



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 02:07 AM UTC

PDB ID : 6D73 / pdb_00006d73
EMDB ID : EMD-7822
Title : Cryo-EM structure of the zebrafish TRPM2 channel in the presence of Ca²⁺
Authors : Yin, Y.; Wu, M.; Borschel, W.F.; Lander, G.C.; Lee, S.-Y.
Deposited on : 2018-04-23
Resolution : 3.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

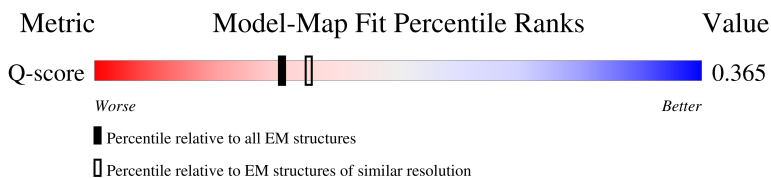
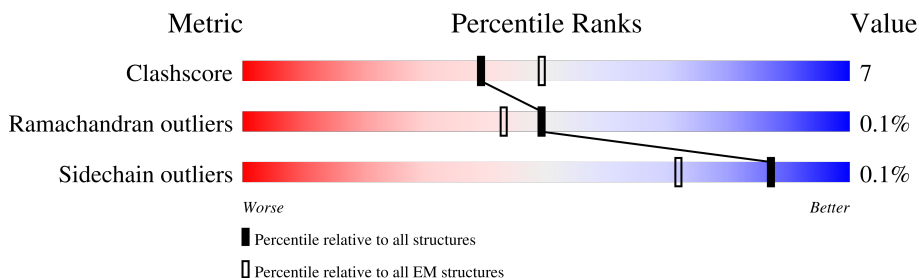
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	1466	
1	B	1466	
1	C	1466	
1	D	1466	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 35340 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 Transient receptor potential cation channel, subfamily M.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1256	Total	C	N	O	S	0	0
			8892	5756	1567	1534	35		
1	A	1227	Total	C	N	O	S	0	0
			8776	5690	1524	1523	39		
1	C	1227	Total	C	N	O	S	0	0
			8776	5690	1524	1523	39		
1	D	1256	Total	C	N	O	S	0	0
			8892	5756	1567	1534	35		

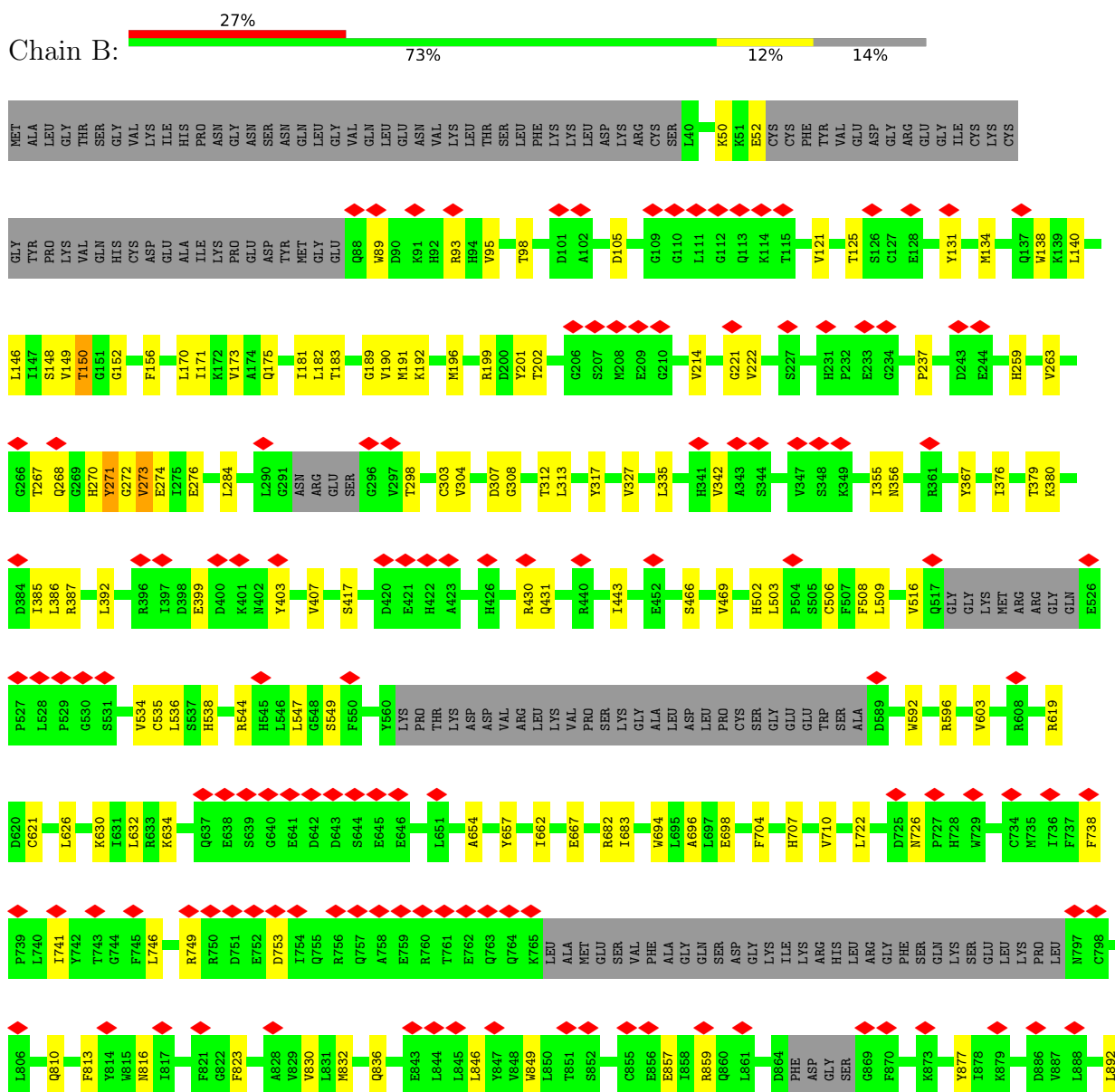
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
2	B	1	Total	Ca	0
			1	1	
2	A	1	Total	Ca	0
			1	1	
2	C	1	Total	Ca	0
			1	1	
2	D	1	Total	Ca	0
			1	1	

3 Residue-property plots

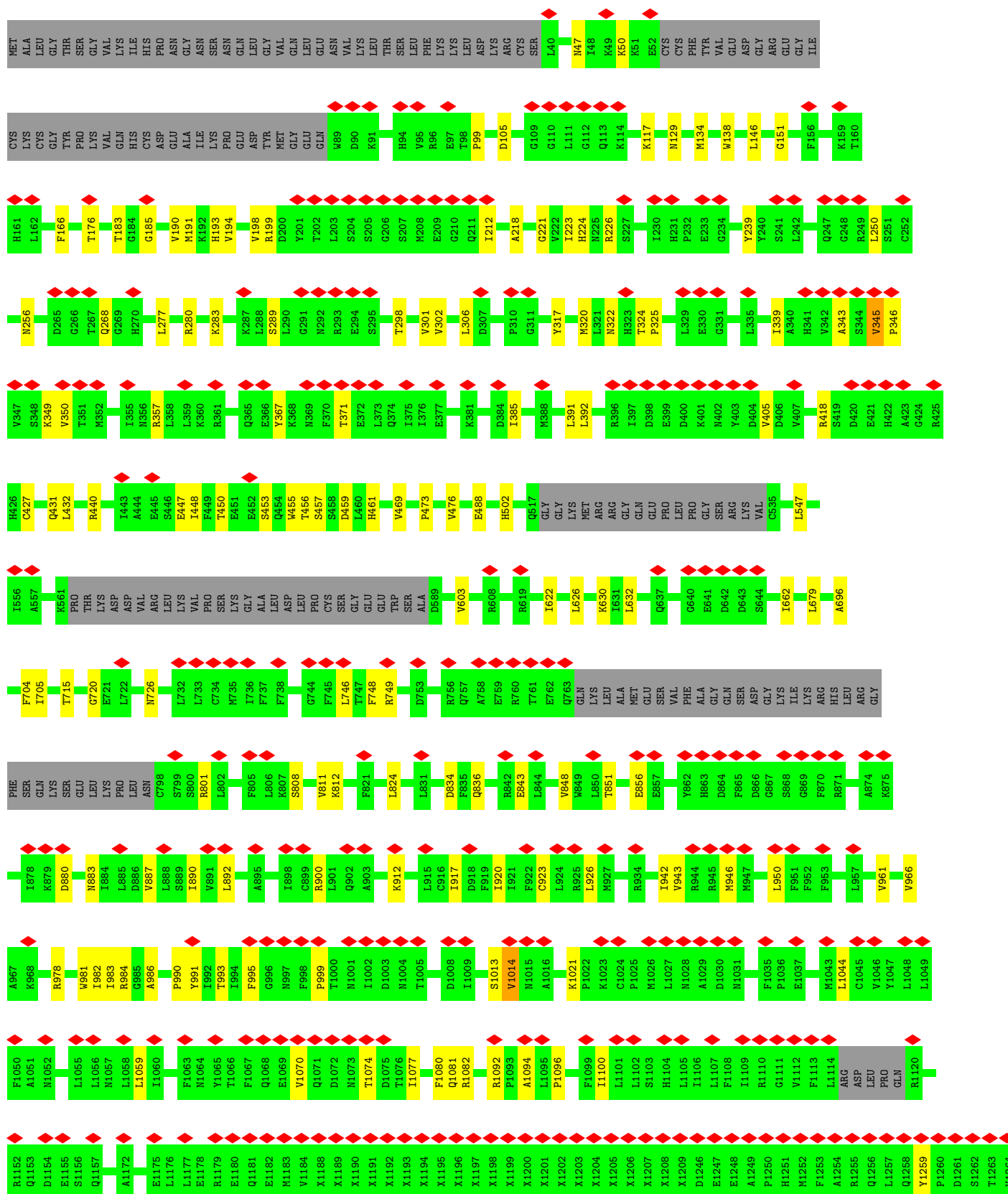
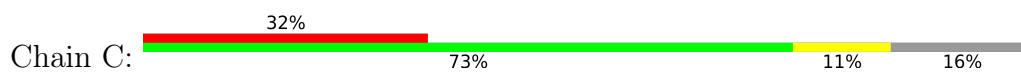
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Transient receptor potential cation channel, subfamily M









