



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:09 AM UTC

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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

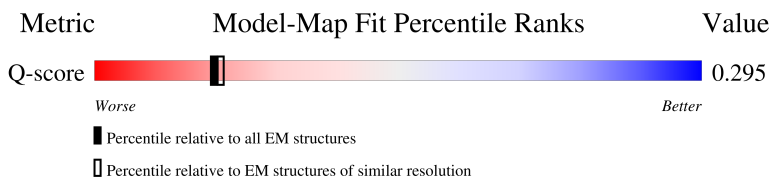
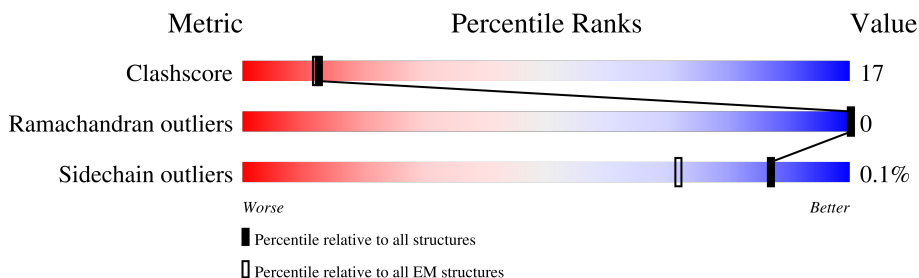
1 Overall quality at a glance

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

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.

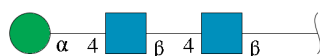
- Molecule 1 is a protein called Phospholipid-transporting ATPase DNF2.

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

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

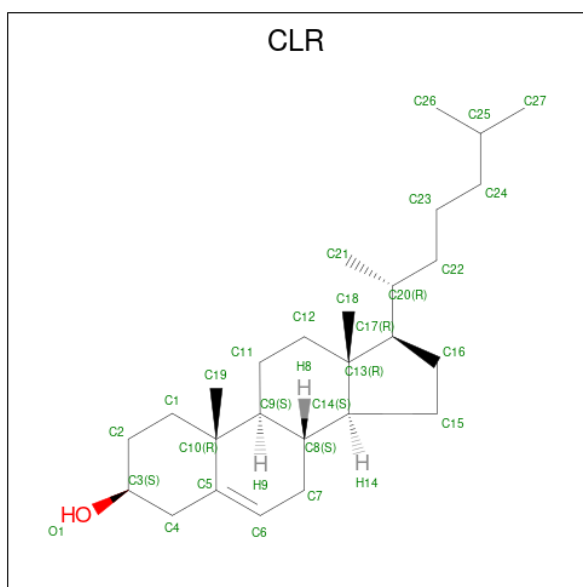
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	369	2974	1908	501	551	14	0	0

- 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.



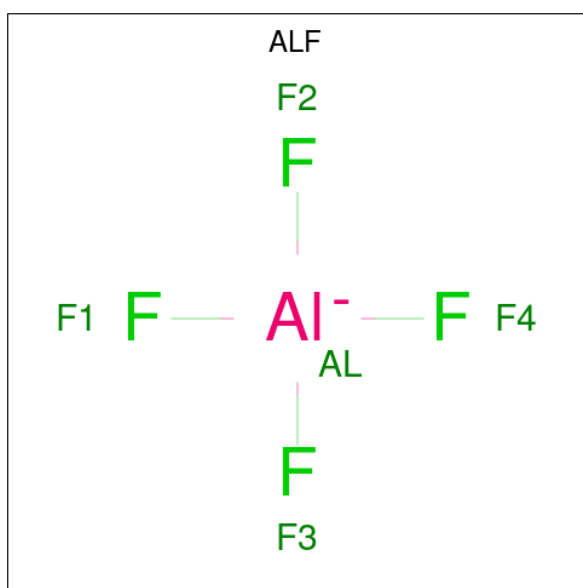
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	3	39	22	2	15	0	0
3	D	3	39	22	2	15	0	0

- 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).

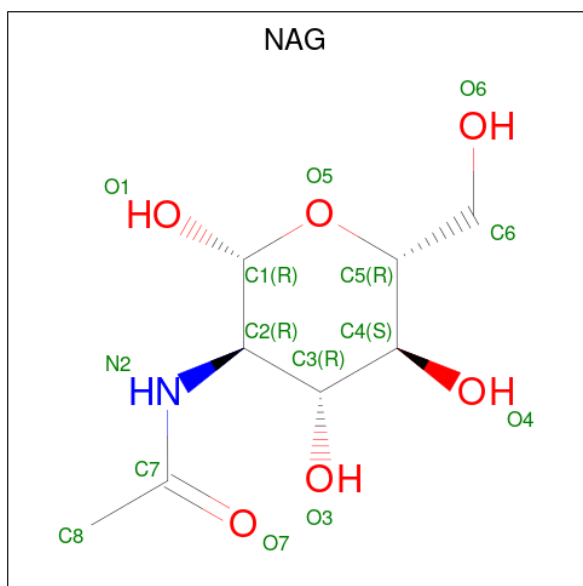


Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	Al	F	0
			5	1	4	

- 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: $C_8H_{15}NO_6$).



