



Full wwPDB EM Validation Report ⓘ

Oct 19, 2024 – 03:32 PM EDT

PDB ID : 8SR9
EMDB ID : EMD-40723
Title : Cryo-EM structure of TRPM2 chanzyme in the presence of Magnesium
Authors : Huang, Y.; Kumar, S.; Lu, W.; Du, J.
Deposited on : 2023-05-05
Resolution : 3.05 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

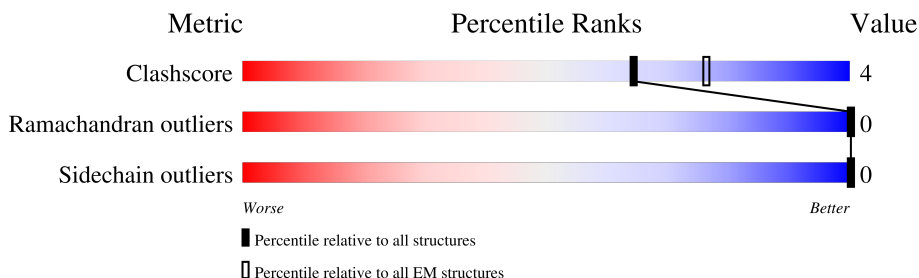
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.05 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1494	
1	B	1494	
1	C	1494	
1	D	1494	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 38176 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.

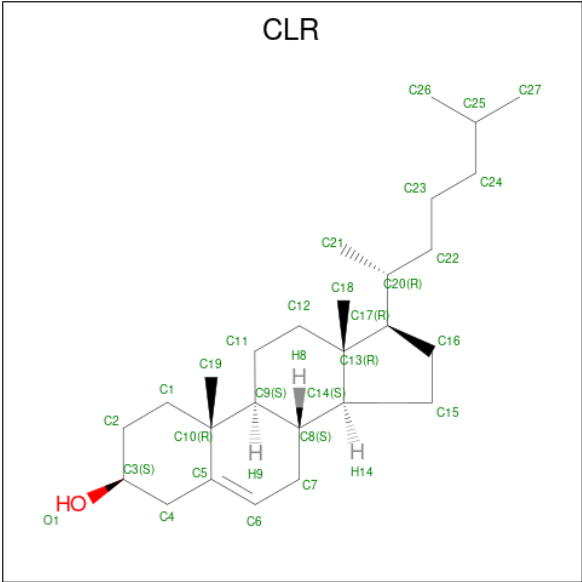
- Molecule 1 is a protein called TRPM2 chanzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1352	Total 9458	C 6068	N 1671	O 1675	S 44	0	0
1	B	1352	Total 9458	C 6068	N 1671	O 1675	S 44	0	0
1	C	1352	Total 9458	C 6068	N 1671	O 1675	S 44	0	0
1	D	1352	Total 9458	C 6068	N 1671	O 1675	S 44	0	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).

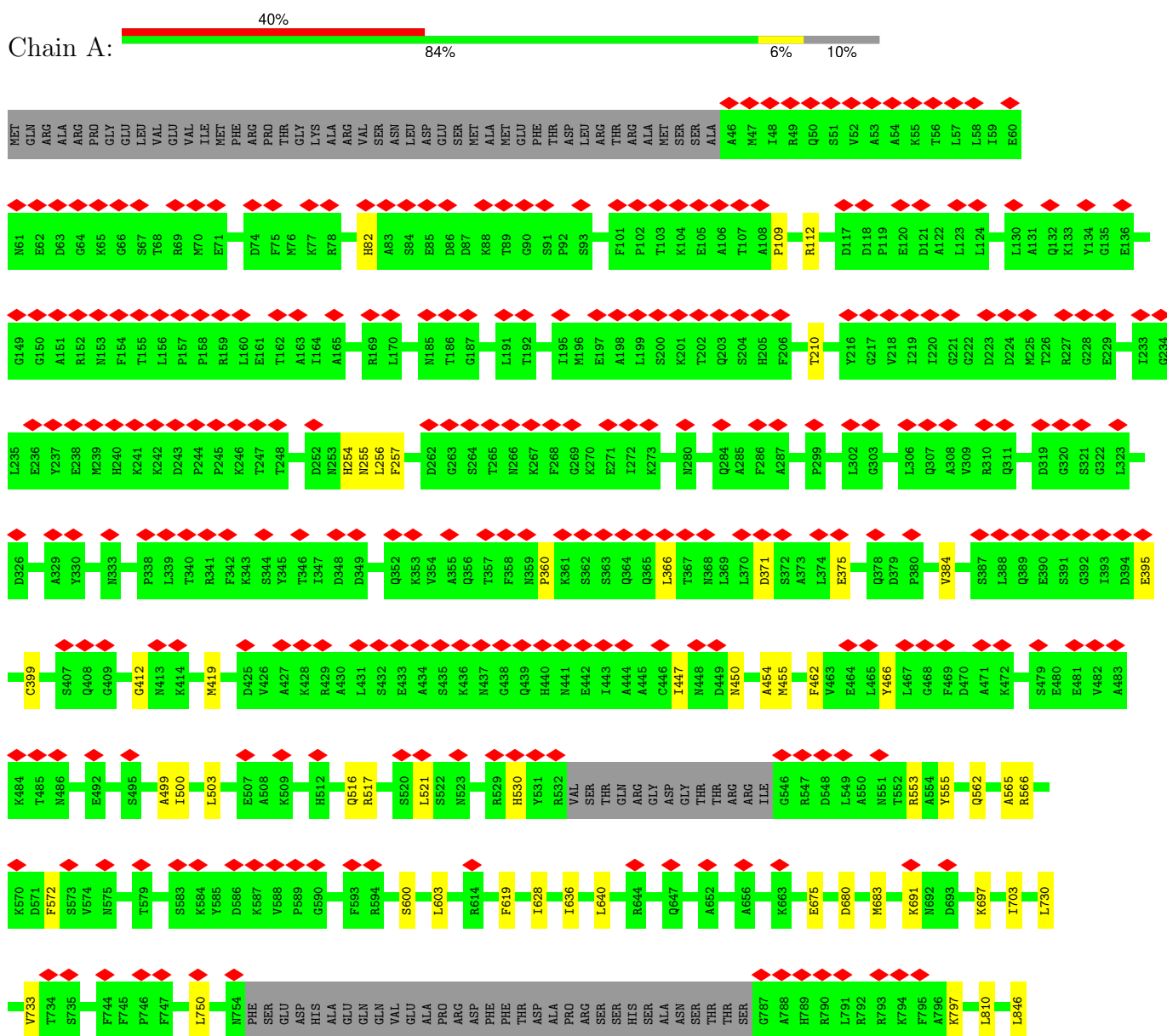


Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	
3	B	1	Total	C	O	0
			28	27	1	
3	B	1	Total	C	O	0
			28	27	1	
3	B	1	Total	C	O	0
			28	27	1	
3	C	1	Total	C	O	0
			28	27	1	
3	C	1	Total	C	O	0
			28	27	1	
3	C	1	Total	C	O	0
			28	27	1	
3	D	1	Total	C	O	0
			28	27	1	
3	D	1	Total	C	O	0
			28	27	1	
3	D	1	Total	C	O	0
			28	27	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: TRPM2 chanzyme





Response	Percentage
Yes	40%
No	85%
Don't know	6%
No answer	10%

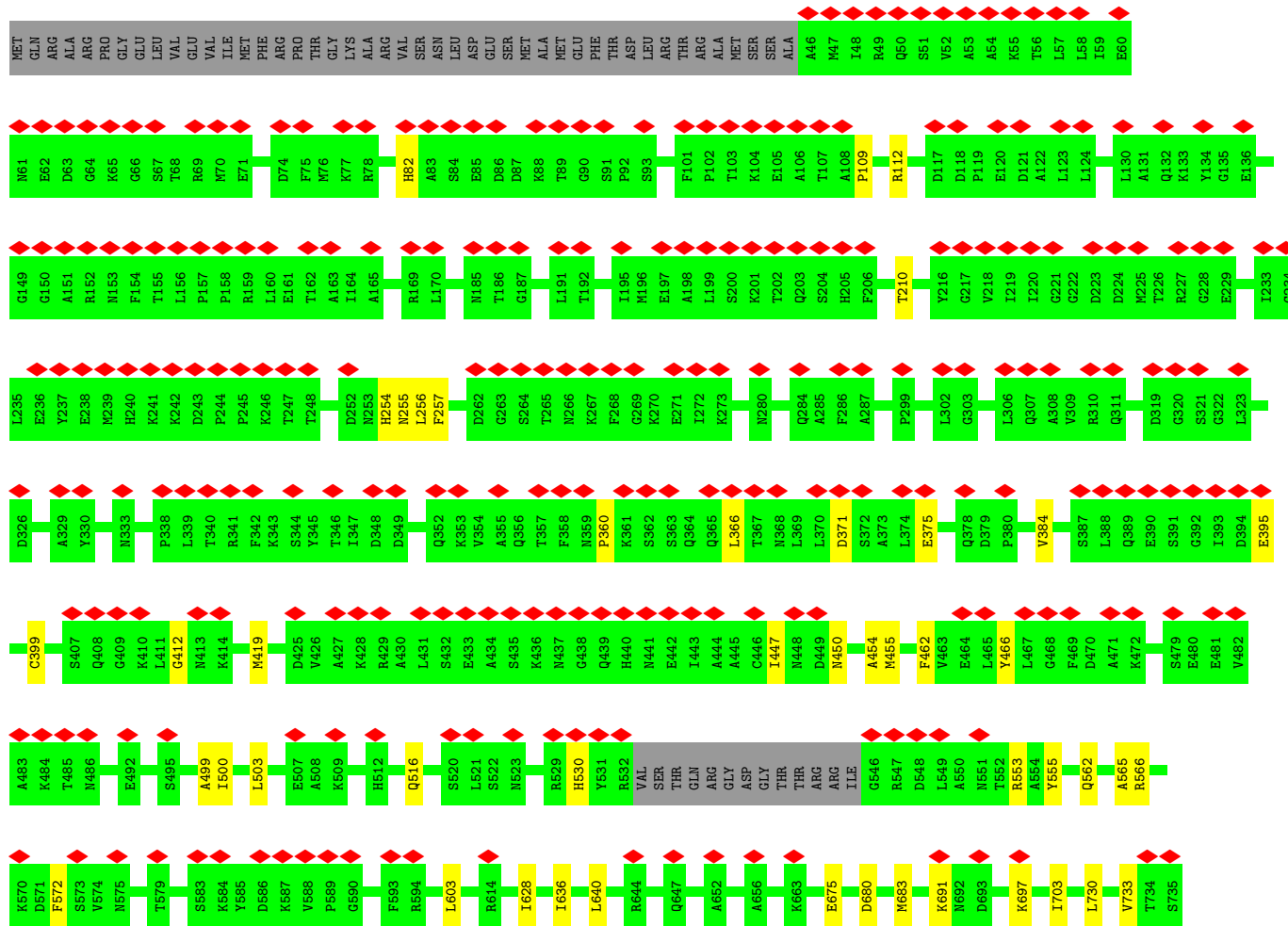
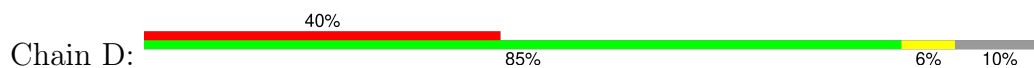








