



Full wwPDB EM Validation Report ⓘ

Sep 28, 2026 – 12:39 PM EDT

PDB ID : 11IM / pdb_000011im
EMDB ID : EMD-75718
Title : Focused Cryo-EM map of a half-region of the human ZNFX1 tetramer
Authors : Wang, F.; He, Q.; Li, H.
Deposited on : 2026-02-25
Resolution : 3.71 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.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.2
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) : 2.51

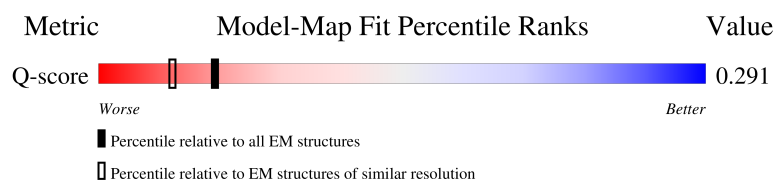
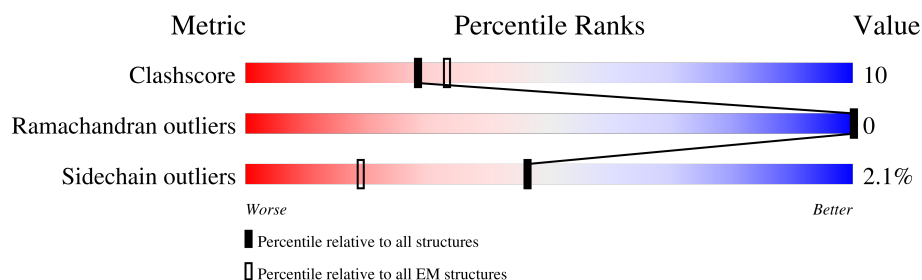
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.71 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	10534 (3.21 - 4.21)

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	1918	10% 53% 14% 33%
1	B	1918	19% 50% 16% 33%
1	C	1918	7% 6% 91%

2 Entry composition [i](#)

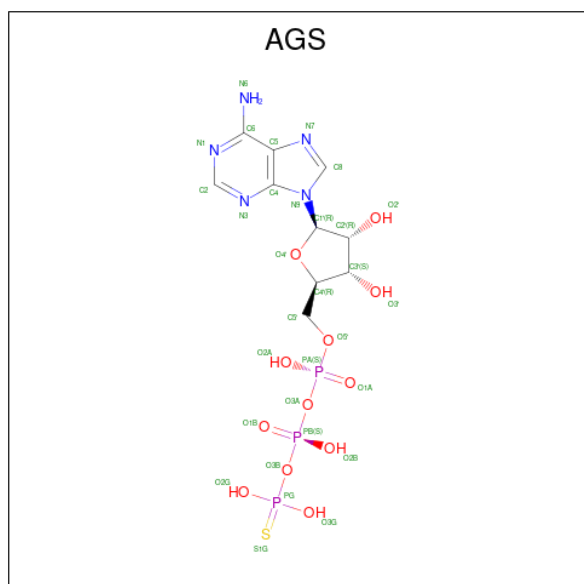
There are 2 unique types of molecules in this entry. The entry contains 22020 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NFX1-type zinc finger-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1282	Total	C	N	O	S	0	0
			10307	6503	1814	1909	81		
1	B	1282	Total	C	N	O	S	0	0
			10307	6503	1814	1909	81		
1	C	172	Total	C	N	O	S	0	0
			1344	855	226	256	7		

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).

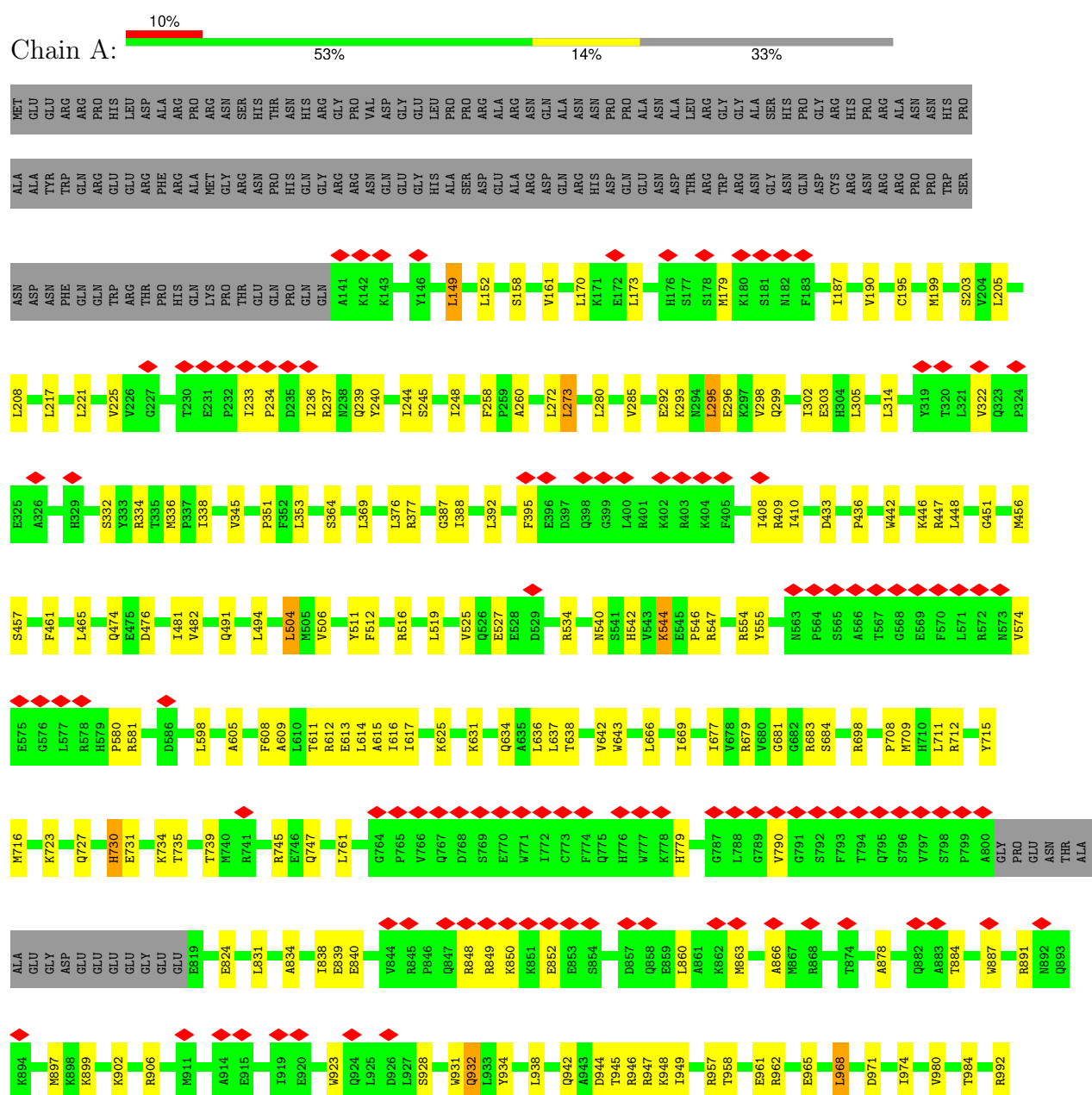


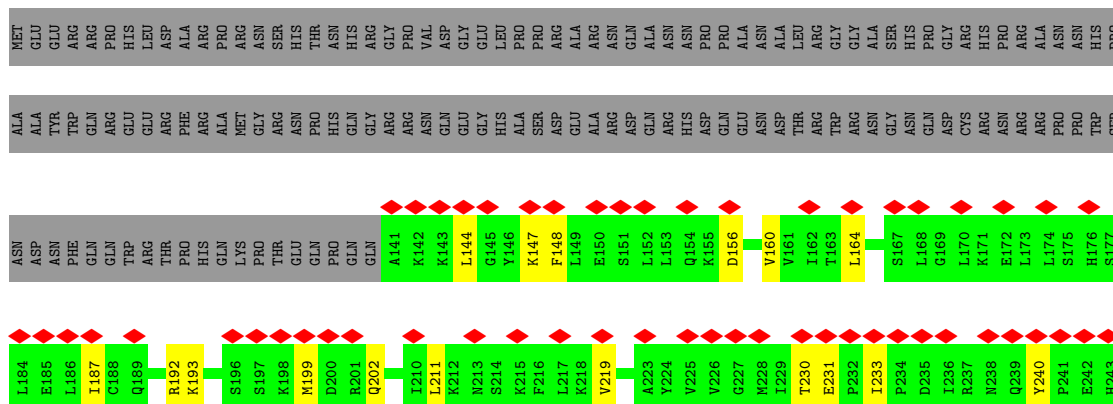
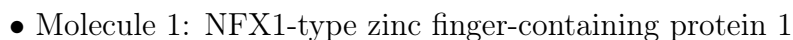
Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

3 Residue-property plots [i](#)

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

- Molecule 1: NFX1-type zinc finger-containing protein 1





CYS	R1354	G1227	M1228	C1372	M130	V1005	L908	E838	V766	R701	I616	V543	I410	Y319	L254
PRO					Q1131	E1006	N909	E839	Q767	E702	P620	Y548	Y411	T320	V255
GLY					H1132	A1008	T910	E840	D768	F703	P621	L549	I416	L321	S256
SER					E1133	A1009	M911	E841	S769	R704	G622	L550	I417	V322	P259
HIS					A1134	L1020	T912	E842	E770	L707	G623	M551	I418	Q323	A260
SER					V1138	V843	A913	V844	W771	W708	G624	R554	M420	P324	
CYS					E1139	V844	A914	V845	W709	W709	Y627	R554	C421	E325	E265
PHE					L1140	V845	E915	V846	L710	L711	V628	F557	S422	A326	T266
ARG					Y1143	P846	A916	Q847	L712	R713	K631	L560	S423	S267	M268
ARG					F1144	Q847	A918	R848	R714	I632	Y633	I561	I426	H329	L269
HIS					L1145	R848	E918	R849	W715	W716	Q634	E562	Y428	V330	V270
GLU					Q1146	R849	I919	R850	Y717	Y717	A635	N563	K429	E331	S271
ARG					Q1147	R850	E920	R851	K778	M719	L636	P564	K435	S332	L272
CYS					E1148	R851	Q924	R852	W779	T720	S641	S565	K438	Y333	L273
GLN					Y1149	R852	Q925	E953	L783	W721	E784	A566	I338	R334	P274
GLN					L1150	E954	L925	E953	W785	Q722	W785	T567		I338	T275
PRO					P1151	E955	D926	E956	L786	K723	I645	G568	N444	L347	S276
CYS					S1152	E956	D926	E957	L787	E724	S646	E569	K446	D348	N278
ARG					Q1153	E957	Q932	E958	G787	S725	L647	F570	K445	A279	L280
ARG					L1157	E958	Q932	E959	L788	E726	Q648	L571	C455	R281	R281
LEU					T1158	E959	Q933	E960	G789	H730	K649	L572	M456	R282	A282
LEU					Q1163	E960	Q934	E961	W790	E731	R650	N573	S457	F351	L277
ILE					L1167	E961	Q935	E962	G791	K734	V654	V574	F461	L353	
SER					L1167	E962	Q936	E963	G792	K735	V655	E575	L465	I357	S283
HIS					Q1168	E963	Q937	E964	W793	L736	V655	E576	L465	G360	Q284
GLN					L1168	E964	Q938	E965	G794	E737	H660	L577	L477	D286	V285
GLU					Q1168	E965	Q939	E966	W795	C738	G668	L578	I481	I287	L287
PRO					G1178	E966	Q940	E967	W796	T739	I669	P580	E488	E288	E290
PRO					V1181	E967	Q941	E968	W797	M740	Y670	R581	Q491	E378	T291
GLY					Q1188	E968	Q942	E969	W798	K741	N671	N582	Q492	D379	E292
CYS					Q1188	E969	Q943	E970	W799	G742	N671	N583	Q492	F380	K293
ARG					L1195	E970	Q944	E971	W800	G743	K674	V584	A495	V381	N294
THR					S1198	E971	Q945	E972	W801	L745	V678	L585	A496	L384	L295
GLN					L1199	E972	Q946	E973	W802	E746	R679	D586	E496	R385	E296
ASN					V1200	E973	Q947	E974	W803	Y748	V680	P587		K297	K297
ARG					M1203	E974	Q948	E975	W804	L749	G681	G588	D501	V298	V298
CYS					Q1204	E975	Q949	E976	W805	K751	S884	Q589	S502	Q299	Q299
CYS					E1205	E976	Q950	E977	W806	K752	S884	W590	F503	T300	T300
VAL					G1206	E977	Q951	E978	W807	Y753	E687	P591	L504	I302	I302
HIS					K1207	E978	Q952	E979	W808	L754	I688	S592	M505	E303	E303
SER					L1213	E979	Q953	E980	W809	S754	I688	K593	V506	H304	H304
GLN					S1214	E980	Q954	E981	W810	P755	I688	E594	T508	L305	L305
CYS					M1215	E981	Q955	E982	W811	K757	K690	E594	T508	K308	K308
CYS					A1224	E982	Q956	E983	W812	W758	T693	A595	R516	R309	R309
GLY					K1225	E983	Q957	E984	W813	E759	L694	L598	H517	R310	R310
					K1226	E984	Q958	E985	W814	S760	R695	D599	L522	R401	R401
						E985	Q959	E986	W815	L761	E696	D600		K402	K402
						E986	Q960	E987	W816	L697	R697	S601		R403	R403
						E987	Q961	E988	W817	M762	R698	Q602		K404	K404
						E988	Q962	E989	W818	G763	M699	M603		D407	D407
						E989	Q963	E990	W819	G764	P765	A609		I408	I408
						E990	Q964	E991	W820	P765		L610		D317	D317
						E991	Q965	E992	W821			R612		T318	T318
						E992	Q966	E993	W822						
						E993	Q967	E994	W823						
						E994	Q968	E995	W824						
						E995	Q969	E996	W825						
						E996	Q970	E997	W826						
						E997	Q971	E998	W827						
						E998	Q972	E999	W828						
						E999	Q973	E1000	W829						
						E1000	Q974	E1001	W830						
						E1001	Q975	E1002	W831						
						E1002	Q976	E1003	W832						
						E1003	Q977	E1004	W833						
						E1004	Q978	E1005	W834						
						E1005	Q979	E1006	W835						
						E1006	Q980	E1007	W836						
						E1007	Q981	E1008	W837						
						E1008	Q982	E1009	W838						
						E1009	Q983	E1010	W839						
						E1010	Q984	E1011	W840						
						E1011	Q985	E1012	W841						
						E1012	Q986	E1013	W842						
						E1013	Q987	E1014	W843						
						E1014	Q988	E1015	W844						
						E1015	Q989	E1016	W845						
						E1016	Q990	E1017	W846						
						E1017	Q991	E1018	W847						
						E1018	Q992	E1019	W848						
						E1019	Q993	E1020	W849						
						E1020	Q994	E1021	W850						
						E1021	Q995	E1022	W851						
						E1022	Q996	E1023	W852						
						E1023	Q997	E1024	W853						
						E1024	Q998	E1025	W854						
						E1025	Q999	E1026	W855						
						E1026	Q1000	E1027	W856						
						E1027	Q1001	E1028	W857						
						E1028	Q1002	E1029	W858						
						E1029	Q1003	E1030	W859						
						E1030	Q1004	E1031	W860						
						E1031	Q1005	E1032	W861						
						E1032	Q1006	E1033	W862						
						E1033	Q1007	E1034	W863						
						E1034	Q1008	E1035	W864						
						E1035	Q1009	E1036	W865						
						E1036	Q1010	E1037	W866						
						E1037	Q1011	E1038	W867						
						E1038	Q1012	E1039	W868						
						E1039	Q1013	E1040	W869						
						E1040	Q1014	E1041	W870						
						E1041	Q1015	E1042	W871						
						E1042	Q1016	E1043	W872						
						E1043	Q1017	E1044	W873						
						E1044	Q1018	E1045	W874						
						E1045	Q1019	E1046	W875						
						E1046	Q1020	E1047	W876						
						E1047	Q1021	E1048	W877						
						E1048	Q1022	E1049	W878						
						E1049	Q1023	E1050	W879						
						E1050	Q1024	E1051	W880						
						E1051	Q1025	E1052	W881						
						E1052	Q1026	E1053	W882						
						E1053	Q1027	E1054	W883						
						E1054	Q1028	E1055	W884						
						E1055	Q1029	E1056	W885						
						E1056	Q1030	E1057	W886						
						E1057	Q1031	E1058	W887						
						E1058	Q1								