ALA	F805	L806	Q810	F813	M816	I817	A818	F821	G822	F823	A828	V829	V830	L831	M832	Q836	E843	L844	L845	L846	Y847	V848	W849	L850	T851	E856	R859	Q860	L861	Y862	H863	D864	PHE	ASP	GLY	SER	G869	F870	K873	K879	D886	V887	L888	L892	F893	I894	A895													
HIS	G896	L897	I898	C899	R900	L901	Q902	A903	S904	Y907	A908	F909	Y909	L915	C916	I917	I920	L924	R934	T935	L936	K939	Y943	R944	M947	L948	F952	L957	A963	E974	R978	L979	R980	W981	A986	P990	T993	I994	F995	G996	N997	F998	P999	T1000	M1001															
HIS	I1002	D1003	N1004	T1005	L1006	F1007	D1008	V1014	N1015	A1016	S1017	D1018	P1019	C1024	P1025	M1026	L1027	N1028	A1029	D1030	N1031	T1032	I1041	F1050	A1051	N1052	T1053	L1054	L1055	L1056	L1059	T1060	F1063	N1064	Y1065	Q1068	E1069	V1070	Q1071	D1072	N1073	T1074	D1075	T1076	I1077	W1078	Q1081	Y1089	H1090	S1091	R1092									
HIS	P1093	A1094	L1095	P1096	F1099	I1100	L1101	L1102	S1103	H1104	L1105	I1106	L1107	F1108	I1109	R1110	G1111	V1112	F1113	L1114	ARG	ASP	LEU	PRO	GLN	R1120	H1121	K1122	N1123	F1124	R1125	L1128	K1144	Y1147	D1154	L1176	L1177	E1178	R1179	E1180	Q1181	E1182	SER	ALA	LEU	ASP	K1303	H1304	R1305	N1306	P1307	G1308	L1309	R1310	T1311					
HIS	X1198	X1199	X1200	X1201	X1202	X1203	X1204	X1205	X1206	X1207	X1208	X1209	ASP	E1247	E1248	A1249	M1252	F1253	R1255	Q1256	L1257	D1261	S1262	R1266	F1267	P1268	W1276	E1277	S1281	Y1288	M1289	Q1290	Q1291	D1292	SER	SER	GLU	SER	ASP	THR	SER	ALA	LEU	ASP	K1303	H1304	R1305	N1306	P1307	G1308	L1309	R1310	T1311							
HIS	G1312	I1313	K1316	G1317	A1318	L1319	N1320	T1321	L1322	N1325	H1326	I1327	L1328	H1329	P1330	I1331	F1332	T1333	R1334	W1335	R1336	D1337	A1338	E1339	H1340	K1341	V1342	L1343	E1344	F1345	L1346	A1347	V1348	W1349	E1350	D1351	A1352	E1353	K1354	R1355	W1356	A1357	L1358	L1359	G1360	G1361	P1362	A1363	Q1364	P1365	D1366	GLU	PRO	L1369	A1370	Q1371	V1372	L1373		
HIS	E1374	R1375	I1376	L1377	G1378	K1379	K1380	L1381	ASN	GLU	LYS	THR	K1386	T1387	L1388	L1389	K1390	A1391	G1392	E1393	E1394	V1395	Y1396	K1397	G1398	Y1399	V1400	D1401	D1402	S1403	R1404	N1405	T1406	D1407	N1408	A1409	W1410	E1411	E1412	T1413	S1414	I1415	I1416	T1417	L1418	H1419	CYS	ASP	LYS	ASN	T1424	P1425	L1426	M1427	A1428	D1429	L1430	N1431	H1432	H1433
HIS	V1434	E1435	S1436	S1437	L1438	S1439	S1440	H1441	Q1442	P1443	L1444	Q1445	W1446	E1447	E1448	V1449	S1450	S1451	D1452	A1453	C1454	R1455	C1456	S1457	Y1458	Q1459	R1460	E1461	A1462	S1463	R1464	Q1465	I1466	A1467	H1468	H1469	H1470	ASN	THR	TYR	PHE	SER	ASN	SER	LEU	GLU	VAL	LEU	PHE	GLN	GLY	PRO	ASP	TYR	LYS	ASP	ASP	ASP	LYS	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	93573	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	63	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.135	Depositor
Minimum map value	-0.062	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	368.0, 368.0, 368.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.29	0/8871	0.60	3/12138 (0.0%)
1	B	0.30	0/8995	0.63	4/12326 (0.0%)
1	C	0.29	0/8871	0.60	3/12138 (0.0%)
1	D	0.30	0/8995	0.63	4/12326 (0.0%)
All	All	0.30	0/35732	0.62	14/48928 (0.0%)

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	2
1	C	0	2
All	All	0	4

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	272	GLY	N-CA-C	12.40	129.49	113.24
1	B	272	GLY	N-CA-C	12.35	129.42	113.24
1	B	502	HIS	N-CA-C	8.87	123.83	112.92
1	D	502	HIS	N-CA-C	8.85	123.80	112.92
1	D	273	VAL	N-CA-C	7.32	118.08	110.62
1	B	273	VAL	N-CA-C	7.27	118.03	110.62
1	D	271	TYR	N-CA-C	6.57	118.53	111.36
1	B	271	TYR	N-CA-C	6.56	118.51	111.36
1	A	1259	TYR	N-CA-C	-5.68	103.49	110.31
1	C	1259	TYR	N-CA-C	-5.64	103.54	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1014	VAL	N-CA-C	5.40	120.57	109.34
1	A	1014	VAL	N-CA-C	5.38	120.52	109.34
1	A	345	VAL	CB-CA-C	-5.13	108.91	114.35
1	C	345	VAL	CB-CA-C	-5.13	108.92	114.35

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1013	SER	Peptide
1	A	1021	LYS	Peptide
1	C	1013	SER	Peptide
1	C	1021	LYS	Peptide

5.2 Too-close contacts ⓘ

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	8776	0	7824	113	0
1	B	8892	0	7798	141	0
1	C	8776	0	7824	108	0
1	D	8892	0	7798	139	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	35340	0	31244	482	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 7.