• Molecule 1: TRPM2 chanzyme



S1488	A1489	L1490	N1491	A1492	Y1493	F1494	R1428	N1429	T1430	D1431	N1432	A1433	W1434	V1435	E1436	T1437	T1438	C1439	V1440	N1441	F1442	H1443	D1444	E1445	S1446	G1447	R1448	H1449	A1450	A1451	R1452	L1453	K1454	L1455	Q1456	G1457	G1458	D1459	D1460	A1461	E1462	H1463	A1464	R1465	W1466	M1467	M1468	V1469	H1470	G1471	G1472	L1473	N1474	L1475	F1476	A1477	S1478	H1479	R1480	T1481	L1482	L1483	Q1484	H1485	V1486	T1487	P1427	D1426	E1425	C1424	Y1423	I1422	R1421	A1420	V1419	I1418	T1417	G1416	S1415	S1414	F1413	L1412	A1411	A1410	L1409	S1408	D1407	K1406	S1405	E1404	A1403	S1402	NET	LEU	ASP	ALA	SER	THR	M1394	G1393	L1392	A1391	E1390	M1389	M1388	F1387	E1386	R1385	G1384	T1382	S1383	W1382	L1381	A1380	V1379	D1378	E1377	G1376	N1375	D1374	V1373	F1372	G1371	G1370	P1369	T1368	W1366	M1365	K1364	N1363	D1362	Q1361	R1360	D1299	I1298	S1297	G1296	S1294	V1293	H1292	C1291	A1290	T1289	R1288	D1287	V1286	W1285	K1284	V1229	G1283	N1282	V1281	E1280	D1279	K1278	V1277	N1276	F1275	K1274	T1273	R1272	K1271	P1270	D1269	A1268	P1267	D1266	A1265	W1264	V1263	P1262	Q1261	VAL	ALA	VAL	HIS	GLY	HIS	THR	ALA	GLU	Q1145	D1141	N1140	T1139	M1138	R1128	E1125	W1124	R1123	R1107	E1104	D1103	Q1101	I1100	K1099	E1098	H1097	Q1096	T1094	V1092	G1091	C1090	L1089	R1088	L1087	L1086	R1085	M1084	F1083	I1074	A1071	D1065	E1062	L1059	F1003	P1002	I982	Y979	F976	D963	L945	W932	L920	R916	N915	F914	R913	ASP	HIS	GLU	ALA	ASP	GLU	PHE	ARG	PRO	ALA	VAL	GLN	GLN	GLU	ALA	GLU	ASP	PHE	THR	THR	SER	THR	THR	SER	G859	D858	C857	L846	L810	K797	F795	K794	R793	L791	R790	H789	A788	G787	S785	S784	L750	F747	F746	F745	F744	I860	A861	D866	D872	D889	Q893	V898	R913	F914	N915	R916	L920	W932	L945	D963	F976	Y979	I982	P1002	F1003	L1059	E1062	D1065	A1071	I1074	F1083	M1084	R1085	L1086	L1087	R1088	C1090	G1091	V1092	H1093	T1094	Q1096	E1096	H1097	P1247	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243	P1240	L1241	G1239	ASP	GLY	LEU	PRO	SER	THR	GLU	THR	PRO	THR	GLY	T1247	P1246	C1245	M1244	S1242	I1243
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	199037	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	52.873	Depositor
Minimum map value	-27.290	Depositor
Average map value	0.140	Depositor
Map value standard deviation	1.387	Depositor
Recommended contour level	11	Depositor
Map size (\AA)	363.44, 363.44, 363.44	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.82600003, 0.82600003, 0.82600003	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: MG, CLR

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	0.54	0/9662	0.78	0/13197
1	B	0.54	0/9662	0.78	0/13197
1	C	0.54	0/9662	0.78	0/13197
1	D	0.54	0/9662	0.78	0/13197
All	All	0.54	0/38648	0.78	0/52788

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	9458	0	8406	74	0
1	B	9458	0	8406	75	0
1	C	9458	0	8406	75	0
1	D	9458	0	8406	74	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	84	0	138	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	84	0	138	4	0
3	C	84	0	138	4	0
3	D	84	0	138	2	0
All	All	38176	0	34176	284	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 4.

