



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 06:48 AM EDT

PDB ID : 7KY5 / pdb_00007ky5
EMDB ID : EMD-23068
Title : Structure of the *S. cerevisiae* phosphatidylcholine flippase Dnf2-Lem3 complex in the E2P transition state
Authors : Bai, L.; You, Q.; Jain, B.K.; Duan, H.D.; Kovach, A.; Graham, T.R.; Li, H.
Deposited on : 2020-12-07
Resolution : 3.98 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

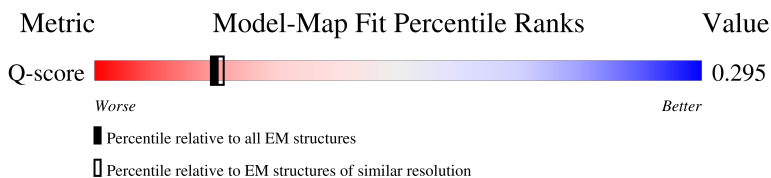
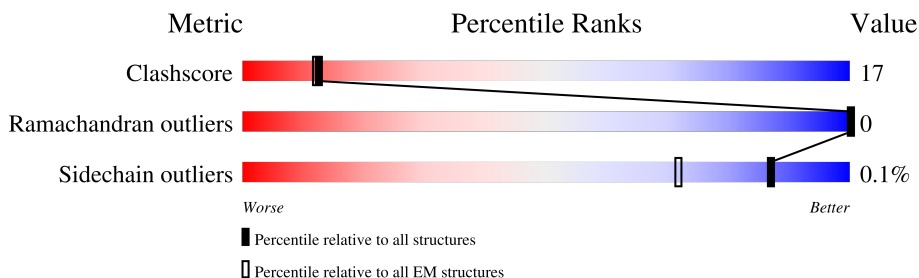
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.98 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	7512 (3.48 - 4.48)

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	1612	31% 47% 25% 28%
2	B	414	18% 59% 30% 11%
3	C	3	100%
3	D	3	100%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12483 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.

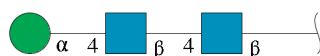
- Molecule 1 is a protein called Phospholipid-transporting ATPase DNF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1165	Total	C	N	O	S	0	0
			9297	5976	1543	1730	48		

- Molecule 2 is a protein called Alkylphosphocholine resistance protein LEM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	369	Total	C	N	O	S	0	0
			2974	1908	501	551	14		

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



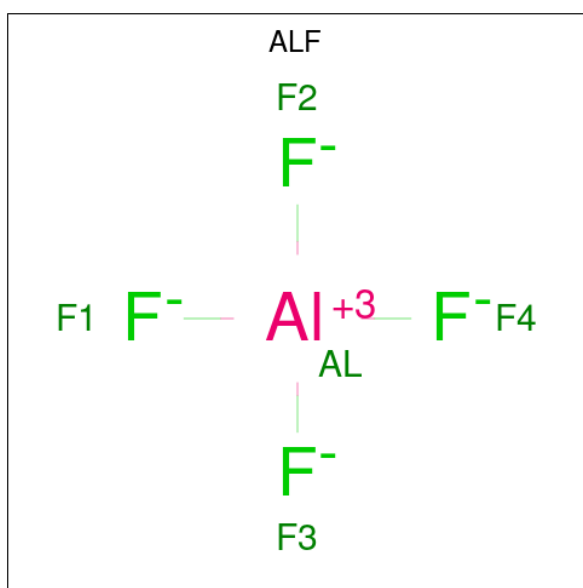
Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	3	Total	C	N	O	0	0
			39	22	2	15		
3	D	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			28	27	1	
4	A	1	Total	C	O	0
			28	27	1	

- Molecule 5 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	Al	F	0
			5	1	4	

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Mg	0
			1	1	

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



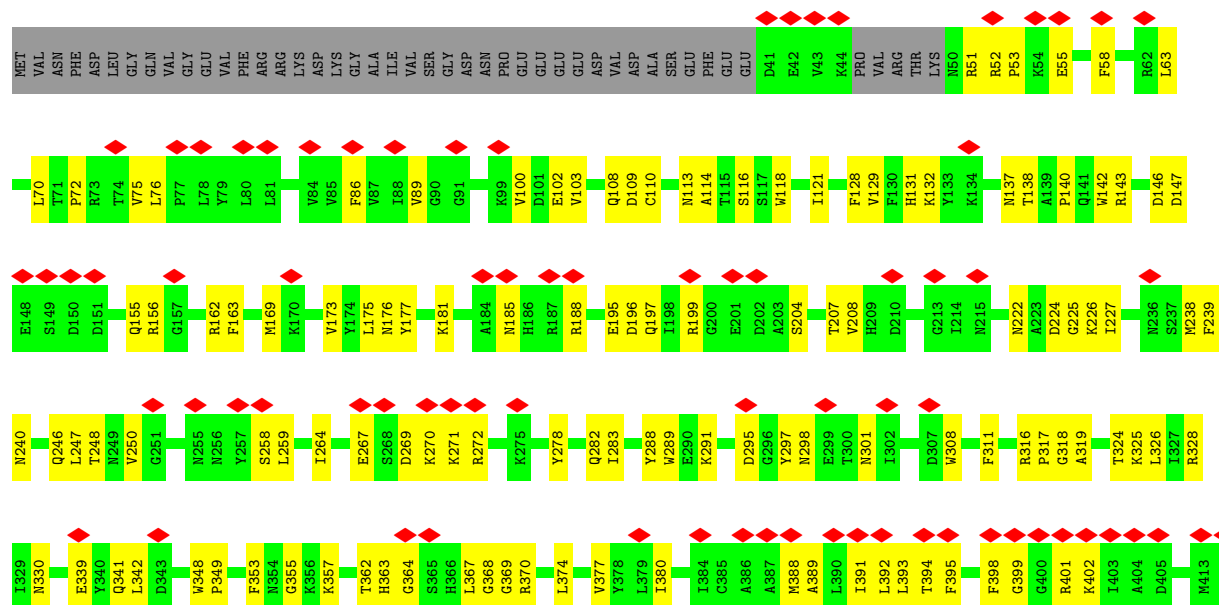
Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			15	8	1	6	
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			15	8	1	6	

ASN	ASN	ASP	A1417	V1340	F1260	G1187	A1119	G1046	N952	D919	G857	D788	E723	F644
PRO	LEU	PHE	Q1418	V1341	E1261	V1188	A1123	N1047	R983	S920	Y858	F844	F724	F644
PRO	GLY	GLY	P1419	T1342	Y1262	G1192	L1124	V1048	E984	V921	S959	L789	K725	W648
ARG	ARG	ILE	W1422	L1346	Y1263	G1193	N1126	L1049	E985	I922	F960	V649	K726	V649
SER	SER	SER	A1423	G1347	T1265	E1194	G1126	N1051	E986	R925	G862	F791	K727	I652
MET	LEU	ASP	V1424	L1348	F1267	G1195	E1127	D1052	N987	L926	S863	V792	I728	L653
ALA	ASP	ASP	V1427	L1349	F1268	G1196	E1128	L1056	D988	D927	S864	K794	I729	L657
SER	SER	THR	G1428	D1349	N1269	M1200	M1129	V1057	K989	R928	K865	E795	Y734	L657
ALA	ALA	THR	V1429	H1350	L1270	C1201	R1130	V1058	V990	T929	K865	E796	G735	V658
GLY	GLY	PHE	L1430	H1351	A1271	S1202	R1131	K1059	T991	Q930	S866	E797	R736	V659
ASN	ASN	ASP	F1431	Y1352	A1272	D1203	K1132	K1060	D992	N931	E798	L741	E740	I660
LYS	LYS	VAL	C1432	F1354	T1273	Y1204	F1133	S1061	V993	D932	S867	L742	A743	S861
LEU	LEU	SER	G1433	G1355	S1274	A1205	L1136	G1062	E995	T934	V870	L800	Y738	Y663
ARG	ARG	HIS	L1434	V1356	G1207	I1206	C1137	E1063	I994	R934	E871	K801	T739	Y664
SER	SER	SER	P1435	F1357	G1208	G1207	L1144	E1064	R996	L935	I872	G802	T739	I664
GLN	GLN	THR	R1436	V1358	F1209	F1208	C1140	D1065	E997	L936	Q873	S903	E740	E667
ASP	ASP	THR	I1439	T1359	F1210	Y1211	K1141	V1065	I998	E937	G874	S904	A741	I668
THR	THR	VAL	V1442	A1360	V1212	V1212	A1142	E1066	L1000	K938	Q876	G905	L742	I669
ARG	ARG	THR	R1443	V1363	V1216	V1216	V1143	E1067	L1001	T939	K877	D806	A743	Q673
GLY	GLY	GLY	K1444	F1368	L1217	L1217	L1144	F1068	G1002	A940	E878	H807	G744	Y678
GLY	GLY	ILE	Y1445	Y1369	V1218	V1218	C1145	G1069	G1003	L941	F879	Q808	L745	A674
MET	MET	PRO	F1446	V1370	H1219	H1219	C1146	S1070	I1006	H942	Q880	Q809	R746	I675
ALA	ALA	MET	Y1447	M1372	K1221	K1221	P1150	D1071	I1007	L943	V881	LYS	L746	I675
SER	SER	ASN	P1448	E1373	W1222	W1222	A1151	D1079	D1008	E944	L882	ARG	Y678	Y678
ILE	ILE	ASN	Y1449	G1374	Y1224	Y1224	Q1152	K1082	R1009	Y946	N884	GLY	V681	V681
LEU	LEU	ASN	D1450	Y1375	K1225	K1225	A1153	E1085	Q1011	A947	L885	V751	V751	V681
ASP	ASP	THR	I1453	R1376	R1226	R1226	A1154	E1086	D1012	T948	E886	D752	D752	K687
THR	THR	GLY	W1377	W1377	E1227	E1227	V1156	F1087	G1013	R952	N888	V753	V753	L688
ARG	ARG	GLN	F1380	G1380	A1228	A1228	V1157	F1088	V1014	R952	F887	E754	E754	D689
VAL	VAL	SER	C1381	C1381	E1229	E1229	K1158	G1089	P1015	C955	R891	A820	A820	P691
ALA	ALA	ARG	G1382	L1383	Q1233	Q1233	M1159	M1090	D1016	L955	K892	L821	L821	C692
ALA	ALA	TYR	L1384	F1384	F1234	F1234	V1160	S1091	S1017	A957	R893	V825	V825	P694
VAL	VAL	ARG	L1387	L1387	F1235	F1235	K1161	E1092	A1019	Q958	M894	K331	K331	I699
SER	SER	SER	G1394	G1394	Y1236	Y1236	D1165	S1093	L1020	R959	I897	D832	D832	S700
LEU	LEU	THR	Y1470	A1390	K1237	K1237	V1166	E1094	A1022	E960	I898	D833	D833	D701
ASP	ASP	THR	P1471	V1391	N1238	N1238	M1167	E1095	E1023	L961	I898	P834	P834	D702
PRO	PRO	LEU	D1472	G1394	F1239	F1239	T1168	E1096	A1024	T962	K999	K335	K335	L703
GLY	GLY	GLY	P1472	G1394	I1240	I1240	L1169	L1097	G1025	W963	I900	K336	K336	G704
ILE	ILE	ARG	T1473	G1394	I1243	I1243	A1170	E1098	G1025	S964	P901	L837	L837	I706
ARG	ARG	ARG	D1474	L1398	L1243	L1243	D1173	A1100	L1028	E965	G902	D838	D838	I709
ASP	ASP	ASP	P1475	W1399	F1246	F1246	G1174	K1101	W1029	Y966	THR	I839	I839	F710
ALA	ALA	LEU	S1476	T1400	Y1247	Y1247	S1175	L1031	V1030	E967	PRO	K340	K340	S711
GLY	GLY	SER	R1477	E1407	Y1248	Y1248	N1176	H1104	L1034	R968	LYS	A841	A841	D712
THR	THR	VAL	P1478	F1408	M1252	M1252	V1177	G1105	D1034	W969	ASP	Q842	Q842	K713
LEU	LEU	THR	R1479	Y1409	F1253	F1253	V1178	L1106	K1035	S970	E908	S943	S943	I771
SER	SER	THR	K1480	K1410	F1254	F1254	A1179	P1107	V1036	K971	P909	P944	P944	I772
GLN	GLN	THR	I1480	P1330	D1255	D1255	M1180	Q1108	E1037	T972	K910	D845	D845	D773
				P1331	G1256	G1256	Q1181	G1109	T1038	Y973	A911	E946	E946	E774
				A1412	S1257	S1257	Q1182	M1110	A1039	D974	L912	S851	S851	T718
				V1415	Y1258	Y1258	D1185	F1111	I1040	V975	L913	S852	S852	Q719
				F1416	L1259	L1259	V1186	I1114	N1041	A976	L914	A853	A853	N720
									F1044	A978	C915	R854	R854	N721
									S1045	S979	K916	Q855	Q855	M722
										V980		L856	L856	M722
										T981				F784

