	2494	0	1248	26	0
2	A	10711	0	10460	170	0
3	C	710	0	668	16	0
All	All	13915	0	12376	200	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 (200) 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)
2:A:32:PHE:O	2:A:42:SER:HA	1.77	0.83
2:A:760:VAL:HA	2:A:956:ILE:O	1.82	0.80
2:A:15:SER:HA	2:A:51:LEU:O	1.82	0.77
2:A:1251:ASP:O	2:A:1255:LYS:HB2	1.90	0.71
2:A:562:LYS:O	2:A:566:GLU:HB3	1.90	0.71
2:A:484:LYS:O	2:A:488:ALA:HB3	1.91	0.71
2:A:191:THR:O	2:A:195:LEU:HB2	1.91	0.70
3:C:70:GLU:O	3:C:73:PHE:HB3	1.92	0.70
2:A:414:ILE:O	2:A:418:GLU:HB2	1.93	0.68
2:A:785:GLU:O	2:A:789:LYS:HB2	1.92	0.68
2:A:1251:ASP:HA	2:A:1254:GLN:HB3	1.76	0.67
2:A:237:LEU:O	2:A:241:LEU:HB2	1.95	0.66
2:A:1205:GLU:HB3	2:A:1346:THR:HB	1.78	0.64
2:A:743:VAL:O	2:A:747:LEU:HB2	1.98	0.63
2:A:1283:ALA:HB1	2:A:1286:ASN:HD22	1.63	0.63
2:A:28:PRO:HB2	2:A:47:LEU:HD12	1.83	0.61
2:A:654:ARG:NH1	2:A:655:ARG:O	2.34	0.60
2:A:212:LEU:HA	2:A:221:ARG:HD3	1.83	0.60
2:A:841:ILE:HG21	2:A:899:ASN:HB3	1.83	0.60
2:A:1045:PHE:HB2	2:A:1064:GLU:HG3	1.84	0.60
1:B:79:C:OP1	2:A:70:ARG:NH2	2.36	0.59
2:A:540:LEU:O	2:A:690:ASN:ND2	2.34	0.59
2:A:777:SER:O	2:A:781:MET:HB2	2.03	0.58
2:A:327:GLU:O	2:A:331:ASP:HB2	2.04	0.58
2:A:783:ARG:NH1	2:A:891:LEU:O	2.36	0.58
2:A:1280:VAL:HG23	2:A:1281:ILE:HD12	1.85	0.58
1:B:20:C:OP1	2:A:407:ASN:ND2	2.37	0.58
2:A:705:LYS:O	2:A:709:GLN:HB2	2.04	0.57
2:A:974:LYS:HE3	2:A:976:ARG:HE	1.69	0.57
2:A:813:LEU:HD23	2:A:816:LEU:HD12	1.86	0.57
2:A:420:HIS:ND1	2:A:441:GLU:OE2	2.37	0.57
2:A:530:VAL:HB	2:A:579:GLU:HB2	1.86	0.57
2:A:353:ASP:OD2	2:A:356:LYS:N	2.37	0.56
2:A:212:LEU:HD22	2:A:246:LEU:HD21	1.87	0.56
2:A:662:LEU:HD22	2:A:666:LEU:HD23	1.88	0.56
2:A:849:ASP:HB3	2:A:854:ASN:HD22	1.70	0.56
2:A:145:SER:O	2:A:425:ARG:NH1	2.38	0.56
2:A:209:LYS:O	2:A:213:SER:CB	2.54	0.56
1:B:15:A:H5''	2:A:70:ARG:HH12	1.71	0.56
1:B:26:A:OP1	2:A:115:ARG:NH2	2.38	0.56
2:A:190:GLN:O	2:A:194:GLN:HB3	2.07	0.55
2:A:1064:GLU:HB2	2:A:1074:TRP:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1295:ASN:OD1	2:A:1298:ARG:NH2	2.40	0.55
3:C:7:ILE:O	3:C:11:LYS:HB2	2.07	0.54
2:A:209:LYS:O	2:A:213:SER:HB2	2.07	0.54
2:A:1018:VAL:HA	2:A:1021:MET:HB2	1.89	0.54
2:A:1139:VAL:HA	2:A:1166:ILE:O	2.07	0.54
3:C:4:ASN:HA	3:C:7:ILE:HB	1.89	0.54
2:A:484:LYS:O	2:A:488:ALA:CB	2.56	0.54
2:A:1101:GLN:HB2	2:A:1140:ALA:HA	1.89	0.54
2:A:190:GLN:O	2:A:194:GLN:CB	2.56	0.54
2:A:1272:GLN:O	2:A:1276:PHE:HB3	2.08	0.54
2:A:772:LYS:O	2:A:776:ASN:ND2	2.40	0.53
2:A:502:LEU:HB2	2:A:666:LEU:HD13	1.89	0.53
2:A:777:SER:O	2:A:781:MET:CB	2.56	0.53
2:A:612:ASN:HA	2:A:615:ILE:HD13	1.91	0.53
2:A:5:TYR:OH	2:A:754:HIS:O	2.26	0.53
2:A:827:GLU:O	2:A:859:ARG:NH2	2.36	0.52
2:A:864:ARG:NH1	2:A:867:SER:O	2.43	0.52
2:A:979:ASN:ND2	2:A:1226:LEU:O	2.43	0.52
2:A:932:ALA:O	2:A:936:ASP:HB2	2.09	0.52
2:A:1148:LYS:HE2	2:A:1159:SER:HB2	1.90	0.52
2:A:680:LEU:HG	2:A:684:LYS:HE2	1.91	0.52
2:A:342:GLN:HE22	2:A:385:GLY:H	1.57	0.52
2:A:1148:LYS:HG2	2:A:1159:SER:HA	1.92	0.52