All (284) 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:D:1473:LEU:HD13	1:D:1475:LEU:HD11	1.49	0.92
1:C:1473:LEU:HD13	1:C:1475:LEU:HD11	1.49	0.92
1:B:1473:LEU:HD13	1:B:1475:LEU:HD11	1.49	0.91
1:A:1473:LEU:HD13	1:A:1475:LEU:HD11	1.49	0.90
1:B:371:ASP:O	1:B:375:GLU:HG3	1.76	0.85
1:A:371:ASP:O	1:A:375:GLU:HG3	1.76	0.85
1:D:371:ASP:O	1:D:375:GLU:HG3	1.76	0.84
1:C:371:ASP:O	1:C:375:GLU:HG3	1.76	0.84
1:D:730:LEU:HD21	1:D:797:LYS:HD3	1.69	0.74
1:B:730:LEU:HD21	1:B:797:LYS:HD3	1.69	0.74
1:A:730:LEU:HD21	1:A:797:LYS:HD3	1.69	0.73
1:C:730:LEU:HD21	1:C:797:LYS:HD3	1.69	0.73
1:D:1332:VAL:HG12	1:D:1334:THR:HG23	1.71	0.73
1:B:1332:VAL:HG12	1:B:1334:THR:HG23	1.71	0.73
1:A:1332:VAL:HG12	1:A:1334:THR:HG23	1.71	0.72
1:C:1332:VAL:HG12	1:C:1334:THR:HG23	1.71	0.71
1:D:384:VAL:HG12	1:D:399:CYS:SG	2.33	0.69
1:C:384:VAL:HG12	1:C:399:CYS:SG	2.32	0.69
1:B:384:VAL:HG12	1:B:399:CYS:SG	2.33	0.68
1:A:384:VAL:HG12	1:A:399:CYS:SG	2.33	0.67
1:B:562:GLN:HB3	1:B:566:ARG:HH12	1.61	0.66
1:D:562:GLN:HB3	1:D:566:ARG:HH12	1.61	0.65
1:D:455:MET:HE3	1:D:603:LEU:HD13	1.79	0.65
1:C:455:MET:HE3	1:C:603:LEU:HD13	1.79	0.65
1:C:562:GLN:HB3	1:C:566:ARG:HH12	1.61	0.65
1:A:562:GLN:HB3	1:A:566:ARG:HH12	1.61	0.64
1:D:733:VAL:O	1:D:733:VAL:HG23	1.99	0.63
1:C:1473:LEU:HB3	1:C:1475:LEU:HG	1.81	0.63
1:B:455:MET:HE3	1:B:603:LEU:HD13	1.80	0.62
1:A:733:VAL:HG23	1:A:733:VAL:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:733:VAL:HG23	1:C:733:VAL:O	1.99	0.62
1:A:455:MET:HE3	1:A:603:LEU:HD13	1.81	0.62
1:B:733:VAL:HG23	1:B:733:VAL:O	1.99	0.62
1:D:1473:LEU:HB3	1:D:1475:LEU:HG	1.81	0.62
1:B:1473:LEU:HB3	1:B:1475:LEU:HG	1.81	0.62
1:B:1475:LEU:H	1:B:1480:ARG:HE	1.48	0.62
1:A:1473:LEU:HB3	1:A:1475:LEU:HG	1.81	0.61
1:A:1475:LEU:H	1:A:1480:ARG:HE	1.48	0.61
1:C:1475:LEU:H	1:C:1480:ARG:HE	1.48	0.60
1:C:384:VAL:CG1	1:C:399:CYS:SG	2.90	0.60
1:D:384:VAL:CG1	1:D:399:CYS:SG	2.90	0.59
1:A:384:VAL:CG1	1:A:399:CYS:SG	2.90	0.59
1:A:109:PRO:HB2	1:A:256:LEU:CD1	2.33	0.59
1:D:109:PRO:HB2	1:D:256:LEU:CD1	2.32	0.59
1:D:1475:LEU:H	1:D:1480:ARG:HE	1.48	0.59
1:B:109:PRO:HB2	1:B:256:LEU:CD1	2.33	0.59
1:B:419:MET:SD	1:B:454:ALA:HA	2.43	0.59
1:B:384:VAL:CG1	1:B:399:CYS:SG	2.90	0.59
1:C:419:MET:SD	1:C:454:ALA:HA	2.43	0.59
1:C:1071:ALA:O	1:C:1074:ILE:HG22	2.03	0.58
1:A:419:MET:SD	1:A:454:ALA:HA	2.43	0.58
1:D:254:HIS:HB2	1:D:257:PHE:CZ	2.39	0.58
1:A:1071:ALA:O	1:A:1074:ILE:HG22	2.03	0.58
1:C:109:PRO:HB2	1:C:256:LEU:CD1	2.33	0.58
1:B:1071:ALA:O	1:B:1074:ILE:HG22	2.03	0.58
1:D:419:MET:SD	1:D:454:ALA:HA	2.43	0.58
1:B:254:HIS:HB2	1:B:257:PHE:CZ	2.39	0.58
1:C:254:HIS:HB2	1:C:257:PHE:CZ	2.39	0.58
1:D:1071:ALA:O	1:D:1074:ILE:HG22	2.03	0.57
1:A:254:HIS:HB2	1:A:257:PHE:CZ	2.39	0.57
1:A:636:ILE:O	1:A:640:LEU:HB2	2.06	0.56
1:A:1331:THR:O	1:A:1331:THR:HG23	2.06	0.56
1:D:636:ILE:O	1:D:640:LEU:HB2	2.06	0.56
1:D:979:TYR:O	1:D:982:ILE:HG12	2.06	0.56
1:B:1331:THR:HG23	1:B:1331:THR:O	2.06	0.56
1:A:979:TYR:O	1:A:982:ILE:HG12	2.06	0.56
1:B:979:TYR:O	1:B:982:ILE:HG12	2.06	0.56
1:C:636:ILE:O	1:C:640:LEU:HB2	2.06	0.56
1:D:1331:THR:HG23	1:D:1331:THR:O	2.06	0.55
1:B:636:ILE:O	1:B:640:LEU:HB2	2.06	0.55
1:C:979:TYR:O	1:C:982:ILE:HG12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1331:THR:HG23	1:C:1331:THR:O	2.06	0.55
1:C:395:GLU:HG2	1:C:395:GLU:O	2.08	0.54
1:B:395:GLU:O	1:B:395:GLU:HG2	2.08	0.54
1:A:395:GLU:O	1:A:395:GLU:HG2	2.08	0.54
1:D:395:GLU:O	1:D:395:GLU:HG2	2.08	0.54
1:B:810:LEU:CD1	1:B:914:PHE:CE1	2.92	0.53
1:D:810:LEU:CD1	1:D:914:PHE:CE1	2.92	0.53
1:B:530:HIS:HB2	1:B:566:ARG:HH21	1.74	0.53
1:C:810:LEU:CD1	1:C:914:PHE:CE1	2.92	0.53
1:A:447:ILE:HD11	1:A:466:TYR:HB3	1.91	0.53
1:B:447:ILE:HD11	1:B:466:TYR:HB3	1.91	0.52
1:C:530:HIS:HB2	1:C:566:ARG:HH21	1.74	0.52
1:A:109:PRO:O	1:A:256:LEU:HD12	2.10	0.52
1:A:810:LEU:CD1	1:A:914:PHE:CE1	2.92	0.52
1:C:109:PRO:O	1:C:256:LEU:HD12	2.10	0.52
1:D:530:HIS:HB2	1:D:566:ARG:HH21	1.74	0.52
1:D:447:ILE:HD11	1:D:466:TYR:HB3	1.91	0.52
1:D:109:PRO:O	1:D:256:LEU:HD12	2.10	0.52
1:C:447:ILE:HD11	1:C:466:TYR:HB3	1.91	0.52
1:D:916:ARG:NH2	1:D:1062:GLU:OE2	2.43	0.52
1:A:916:ARG:NH2	1:A:1062:GLU:OE2	2.43	0.51
1:B:916:ARG:NH2	1:B:1062:GLU:OE2	2.43	0.51
1:C:916:ARG:NH2	1:C:1062:GLU:OE2	2.43	0.51
1:A:530:HIS:HB2	1:A:566:ARG:HH21	1.74	0.51
1:B:109:PRO:O	1:B:256:LEU:HD12	2.10	0.51
1:C:920:LEU:CD1	1:C:1059:LEU:HD13	2.41	0.51
1:D:920:LEU:CD1	1:D:1059:LEU:HD13	2.41	0.51
1:A:500:ILE:HG12	1:A:603:LEU:HD21	1.93	0.50
1:D:500:ILE:HG12	1:D:603:LEU:HD21	1.93	0.50
1:C:1002:PRO:HG2	1:D:976:PHE:CE2	2.47	0.50
1:B:920:LEU:CD1	1:B:1059:LEU:HD13	2.41	0.50
1:A:920:LEU:CD1	1:A:1059:LEU:HD13	2.41	0.50
1:A:976:PHE:CE2	1:D:1002:PRO:HG2	2.47	0.50
1:B:1002:PRO:HG2	1:C:976:PHE:CE2	2.47	0.50
1:B:1474:ASN:HA	1:B:1480:ARG:HH21	1.77	0.50
1:A:1002:PRO:HG2	1:B:976:PHE:CE2	2.47	0.49
1:C:1474:ASN:HA	1:C:1480:ARG:HH21	1.77	0.49
1:D:1473:LEU:HD13	1:D:1475:LEU:CD1	2.34	0.49
1:A:893:GLN:NE2	1:D:963:ASP:OD2	2.46	0.49
1:A:628:ILE:HG23	1:A:703:ILE:HG21	1.94	0.49
1:B:628:ILE:HG23	1:B:703:ILE:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:628:ILE:HG23	1:C:703:ILE:HG21	1.94	0.49
1:C:963:ASP:OD2	1:D:893:GLN:NE2	2.45	0.49
1:B:500:ILE:HG12	1:B:603:LEU:HD21	1.93	0.49
1:D:628:ILE:HG23	1:D:703:ILE:HG21	1.94	0.49
1:A:963:ASP:OD2	1:B:893:GLN:NE2	2.44	0.49
1:A:810:LEU:HD11	1:A:914:PHE:CE1	2.48	0.49
1:D:810:LEU:HD11	1:D:914:PHE:CE1	2.48	0.49
1:A:730:LEU:HD21	1:A:797:LYS:CD	2.41	0.49
1:C:500:ILE:HG12	1:C:603:LEU:HD21	1.93	0.49
1:B:963:ASP:OD2	1:C:893:GLN:NE2	2.45	0.48
1:D:846:LEU:HD21	1:D:1071:ALA:HB1	1.95	0.48
1:A:680:ASP:HB3	1:A:683:MET:HB2	1.96	0.48
1:D:1474:ASN:HA	1:D:1480:ARG:HH21	1.77	0.48
1:C:810:LEU:HD11	1:C:914:PHE:CE1	2.48	0.48
1:D:730:LEU:HD21	1:D:797:LYS:CD	2.41	0.48
1:A:846:LEU:HD21	1:A:1071:ALA:HB1	1.95	0.48
1:A:1474:ASN:HA	1:A:1480:ARG:HH21	1.77	0.48
1:B:680:ASP:HB3	1:B:683:MET:HB2	1.96	0.48
1:C:730:LEU:CD2	1:C:797:LYS:HD3	2.42	0.48
1:C:846:LEU:HD21	1:C:1071:ALA:HB1	1.95	0.48
1:D:680:ASP:HB3	1:D:683:MET:HB2	1.96	0.48
1:C:730:LEU:HD21	1:C:797:LYS:CD	2.41	0.48
1:B:810:LEU:HD11	1:B:914:PHE:CE1	2.48	0.48
1:B:846:LEU:HD21	1:B:1071:ALA:HB1	1.95	0.48
1:A:810:LEU:HD12	1:A:914:PHE:CE1	2.49	0.47
1:B:810:LEU:HD12	1:B:914:PHE:CE1	2.49	0.47
1:A:1338:ARG:NH2	1:A:1445:GLU:O	2.47	0.47
1:C:680:ASP:HB3	1:C:683:MET:HB2	1.96	0.47
1:C:810:LEU:HD12	1:C:914:PHE:CE1	2.49	0.47
1:B:730:LEU:CD2	1:B:797:LYS:HD3	2.42	0.47
1:B:1338:ARG:NH2	1:B:1445:GLU:O	2.47	0.47
1:D:810:LEU:HD12	1:D:914:PHE:CE1	2.49	0.47
1:D:730:LEU:CD2	1:D:797:LYS:HD3	2.42	0.47
1:A:730:LEU:CD2	1:A:797:LYS:HD3	2.42	0.47
1:C:82:HIS:O	1:C:112:ARG:NH2	2.48	0.47
1:A:82:HIS:O	1:A:112:ARG:NH2	2.48	0.46
1:A:810:LEU:HD11	1:A:914:PHE:CZ	2.50	0.46
1:C:565:ALA:HB1	1:C:572:PHE:O	2.15	0.46
1:D:810:LEU:HD11	1:D:914:PHE:CZ	2.50	0.46
1:C:810:LEU:HD11	1:C:914:PHE:CZ	2.50	0.46
1:D:82:HIS:O	1:D:112:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:565:ALA:HB1	1:D:572:PHE:O	2.15	0.46
1:A:1473:LEU:HD13	1:A:1475:LEU:CD1	2.34	0.46
1:C:691:LYS:HE3	1:C:697:LYS:HB3	1.97	0.46
1:C:1338:ARG:NH2	1:C:1445:GLU:O	2.47	0.46
1:B:82:HIS:O	1:B:112:ARG:NH2	2.48	0.46
1:B:730:LEU:HD21	1:B:797:LYS:CD	2.41	0.46
1:B:565:ALA:HB1	1:B:572:PHE:O	2.15	0.46
1:D:691:LYS:HE3	1:D:697:LYS:HB3	1.97	0.46
1:A:565:ALA:HB1	1:A:572:PHE:O	2.15	0.46
1:B:691:LYS:HE3	1:B:697:LYS:HB3	1.97	0.46
1:D:1332:VAL:HG12	1:D:1334:THR:CG2	2.44	0.46
1:A:691:LYS:HE3	1:A:697:LYS:HB3	1.97	0.46
1:C:419:MET:HA	1:C:462:PHE:CZ	2.51	0.45
1:B:810:LEU:HD11	1:B:914:PHE:CZ	2.50	0.45
1:A:1003:PHE:HB2	3:A:3004:CLR:H41	1.99	0.45
1:D:675:GLU:OE1	1:D:1123:ARG:NH2	2.50	0.45
1:A:419:MET:HA	1:A:462:PHE:CZ	2.51	0.45
1:A:447:ILE:HD11	1:A:466:TYR:CB	2.47	0.45
1:A:931:MET:HE3	1:A:931:MET:HB3	1.82	0.45
1:B:419:MET:HA	1:B:462:PHE:CZ	2.51	0.45
1:B:1003:PHE:HB2	3:B:3004:CLR:H41	1.99	0.45