[illegible]

- Molecule 1: NFX1-type zinc finger-containing protein 1



LEU	GLN	LYS	LEU	R309	T244	F183	ASN	ALA	MET
SER	GLN	VAL	ASP	R310	T247	L184	ASP	ALA	GLU
GLN	GLN	GLN	THR	E311	T248	L185	ASN	ALA	GLU
GLY	GLN	PHE	PHE	G312	T249	L186	PHE	TRP	ARG
ARG	LEU	THR	ARG	THR	T250	L187	GLN	ARG	PRO
TYR	ALA	LYS	LEU	LEU	T251	G188	TRP	GLU	PRO
ASP	GLU	PRO	LEU	ARG	T252	G189	ARG	GLU	LEU
PHE	VAL	LEU	ARG	VAL	Q253	Q189	THR	ASP	ASP
THR	GLN	LEU	GLU	ASP	D253	V190	PRO	PHE	ALA
PRO	PRO	PHE	ASP	THR	L254	L191	HIS	ARG	ARG
LEU	SER	VAL	PHE	TYR	T255	R192	GLN	ALA	PRO
ILE	ASP	ARG	VAL	THR	T256	G192	LYS	MET	ARG
GLU	GLU	TRP	ARG	LEU	T257	K193	THR	ARG	ASN
ASN	PHE	GLN	PRO	VAL	V257	A194	PRO	GLY	SER
PRO	LEU	ASN	GLN	GLN	F258	C195	GLU	ASN	HIS
SER	MET	SER	ARG	PRO	P259	S196	GLN	THR	PRO
ALA	VAL	LYS	GLU	GLU	A260	S197	PRO	HIS	ASN
THR	GLU	ARG	GLY	ALA	S261	S197	GLN	GLN	HIS
GLY	THR	LEU	ILE	GLU	T262	M198	GLN	GLY	ASN
GLU	LEU	TYR	GLU	ASP	S262	G198	VAL	ARG	ASN
PHE	ALA	LEU	GLU	HIS	T263	D200	VAL	ASN	PRO
LEU	GLY	GLY	LEU	VAL	Q264	R201	GLN	ASN	ASP
ARG	PHE	SER	LEU	GLU	E265	Q202	GLY	GLU	GLY
ASN	GLU	LEU	GLN	SER	T266	S203	GLY	LEU	LEU
VAL	ALA	VAL	PHE	TYR	G267	V204	ALA	ALA	ALA
GLY	TYR	CYS	ASP	ARG	T268	S205	PRO	SER	PRO
GLY	ARG	MET	ASP	THR	S267	H206	K147	ASP	ARG
LEU	HIS	LYS	GLN	PRO	L269	L205	F148	GLU	ARG
ARG	VAL	ASP	GLY	ILE	T270	V207	E150	ALA	ARG
HIS	LEU	GLY	LEU	TYR	S271	L208	ASP	GLN	GLN
PRO	GLU	ASN	LEU	PRO	T276	G209	S151	GLN	ALA
ARG	GLY	PHE	ARG	THR	S277	T210	L152	ARG	ASN
ILE	LEU	THR	LYS	TYR	L277	L211	L153	HIS	ASN
ASN	GLU	PHE	LYS	ASN	M278	K212	Q154	ASP	PRO
VAL	VAL	LEU	PHE	GLU	A279	G213	K155	GLN	PRO
GLN	GLU	PHE	ASP	HIS	T280	L213	D156	GLU	ALA
GLY	GLU	THR	ILE	LEU	L281	G214	P157	ASN	ASN
GLN	ASP	VAL	ARG	ASP	R281	S215	G157	ASP	ALA
GLY	VAL	SER	ILE	GLU	A282	K215	S158	THR	LEU
TRP	PRO	ASN	TYR	ARG	G283	F216	E159	ARG	LEU
PRO	PHE	ARG	PHE	PRO	G284	L217	G159	TRP	GLY
SER	GLN	GLU	ASP	PHE	T285	K218	V160	GLY	GLY
GLU	ARG	GLN	THR	LEU	G286	V219	V161	ASN	SER
ALA	ASN	GLU	ARG	ARG	T287	G220	G162	GLY	ALA
LEU	ILE	ASP	ILE	PRO	E288	L221	T163	ASN	HIS
LYS	VAL	LEU	ILE	ASN	T287	P222	L164	GLN	PRO
LEU	GLU	CYS	THR	ILE	E288	G223	A165	ASN	GLY
ASP	CYS	ARG	PRO	ILE	T289	A223	G165	CYS	ARG
ASN	ASN	GLY	MET	SER	E290	G224	T166	ARG	HIS
SER	SER	ILE	CYS	GLY	T291	G225	S167	ASN	PRO
SER	THR	VAL	SER	LYS	E292	G227	L168	ARG	ALA
GLN	HIS	GLN	SER	TYR	G293	L229	G169	ARG	ALA
MET	VAL	LEU	SER	ASP	M294	T230	T170	PRO	ASN
GLY	LYS	LEU	LEU	THR	L295	E231	G171	PRO	ASN
ALA	GLU	PHE	ILE	THR	E296	G231	G172	TRP	HIS
LEU	ARG	GLU	VAL	ILE	T297	G232	G173	SER	PRO
GLN	THR	THR	THR	THR	E297	G233	G174	ALA	ALA



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	258760	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.060	Depositor
Minimum map value	-0.676	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.07	Depositor
Map size ($\text{\AA}$)	331.2, 331.2, 331.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.828, 0.828, 0.828	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: AGS

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	0.18	0/10508	0.47	0/14189
1	B	0.23	0/10508	0.51	0/14189
1	C	0.19	0/1361	0.53	0/1836
All	All	0.21	0/22377	0.49	0/30214

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	10307	0	10368	171	0
1	B	10307	0	10368	220	0
1	C	1344	0	1417	36	0
2	A	31	0	12	2	0
2	B	31	0	12	8	0
All	All	22020	0	22177	421	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 10.