2:A:850:ASP:HA	2:A:855:LYS:HE3	1.92	0.51
2:A:220:ARG:O	2:A:224:ASN:ND2	2.44	0.51
2:A:1144:LEU:HB3	2:A:1196:ILE:HB	1.91	0.51
2:A:1161:LYS:NZ	2:A:1362:LEU:O	2.42	0.51
2:A:485:GLY:O	2:A:489:GLN:HB2	2.10	0.51
2:A:337:ALA:O	2:A:341:GLN:HB2	2.10	0.51
2:A:920:GLN:HE22	2:A:1041:ASN:HA	1.75	0.51
2:A:563:GLN:O	2:A:567:ASP:HB2	2.11	0.51
2:A:893:THR:HG23	2:A:896:LYS:H	1.76	0.51
2:A:672:ASP:HB3	2:A:675:SER:HB2	1.92	0.51
2:A:1091:GLN:NE2	2:A:1093:ASN:OD1	2.40	0.51
2:A:562:LYS:O	2:A:566:GLU:CB	2.57	0.50
2:A:1138:THR:OG1	3:C:36:ASN:ND2	2.43	0.50
1:B:15:A:H4'	2:A:454:PRO:HD3	1.93	0.50
2:A:629:ARG:O	2:A:632:ILE:HB	2.12	0.50
2:A:49:GLY:HA3	2:A:1093:ASN:HB2	1.94	0.50
2:A:508:LEU:HD21	2:A:664:ARG:HB2	1.94	0.50
2:A:987:ALA:HA	2:A:990:ASN:HD22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:138:LEU:HD11	2:A:153:LEU:HD21	1.93	0.50
2:A:273:ASP:O	2:A:276:ASP:HB2	2.11	0.50
2:A:400:ARG:NH2	2:A:406:ASP:OD2	2.44	0.50
2:A:474:THR:OG1	2:A:477:ASN:OD1	2.27	0.50
2:A:645:ASP:HA	2:A:648:MET:HB2	1.94	0.50
2:A:988:TYR:HE2	2:A:1083:VAL:HG13	1.76	0.49
2:A:1222:LYS:HE2	2:A:1321:PRO:HG3	1.94	0.49
2:A:282:ILE:HD12	2:A:286:TYR:HD2	1.77	0.49
2:A:627:GLU:OE1	2:A:655:ARG:NE	2.45	0.49
2:A:456:ALA:O	2:A:467:ARG:NH2	2.45	0.49
1:B:31:U:H2'	1:B:32:A:H8	1.78	0.49
2:A:686:ASP:HB3	2:A:690:ASN:HA	1.95	0.49
2:A:1215:ALA:HB2	2:A:1221:GLN:HG3	1.95	0.49
3:C:33:ARG:HA	3:C:40:GLU:HA	1.95	0.49
2:A:103:GLU:OE2	2:A:112:LYS:NZ	2.40	0.49
2:A:275:LEU:O	2:A:279:LEU:N	2.44	0.49
3:C:30:LEU:HD22	3:C:51:ILE:HD11	1.94	0.49
2:A:1052:LEU:HB2	2:A:1056:GLU:HB2	1.95	0.48
2:A:1306:ALA:HA	2:A:1309:ILE:HD12	1.94	0.48
2:A:9:LEU:HA	2:A:17:GLY:O	2.13	0.48
2:A:1065:THR:HG22	2:A:1072:ILE:HA	1.94	0.48
3:C:53:GLU:O	3:C:57:SER:HB3	2.13	0.48
2:A:1108:GLU:N	3:C:14:ASP:OD2	2.47	0.48
2:A:1148:LYS:HD3	2:A:1157:LEU:HB3	1.97	0.47
2:A:629:ARG:HA	2:A:632:ILE:HD12	1.96	0.47
2:A:960:SER:O	2:A:964:SER:CB	2.61	0.47
2:A:777:SER:HB2	2:A:806:LEU:HD23	1.96	0.47
2:A:1211:LYS:N	2:A:1224:ASN:OD1	2.42	0.47
1:B:45:A:H3'	1:B:46:A:C8	2.50	0.47
2:A:1245:LEU:HD13	2:A:1252:ASN:HA	1.97	0.47
2:A:1252:ASN:O	2:A:1256:GLN:CB	2.63	0.47
1:B:1:GTP:O1G	2:A:976:ARG:NH2	2.41	0.47
2:A:1206:LEU:HB2	2:A:1210:ARG:HB3	1.97	0.47
2:A:1250:GLU:O	2:A:1254:GLN:CB	2.63	0.46
2:A:1115:ASN:HA	2:A:1129:LYS:HG2	1.97	0.46
2:A:94:ASP:OD2	2:A:100:ARG:NH2	2.48	0.46
2:A:1237:TYR:O	2:A:1240:SER:OG	2.33	0.46
1:B:25:U:H2'	1:B:26:A:H8	1.79	0.46
1:B:3:C:H4'	1:B:4:G:H5'	1.97	0.46
2:A:1307:GLU:O	2:A:1311:HIS:ND1	2.43	0.46
3:C:10:ILE:HD11	3:C:80:ILE:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:79:ILE:HD11	2:A:163:LYS:HG3	1.97	0.46
2:A:540:LEU:HB2	2:A:545:LYS:HE3	1.98	0.45
2:A:1272:GLN:O	2:A:1276:PHE:CB	2.64	0.45
1:B:1:GTP:H2'	1:B:2:G:C8	2.52	0.45
2:A:149:ALA:HB3	2:A:154:ILE:HD11	1.99	0.45
2:A:521:TYR:HB3	2:A:683:LEU:HB3	1.98	0.45
2:A:89:GLU:O	2:A:92:LYS:HB3	2.17	0.45
2:A:1179:ILE:HG22	2:A:1190:VAL:HG11	1.99	0.45
2:A:369:GLN:HE22	2:A:400:ARG:HH11	1.65	0.44
2:A:1198:LEU:HD13	2:A:1204:PHE:HZ	1.83	0.44