All (482) 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:C:346:PRO:HB2	1:C:349:LYS:CB	1.43	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:PRO:HB2	1:A:349:LYS:CB	1.43	1.44
1:D:156:PHE:HE1	1:D:189:GLY:C	1.46	1.23
1:B:156:PHE:HE1	1:B:189:GLY:C	1.46	1.21
1:C:367:TYR:O	1:C:371:THR:HG23	1.40	1.20
1:B:156:PHE:HE1	1:B:189:GLY:CA	1.57	1.18
1:D:156:PHE:HE1	1:D:189:GLY:CA	1.57	1.16
1:A:367:TYR:O	1:A:371:THR:HG23	1.40	1.14
1:D:156:PHE:CE1	1:D:189:GLY:C	2.27	1.13
1:B:156:PHE:CE1	1:B:189:GLY:C	2.27	1.12
1:C:346:PRO:CB	1:C:349:LYS:CB	2.27	1.12
1:A:346:PRO:CB	1:A:349:LYS:CB	2.27	1.12
1:D:149:VAL:HG22	1:D:304:VAL:CG2	1.80	1.11
1:B:149:VAL:HG22	1:B:304:VAL:CG2	1.80	1.10
1:D:149:VAL:HG22	1:D:304:VAL:HG22	1.34	1.08
1:B:222:VAL:HG11	1:B:271:TYR:CE1	1.91	1.06
1:D:222:VAL:HG11	1:D:271:TYR:CE1	1.91	1.05
1:B:149:VAL:HG22	1:B:304:VAL:HG22	1.34	1.02
1:B:156:PHE:CE1	1:B:189:GLY:HA2	1.97	1.00
1:D:156:PHE:CE1	1:D:189:GLY:HA2	1.97	0.99
1:C:367:TYR:CD1	1:C:371:THR:HG22	1.98	0.99
1:B:156:PHE:CE1	1:B:189:GLY:CA	2.45	0.98
1:D:50:LYS:HB3	1:D:98:THR:O	1.64	0.98
1:B:156:PHE:CE1	1:B:190:VAL:N	2.32	0.98
1:A:367:TYR:CD1	1:A:371:THR:HG22	1.97	0.97
1:D:156:PHE:CE1	1:D:189:GLY:CA	2.45	0.97
1:D:156:PHE:CE1	1:D:190:VAL:N	2.32	0.97
1:B:50:LYS:HB3	1:B:98:THR:O	1.64	0.95
1:B:156:PHE:HE1	1:B:189:GLY:HA2	1.31	0.92
1:A:367:TYR:O	1:A:371:THR:CG2	2.18	0.92
1:C:367:TYR:O	1:C:371:THR:CG2	2.18	0.90
1:D:156:PHE:HE1	1:D:189:GLY:HA2	1.31	0.90
1:D:222:VAL:CG1	1:D:271:TYR:CE1	2.57	0.88
1:B:222:VAL:CG1	1:B:271:TYR:CE1	2.56	0.88
1:D:105:ASP:O	1:D:237:PRO:HA	1.74	0.87
1:B:105:ASP:O	1:B:237:PRO:HA	1.74	0.86
1:B:152:GLY:H	1:B:308:GLY:HA2	1.40	0.86
1:D:152:GLY:H	1:D:308:GLY:HA2	1.40	0.85
1:A:991:TYR:HD1	1:A:995:PHE:CZ	1.96	0.84
1:C:991:TYR:HD1	1:C:995:PHE:CZ	1.96	0.82
1:C:367:TYR:CD1	1:C:371:THR:CG2	2.65	0.80
1:A:367:TYR:CD1	1:A:371:THR:CG2	2.65	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:VAL:HG13	1:B:304:VAL:HG23	1.65	0.77
1:D:149:VAL:HG13	1:D:304:VAL:HG23	1.65	0.76
1:C:350:VAL:HG12	1:C:350:VAL:O	1.86	0.76
1:A:367:TYR:CE1	1:A:371:THR:HG22	2.21	0.75
1:D:148:SER:O	1:D:303:CYS:HA	1.86	0.75
1:C:367:TYR:CE1	1:C:371:THR:HG22	2.21	0.75
1:B:148:SER:O	1:B:303:CYS:HA	1.86	0.74
1:A:350:VAL:HG12	1:A:350:VAL:O	1.86	0.74
1:A:367:TYR:CE1	1:A:371:THR:CG2	2.74	0.70
1:D:267:THR:HG22	1:D:270:HIS:CE1	2.27	0.70
1:C:367:TYR:CE1	1:C:371:THR:CG2	2.74	0.69
1:B:267:THR:HG22	1:B:270:HIS:CE1	2.27	0.69
1:D:506:CYS:SG	1:D:508:PHE:HB3	2.34	0.68
1:D:1006:LEU:HD12	1:D:1008:ASP:H	1.59	0.68
1:B:832:MET:HE3	1:C:966:VAL:HG23	1.76	0.68
1:A:345:VAL:N	1:A:346:PRO:HD2	2.09	0.68
1:C:345:VAL:N	1:C:346:PRO:HD2	2.09	0.68
1:B:152:GLY:N	1:B:308:GLY:HA2	2.08	0.67
1:B:506:CYS:SG	1:B:508:PHE:HB3	2.34	0.67
1:D:317:TYR:HA	1:D:385:ILE:HD11	1.76	0.67
1:D:152:GLY:N	1:D:308:GLY:HA2	2.08	0.67
1:B:1006:LEU:HD12	1:B:1008:ASP:H	1.59	0.66
1:B:317:TYR:HA	1:B:385:ILE:HD11	1.77	0.66
1:C:961:VAL:HG11	1:C:991:TYR:CE2	2.32	0.65
1:C:47:ASN:HB3	1:C:129:ASN:HD21	1.61	0.65
1:D:222:VAL:HG11	1:D:271:TYR:HE1	1.59	0.65
1:A:47:ASN:HB3	1:A:129:ASN:HD21	1.61	0.65
1:B:222:VAL:HG11	1:B:271:TYR:HE1	1.59	0.64
1:A:961:VAL:HG11	1:A:991:TYR:CE2	2.32	0.64
1:C:1077:ILE:HG22	1:C:1081:GLN:HE22	1.61	0.64
1:A:1077:ILE:HG22	1:A:1081:GLN:HE22	1.61	0.64
1:A:339:ILE:O	1:A:343:ALA:HB2	1.98	0.64
1:C:339:ILE:O	1:C:343:ALA:HB2	1.98	0.63
1:B:52:GLU:O	1:B:95:VAL:HA	1.98	0.63
1:D:52:GLU:O	1:D:95:VAL:HA	1.98	0.62
1:D:267:THR:HG22	1:D:270:HIS:HE1	1.64	0.62
1:D:156:PHE:CZ	1:D:190:VAL:HA	2.35	0.62
1:C:289:SER:HA	1:C:298:THR:HA	1.81	0.62
1:D:1426:LEU:O	1:D:1431:ASN:ND2	2.33	0.62
1:B:1333:THR:HG23	1:B:1419:HIS:HB2	1.82	0.62
1:B:267:THR:CG2	1:B:270:HIS:CE1	2.83	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:VAL:CG2	1:D:304:VAL:CG2	2.69	0.62
1:A:978:ARG:HD2	1:A:981:TRP:HB2	1.81	0.61
1:C:978:ARG:HD2	1:C:981:TRP:HB2	1.81	0.61
1:B:1095:LEU:HD23	1:B:1103:SER:HB3	1.83	0.61
1:D:1095:LEU:HD23	1:D:1103:SER:HB3	1.82	0.61
1:B:156:PHE:CZ	1:B:190:VAL:HA	2.35	0.61
1:D:267:THR:CG2	1:D:270:HIS:CE1	2.83	0.61
1:D:156:PHE:HB2	1:D:307:ASP:CB	2.31	0.61
1:B:267:THR:HG22	1:B:270:HIS:HE1	1.64	0.61
1:B:1426:LEU:O	1:B:1431:ASN:ND2	2.33	0.61
1:A:961:VAL:HG22	1:A:990:PRO:HB2	1.83	0.61
1:B:156:PHE:HB2	1:B:307:ASP:CB	2.31	0.61
1:C:961:VAL:HG22	1:C:990:PRO:HB2	1.83	0.61
1:D:1333:THR:HG23	1:D:1419:HIS:HB2	1.82	0.60
1:A:289:SER:HA	1:A:298:THR:HA	1.81	0.60
1:B:974:GLU:O	1:A:912:LYS:NZ	2.35	0.59
1:C:843:GLU:OE2	1:C:900:ARG:NH1	2.35	0.59
1:A:991:TYR:CD1	1:A:995:PHE:CZ	2.86	0.59
1:C:912:LYS:NZ	1:D:974:GLU:O	2.34	0.59
1:D:694:TRP:O	1:D:698:GLU:HB2	2.02	0.59
1:C:357:ARG:NH1	1:C:367:TYR:OH	2.35	0.59
1:C:991:TYR:CD1	1:C:995:PHE:CZ	2.86	0.59
1:B:694:TRP:O	1:B:698:GLU:HB2	2.02	0.59
1:A:843:GLU:OE2	1:A:900:ARG:NH1	2.35	0.59
1:B:892:LEU:HD21	1:B:917:ILE:HG23	1.85	0.59
1:B:990:PRO:HA	1:B:993:THR:HG22	1.85	0.59
1:D:313:LEU:HD13	1:D:335:LEU:HD11	1.85	0.59
1:C:190:VAL:HA	1:C:193:HIS:HD2	1.67	0.59
1:C:1059:LEU:HG	1:D:1060:ILE:HD11	1.85	0.59
1:D:662:ILE:HG22	1:D:704:PHE:HD1	1.68	0.59
1:D:990:PRO:HA	1:D:993:THR:HG22	1.85	0.59
1:B:149:VAL:CG2	1:B:304:VAL:CG2	2.69	0.59
1:A:357:ARG:NH1	1:A:367:TYR:OH	2.35	0.58
1:C:715:THR:OG1	1:C:1082:ARG:NH2	2.36	0.58
1:B:662:ILE:HG22	1:B:704:PHE:HD1	1.68	0.58
1:A:715:THR:OG1	1:A:1082:ARG:NH2	2.36	0.58
1:D:978:ARG:NH1	1:D:1015:ASN:O	2.36	0.58
1:C:185:GLY:HA3	1:C:218:ALA:HB2	1.86	0.58
1:C:350:VAL:O	1:C:350:VAL:CG1	2.52	0.58
1:B:313:LEU:HD13	1:B:335:LEU:HD11	1.85	0.58
1:B:978:ARG:NH1	1:B:1015:ASN:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:ILE:O	1:D:175:GLN:HB2	2.04	0.57
1:B:1060:ILE:HD11	1:A:1059:LEU:HG	1.86	0.57
1:A:190:VAL:HA	1:A:193:HIS:HD2	1.67	0.57
1:A:720:GLY:O	1:A:749:ARG:NH1	2.37	0.57
1:D:836:GLN:O	1:D:900:ARG:NH2	2.36	0.57
1:A:457:SER:O	1:A:461:HIS:ND1	2.37	0.57
1:C:720:GLY:O	1:C:749:ARG:NH1	2.37	0.57
1:B:171:ILE:O	1:B:175:GLN:HB2	2.04	0.57
1:A:418:ARG:NH1	1:A:447:GLU:OE2	2.38	0.57
1:A:982:ILE:O	1:A:986:ALA:HB2	2.04	0.57
1:D:892:LEU:HD21	1:D:917:ILE:HG23	1.85	0.57
1:C:982:ILE:O	1:C:986:ALA:HB2	2.04	0.57
1:D:1096:PRO:O	1:D:1100:ILE:N	2.38	0.57
1:A:221:GLY:HA3	1:A:268:GLN:HA	1.87	0.57
1:A:836:GLN:O	1:A:900:ARG:NH2	2.38	0.57
1:C:418:ARG:NH1	1:C:447:GLU:OE2	2.38	0.57
1:C:920:ILE:HG22	1:D:963:ALA:HB1	1.86	0.57
1:C:151:GLY:HA3	1:C:190:VAL:HG11	1.87	0.56
1:D:171:ILE:HD12	1:D:201:TYR:HB2	1.87	0.56
1:A:185:GLY:HA3	1:A:218:ALA:HB2	1.86	0.56
1:B:171:ILE:HD12	1:B:201:TYR:HB2	1.87	0.56
1:B:626:LEU:HD13	1:B:696:ALA:HB2	1.88	0.56
1:B:816:ASN:ND2	1:B:1089:TYR:OH	2.37	0.56
1:B:963:ALA:HB1	1:A:920:ILE:HG22	1.87	0.56
1:A:350:VAL:O	1:A:350:VAL:CG1	2.52	0.56
1:D:222:VAL:HG13	1:D:271:TYR:CZ	2.39	0.56
1:B:222:VAL:HG13	1:B:271:TYR:CZ	2.39	0.56
1:C:221:GLY:HA3	1:C:268:GLN:HA	1.87	0.56
1:D:816:ASN:ND2	1:D:1089:TYR:OH	2.37	0.56
1:B:1096:PRO:O	1:B:1100:ILE:N	2.38	0.56
1:A:301:VAL:O	1:A:324:THR:OG1	2.22	0.56
1:D:503:LEU:O	1:D:509:LEU:HD12	2.06	0.55
1:C:836:GLN:O	1:C:900:ARG:NH2	2.38	0.55
1:D:667:GLU:HG3	1:D:1147:TYR:HB2	1.87	0.55
1:B:503:LEU:O	1:B:509:LEU:HD12	2.06	0.55
1:A:151:GLY:HA3	1:A:190:VAL:HG11	1.87	0.55
1:D:626:LEU:HD13	1:D:696:ALA:HB2	1.88	0.55
1:B:667:GLU:HG3	1:B:1147:TYR:HB2	1.88	0.55
1:D:156:PHE:CZ	1:D:190:VAL:CA	2.90	0.55
1:B:619:ARG:NH2	1:C:239:TYR:OH	2.38	0.55
1:D:150:THR:OG1	1:D:312:THR:HA	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:836:GLN:O	1:B:900:ARG:NH2	2.36	0.54
1:D:1252:MET:HA	1:D:1255:ARG:HD3	1.89	0.54
1:B:131:TYR:HB2	1:B:284:LEU:HD21	1.90	0.54
1:A:1026:MET:HE3	1:D:909:TYR:CE1	2.43	0.54
1:B:170:LEU:HA	1:B:173:VAL:HG22	1.90	0.54
1:D:222:VAL:HG13	1:D:271:TYR:CE1	2.43	0.54
1:B:156:PHE:CZ	1:B:190:VAL:CA	2.90	0.54
1:D:192:LYS:HG2	1:D:196:MET:HE2	1.89	0.54
1:B:1041:ILE:HD11	1:A:983:ILE:HG23	1.89	0.54
1:C:983:ILE:HG23	1:D:1041:ILE:HD11	1.89	0.53
1:B:150:THR:OG1	1:B:312:THR:HA	2.07	0.53
1:B:192:LYS:HG2	1:B:196:MET:HE2	1.89	0.53
1:A:432:LEU:HD13	1:A:448:ILE:HD11	1.91	0.53
1:C:301:VAL:O	1:C:324:THR:OG1	2.22	0.53
1:C:1096:PRO:O	1:C:1100:ILE:N	2.41	0.53
1:D:170:LEU:HA	1:D:173:VAL:HG22	1.90	0.53
1:D:1095:LEU:HD12	1:D:1096:PRO:HD2	1.91	0.53
1:D:547:LEU:O	1:D:630:LYS:NZ	2.39	0.53
1:B:1252:MET:HA	1:B:1255:ARG:HD3	1.89	0.53
1:A:1026:MET:HE3	1:D:909:TYR:HE1	1.74	0.53
1:B:1257:LEU:HA	1:B:1266:ARG:HG2	1.90	0.53
1:C:824:LEU:HD11	1:C:926:LEU:HD11	1.91	0.53
1:A:1096:PRO:O	1:A:1100:ILE:N	2.41	0.52
1:D:830:VAL:HG11	1:D:846:LEU:HD22	1.91	0.52
1:A:277:LEU:HA	1:A:280:ARG:HG2	1.91	0.52
1:C:432:LEU:HD13	1:C:448:ILE:HD11	1.91	0.52
1:D:131:TYR:HB2	1:D:284:LEU:HD21	1.90	0.52
1:B:830:VAL:HG11	1:B:846:LEU:HD22	1.91	0.52
1:C:457:SER:O	1:C:461:HIS:ND1	2.37	0.52
1:B:1095:LEU:HD12	1:B:1096:PRO:HD2	1.91	0.52
1:A:547:LEU:O	1:A:630:LYS:NZ	2.43	0.52
1:A:1070:VAL:O	1:A:1074:THR:HB	2.10	0.52
1:B:222:VAL:HG13	1:B:271:TYR:CE1	2.43	0.52
1:B:149:VAL:HG22	1:B:304:VAL:HG23	1.85	0.52
1:B:1006:LEU:HD21	1:B:1032:THR:CB	2.40	0.52
1:D:1006:LEU:HD21	1:D:1032:THR:CB	2.40	0.52
1:B:140:LEU:HD21	1:B:259:HIS:HE1	1.75	0.52
1:A:1319:LEU:HD23	1:A:1325:ASN:HD22	1.75	0.52
1:A:824:LEU:HD11	1:A:926:LEU:HD11	1.91	0.52
1:C:277:LEU:HA	1:C:280:ARG:HG2	1.92	0.52
1:B:813:PHE:HD1	1:B:1089:TYR:HE2	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:503:LEU:O	1:D:509:LEU:CD1	2.58	0.52
1:D:547:LEU:HD12	1:D:630:LYS:HD3	1.92	0.52
1:D:1257:LEU:HA	1:D:1266:ARG:HG2	1.90	0.52
1:C:456:THR:HG23	1:C:459:ASP:H	1.75	0.51
1:C:1070:VAL:O	1:C:1074:THR:HB	2.10	0.51
1:B:156:PHE:CZ	1:B:189:GLY:C	2.86	0.51
1:B:342:VAL:HG12	1:B:386:LEU:HD22	1.93	0.51
1:C:547:LEU:O	1:C:630:LYS:NZ	2.43	0.51
1:C:892:LEU:HD21	1:C:917:ILE:HG23	1.92	0.51
1:B:503:LEU:O	1:B:509:LEU:CD1	2.58	0.51
1:A:367:TYR:CE1	1:A:371:THR:HG21	2.45	0.51
1:D:148:SER:O	1:D:303:CYS:CA	2.58	0.51
1:A:812:LYS:HE2	1:A:1094:ALA:HB2	1.92	0.51
1:C:812:LYS:HE2	1:C:1094:ALA:HB2	1.92	0.51
1:A:456:THR:HG23	1:A:459:ASP:H	1.75	0.51
1:D:298:THR:OG1	1:D:430:ARG:NH1	2.44	0.51
1:D:738:PHE:HA	1:D:741:ILE:HD12	1.93	0.51
1:A:990:PRO:O	1:A:993:THR:HG22	2.11	0.51
1:D:121:VAL:HB	1:D:125:THR:HG21	1.93	0.51
1:C:880:ASP:OD2	1:C:883:ASN:ND2	2.44	0.51
1:C:990:PRO:O	1:C:993:THR:HG22	2.11	0.51
1:D:342:VAL:HG12	1:D:386:LEU:HD22	1.93	0.51
1:B:298:THR:OG1	1:B:430:ARG:NH1	2.44	0.51
1:C:622:ILE:HD12	1:C:679:LEU:HD23	1.93	0.51
1:D:140:LEU:HD21	1:D:259:HIS:HE1	1.75	0.51
1:B:547:LEU:HD12	1:B:630:LYS:HD3	1.92	0.50
1:B:1053:ILE:HD13	1:A:950:LEU:HD13	1.92	0.50
1:B:1396:TYR:HB2	1:B:1415:ILE:HG23	1.94	0.50
1:A:223:ILE:O	1:A:226:ARG:NH1	2.42	0.50
1:C:367:TYR:CE1	1:C:371:THR:HG21	2.45	0.50
1:C:950:LEU:HD13	1:D:1053:ILE:HD13	1.94	0.50
1:A:892:LEU:HD21	1:A:917:ILE:HG23	1.92	0.50
1:A:943:VAL:HA	1:A:946:MET:HG2	1.94	0.50
1:C:1319:LEU:HD23	1:C:1325:ASN:HD22	1.75	0.50
1:D:221:GLY:HA3	1:D:268:GLN:HA	1.93	0.50
1:B:221:GLY:HA3	1:B:268:GLN:HA	1.93	0.50
1:A:1070:VAL:O	1:A:1074:THR:CB	2.60	0.50
1:B:121:VAL:HB	1:B:125:THR:HG21	1.93	0.50
1:B:1318:ALA:HB3	1:B:1404:ARG:HD2	1.94	0.50