All (421) 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:B:621:PRO:HG3	1:B:1035:GLN:HE21	1.28	0.94
1:B:621:PRO:HG3	1:B:1035:GLN:NE2	1.93	0.84
1:A:1068:ARG:HH22	1:A:1090:ASP:H	1.27	0.82
1:B:1068:ARG:HH22	1:B:1089:GLN:H	1.27	0.81
1:A:554:ARG:HD2	1:A:581:ARG:HB3	1.65	0.78
1:B:621:PRO:CG	1:B:1035:GLN:HE21	1.97	0.77
1:C:217:LEU:HA	1:C:221:LEU:HD23	1.67	0.76
1:B:654:VAL:HG12	1:B:1004:ILE:HG12	1.68	0.76
1:B:680:VAL:HG12	1:B:694:LEU:HD21	1.70	0.74
1:A:410:ILE:HG22	1:A:506:VAL:HG12	1.71	0.73
1:B:653:LEU:HB3	1:B:1003:VAL:HG12	1.72	0.72
1:B:709:MET:HA	1:B:712:ARG:HD3	1.71	0.71
1:A:709:MET:HE3	1:A:709:MET:H	1.53	0.71
1:A:260:ALA:HA	1:A:314:LEU:HD21	1.72	0.70
1:B:867:MET:HE1	1:B:901:VAL:HG11	1.72	0.70
1:B:884:THR:HG21	1:B:891:ARG:HG3	1.74	0.69
1:B:749:LEU:HD11	1:B:937:TRP:HB3	1.74	0.69
1:A:544:LYS:HD3	1:A:547:ARG:HH12	1.57	0.69
1:B:984:THR:HG23	1:B:987:GLY:H	1.56	0.69
1:B:1224:ALA:HB2	1:B:1228:MET:HB2	1.75	0.69
1:A:248:ILE:HD11	1:A:298:VAL:HG21	1.74	0.68
1:B:655:VAL:HB	1:B:1005:VAL:HG22	1.75	0.68
1:B:192:ARG:HH22	1:B:193:LYS:HE2	1.58	0.68
1:B:1130:ASN:HB2	1:B:1163:GLN:HE21	1.59	0.68
1:A:345:VAL:HG13	1:A:388:ILE:HG21	1.75	0.67
1:A:1418:HIS:HA	1:A:1427:LEU:HD21	1.76	0.67
1:B:505:MET:HE1	1:B:507:GLU:HB3	1.77	0.66
1:B:624:GLY:HA3	2:B:2000:AGS:H8	1.77	0.66
1:B:275:THR:HG21	1:C:271:SER:HB2	1.76	0.66
1:B:1272:THR:HG21	1:B:1283:VAL:HG11	1.78	0.66
1:A:376:LEU:HB3	1:A:519:LEU:HD21	1.79	0.65
1:B:408:ILE:HD11	1:B:508:THR:HB	1.78	0.65
1:B:1122:ILE:HG23	1:B:1124:GLU:H	1.61	0.65
1:B:288:GLU:HG2	1:B:291:THR:H	1.61	0.65
1:B:338:ILE:HG21	1:B:516:ARG:HG2	1.78	0.65
1:A:947:ARG:HH21	1:A:948:LYS:HG2	1.62	0.64
1:B:788:LEU:HB3	1:B:897:MET:HE2	1.80	0.64
1:A:887:TRP:CD1	1:A:891:ARG:HB2	2.33	0.64
1:B:302:ILE:HA	1:B:305:LEU:HG	1.78	0.64
1:B:636:LEU:HD13	1:B:1002:ILE:HD13	1.80	0.64
1:B:270:VAL:HG21	1:B:302:ILE:HG21	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1105:GLY:HA2	1:B:1263:CYS:O	1.99	0.63
1:A:448:LEU:HD12	1:A:482:VAL:HG21	1.80	0.63
1:A:299:GLN:O	1:A:303:GLU:HG3	1.99	0.62
1:B:621:PRO:HB3	2:B:2000:AGS:O3G	1.99	0.62
1:B:1140:LEU:HG	1:B:1144:PHE:HE2	1.64	0.62
1:B:411:TYR:HB2	1:B:505:MET:HG3	1.82	0.62
1:B:624:GLY:HA2	2:B:2000:AGS:O5'	1.98	0.62
1:A:1322:CYS:HB2	1:A:1337:CYS:HA	1.82	0.62
1:B:868:ARG:O	1:B:898:LYS:HE2	2.00	0.61
1:A:442:TRP:HB2	1:A:474:GLN:HE22	1.65	0.61
1:B:1163:GLN:HE22	1:B:1200:VAL:HA	1.65	0.61
1:A:614:LEU:HD21	1:A:1059:LEU:HD21	1.82	0.61
1:A:683:ARG:HG2	1:A:834:ALA:HB1	1.81	0.61
1:A:730:HIS:O	1:A:734:LYS:HG3	2.00	0.61
1:A:848:ARG:HE	1:A:850:LYS:HE2	1.63	0.61
1:B:455:CYS:HA	1:B:465:LEU:O	1.99	0.61
1:A:938:LEU:O	1:A:942:GLN:HG2	2.01	0.61
1:A:945:THR:HA	1:A:948:LYS:HE2	1.83	0.60
1:B:1005:VAL:HG12	1:B:1008:ALA:HB2	1.83	0.60
1:B:488:GLU:HA	1:B:491:GLN:HB3	1.81	0.60
1:A:1384:HIS:HB3	1:A:1400:GLU:HG3	1.83	0.60
1:A:708:PRO:HD2	1:A:711:LEU:HD12	1.84	0.60
1:B:1134:ALA:O	1:B:1138:VAL:HG22	2.03	0.59
1:A:273:LEU:HB3	1:A:295:LEU:HD11	1.85	0.59
1:A:745:ARG:HH22	1:A:866:ALA:H	1.50	0.59
1:B:1068:ARG:HH12	1:B:1089:GLN:HB3	1.67	0.59
1:A:225:VAL:HG11	1:A:272:LEU:HB3	1.84	0.59
1:B:305:LEU:HA	1:B:308:LYS:HE2	1.84	0.59
1:B:598:LEU:HB2	1:B:603:MET:HE1	1.85	0.58
1:B:971:ASP:HA	1:B:974:ILE:HG12	1.84	0.58
1:B:1103:ILE:HD11	1:B:1226:LYS:HB3	1.86	0.58
1:C:186:LEU:HD12	1:C:189:GLN:HE21	1.67	0.58
1:B:610:LEU:HD21	1:B:636:LEU:HD21	1.85	0.58
1:A:574:VAL:HG11	1:A:580:PRO:HD3	1.84	0.58
1:A:731:GLU:O	1:A:735:THR:HG23	2.03	0.57
1:A:636:LEU:HD13	1:A:1002:ILE:HD13	1.85	0.57
1:A:928:SER:O	1:A:932:GLN:HG2	2.03	0.57
1:A:387:GLY:HA3	1:A:408:ILE:HD11	1.86	0.57
1:A:1165:PHE:HE2	1:A:1169:LYS:HE3	1.68	0.57
1:A:1401:MET:HE3	1:A:1402:VAL:N	2.20	0.57
1:B:408:ILE:HG12	1:B:507:GLU:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:823:ILE:HG23	1:B:825:ILE:HG23	1.86	0.57
1:B:457:SER:O	1:B:503:PHE:HA	2.05	0.57
1:B:999:GLU:HB3	1:B:1023:ALA:HB3	1.87	0.57
1:B:1062:VAL:HG23	1:B:1064:ILE:HG12	1.85	0.57
1:B:321:LEU:HD12	1:B:324:PRO:HB3	1.86	0.56
1:A:1134:ALA:O	1:A:1138:VAL:HG12	2.05	0.56
1:A:1259:MET:HG3	1:A:1273:LEU:HG	1.87	0.56
1:B:199:MET:HE1	1:B:993:GLN:HG3	1.87	0.56
1:B:582:ILE:HB	1:B:589:GLN:HG3	1.86	0.56
1:C:211:LEU:HD11	1:C:217:LEU:HD21	1.86	0.56
1:A:534:ARG:HH22	1:A:542:HIS:HB3	1.70	0.56
1:B:292:GLU:HA	1:B:295:LEU:HG	1.88	0.56
1:A:1247:ILE:HG23	1:A:1256:ILE:HD13	1.88	0.55
1:A:1073:HIS:CD2	2:A:2000:AGS:C8	2.90	0.55
1:B:1240:VAL:HB	1:B:1243:TRP:HB2	1.88	0.55
1:A:1042:VAL:HG12	1:A:1045:LEU:H	1.70	0.55
1:A:968:LEU:HG	1:A:994:ILE:HD11	1.89	0.55
1:B:1147:GLN:HE21	1:B:1147:GLN:HA	1.72	0.55
1:B:593:LYS:HB2	1:B:603:MET:HE3	1.88	0.55
1:C:229:ILE:HD11	1:C:276:SER:HA	1.88	0.55
1:B:219:VAL:HG11	1:C:219:VAL:HG22	1.88	0.55
1:B:598:LEU:HD23	2:B:2000:AGS:N6	2.22	0.55
1:A:158:SER:HB2	1:A:199:MET:HE3	1.88	0.54
1:A:456:MET:HA	1:A:504:LEU:O	2.07	0.54
1:A:457:SER:HB3	1:A:461:PHE:CD2	2.42	0.54
1:B:822:LEU:HD23	1:B:1168:ARG:HH12	1.72	0.54
1:B:972:LEU:HD12	1:B:994:ILE:HG12	1.90	0.54
1:C:240:TYR:O	1:C:244:ILE:HG12	2.08	0.54
1:B:1203:ASN:C	1:B:1203:ASN:HD22	2.12	0.54
1:A:735:THR:O	1:A:739:THR:HG23	2.07	0.54
1:B:823:ILE:HG22	1:B:1168:ARG:HD2	1.90	0.54
1:A:1142:LYS:HB3	1:A:1176:PHE:CZ	2.43	0.53
1:A:1165:PHE:CE2	1:A:1169:LYS:HE3	2.43	0.53
1:B:616:ILE:HD11	1:B:1059:LEU:HG	1.89	0.53
1:A:1138:VAL:HG11	1:A:1170:LEU:HG	1.90	0.53
1:B:943:ALA:O	1:B:947:ARG:HG2	2.08	0.53
1:B:620:PRO:HD2	1:B:623:THR:HG21	1.91	0.53
1:B:654:VAL:HG23	1:B:982:GLY:HA2	1.91	0.53
1:A:244:ILE:HD12	1:A:273:LEU:HD11	1.91	0.53
1:A:1113:VAL:HG11	1:A:1260:LEU:HD23	1.91	0.53
1:B:929:SER:HA	1:B:932:GLN:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:621:PRO:CD	1:B:1035:GLN:HE21	2.21	0.53
1:B:719:MET:HE3	1:B:719:MET:HA	1.90	0.53
1:B:259:PRO:HD2	1:B:317:ASP:HB3	1.91	0.53
1:B:560:LEU:HD11	1:B:635:ALA:HB2	1.91	0.53
1:B:1006:GLU:HA	1:B:1030:ILE:HB	1.89	0.53
1:A:369:LEU:HD21	1:A:525:VAL:HG12	1.91	0.52
1:B:408:ILE:HG23	1:B:507:GLU:O	2.09	0.52
1:B:248:ILE:HA	1:B:251:LEU:HG	1.91	0.52
1:B:384:LEU:N	1:B:408:ILE:HD12	2.24	0.52
1:A:1112:PHE:HD2	1:A:1234:MET:HE2	1.74	0.52
1:A:666:LEU:HA	1:A:669:ILE:HG22	1.90	0.52
1:A:1078:GLU:HA	1:A:1081:ARG:HH12	1.75	0.52
1:B:378:GLU:HA	1:B:381:VAL:HG22	1.92	0.52
1:C:240:TYR:HA	1:C:243:HIS:NE2	2.24	0.52
1:C:306:GLN:O	1:C:310:ARG:HG2	2.10	0.52
1:B:408:ILE:HG12	1:B:508:THR:HA	1.92	0.52
1:A:388:ILE:HG12	1:A:461:PHE:CE1	2.45	0.52
1:A:1171:MET:HB2	1:A:1176:PHE:CD1	2.44	0.52
1:A:546:PRO:HD3	1:A:613:GLU:HB3	1.92	0.52
1:B:416:ILE:HD11	1:B:456:MET:HE1	1.91	0.52
1:B:707:LEU:HB3	1:B:711:LEU:HD11	1.92	0.52
1:A:512:PHE:O	1:A:516:ARG:HB2	2.10	0.52
1:B:557:PHE:HB3	1:B:560:LEU:HD12	1.92	0.51
1:B:1279:ASP:HA	1:B:1282:LYS:HD3	1.92	0.51
1:A:1168:ARG:HH11	1:A:1168:ARG:HG2	1.76	0.51
1:B:1079:ILE:HG12	1:B:1110:LEU:HD13	1.92	0.51
1:A:534:ARG:HH11	1:A:544:LYS:NZ	2.08	0.51
1:B:764:GLY:HA3	1:B:771:TRP:CD1	2.46	0.51
1:A:555:TYR:CE2	1:A:642:VAL:HG11	2.46	0.51
1:B:418:THR:HG23	1:B:420:MET:HE1	1.92	0.51
1:B:1213:ILE:HD11	1:B:1215:ASN:HD21	1.75	0.51
1:A:1288:CYS:H	1:A:1306:CYS:HB3	1.76	0.51
1:A:849:ARG:HG3	1:A:852:GLU:HB3	1.92	0.50
1:A:611:THR:HG22	1:A:612:ARG:HD3	1.92	0.50
1:A:1102:LYS:HZ1	1:A:1105:GLY:H	1.59	0.50
1:B:838:ILE:HD13	1:B:990:LYS:HE3	1.93	0.50
1:B:1378:LYS:HD3	1:B:1379:SER:H	1.76	0.50
1:C:297:LYS:O	1:C:301:ILE:HG12	2.12	0.50
1:C:170:LEU:O	1:C:174:LEU:HB3	2.11	0.50
1:B:160:VAL:O	1:B:164:LEU:HG	2.11	0.50
1:B:598:LEU:HB3	1:B:602:GLN:OE1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:987:GLY:O	1:B:991:TYR:HB2	2.11	0.50
1:A:392:LEU:HA	1:A:395:PHE:HD2	1.77	0.50
1:B:230:THR:HG23	1:C:309:ARG:HH12	1.75	0.50
1:B:1035:GLN:NE2	2:B:2000:AGS:S1G	2.85	0.50
1:A:971:ASP:HA	1:A:974:ILE:HD12	1.93	0.50
1:A:958:THR:O	1:A:962:ARG:HG3	2.12	0.49
1:B:144:LEU:HD13	1:B:148:PHE:HE1	1.77	0.49
1:B:1352:ILE:HG22	1:B:1354:ARG:H	1.76	0.49
1:A:1150:LEU:HD12	1:A:1150:LEU:H	1.77	0.49
1:A:1351:THR:HA	1:A:1358:GLU:HA	1.94	0.49
1:B:543:VAL:HG21	1:B:612:ARG:HB3	1.94	0.49
1:A:1128:HIS:CD2	1:A:1201:ARG:HE	2.31	0.49
1:A:679:ARG:NH1	1:A:684:SER:HB2	2.28	0.49
1:B:273:LEU:O	1:B:277:LEU:HG	2.12	0.49
1:B:1276:LYS:HE2	1:B:1277:ALA:H	1.78	0.49
1:A:409:ARG:HD3	1:A:447:ARG:HG2	1.94	0.49
1:A:994:ILE:O	1:A:998:VAL:HG23	2.13	0.49
1:B:1205:GLU:HG3	1:B:1207:LYS:H	1.76	0.49
1:C:251:LEU:HA	1:C:254:LEU:HG	1.94	0.49
1:A:838:ILE:HG23	1:A:840:GLU:OE1	2.13	0.49
1:A:1193:ASP:HA	1:A:1225:LYS:HB2	1.94	0.49
1:B:309:ARG:HH12	1:C:232:PRO:HG3	1.78	0.49
1:A:831:LEU:HD13	1:A:1186:LYS:HG3	1.95	0.48
1:B:1130:ASN:H	1:B:1163:GLN:HG3	1.77	0.48
1:A:681:GLY:HA3	1:A:984:THR:HG23	1.93	0.48
1:A:860:LEU:HD12	1:A:863:MET:SD	2.54	0.48
1:B:429:LYS:NZ	1:B:481:ILE:HD12	2.28	0.48
1:C:187:ILE:HA	1:C:190:VAL:HG22	1.94	0.48
1:A:1055:LEU:O	1:A:1059:LEU:HB2	2.13	0.48
1:B:554:ARG:HB3	1:B:581:ARG:HB3	1.96	0.48
1:B:1352:ILE:HD13	1:B:1372:CYS:SG	2.54	0.48
1:B:1036:LEU:HD12	1:B:1188:GLN:HB2	1.95	0.48
1:B:1150:LEU:HB2	1:B:1153:GLN:HG3	1.95	0.48
1:A:236:ILE:HD12	1:A:239:GLN:HG3	1.94	0.48
1:A:634:GLN:O	1:A:638:THR:HG23	2.14	0.48
1:B:183:PHE:O	1:B:187:ILE:HG12	2.13	0.48
1:A:280:LEU:HD22	1:A:285:VAL:HG11	1.96	0.48
1:A:878:ALA:HB1	1:A:891:ARG:HD2	1.96	0.48
1:A:1139:GLU:HA	1:A:1142:LYS:HG2	1.96	0.48
1:A:1291:PRO:HA	1:A:1305:ALA:HA	1.96	0.48
1:A:1318:CYS:HB3	1:A:1337:CYS:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:GLU:O	1:A:296:GLU:HG2	2.13	0.48
1:A:1248:HIS:O	1:A:1252:GLU:HG3	2.14	0.48
1:B:779:HIS:CE1	1:B:783:LEU:HD23	2.49	0.48
1:B:1163:GLN:OE1	1:B:1200:VAL:HG22	2.13	0.48
1:A:1014:ALA:HA	1:A:1017:ILE:HG22	1.96	0.47
1:B:584:VAL:HG11	1:B:610:LEU:HB3	1.95	0.47
1:B:363:ASP:HB2	1:B:367:ILE:HG21	1.96	0.47
1:B:762:MET:HE3	1:B:762:MET:O	2.14	0.47
1:A:608:PHE:HE1	1:A:616:ILE:H	1.62	0.47
