



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 07:34 PM UTC

PDB ID : 7M7F / pdb_00007m7f
EMDB ID : EMD-23711
Title : 6-Deoxyerythronolide B synthase (DEBS) module 1 in complex with antibody fragment 1B2: State 1
Authors : Cogan, D.P.; Zhang, K.; Chiu, W.; Khosla, C.
Deposited on : 2021-03-28
Resolution : 3.20 Å(reported)

This is a wwPDB EM Validation Summary 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:

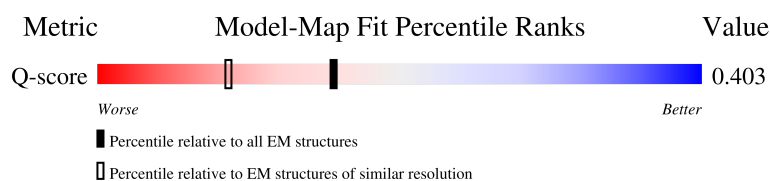
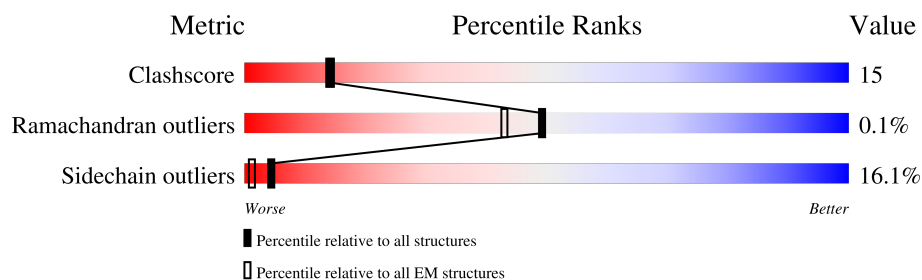
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	1784	11% 46% 26% • • 22%
1	B	1784	6% 33% 20% • 44%
2	C	249	• 44% 29% 8% • 18%
2	E	249	• 43% 31% 8% • 18%

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Mol	Chain	Length	Quality of chain
3	D	236	
3	F	236	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23971 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 EryAI,6-deoxyerythronolide-B synthase EryA3, modules 5 and 6 chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	999	Total	C	N	O	S	0	0
			7417	4613	1363	1414	27		
1	A	1390	Total	C	N	O	S	0	0
			10319	6413	1899	1972	35		

There are 106 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	expression tag	UNP Q5UNP6
B	2	ALA	-	expression tag	UNP Q5UNP6
B	3	SER	-	expression tag	UNP Q5UNP6
B	4	THR	-	expression tag	UNP Q5UNP6
B	5	ASP	-	expression tag	UNP Q5UNP6
B	6	SER	-	expression tag	UNP Q5UNP6
B	7	GLU	-	expression tag	UNP Q5UNP6
B	8	LYS	-	expression tag	UNP Q5UNP6
B	9	VAL	-	expression tag	UNP Q5UNP6
B	10	ALA	-	expression tag	UNP Q5UNP6
B	11	GLU	-	expression tag	UNP Q5UNP6
B	12	TYR	-	expression tag	UNP Q5UNP6
B	13	LEU	-	expression tag	UNP Q5UNP6
B	14	ARG	-	expression tag	UNP Q5UNP6
B	15	ARG	-	expression tag	UNP Q5UNP6
B	16	ALA	-	expression tag	UNP Q5UNP6
B	17	THR	-	expression tag	UNP Q5UNP6
B	18	LEU	-	expression tag	UNP Q5UNP6
B	19	ASP	-	expression tag	UNP Q5UNP6
B	20	LEU	-	expression tag	UNP Q5UNP6
B	21	ARG	-	expression tag	UNP Q5UNP6
B	22	ALA	-	expression tag	UNP Q5UNP6
B	23	ALA	-	expression tag	UNP Q5UNP6
B	24	ARG	-	expression tag	UNP Q5UNP6
B	25	GLN	-	expression tag	UNP Q5UNP6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	26	ARG	-	expression tag	UNP Q5UNP6
B	27	ILE	-	expression tag	UNP Q5UNP6
B	28	ARG	-	expression tag	UNP Q5UNP6
B	29	GLU	-	expression tag	UNP Q5UNP6
B	30	LEU	-	expression tag	UNP Q5UNP6
B	31	GLU	-	expression tag	UNP Q5UNP6
B	1486	THR	-	linker	UNP Q5UNP6
B	1487	SER	-	linker	UNP Q5UNP6
B	1488	GLU	-	linker	UNP Q5UNP6
B	1489	LEU	-	linker	UNP Q5UNP6
B	1490	GLY	-	linker	UNP Q5UNP6
B	1768	SER	-	expression tag	UNP Q03133
B	1769	SER	-	expression tag	UNP Q03133
B	1770	VAL	-	expression tag	UNP Q03133
B	1771	ASP	-	expression tag	UNP Q03133
B	1772	LYS	-	expression tag	UNP Q03133
B	1773	LEU	-	expression tag	UNP Q03133
B	1774	ALA	-	expression tag	UNP Q03133
B	1775	ALA	-	expression tag	UNP Q03133
B	1776	ALA	-	expression tag	UNP Q03133
B	1777	LEU	-	expression tag	UNP Q03133
B	1778	GLU	-	expression tag	UNP Q03133
B	1779	HIS	-	expression tag	UNP Q03133
B	1780	HIS	-	expression tag	UNP Q03133
B	1781	HIS	-	expression tag	UNP Q03133
B	1782	HIS	-	expression tag	UNP Q03133
B	1783	HIS	-	expression tag	UNP Q03133
B	1784	HIS	-	expression tag	UNP Q03133
A	1	MET	-	expression tag	UNP Q5UNP6
A	2	ALA	-	expression tag	UNP Q5UNP6
A	3	SER	-	expression tag	UNP Q5UNP6
A	4	THR	-	expression tag	UNP Q5UNP6
A	5	ASP	-	expression tag	UNP Q5UNP6
A	6	SER	-	expression tag	UNP Q5UNP6
A	7	GLU	-	expression tag	UNP Q5UNP6
A	8	LYS	-	expression tag	UNP Q5UNP6
A	9	VAL	-	expression tag	UNP Q5UNP6
A	10	ALA	-	expression tag	UNP Q5UNP6
A	11	GLU	-	expression tag	UNP Q5UNP6
A	12	TYR	-	expression tag	UNP Q5UNP6
A	13	LEU	-	expression tag	UNP Q5UNP6
A	14	ARG	-	expression tag	UNP Q5UNP6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ARG	-	expression tag	UNP Q5UNP6
A	16	ALA	-	expression tag	UNP Q5UNP6
A	17	THR	-	expression tag	UNP Q5UNP6
A	18	LEU	-	expression tag	UNP Q5UNP6
A	19	ASP	-	expression tag	UNP Q5UNP6
A	20	LEU	-	expression tag	UNP Q5UNP6
A	21	ARG	-	expression tag	UNP Q5UNP6
A	22	ALA	-	expression tag	UNP Q5UNP6
A	23	ALA	-	expression tag	UNP Q5UNP6
A	24	ARG	-	expression tag	UNP Q5UNP6
A	25	GLN	-	expression tag	UNP Q5UNP6
A	26	ARG	-	expression tag	UNP Q5UNP6
A	27	ILE	-	expression tag	UNP Q5UNP6
A	28	ARG	-	expression tag	UNP Q5UNP6
A	29	GLU	-	expression tag	UNP Q5UNP6
A	30	LEU	-	expression tag	UNP Q5UNP6
A	31	GLU	-	expression tag	UNP Q5UNP6
A	1486	THR	-	linker	UNP Q5UNP6
A	1487	SER	-	linker	UNP Q5UNP6
A	1488	GLU	-	linker	UNP Q5UNP6
A	1489	LEU	-	linker	UNP Q5UNP6
A	1490	GLY	-	linker	UNP Q5UNP6
A	1768	SER	-	expression tag	UNP Q03133
A	1769	SER	-	expression tag	UNP Q03133
A	1770	VAL	-	expression tag	UNP Q03133
A	1771	ASP	-	expression tag	UNP Q03133
A	1772	LYS	-	expression tag	UNP Q03133
A	1773	LEU	-	expression tag	UNP Q03133
A	1774	ALA	-	expression tag	UNP Q03133
A	1775	ALA	-	expression tag	UNP Q03133
A	1776	ALA	-	expression tag	UNP Q03133
A	1777	LEU	-	expression tag	UNP Q03133
A	1778	GLU	-	expression tag	UNP Q03133
A	1779	HIS	-	expression tag	UNP Q03133
A	1780	HIS	-	expression tag	UNP Q03133
A	1781	HIS	-	expression tag	UNP Q03133
A	1782	HIS	-	expression tag	UNP Q03133
A	1783	HIS	-	expression tag	UNP Q03133
A	1784	HIS	-	expression tag	UNP Q03133