2:A:1250:GLU:O	2:A:1254:GLN:HB2	2.17	0.44
2:A:833:LEU:HD23	2:A:836:TYR:HD2	1.82	0.44
1:B:96:A:H2'	1:B:97:G:H8	1.82	0.44
2:A:265:GLN:HG2	2:A:268:LYS:H	1.83	0.44
2:A:560:THR:HG23	2:A:563:GLN:H	1.83	0.44
1:B:67:A:N3	2:A:1122:ARG:NH2	2.61	0.44
2:A:172:GLY:O	2:A:413:GLN:NE2	2.49	0.44
2:A:920:GLN:NE2	2:A:1040:SER:O	2.50	0.44
3:C:71:GLU:HA	3:C:74:TYR:HD2	1.83	0.44
2:A:1074:TRP:HE1	2:A:1076:LYS:HD3	1.82	0.44
1:B:101:C:H2'	1:B:102:A:C8	2.53	0.44
1:B:107:G:N1	2:A:1272:GLN:OE1	2.47	0.44
2:A:58:THR:HA	2:A:731:PRO:HG2	1.99	0.44
2:A:337:ALA:O	2:A:341:GLN:CB	2.66	0.44
3:C:7:ILE:O	3:C:11:LYS:CB	2.65	0.44
1:B:2:G:O2'	1:B:4:G:O4'	2.36	0.44
1:B:101:C:H2'	1:B:102:A:H8	1.83	0.43
3:C:63:TRP:O	3:C:65:GLN:N	2.49	0.43
2:A:327:GLU:O	2:A:331:ASP:CB	2.66	0.43
2:A:866:LYS:O	2:A:1054:ASN:ND2	2.48	0.43
2:A:1249:PRO:HA	2:A:1252:ASN:HB2	1.99	0.43
2:A:777:SER:HB3	2:A:807:GLN:HE21	1.83	0.43
1:B:25:U:H2'	1:B:26:A:C8	2.54	0.43
2:A:909:SER:OG	2:A:910:GLU:N	2.51	0.43
2:A:339:VAL:O	2:A:343:LEU:N	2.44	0.43
2:A:194:GLN:NE2	2:A:557:ARG:HH12	2.17	0.43
2:A:761:ILE:HD11	2:A:935:LEU:HD12	2.00	0.43
2:A:1221:GLN:NE2	3:C:40:GLU:OE2	2.43	0.43
2:A:1347:LEU:HD23	2:A:1360:ILE:HB	2.00	0.43
2:A:391:VAL:O	2:A:395:ARG:CB	2.66	0.43
2:A:693:PHE:HA	2:A:696:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:53:GLU:O	3:C:57:SER:CB	2.67	0.42
2:A:677:LYS:NZ	2:A:685:SER:O	2.38	0.42
3:C:15:TYR:OH	3:C:76:ASP:OD2	2.30	0.42
1:B:109:C:H2'	1:B:110:G:H8	1.85	0.42
2:A:191:THR:O	2:A:195:LEU:CB	2.65	0.42
2:A:212:LEU:HD23	2:A:221:ARG:HD3	2.02	0.42
2:A:279:LEU:HD11	2:A:287:ALA:HB2	2.00	0.42
2:A:785:GLU:O	2:A:789:LYS:CB	2.63	0.42
1:B:59:A:OP1	2:A:340:ARG:NH2	2.47	0.42
2:A:15:SER:HB3	2:A:52:LEU:HD23	2.02	0.42
2:A:194:GLN:HE22	2:A:557:ARG:HH12	1.66	0.42
2:A:490:SER:O	2:A:494:ARG:N	2.42	0.42
2:A:516:GLU:HA	2:A:519:THR:HG22	2.01	0.42
1:B:31:U:H2'	1:B:32:A:C8	2.54	0.42
2:A:389:LEU:HD13	2:A:389:LEU:HA	1.88	0.42
1:B:1:GTP:H2'	1:B:2:G:H8	1.85	0.42
3:C:80:ILE:HA	3:C:80:ILE:HD12	1.80	0.42
2:A:560:THR:OG1	2:A:585:ASP:OD1	2.30	0.41
2:A:324:ARG:HH21	2:A:400:ARG:HG2	1.84	0.41
1:B:109:C:H2'	1:B:110:G:C8	2.55	0.41
1:B:11:G:H1'	1:B:12:A:C8	2.55	0.41
2:A:138:LEU:HD21	2:A:153:LEU:HG	2.03	0.41
2:A:226:ILE:HD13	2:A:234:LYS:HA	2.02	0.41
2:A:548:ILE:HG23	2:A:552:LEU:HD12	2.01	0.41
2:A:30:LYS:HE2	2:A:32:PHE:HE1	1.85	0.41
2:A:82:LEU:HD22	2:A:162:ILE:HD12	2.03	0.41
2:A:21:ILE:HD11	2:A:995:THR:HG21	2.03	0.40
2:A:960:SER:O	2:A:964:SER:HB3	2.20	0.40
2:A:1004:LEU:HD11	2:A:1021:MET:HG3	2.03	0.40
2:A:801:VAL:HG11	2:A:811:LEU:HD21	2.03	0.40
1:B:37:G:N2	1:B:50:C:H41	2.19	0.40
2:A:1328:ASP:OD1	2:A:1328:ASP:N	2.54	0.40
1:B:88:C:H2'	1:B:89:U:H6	1.86	0.40
2:A:419:LEU:HD21	2:A:440:ILE:HG22	2.03	0.40
2:A:704:PHE:HA	2:A:707:ASP:HB2	2.04	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	
2	A	1362/1369 (100%)	1256 (92%)	106 (8%)	0	100	100
3	C	85/87 (98%)	70 (82%)	15 (18%)	0	100	100
All	All	1447/1456 (99%)	1326 (92%)	121 (8%)	0	100	100