1:B:252:GLN:HA	1:B:255:VAL:HG12	1.97	0.47
1:B:1251:ARG:HH21	1:B:1256:ILE:HD13	1.79	0.47
1:A:605:ALA:HB1	1:A:617:ILE:HD13	1.96	0.47
1:A:779:HIS:CE1	1:A:790:VAL:HG23	2.49	0.47
2:A:2000:AGS:O2A	2:A:2000:AGS:O3'	2.33	0.47
1:B:679:ARG:NH1	1:B:684:SER:HB3	2.29	0.47
1:B:715:TYR:HD2	1:B:716:MET:HE2	1.79	0.47
1:A:476:ASP:HB3	1:A:481:ILE:HB	1.97	0.47
1:A:1321:PRO:HA	1:A:1336:VAL:HA	1.96	0.47
1:A:1296:LEU:HD21	1:A:1302:CYS:HB2	1.96	0.47
1:B:704:ARG:HH12	1:B:712:ARG:CZ	2.28	0.47
1:B:887:TRP:HB3	1:B:891:ARG:HG2	1.97	0.47
1:B:1115:HIS:HB2	1:B:1132:HIS:HE1	1.79	0.47
1:A:555:TYR:HE2	1:A:642:VAL:HG11	1.80	0.47
1:A:824:GLU:HA	1:A:1168:ARG:CZ	2.45	0.47
1:B:715:TYR:O	1:B:719:MET:HG2	2.15	0.47
1:A:237:ARG:HA	1:A:240:TYR:CD2	2.49	0.47
1:A:351:PRO:HG2	1:A:353:LEU:HD21	1.97	0.47
1:A:1403:THR:HA	1:A:1413:PRO:HA	1.96	0.47
1:B:1130:ASN:HB2	1:B:1163:GLN:NE2	2.27	0.47
1:B:1143:TYR:CE1	1:B:1262:LEU:HD13	2.49	0.47
1:C:228:MET:HB2	1:C:280:LEU:HD21	1.97	0.47
1:C:224:TYR:HE2	1:C:247:ILE:HG21	1.80	0.47
1:B:240:TYR:O	1:B:244:ILE:HG12	2.15	0.46
1:A:534:ARG:HH21	1:A:540:ASN:CG	2.24	0.46
1:B:896:LYS:HA	1:B:899:LYS:HE3	1.96	0.46
1:B:410:ILE:HG12	1:B:506:VAL:HG12	1.98	0.46
1:B:384:LEU:HD13	1:B:408:ILE:HD13	1.98	0.46
1:B:409:ARG:HB2	1:B:507:GLU:CG	2.46	0.46
1:B:678:VAL:HB	1:B:981:VAL:HG12	1.97	0.46
1:B:721:GLN:HA	1:B:724:GLU:OE1	2.15	0.46
1:B:332:SER:O	1:B:334:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:548:TYR:HA	1:B:551:MET:HE1	1.97	0.46
1:B:660:HIS:CD2	1:B:1190:GLU:HG3	2.50	0.46
1:B:737:GLU:HA	1:B:740:MET:HG3	1.96	0.46
1:C:298:VAL:O	1:C:302:ILE:HG12	2.16	0.46
1:A:723:LYS:HE3	1:A:723:LYS:HA	1.98	0.46
1:C:211:LEU:HG	1:C:217:LEU:HD11	1.98	0.46
1:C:244:ILE:O	1:C:248:ILE:HG22	2.16	0.46
1:A:442:TRP:HB2	1:A:474:GLN:NE2	2.32	0.45
1:A:745:ARG:HG3	1:A:747:GLN:H	1.80	0.45
1:B:147:LYS:HD2	1:B:147:LYS:C	2.41	0.45
1:B:329:HIS:O	1:B:329:HIS:ND1	2.48	0.45
1:A:712:ARG:O	1:A:716:MET:HG3	2.15	0.45
1:B:744:LEU:HD11	1:B:749:LEU:HB2	1.98	0.45
1:B:1251:ARG:HE	1:B:1256:ILE:HG23	1.80	0.45
1:B:860:LEU:HA	1:B:863:MET:HG3	1.99	0.45
1:C:267:SER:HA	1:C:270:VAL:HG12	1.97	0.45
1:B:351:PRO:HG2	1:B:353:LEU:HD21	1.98	0.45
1:C:212:LYS:HD2	1:C:262:SER:HB3	1.97	0.45
1:B:385:ARG:O	1:B:388:ILE:HG22	2.17	0.45
1:B:687:GLU:HA	1:B:690:LYS:HG2	1.99	0.45
1:B:897:MET:HB3	1:B:900:ARG:HH21	1.81	0.45
1:A:338:ILE:HG21	1:A:516:ARG:HG2	1.98	0.45
1:A:727:GLN:O	1:A:731:GLU:HG2	2.17	0.45
1:A:902:LYS:O	1:A:906:ARG:HG3	2.17	0.45
1:B:272:LEU:HD21	1:C:268:MET:HG2	1.99	0.45
1:B:293:LYS:HA	1:B:296:GLU:OE1	2.17	0.45
1:B:599:ASP:O	1:B:603:MET:HE2	2.17	0.45
1:B:1189:GLY:HA2	2:B:2000:AGS:O2G	2.16	0.45
1:B:1105:GLY:HA3	1:B:1147:GLN:OE1	2.17	0.44
1:B:1416:CYS:O	1:B:1419:VAL:HB	2.16	0.44
1:B:1380:LEU:HD13	1:B:1398:CYS:HA	2.00	0.44
1:A:199:MET:H	1:A:199:MET:HG2	1.59	0.44
1:A:928:SER:HA	1:A:931:TRP:CE3	2.52	0.44
1:B:305:LEU:HA	1:B:308:LYS:CE	2.47	0.44
1:B:1009:ALA:O	1:B:1038:PRO:HD3	2.18	0.44
1:B:881:GLU:HG2	1:B:882:GLN:HG2	1.99	0.44
1:B:1112:PHE:HE1	1:B:1228:MET:HE1	1.82	0.44
1:B:1199:LEU:HD13	1:B:1237:LEU:HD22	1.99	0.44
1:A:195:CYS:SG	1:A:208:LEU:HD21	2.57	0.44
1:A:208:LEU:HB3	1:A:258:PHE:HE2	1.82	0.44
1:A:1197:LEU:O	1:A:1230:CYS:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1096:SER:HA	1:B:1099:LYS:HZ3	1.83	0.44
1:A:711:LEU:O	1:A:715:TYR:HB2	2.18	0.44
1:A:942:GLN:HB2	1:A:946:ARG:NH2	2.33	0.44
1:B:249:SER:O	1:B:252:GLN:HG2	2.17	0.44
1:B:291:THR:O	1:B:295:LEU:HG	2.17	0.44
1:B:1078:GLU:HA	1:B:1081:ARG:HH11	1.83	0.44
1:B:648:GLN:HB2	1:B:650:PHE:CE1	2.53	0.44
1:B:628:VAL:HA	1:B:631:LYS:HZ2	1.83	0.44
1:A:1298:CYS:HB2	1:A:1337:CYS:SG	2.58	0.43
1:B:688:ILE:HD12	1:B:688:ILE:H	1.83	0.43
1:B:1074:ARG:NH1	2:B:2000:AGS:O3G	2.51	0.43
1:C:161:VAL:HB	1:C:194:ALA:HB1	2.00	0.43
1:C:184:LEU:HD13	1:C:224:TYR:HB2	2.00	0.43
1:A:433:ASP:OD2	1:A:436:PRO:HD2	2.19	0.43
1:C:193:LYS:HB3	1:C:193:LYS:HE3	1.73	0.43
1:A:248:ILE:HG12	1:A:295:LEU:HD22	1.99	0.43
1:A:388:ILE:HG12	1:A:461:PHE:HE1	1.84	0.43
1:A:1218:CYS:O	1:A:1222:SER:HB3	2.19	0.43
1:B:179:MET:HE2	1:B:179:MET:HA	2.00	0.43
1:B:870:ASP:N	1:B:898:LYS:HD3	2.33	0.43
1:A:244:ILE:HD13	1:A:244:ILE:HA	1.76	0.43
1:A:643:TRP:H	1:A:643:TRP:CD1	2.36	0.43
1:B:1095:PRO:HA	1:B:1098:LEU:HG	2.00	0.43
1:B:1378:LYS:HD3	1:B:1379:SER:N	2.32	0.43
1:C:212:LYS:HA	1:C:217:LEU:HD12	2.00	0.43
1:A:161:VAL:HG22	1:A:203:SER:OG	2.19	0.43
1:A:609:ALA:HB2	1:A:617:ILE:HD11	2.00	0.43
1:A:849:ARG:HD2	1:A:849:ARG:HA	1.79	0.43
1:A:884:THR:HG21	1:A:891:ARG:HB3	1.99	0.43
1:B:1203:ASN:C	1:B:1203:ASN:ND2	2.76	0.43
1:B:745:ARG:HD2	1:B:747:GLN:OE1	2.18	0.43
1:B:298:VAL:HA	1:B:301:ILE:HG12	2.01	0.42
1:B:693:THR:O	1:B:697:LEU:HD13	2.19	0.42
1:B:976:LYS:HG2	1:B:998:VAL:HG12	2.01	0.42
1:B:267:SER:HA	1:B:270:VAL:HG22	2.00	0.42
1:B:435:LYS:HA	1:B:438:LYS:HE3	2.00	0.42
1:B:758:TRP:CE3	1:B:761:LEU:HB3	2.54	0.42
1:A:1073:HIS:HD1	1:A:1094:HIS:HB2	1.84	0.42
1:B:423:SER:HB3	1:B:842:GLU:OE2	2.19	0.42
1:B:1077:PRO:HA	1:B:1080:ALA:HB3	2.01	0.42
1:A:149:LEU:HD12	1:A:190:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:SER:O	1:A:334:ARG:HG2	2.19	0.42
1:A:679:ARG:HH12	1:A:684:SER:HB2	1.84	0.42
1:A:945:THR:O	1:A:949:ILE:HG22	2.19	0.42
1:B:557:PHE:CE2	1:B:582:ILE:HD11	2.53	0.42
1:B:1145:LEU:HD21	1:B:1151:PRO:HA	2.00	0.42
1:B:1385:ARG:HA	1:B:1385:ARG:HD3	1.82	0.42
1:A:1113:VAL:HA	1:A:1257:GLY:O	2.19	0.42
1:B:422:SER:OG	1:B:423:SER:N	2.52	0.42
1:B:624:GLY:CA	2:B:2000:AGS:H8	2.48	0.42
1:B:881:GLU:HG2	1:B:882:GLN:H	1.84	0.42
1:A:1208:VAL:HB	1:A:1212:GLN:HG3	2.00	0.42
1:C:177:SER:HB2	1:C:219:VAL:HG11	2.02	0.42
1:A:451:GLY:HA3	1:A:511:TYR:CE1	2.55	0.42
1:A:961:GLU:O	1:A:965:GLU:HG2	2.19	0.42
1:A:1110:LEU:HD11	1:A:1112:PHE:HE1	1.84	0.42
1:B:610:LEU:HD23	1:B:610:LEU:HA	1.87	0.42
1:B:679:ARG:HH12	1:B:684:SER:HB3	1.84	0.42
1:B:1097:VAL:HG23	1:B:1100:TYR:CE2	2.54	0.42
1:A:336:MET:HE2	1:A:377:ARG:HE	1.85	0.42
1:A:677:ILE:HD12	1:A:980:VAL:HB	2.01	0.42
1:B:579:HIS:HB3	1:B:581:ARG:HH22	1.85	0.42
1:B:891:ARG:HD3	1:B:891:ARG:HA	1.77	0.42
1:A:934:TYR:CZ	1:A:938:LEU:HD21	2.54	0.42
1:B:444:ASN:HA	1:B:827:GLU:OE2	2.20	0.42
1:B:1103:ILE:HB	1:B:1106:VAL:HG21	2.01	0.42
1:A:491:GLN:HE21	1:A:957:ARG:HD2	1.85	0.42
1:A:899:LYS:HD3	1:B:880:GLN:HG3	2.01	0.42
1:A:944:ASP:O	1:A:948:LYS:HG3	2.20	0.42
1:B:1036:LEU:HD23	1:B:1036:LEU:HA	1.81	0.42
1:B:1157:LEU:HD23	1:B:1195:ILE:HG23	2.02	0.41
1:A:217:LEU:HD12	1:A:221:LEU:HD12	2.02	0.41
1:C:208:LEU:HA	1:C:211:LEU:HB3	2.02	0.41
1:A:302:ILE:HA	1:A:305:LEU:HG	2.02	0.41
1:A:1213:ILE:HD12	1:A:1213:ILE:H	1.84	0.41
1:B:179:MET:SD	1:B:183:PHE:HB3	2.60	0.41
1:B:231:GLU:HG3	1:B:233:ILE:HG12	2.01	0.41
1:B:446:LYS:HB3	1:B:446:LYS:HE2	1.81	0.41
1:B:719:MET:O	1:B:723:LYS:HG3	2.21	0.41
1:B:723:LYS:O	1:B:726:GLU:HG2	2.19	0.41
1:A:698:ARG:HB2	1:A:974:ILE:HD11	2.01	0.41
1:A:1110:LEU:HD11	1:A:1112:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:LYS:HA	1:B:293:LYS:HD2	1.86	0.41
1:B:587:PRO:HA	1:B:590:TRP:CE2	2.56	0.41
1:B:749:LEU:HA	1:B:941:TYR:HE2	1.85	0.41
1:B:1103:ILE:HB	1:B:1106:VAL:CG2	2.50	0.41
1:B:1267:HIS:HB2	1:B:1270:THR:OG1	2.21	0.41
1:A:170:LEU:HD12	1:A:173:LEU:HD23	2.02	0.41
1:A:992:ARG:NH2	1:A:993:GLN:HG3	2.36	0.41
1:A:1380:LEU:HD21	1:A:1386:CYS:HB2	2.02	0.41
1:B:457:SER:HB2	1:B:461:PHE:CE1	2.55	0.41
1:A:152:LEU:HD23	1:A:152:LEU:HA	1.90	0.41
1:A:221:LEU:HD23	1:A:221:LEU:HA	1.81	0.41
1:A:446:LYS:H	1:A:446:LYS:HG2	1.77	0.41
1:B:761:LEU:HD13	1:B:785:TRP:HZ3	1.85	0.41
1:B:587:PRO:HA	1:B:590:TRP:CD2	2.55	0.41
1:C:184:LEU:HD21	1:C:221:LEU:HD13	2.03	0.41
1:C:254:LEU:HA	1:C:257:VAL:HG12	2.03	0.41
1:A:173:LEU:HD21	1:A:187:ILE:HD11	2.02	0.41
1:A:245:SER:HA	1:A:248:ILE:HG22	2.03	0.41
1:A:293:LYS:HE2	1:A:293:LYS:HB2	1.92	0.41
1:A:761:LEU:HA	1:A:923:TRP:HE1	1.85	0.41
1:A:779:HIS:HE1	1:A:790:VAL:HG23	1.86	0.41
1:A:838:ILE:HG13	1:A:839:GLU:H	1.86	0.41
1:A:1189:GLY:H	1:A:1223:ARG:HH12	1.68	0.41
1:B:308:LYS:HE3	1:B:322:VAL:HG21	2.02	0.41
1:B:881:GLU:HG2	1:B:882:GLN:N	2.36	0.41
1:B:1096:SER:HA	1:B:1099:LYS:NZ	2.36	0.41
1:B:1145:LEU:HD23	1:B:1145:LEU:HA	1.83	0.41
1:C:157:PRO:HB3	1:C:194:ALA:HA	2.03	0.41
1:C:183:PHE:O	1:C:187:ILE:HG22	2.21	0.41
1:B:704:ARG:HH12	1:B:712:ARG:NE	2.19	0.41
1:B:1009:ALA:O	1:B:1037:ARG:HA	2.21	0.41
1:B:1158:THR:HG22	1:B:1198:SER:HB3	2.03	0.41
1:C:219:VAL:C	1:C:222:PRO:HD2	2.47	0.41
1:A:456:MET:O	1:A:465:LEU:HB2	2.22	0.40
1:A:1171:MET:HB2	1:A:1176:PHE:CE1	2.56	0.40
1:B:202:GLN:HG2	1:B:961:GLU:HB2	2.03	0.40
1:A:1273:LEU:HD12	1:A:1273:LEU:HA	1.97	0.40
1:B:230:THR:HA	1:C:309:ARG:NH1	2.36	0.40
1:B:1037:ARG:HD2	1:B:1215:ASN:HD21	1.86	0.40
1:A:233:ILE:HA	1:A:234:PRO:HD3	1.97	0.40
1:A:1168:ARG:HG2	1:A:1168:ARG:NH1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1208:VAL:HG12	1:A:1211:LEU:HB2	2.03	0.40
1:B:299:GLN:HA	1:B:302:ILE:HG22	2.03	0.40
1:C:152:LEU:HD22	1:C:160:VAL:HG12	2.04	0.40
1:A:615:ALA:HB3	1:A:1028:ILE:HG12	2.03	0.40
1:A:637:LEU:HA	1:A:637:LEU:HD23	1.90	0.40
1:A:902:LYS:O	1:A:902:LYS:HD3	2.21	0.40
1:B:156:ASP:O	1:B:160:VAL:HG13	2.21	0.40
1:B:849:ARG:HD2	1:B:849:ARG:HA	1.78	0.40
1:B:1149:TYR:HD2	1:B:1149:TYR:HA	1.79	0.40
1:A:625:LYS:HE3	1:A:1031:GLY:HA2	2.04	0.40
1:B:655:VAL:HA	1:B:983:MET:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1278/1918 (67%)	1221 (96%)	57 (4%)	0	100	100
1	B	1278/1918 (67%)	1232 (96%)	46 (4%)	0	100	100
1	C	170/1918 (9%)	163 (96%)	7 (4%)	0	100	100
All	All	2726/5754 (47%)	2616 (96%)	110 (4%)	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	
1	A	1162/1726 (67%)	1139 (98%)	23 (2%)	48	64
1	B	1162/1726 (67%)	1134 (98%)	28 (2%)	43	62
1	C	159/1726 (9%)	157 (99%)	2 (1%)	61	71
All	All	2483/5178 (48%)	2430 (98%)	53 (2%)	46	64