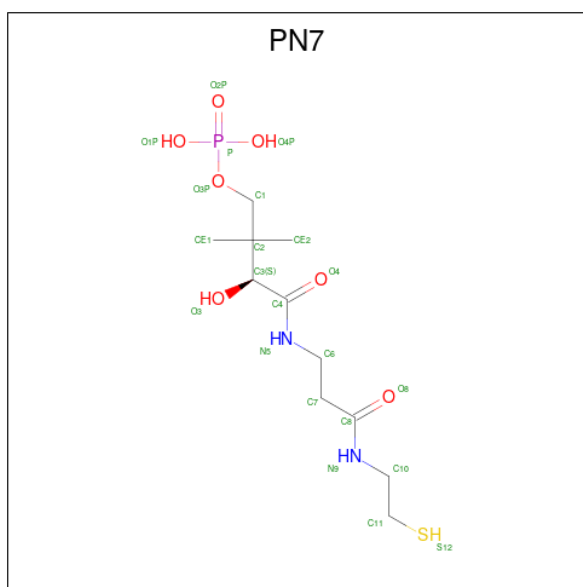
- Molecule 2 is a protein called 1B2 (heavy chain).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	205	Total	C	N	O	S	0	0
			1539	978	257	298	6		
2	E	205	Total	C	N	O	S	0	0
			1539	978	257	298	6		

- Molecule 3 is a protein called 1B2 (light chain).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	206	Total	C	N	O	S	0	0
			1568	983	262	317	6		
3	F	206	Total	C	N	O	S	0	0
			1568	984	262	316	6		

- Molecule 4 is N 3 -[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-N-(2-sulfanylet hyl)-beta-alaninamide (CCD ID: PN7) (formula: C₁₁H₂₃N₂O₇PS).

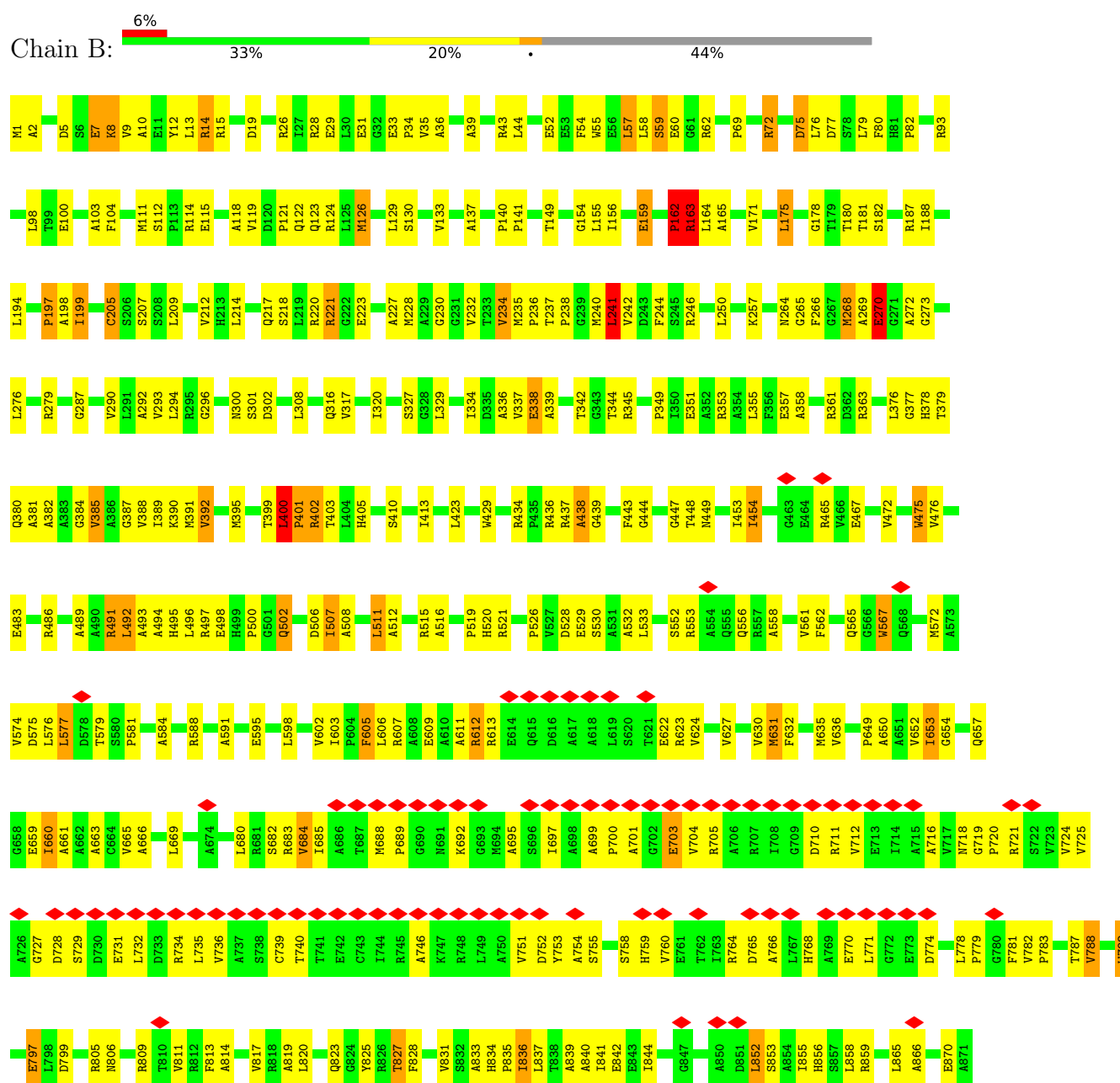


Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	S
			21	11	2	6	1	1
								0

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: EryAI,6-deoxyerythronolide-B synthase EryA3, modules 5 and 6 chimera