ARG
SER
ARG
ASP
ARG

• Molecule 2: Alkylphosphocholine resistance protein LEM3

Chain B: 

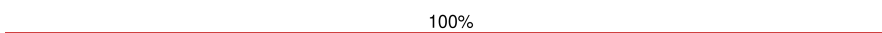


• Molecule 3: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 

MAG1
MAG2
MAN3

• Molecule 3: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 

MAG1
MAG2
MAN3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	127442	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 ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.037	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.012	Depositor
Map size ($\text{\AA}$)	231.28, 231.28, 231.28	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.826, 0.826, 0.826	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, MAN, NAG, CLR, ALF

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	0.15	0/9490	0.41	1/12865 (0.0%)
2	B	0.14	0/3055	0.36	0/4153
All	All	0.14	0/12545	0.40	1/17018 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	699	ILE	N-CA-C	5.49	115.15	106.32

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	9297	0	9301	332	0
2	B	2974	0	2868	115	0
3	C	39	0	34	3	0
3	D	39	0	32	3	0
4	A	56	0	92	2	0
5	A	5	0	0	0	0
6	A	1	0	0	0	0
7	B	72	0	69	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12483	0	12396	419	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 17.

All (419) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1409:TYR:HD1	2:B:272:ARG:NH2	1.45	1.12
1:A:1127:GLU:HG2	1:A:1130:ARG:HH11	1.02	1.09
1:A:941:LEU:HA	1:A:944:GLU:OE1	1.54	1.08
1:A:941:LEU:HA	1:A:944:GLU:CD	1.78	1.08
1:A:1409:TYR:CD1	2:B:272:ARG:NH2	2.20	1.06
1:A:1127:GLU:HG2	1:A:1130:ARG:NH1	1.70	1.06
1:A:861:VAL:O	1:A:869:ILE:HB	1.56	1.06
1:A:1308:TRP:HD1	1:A:1312:LYS:HZ1	1.15	0.94
1:A:1127:GLU:CG	1:A:1130:ARG:NH1	2.32	0.92
1:A:941:LEU:O	1:A:944:GLU:HG2	1.77	0.84
1:A:1096:GLU:HA	1:A:1099:GLU:CD	2.04	0.82
1:A:1409:TYR:HD1	2:B:272:ARG:HH21	0.85	0.81
2:B:175:LEU:HB3	2:B:328:ARG:HB2	1.62	0.81
1:A:1410:LYS:CG	2:B:269:ASP:OD1	2.32	0.78
2:B:222:ASN:HD21	2:B:226:LYS:HB2	1.49	0.77
1:A:781:ASN:HB3	1:A:784:PHE:HB2	1.67	0.76
1:A:1237:LYS:HE3	1:A:1273:THR:HG23	1.70	0.73
1:A:468:SER:OG	1:A:507:ILE:CD1	2.38	0.72
1:A:557:LEU:HD21	1:A:560:THR:HB	1.70	0.72
1:A:888:ASN:HB2	1:A:891:ARG:HB2	1.70	0.71
1:A:1400:THR:HG21	1:A:1412:ALA:H	1.55	0.71
2:B:173:VAL:HB	2:B:330:ASN:HB3	1.72	0.71
1:A:1308:TRP:CD1	1:A:1312:LYS:HZ1	2.05	0.71
1:A:894:MET:HB3	1:A:916:LYS:HE3	1.73	0.70
1:A:735:GLY:H	1:A:793:SER:HB3	1.57	0.69
1:A:532:TRP:NE1	1:A:541:ARG:HE	1.89	0.69
1:A:690:TYR:HA	2:B:51:ARG:HH22	1.58	0.69
1:A:318:LEU:HD11	1:A:436:CYS:HB2	1.75	0.69
1:A:681:VAL:HG12	2:B:53:PRO:HB2	1.75	0.69
1:A:941:LEU:CA	1:A:944:GLU:OE1	2.38	0.69
2:B:102:GLU:HG3	2:B:129:VAL:HG22	1.75	0.69
1:A:681:VAL:HG11	2:B:55:GLU:HG2	1.73	0.69
1:A:627:ARG:HH12	2:B:188:ARG:HB3	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:PRO:HB3	1:A:1204:TYR:CE1	2.28	0.68
1:A:468:SER:OG	1:A:507:ILE:HD13	1.94	0.68
2:B:246:GLN:HA	2:B:258:SER:HA	1.76	0.68
1:A:602:PHE:HE1	1:A:658:VAL:HG21	1.59	0.68
1:A:285:LEU:HD22	1:A:660:ILE:HD12	1.77	0.67
1:A:501:ILE:HD12	1:A:507:ILE:HG12	1.75	0.67
1:A:322:LYS:H	1:A:322:LYS:HD2	1.60	0.66
1:A:1430:LEU:HD11	2:B:86:PHE:HD2	1.59	0.66
2:B:297:TYR:HA	2:B:301:ASN:HD21	1.60	0.66
2:B:238:MET:HB3	2:B:289:TRP:HE1	1.61	0.66
2:B:86:PHE:HA	2:B:89:VAL:HG12	1.78	0.66
1:A:1234:PHE:HD2	1:A:1237:LYS:HD3	1.60	0.65
1:A:211:ASN:HB2	1:A:511:LYS:HA	1.78	0.65
1:A:463:ASP:HB2	1:A:569:PHE:HB2	1.79	0.65
1:A:260:TYR:HA	1:A:263:ILE:HG12	1.78	0.65
2:B:108:GLN:HB3	2:B:357:LYS:H	1.61	0.65
1:A:1127:GLU:HG3	1:A:1130:ARG:NH1	2.12	0.65
1:A:1096:GLU:HA	1:A:1099:GLU:OE1	1.97	0.64
1:A:724:PHE:HB3	1:A:852:THR:HG21	1.78	0.64
1:A:481:LYS:NZ	1:A:486:GLU:O	2.29	0.64
1:A:520:HIS:HD2	1:A:522:ASN:HD22	1.44	0.64
1:A:927:ASP:O	1:A:931:ASN:ND2	2.31	0.64
1:A:1350:HIS:HB3	1:A:1353:PHE:HD2	1.63	0.64
1:A:532:TRP:HE1	1:A:541:ARG:HE	1.43	0.64
2:B:100:VAL:O	2:B:370:ARG:NH1	2.30	0.64
2:B:114:ALA:HB2	2:B:142:TRP:CZ3	2.33	0.64
1:A:770:THR:HG23	1:A:794:LYS:HD3	1.80	0.64
1:A:1369:TYR:HE1	1:A:1436:ARG:HG2	1.63	0.63
2:B:121:ILE:HG12	2:B:142:TRP:CD1	2.33	0.63
1:A:1410:LYS:HG3	2:B:269:ASP:OD1	1.97	0.63
2:B:226:LYS:HD2	2:B:282:GLN:HA	1.80	0.63
1:A:232:ASN:ND2	1:A:443:TRP:O	2.29	0.62
2:B:52:ARG:NH1	2:B:55:GLU:OE2	2.32	0.62
1:A:922:ILE:HG13	1:A:955:CYS:HB2	1.81	0.62
1:A:900:ILE:O	1:A:909:PRO:HA	2.00	0.62
2:B:246:GLN:HE22	2:B:248:THR:HG23	1.65	0.61
1:A:1375:TYR:O	1:A:1455:ARG:NH1	2.33	0.61
1:A:1018:ILE:HG23	1:A:1028:LEU:HD21	1.82	0.61
1:A:1130:ARG:HD2	1:A:1159:LEU:HD13	1.83	0.61
1:A:1338:ASN:HB2	1:A:1340:VAL:HG12	1.82	0.61
1:A:1419:PRO:HA	1:A:1422:TRP:HD1	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1154:ALA:HB2	1:A:1179:ALA:HB1	1.83	0.61
1:A:726:LYS:HE2	1:A:736:ARG:HA	1.84	0.60
2:B:240:ASN:H	2:B:348:TRP:HB2	1.66	0.60
1:A:207:THR:HA	1:A:514:VAL:O	2.01	0.60
1:A:1226:ARG:HG2	1:A:1284:ASP:HB3	1.82	0.60
1:A:821:LEU:HD23	1:A:914:ILE:HD11	1.82	0.60
1:A:295:LYS:NZ	1:A:296:ASP:OD1	2.34	0.60
1:A:699:ILE:O	1:A:699:ILE:HG22	2.00	0.60
1:A:1343:GLU:H	2:B:368:GLY:HA2	1.66	0.60
2:B:185:ASN:ND2	2:B:319:ALA:O	2.35	0.60
1:A:582:VAL:HG22	1:A:582:VAL:O	2.01	0.59
2:B:238:MET:HE2	2:B:311:PHE:HD1	1.68	0.59
1:A:1252:ASN:ND2	2:B:185:ASN:O	2.34	0.59
1:A:772:ILE:HG12	1:A:789:LEU:HD23	1.85	0.59
1:A:1187:GLY:HA3	1:A:1203:ASP:H	1.68	0.59
1:A:1260:PHE:HB3	1:A:1264:TYR:HD2	1.68	0.59
1:A:1375:TYR:HB3	1:A:1455:ARG:HH12	1.67	0.59
1:A:1261:GLU:OE2	1:A:1399:TRP:NE1	2.35	0.59
1:A:468:SER:CB	1:A:507:ILE:CD1	2.80	0.59
1:A:806:ASP:OD1	1:A:807:HIS:N	2.35	0.59
1:A:1125:ASN:OD1	1:A:1126:GLY:N	2.35	0.58
1:A:929:THR:HG23	1:A:930:GLN:OE1	2.03	0.58
2:B:146:ASP:OD1	2:B:156:ARG:NH2	2.36	0.58
1:A:980:VAL:HG12	1:A:981:THR:H	1.68	0.58
1:A:1018:ILE:HG21	1:A:1048:VAL:HG22	1.85	0.58
2:B:155:GLN:HG3	2:B:349:PRO:HA	1.85	0.58
1:A:796:ILE:HD11	1:A:816:LEU:HD11	1.85	0.58
2:B:208:VAL:HG21	2:B:227:ILE:HD11	1.85	0.57
1:A:1331:PRO:HG2	1:A:1358:VAL:HG12	1.85	0.57
1:A:479:GLU:OE2	1:A:489:LEU:HD13	2.03	0.57
1:A:825:VAL:HG11	1:A:850:VAL:HG21	1.85	0.57
1:A:1153:LYS:HA	1:A:1156:VAL:HG12	1.86	0.57
1:A:1348:LEU:O	1:A:1349:ASP:CB	2.52	0.57
1:A:821:LEU:HD21	1:A:898:ILE:HG21	1.87	0.56
2:B:267:GLU:HA	2:B:270:LYS:HE2	1.87	0.56
1:A:1056:LEU:HB2	1:A:1113:VAL:HG12	1.86	0.56
2:B:301:ASN:HD22	3:D:1:NAG:C7	2.18	0.56
1:A:468:SER:OG	1:A:507:ILE:HD11	2.05	0.56
1:A:860:PHE:HE1	1:A:868:LEU:HB3	1.69	0.56
1:A:605:LEU:HD12	1:A:657:LEU:HD12	1.87	0.56
1:A:678:TYR:HE1	1:A:693:THR:HG22	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1187:GLY:O	1:A:1204:TYR:N	2.29	0.56
1:A:772:ILE:O	1:A:776:ARG:HG2	2.06	0.56
1:A:1096:GLU:O	1:A:1099:GLU:HG2	2.06	0.56
2:B:271:LYS:HA	2:B:271:LYS:HE3	1.88	0.56
2:B:394:THR:OG1	2:B:398:PHE:CD2	2.59	0.56
1:A:468:SER:CB	1:A:507:ILE:HD11	2.36	0.56