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	LEU
1	A	179	MET
1	A	205	LEU
1	A	273	LEU
1	A	295	LEU
1	A	322	VAL
1	A	364	SER
1	A	494	LEU
1	A	504	LEU
1	A	527	GLU
1	A	544	LYS
1	A	598	LEU
1	A	631	LYS
1	A	730	HIS
1	A	897	MET
1	A	932	GLN
1	A	968	LEU
1	A	1020	LEU
1	A	1175	THR
1	A	1213	ILE
1	A	1219	VAL
1	A	1274	VAL
1	A	1319	MET
1	B	211	LEU
1	B	329	HIS
1	B	380	PHE
1	B	408	ILE
1	B	418	THR
1	B	427	VAL
1	B	477	LEU
1	B	517	HIS
1	B	522	LEU

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Mol	Chain	Res	Type
1	B	543	VAL
1	B	584	VAL
1	B	627	TYR
1	B	744	LEU
1	B	819	GLU
1	B	838	ILE
1	B	868	ARG
1	B	1004	ILE
1	B	1028	ILE
1	B	1043	TYR
1	B	1110	LEU
1	B	1132	HIS
1	B	1147	GLN
1	B	1181	VAL
1	B	1203	ASN
1	B	1230	CYS
1	B	1252	GLU
1	B	1260	LEU
1	B	1348	VAL
1	C	263	VAL
1	C	291	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	474	GLN
1	A	483	GLN
1	A	491	GLN
1	A	535	ASN
1	A	659	ASN
1	A	660	HIS
1	A	664	GLN
1	A	685	ASN
1	A	747	GLN
1	A	779	HIS
1	A	847	GLN
1	A	996	GLN
1	A	1089	GLN
1	A	1203	ASN
1	A	1235	GLN
1	A	1253	ASN
1	A	1265	GLN

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Mol	Chain	Res	Type
1	A	1345	GLN
1	A	1359	GLN
1	A	1412	GLN
1	B	579	HIS
1	B	589	GLN
1	B	634	GLN
1	B	660	HIS
1	B	685	ASN
1	B	847	GLN
1	B	1035	GLN
1	B	1147	GLN
1	B	1163	GLN
1	B	1317	GLN
1	C	189	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AGS	B	2000	-	32,33,33	0.68	1 (3%)	45,52,52	0.56	0
2	AGS	A	2000	-	32,33,33	0.64	0	45,52,52	0.76	1 (2%)

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
2	AGS	B	2000	-	-	2/21/38/38	0/3/3/3
2	AGS	A	2000	-	-	5/21/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2000	AGS	PG-S1G	2.01	1.95	1.90

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2000	AGS	PB-O3B-PG	-2.75	123.12	133.17

There are no chirality outliers.

All (7) torsion outliers are listed below:

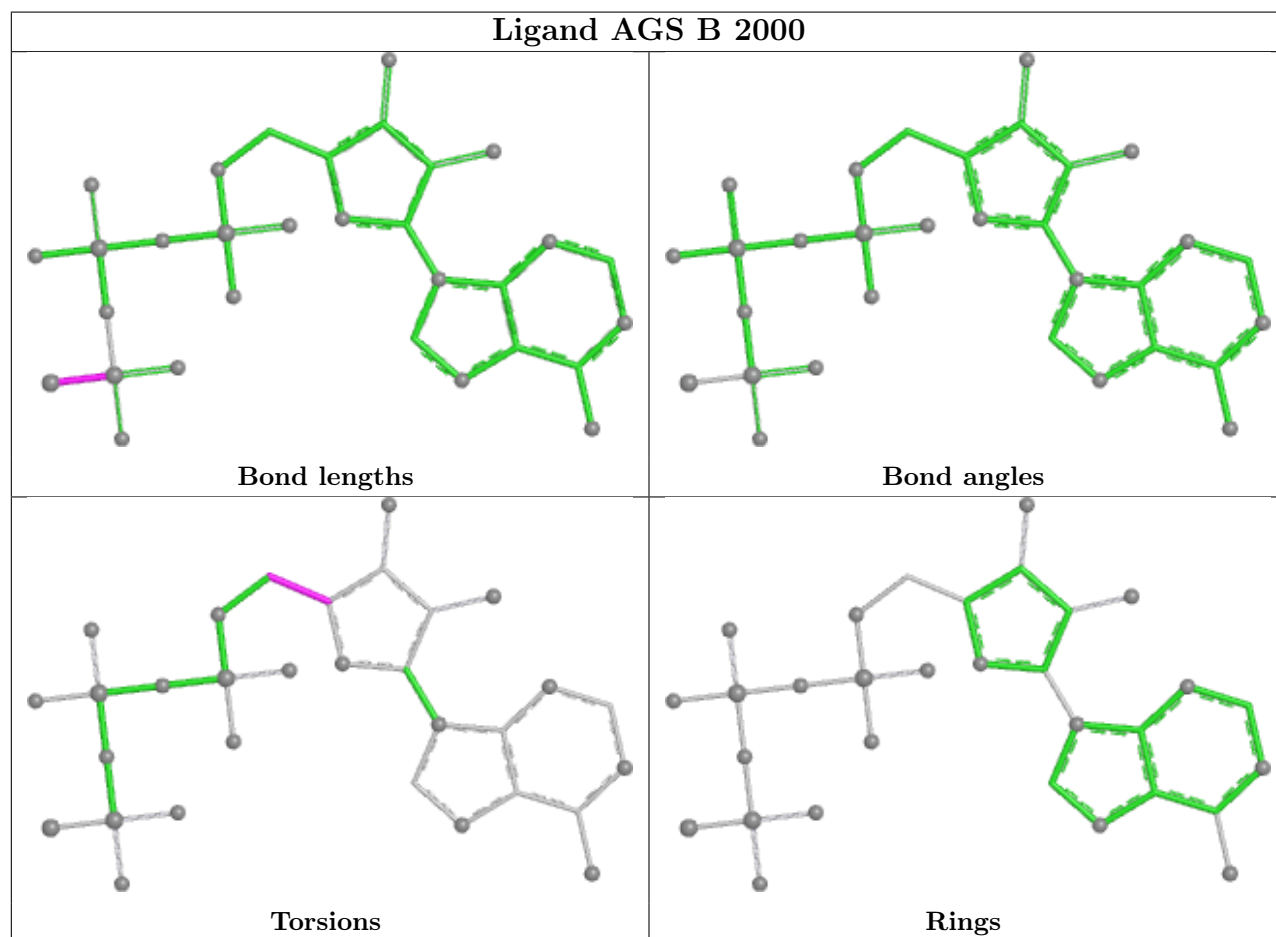
Mol	Chain	Res	Type	Atoms
2	A	2000	AGS	C5'-O5'-PA-O2A
2	A	2000	AGS	C5'-O5'-PA-O3A
2	A	2000	AGS	C4'-C5'-O5'-PA
2	A	2000	AGS	C3'-C4'-C5'-O5'
2	A	2000	AGS	O4'-C4'-C5'-O5'
2	B	2000	AGS	O4'-C4'-C5'-O5'
2	B	2000	AGS	C3'-C4'-C5'-O5'

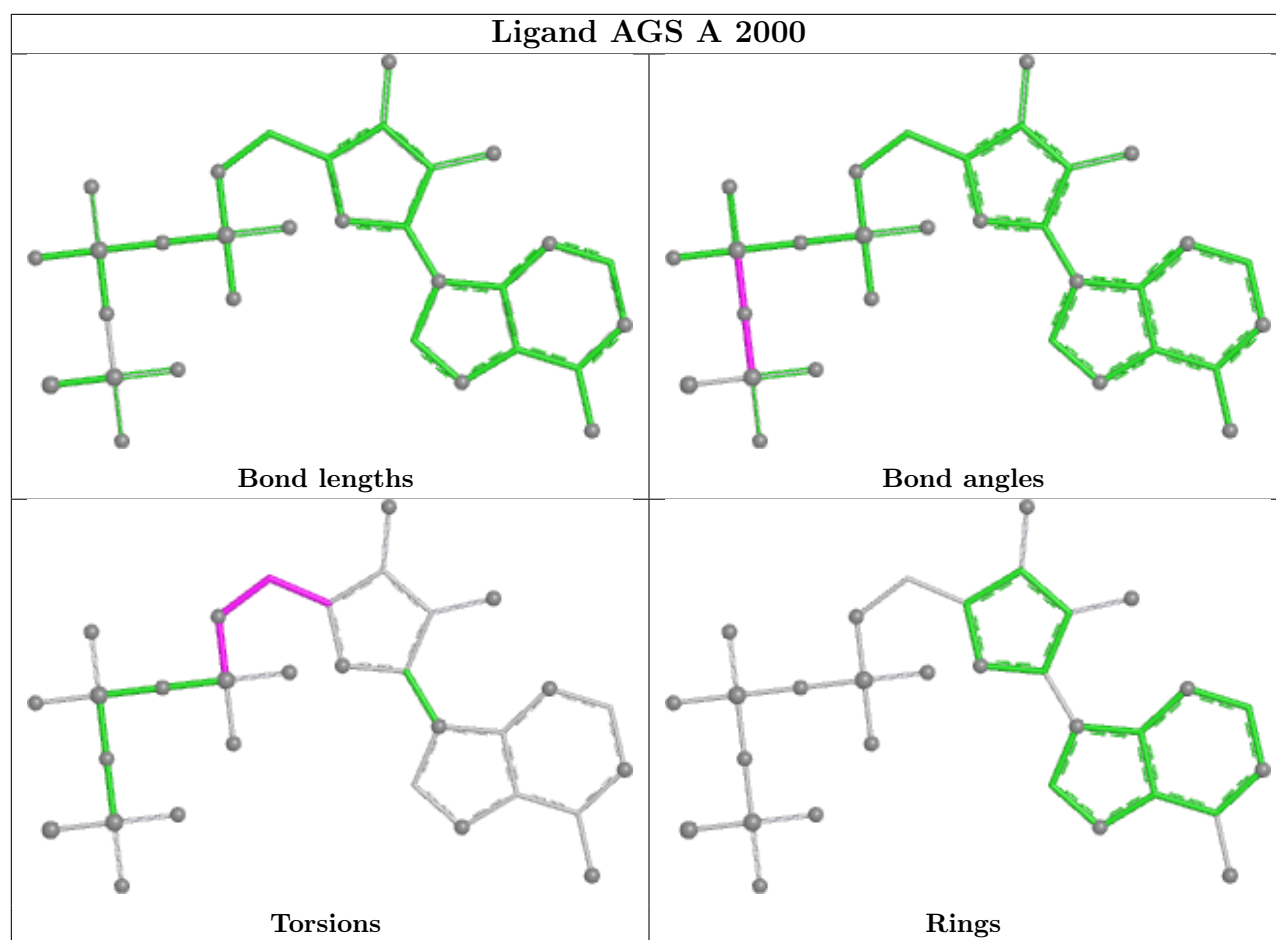
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2000	AGS	8	0
2	A	2000	AGS	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.