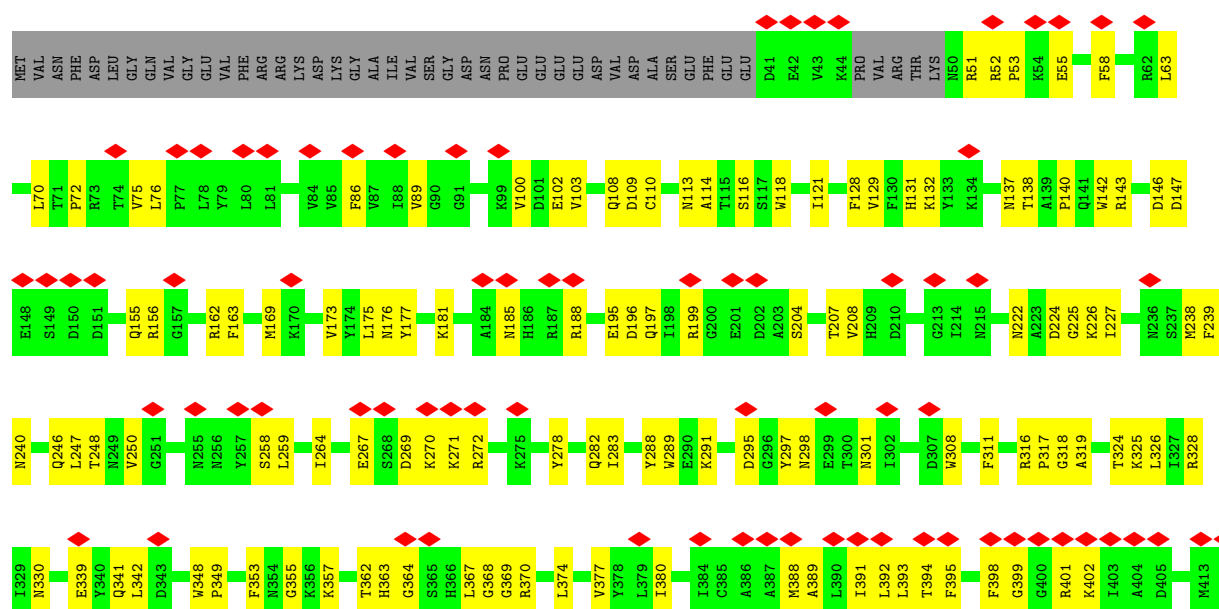
Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			15	8	1	6	
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			15	8	1	6	

ASN	ASN	ASP	A1417	V1340	F1260	G1187	A1119	G1046	N952	D919	G857	D788	E723	F644
LEU	LEU	PHE	Q1418	V1341	E1261	V1188	A1123	N1047	R983	S920	N588	D789	F724	F644
PRO	PRO	GLY	P1419	T1342	Y1262	G1192	L1124	V1048	E984	V921	S959	L789	K725	W648
ARG	ARG	ILE	W4422	L1346	Y1263	G1193	N1126	L1049	E985	I922	F960	K726	K726	V649
SER	SER	SER	A1423	G1347	T1265	E1194	G1126	N1051	E986	R925	G862	F791	C727	I652
MET	MET	LEU	V1424	L1348	F1267	G1195	E1127	D1052	N987	L926	S863	V792	I728	L653
ALA	ALA	ASP	V1427	L1349	F1268	M1200	E1128	L1056	D988	D927	S864	K794	N730	
SER	SER	THR	G1428	D1349	N1269	C1201	M1129	V1057	K989	R928	K865	E795	Y734	L657
ALA	ALA	HIS	V1429	H1350	L1270	C1202	R1130	V1058	V990	T929	K865	E796	G735	V658
GLY	GLY	PHE	L1430	R1351	A1271	D1203	R1131	K1059	T991	Q930	S866	E797	R736	P659
ASN	ASN	ASP	F1431	Y1352	A1272	Y1204	K1132	K1060	D992	N931	E798	L741	G736	I660
VAL	VAL	GLY	C1432	F1354	T1273	A1205	F1133	S1061	V993	D932	S867	L742	I729	S861
LEU	LEU	VAL	L1433	G1355	S1274	I1206	L1136	G1062	I994	A933	L868	A743	T729	Y663
SER	SER	SER	L1434	V1356		G1207	C1137	E1063	E995	T934	V870	L800	I738	Y663
THR	THR	SER	P1435	F1357	L1278	G1208	L1137	E1064	R996	L935	E871	K801	T739	I664
SER	SER	GLN	R1436	V1358	L1279	F1209	C1140	D1065	E997	L936	Q873	G802	E740	E667
ASP	ASP	THR	A1360	T1359	A1281	Y1211	K1141	V1065	L998	E937	G874	S903	A741	I668
THR	THR	ILE	V1363	A1360	L1282	V1212	A1142	E1066	I999	K938	Q876	G905	L742	I669
ARG	ARG	VAL			V1216		V1143	E1067	L1000	T939	K877	D806	A743	Q673
THR	THR	THR			L1217		L1144	F1068	L1001	A940	E878	H807	G744	A674
GLY	GLY	GLY			L1218		L1145	G1069	G1002	L941	F879	Q808	L745	I675
GLY	GLY	GLY			V1219		C1146	S1070	I1006	H942	Q880	K909	R746	Y678
ILE	ILE	MET			G1220		C1147	D1071	I1007	L943	V881	ARG	LVS	
ASN	ASN	SER			K1221		V1148		D1008	E944	L882	K810	GLN	
LEU	LEU	ILE			W1222		P1150	L1079	R1009	E945	N884	H814	GLY	
ASN	ASN	THR			Y1224		A1151	K1082	I1010	Y946	N884	F815	V751	V681
ASP	ASP	GLY			K1225		K1153	R1085	D1011	A947	L885	L816	D752	K887
THR	THR	GLY			R1226		A1154	E1086	D1012	T948	E886	A818	V753	L688
GLN	GLN	GLY			L1227		V1156	F1087	G1013	R952	N888	L819	E754	D689
GLY	GLY	THR			A1228		V1157	F1088	V1014	R952	S889	A820	S755	Y690
SER	SER	ARG			E1229		K1158	G1089	D1015	C955	S890	L821	E756	P691
ARG	ARG	ARG			Q1233		V1159	M1090	D1016	L955	R891	V825	G757	C892
GLY	GLY	TYR			F1234		V1160	S1091	S1017	A957	K892	R758	G758	T693
ALA	ALA	ARG			F1235		K1161	E1094	I1018	N957	R893	P694	P694	P694
VAL	VAL	VAL			Y1236		D1165	G1092	A1019	Q958	M894	K331	E760	I699
SER	SER	SER			K1237		V1166	E1093	L1020	R959	I897	D832	K761	S700
THR	THR	THR			N1238		T1168	E1095	L1021	E960	I898	D833	D701	D701
ASP	ASP	THR			V1239		M1167	E1096	E1022	L961	I898	P834	L702	D702
LEU	LEU	LEU			I1240		L1169	L1097	E1023	T962	K999	K335	I764	L703
GLY	GLY	GLY					A1170	K1098	A1024	W963	I900	K336	G704	G704
ARG	ARG	ARG						E1099	G1025	S964	P901	L837	Q705	I706
ARG	ARG	ARG								E965	G902	D838	A765	I706
ASP	ASP	ASP								Y966	THR	I839	D767	I709
GLN	GLN	GLN								E967	THR	K340	R768	F710
LEU	LEU	LEU								R968	LYS	A841	S711	D712
SER	SER	SER									ASP	Q842	T770	D712
PRO	PRO	PRO									ASP	M771	I772	K713
VAL	VAL	VAL									E908	S943	D773	L717
LEU	LEU	THR									P909	P944	E774	Q719
LEU	LEU	THR									K910	D845	L775	Q719
SER	SER	THR									A911	E946	R776	N720
GLN	GLN	THR									L912	S851	S777	V721
		THR									L913	V850	M778	N720
		THR									I914	T852	D779	V721
		THR									A953	A854	S779	M722
		THR									C915	Q855	T782	
		THR									K916	L856	Q783	
		THR											F784	