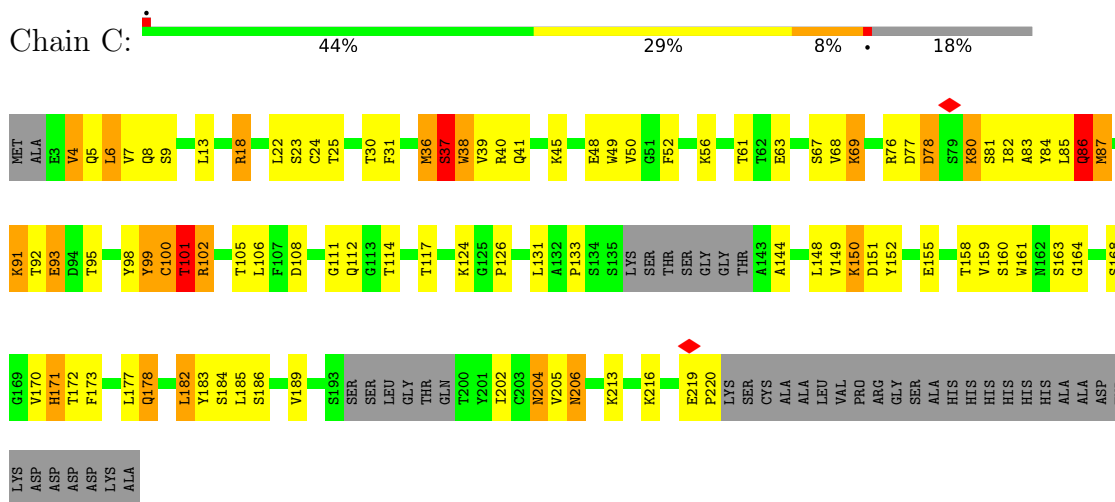




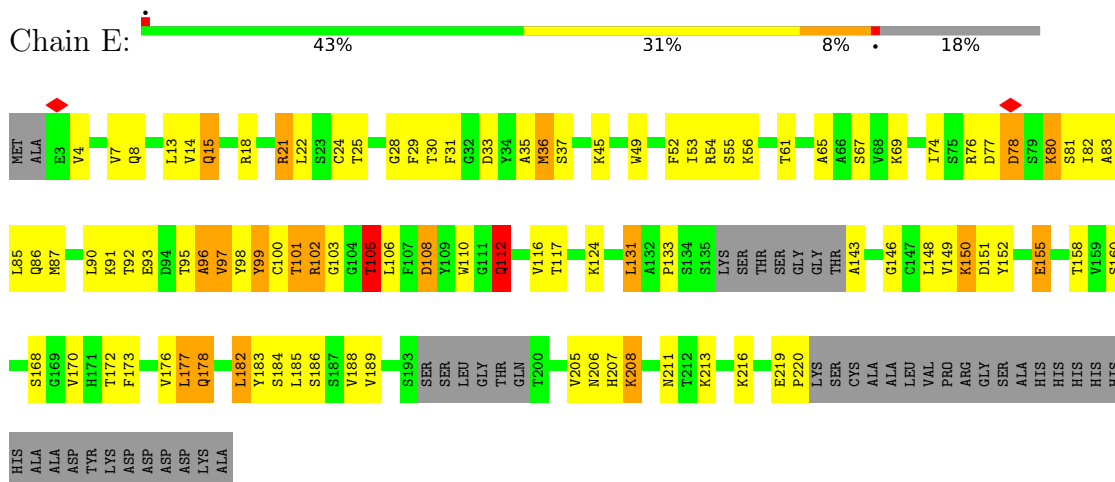
G1325	P1326	V1327	R1330	F1331	R1332	R1333	H1334	V1335	V1336	I1337	E1338	M1339	P1340	P1341	E1342	V1357	T1360	V1361	D1362	D1363	V1364	R1365	W1366	D1367	F1369	L1370	L1371	Q1376	R1377	P1378	T1379	R1380	D1383	E1384	I1385	R1389	R1390	ALA	ALA	PRO	GLN	ALA	ALA	ALA	GLU	PRO	ARG	VAL	GLY	ALA	LEU	ALA								
E1242	R1243	I1244	A1247	S1248	R1249	A1250	K1251	V1252	L1253	P1176	D1177	A1178	D1179	E1183	L1184	L1188	E1189	A1190	R1194	T1195	T1196	L1197	A1198	A1199	C1200	D1201	V1202	E1206	R1209	E1210	L1211	Q1301	R1302	S1303	S1304	D1305	G1306	L1307	P1308	A1309	T1310	A1311	V1312	A1313	W1317	A1318	G1321	M1322	A1323	E1324										
G1164	A1165	P1166	H1167	L1168	L1169	L1170	V1171	S1172	R1173	P1176	D1177	A1178	D1179	E1183	L1184	L1188	E1189	A1190	R1194	T1195	T1196	L1197	A1198	A1199	C1200	D1201	V1202	E1206	R1209	E1210	L1211	Q1301	R1302	S1303	S1304	D1305	G1306	L1307	P1308	A1309	T1310	A1311	V1312	A1313	W1317	A1318	G1321	M1322	A1323	E1324										
W1068	G1069	V1070	G1071	R1072	V1073	I1074	A1075	N1078	P1079	A1080	V1081	W1082	L1085	V1086	D1087	V1088	F1089	A1090	V1093	L1096	L1100	S1105	E1110	Q1111	Q1112	L1113	A1114	W1125	A1129	D1135	E1136	W1137	P1139	V1143	L1144	V1145	V1152	Q1155	A1157	R1158	W1159	L1160	R1163																	
G869	E870	V880	A881	V882	D883	V884	R894	R895	V896	P897	L898	P899	R905	E906	R907	V908	W909	E911	K913	P914	V915	V916	R917	R918	S919	L928	R929	Y930	R931	T932	A943	R944	L945	I944	G946	D946	G947	T948	W949	L950	A955	G956	T957	A958	D959	E960	T961	R966	L969	A972										
V976	R977	E978	L979	V980	V981	D982	L990	G998	E999	V1000	A1001	G1002	V1003	L1004	L1007	D1010	E1013	P1014	E1015	L1019	A1025	L1028	S1029	L1030	V1031	Q1032	A1033	M1034	A1037	E1038	L1039	L1043	W1044	E1048	S1049	G1054	P1055	F1056	R1060	M1061	A1062	A1063	A1066	L1067																
L798	D799	A800	G801	Y802	W803	Y804	R805	N806	L807	R808	R809	T810	V811	R812	F813	A814	D815	A816	V817	L820	A821	E822	R826	L829	E830	V831	L837	T838	A839	A840	T841	E842	E843	I844	G845	D846	G847	S848	R849	A850	D851	L852	S853	A854	I855	H856	R859	R860	G861	L865	A866	D867	F868							
R734	L735	V736	A737	S738	C739	T740	T741	E742	C743	I744	R745	A746	K747	R748	L749	A750	V751	D752	A754	S755	H756	S757	S758	H759	V760	T761	T762	I763	R764	D765	A766	L767	H768	A769	E770	L771	G772	E773	D774	F775	H776	P777	L778	P779	G780	F781	V782	P783	F784	F785	S786	W792	T793	Q794	P795	D796	E797			
D673	A674	A675	R676	A679	L680	R681	S682	R683	V684	V685	A686	T687	M688	G689	N691	K692	G693	M694	A695	S696	I697	A698	A699	F700	G701	A701	G702	E703	V704	R705	A706	R707	I708	G709	D710	R711	V712	E713	I714	A715	A716	H655	S656	W717	N718	G719	P720	R721	S722	V723	V724	V725	A726	G727	D728	S729	D730	E731	L732	D733
E601	V602	I603	P604	F605	L606	R607	A608	E609	G610	A611	R612	R613	E614	Q615	D616	A617	A618	L619	S620	T621	E622	R623	R624	D625	V626	G627	M628	P629	V630	M631	M635	L638	A639	S640	M641	W642	R643	G646	V647	E648	V652	I653	G654	H655	S656	Q657	G658	E659	I660	A666	G667	A668	D672							
L518	A522	A523	F524	P526	V527	E529	S530	A531	A532	L533	R534	V535	L536	L539	Q555	Q556	R557	A558	V561	F562	Q565	Q568	V569	A570	G571	M572	A573	V574	L576	L577	L485	Q488	L492	A493	A494	H495	R497	E498	R505	D506	S510	L511	L512	R515	L516	A517	D599	F600												
I413	I420	S421	L422	R437	A438	G439	V440	S441	S442	F443	N449	I453	I454	E455	V460	V461	E462	G463	E464	R465	V466	E467	V471	V476	L477	S478	A479	S480	L485	Q488	L492	A493	A494	H495	R497	E498	R505	D506	S510	L511	L512	R515	L516	A517																
N312	A315	Q316	V317	R318	V319	L329	G330	E331	I334	V337	E338	A339	H340	G341	T342	T344	P349	I350	A358	Y359	R363	L367	H368	L369	V372	K373	S374	N375	L376	Q380	A381	V385	V388	I389	K390	W391	V392	L393	P401	R402	W403	L404	H405	A406																
D202	T203	S207	S208	L209	R220	R221	G222	E223	S224	S225	L226	A227	M228	V232	T233	V234	M235	P236	M240	L241	V242	D243	F244	M247	L260	D253	G254	R255	G265	F266	M268	A269	E270	G271	A272	L276	L277	E278	V283	D302	S305	W306	G307	L308	P311															