There are no Ramachandran outliers to report.

### 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	
2	A	1118/1228 (91%)	1112 (100%)	6 (0%)	88	93
3	C	82/83 (99%)	79 (96%)	3 (4%)	34	60
All	All	1200/1311 (92%)	1191 (99%)	9 (1%)	82	89

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	152	ARG
2	A	255	ASN
2	A	437	ARG
2	A	522	ASN
2	A	664	ARG
2	A	767	ASN
3	C	2	ASN
3	C	12	ASN

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Mol	Chain	Res	Type
3	C	25	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	99	HIS
2	A	137	HIS
2	A	194	GLN
2	A	224	ASN
2	A	522	ASN
2	A	595	HIS
2	A	767	ASN
2	A	863	ASN
2	A	899	ASN
2	A	1286	ASN
2	A	1317	ASN
3	C	2	ASN
3	C	12	ASN
3	C	25	ASN
3	C	75	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	114/118 (96%)	43 (37%)	4 (3%)

All (43) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	3	C
1	B	5	C
1	B	6	A
1	B	7	U
1	B	9	A
1	B	10	A
1	B	12	A
1	B	13	U
1	B	14	G
1	B	20	C
1	B	27	G

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Mol	Chain	Res	Type
1	B	28	A
1	B	29	G
1	B	36	U
1	B	37	G
1	B	41	U
1	B	44	A
1	B	45	A
1	B	46	A
1	B	47	A
1	B	48	A
1	B	49	A
1	B	50	C
1	B	57	G
1	B	60	A
1	B	61	G
1	B	62	U
1	B	64	A
1	B	69	A
1	B	74	U
1	B	77	U
1	B	81	U
1	B	86	A
1	B	87	A
1	B	90	U
1	B	95	A
1	B	99	G
1	B	100	G
1	B	102	A
1	B	107	G
1	B	108	U
1	B	109	C
1	B	116	U

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	27	G
1	B	35	C
1	B	47	A
1	B	86	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.

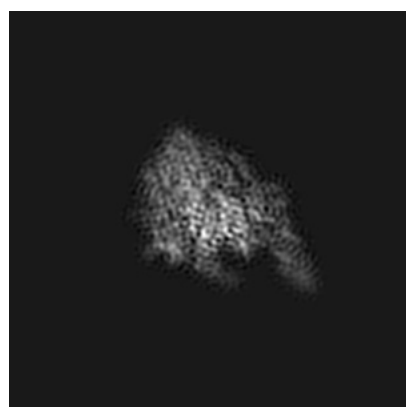
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8749. These allow visual inspection of the internal detail of the map and identification of artifacts.

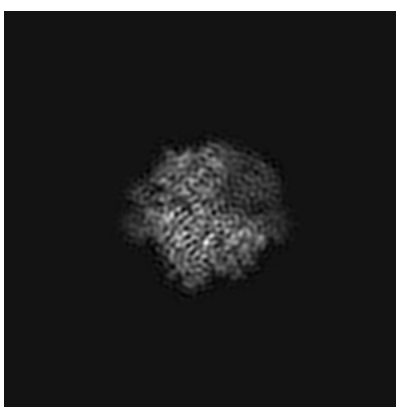
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