ARG
SER
ARG
ASP
ARG

• Molecule 2: Alkylphosphocholine resistance protein LEM3

Chain B: 

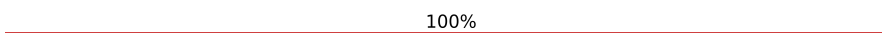


• Molecule 3: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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: ALF, NAG, MG, MAN, 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	0.15	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	3,2	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	3,2	-	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:

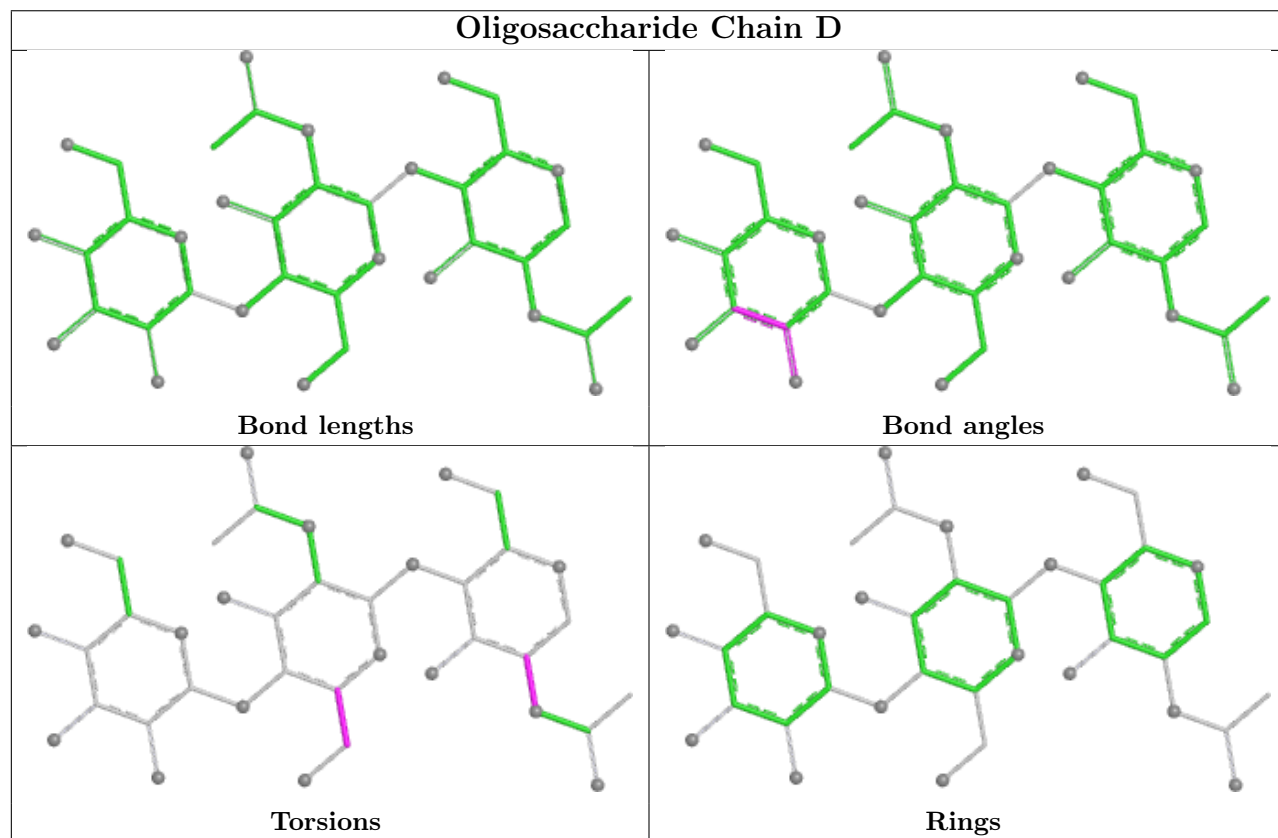
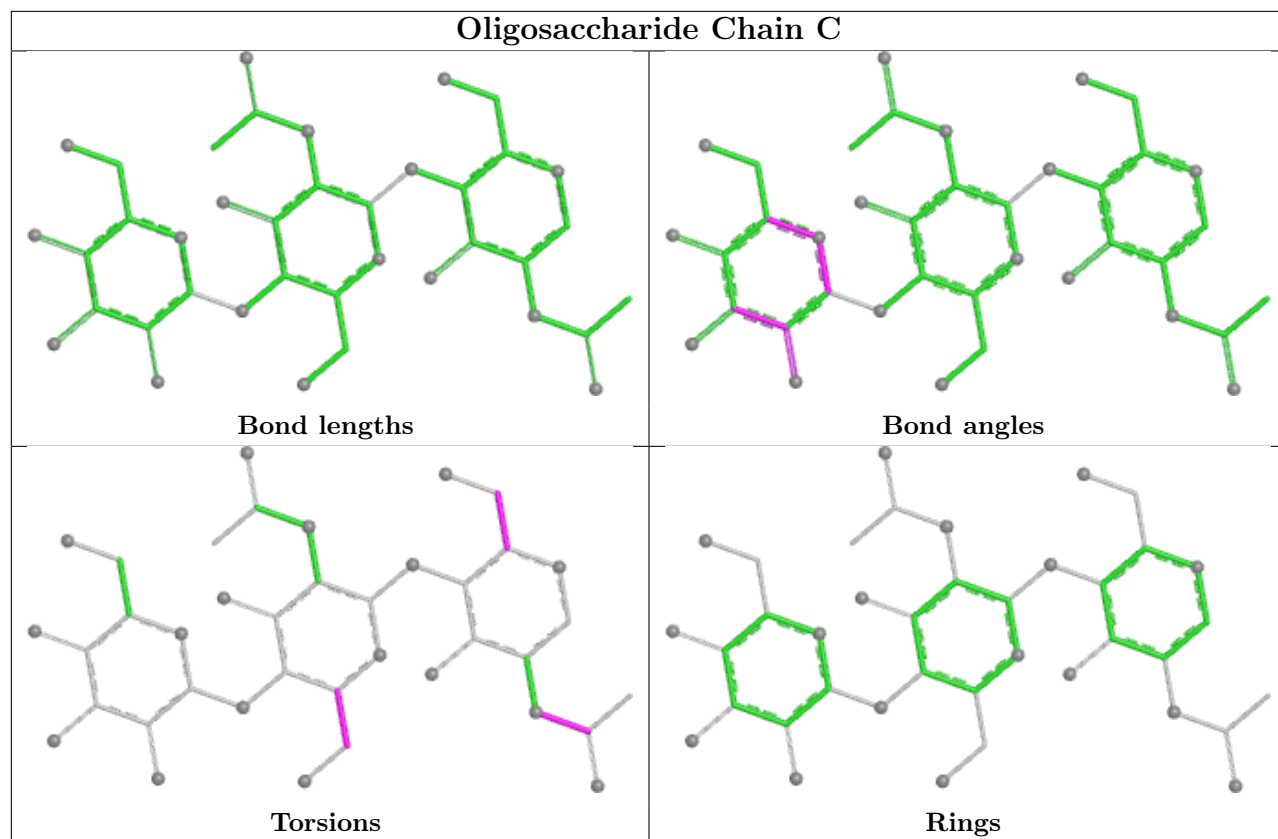
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	D	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	D	1	NAG	C1-C2-N2-C7
3	D	1	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	3	0
3	C	2	NAG	2	0
3	D	2	NAG	1	0
3	C	1	NAG	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 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	504	2	14,14,15	0.22	0	17,19,21	0.38	0
7	NAG	B	505	-	15,15,15	0.10	0	21,21,21	0.11	0
7	NAG	B	503	-	15,15,15	0.11	0	21,21,21	0.10	0
4	CLR	A	1702	-	31,31,31	0.52	0	48,48,48	1.36	5 (10%)
7	NAG	B	502	2	14,14,15	0.28	0	17,19,21	0.42	0
5	ALF	A	1703	-	4,4,4	1.38	0	-		
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%)

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	504	2	-	1/6/23/26	0/1/1/1
7	NAG	B	505	-	-	0/6/26/26	0/1/1/1
7	NAG	B	503	-	-	2/6/26/26	0/1/1/1
4	CLR	A	1702	-	-	7/10/68/68	0/4/4/4
7	NAG	B	502	2	-	2/6/23/26	0/1/1/1
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

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:

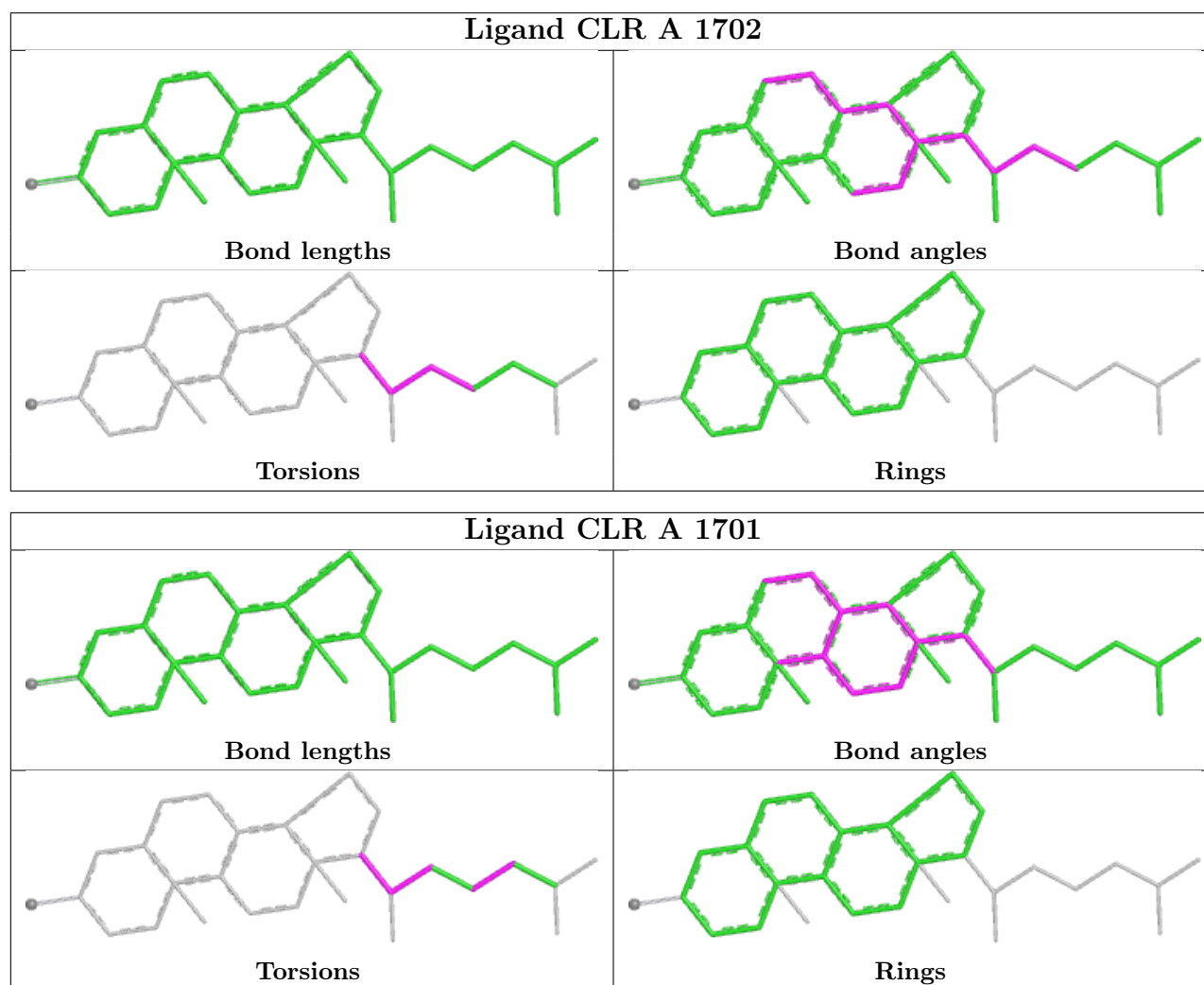
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1702	CLR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1701	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.

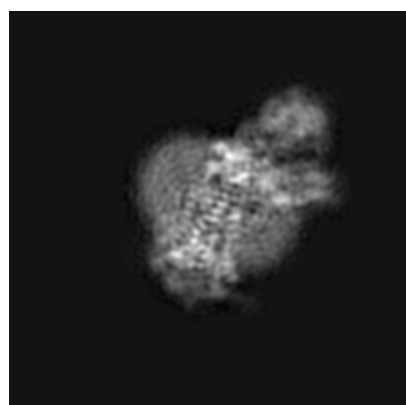
6 Map visualisation [i](#)

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.

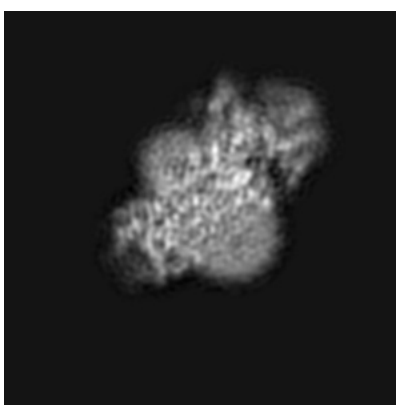
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

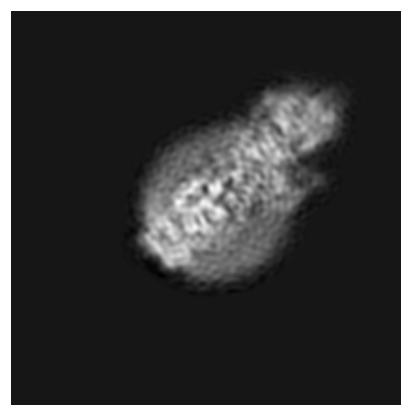
6.1.1 Primary map



X



Y

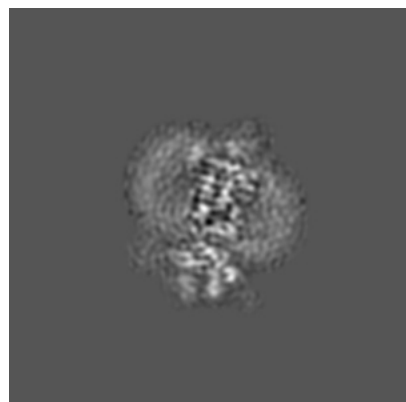


Z

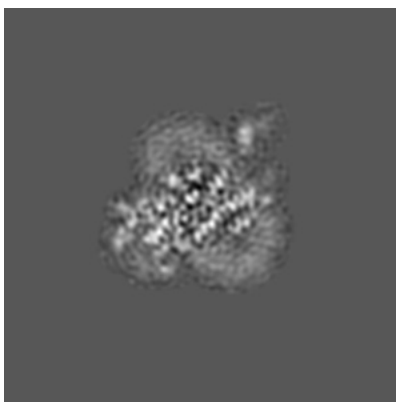
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