1:A:754:GLU:HB2	1:A:1475:PRO:HB2	1.87	0.55
1:A:1323:GLN:HE22	1:A:1432:CYS:HA	1.70	0.55
1:A:694:PRO:HB3	1:A:1204:TYR:HE1	1.70	0.55
1:A:936:LEU:HG	1:A:1000:LEU:HD21	1.89	0.55
1:A:1038:THR:HA	1:A:1041:ASN:HD21	1.71	0.55
1:A:935:LEU:HA	1:A:938:LYS:HE2	1.89	0.54
1:A:1374:GLN:OE1	1:A:1376:ARG:N	2.39	0.54
2:B:401:ARG:NH2	2:B:402:LYS:O	2.40	0.54
1:A:965:GLU:O	1:A:968:ARG:HD3	2.07	0.54
1:A:1127:GLU:CG	1:A:1130:ARG:HH11	1.87	0.54
1:A:474:GLY:O	1:A:494:SER:N	2.40	0.54
1:A:1300:ARG:HA	1:A:1303:ILE:HD12	1.88	0.54
1:A:1234:PHE:CD2	1:A:1237:LYS:HD3	2.41	0.54
1:A:1278:ILE:O	1:A:1282:VAL:HG12	2.08	0.54
1:A:1238:ASN:OD1	1:A:1239:VAL:N	2.41	0.54
1:A:972:THR:HA	1:A:975:VAL:HG12	1.88	0.53
2:B:196:ASP:OD1	2:B:197:GLN:N	2.42	0.53
1:A:477:TYR:HB3	1:A:489:LEU:HD12	1.91	0.53
2:B:248:THR:OG1	2:B:341:GLN:O	2.24	0.53
1:A:457:ASN:HA	1:A:558:ARG:HH21	1.72	0.53
1:A:1350:HIS:CD2	2:B:317:PRO:HD2	2.43	0.53
1:A:249:ILE:O	1:A:253:PHE:N	2.37	0.53
1:A:1400:THR:OG1	1:A:1411:GLY:N	2.32	0.53
1:A:1352:TYR:HB3	1:A:1408:PHE:CZ	2.44	0.53
2:B:278:TYR:HD1	2:B:282:GLN:HE21	1.57	0.53
1:A:211:ASN:ND2	1:A:510:THR:O	2.42	0.52
1:A:1118:ASP:OD1	1:A:1119:ALA:N	2.42	0.52
1:A:1212:VAL:O	1:A:1216:VAL:HG12	2.09	0.52
1:A:549:ASN:O	1:A:549:ASN:ND2	2.43	0.52
1:A:1304:LEU:HB2	1:A:1306:LYS:HZ2	1.75	0.52
1:A:1371:PHE:O	1:A:1377:TRP:NE1	2.42	0.52
1:A:1350:HIS:HB3	1:A:1353:PHE:CD2	2.42	0.52
1:A:653:LEU:HD22	1:A:1256:GLY:HA2	1.92	0.52
1:A:1430:LEU:HD11	2:B:86:PHE:CD2	2.42	0.52
2:B:140:PRO:HB3	2:B:163:PHE:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:ASN:OD1	2:B:326:LEU:HA	2.09	0.51
1:A:1448:PRO:HB2	1:A:1453:ILE:HD11	1.92	0.51
1:A:437:ARG:HE	1:A:438:PHE:H	1.58	0.51
1:A:594:LEU:HD21	1:A:662:LEU:HD21	1.92	0.51
1:A:1140:CYS:SG	1:A:1141:LYS:N	2.82	0.51
1:A:1200:MET:HA	1:A:1200:MET:HE3	1.93	0.51
1:A:447:LYS:HD3	1:A:448:VAL:N	2.26	0.51
2:B:110:CYS:HA	2:B:142:TRP:HZ3	1.76	0.51
2:B:291:LYS:HE2	3:C:2:NAG:C6	2.40	0.51
1:A:1124:LEU:O	1:A:1130:ARG:NH2	2.38	0.51
1:A:718:THR:OG1	1:A:1009:ARG:O	2.26	0.51
1:A:925:ARG:HH21	1:A:992:ASP:HA	1.76	0.50
1:A:704:GLY:HA3	1:A:1224:TYR:HB2	1.92	0.50
1:A:783:GLN:H	1:A:854:ARG:NH1	2.09	0.50
1:A:1235:PHE:HD2	1:A:1313:PHE:CZ	2.28	0.50
1:A:477:TYR:HE2	1:A:491:VAL:HG12	1.75	0.50
1:A:1110:ASN:H	1:A:1141:LYS:HE2	1.76	0.50
1:A:1298:LEU:O	1:A:1301:VAL:HG22	2.10	0.50
1:A:1341:VAL:HA	2:B:368:GLY:HA3	1.93	0.50
1:A:464:MET:HE2	1:A:464:MET:HA	1.94	0.50
2:B:316:ARG:O	2:B:325:LYS:NZ	2.35	0.50
1:A:1410:LYS:HG2	2:B:269:ASP:OD1	2.12	0.50
2:B:116:SER:O	2:B:143:ARG:NH2	2.45	0.50
2:B:297:TYR:HA	2:B:301:ASN:ND2	2.26	0.50
1:A:710:PHE:HD1	1:A:1029:TRP:HB2	1.76	0.50
2:B:308:TRP:CD1	2:B:311:PHE:H	2.30	0.50
1:A:462:ALA:HA	1:A:553:ARG:HD3	1.94	0.50
1:A:814:HIS:CD2	1:A:1001:LEU:HD22	2.47	0.50
1:A:484:ASP:OD1	1:A:485:GLY:N	2.44	0.49
1:A:507:ILE:HG22	1:A:507:ILE:O	2.12	0.49
1:A:745:LEU:HD12	1:A:746:ARG:HG2	1.94	0.49
1:A:703:LEU:O	1:A:1299:TYR:OH	2.29	0.49
1:A:939:THR:O	1:A:943:LEU:HD23	2.12	0.49
1:A:1012:ASP:N	1:A:1012:ASP:OD1	2.44	0.49
1:A:1330:PHE:HE1	1:A:1427:VAL:HG22	1.78	0.49
2:B:76:LEU:HG	2:B:393:LEU:HD21	1.95	0.49
1:A:520:HIS:CD2	1:A:522:ASN:HD22	2.29	0.49
1:A:706:ILE:HD12	1:A:1169:LEU:HB2	1.95	0.49
1:A:1079:LEU:HA	1:A:1082:LYS:HE2	1.94	0.49
1:A:1157:VAL:HA	1:A:1160:VAL:HG12	1.95	0.49
1:A:1013:GLY:O	1:A:1017:SER:OG	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:891:ARG:HH11	1:A:893:ARG:HG3	1.78	0.49
3:D:1:NAG:H4	3:D:2:NAG:H2	1.63	0.49
1:A:882:LEU:HD11	1:A:899:LYS:HB2	1.95	0.49
1:A:1101:LYS:NZ	1:A:1165:ASP:OD1	2.45	0.49
1:A:1137:CYS:HB2	1:A:1143:VAL:HG21	1.95	0.49
2:B:121:ILE:HA	2:B:142:TRP:NE1	2.28	0.49
1:A:259:ILE:O	1:A:263:ILE:HG23	2.12	0.48
1:A:1252:ASN:ND2	1:A:1257:SER:OG	2.46	0.48
2:B:113:ASN:HB2	2:B:142:TRP:HH2	1.77	0.48
1:A:1450:ASP:O	1:A:1454:VAL:HG13	2.13	0.48
1:A:891:ARG:HE	1:A:893:ARG:HG3	1.77	0.48
1:A:1182:GLN:NE2	1:A:1201:CYS:SG	2.86	0.48
1:A:306:LEU:O	1:A:309:GLU:HG3	2.14	0.48
1:A:726:LYS:HA	1:A:734:TYR:O	2.13	0.48
1:A:1348:LEU:O	1:A:1349:ASP:HB3	2.14	0.48
1:A:911:ALA:HB3	1:A:961:LEU:HB2	1.96	0.48
1:A:649:VAL:HA	1:A:652:ILE:HG22	1.96	0.48
1:A:1128:GLU:HG3	1:A:1132:LYS:HE2	1.95	0.48
1:A:1280:LEU:O	1:A:1284:ASP:HB2	2.13	0.48
1:A:867:GLY:H	1:A:881:VAL:HG12	1.78	0.48
1:A:887:PHE:HB2	1:A:894:MET:HB2	1.94	0.48
1:A:1014:VAL:O	1:A:1018:ILE:HG12	2.13	0.48
1:A:1176:ASN:OD1	1:A:1177:ASP:N	2.46	0.48
2:B:103:VAL:HG23	2:B:128:PHE:CD1	2.48	0.48
1:A:507:ILE:CD1	1:A:564:MET:HE2	2.44	0.48
1:A:980:VAL:HG12	1:A:981:THR:N	2.27	0.48
2:B:110:CYS:HA	2:B:142:TRP:CZ3	2.49	0.48
1:A:288:ILE:HG22	1:A:664:ILE:HD12	1.96	0.48
1:A:1034:ASP:OD1	1:A:1034:ASP:N	2.47	0.48
1:A:1169:LEU:HD11	1:A:1188:VAL:HG12	1.96	0.47
2:B:195:GLU:OE1	2:B:199:ARG:NH1	2.41	0.47
1:A:814:HIS:HE1	1:A:912:LEU:HD21	1.79	0.47
1:A:1353:PHE:HA	1:A:1356:VAL:HG12	1.96	0.47
1:A:1229:GLU:O	1:A:1233:GLN:HG2	2.14	0.47
1:A:1400:THR:HG21	1:A:1412:ALA:N	2.28	0.47
2:B:162:ARG:HG2	2:B:341:GLN:HB2	1.97	0.47
2:B:391:ILE:HG13	2:B:395:PHE:CE2	2.50	0.47
1:A:265:LEU:HD11	1:A:285:LEU:HD23	1.95	0.47
1:A:712:ASP:OD1	1:A:713:LYS:N	2.42	0.47
1:A:1208:GLN:HE21	1:A:1210:ARG:HB3	1.80	0.47
1:A:1223:CYS:HA	1:A:1226:ARG:HE	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1308:TRP:HD1	1:A:1312:LYS:NZ	1.99	0.47
1:A:1341:VAL:HG13	1:A:1341:VAL:O	2.15	0.47
1:A:1444:LYS:HG3	2:B:70:LEU:HD11	1.97	0.47
1:A:859:SER:OG	1:A:871:GLU:HB2	2.15	0.47
1:A:897:ILE:HG13	1:A:913:LEU:HD13	1.97	0.47
1:A:937:GLU:N	1:A:937:GLU:OE1	2.46	0.47
1:A:1050:ASN:ND2	1:A:1052:ASP:OD1	2.48	0.47
4:A:1702:CLR:H183	4:A:1702:CLR:H20	1.79	0.47
2:B:291:LYS:HE2	3:C:2:NAG:H61	1.96	0.47
1:A:678:TYR:CE1	1:A:693:THR:HG22	2.49	0.47
1:A:796:ILE:HA	1:A:799:ASP:OD2	2.15	0.47
1:A:854:ARG:NH2	1:A:854:ARG:O	2.48	0.47
1:A:551:LEU:HD23	1:A:552:LEU:O	2.15	0.47
1:A:1424:VAL:HA	1:A:1427:VAL:HG12	1.97	0.47
1:A:1342:THR:HB	1:A:1348:LEU:HD12	1.97	0.47
1:A:1409:TYR:CB	2:B:272:ARG:HH21	2.27	0.47
2:B:181:LYS:HB2	2:B:355:GLY:HA2	1.96	0.47
2:B:298:ASN:H	2:B:301:ASN:ND2	2.13	0.46
1:A:814:HIS:HD2	1:A:1001:LEU:HD22	1.79	0.46
2:B:102:GLU:HG3	2:B:129:VAL:CG2	2.45	0.46
2:B:391:ILE:HA	2:B:394:THR:HG22	1.98	0.46
1:A:1058:VAL:HG22	1:A:1079:LEU:HD21	1.96	0.46
1:A:1237:LYS:NZ	1:A:1274:SER:HA	2.30	0.46
2:B:388:MET:HA	2:B:391:ILE:HG22	1.97	0.46
1:A:1206:ILE:HD13	1:A:1212:VAL:HG23	1.97	0.46
1:A:1409:TYR:CD1	2:B:272:ARG:CZ	2.97	0.46
1:A:1352:TYR:CD2	1:A:1407:GLU:HG2	2.50	0.46
1:A:1410:LYS:HG3	2:B:269:ASP:CG	2.41	0.46
1:A:1435:PRO:O	1:A:1439:ILE:HG12	2.15	0.46
1:A:474:GLY:HA3	1:A:494:SER:HB3	1.98	0.46
1:A:938:LYS:O	1:A:941:LEU:HG	2.16	0.46
1:A:1165:ASP:OD1	1:A:1165:ASP:N	2.48	0.46
1:A:457:ASN:HA	1:A:558:ARG:NH2	2.31	0.46
1:A:1058:VAL:N	1:A:1114:ILE:O	2.31	0.46
1:A:1268:TYR:HA	1:A:1272:PHE:CD2	2.51	0.46
1:A:520:HIS:HD2	1:A:522:ASN:ND2	2.12	0.45
1:A:771:MET:HE3	1:A:775:LEU:HD21	1.97	0.45