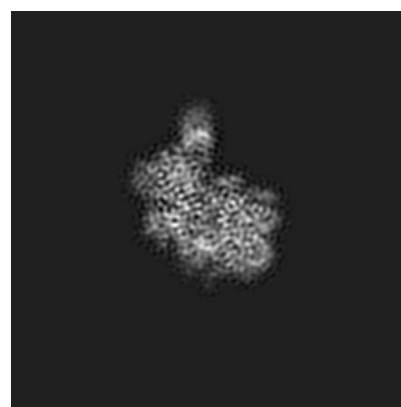
#### 6.1.1 Primary map



X



Y

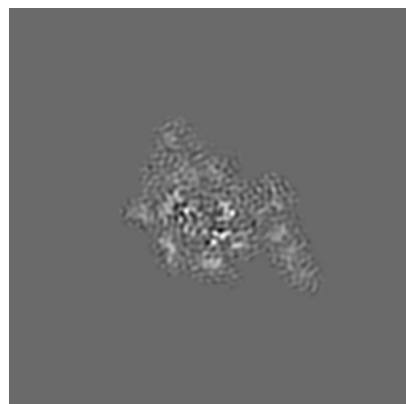


Z

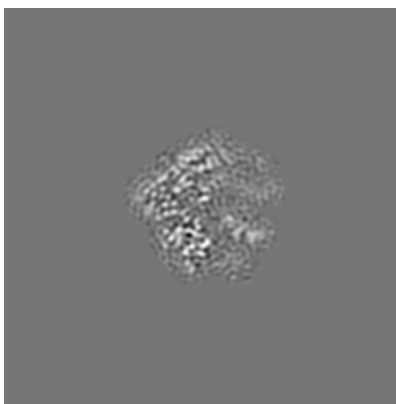
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

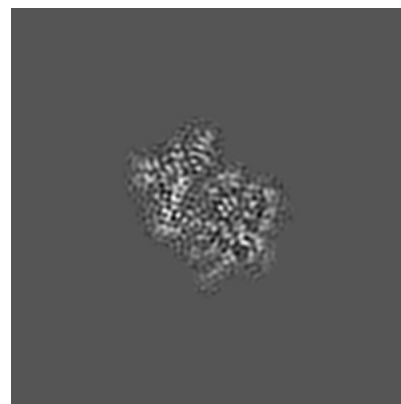
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

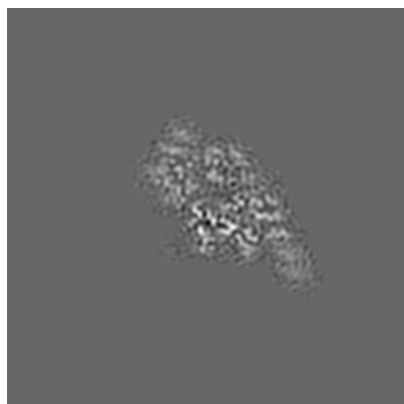


Z Index: 128

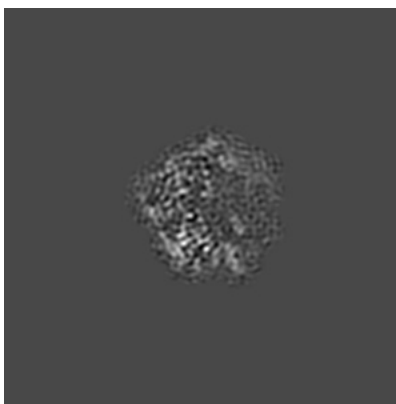
The images above show central slices of the map in three orthogonal directions.

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

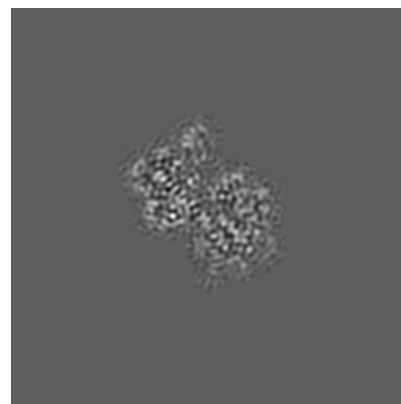
### 6.3.1 Primary map



X Index: 110



Y Index: 124



Z Index: 120

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

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

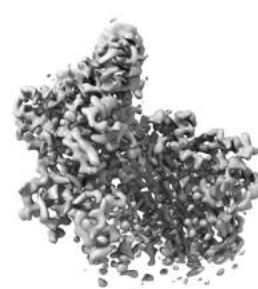
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