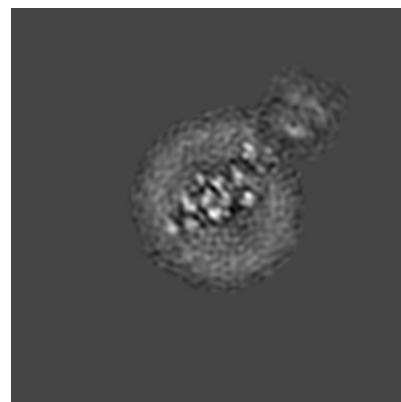
6.2.1 Primary map



X Index: 140



Y Index: 140

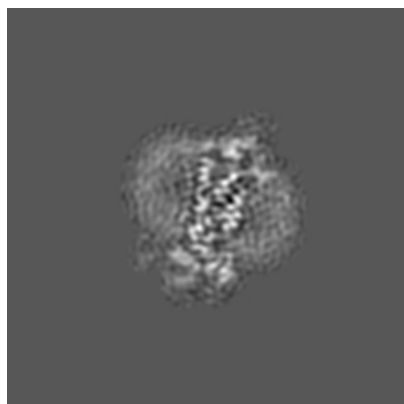


Z Index: 140

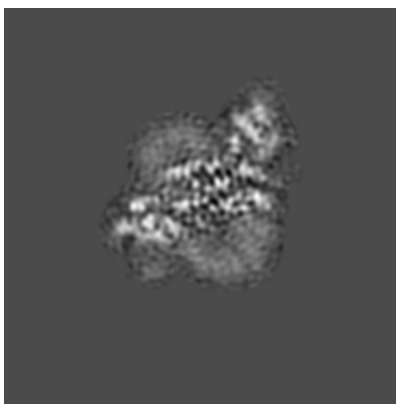
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 144



Y Index: 154

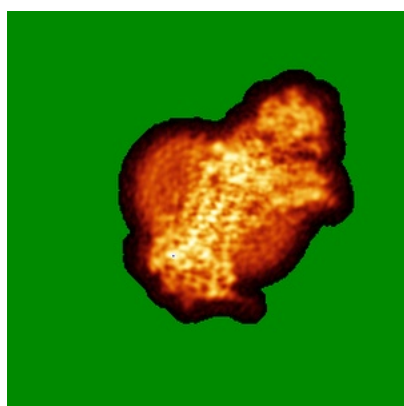


Z Index: 163

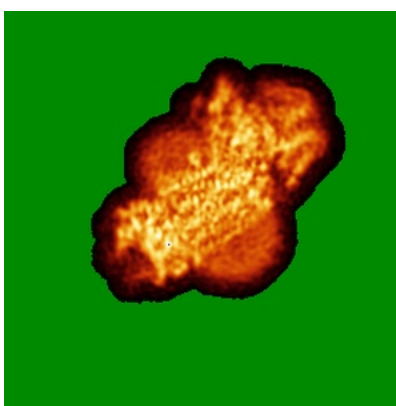
The images above show the largest variance slices of the map in three orthogonal directions.

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

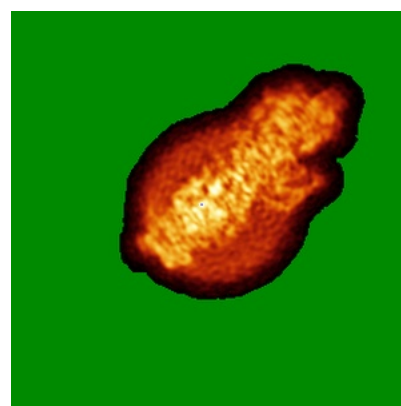
6.4.1 Primary map



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

This section was not generated.