ASN	SER	SER	GLY	PRO	PRO	GLN	SER	ARG	SER
SER	SER	GLY	LEU	ARG	GLN	GLY	ASP	LEU	PRO
SER	PRO	GLY	THR	PRO	PRO	PRO	PHE	PRO	ALA
VAL	VAL	VAL	LEU	VAL	TYR	TYR	GLU	THR	THR
ASP	ASP	LEU	LEU	LEU	GLU	GLU	HIS	THR	GLU
LYS	VAL	VAL	VAL	ILE	GLY	GLY	PHE	VAL	ARG
LEU	SER	SER	ASP	ASP	GLY	GLY	ASP	PHE	GLU
ALA	ALA	ALA	ALA	VAL	GLU	GLU	GLY	ASP	LYS
ALA	ALA	GLY	GLY	TYR	PRO	PRO	SER	HIS	LEU
ALA	GLU	GLU	GLU	PRO	PRO	PRO	GLY	ASP	ASP
LEU	LEU	PRO	PRO	PRO	SER	SER	PHE	VAL	GLU
GLU	GLU	GLY	GLY	GLY	SER	SER	GLY	ARG	VAL
HIS	HIS	HIS	HIS	HIS	GLN	GLN	LEU	THR	LEU
HIS	HIS	TRP	TRP	ASP	ALA	ALA	LEU	LEU	SER
HIS	ASP	PRO	PRO	ALA	VAL	VAL	VAL	ALA	HIS
HIS	ASP	ASN	MET	MET	ALA	ALA	ASP	HIS	ALA
	SER	SER	ALA	ALA	ALA	ALA	MET	LEU	ALA
	TRP	TRP	LEU	VAL	GLN	GLN	ASP	THR	ALA
	PRO	LYS	GLY	GLY	ASP	ASP	GLY	GLU	VAL
	THR	THR	THR	GLU	ASP	ASP	GLY	LEU	GLY
	PRO	THR	TRP	LEU	ALA	ALA	GLY	GLY	HIS
	THR	PHE	THR	THR	ILE	ILE	VAL	THR	ALA
	GLU	GLY	GLU	THR	ARG	ARG	THR	THR	ALA
	HIS	HIS	LEU	THR	THR	GLN	VAL	PRO	GLU
	ASP	THR	ASP	PHE	GLN	GLY	CYS	ALA	ARG
	THR	VAL	ARG	ARG	ASP	ASP	PRO	GLU	VAL
	ALA	ALA	GLU	GLY	LYS	LYS	ALA	ALA	ALA
	VAL	VAL	VAL	THR	PRO	PRO	GLY	SER	ASP
	PRO	PRO	VAL	VAL	PHE	PHE	THR	SER	GLN
	GLY	GLY	ARG	VAL	VAL	ALA	ALA	ALA	ALA
	ASP	ASP	MET	MET	VAL	VAL	ALA	LEU	PHE
	HIS	PHE	ASP	ASP	ALA	ALA	ILE	ARG	ALA
	THR	THR	THR	THR	HIS	HIS	GLY	ASP	GLU
	MET	MET	THR	THR	ASP	ASP	GLY	THR	LEU
	VAL	VAL	VAL	LEU	ALA	ALA	PRO	ARG	VAL
	GLN	GLU	GLU	THR	GLY	GLY	HIS	GLN	ASP
	GLU	HIS	GLY	ALA	ALA	ALA	PHE	ALA	SER
	ALA	ALA	LEU	LEU	MET	MET	ARG	VAL	GLY
	ASP	ALA	ALA	TYR	TYR	ALA	LEU	SER	ALA
	ILE	ILE	ASP	ASP	ALA	ALA	GLY	GLY	LEU
	ARG	ARG	ARG	LEU	ALA	LEU	ARG	ARG	GLU
	HIS	HIS	THR	THR	THR	THR	ARG	SER	ASN
	ILE	ILE	THR	GLY	GLY	GLY	GLY	TYR	LEU
	ASP	ASP	GLN	GLN	LEU	LEU	ILE	LEU	GLY
	ALA	ALA	TRP	TRP	LEU	LEU	ASP	ASP	GLY
	TRP	TRP	LEU	ARG	ASP	ASP	PRO	LEU	ALA
	LEU	LEU	GLY	ARG	GLY	GLY	VAL	LEU	ALA
	GLY	GLY	GLY	ARG	HIS	ARG	ALA	THR	GLY
	GLY	GLY	THR	THR	PRO	PRO	ALA	LEU	VAL

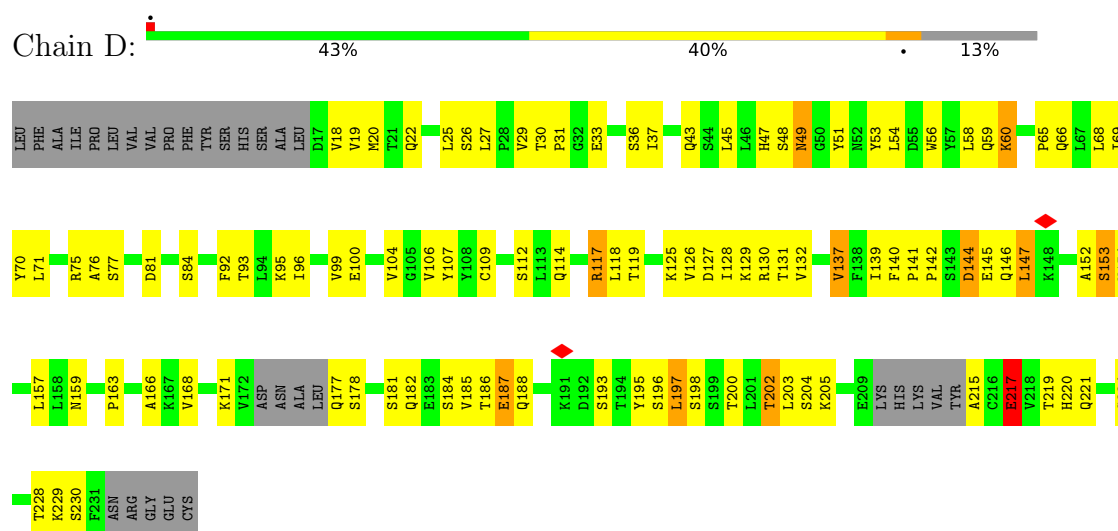
- Molecule 2: 1B2 (heavy chain)



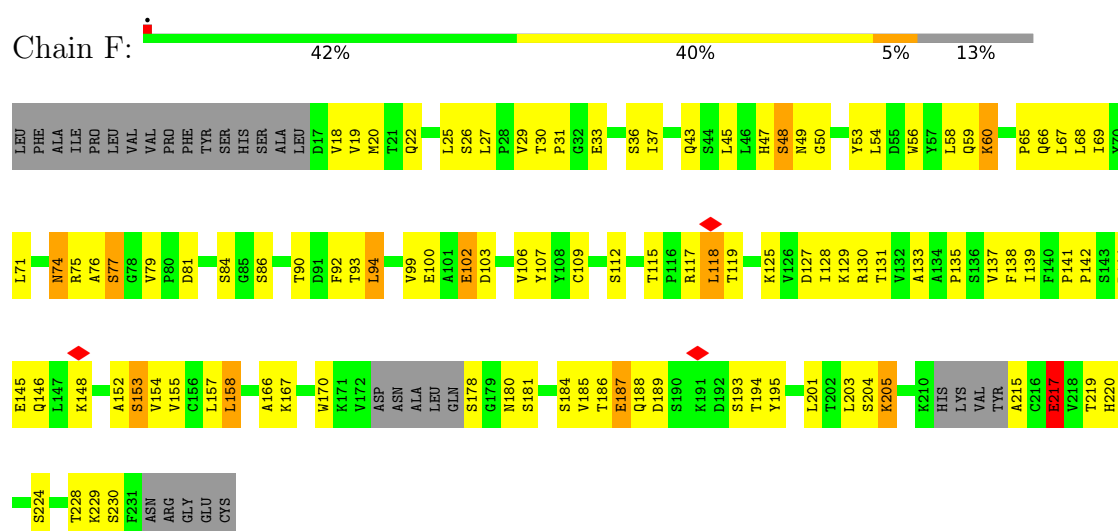
- Molecule 2: 1B2 (heavy chain)



- Molecule 3: 1B2 (light chain)



- Molecule 3: 1B2 (light chain)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	172352	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	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	7.734	Depositor
Minimum map value	-4.602	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.138	Depositor
Recommended contour level	0.53	Depositor
Map size (Å)	336.0, 336.0, 336.0	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PN7

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	0.94	64/10522 (0.6%)	1.20	101/14323 (0.7%)
1	B	0.93	50/7566 (0.7%)	1.18	84/10293 (0.8%)
2	C	0.86	9/1575 (0.6%)	1.12	12/2141 (0.6%)
2	E	0.81	5/1575 (0.3%)	1.18	10/2141 (0.5%)
3	D	0.58	0/1601	0.97	7/2175 (0.3%)
3	F	0.70	5/1601 (0.3%)	1.05	12/2174 (0.6%)
All	All	0.89	133/24440 (0.5%)	1.17	226/33247 (0.7%)