1:B:1409:LEU:HD13	1:B:1453:LEU:HD21	1.99	0.45
1:A:1138:MET:CE	1:D:1140:ASN:HD21	2.30	0.45
1:C:447:ILE:HD11	1:C:466:TYR:CB	2.47	0.45
1:C:920:LEU:HD12	1:C:1059:LEU:HD13	1.99	0.45
1:C:1003:PHE:HB2	3:C:3004:CLR:H41	1.99	0.45
1:D:419:MET:HA	1:D:462:PHE:CZ	2.51	0.45
1:B:675:GLU:OE1	1:B:1123:ARG:NH2	2.50	0.45
1:D:1338:ARG:NH2	1:D:1445:GLU:O	2.47	0.45
1:B:1140:ASN:HD21	1:C:1138:MET:CE	2.30	0.45
1:C:945:LEU:HD21	1:C:982:ILE:HD13	1.99	0.45
1:B:447:ILE:HD11	1:B:466:TYR:CB	2.47	0.44
1:A:210:THR:H	1:A:255:ASN:HB2	1.82	0.44
1:A:1140:ASN:HD21	1:B:1138:MET:CE	2.30	0.44
1:B:898:VAL:HG22	3:B:3003:CLR:H21	1.99	0.44
1:B:945:LEU:HD21	1:B:982:ILE:HD13	2.00	0.44
3:B:3003:CLR:H162	3:B:3003:CLR:H222	1.66	0.44
1:C:210:THR:H	1:C:255:ASN:HB2	1.82	0.44
1:A:675:GLU:OE1	1:A:1123:ARG:NH2	2.50	0.44
1:B:920:LEU:HD12	1:B:1059:LEU:HD13	1.99	0.44
1:C:1140:ASN:HD21	1:D:1138:MET:CE	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:898:VAL:HG22	3:A:3003:CLR:H21	1.99	0.44
1:A:920:LEU:HD12	1:A:1059:LEU:HD13	1.99	0.44
1:C:675:GLU:OE1	1:C:1123:ARG:NH2	2.50	0.44
1:D:920:LEU:HD12	1:D:1059:LEU:HD13	1.99	0.44
1:D:1003:PHE:HB2	3:D:6001:CLR:H41	2.00	0.44
1:C:500:ILE:HG12	1:C:603:LEU:CD2	2.48	0.44
1:D:210:THR:H	1:D:255:ASN:HB2	1.82	0.44
1:D:500:ILE:HG12	1:D:603:LEU:CD2	2.48	0.44
1:C:750:LEU:HD12	1:C:750:LEU:HA	1.88	0.44
1:D:447:ILE:HD11	1:D:466:TYR:CB	2.47	0.44
1:D:945:LEU:HD21	1:D:982:ILE:HD13	2.00	0.44
1:A:945:LEU:HD21	1:A:982:ILE:HD13	2.00	0.43
3:A:3003:CLR:H222	3:A:3003:CLR:H162	1.66	0.43
1:B:210:THR:H	1:B:255:ASN:HB2	1.82	0.43
1:D:898:VAL:HG22	3:D:6005:CLR:H21	1.99	0.43
1:D:1087:LEU:HD12	1:D:1087:LEU:HA	1.87	0.43
1:A:553:ARG:HE	1:A:553:ARG:HB3	1.64	0.43
1:A:1409:LEU:HD13	1:A:1453:LEU:HD21	1.99	0.43
1:B:500:ILE:HG12	1:B:603:LEU:CD2	2.48	0.43
1:B:1087:LEU:HD12	1:B:1087:LEU:HA	1.87	0.43
1:D:1409:LEU:HD13	1:D:1453:LEU:HD21	1.99	0.43
1:A:109:PRO:HB2	1:A:256:LEU:HD12	2.01	0.43
1:C:553:ARG:HE	1:C:553:ARG:HB3	1.64	0.43
1:D:109:PRO:HB2	1:D:256:LEU:HD12	2.01	0.43
1:C:1013:MET:HE3	1:C:1013:MET:HB3	1.85	0.43
1:A:500:ILE:HG12	1:A:603:LEU:CD2	2.48	0.43
1:A:1332:VAL:HG12	1:A:1334:THR:CG2	2.44	0.43
1:C:898:VAL:HG22	3:C:3003:CLR:H21	1.99	0.43
1:D:750:LEU:HD12	1:D:750:LEU:HA	1.88	0.43
1:B:256:LEU:HG	1:B:257:PHE:N	2.34	0.43
1:C:1409:LEU:HD13	1:C:1453:LEU:HD21	1.99	0.43
1:D:412:GLY:HA2	1:D:450:ASN:HD21	1.84	0.43
1:B:109:PRO:HB2	1:B:256:LEU:HD12	2.01	0.42
1:B:1332:VAL:HG12	1:B:1334:THR:CG2	2.44	0.42
1:B:360:PRO:HG2	1:B:366:LEU:HB2	2.01	0.42
1:B:750:LEU:HD12	1:B:750:LEU:HA	1.88	0.42
1:A:256:LEU:HG	1:A:257:PHE:N	2.34	0.42
1:A:1157:MET:HE2	1:B:1156:HIS:HB3	2.01	0.42
1:B:412:GLY:HA2	1:B:450:ASN:HD21	1.84	0.42
1:C:256:LEU:HG	1:C:257:PHE:N	2.34	0.42
1:C:1473:LEU:HD13	1:C:1475:LEU:CD1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1013:MET:HB3	1:B:1013:MET:HE3	1.84	0.42
3:B:3004:CLR:H272	3:B:3004:CLR:H231	1.84	0.42
1:C:1328:ALA:HB3	1:C:1437:THR:HG22	2.02	0.42
3:C:3003:CLR:H222	3:C:3003:CLR:H162	1.66	0.42
1:C:708:LYS:HD2	1:C:708:LYS:HA	1.92	0.42
1:D:516:GLN:OE1	1:D:555:TYR:OH	2.38	0.42
1:D:1328:ALA:HB3	1:D:1437:THR:HG22	2.02	0.42
1:C:499:ALA:O	1:C:503:LEU:HG	2.20	0.42
3:C:3004:CLR:H272	3:C:3004:CLR:H231	1.84	0.42
1:A:516:GLN:OE1	1:A:555:TYR:OH	2.38	0.41
1:B:553:ARG:HE	1:B:553:ARG:HB3	1.64	0.41
1:B:562:GLN:HB3	1:B:566:ARG:NH1	2.33	0.41
1:C:412:GLY:HA2	1:C:450:ASN:HD21	1.84	0.41
1:D:256:LEU:HG	1:D:257:PHE:N	2.34	0.41
1:D:360:PRO:HG2	1:D:366:LEU:HB2	2.01	0.41
1:D:553:ARG:HE	1:D:553:ARG:HB3	1.64	0.41
1:A:360:PRO:HG2	1:A:366:LEU:HB2	2.01	0.41
1:C:360:PRO:HG2	1:C:366:LEU:HB2	2.01	0.41
1:D:499:ALA:O	1:D:503:LEU:HG	2.20	0.41
1:A:750:LEU:HD12	1:A:750:LEU:HA	1.88	0.41
1:D:530:HIS:HB2	1:D:566:ARG:NH2	2.36	0.41
1:C:1332:VAL:HG12	1:C:1334:THR:CG2	2.44	0.41
1:D:562:GLN:HB3	1:D:566:ARG:NH1	2.33	0.41
1:A:412:GLY:HA2	1:A:450:ASN:HD21	1.84	0.41
1:A:530:HIS:HB2	1:A:566:ARG:NH2	2.35	0.41
1:B:516:GLN:OE1	1:B:555:TYR:OH	2.38	0.41
1:A:1328:ALA:HB3	1:A:1437:THR:HG22	2.02	0.41
1:C:1157:MET:CE	1:D:1156:HIS:HB3	2.51	0.41
1:A:499:ALA:O	1:A:503:LEU:HG	2.20	0.41
1:A:1157:MET:CE	1:B:1156:HIS:HB3	2.51	0.41
1:B:1157:MET:CE	1:C:1156:HIS:HB3	2.51	0.41
1:B:1328:ALA:HB3	1:B:1437:THR:HG22	2.02	0.41
1:C:1331:THR:O	1:C:1331:THR:CG2	2.69	0.41
1:C:621:LEU:HD12	1:C:621:LEU:HA	1.87	0.41
1:A:517:ARG:O	1:A:521:LEU:HB2	2.21	0.40
1:B:499:ALA:O	1:B:503:LEU:HG	2.20	0.40
1:C:109:PRO:HB2	1:C:256:LEU:HD12	2.01	0.40
1:C:516:GLN:OE1	1:C:555:TYR:OH	2.38	0.40
1:A:1156:HIS:HB3	1:D:1157:MET:CE	2.51	0.40
1:B:600:SER:OG	1:B:619:PHE:O	2.40	0.40
1:B:708:LYS:HD2	1:B:708:LYS:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:THR:HB	1:B:255:ASN:H	1.86	0.40
1:D:872:ASP:OD1	1:D:913:ARG:NE	2.54	0.40
1:A:1153:LEU:HD12	1:D:1157:MET:SD	2.61	0.40
1:C:530:HIS:HB2	1:C:566:ARG:NH2	2.35	0.40
1:C:872:ASP:OD1	1:C:913:ARG:NE	2.54	0.40
1:C:1157:MET:HE2	1:D:1156:HIS:HB3	2.03	0.40
1:A:600:SER:OG	1:A:619:PHE:O	2.40	0.40
1:B:1473:LEU:HD13	1:B:1475:LEU:CD1	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1342/1494 (90%)	1308 (98%)	34 (2%)	0	100	100
1	B	1342/1494 (90%)	1308 (98%)	34 (2%)	0	100	100
1	C	1342/1494 (90%)	1308 (98%)	34 (2%)	0	100	100
1	D	1342/1494 (90%)	1308 (98%)	34 (2%)	0	100	100
All	All	5368/5976 (90%)	5232 (98%)	136 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	786/1276 (62%)	786 (100%)	0	100	100
1	B	786/1276 (62%)	786 (100%)	0	100	100
1	C	786/1276 (62%)	786 (100%)	0	100	100
1	D	786/1276 (62%)	786 (100%)	0	100	100
All	All	3144/5104 (62%)	3144 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	457	HIS
1	A	1140	ASN
1	A	1441	ASN
1	B	457	HIS
1	B	1140	ASN
1	B	1441	ASN
1	C	457	HIS
1	C	1140	ASN
1	C	1441	ASN
1	D	457	HIS
1	D	1140	ASN
1	D	1441	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 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	CLR	C	3004	-	31,31,31	0.31	0	48,48,48	0.48	0
3	CLR	D	6001	-	31,31,31	0.31	0	48,48,48	0.48	0
3	CLR	B	3003	-	31,31,31	0.28	0	48,48,48	0.47	0
3	CLR	A	3003	-	31,31,31	0.28	0	48,48,48	0.47	0
3	CLR	D	6005	-	31,31,31	0.28	0	48,48,48	0.47	0
3	CLR	C	3003	-	31,31,31	0.28	0	48,48,48	0.47	0
3	CLR	B	3005	-	31,31,31	0.28	0	48,48,48	0.58	0
3	CLR	A	3005	-	31,31,31	0.28	0	48,48,48	0.58	0
3	CLR	B	3004	-	31,31,31	0.31	0	48,48,48	0.48	0
3	CLR	D	6002	-	31,31,31	0.28	0	48,48,48	0.58	0
3	CLR	A	3004	-	31,31,31	0.31	0	48,48,48	0.48	0
3	CLR	C	3005	-	31,31,31	0.28	0	48,48,48	0.58	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLR	C	3004	-	-	2/10/68/68	0/4/4/4
3	CLR	D	6001	-	-	2/10/68/68	0/4/4/4
3	CLR	B	3003	-	-	5/10/68/68	0/4/4/4
3	CLR	A	3003	-	-	5/10/68/68	0/4/4/4
3	CLR	D	6005	-	-	5/10/68/68	0/4/4/4
3	CLR	C	3003	-	-	5/10/68/68	0/4/4/4
3	CLR	B	3005	-	-	0/10/68/68	0/4/4/4
3	CLR	A	3005	-	-	0/10/68/68	0/4/4/4
3	CLR	B	3004	-	-	2/10/68/68	0/4/4/4
3	CLR	D	6002	-	-	0/10/68/68	0/4/4/4
3	CLR	A	3004	-	-	2/10/68/68	0/4/4/4
3	CLR	C	3005	-	-	0/10/68/68	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3003	CLR	C16-C17-C20-C21
3	B	3003	CLR	C16-C17-C20-C21
3	C	3003	CLR	C16-C17-C20-C21
3	D	6005	CLR	C16-C17-C20-C21
3	A	3003	CLR	C13-C17-C20-C21
3	B	3003	CLR	C13-C17-C20-C21
3	C	3003	CLR	C13-C17-C20-C21
3	D	6005	CLR	C13-C17-C20-C21
3	A	3003	CLR	C13-C17-C20-C22
3	B	3003	CLR	C13-C17-C20-C22
3	C	3003	CLR	C13-C17-C20-C22
3	D	6005	CLR	C13-C17-C20-C22
3	A	3003	CLR	C16-C17-C20-C22
3	B	3003	CLR	C16-C17-C20-C22
3	C	3003	CLR	C16-C17-C20-C22
3	D	6005	CLR	C16-C17-C20-C22
3	A	3004	CLR	C22-C23-C24-C25
3	B	3004	CLR	C22-C23-C24-C25
3	C	3004	CLR	C22-C23-C24-C25
3	D	6001	CLR	C22-C23-C24-C25
3	A	3004	CLR	C23-C24-C25-C27
3	B	3004	CLR	C23-C24-C25-C27
3	C	3004	CLR	C23-C24-C25-C27
3	D	6001	CLR	C23-C24-C25-C27
3	A	3003	CLR	C23-C24-C25-C27
3	B	3003	CLR	C23-C24-C25-C27
3	D	6005	CLR	C23-C24-C25-C27
3	C	3003	CLR	C23-C24-C25-C27