1:A:1282:VAL:HG22	1:A:1283:LEU:HD22	1.98	0.45
1:A:1383:LEU:O	1:A:1387:LEU:HD23	2.16	0.45
1:A:1085:ARG:NE	1:A:1091:SER:OG	2.49	0.45
1:A:464:MET:HB3	1:A:551:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:942:HIS:O	1:A:945:GLU:HG2	2.15	0.45
2:B:377:VAL:HA	2:B:380:ILE:HG22	1.98	0.45
2:B:247:LEU:HD21	2:B:259:LEU:HD11	1.98	0.45
1:A:322:LYS:HD2	1:A:322:LYS:N	2.28	0.45
1:A:758:ARG:O	1:A:762:GLU:HG2	2.16	0.45
1:A:854:ARG:NH2	1:A:859:SER:HB3	2.32	0.45
1:A:1124:LEU:HD12	1:A:1130:ARG:HG2	1.98	0.45
1:A:1234:PHE:HA	1:A:1237:LYS:HD3	1.99	0.45
1:A:1339:MET:HB2	2:B:324:THR:HG22	1.97	0.45
2:B:109:ASP:OD1	2:B:109:ASP:N	2.48	0.45
2:B:118:TRP:CD2	2:B:143:ARG:HD3	2.52	0.45
1:A:1161:LYS:HZ1	1:A:1167:MET:HA	1.82	0.45
2:B:169:MET:SD	2:B:363:HIS:HB2	2.57	0.45
2:B:295:ASP:OD2	2:B:295:ASP:N	2.48	0.45
1:A:1248:TYR:HA	1:A:1328:PHE:CE2	2.51	0.45
4:A:1701:CLR:H221	4:A:1701:CLR:H162	1.57	0.45
2:B:288:TYR:HB3	3:C:1:NAG:H62	1.98	0.45
2:B:362:THR:HG22	2:B:364:GLY:H	1.81	0.45
1:A:259:ILE:HG13	1:A:260:TYR:CD1	2.52	0.44
1:A:1173:ASP:OD1	1:A:1195:GLY:HA3	2.17	0.44
1:A:1226:ARG:HD2	1:A:1281:ALA:O	2.16	0.44
1:A:284:PRO:HA	1:A:287:VAL:HG22	1.98	0.44
1:A:477:TYR:CE2	1:A:491:VAL:HG12	2.52	0.44
1:A:959:ARG:HB2	1:A:998:LEU:HD23	1.99	0.44
1:A:1235:PHE:HD2	1:A:1313:PHE:CE2	2.35	0.44
1:A:1350:HIS:NE2	1:A:1407:GLU:OE2	2.50	0.44
1:A:710:PHE:CD1	1:A:1029:TRP:HB2	2.52	0.44
1:A:545:VAL:HG13	1:A:549:ASN:HB3	2.00	0.44
1:A:689:ASP:O	2:B:51:ARG:NH2	2.51	0.44
1:A:794:LYS:O	1:A:797:VAL:HG22	2.17	0.44
1:A:913:LEU:O	1:A:958:GLN:HA	2.17	0.44
1:A:1016:ASP:OD1	1:A:1017:SER:N	2.51	0.44
1:A:1150:PRO:HA	1:A:1153:LYS:HE2	1.98	0.44
1:A:287:VAL:HA	1:A:290:ILE:HG12	1.98	0.44
1:A:867:GLY:N	1:A:881:VAL:HG12	2.33	0.44
1:A:1031:LEU:HD22	1:A:1145:CYS:HB2	2.00	0.44
2:B:222:ASN:OD1	2:B:226:LYS:N	2.50	0.44
1:A:724:PHE:O	1:A:790:THR:OG1	2.33	0.44
1:A:1458:TRP:HD1	1:A:1463:PHE:HB2	1.82	0.44
2:B:298:ASN:H	2:B:301:ASN:HD21	1.66	0.44
1:A:727:CYS:SG	1:A:734:TYR:HB2	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:VAL:HG23	1:A:648:TRP:HE1	1.83	0.43
1:A:288:ILE:HG13	1:A:289:VAL:N	2.33	0.43
1:A:468:SER:CB	1:A:507:ILE:HD13	2.47	0.43
1:A:590:ILE:HG13	1:A:1308:TRP:CH2	2.53	0.43
1:A:859:SER:HG	1:A:871:GLU:HB2	1.83	0.43
1:A:1219:HIS:O	1:A:1220:GLY:C	2.60	0.43
2:B:177:TYR:HE2	2:B:239:PHE:CE2	2.36	0.43
1:A:593:GLU:HB2	1:A:1308:TRP:CH2	2.53	0.43
1:A:690:TYR:OH	1:A:1205:ALA:HB3	2.18	0.43
2:B:72:PRO:HA	2:B:75:VAL:HG22	1.99	0.43
1:A:1088:PHE:HB2	1:A:1090:MET:HE3	1.99	0.43
2:B:301:ASN:HB3	3:D:1:NAG:H2	2.01	0.43
1:A:664:ILE:O	1:A:667:GLU:HG3	2.18	0.43
1:A:774:GLU:O	1:A:778:MET:HG3	2.18	0.43
1:A:1093:SER:HB3	1:A:1131:ARG:HD2	1.98	0.43
1:A:1206:ILE:HD12	1:A:1208:GLN:O	2.18	0.43
1:A:1221:LYS:O	1:A:1222:TRP:C	2.61	0.43
2:B:224:ASP:OD1	2:B:225:GLY:N	2.52	0.43
2:B:324:THR:O	2:B:325:LYS:HD3	2.18	0.43
2:B:401:ARG:CD	2:B:401:ARG:H	2.31	0.43
1:A:314:ARG:HH12	1:A:438:PHE:HE2	1.65	0.43
1:A:514:VAL:HG13	1:A:530:PHE:HE1	1.83	0.43
1:A:942:HIS:HA	1:A:945:GLU:HG2	2.00	0.43
1:A:1108:GLN:N	1:A:1141:LYS:HD3	2.34	0.43
1:A:1037:GLU:O	1:A:1041:ASN:ND2	2.51	0.43
1:A:882:LEU:HD13	1:A:966:TYR:CE1	2.54	0.43
1:A:1149:SER:O	1:A:1153:LYS:HG2	2.19	0.43
1:A:691:PRO:HD2	2:B:51:ARG:HH12	1.83	0.43
1:A:758:ARG:NH2	1:A:1476:SER:HB3	2.33	0.43
1:A:760:GLU:O	1:A:764:ILE:HG12	2.18	0.43
1:A:815:PHE:O	1:A:819:LEU:HG	2.19	0.43
2:B:121:ILE:HG12	2:B:142:TRP:HD1	1.82	0.43
1:A:1096:GLU:OE2	1:A:1096:GLU:N	2.52	0.42
1:A:478:VAL:HG23	1:A:490:LYS:HB3	2.00	0.42
1:A:742:LEU:HD23	1:A:742:LEU:H	1.84	0.42
1:A:825:VAL:HG23	1:A:841:ALA:HA	1.99	0.42
1:A:1429:VAL:HA	1:A:1432:CYS:SG	2.58	0.42
1:A:795:GLU:HA	1:A:798:GLU:CD	2.45	0.42
1:A:673:GLN:NE2	1:A:700:SER:O	2.51	0.42
1:A:709:ILE:HD13	1:A:1169:LEU:HB3	2.00	0.42
2:B:147:ASP:O	2:B:156:ARG:NH2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:612:ALA:O	1:A:1254:PHE:HD2	2.03	0.42
1:A:1357:PHE:CE1	1:A:1415:VAL:HG22	2.54	0.42
1:A:1380:PHE:CE1	1:A:1384:PHE:HE2	2.37	0.42
1:A:885:LEU:HD12	1:A:987:LEU:HD21	2.02	0.42
2:B:70:LEU:HD23	2:B:70:LEU:H	1.85	0.42
2:B:401:ARG:H	2:B:401:ARG:HD3	1.84	0.42
1:A:514:VAL:HG22	1:A:530:PHE:CE1	2.55	0.42
1:A:691:PRO:HD2	2:B:51:ARG:NH1	2.35	0.42
1:A:501:ILE:CD1	1:A:507:ILE:HG12	2.47	0.42
1:A:616:ASN:HA	1:A:619:TYR:CE1	2.55	0.42
1:A:882:LEU:HD12	1:A:897:ILE:HG22	2.02	0.42
2:B:204:SER:N	2:B:207:THR:OG1	2.51	0.42
1:A:659:PRO:HD2	1:A:1238:ASN:HD22	1.85	0.42
1:A:1038:THR:HA	1:A:1041:ASN:ND2	2.33	0.42
2:B:259:LEU:HD13	2:B:328:ARG:HB3	2.02	0.42
2:B:389:ALA:O	2:B:392:LEU:HG	2.20	0.42
1:A:507:ILE:HD12	1:A:564:MET:HE2	2.01	0.42
1:A:742:LEU:HA	1:A:745:LEU:HD23	2.02	0.42
1:A:919:ASP:N	1:A:919:ASP:OD1	2.53	0.42
1:A:1409:TYR:HB2	2:B:272:ARG:NH2	2.35	0.42
2:B:131:HIS:CE1	2:B:132:LYS:HG2	2.55	0.42
2:B:283:ILE:HG22	2:B:297:TYR:CD1	2.55	0.42
1:A:1017:SER:O	1:A:1021:LEU:HD23	2.20	0.41
1:A:1024:ALA:HB2	1:A:1296:PRO:HB2	2.02	0.41
1:A:1346:LEU:HD12	2:B:264:ILE:O	2.20	0.41
2:B:58:PHE:HA	2:B:63:LEU:HD11	2.02	0.41
1:A:315:THR:HG1	1:A:443:TRP:CD1	2.38	0.41
2:B:137:ASN:OD1	2:B:138:THR:N	2.41	0.41
1:A:306:LEU:HG	1:A:1200:MET:HE1	2.02	0.41
1:A:1343:GLU:H	2:B:368:GLY:CA	2.32	0.41
1:A:502:LYS:HE2	1:A:502:LYS:HB3	1.84	0.41
2:B:395:PHE:O	2:B:399:GLY:C	2.62	0.41
1:A:799:ASP:O	1:A:809:GLN:HG2	2.19	0.41
1:A:814:HIS:NE2	1:A:958:GLN:OE1	2.53	0.41
1:A:1128:GLU:OE1	1:A:1131:ARG:NH1	2.49	0.41
1:A:800:LEU:HD21	1:A:816:LEU:HD12	2.02	0.41
1:A:1360:ALA:HA	1:A:1363:VAL:HG12	2.02	0.41
1:A:1398:ILE:HD12	1:A:1398:ILE:HA	1.92	0.41
1:A:615:VAL:O	1:A:618:VAL:HG22	2.21	0.41
1:A:624:PRO:HB3	2:B:353:PHE:HB2	2.03	0.41
1:A:1341:VAL:HG23	2:B:367:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:ARG:HH21	1:A:438:PHE:HD1	1.69	0.41
1:A:501:ILE:HD12	1:A:507:ILE:CG1	2.48	0.41
1:A:673:GLN:CD	1:A:700:SER:HB3	2.46	0.41
1:A:1094:GLU:O	1:A:1098:LYS:HG2	2.21	0.41
1:A:1289:ASP:OD1	1:A:1289:ASP:N	2.54	0.41
1:A:1349:ASP:OD1	2:B:318:GLY:HA2	2.21	0.41
2:B:308:TRP:CE2	2:B:311:PHE:HB2	2.55	0.41
2:B:367:LEU:HD11	2:B:374:LEU:HD12	2.02	0.41
1:A:587:LYS:HD3	1:A:588:SER:O	2.20	0.41
1:A:1316:TYR:OH	1:A:1436:ARG:NH1	2.54	0.41
1:A:201:ARG:HG3	1:A:518:GLY:HA3	2.03	0.40
1:A:507:ILE:HD12	1:A:564:MET:CE	2.51	0.40
2:B:391:ILE:HG13	2:B:395:PHE:HE2	1.83	0.40
1:A:893:ARG:HD3	1:A:921:VAL:HG21	2.03	0.40
1:A:1341:VAL:HA	2:B:369:GLY:H	1.86	0.40
2:B:163:PHE:HE1	2:B:342:LEU:HD23	1.85	0.40
2:B:250:VAL:HB	2:B:339:GLU:HB3	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	1155/1612 (72%)	1077 (93%)	78 (7%)	0	100	100
2	B	365/414 (88%)	343 (94%)	22 (6%)	0	100	100
All	All	1520/2026 (75%)	1420 (93%)	100 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1027/1426 (72%)	1026 (100%)	1 (0%)	88	89
2	B	320/364 (88%)	320 (100%)	0	100	100
All	All	1347/1790 (75%)	1346 (100%)	1 (0%)	87	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1099	GLU