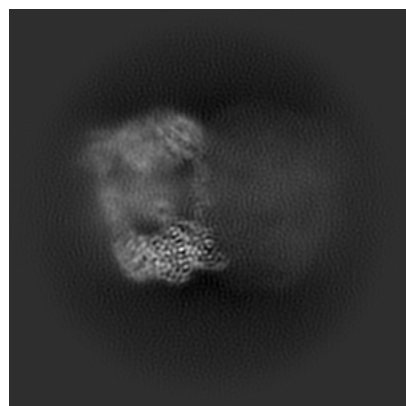
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75718. These allow visual inspection of the internal detail of the map and identification of artifacts.

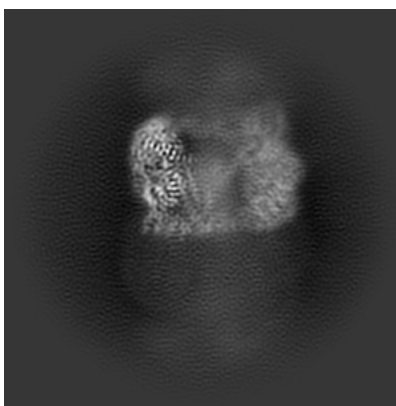
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

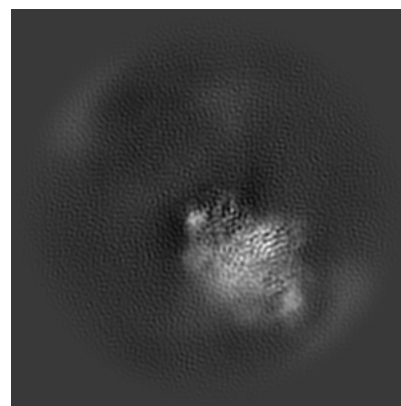
6.1.1 Primary map



X

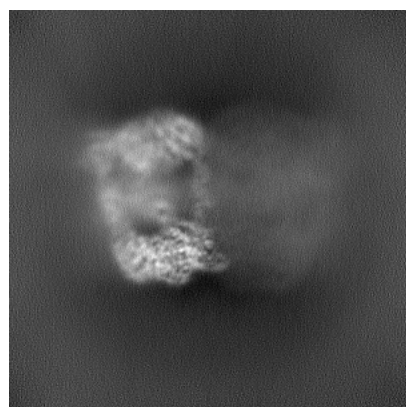


Y

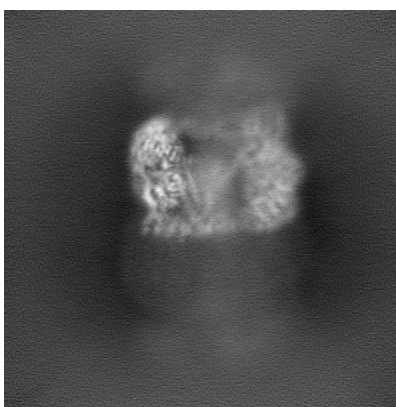


Z

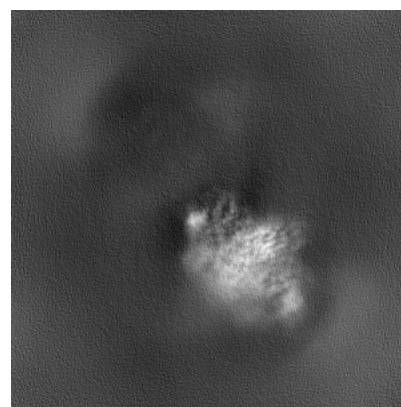
6.1.2 Raw map



X



Y

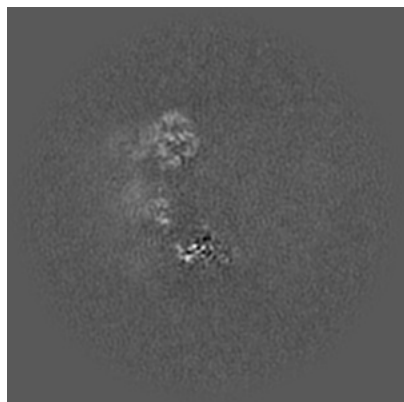


Z

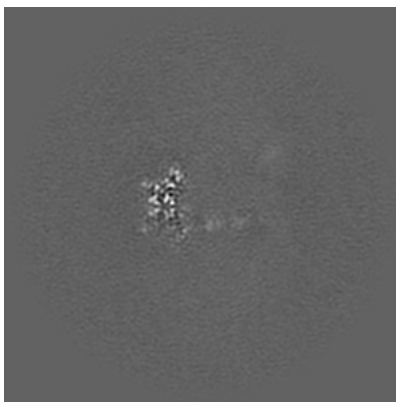
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

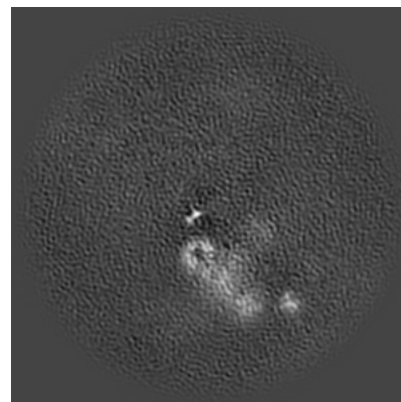
6.2.1 Primary map



X Index: 200



Y Index: 200

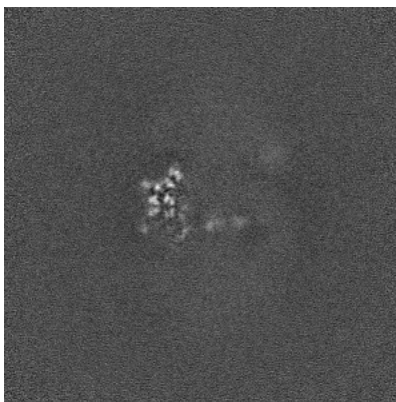


Z Index: 200

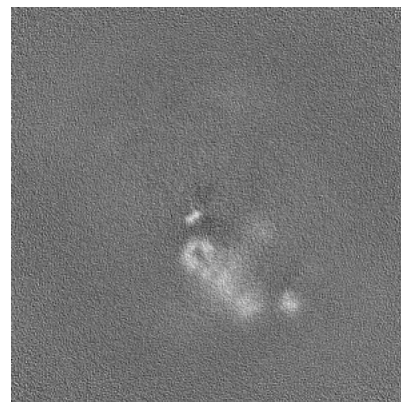
6.2.2 Raw map



X Index: 200



Y Index: 200

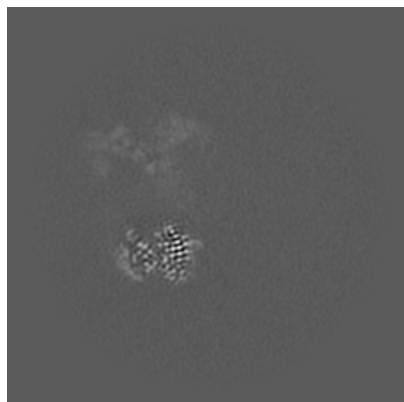


Z Index: 200

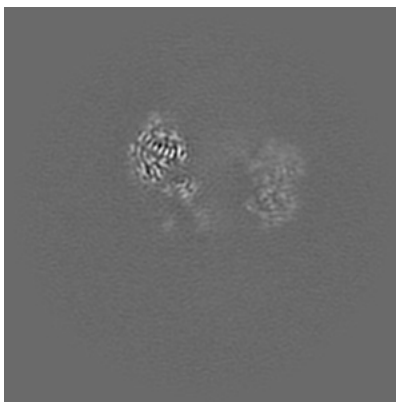
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

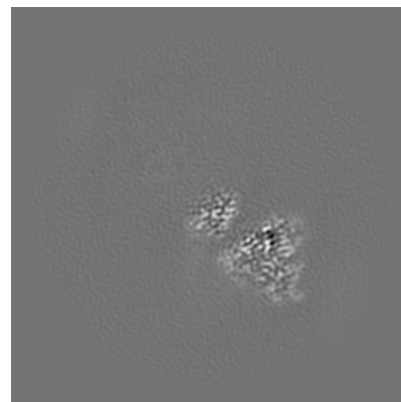
6.3.1 Primary map



X Index: 258

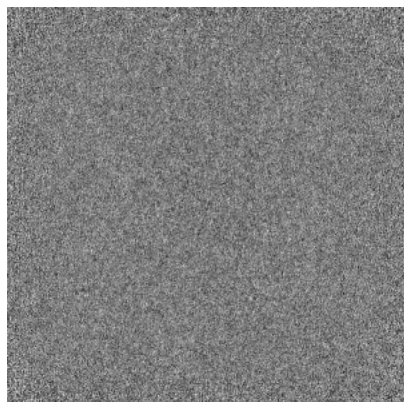


Y Index: 164

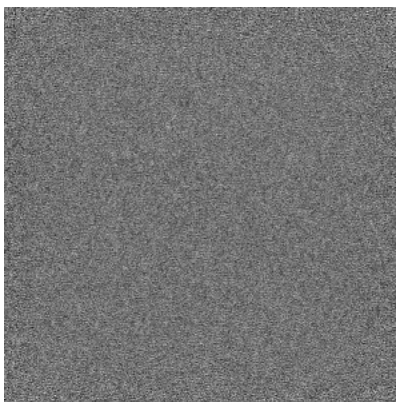


Z Index: 156

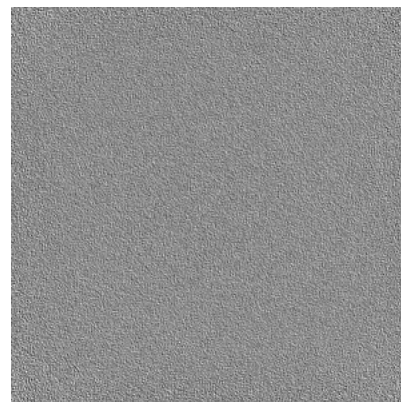
6.3.2 Raw map



X Index: 0



Y Index: 0

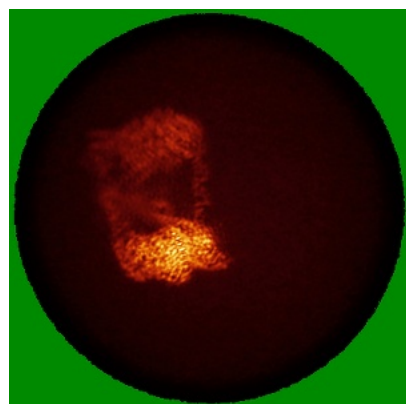


Z Index: 0

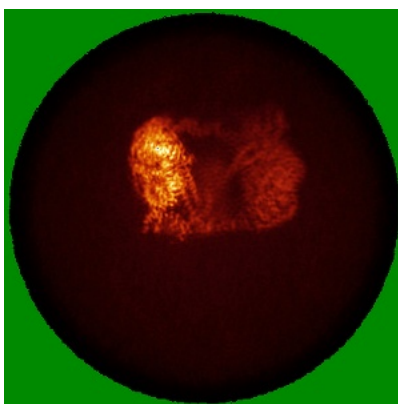
The images above show the largest variance slices of the map in three orthogonal directions.

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

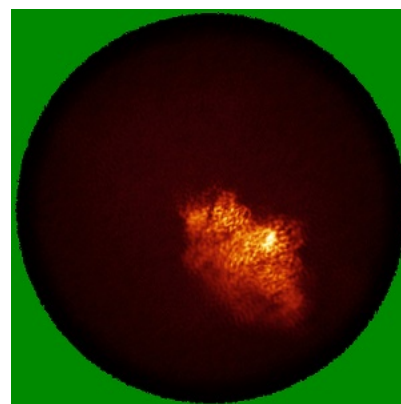
6.4.1 Primary map



X

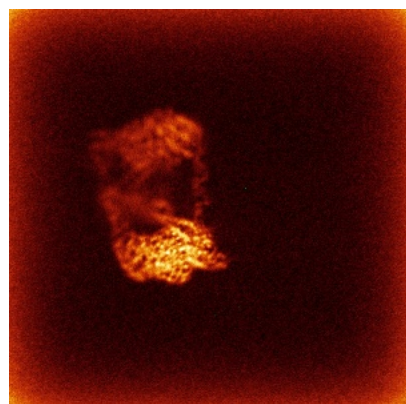


Y

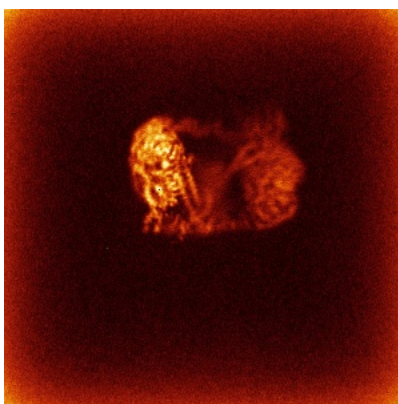


Z

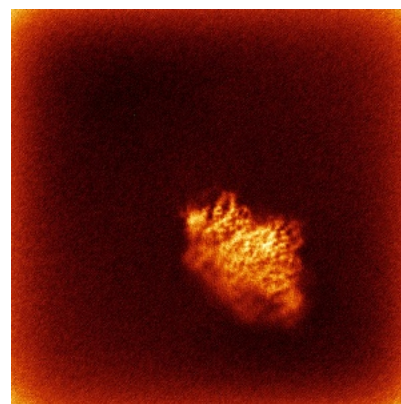
6.4.2 Raw map



X



Y

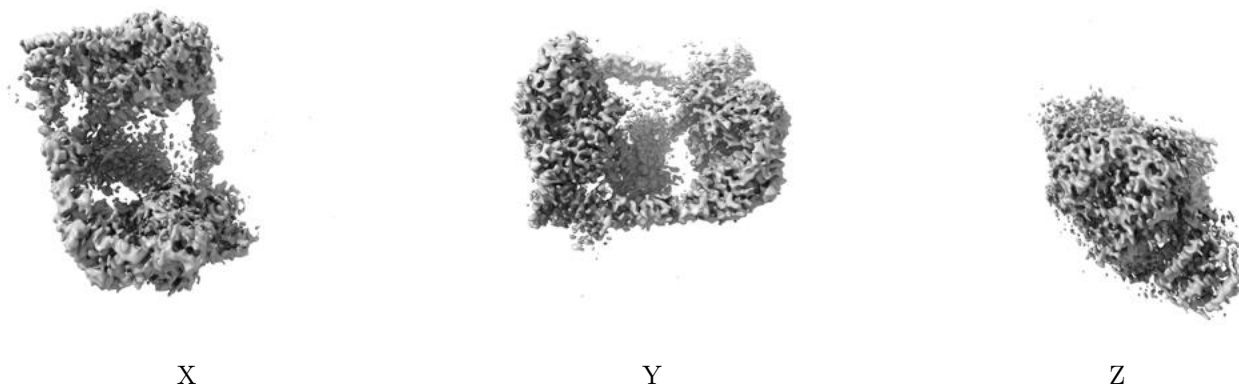


Z

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.