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
1	A	0	1
2	C	0	1
2	E	0	3
3	F	0	1
All	All	0	6

The worst 5 of 133 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	442	SER	CA-CB	-14.41	1.30	1.53
1	A	43	ARG	C-O	-14.33	1.07	1.24
1	A	207	SER	CA-CB	-14.15	1.28	1.53
1	B	197	PRO	C-O	-13.30	1.06	1.24
1	B	908	VAL	C-O	-12.62	1.08	1.23

The worst 5 of 226 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	PRO	N-CA-CB	-23.65	83.45	103.32
1	A	159	GLU	CB-CA-C	-19.80	78.12	110.19
1	B	883	ASP	CB-CA-C	-18.93	78.51	109.75
1	B	266	PHE	CA-CB-CG	17.75	131.55	113.80
1	A	43	ARG	CB-CA-C	-17.11	83.20	110.74

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1301	GLN	Mainchain
2	C	155	GLU	Peptide
2	E	155	GLU	Peptide
2	E	21	ARG	Sidechain
2	E	96	ALA	Mainchain

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	10319	0	10164	317	0
1	B	7417	0	7306	220	0
2	C	1539	0	1511	61	0
2	E	1539	0	1511	62	0
3	D	1568	0	1528	55	0
3	F	1568	0	1533	62	0
4	B	21	0	22	2	0
All	All	23971	0	23575	736	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 15.

The worst 5 of 736 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:777:PRO:HB3	1:A:796:ASP:HA	1.54	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:86:GLN:HA	2:C:86:GLN:HE21	1.38	0.87
2:E:108:ASP:CG	3:F:67:LEU:CD2	2.60	0.75
2:E:108:ASP:CG	3:F:67:LEU:HD23	2.11	0.75
1:B:567:TRP:HB3	1:B:834:HIS:HB3	1.68	0.74

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	1388/1784 (78%)	1264 (91%)	123 (9%)	1 (0%)	48	79
1	B	995/1784 (56%)	915 (92%)	78 (8%)	2 (0%)	43	73
2	C	199/249 (80%)	179 (90%)	20 (10%)	0	100	100
2	E	199/249 (80%)	176 (88%)	23 (12%)	0	100	100
3	D	200/236 (85%)	184 (92%)	16 (8%)	0	100	100
3	F	200/236 (85%)	187 (94%)	13 (6%)	0	100	100
All	All	3181/4538 (70%)	2905 (91%)	273 (9%)	3 (0%)	49	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1449	SER
1	B	720	PRO
1	A	779	PRO

5.3.2 Protein sidechains [i](#)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1028/1325 (78%)	873 (85%)	155 (15%)	3	14
1	B	746/1325 (56%)	651 (87%)	95 (13%)	4	20
2	C	170/203 (84%)	133 (78%)	37 (22%)	1	6
2	E	170/203 (84%)	135 (79%)	35 (21%)	1	7
3	D	182/208 (88%)	143 (79%)	39 (21%)	1	6
3	F	182/208 (88%)	145 (80%)	37 (20%)	1	7
All	All	2478/3472 (71%)	2080 (84%)	398 (16%)	4	13

5 of 398 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1307	LEU
2	C	219	GLU
1	A	1357	VAL
2	C	69	LYS
3	D	96	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	52	ASN
3	F	52	ASN
3	D	111	GLN
3	D	188	GLN
3	F	111	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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
4	PN7	B	1801	1	14,20,21	2.13	4 (28%)	18,26,29	1.42	5 (27%)

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
4	PN7	B	1801	1	-	12/24/26/27	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1801	PN7	C8-N9	4.99	1.45	1.33
4	B	1801	PN7	C4-N5	4.97	1.45	1.33
4	B	1801	PN7	O4-C4	-2.36	1.18	1.23
4	B	1801	PN7	O8-C8	-2.15	1.19	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1801	PN7	C6-C7-C8	2.43	116.44	112.39
4	B	1801	PN7	C6-N5-C4	-2.25	118.50	122.55
4	B	1801	PN7	CE2-C2-C3	2.20	112.52	108.77
4	B	1801	PN7	C11-C10-N9	-2.04	107.68	112.31
4	B	1801	PN7	C3-C4-N5	2.03	120.34	116.48

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

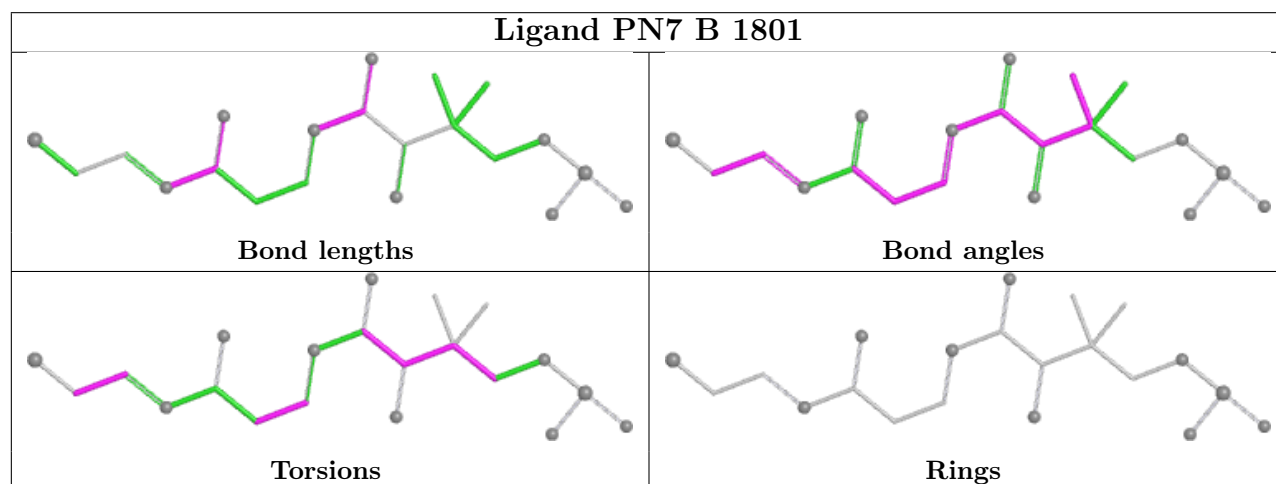
Mol	Chain	Res	Type	Atoms
4	B	1801	PN7	C1-C2-C3-O3
4	B	1801	PN7	C1-C2-C3-C4
4	B	1801	PN7	CE1-C2-C3-O3
4	B	1801	PN7	CE1-C2-C3-C4
4	B	1801	PN7	CE2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1801	PN7	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

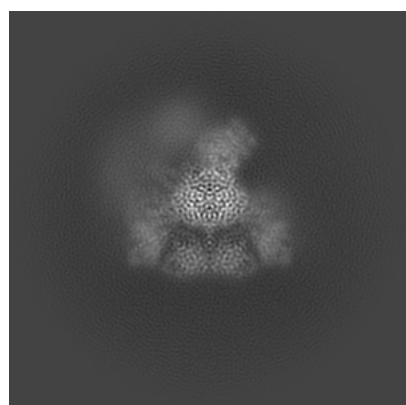
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23711. These allow visual inspection of the internal detail of the map and identification of artifacts.