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

Mol	Chain	Res	Type
1	A	255	ASN
1	A	277	ASN
1	A	520	HIS
1	A	616	ASN
1	A	698	ASN
1	A	855	GLN
1	A	888	ASN
1	A	1011	GLN
1	A	1041	ASN
1	A	1252	ASN
1	A	1323	GLN
2	B	131	HIS
2	B	246	GLN
2	B	282	GLN
2	B	301	ASN

5.3.3 RNA ⓘ

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](#)

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	1	3	14,14,15	0.29	0	17,19,21	0.56	0
3	NAG	C	2	3	14,14,15	0.24	0	17,19,21	0.40	0
3	MAN	C	3	3	11,11,12	0.63	0	15,15,17	1.06	2 (13%)
3	NAG	D	1	2,3	14,14,15	0.47	0	17,19,21	0.49	0
3	NAG	D	2	3	14,14,15	0.32	0	17,19,21	0.49	0
3	MAN	D	3	3	11,11,12	0.64	0	15,15,17	0.90	1 (6%)

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	NAG	C	1	3	-	3/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	MAN	C	3	3	-	0/2/19/22	0/1/1/1
3	NAG	D	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	MAN	D	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	MAN	C1-O5-C5	2.77	115.90	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	MAN	O2-C2-C3	-2.18	105.64	110.15
3	C	3	MAN	O2-C2-C3	-2.17	105.65	110.15

There are no chirality outliers.

All (9) torsion outliers are listed below:

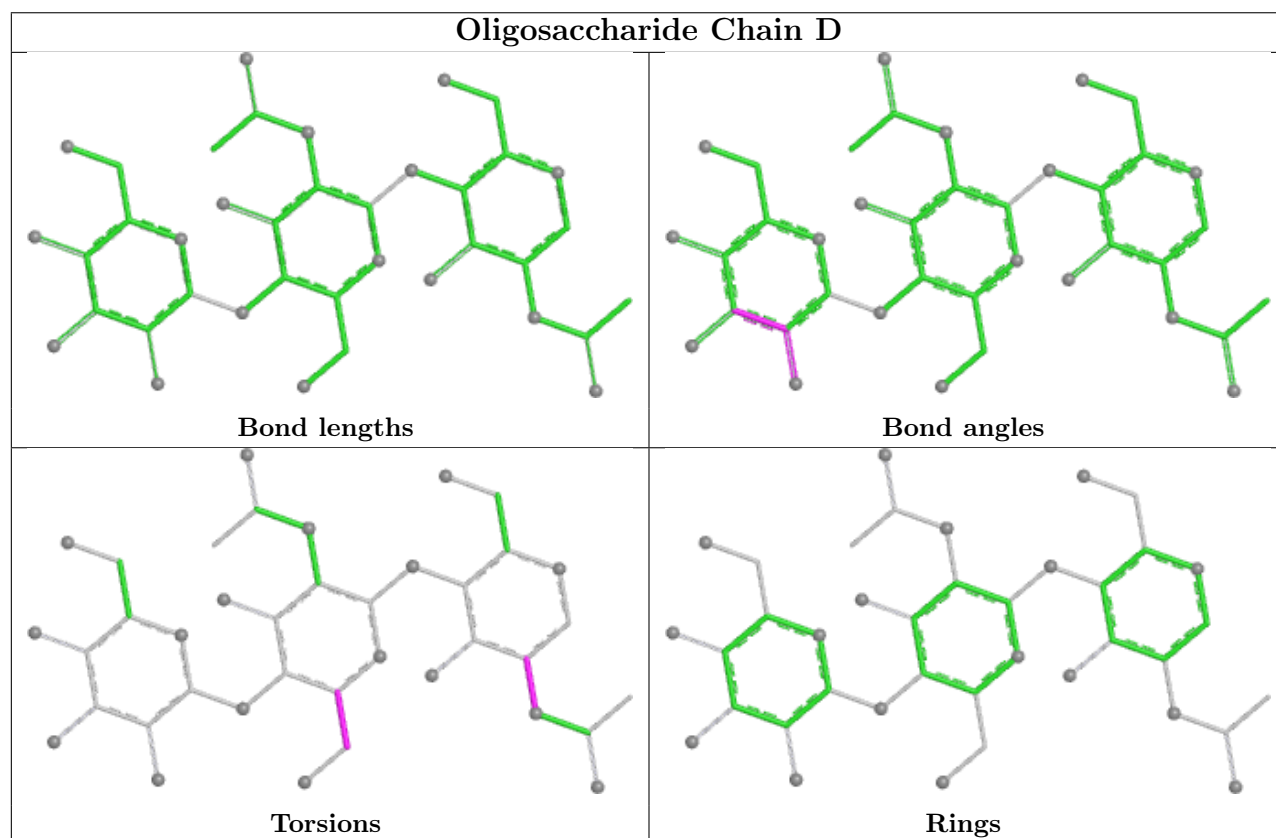
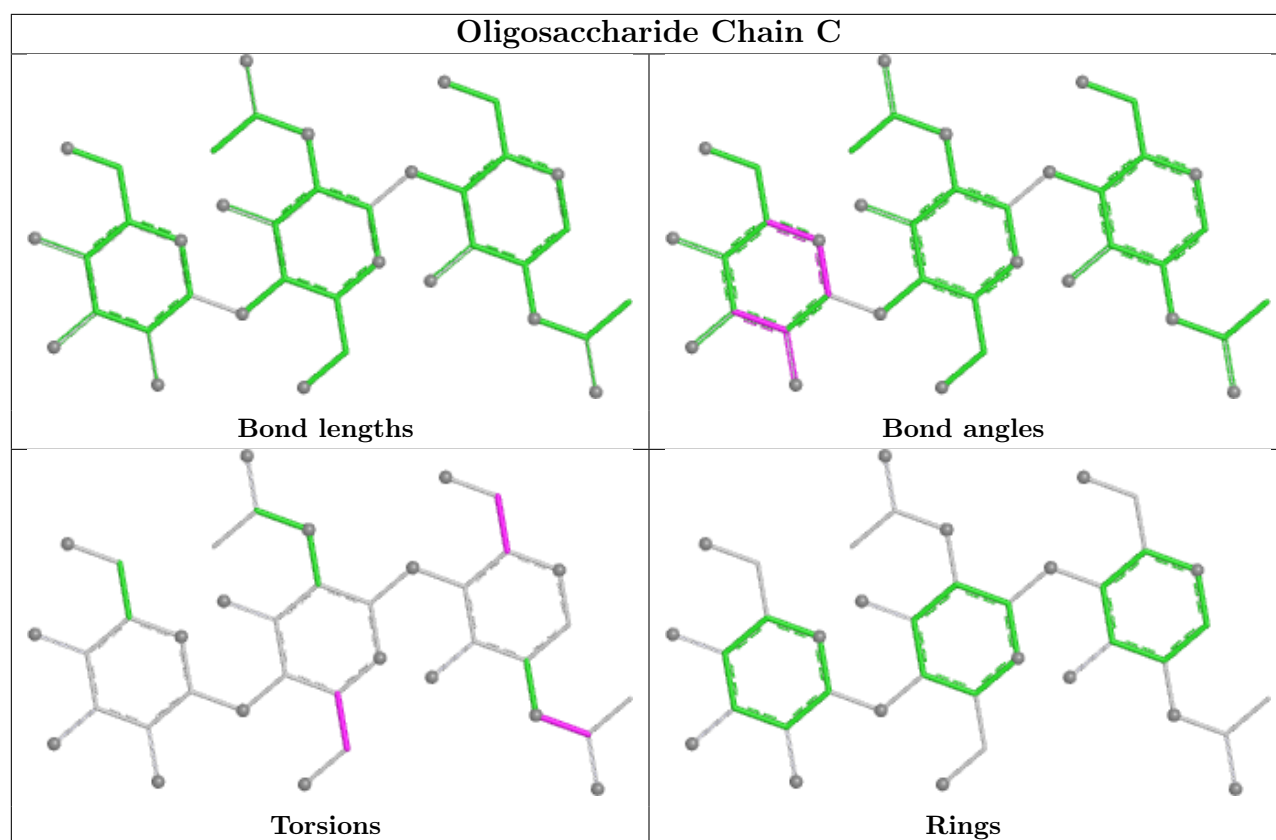
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	D	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	D	1	NAG	C1-C2-N2-C7
3	D	1	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	NAG	1	0
3	C	1	NAG	1	0
3	C	2	NAG	2	0
3	D	1	NAG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\# Z > 2$
7	NAG	B	501	2	14,14,15	0.21	0	17,19,21	0.42	0
4	CLR	A	1701	-	31,31,31	0.54	0	48,48,48	1.33	6 (12%)
5	ALF	A	1703	-	4,4,4	1.38	0	-		
4	CLR	A	1702	-	31,31,31	0.52	0	48,48,48	1.36	5 (10%)
7	NAG	B	503	-	15,15,15	0.11	0	21,21,21	0.10	0
7	NAG	B	505	-	15,15,15	0.10	0	21,21,21	0.11	0
7	NAG	B	504	2	14,14,15	0.22	0	17,19,21	0.38	0
7	NAG	B	502	2	14,14,15	0.28	0	17,19,21	0.42	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
7	NAG	B	501	2	-	2/6/23/26	0/1/1/1
4	CLR	A	1701	-	-	7/10/68/68	0/4/4/4
4	CLR	A	1702	-	-	7/10/68/68	0/4/4/4
7	NAG	B	503	-	-	2/6/26/26	0/1/1/1
7	NAG	B	505	-	-	0/6/26/26	0/1/1/1
7	NAG	B	504	2	-	1/6/23/26	0/1/1/1
7	NAG	B	502	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1702	CLR	C13-C17-C20	-4.49	112.56	119.50
4	A	1701	CLR	C13-C17-C20	-4.35	112.77	119.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1701	CLR	C13-C14-C8	-2.92	110.26	114.41
4	A	1702	CLR	C13-C14-C8	-2.92	110.28	114.41
4	A	1702	CLR	C8-C7-C6	-2.48	109.33	112.76
4	A	1702	CLR	C23-C22-C20	-2.26	108.74	115.08
4	A	1701	CLR	C11-C9-C10	-2.26	110.30	113.08
4	A	1701	CLR	C10-C9-C8	-2.26	109.41	112.71
4	A	1701	CLR	C8-C7-C6	-2.11	109.84	112.76
4	A	1701	CLR	C11-C12-C13	-2.11	109.18	112.74
4	A	1702	CLR	C11-C12-C13	-2.05	109.28	112.74