1:D:1318:ALA:HB3	1:D:1404:ARG:HD2	1.94	0.50
1:D:813:PHE:HD1	1:D:1089:TYR:HE2	1.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:ILE:HD12	1:A:679:LEU:HD23	1.93	0.50
1:A:880:ASP:OD2	1:A:883:ASN:ND2	2.44	0.50
1:B:385:ILE:HG22	1:B:392:LEU:HD11	1.94	0.50
1:C:345:VAL:N	1:C:346:PRO:CD	2.75	0.50
1:C:943:VAL:HA	1:C:946:MET:HG2	1.94	0.50
1:B:148:SER:O	1:B:303:CYS:CA	2.58	0.49
1:A:345:VAL:N	1:A:346:PRO:CD	2.75	0.49
1:A:450:THR:O	1:A:453:SER:OG	2.29	0.49
1:C:473:PRO:HA	1:C:476:VAL:HG12	1.94	0.49
1:D:149:VAL:CG1	1:D:304:VAL:HG23	2.40	0.49
1:D:385:ILE:HG22	1:D:392:LEU:HD11	1.95	0.49
1:D:1396:TYR:HB2	1:D:1415:ILE:HG23	1.94	0.49
1:B:738:PHE:HA	1:B:741:ILE:HD12	1.93	0.49
1:A:183:THR:HG22	1:A:191:MET:HG3	1.94	0.49
1:A:1272:GLU:HG3	1:A:1273:LYS:HG2	1.94	0.49
1:C:1070:VAL:O	1:C:1074:THR:CB	2.60	0.49
1:C:183:THR:HG22	1:C:191:MET:HG3	1.94	0.49
1:C:942:ILE:HG13	1:C:1074:THR:HG21	1.94	0.49
1:A:239:TYR:OH	1:D:487:ARG:NH2	2.46	0.49
1:A:942:ILE:HG13	1:A:1074:THR:HG21	1.94	0.49
1:C:166:PHE:HA	1:C:405:VAL:HG21	1.95	0.49
1:A:166:PHE:HA	1:A:405:VAL:HG21	1.95	0.49
1:A:1273:LYS:HD2	1:A:1280:PHE:HB3	1.95	0.49
1:C:224:HIS:HA	1:C:250:LEU:HD12	1.95	0.49
1:C:1272:GLU:HG3	1:C:1273:LYS:HG2	1.94	0.49
1:D:823:PHE:HB2	1:D:849:TRP:CZ2	2.48	0.49
1:A:473:PRO:HA	1:A:476:VAL:HG12	1.94	0.49
1:D:156:PHE:CZ	1:D:189:GLY:C	2.86	0.49
1:B:149:VAL:CG1	1:B:304:VAL:HG23	2.40	0.48
1:A:982:ILE:HD11	1:D:832:MET:HB3	1.95	0.48
1:D:149:VAL:HA	1:D:304:VAL:O	2.13	0.48
1:D:149:VAL:HG22	1:D:304:VAL:HG23	1.86	0.48
1:B:149:VAL:HA	1:B:304:VAL:O	2.13	0.48
1:C:226:ARG:HH22	1:C:268:GLN:HE21	1.62	0.48
1:A:151:GLY:HA2	1:A:306:LEU:H	1.79	0.48
1:B:823:PHE:HB2	1:B:849:TRP:CZ2	2.48	0.48
1:D:156:PHE:CD1	1:D:189:GLY:HA2	2.48	0.48
1:B:138:TRP:HB3	1:B:140:LEU:HD23	1.95	0.47
1:A:224:HIS:HA	1:A:250:LEU:HD12	1.95	0.47
1:A:226:ARG:HH22	1:A:268:GLN:HE21	1.62	0.47
1:C:961:VAL:HG22	1:C:990:PRO:CB	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:PHE:CZ	1:D:190:VAL:N	2.81	0.47
1:B:356:ASN:OD1	1:B:367:TYR:OH	2.30	0.47
1:C:1328:LEU:HD11	1:C:1369:LEU:HD12	1.97	0.47
1:A:961:VAL:HG22	1:A:990:PRO:CB	2.43	0.47
1:C:1273:LYS:HD2	1:C:1280:PHE:HB3	1.95	0.47
1:A:302:VAL:HG23	1:A:325:PRO:HG2	1.96	0.47
1:A:1395:VAL:N	1:A:1415:ILE:O	2.48	0.47
1:C:705:ILE:HD13	1:C:1080:PHE:HA	1.96	0.47
1:D:859:ARG:HG2	1:D:1104:HIS:HE1	1.79	0.47
1:B:547:LEU:O	1:B:630:LYS:NZ	2.39	0.47
1:B:191:MET:SD	1:B:191:MET:N	2.87	0.47
1:D:138:TRP:HB3	1:D:140:LEU:HD23	1.95	0.47
1:D:544:ARG:HE	1:D:549:SER:HA	1.80	0.47
1:B:682:ARG:HG2	1:B:1128:LEU:HD23	1.97	0.47
1:A:887:VAL:HA	1:A:890:ILE:HG22	1.97	0.47
1:C:469:VAL:HG23	1:C:502:HIS:HB3	1.97	0.47
1:A:283:LYS:HB3	1:A:322:ASN:HD21	1.80	0.47
1:D:978:ARG:HH21	1:D:981:TRP:CD1	2.33	0.47
1:B:859:ARG:HG2	1:B:1104:HIS:HE1	1.80	0.47
1:B:1090:HIS:HE1	1:B:1123:ASN:HD22	1.62	0.47
1:A:705:ILE:HD13	1:A:1080:PHE:HA	1.96	0.47
1:A:923:CYS:HA	1:A:926:LEU:HD13	1.97	0.47
1:B:183:THR:HG22	1:B:191:MET:HG3	1.98	0.46
1:B:417:SER:HB3	1:B:431:GLN:HE22	1.79	0.46
1:A:856:GLU:OE2	1:A:1092:ARG:NE	2.49	0.46
1:A:1328:LEU:HD11	1:A:1369:LEU:HD12	1.97	0.46
1:C:302:VAL:HG23	1:C:325:PRO:HG2	1.96	0.46
1:A:134:MET:O	1:A:138:TRP:HB2	2.15	0.46
1:A:986:ALA:O	1:A:990:PRO:HG2	2.16	0.46
1:C:283:LYS:HB3	1:C:322:ASN:HD21	1.80	0.46
1:D:417:SER:HB3	1:D:431:GLN:HE22	1.80	0.46
1:A:427:CYS:SG	1:A:431:GLN:NE2	2.89	0.46
1:C:198:VAL:HG23	1:C:212:ILE:HD11	1.97	0.46
1:C:223:ILE:O	1:C:226:ARG:NH1	2.42	0.46
1:C:427:CYS:SG	1:C:431:GLN:NE2	2.89	0.46
1:C:887:VAL:HA	1:C:890:ILE:HG22	1.97	0.46
1:B:387:ARG:NH1	1:B:1252:MET:SD	2.87	0.46
1:D:682:ARG:HG2	1:D:1128:LEU:HD23	1.97	0.46
1:C:450:THR:O	1:C:453:SER:OG	2.29	0.46
1:C:151:GLY:HA2	1:C:306:LEU:H	1.79	0.46
1:C:856:GLU:OE2	1:C:1092:ARG:NE	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ILE:HB	1:B:214:VAL:HG12	1.98	0.46
1:B:978:ARG:HH21	1:B:981:TRP:CD1	2.33	0.46
1:A:626:LEU:HD13	1:A:696:ALA:HB2	1.98	0.46
1:C:134:MET:O	1:C:138:TRP:HB2	2.15	0.46
1:C:986:ALA:O	1:C:990:PRO:HG2	2.16	0.46
1:B:544:ARG:HE	1:B:549:SER:HA	1.80	0.46
1:B:726:ASN:HD22	1:B:746:LEU:HD23	1.81	0.46
1:A:198:VAL:HG23	1:A:212:ILE:HD11	1.97	0.46
1:A:999:PRO:HB2	1:A:1044:LEU:HD21	1.98	0.46
1:D:183:THR:HG22	1:D:191:MET:HG3	1.98	0.46
1:B:156:PHE:CZ	1:B:190:VAL:N	2.81	0.46
1:C:1395:VAL:N	1:C:1415:ILE:O	2.48	0.46
1:D:506:CYS:SG	1:D:509:LEU:N	2.89	0.45
1:C:923:CYS:HA	1:C:926:LEU:HD13	1.97	0.45
1:C:999:PRO:HB2	1:C:1044:LEU:HD21	1.98	0.45
1:D:1090:HIS:HE1	1:D:1123:ASN:HD22	1.62	0.45
1:A:469:VAL:HG23	1:A:502:HIS:HB3	1.97	0.45
1:C:626:LEU:HD13	1:C:696:ALA:HB2	1.98	0.45
1:D:1322:LEU:HA	1:D:1409:ALA:HB2	1.98	0.45
1:D:726:ASN:HD22	1:D:746:LEU:HD23	1.81	0.45
1:B:592:TRP:O	1:B:596:ARG:NH1	2.50	0.45
1:B:506:CYS:SG	1:B:509:LEU:N	2.89	0.45
1:D:148:SER:O	1:D:304:VAL:N	2.48	0.45
1:D:181:ILE:HB	1:D:214:VAL:HG12	1.98	0.45
1:D:683:ILE:HD13	1:D:1125:ARG:HE	1.82	0.45
1:B:273:VAL:O	1:B:276:GLU:N	2.43	0.45
1:D:722:LEU:HD23	1:D:810:GLN:HE21	1.82	0.45
1:B:1347:ALA:HA	1:B:1358:LEU:HA	1.99	0.44
1:B:722:LEU:HD21	1:B:726:ASN:HD21	1.83	0.44
1:D:1347:ALA:HA	1:D:1358:LEU:HA	1.99	0.44
1:D:407:VAL:HG22	1:D:443:ILE:HD11	1.99	0.44
1:D:1346:LEU:HA	1:D:1446:TRP:HA	2.00	0.44
1:B:263:VAL:HG21	1:B:274:GLU:HA	1.99	0.44
1:B:1322:LEU:HA	1:B:1409:ALA:HB2	1.99	0.44
1:B:273:VAL:O	1:B:274:GLU:C	2.60	0.44
1:C:1334:ARG:NE	1:C:1344:GLU:OE1	2.41	0.44
1:D:263:VAL:HG21	1:D:274:GLU:HA	1.99	0.44
1:B:1346:LEU:HA	1:B:1446:TRP:HA	2.00	0.44
1:B:407:VAL:HG22	1:B:443:ILE:HD11	1.99	0.44
1:B:722:LEU:HD23	1:B:810:GLN:HE21	1.82	0.44
1:C:385:ILE:HG22	1:C:392:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1090:HIS:CE1	1:B:1123:ASN:HD22	2.36	0.43
1:D:621:CYS:SG	1:D:1144:LYS:HD2	2.58	0.43
1:B:621:CYS:SG	1:B:1144:LYS:HD2	2.58	0.43
1:B:632:LEU:HB3	1:B:654:ALA:HB2	2.00	0.43
1:D:273:VAL:O	1:D:274:GLU:C	2.60	0.43
1:D:722:LEU:HD21	1:D:726:ASN:HD21	1.83	0.43
1:D:191:MET:SD	1:D:191:MET:N	2.87	0.43
1:D:592:TRP:O	1:D:596:ARG:NH1	2.50	0.43
1:A:183:THR:HG21	1:A:194:VAL:HG11	2.01	0.43
1:C:1394:GLU:HA	1:C:1416:ILE:HA	2.01	0.43
1:B:857:GLU:OE1	1:B:877:TYR:OH	2.33	0.43
1:A:199:ARG:CZ	1:A:256:ASN:HD21	2.32	0.43
1:D:632:LEU:HB3	1:D:654:ALA:HB2	2.00	0.43
1:D:657:TYR:HD1	1:D:657:TYR:HA	1.68	0.43
1:D:1090:HIS:CE1	1:D:1123:ASN:HD22	2.37	0.43
1:B:89:TRP:O	1:B:93:ARG:CB	2.67	0.43
1:B:694:TRP:O	1:B:698:GLU:CB	2.67	0.43
1:C:199:ARG:CZ	1:C:256:ASN:HD21	2.31	0.43
1:B:148:SER:O	1:B:304:VAL:N	2.48	0.43
1:B:535:CYS:H	1:B:538:HIS:HD2	1.66	0.43
1:B:904:SER:HB2	1:B:907:VAL:HG22	2.01	0.43
1:A:453:SER:HB3	1:A:455:TRP:CD1	2.54	0.43
1:D:466:SER:HA	1:D:469:VAL:HG12	2.01	0.43
1:D:707:HIS:HB3	1:D:710:VAL:HG12	2.00	0.43
1:D:904:SER:HB2	1:D:907:VAL:HG22	2.01	0.43
1:B:683:ILE:HD13	1:B:1125:ARG:HE	1.82	0.43
1:D:146:LEU:HD11	1:D:182:LEU:HB2	2.01	0.43
1:C:461:HIS:NE2	1:C:488:GLU:O	2.52	0.43
1:C:808:SER:HB2	1:C:811:VAL:HG12	2.00	0.43
1:B:376:ILE:HG23	1:B:1268:PRO:HG2	2.01	0.42
1:A:848:VAL:HA	1:A:851:THR:HG22	2.01	0.42
1:A:1333:THR:HG22	1:A:1345:PHE:HB3	2.01	0.42
1:C:183:THR:HG21	1:C:194:VAL:HG11	2.01	0.42
1:C:848:VAL:HA	1:C:851:THR:HG22	2.01	0.42
1:C:984:ARG:NE	1:D:1003:ASP:O	2.52	0.42
1:D:273:VAL:O	1:D:276:GLU:N	2.43	0.42
1:A:808:SER:HB2	1:A:811:VAL:HG12	2.00	0.42
1:D:199:ARG:HA	1:D:202:THR:HG22	2.01	0.42
1:B:156:PHE:CD1	1:B:189:GLY:HA2	2.48	0.42
1:B:466:SER:HA	1:B:469:VAL:HG12	2.01	0.42
1:B:707:HIS:HB3	1:B:710:VAL:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1333:THR:HG22	1:C:1345:PHE:HB3	2.01	0.42
1:D:694:TRP:O	1:D:698:GLU:CB	2.67	0.42
1:B:380:LYS:HD2	1:B:1257:LEU:HD11	2.01	0.42
1:A:385:ILE:HG22	1:A:392:LEU:HD11	2.00	0.42
1:D:89:TRP:O	1:D:93:ARG:CB	2.67	0.42
1:D:387:ARG:NH1	1:D:1252:MET:SD	2.87	0.42
1:B:603:VAL:HG22	1:B:632:LEU:HD21	2.01	0.42
1:C:726:ASN:HD22	1:C:746:LEU:HD22	1.85	0.42
1:D:356:ASN:OD1	1:D:367:TYR:OH	2.30	0.42
1:D:376:ILE:HG23	1:D:1268:PRO:HG2	2.01	0.42
1:D:859:ARG:HG2	1:D:1104:HIS:CE1	2.54	0.42
1:B:1003:ASP:O	1:A:984:ARG:NE	2.52	0.42
1:B:199:ARG:HA	1:B:202:THR:HG22	2.02	0.42
1:B:619:ARG:HH22	1:C:239:TYR:HH	1.65	0.42
1:B:657:TYR:HD1	1:B:657:TYR:HA	1.68	0.42
1:A:461:HIS:NE2	1:A:488:GLU:O	2.52	0.42
1:C:176:THR:HG21	1:C:440:ARG:HH11	1.85	0.42
1:A:346:PRO:HB3	1:A:349:LYS:CB	2.40	0.42
1:A:1394:GLU:HA	1:A:1416:ILE:HA	2.01	0.42
1:C:453:SER:HB3	1:C:455:TRP:CD1	2.54	0.42
1:D:399:GLU:H	1:D:403:TYR:HB2	1.85	0.42
1:D:535:CYS:SG	1:D:536:LEU:N	2.93	0.42
1:A:146:LEU:HB3	1:A:301:VAL:HG22	2.02	0.41
1:A:748:PHE:HE2	1:A:801:ARG:HG3	1.85	0.41
1:D:380:LYS:HD2	1:D:1257:LEU:HD11	2.01	0.41
1:B:535:CYS:SG	1:B:536:LEU:N	2.93	0.41
1:C:50:LYS:N	1:C:99:PRO:O	2.53	0.41
1:D:304:VAL:HG12	1:D:327:VAL:HB	2.02	0.41
1:C:705:ILE:HG21	1:C:1080:PHE:HD1	1.85	0.41
1:A:320:MET:HE1	1:A:391:LEU:HB2	2.01	0.41
1:B:634:LYS:HA	1:B:634:LYS:HD2	1.91	0.41
1:A:50:LYS:N	1:A:99:PRO:O	2.53	0.41
1:D:535:CYS:H	1:D:538:HIS:HD2	1.66	0.41
1:A:176:THR:HG21	1:A:440:ARG:HH11	1.85	0.41
1:A:705:ILE:HG21	1:A:1080:PHE:HD1	1.85	0.41
1:C:320:MET:HE1	1:C:391:LEU:HB2	2.01	0.41
1:D:603:VAL:HG22	1:D:632:LEU:HD21	2.01	0.41
1:D:1276:TRP:NE1	1:D:1306:ASN:O	2.40	0.41
1:B:304:VAL:HG12	1:B:327:VAL:HB	2.03	0.41
1:B:749:ARG:O	1:B:753:ASP:CB	2.69	0.41
1:B:859:ARG:HG2	1:B:1104:HIS:CE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:TYR:HA	1:A:385:ILE:HD11	2.03	0.41
1:C:105:ASP:HA	1:C:117:LYS:HA	2.03	0.41
1:B:146:LEU:HD11	1:B:182:LEU:HB2	2.01	0.41
1:D:749:ARG:O	1:D:753:ASP:CB	2.69	0.41
1:B:134:MET:HA	1:B:138:TRP:CE3	2.56	0.41
1:B:399:GLU:H	1:B:403:TYR:HB2	1.85	0.41
1:A:603:VAL:HG22	1:A:632:LEU:HD21	2.03	0.41
1:A:726:ASN:HD22	1:A:746:LEU:HD22	1.85	0.41
1:C:146:LEU:HB3	1:C:301:VAL:HG22	2.02	0.41
1:C:603:VAL:HG22	1:C:632:LEU:HD21	2.03	0.41
1:C:748:PHE:HE2	1:C:801:ARG:HG3	1.85	0.41
1:D:1399:TYR:HA	1:D:1412:GLU:HG2	2.02	0.41
1:A:662:ILE:HG22	1:A:704:PHE:HD1	1.86	0.40
1:D:335:LEU:HD13	1:D:378:TRP:HZ3	1.86	0.40
1:B:50:LYS:CB	1:B:98:THR:O	2.53	0.40
1:B:516:VAL:HG21	1:B:534:VAL:HG12	2.03	0.40
1:B:1399:TYR:HA	1:B:1412:GLU:HG2	2.02	0.40
1:A:823:PHE:HB2	1:A:849:TRP:CE2	2.57	0.40
1:C:317:TYR:HA	1:C:385:ILE:HD11	2.03	0.40
1:C:662:ILE:HG22	1:C:704:PHE:HD1	1.86	0.40
1:B:355:ILE:HD13	1:B:379:THR:HA	2.03	0.40
1:A:105:ASP:HA	1:A:117:LYS:HA	2.03	0.40
1:A:834:ASP:OD1	1:A:834:ASP:N	2.54	0.40
1:A:1077:ILE:O	1:A:1081:GLN:NE2	2.54	0.40
1:C:834:ASP:N	1:C:834:ASP:OD1	2.54	0.40
1:B:630:LYS:HZ2	1:B:698:GLU:CD	2.29	0.40
1:A:741:ILE:HD12	1:A:801:ARG:HG2	2.04	0.40
1:A:1121:HIS:HD2	1:A:1124:PHE:HB2	1.87	0.40
1:D:105:ASP:OD1	1:D:105:ASP:N	2.52	0.40
1:D:516:VAL:HG21	1:D:534:VAL:HG12	2.03	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	1177/1466 (80%)	1102 (94%)	74 (6%)	1 (0%)	48	79
1	B	1208/1466 (82%)	1127 (93%)	80 (7%)	1 (0%)	48	79
1	C	1177/1466 (80%)	1103 (94%)	73 (6%)	1 (0%)	48	79
1	D	1208/1466 (82%)	1128 (93%)	79 (6%)	1 (0%)	48	79
All	All	4770/5864 (81%)	4460 (94%)	306 (6%)	4 (0%)	49	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1014	VAL
1	C	1014	VAL
1	B	1024	CYS
1	D	1024	CYS