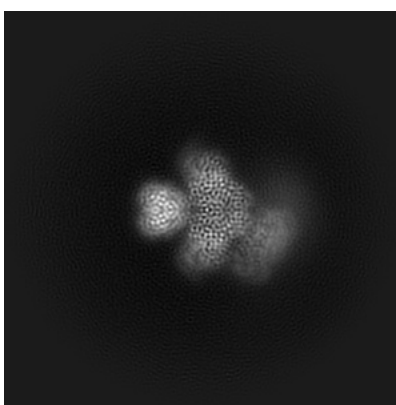
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

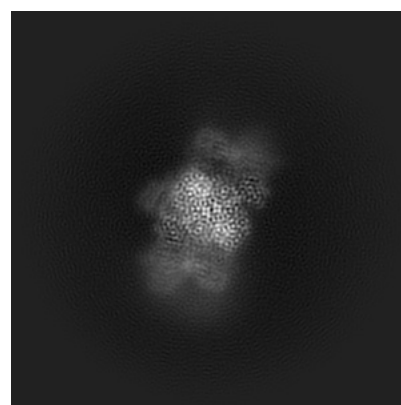
6.1.1 Primary map



X



Y

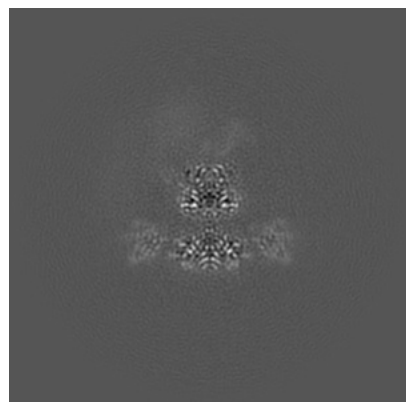


Z

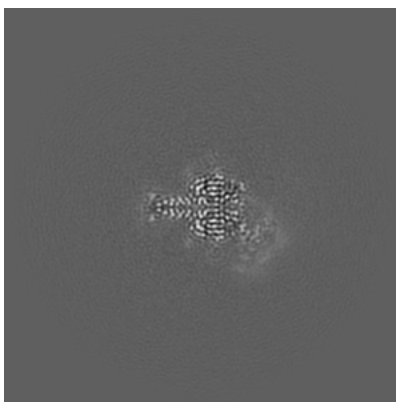
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

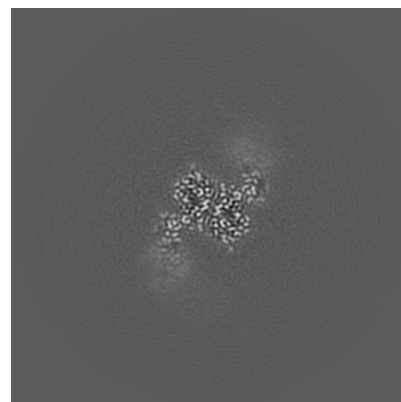
6.2.1 Primary map



X Index: 168



Y Index: 168

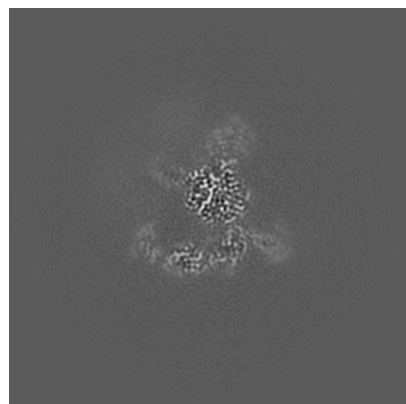


Z Index: 168

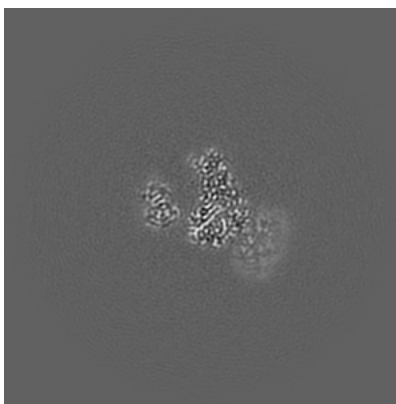
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

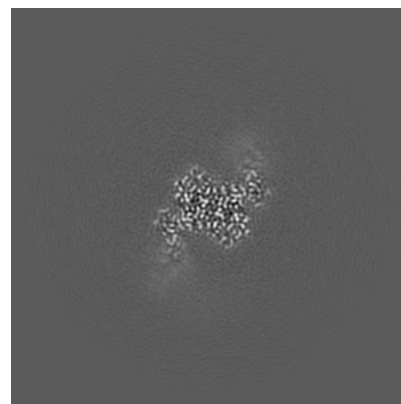
6.3.1 Primary map



X Index: 157



Y Index: 181

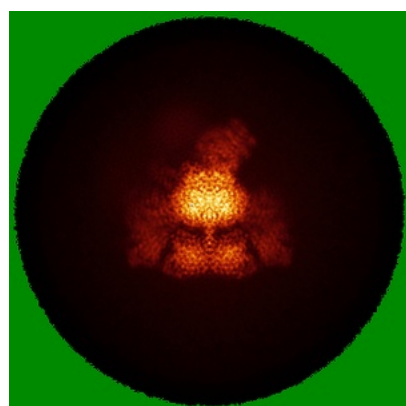


Z Index: 173

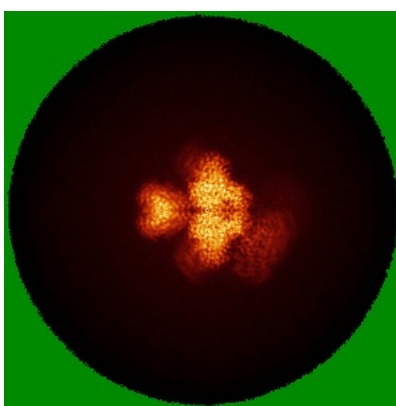
The images above show the largest variance slices of the map in three orthogonal directions.

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

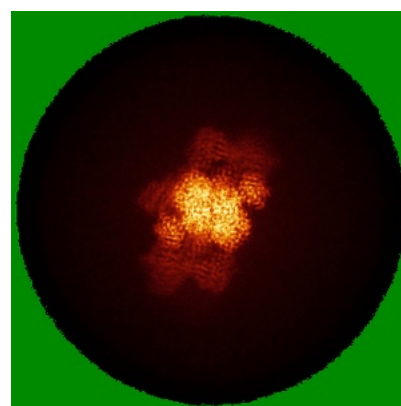
6.4.1 Primary map



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



The images above show the 3D surface view of the map at the recommended contour level 0.53. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

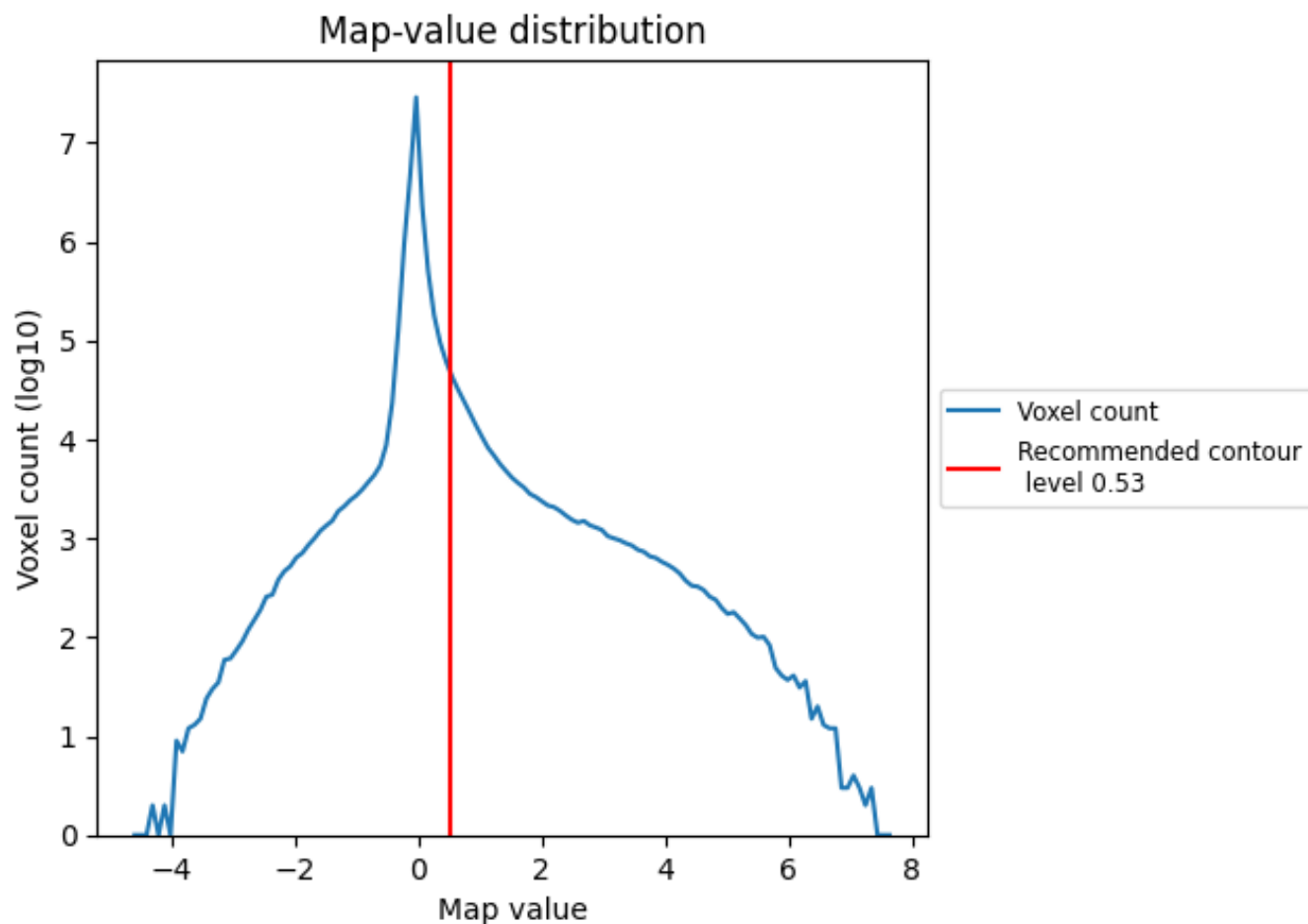
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