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1702	CLR	C13-C17-C20-C21
4	A	1702	CLR	C16-C17-C20-C21
4	A	1701	CLR	C13-C17-C20-C21
4	A	1701	CLR	C13-C17-C20-C22
4	A	1702	CLR	C13-C17-C20-C22
4	A	1702	CLR	C16-C17-C20-C22
4	A	1702	CLR	C17-C20-C22-C23
4	A	1702	CLR	C21-C20-C22-C23
4	A	1701	CLR	C17-C20-C22-C23
4	A	1701	CLR	C16-C17-C20-C21
7	B	501	NAG	C8-C7-N2-C2
7	B	501	NAG	O7-C7-N2-C2
7	B	503	NAG	C4-C5-C6-O6
7	B	502	NAG	O5-C5-C6-O6
4	A	1701	CLR	C21-C20-C22-C23
4	A	1701	CLR	C16-C17-C20-C22
4	A	1702	CLR	C20-C22-C23-C24
7	B	503	NAG	O5-C5-C6-O6
7	B	504	NAG	O5-C5-C6-O6
4	A	1701	CLR	C22-C23-C24-C25
7	B	502	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

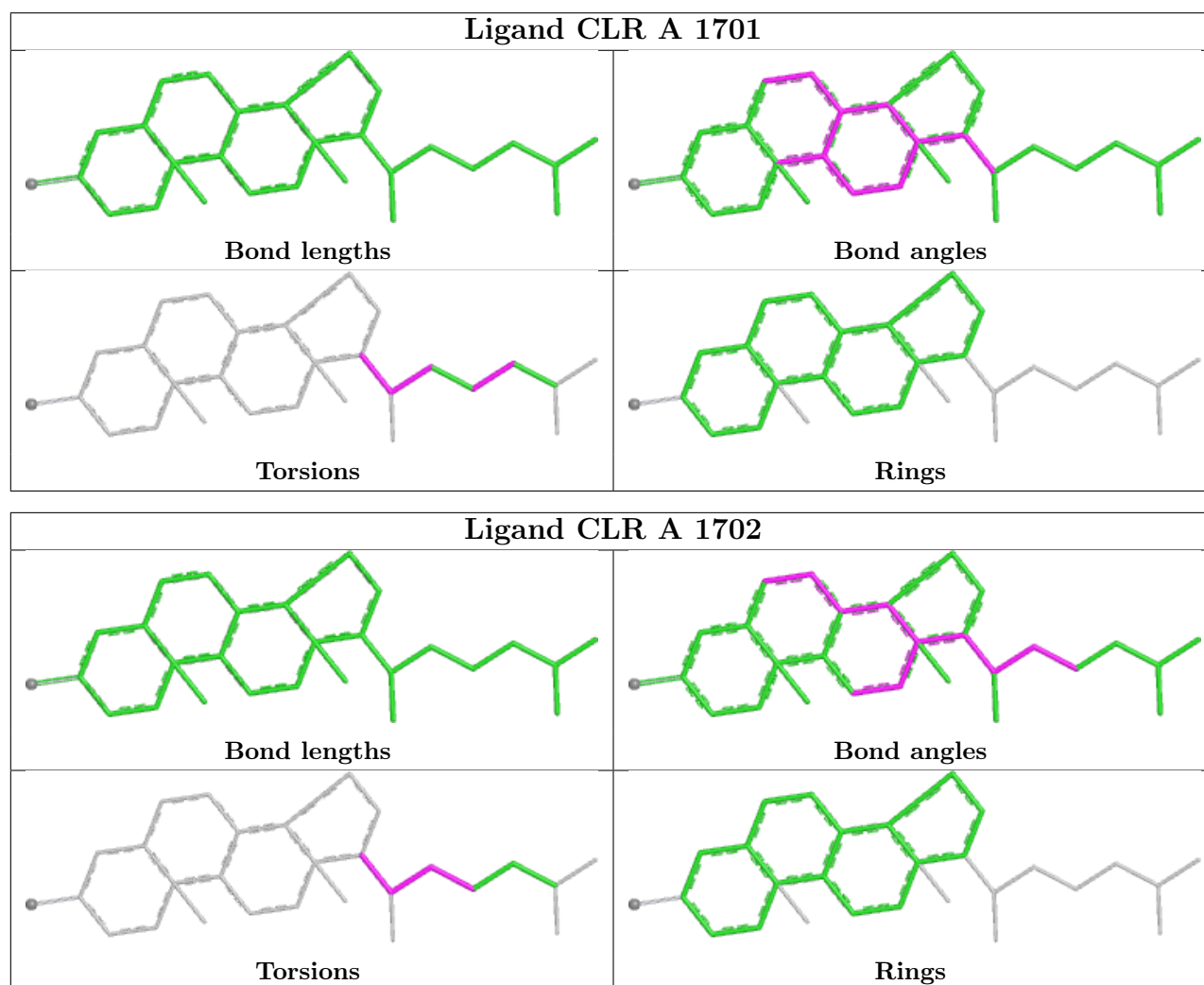
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1701	CLR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1702	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

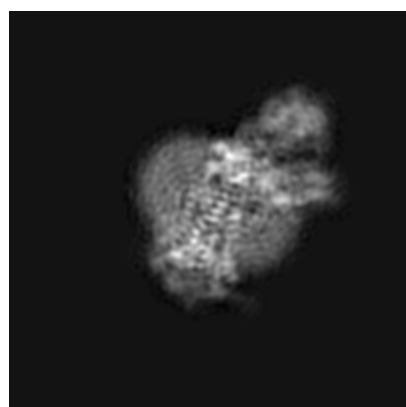
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23068. These allow visual inspection of the internal detail of the map and identification of artifacts.

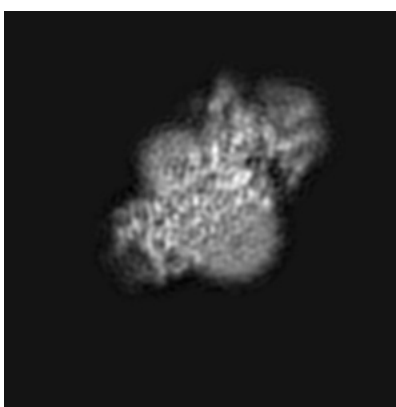
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

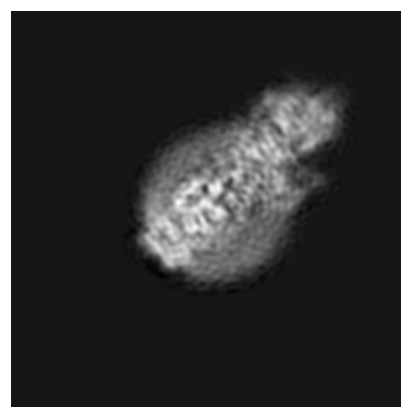
6.1.1 Primary map



X



Y

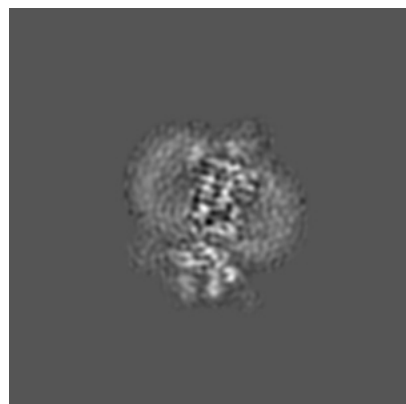


Z

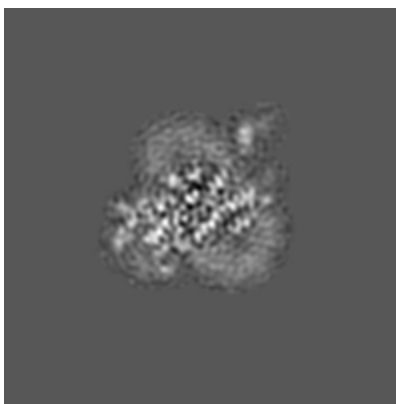
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

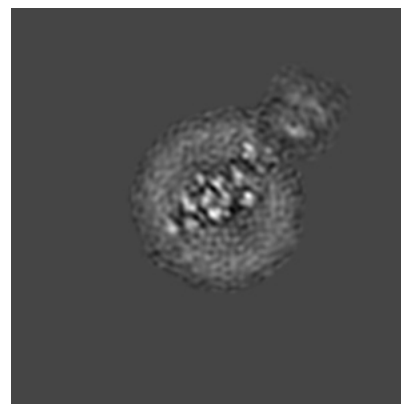
6.2.1 Primary map



X Index: 140



Y Index: 140

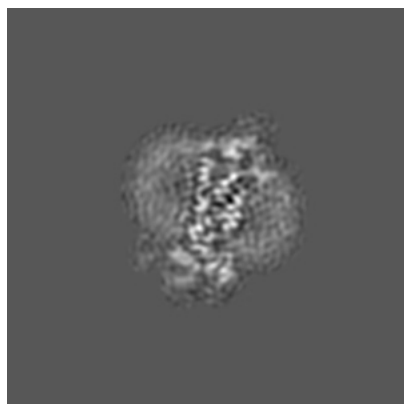


Z Index: 140

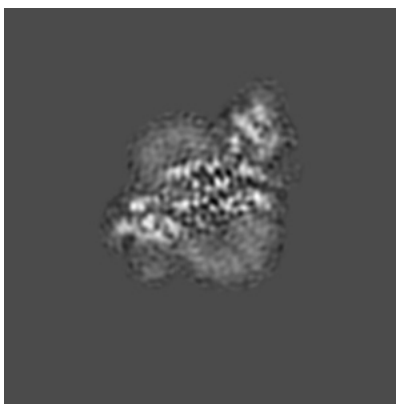
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 144