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	760/1277 (60%)	760 (100%)	0	100	100
1	B	743/1277 (58%)	742 (100%)	1 (0%)	88	89
1	C	760/1277 (60%)	760 (100%)	0	100	100
1	D	743/1277 (58%)	742 (100%)	1 (0%)	88	89
All	All	3006/5108 (59%)	3004 (100%)	2 (0%)	87	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	150	THR
1	D	150	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59)

such sidechains are listed below:

Mol	Chain	Res	Type
1	B	187	HIS
1	B	231	HIS
1	B	259	HIS
1	B	431	GLN
1	B	538	HIS
1	B	816	ASN
1	B	1001	ASN
1	B	1064	ASN
1	B	1090	HIS
1	B	1104	HIS
1	B	1146	ASN
1	B	1161	HIS
1	B	1405	ASN
1	A	129	ASN
1	A	187	HIS
1	A	193	HIS
1	A	256	ASN
1	A	259	HIS
1	A	268	GLN
1	A	270	HIS
1	A	314	ASN
1	A	431	GLN
1	A	656	HIS
1	A	816	ASN
1	A	1073	ASN
1	A	1081	GLN
1	A	1104	HIS
1	A	1121	HIS
1	A	1146	ASN
1	A	1325	ASN
1	C	129	ASN
1	C	187	HIS
1	C	256	ASN
1	C	259	HIS
1	C	268	GLN
1	C	270	HIS
1	C	314	ASN
1	C	431	GLN
1	C	656	HIS
1	C	816	ASN
1	C	1073	ASN
1	C	1081	GLN

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Mol	Chain	Res	Type
1	C	1104	HIS
1	C	1121	HIS
1	C	1146	ASN
1	C	1325	ASN
1	D	187	HIS
1	D	231	HIS
1	D	259	HIS
1	D	431	GLN
1	D	538	HIS
1	D	816	ASN
1	D	1001	ASN
1	D	1064	ASN
1	D	1090	HIS
1	D	1104	HIS
1	D	1146	ASN
1	D	1161	HIS
1	D	1405	ASN

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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
1	C	2
1	B	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1209:UNK	C	1246:ASP	N	42.80
1	C	1209:UNK	C	1246:ASP	N	42.80
1	B	1184:VAL	C	1188:UNK	N	10.31
1	D	1184:VAL	C	1188:UNK	N	10.31
1	A	1184:VAL	C	1188:UNK	N	9.14
1	C	1184:VAL	C	1188:UNK	N	9.14

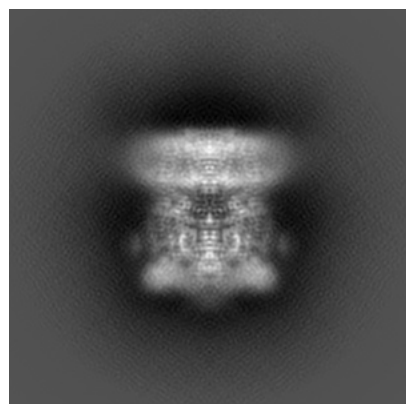
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7822. These allow visual inspection of the internal detail of the map and identification of artifacts.