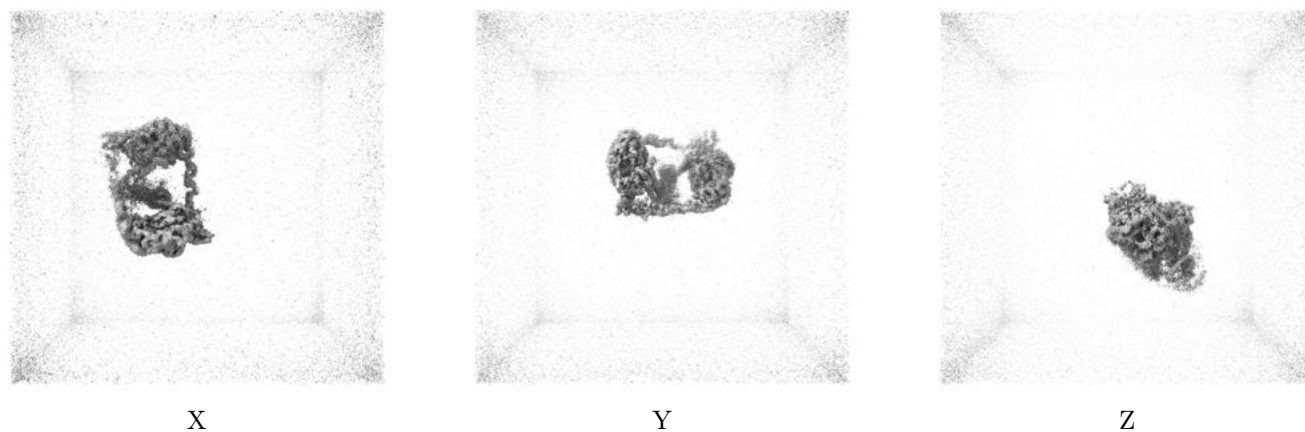
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. 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.

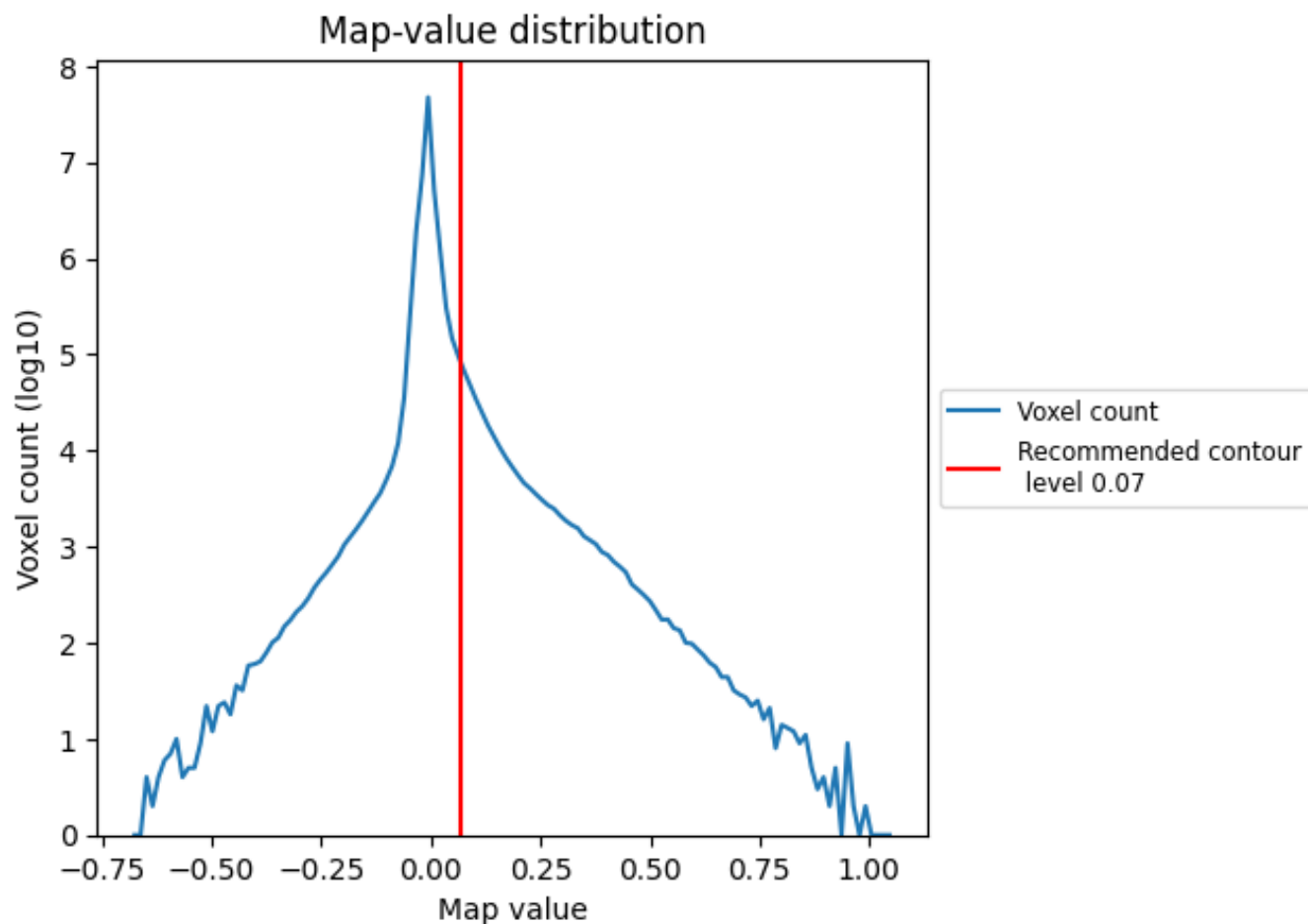
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

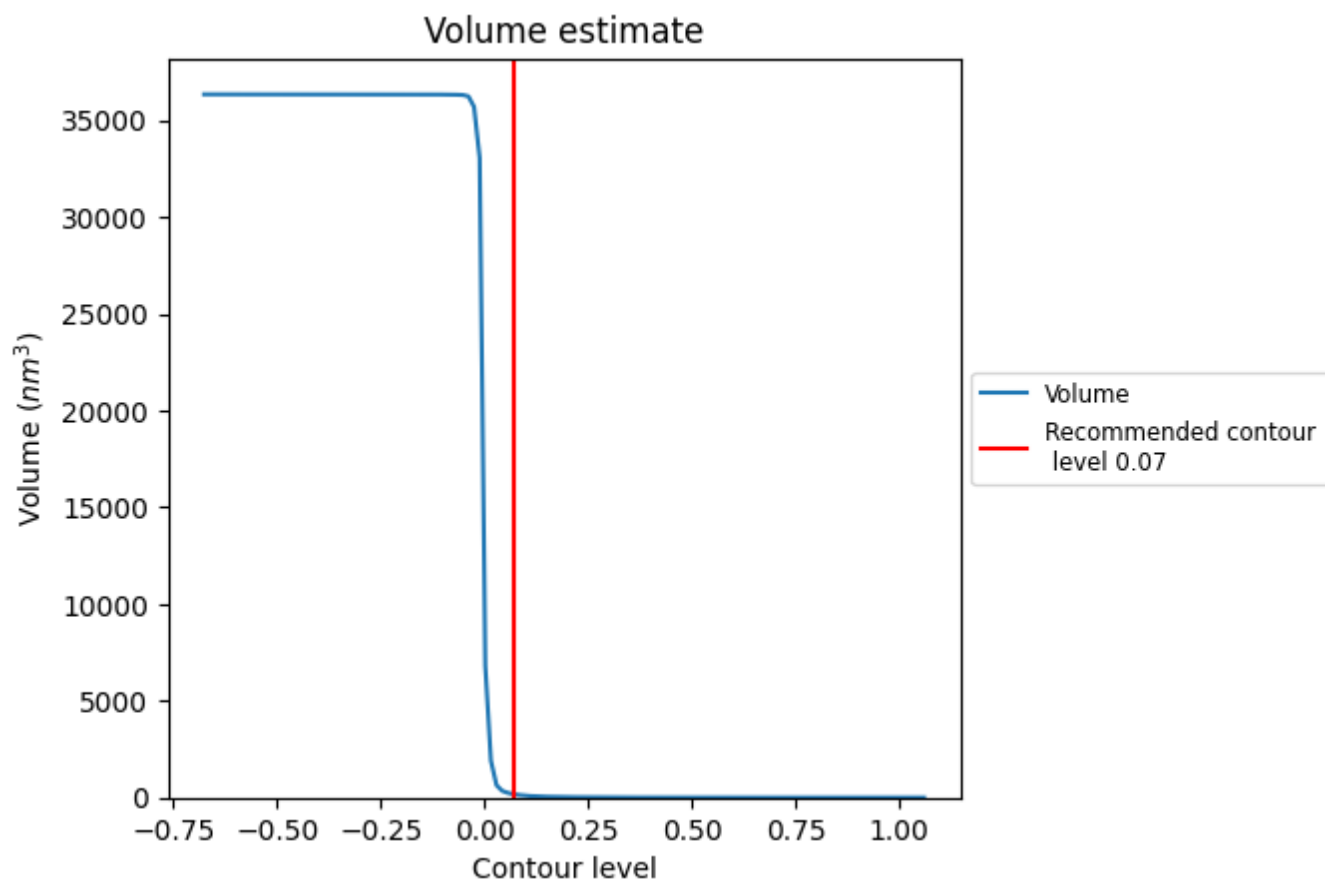
This section contains the results of statistical analysis of the map.

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.

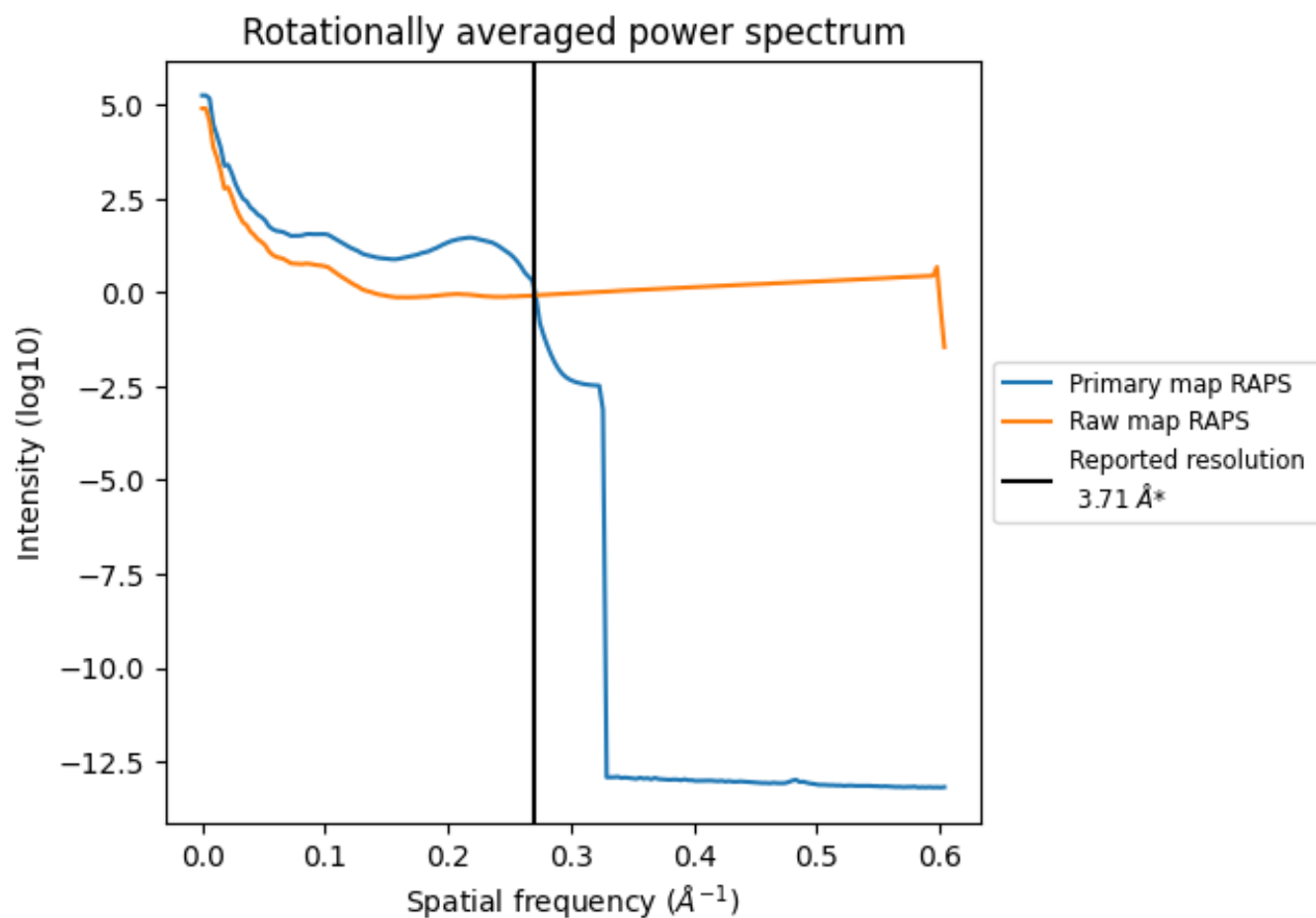
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 177 nm³; this corresponds to an approximate mass of 160 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 ⓘ