Y Index: 154

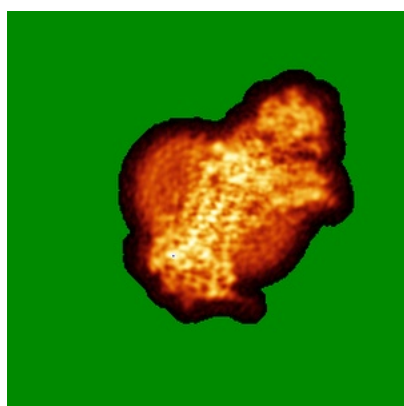


Z Index: 163

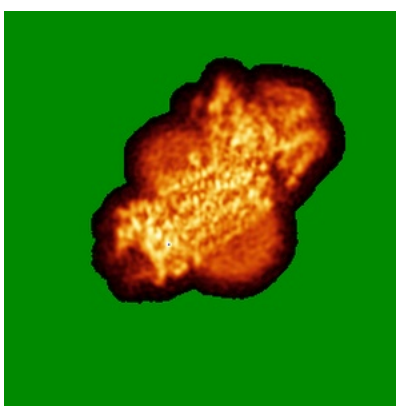
The images above show the largest variance slices of the map in three orthogonal directions.

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

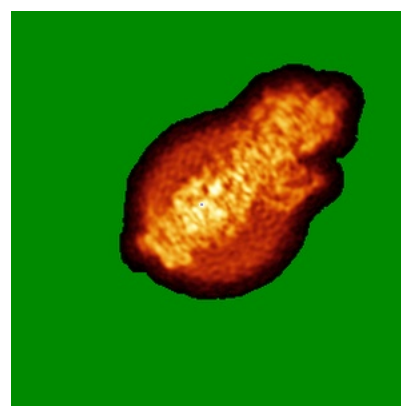
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

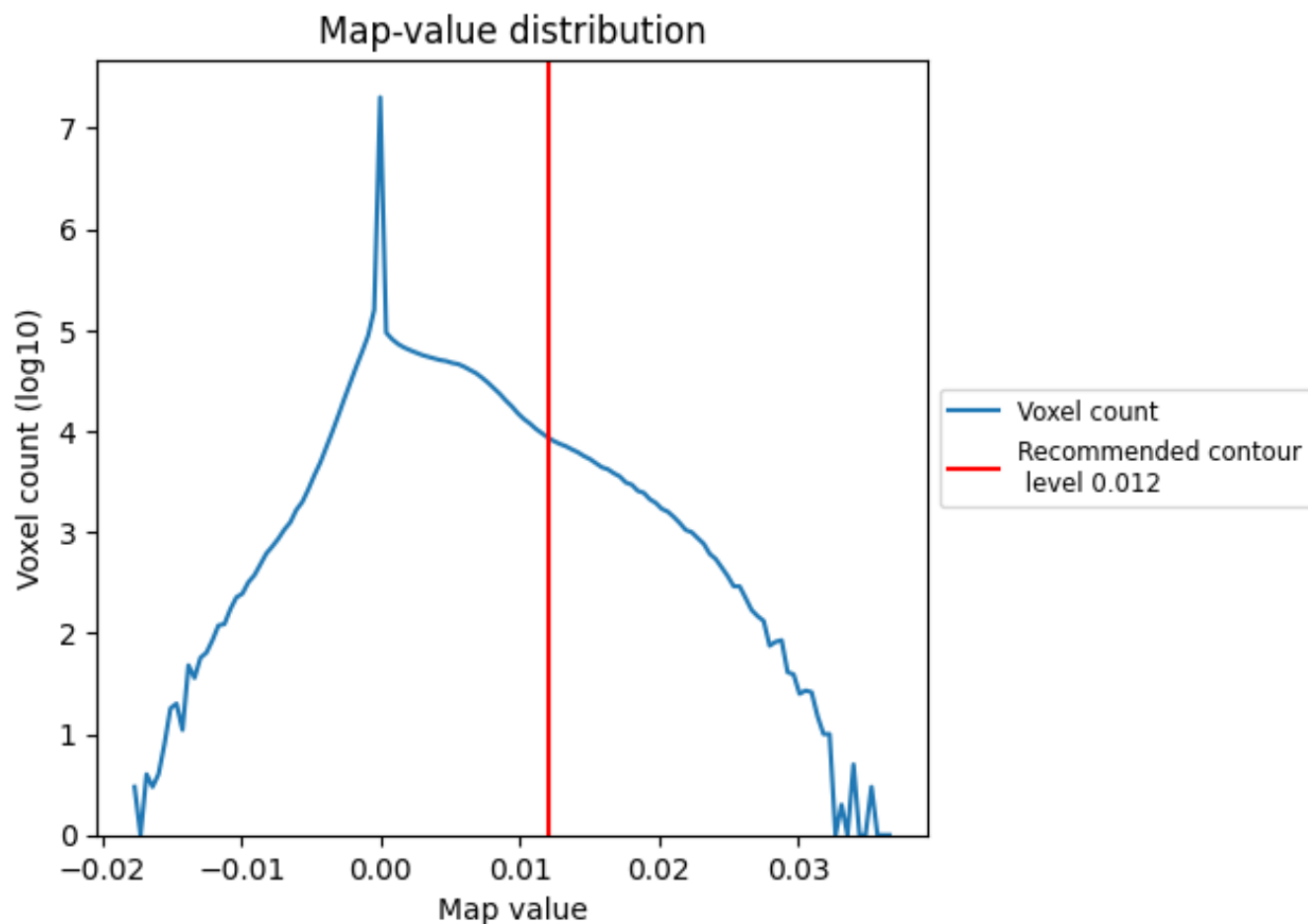
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

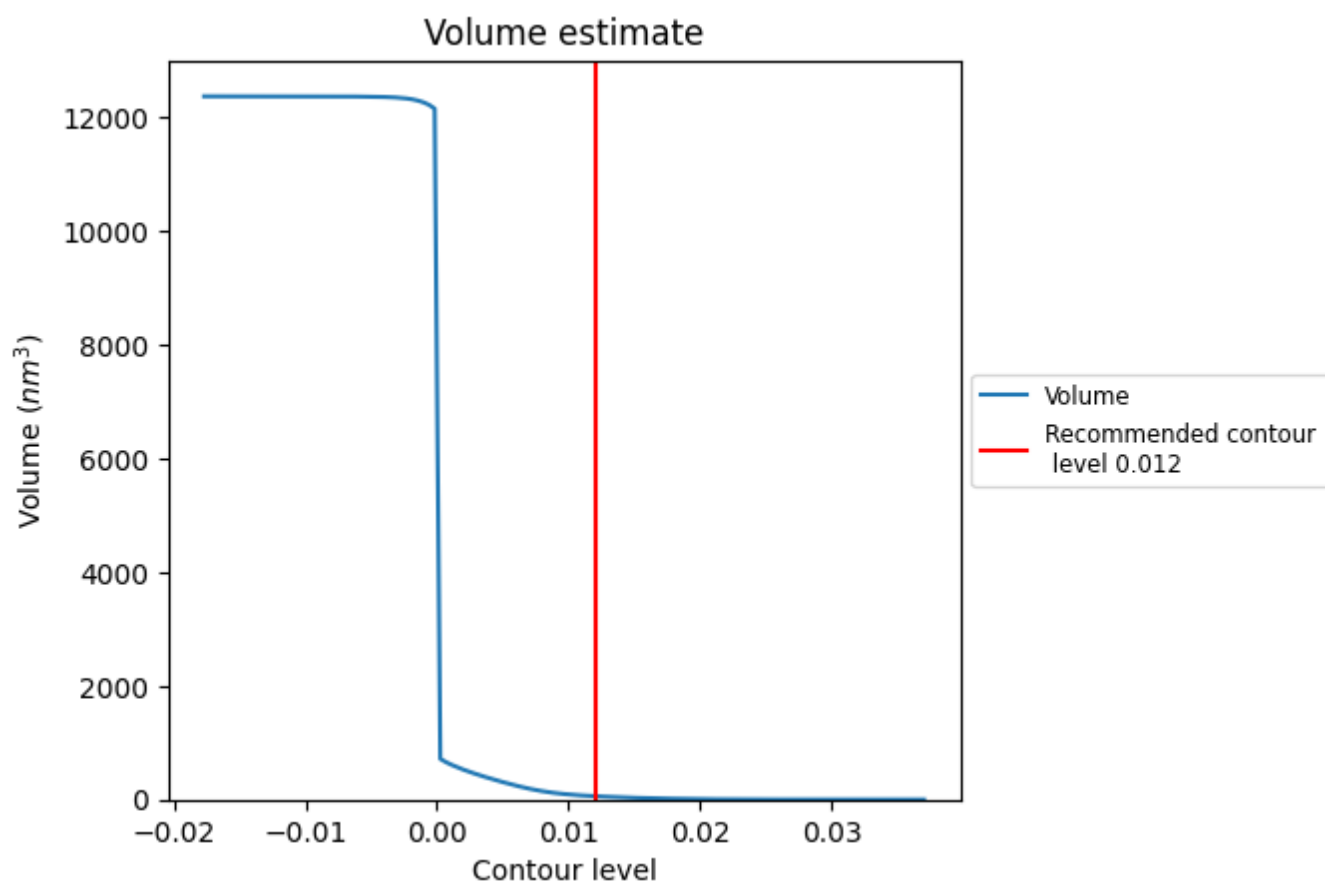
This section contains the results of statistical analysis of the map.

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.