There are no ring outliers.

8 monomers are involved in 13 short contacts:

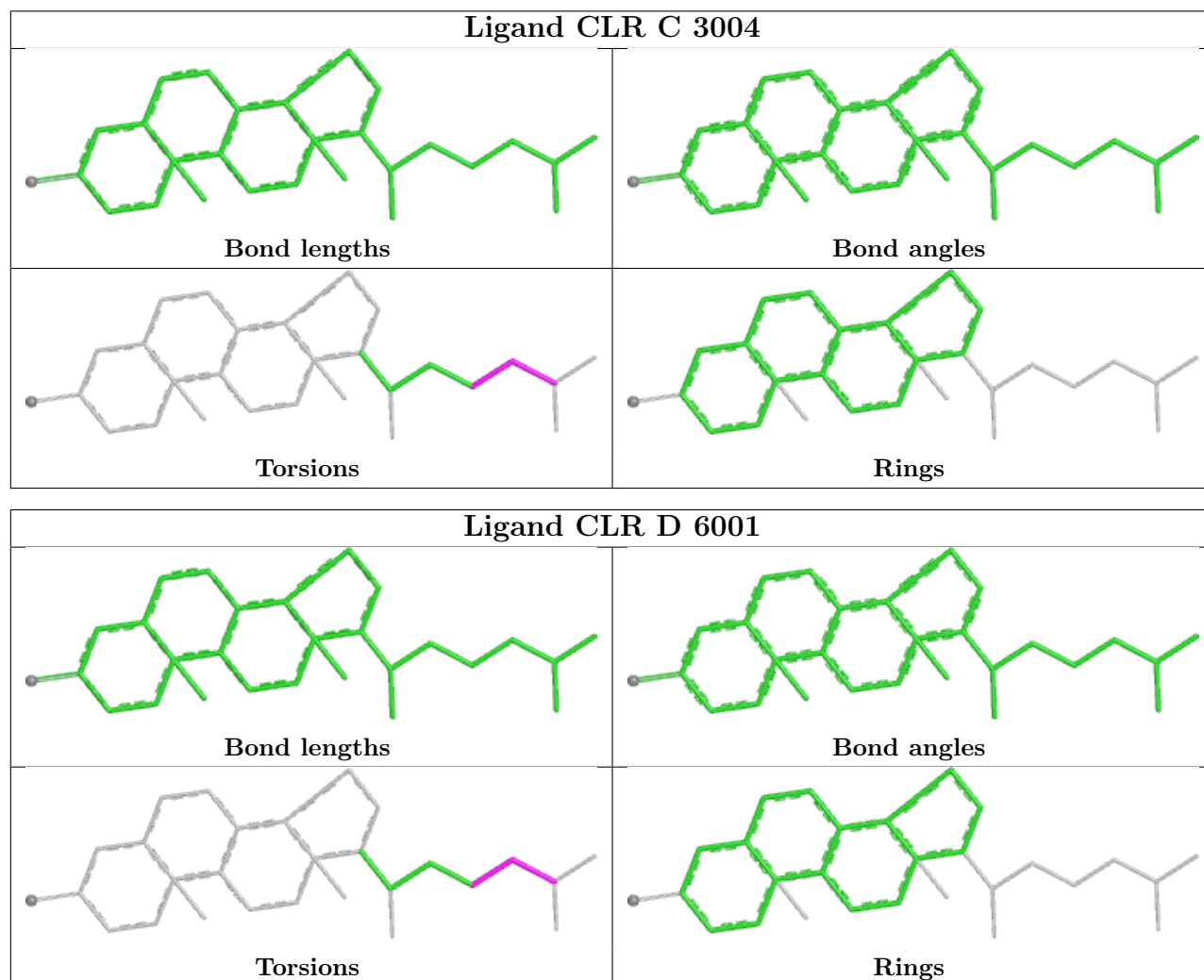
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3004	CLR	2	0
3	D	6001	CLR	1	0
3	B	3003	CLR	2	0
3	A	3003	CLR	2	0
3	D	6005	CLR	1	0

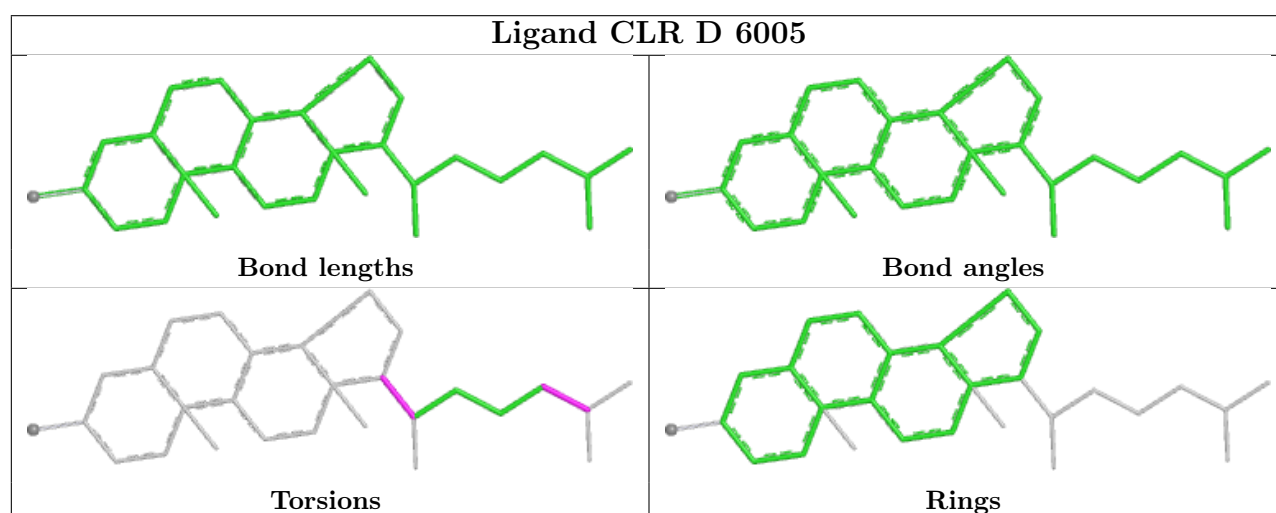
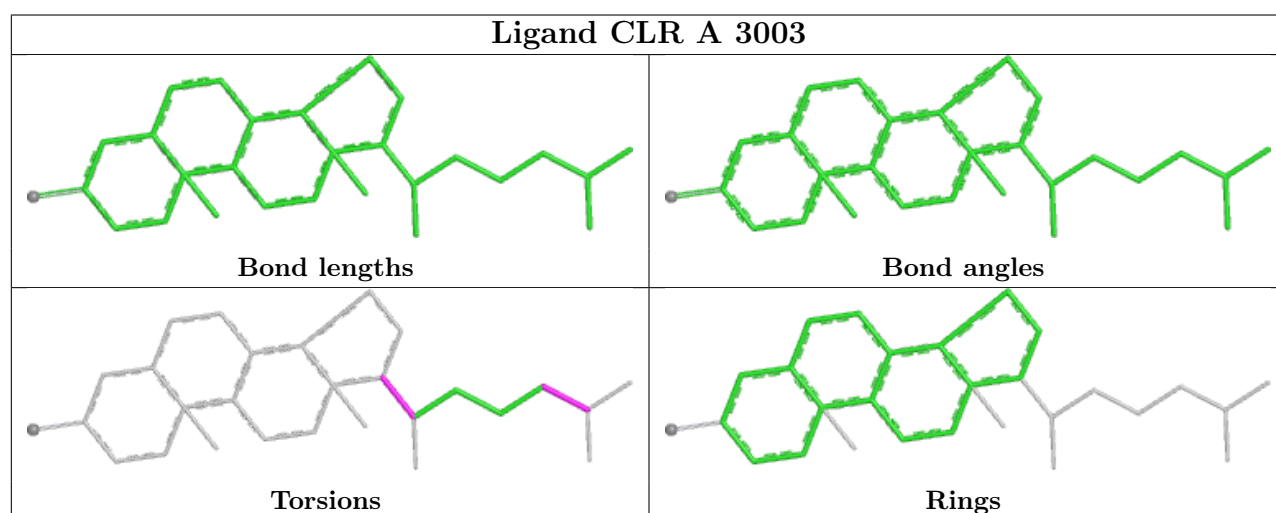
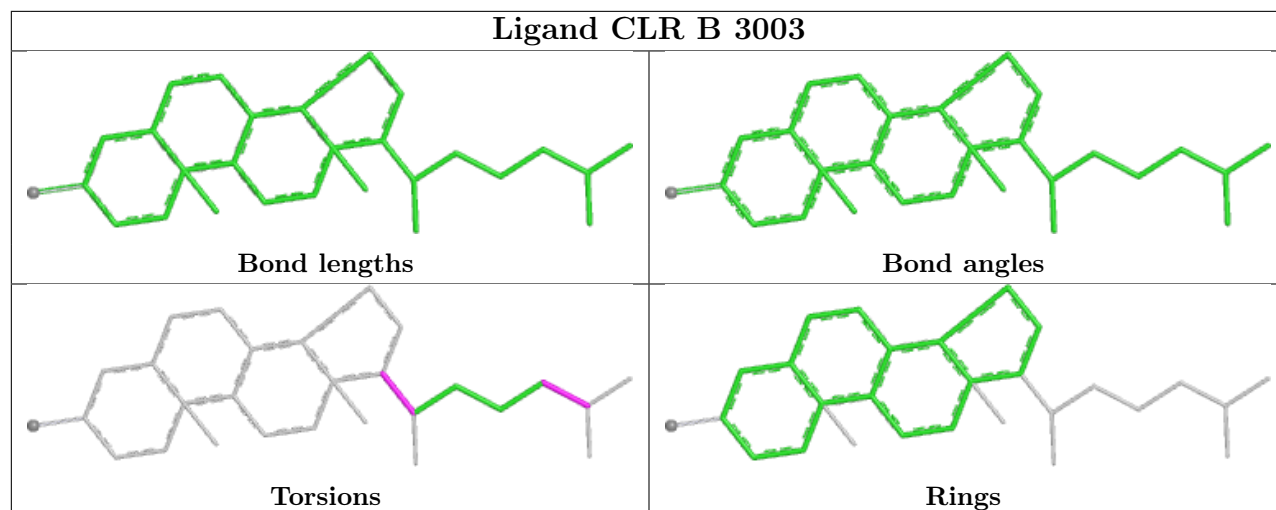
Continued on next page...