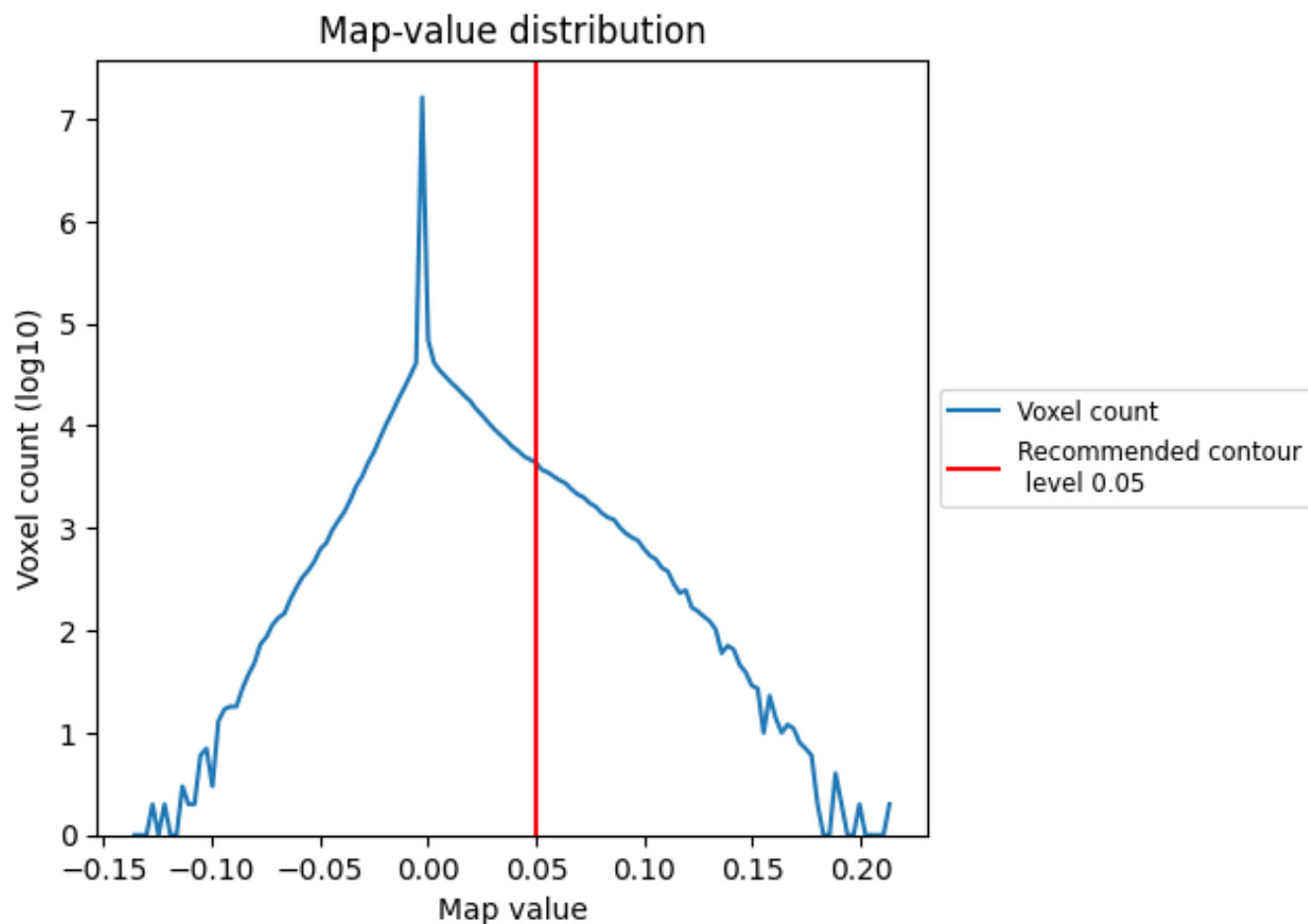
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

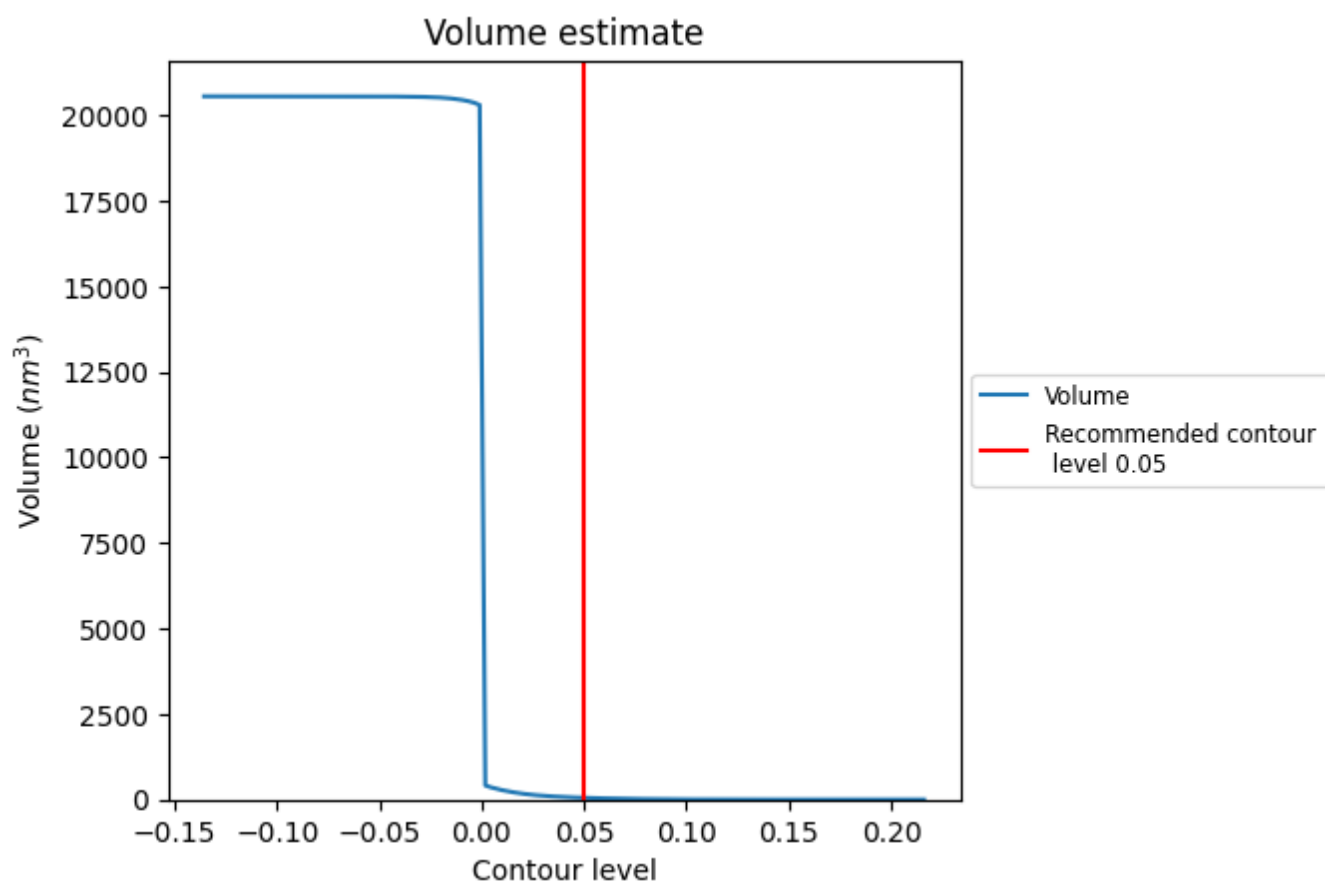
This section contains the results of statistical analysis of the map.