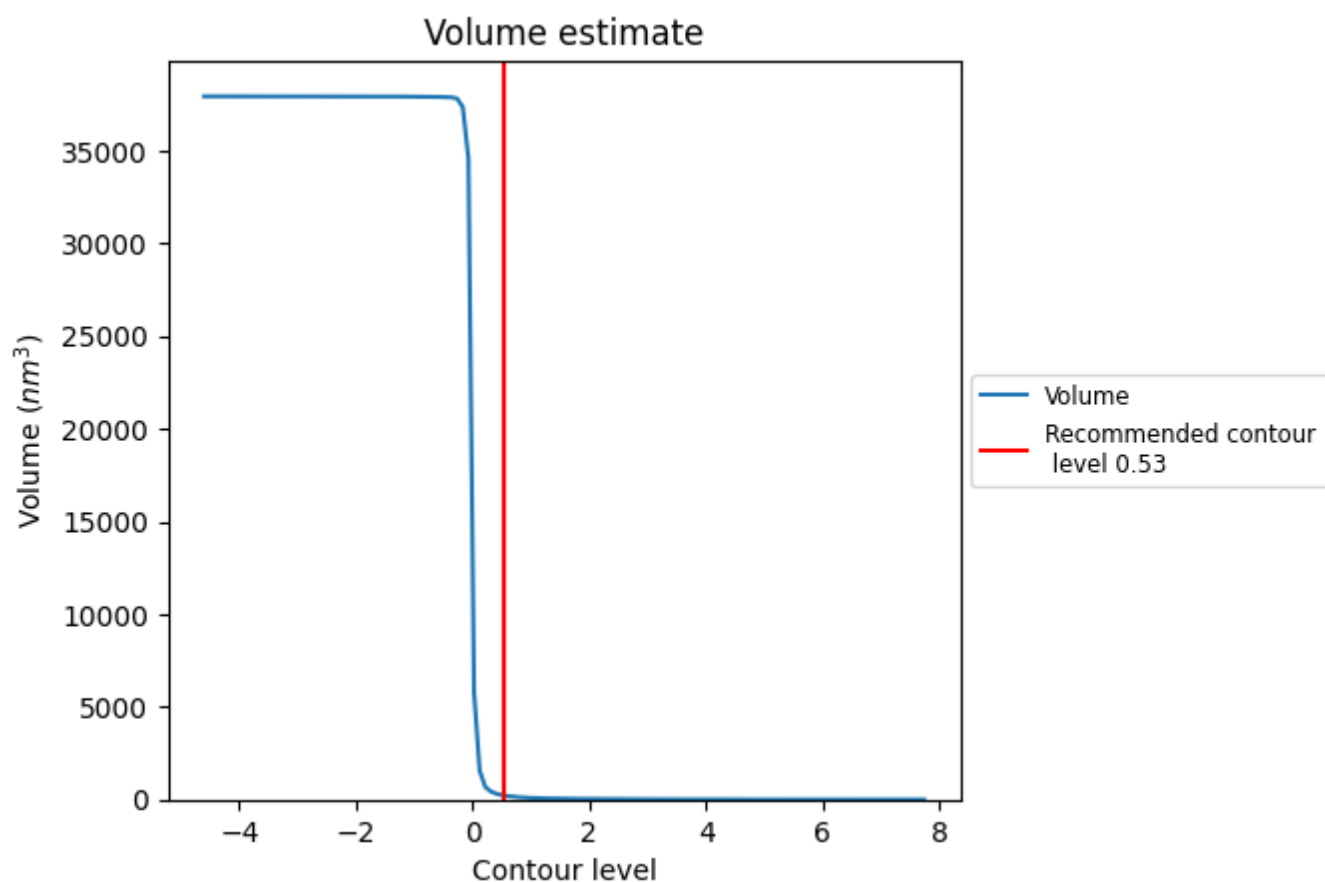
This section contains the results of statistical analysis of the map.

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.

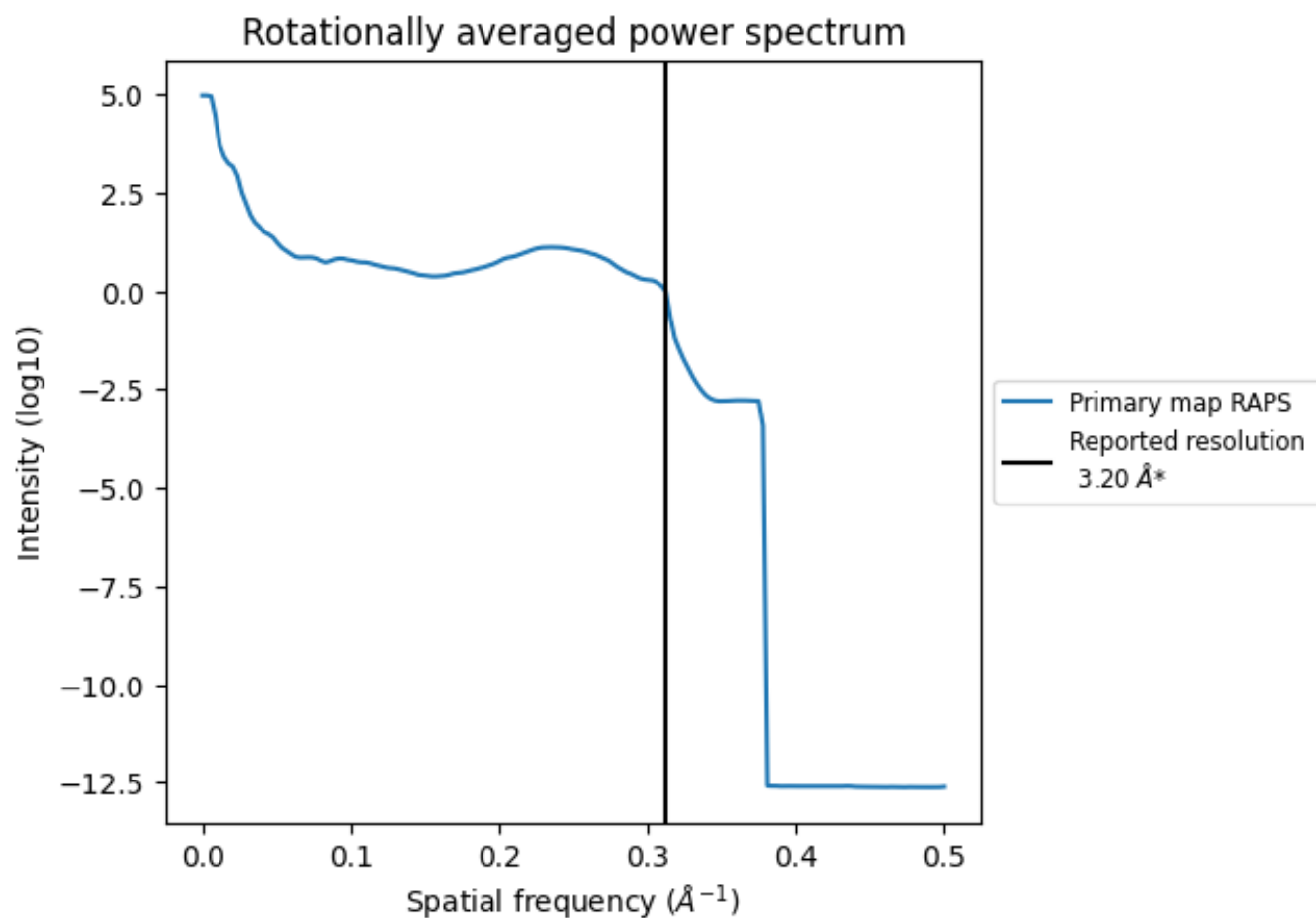
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 226 nm³; this corresponds to an approximate mass of 204 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 0.312 Å⁻¹