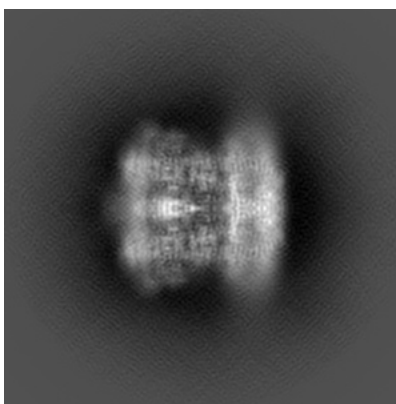
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

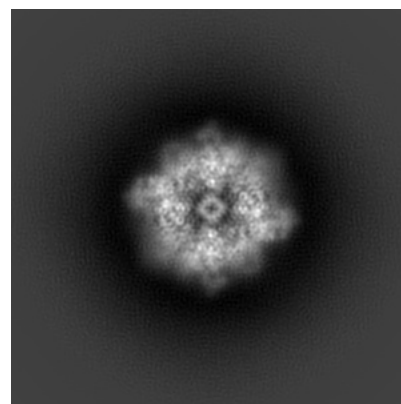
6.1.1 Primary map



X

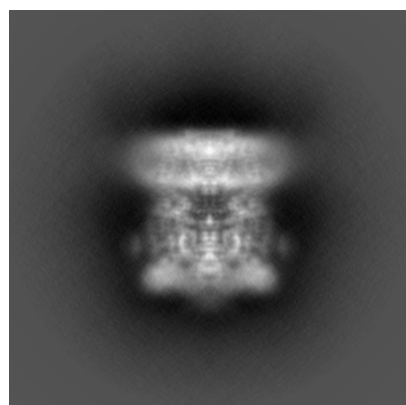


Y

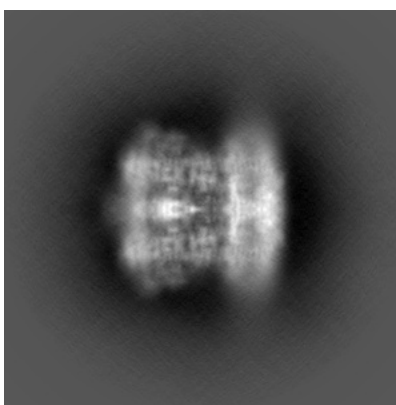


Z

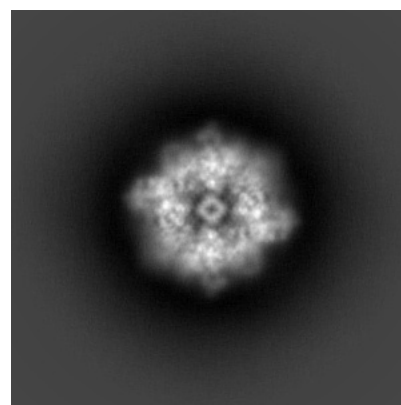
6.1.2 Raw map



X



Y

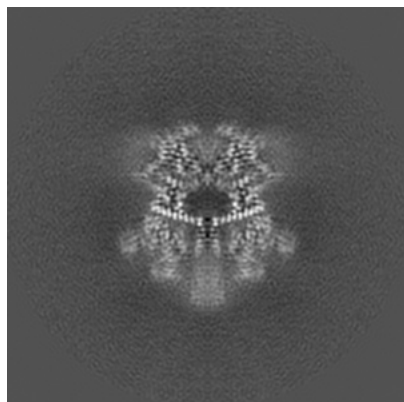


Z

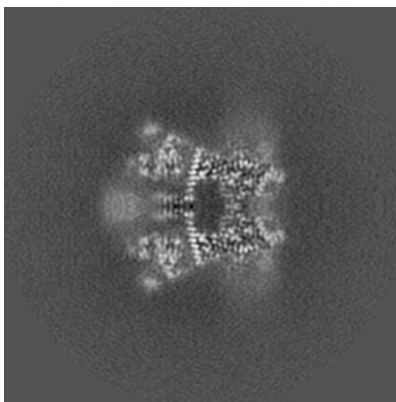
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

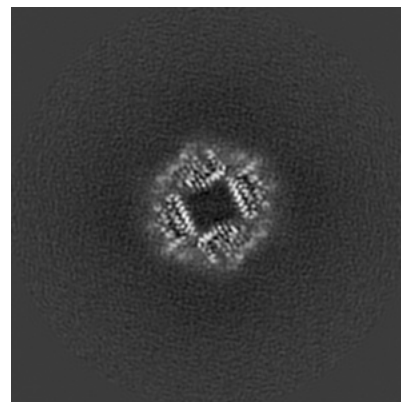
6.2.1 Primary map



X Index: 160

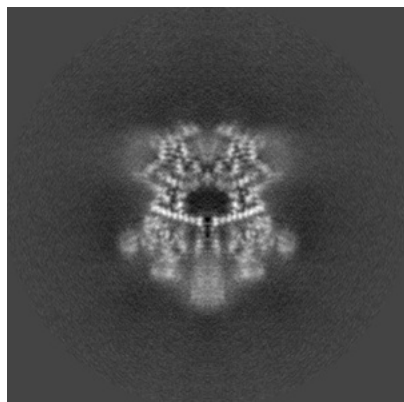


Y Index: 160

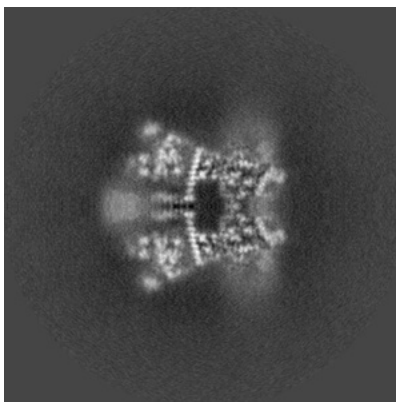


Z Index: 160

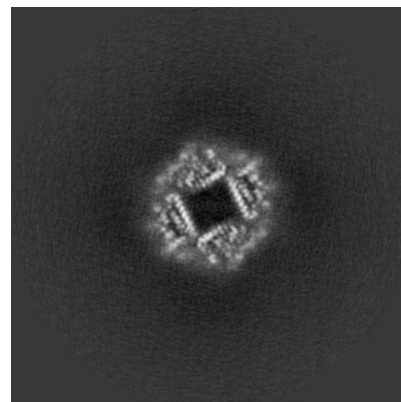
6.2.2 Raw map



X Index: 160



Y Index: 160

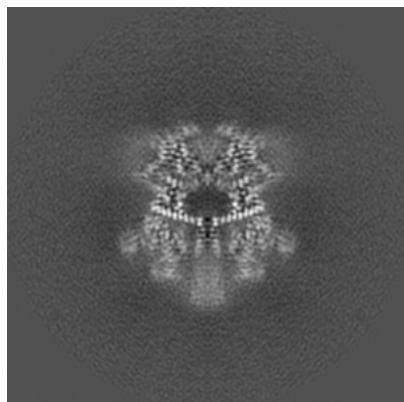


Z Index: 160

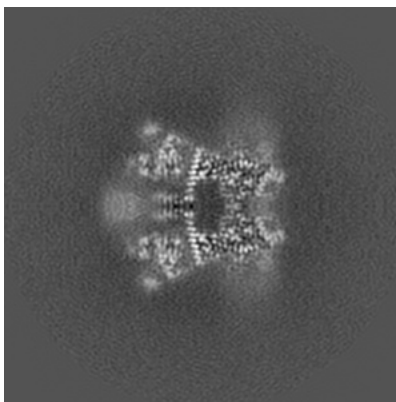
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

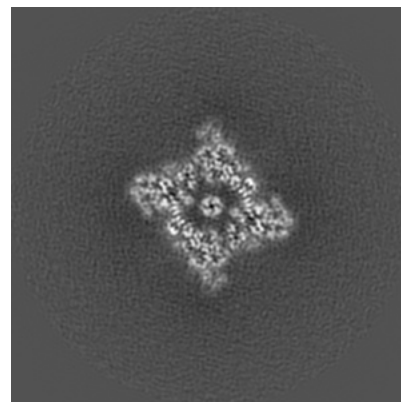
6.3.1 Primary map



X Index: 160

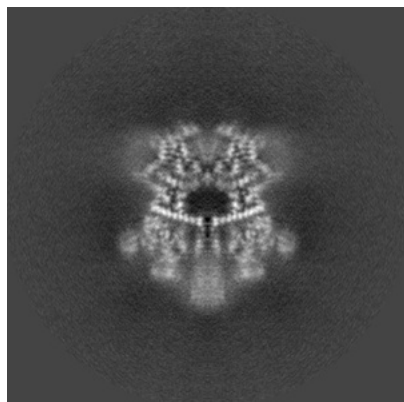


Y Index: 160

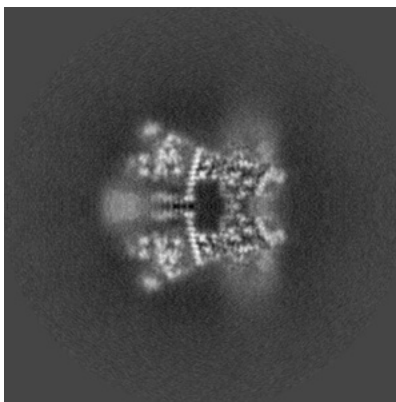


Z Index: 137

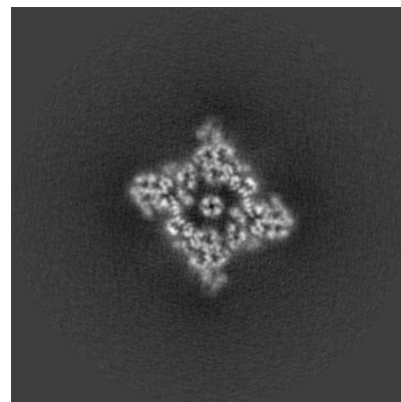
6.3.2 Raw map



X Index: 160



Y Index: 160

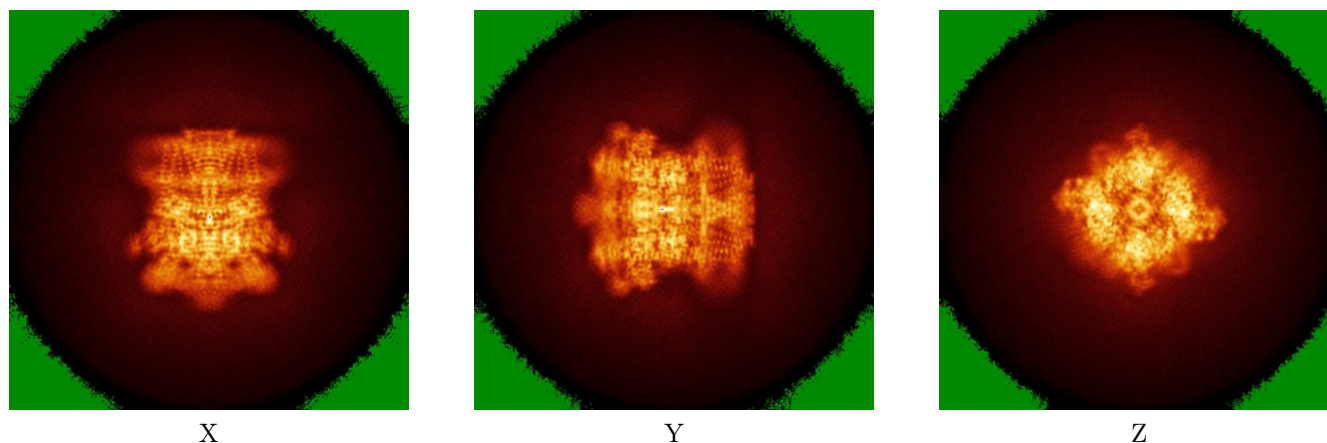


Z Index: 137

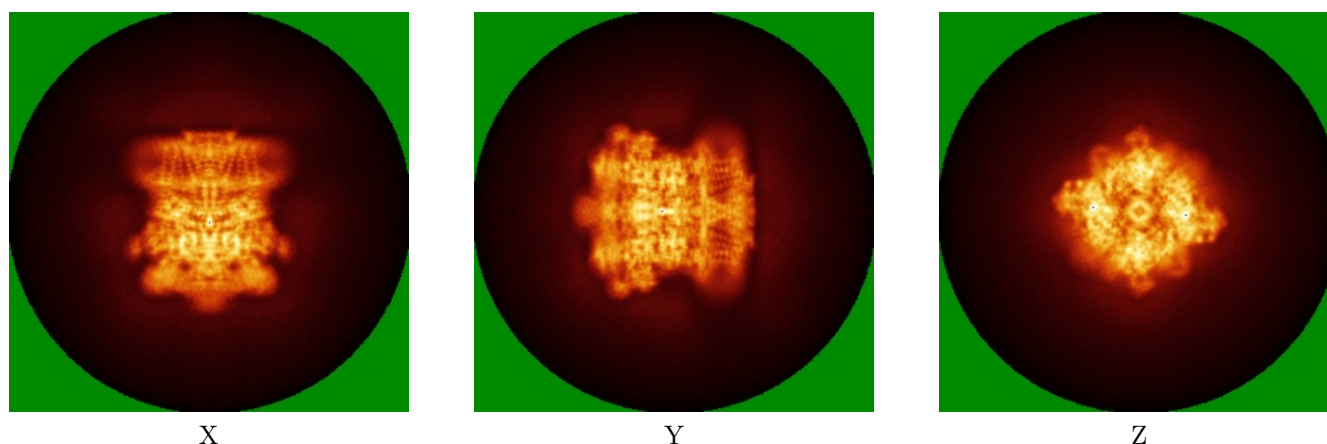
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