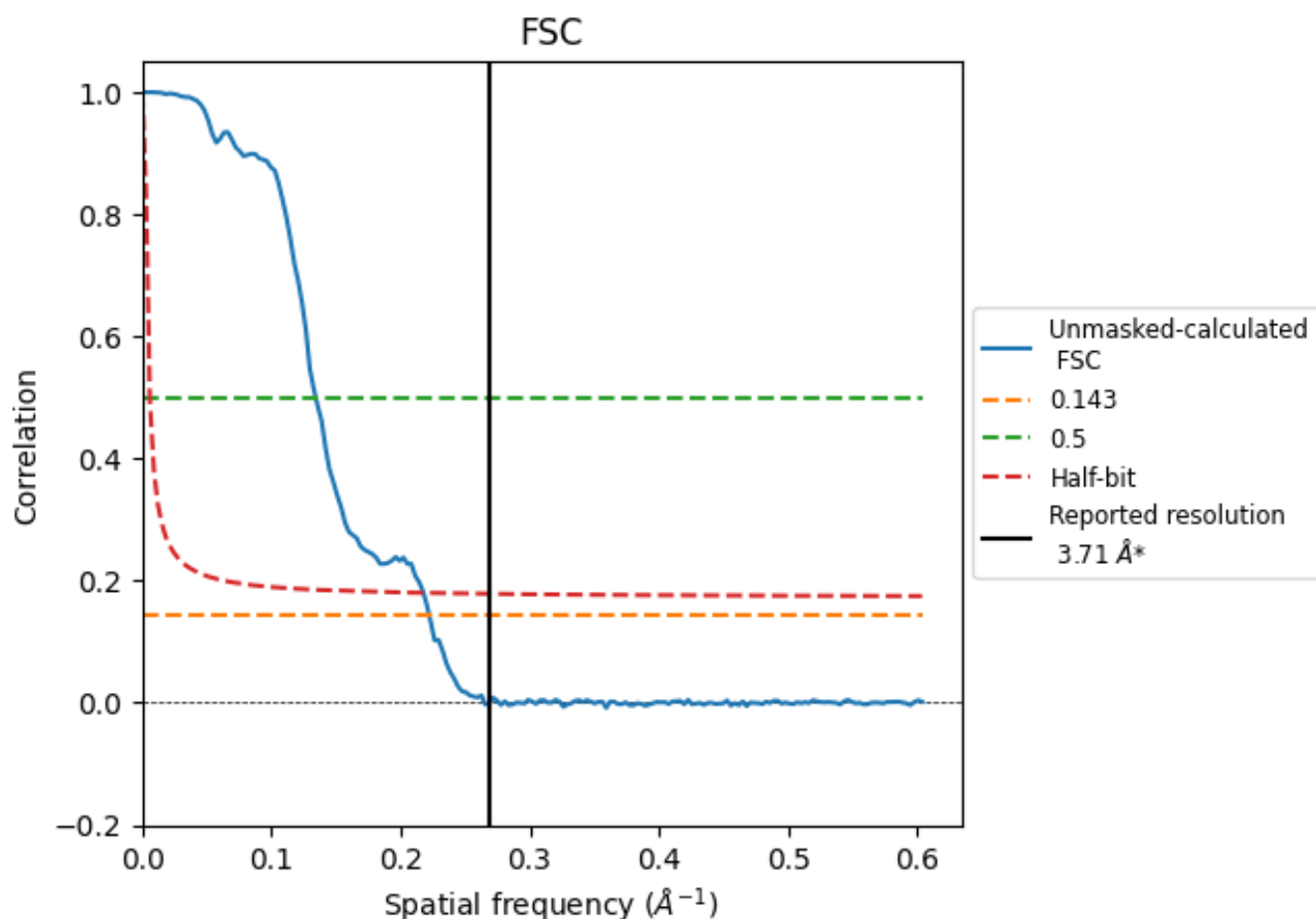


*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

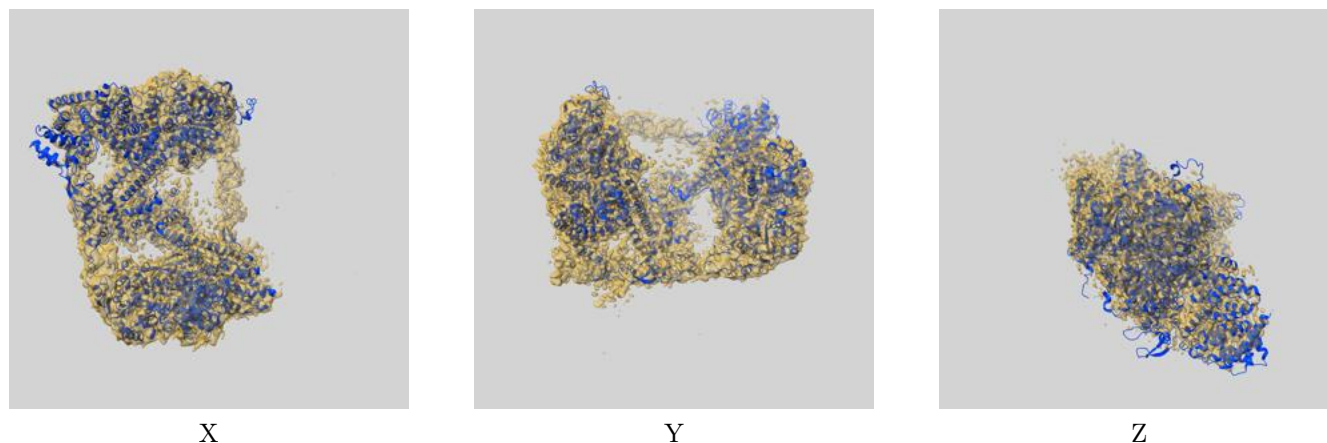
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.71	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.50	7.45	4.59

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.50 differs from the reported value 3.71 by more than 10 %

9 Map-model fit [i](#)

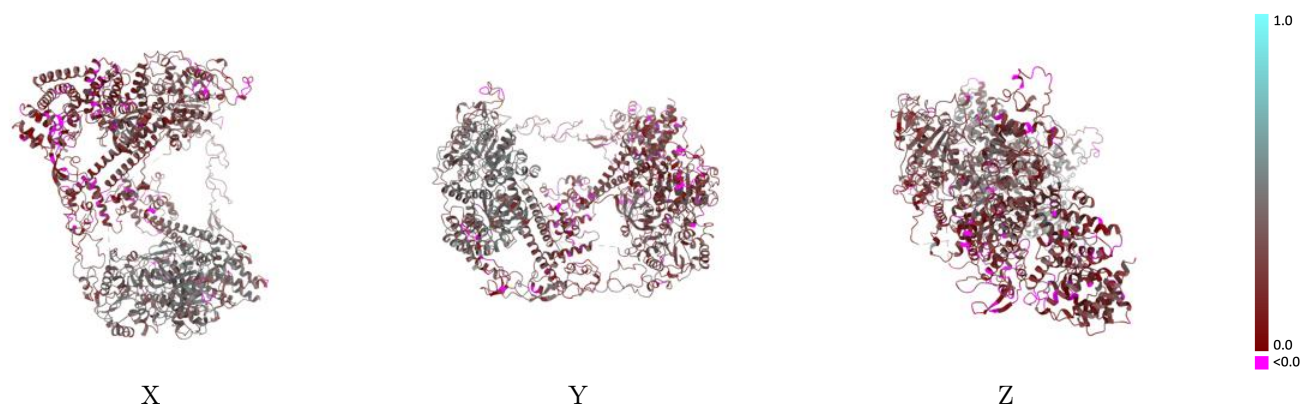
This section contains information regarding the fit between EMDB map EMD-75718 and PDB model 11IM. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



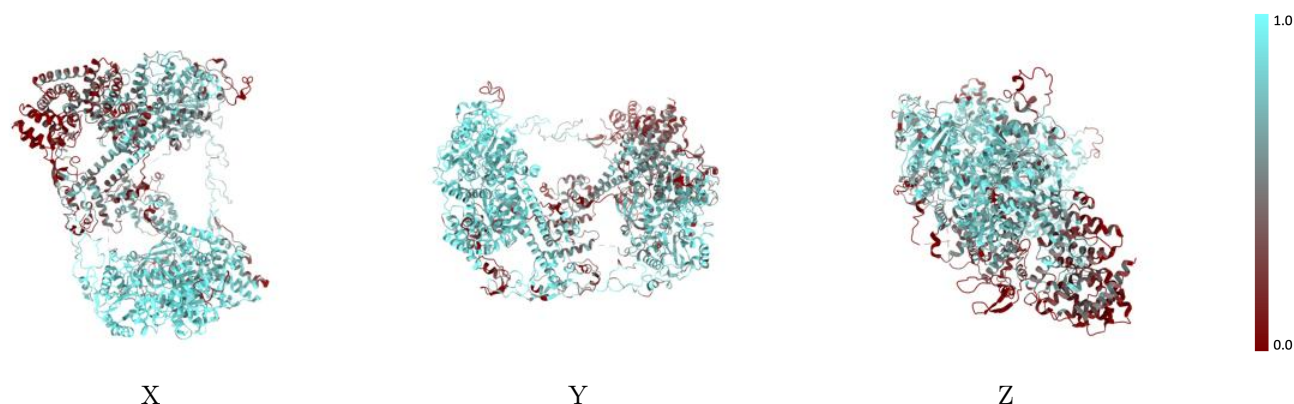
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



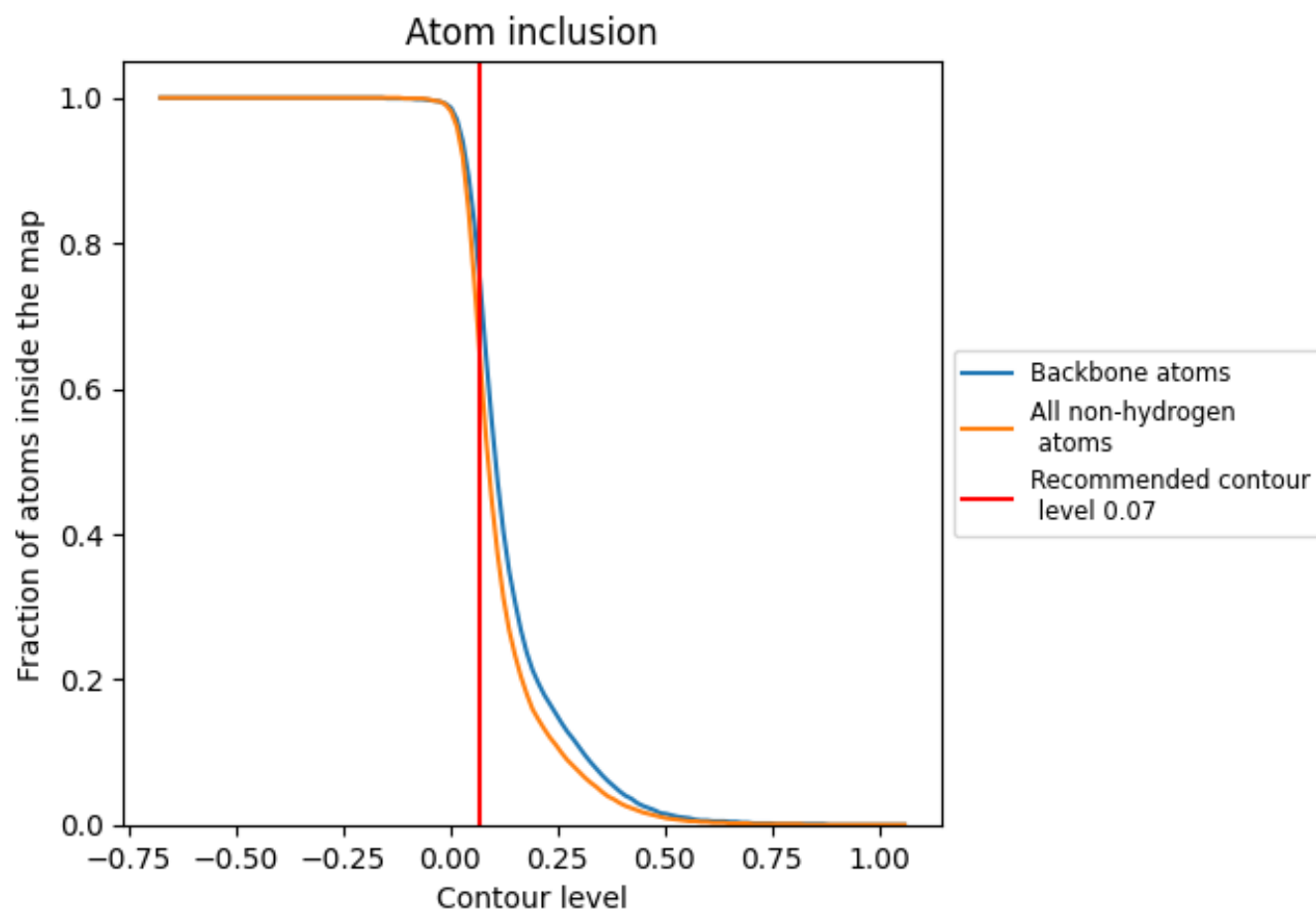
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 64% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6350	0.2910
A	0.7510	0.3560
B	0.5710	0.2380
C	0.2280	0.2000