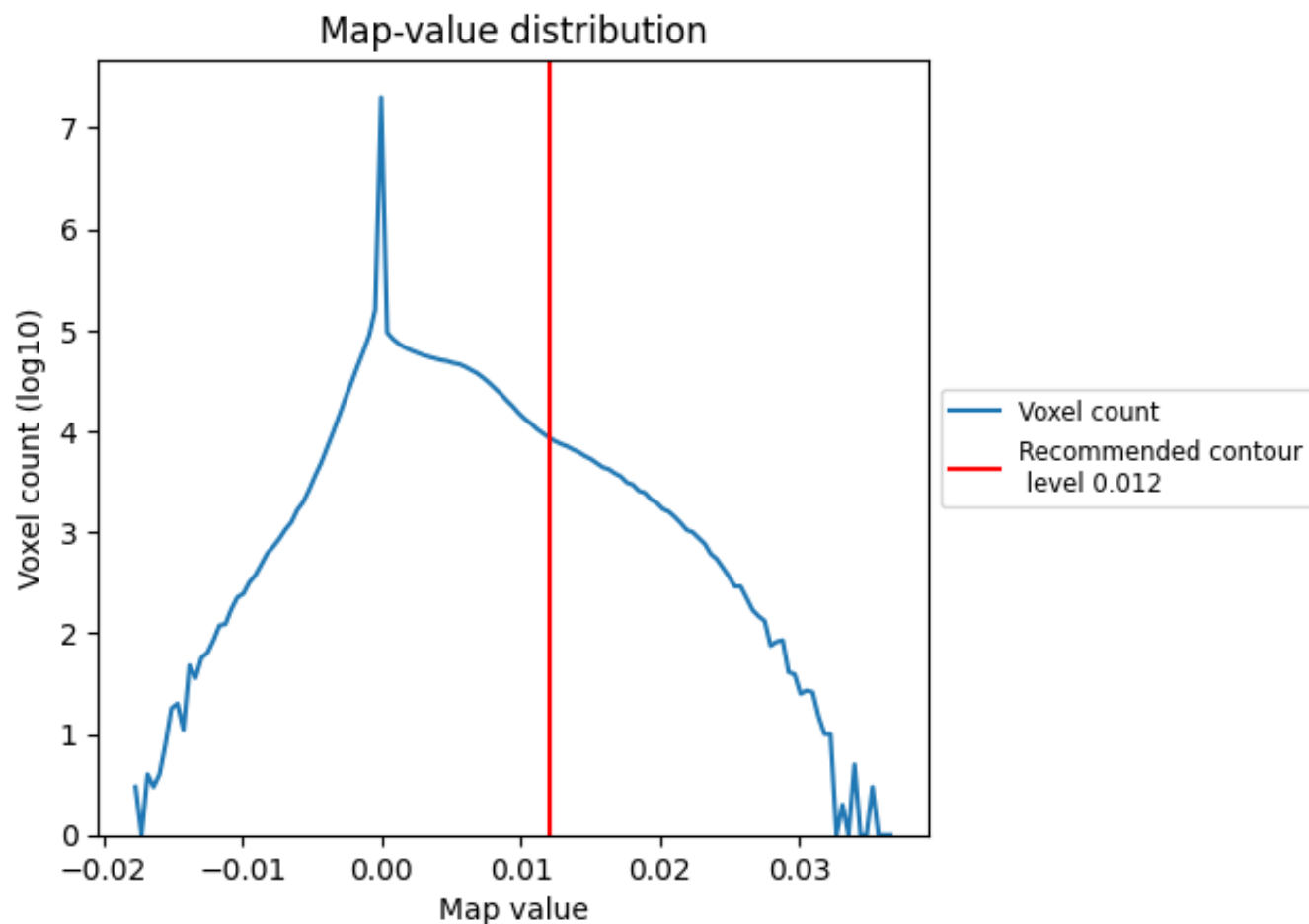
6.6 Mask visualisation

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

7 Map analysis [i](#)

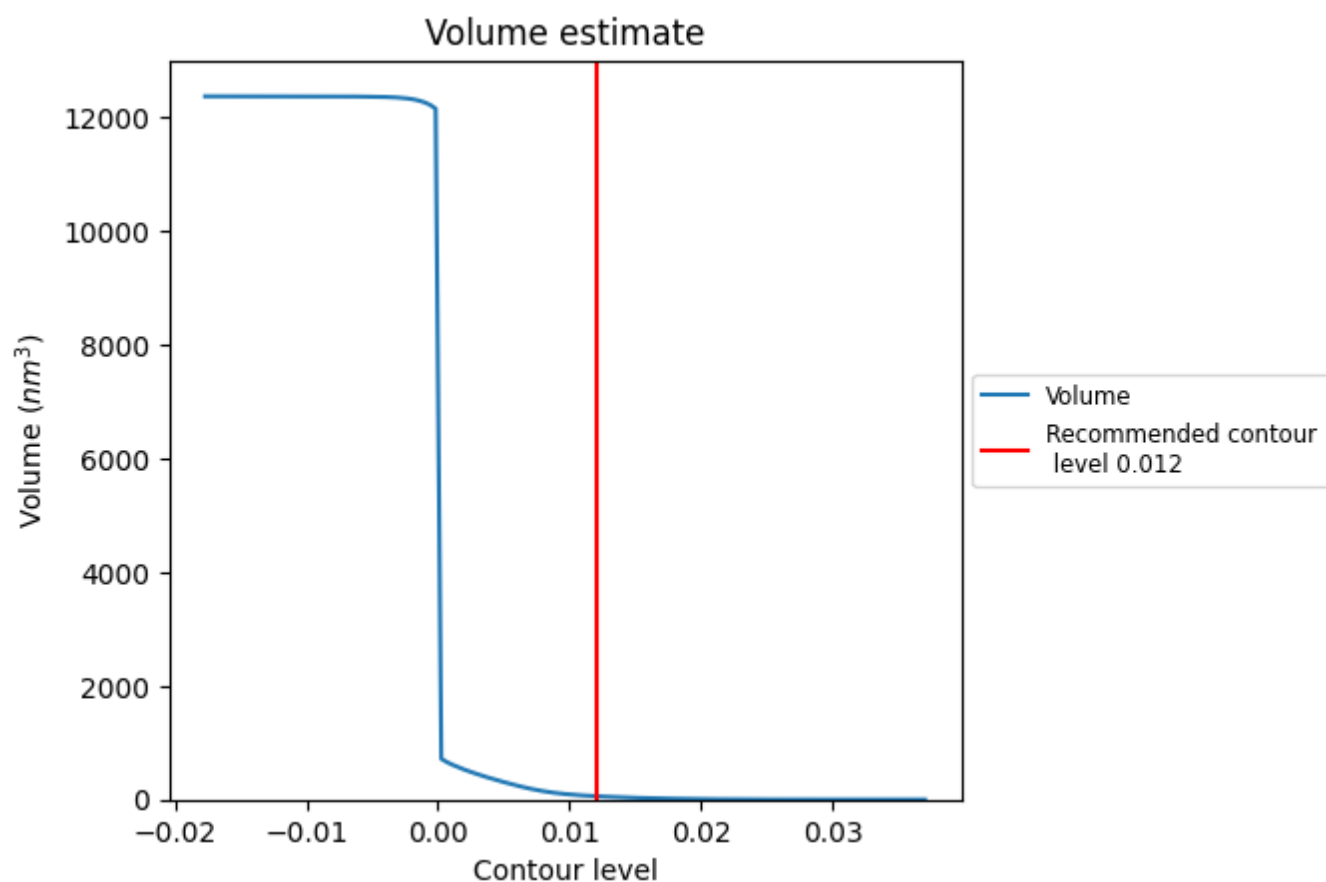
This section contains the results of statistical analysis of the map.

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.