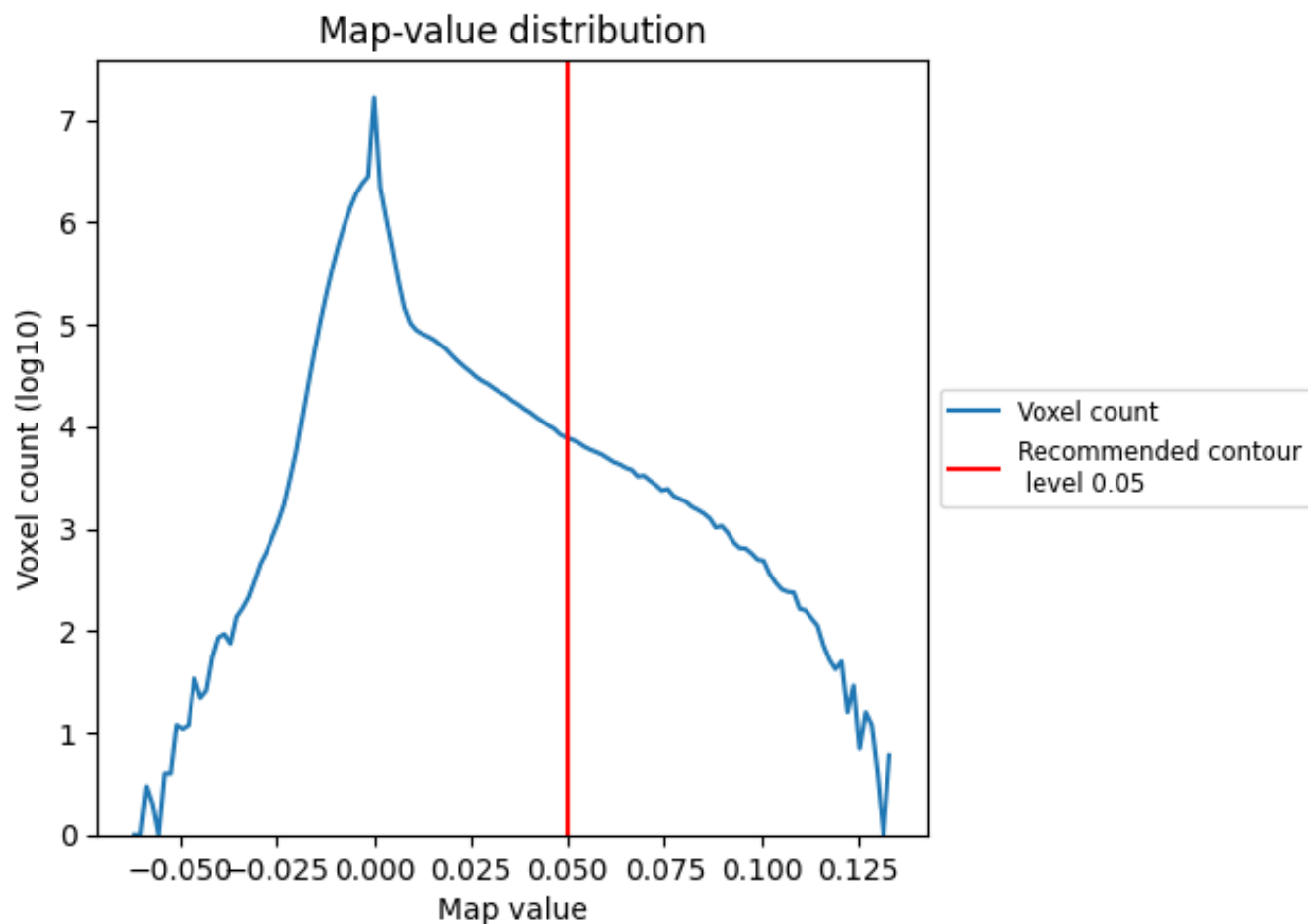
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

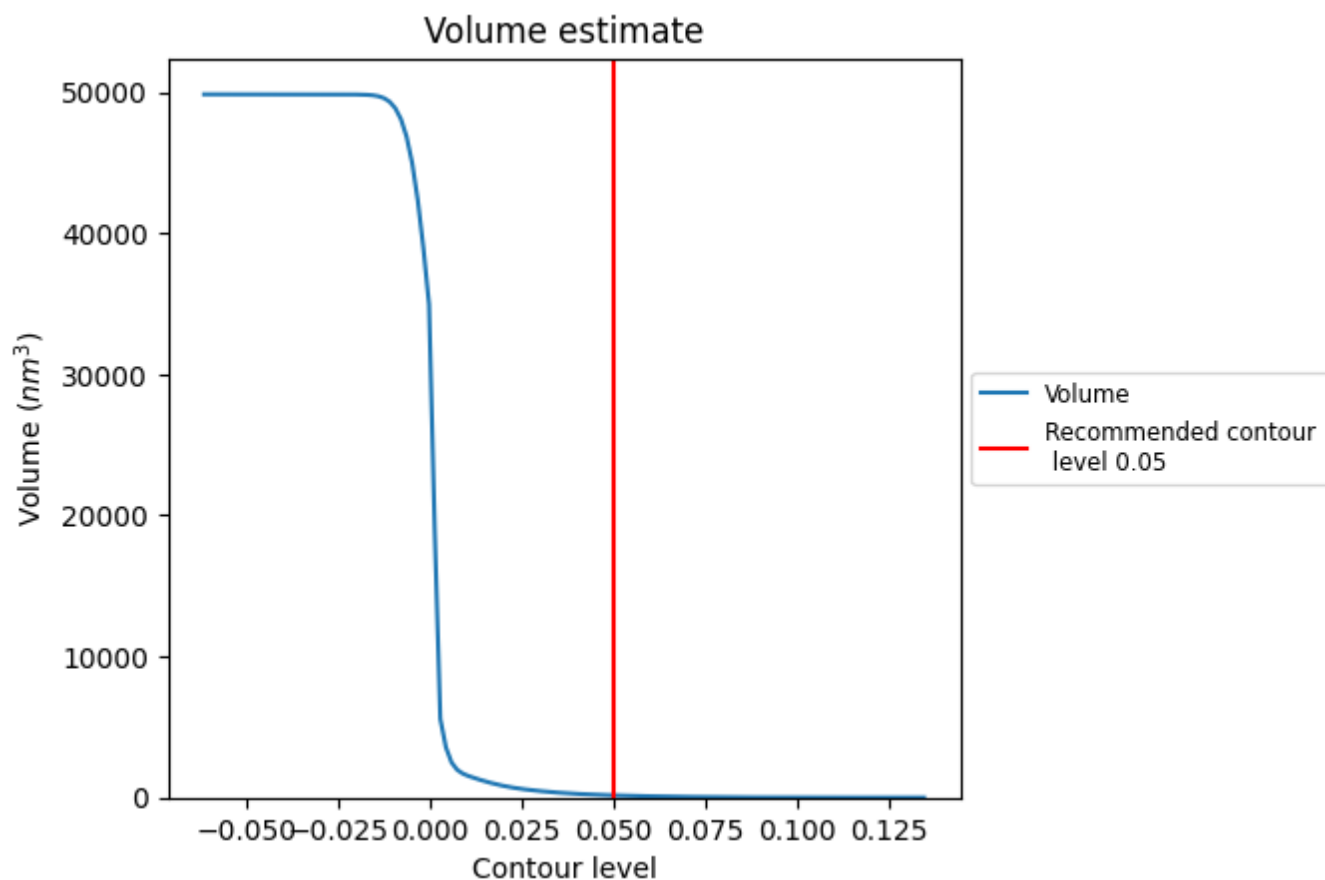
This section contains the results of statistical analysis of the map.

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.

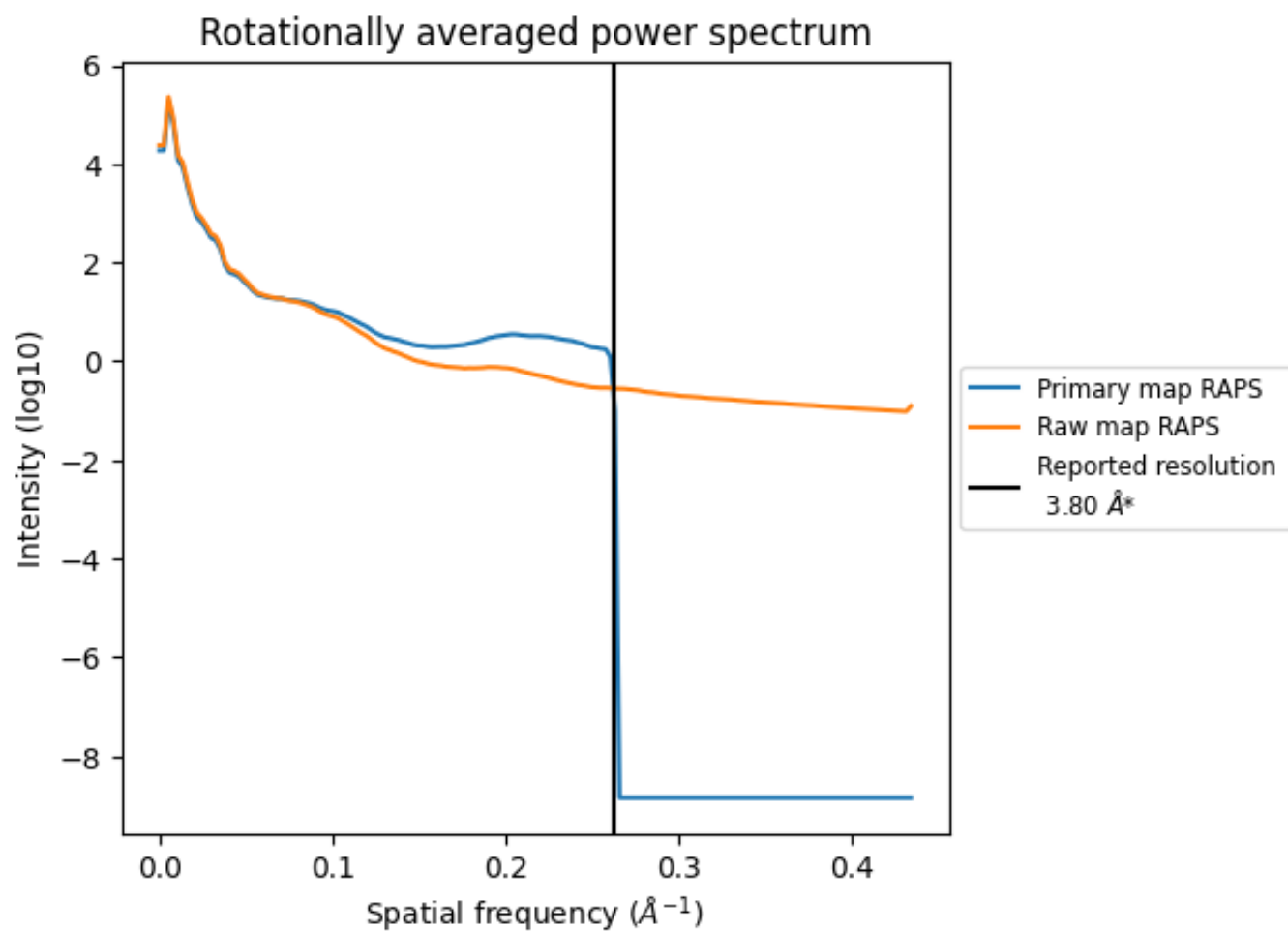
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 155 nm³; this corresponds to an approximate mass of 140 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 ⓘ