### 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.

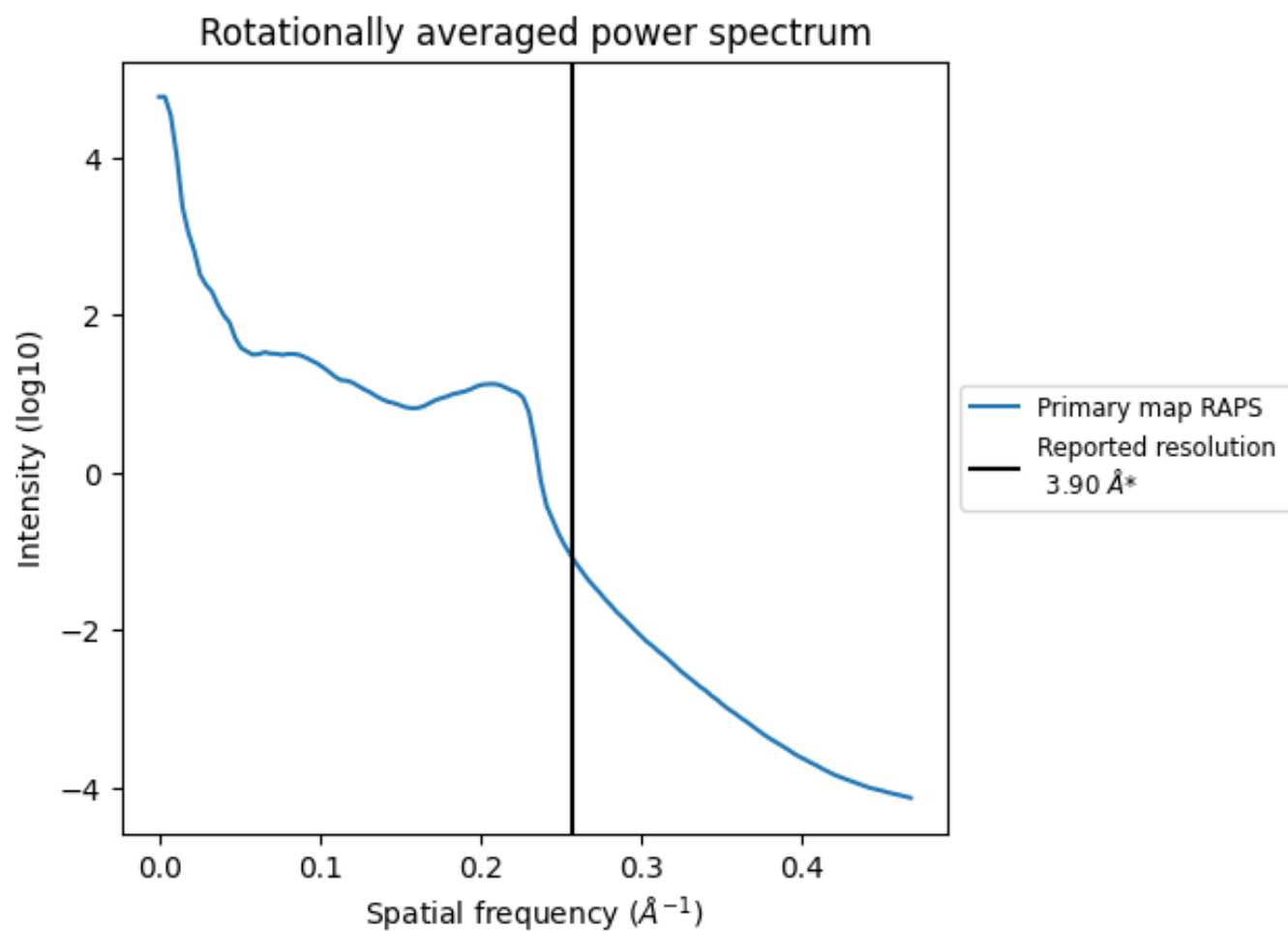
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 51 nm<sup>3</sup>; this corresponds to an approximate mass of 46 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 0.256 Å<sup>-1</sup>