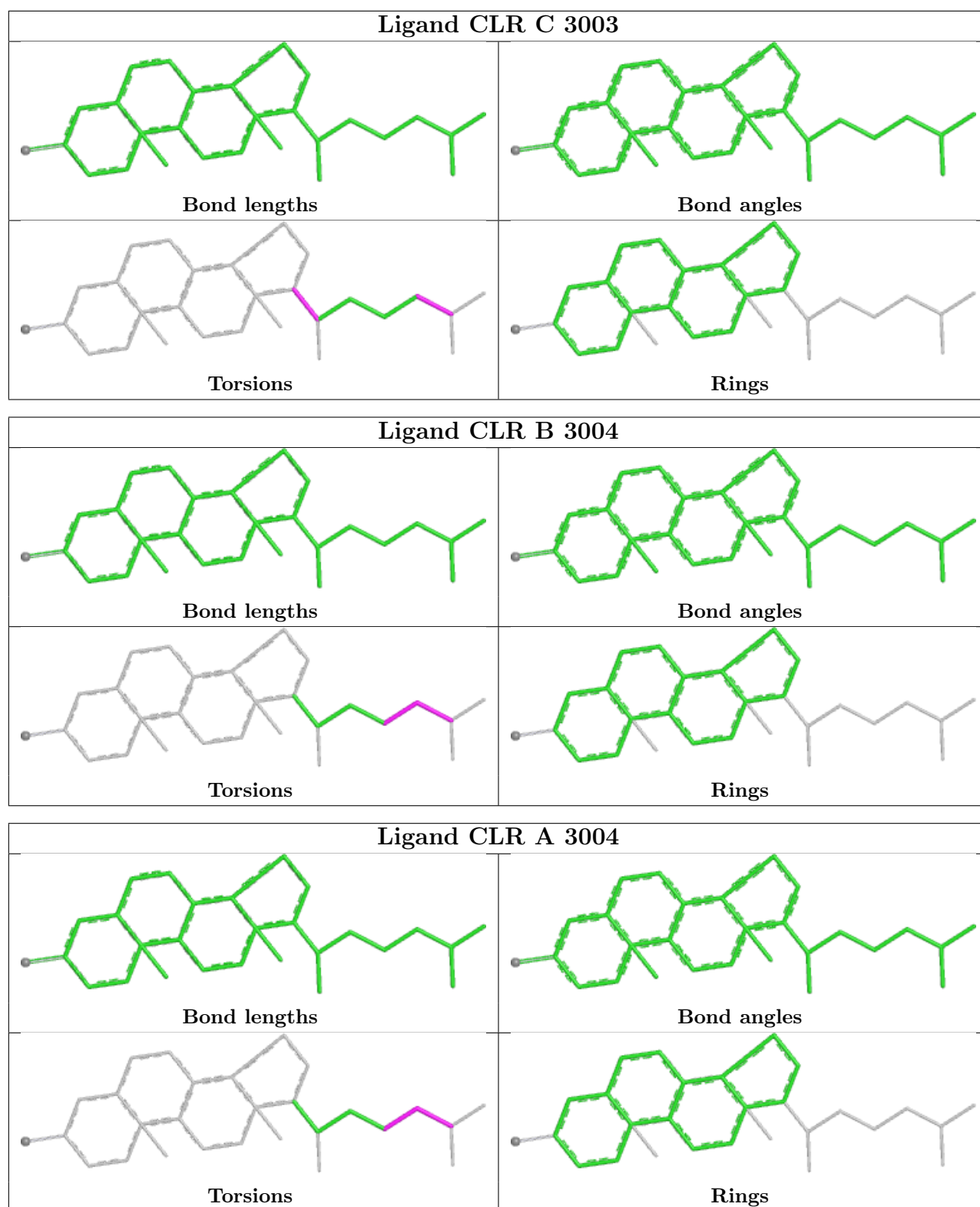
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3003	CLR	2	0
3	B	3004	CLR	2	0
3	A	3004	CLR	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

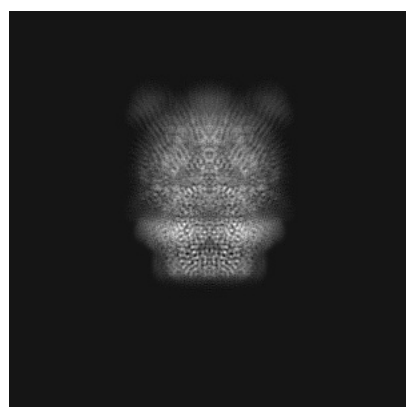
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40723. These allow visual inspection of the internal detail of the map and identification of artifacts.

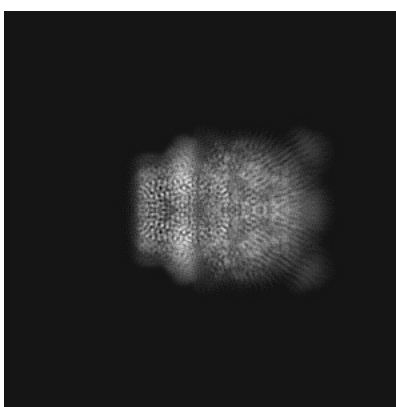
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

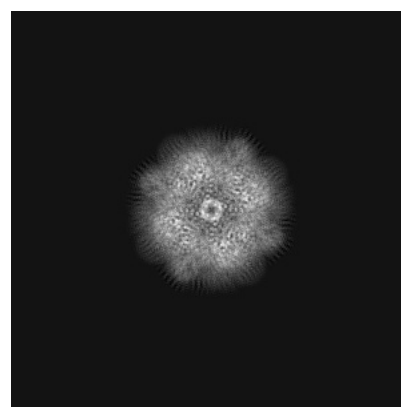
6.1.1 Primary map



X



Y



Z

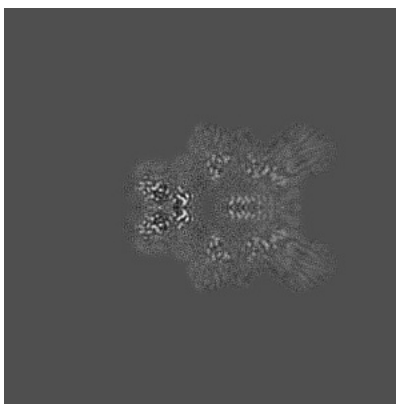
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

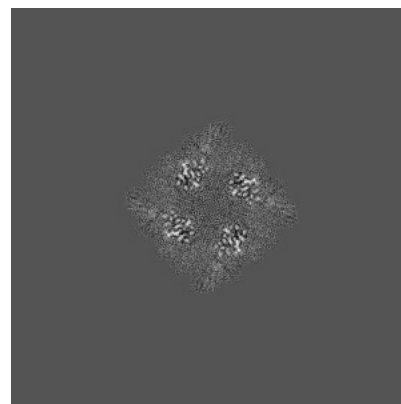
6.2.1 Primary map



X Index: 220



Y Index: 220



Z Index: 220

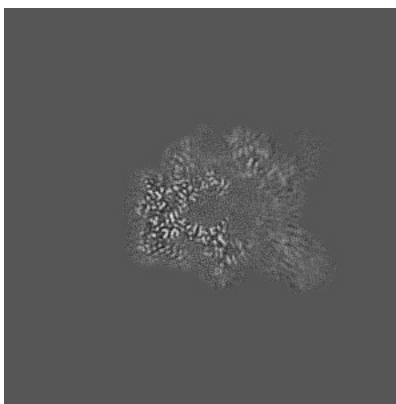
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

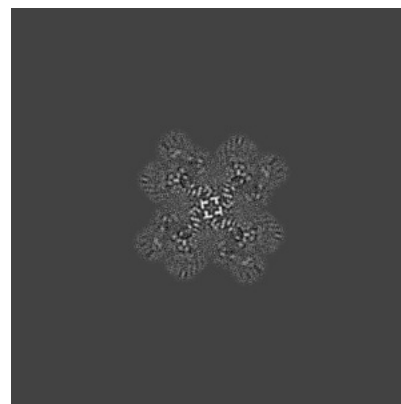
6.3.1 Primary map



X Index: 240



Y Index: 200

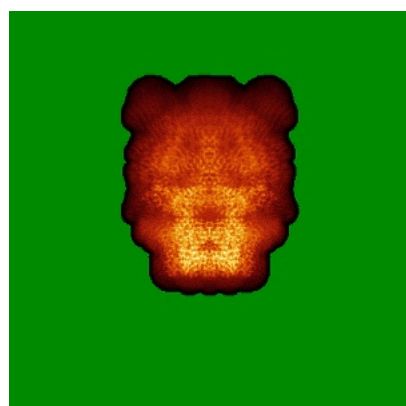


Z Index: 196

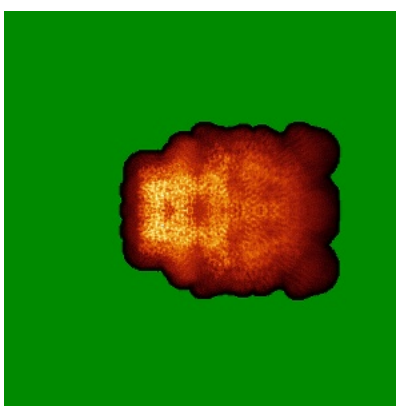
The images above show the largest variance slices of the map in three orthogonal directions.