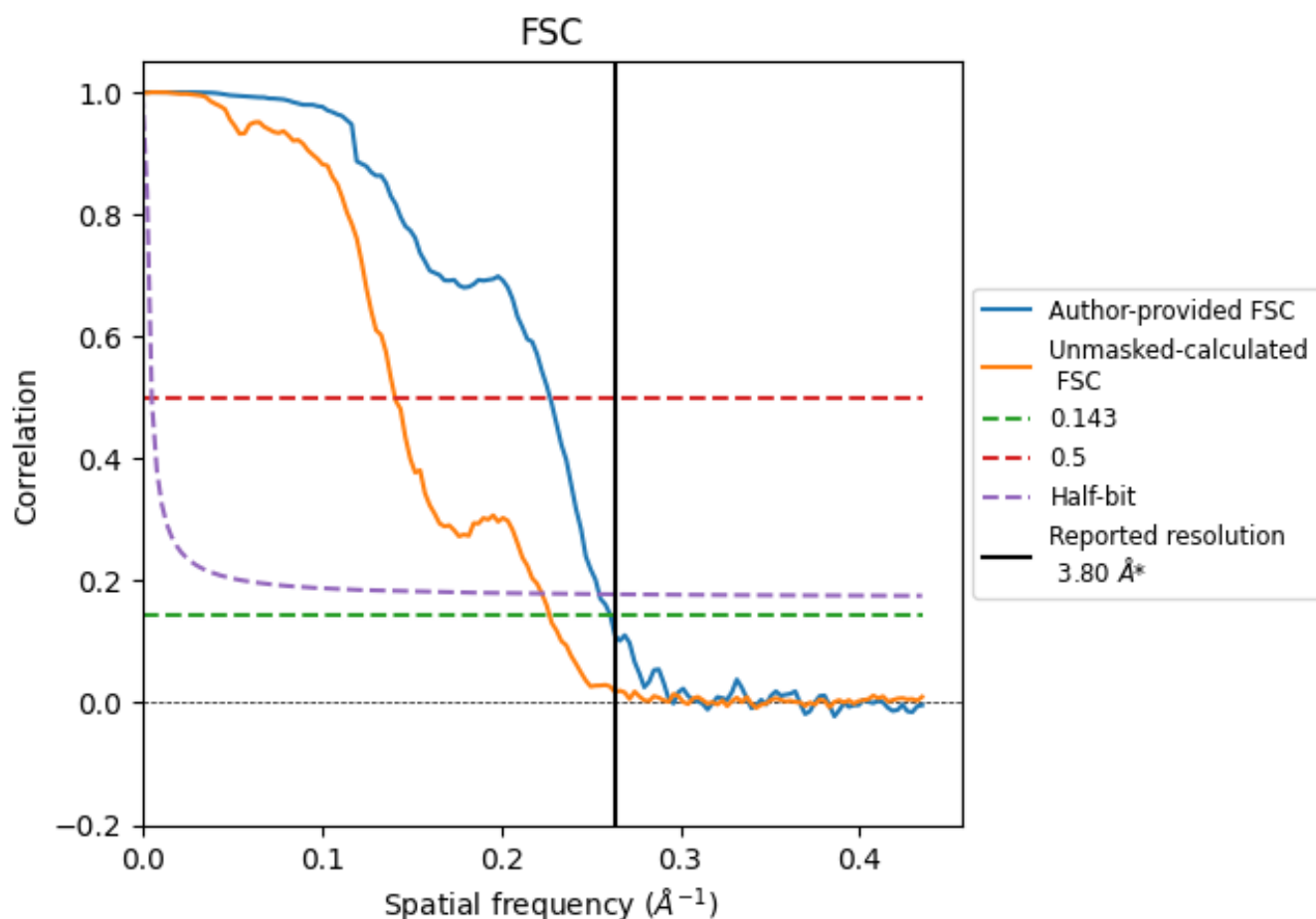


*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

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 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates

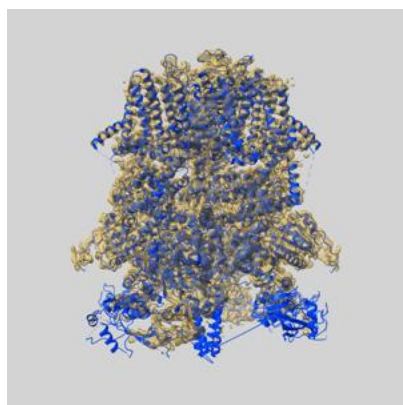
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.83	4.40	3.92
Unmasked-calculated*	4.40	7.10	4.49

*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 4.40 differs from the reported value 3.8 by more than 10 %

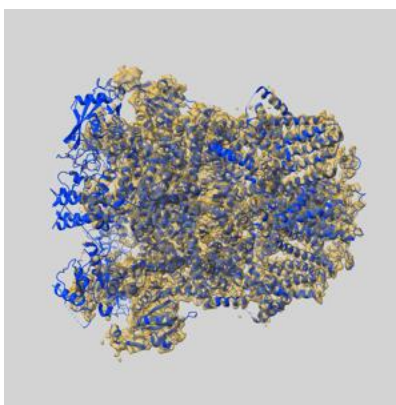
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7822 and PDB model 6D73. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

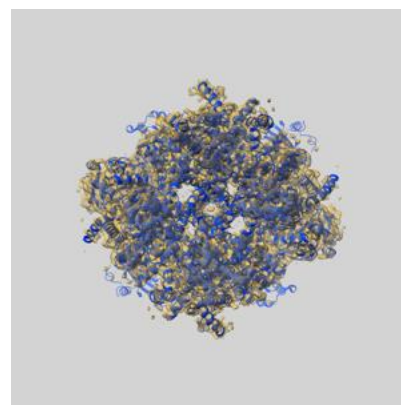
9.1 Map-model overlay [i](#)



X



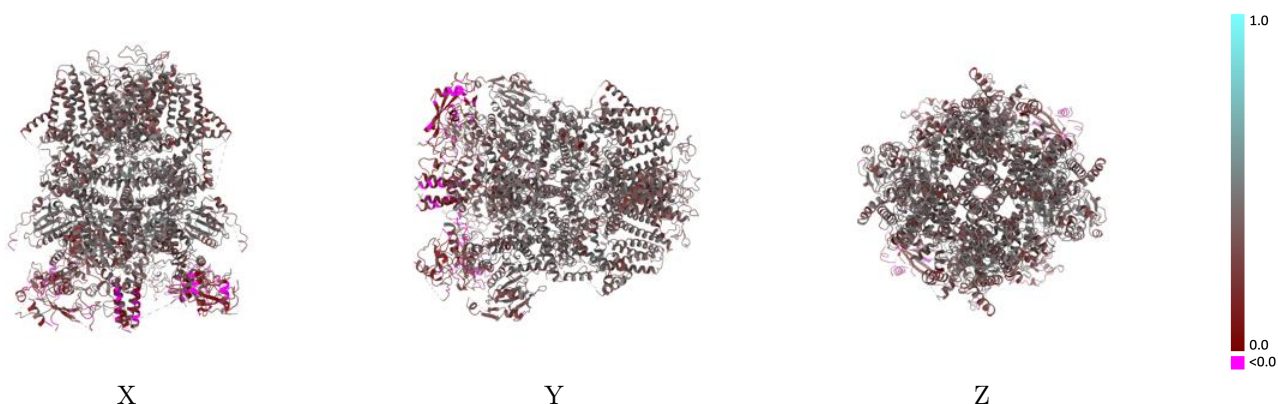
Y



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](#)

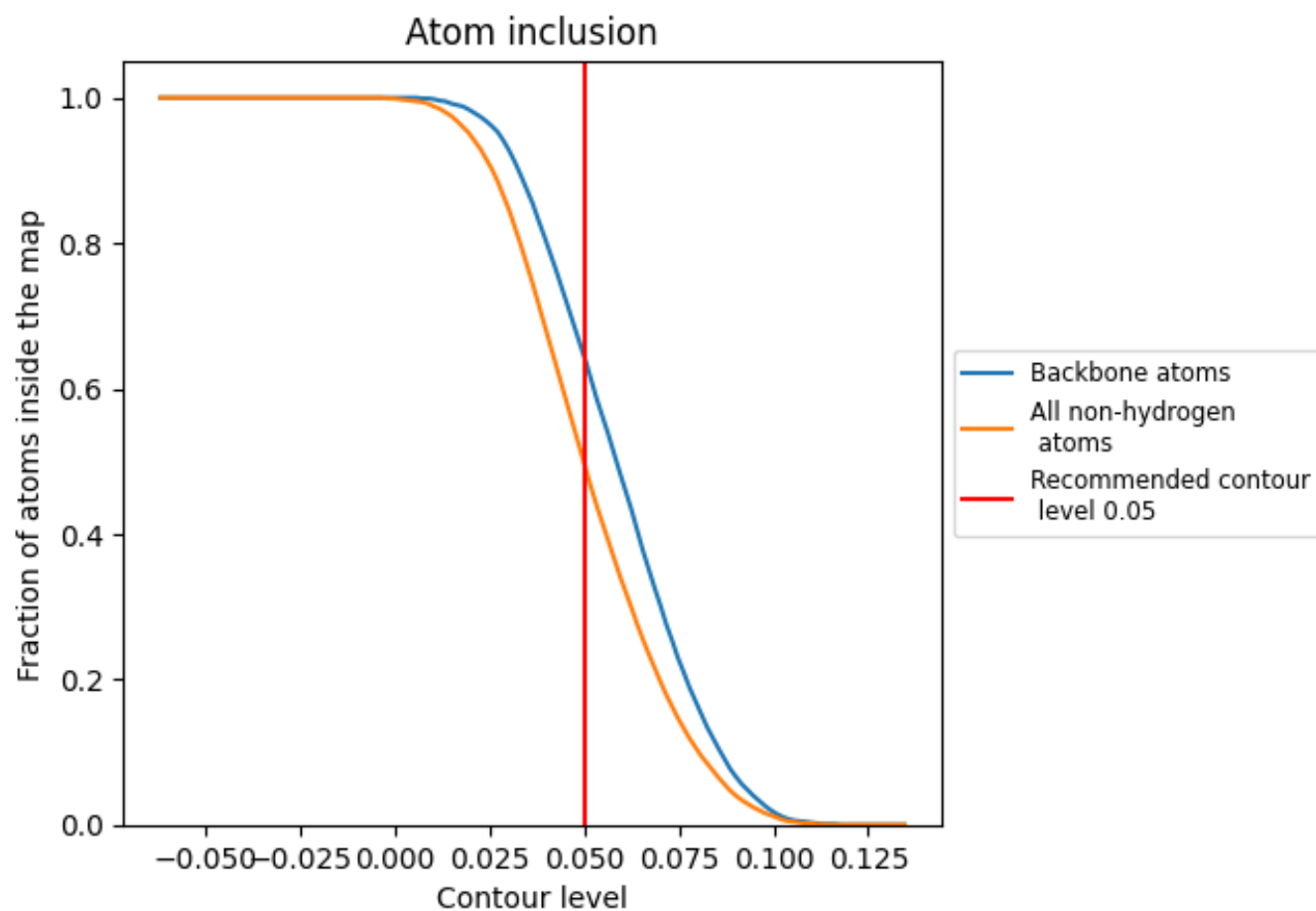


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 64% of all backbone atoms, 50% 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	0.4970	0.3650
A	0.4770	0.3590
B	0.5160	0.3710
C	0.4770	0.3580
D	0.5160	0.3710