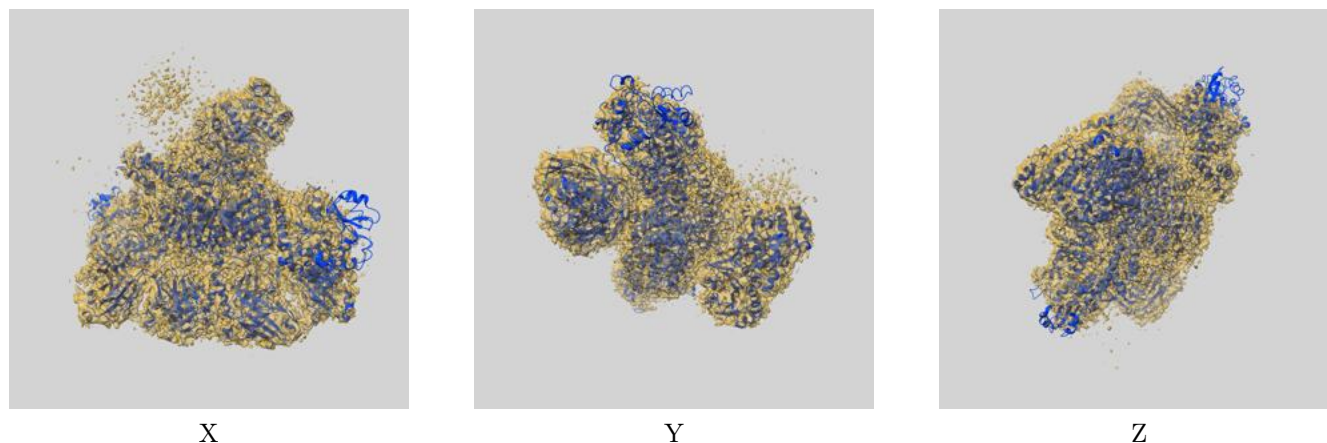
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

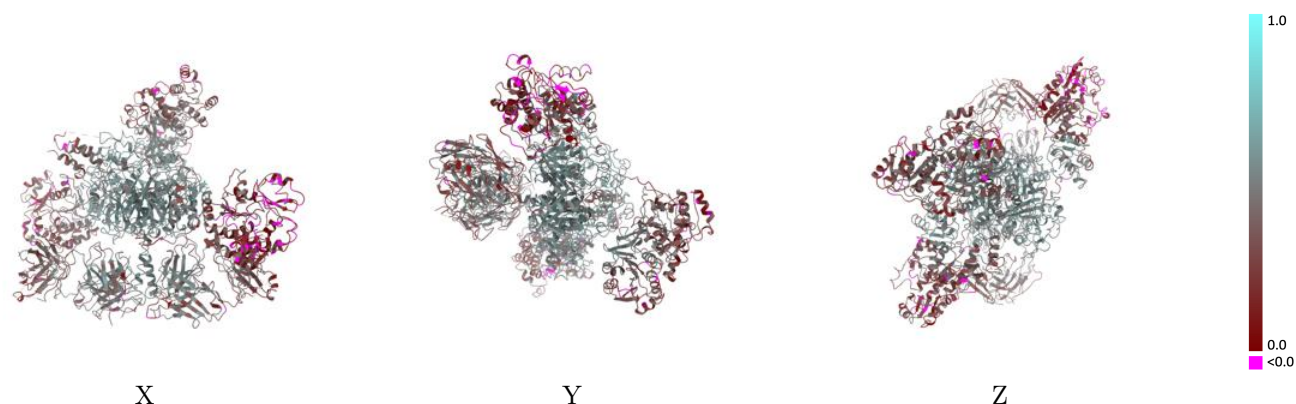
This section contains information regarding the fit between EMDB map EMD-23711 and PDB model 7M7F. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.53 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](#)

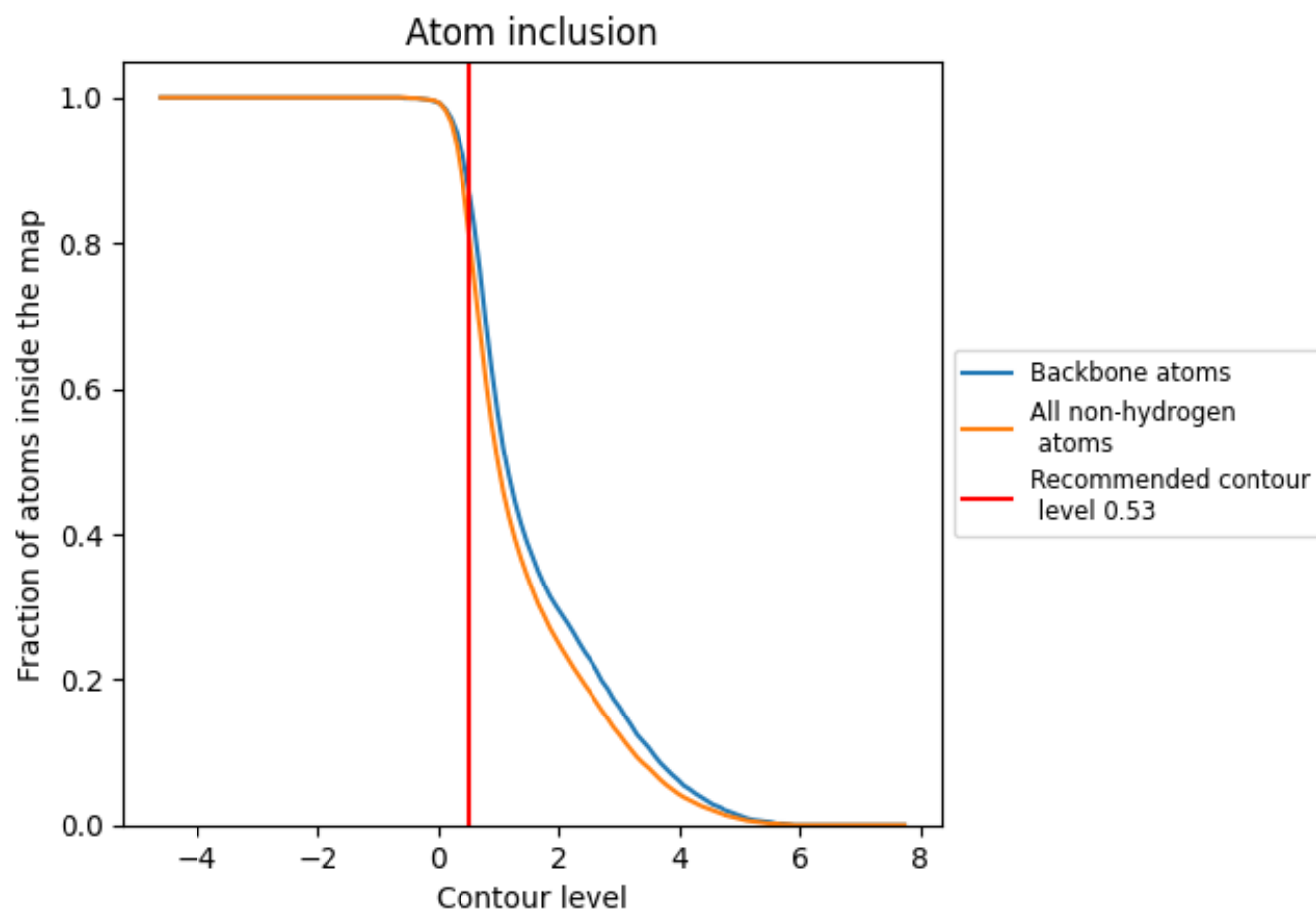


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 80% 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 (0.53) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8030	0.4030
A	0.7710	0.3800
B	0.8070	0.4320
C	0.8310	0.3850
D	0.8630	0.4110
E	0.8640	0.4200
F	0.8520	0.4070

1.0

0.0

<0.0