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

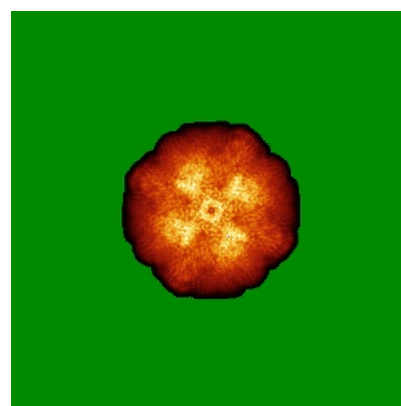
6.4.1 Primary map



X



Y

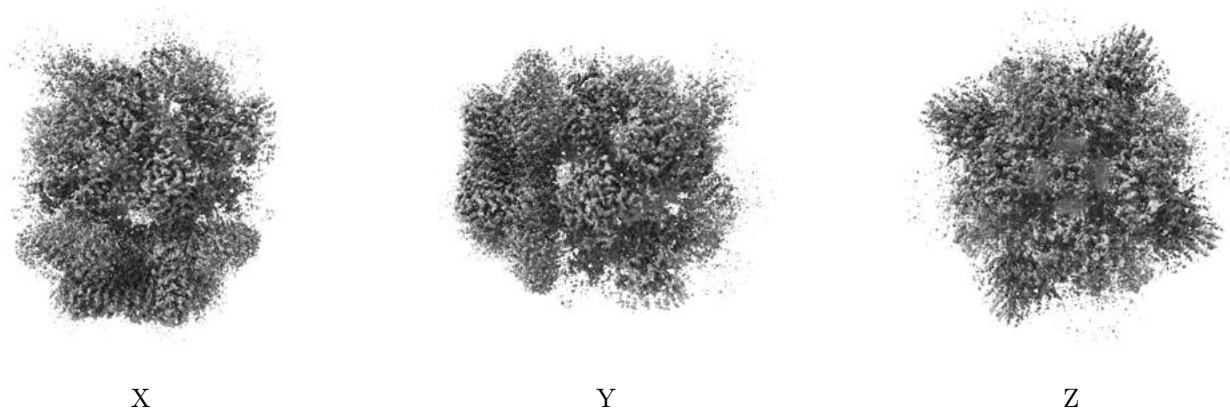


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 11.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

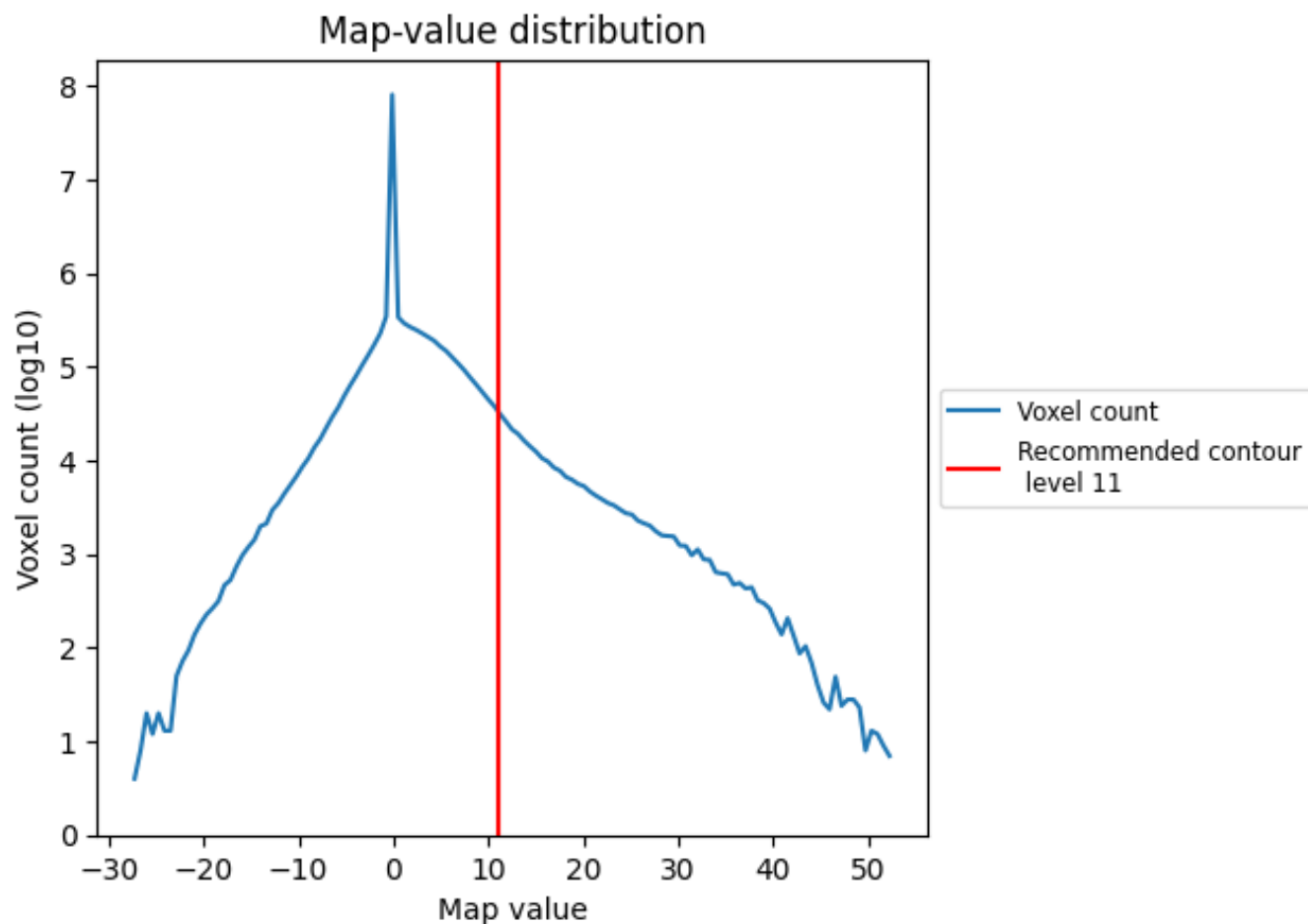
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

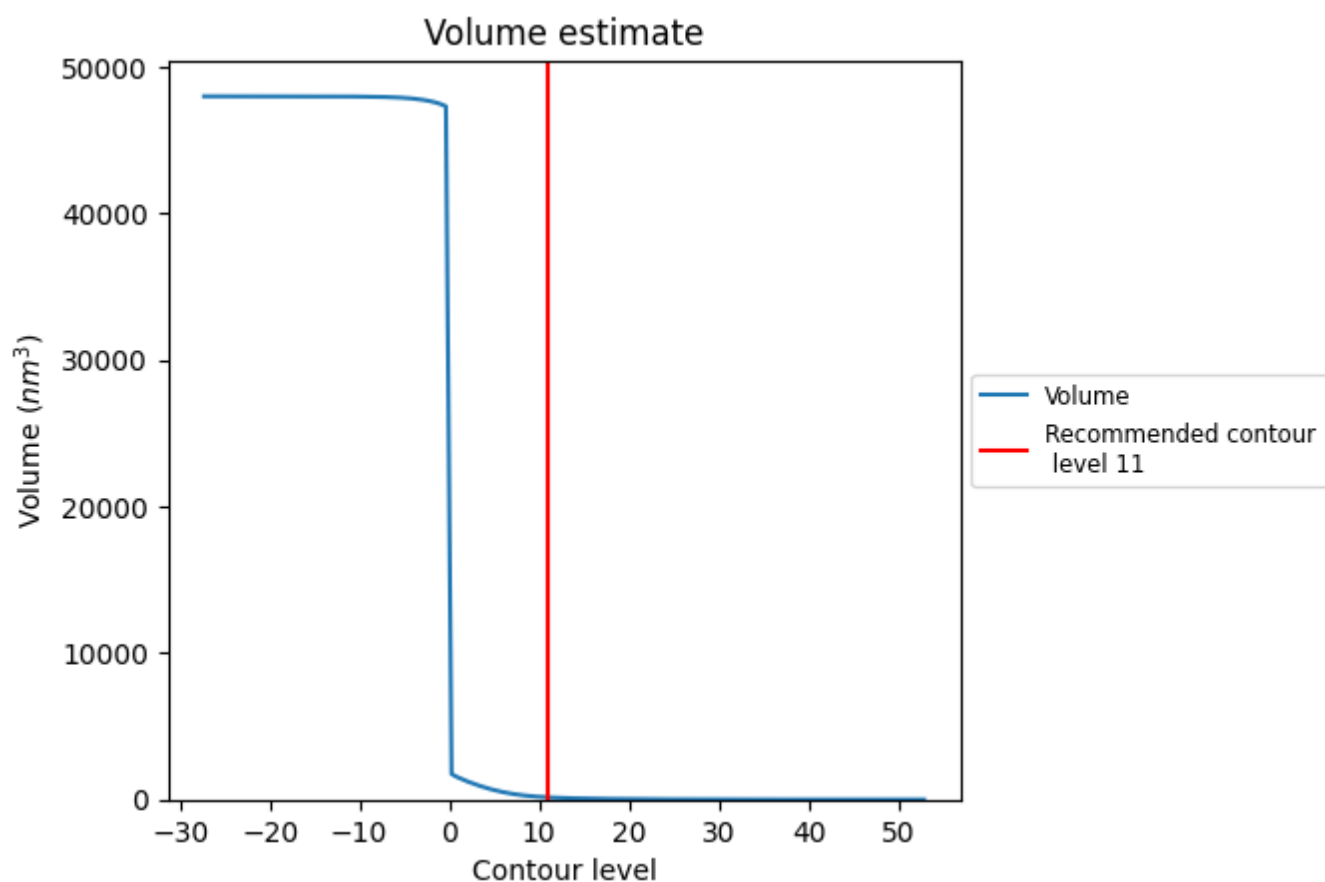
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

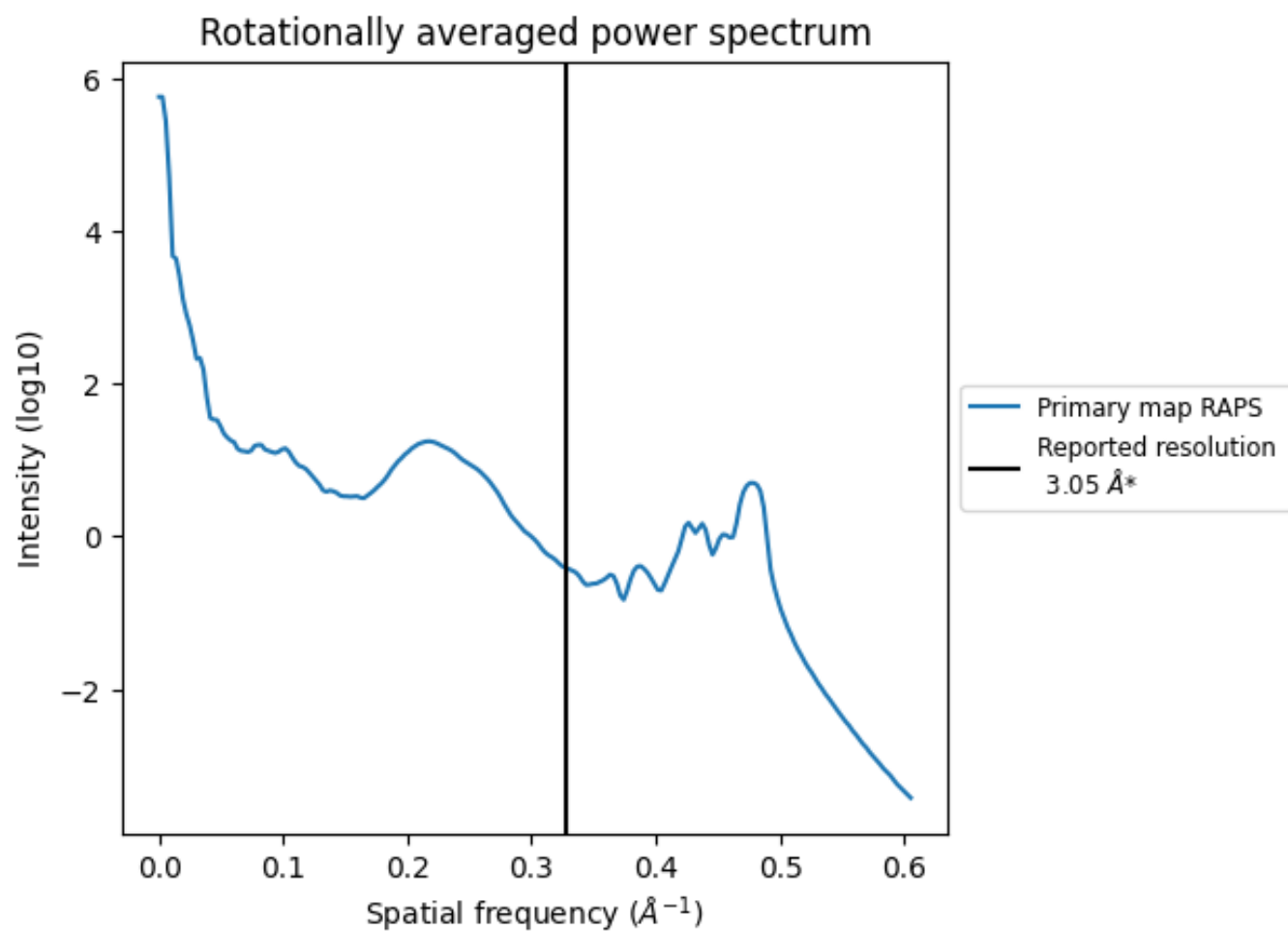
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 151 nm³; this corresponds to an approximate mass of 136 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 0.328 Å⁻¹