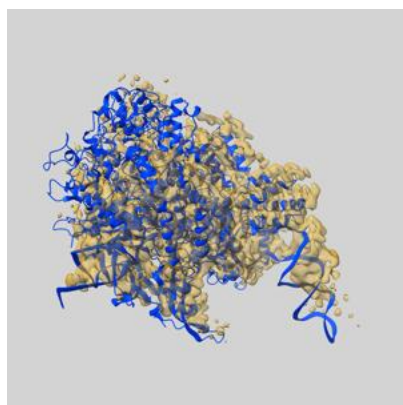
## 8 Fourier-Shell correlation

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

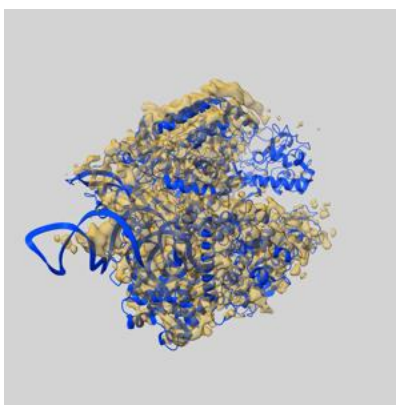
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8749 and PDB model 5VZL. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

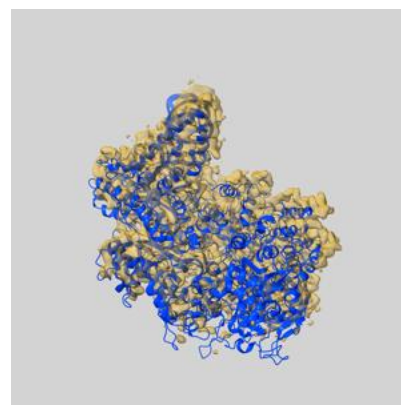
### 9.1 Map-model overlay [i](#)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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](#)



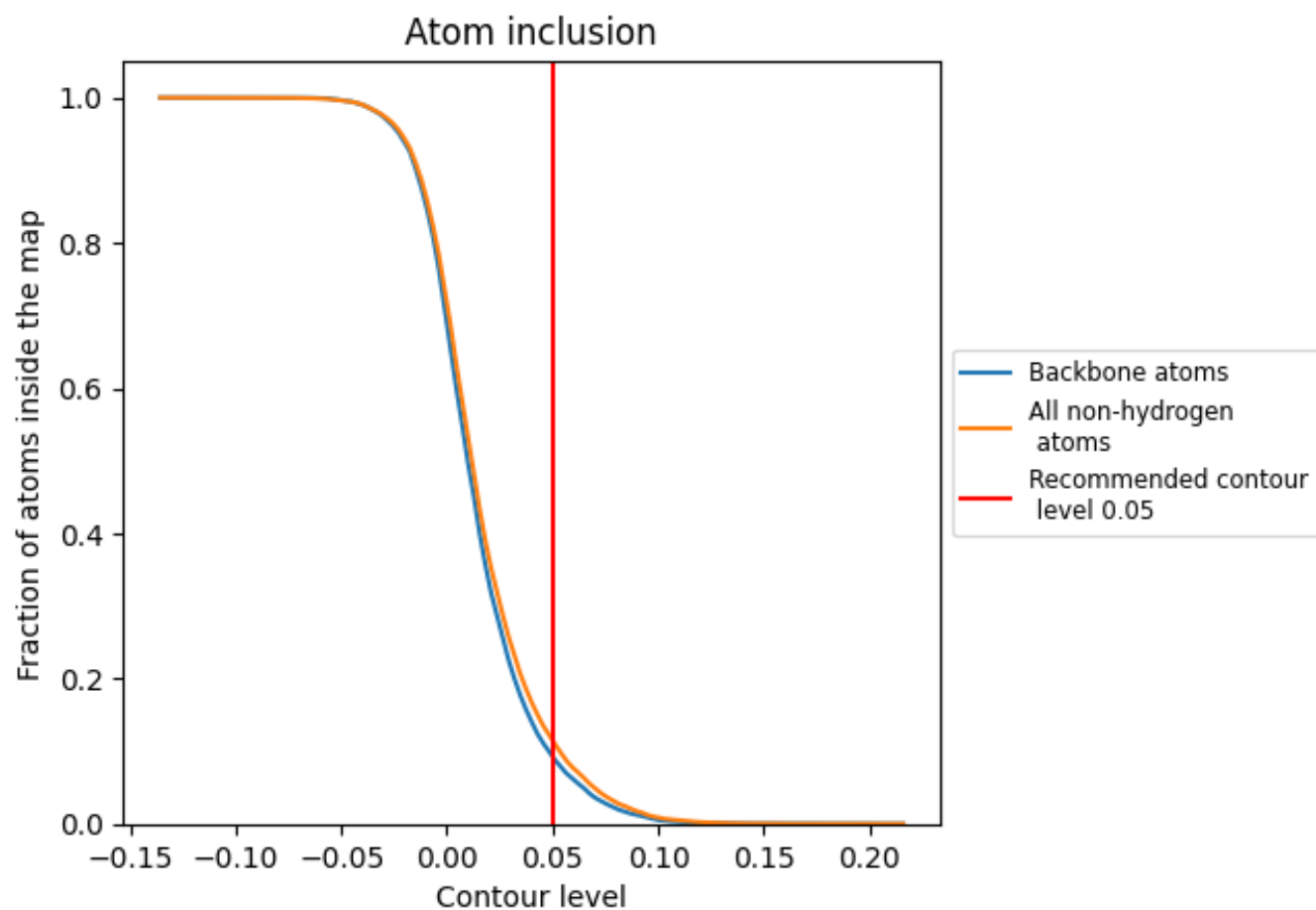
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 9% of all backbone atoms, 12% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.1151	<div></div> 0.0060
A	<div></div> 0.1082	<div></div> 0.0040
B	<div></div> 0.1403	<div></div> 0.0200
C	<div></div> 0.1284	<div></div> -0.0130