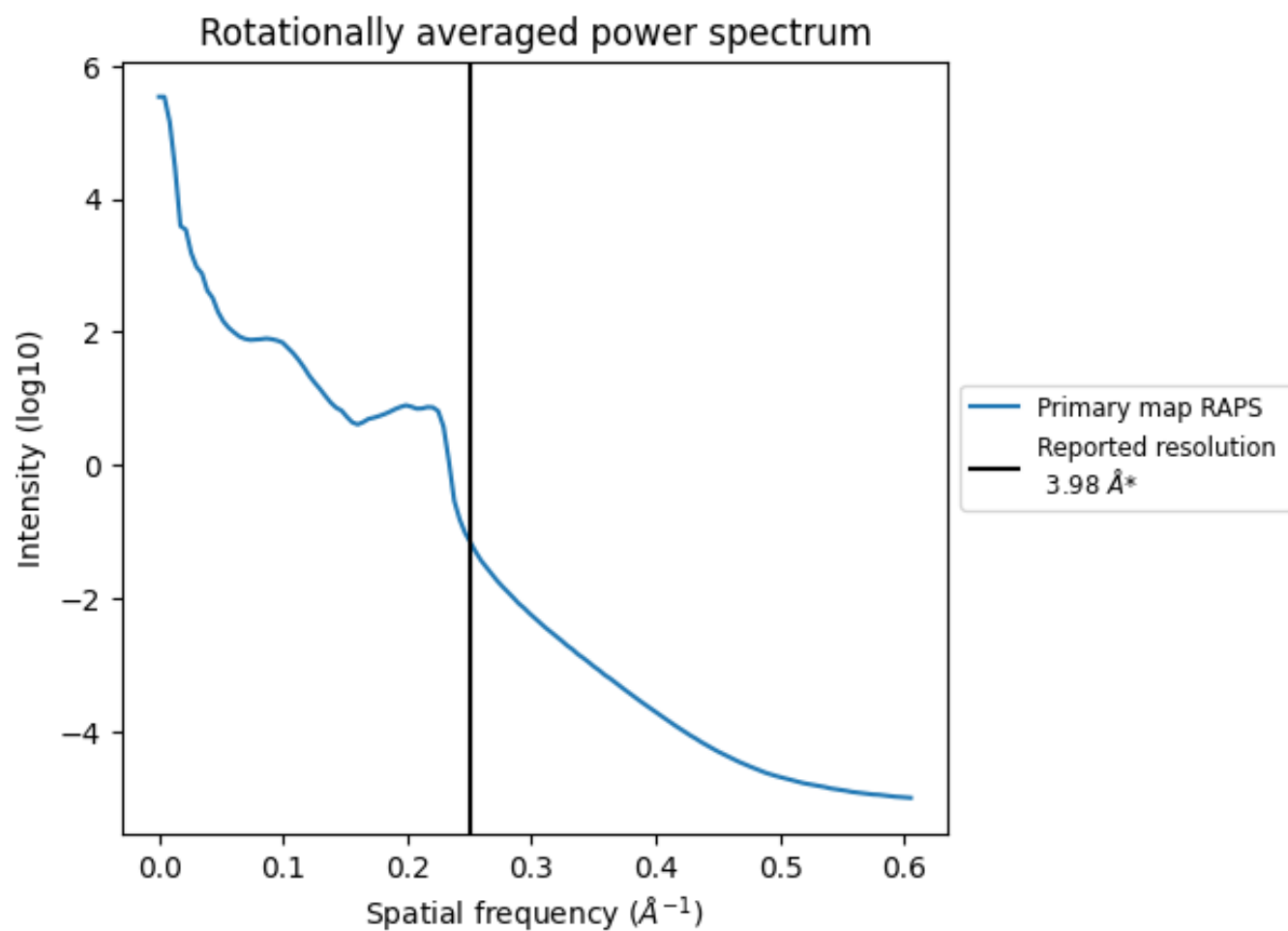
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 59 nm³; this corresponds to an approximate mass of 53 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 0.251 $\text{\AA}^{-1}$

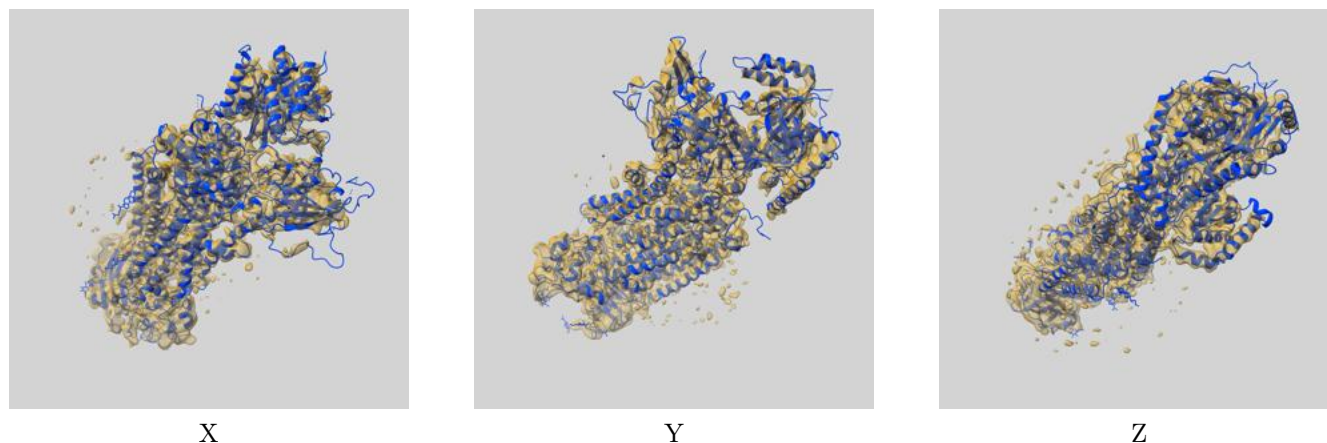
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

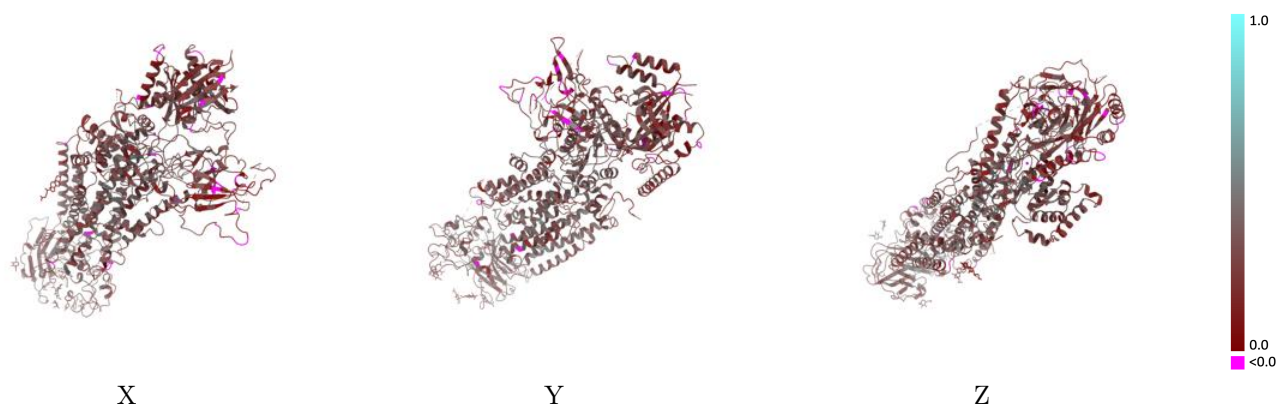
This section contains information regarding the fit between EMDB map EMD-23068 and PDB model 7KY5. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



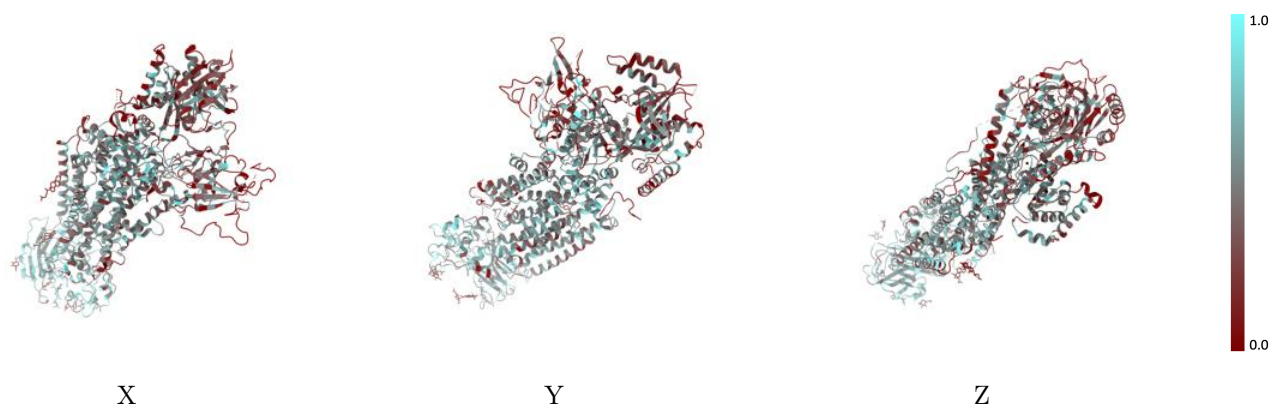
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



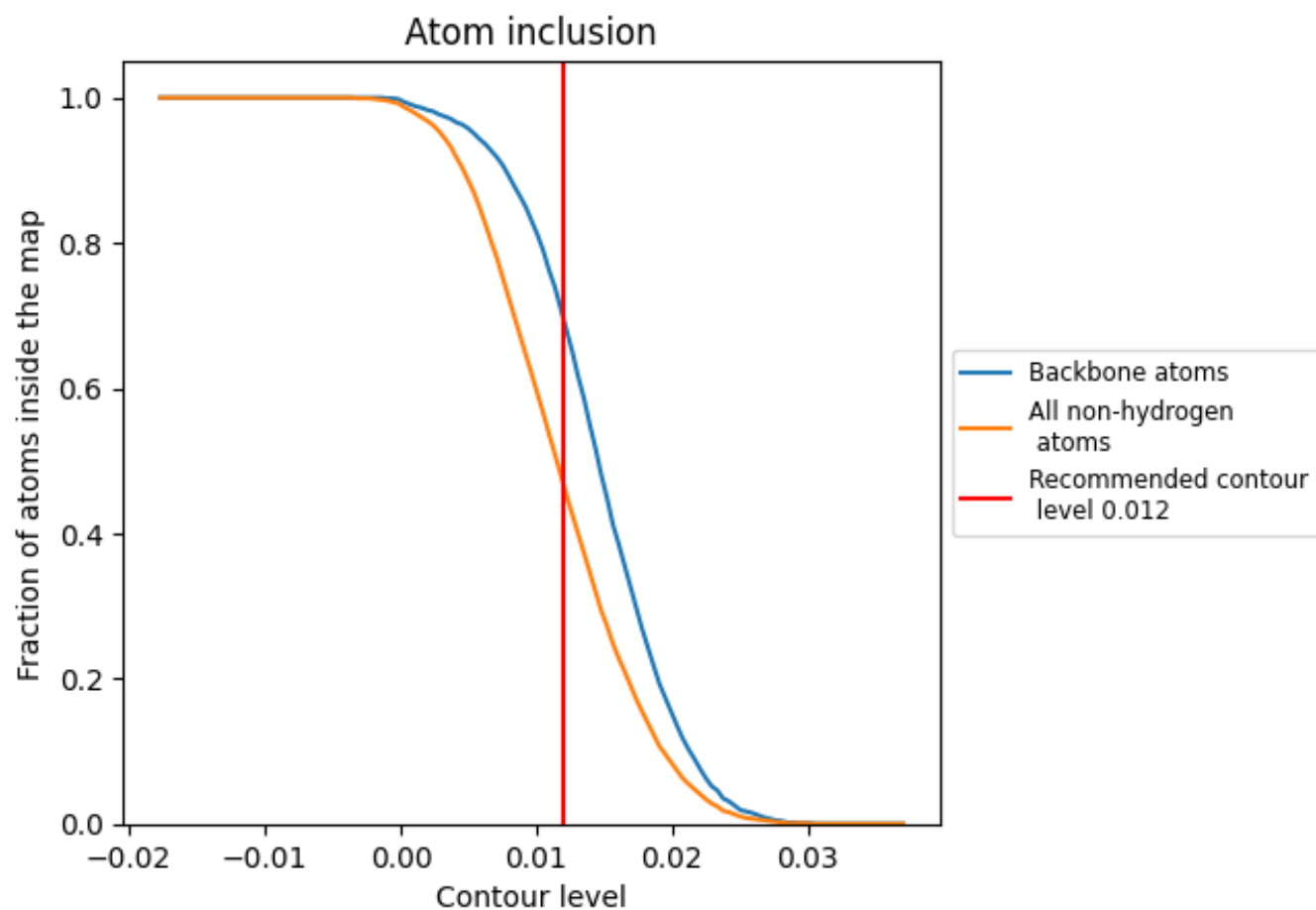
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 47% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4670	0.2950
A	0.4320	0.2850
B	0.5740	0.3260
C	0.6150	0.3380
D	0.2310	0.2730