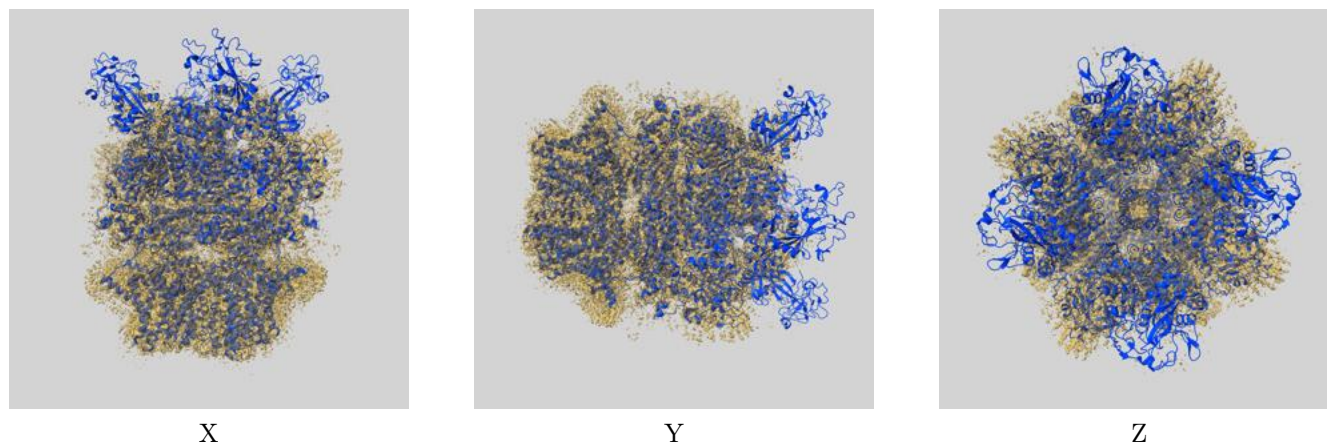
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

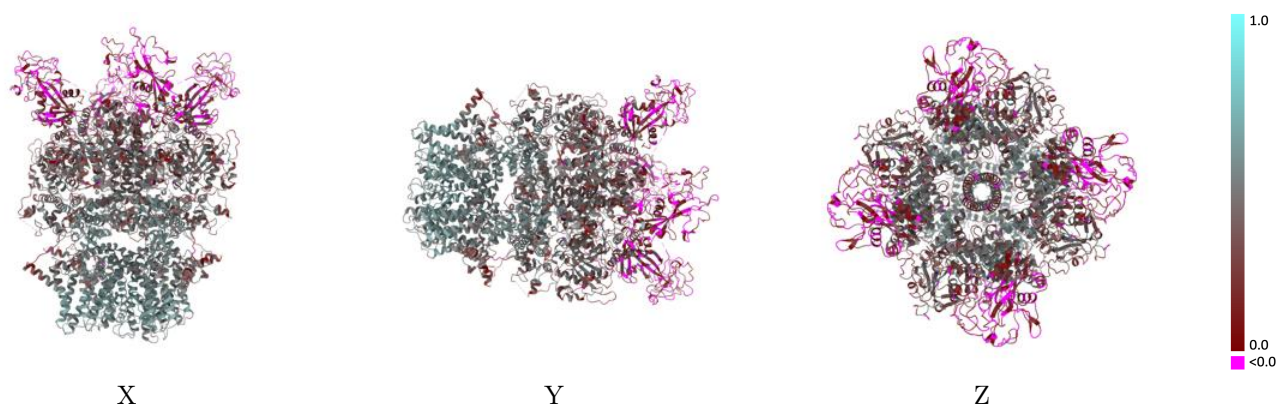
This section contains information regarding the fit between EMDB map EMD-40723 and PDB model 8SR9. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



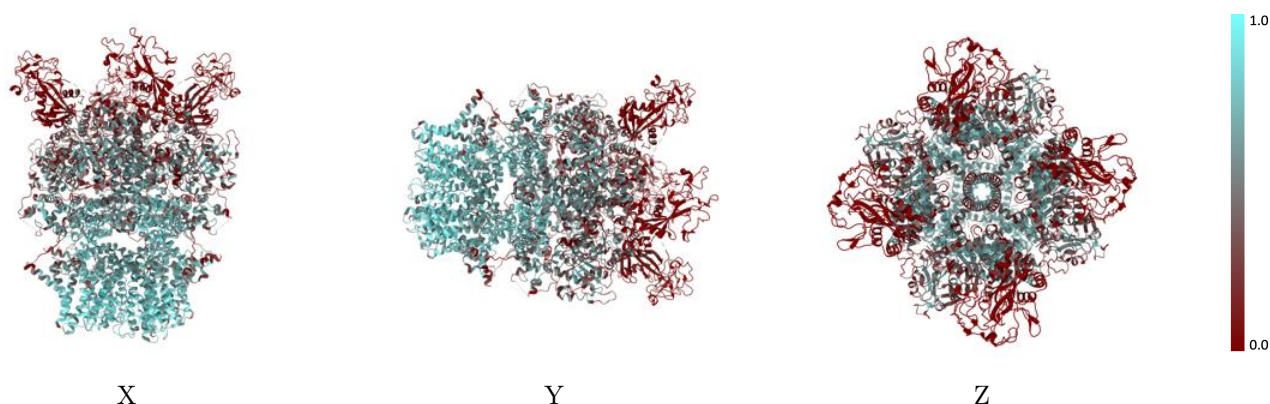
The images above show the 3D surface view of the map at the recommended contour level 11.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



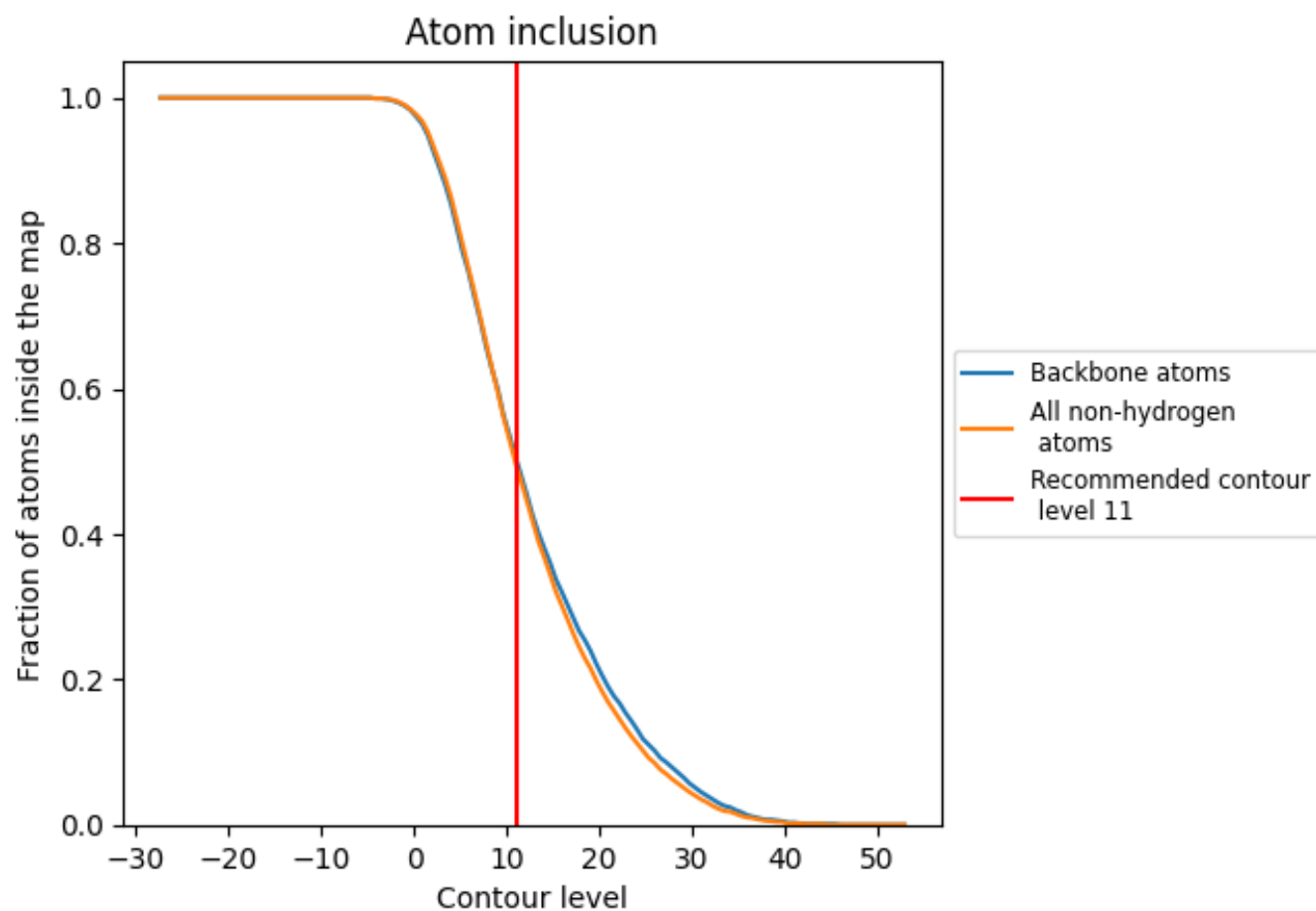
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (11).

9.4 Atom inclusion [i](#)



At the recommended contour level, 50% 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 (11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4960	<div></div> 0.3880
A	<div></div> 0.4970	<div></div> 0.3890
B	<div></div> 0.4960	<div></div> 0.3880
C	<div></div> 0.4960	<div></div> 0.3870
D	<div></div> 0.4960	<div></div> 0.3890