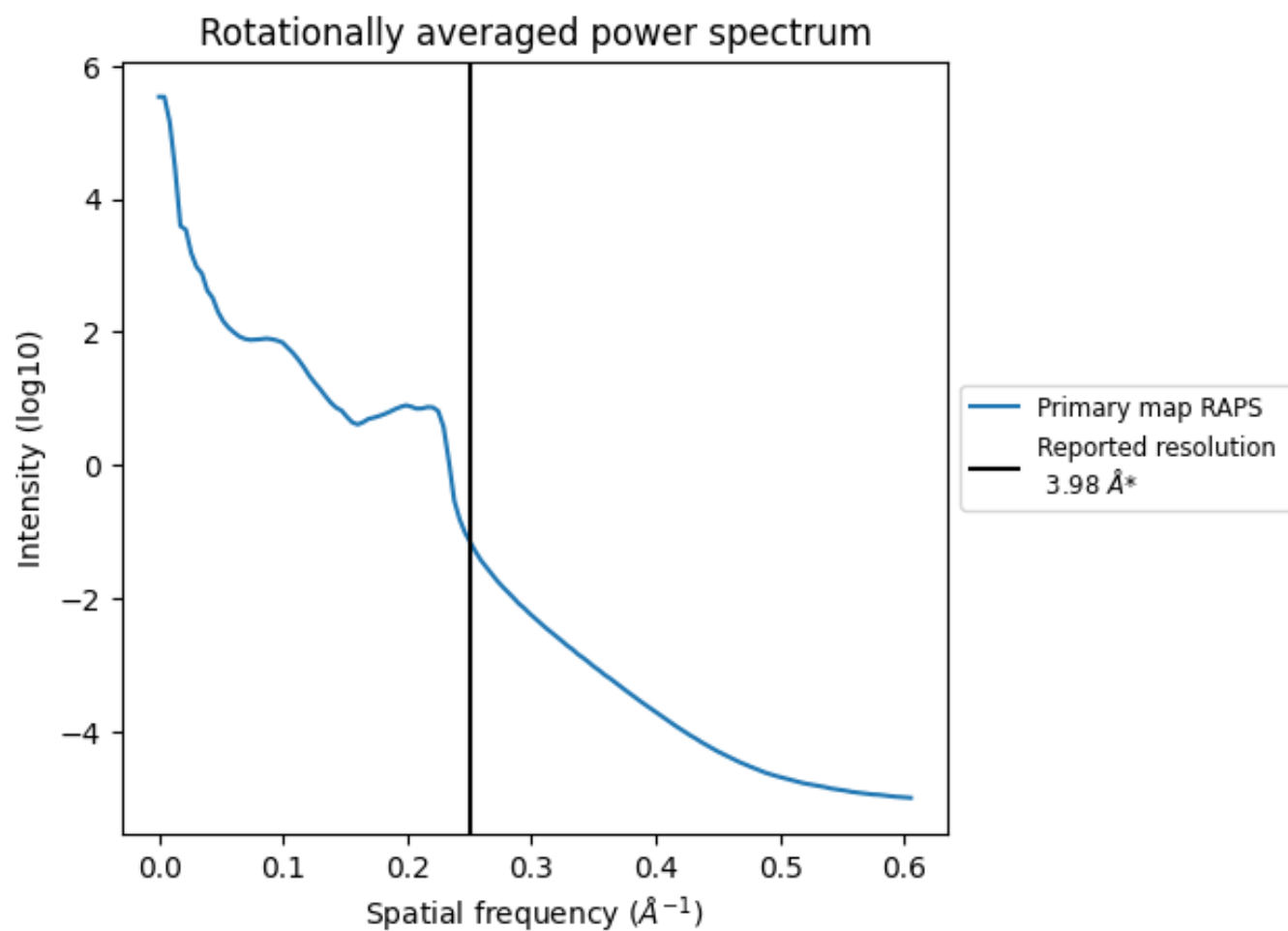
7.2 Volume estimate [i](#)



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

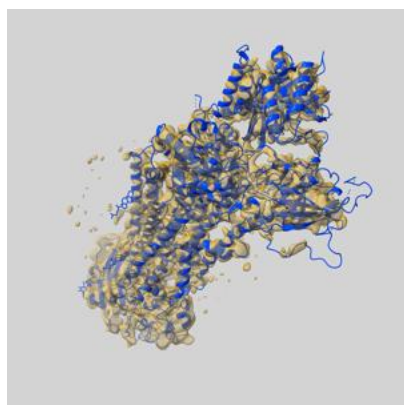
8 Fourier-Shell correlation

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

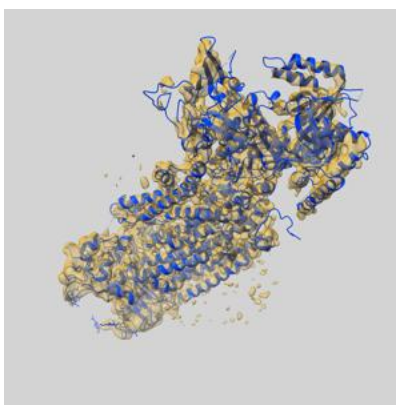
9 Map-model fit [i](#)

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](#).

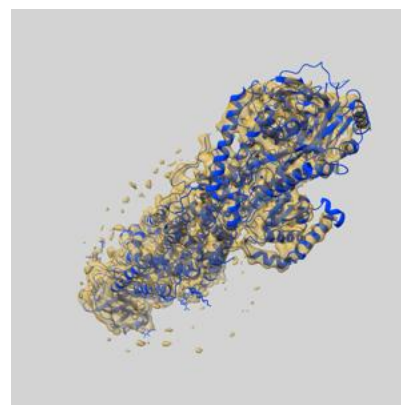
9.1 Map-model overlay [i](#)



X



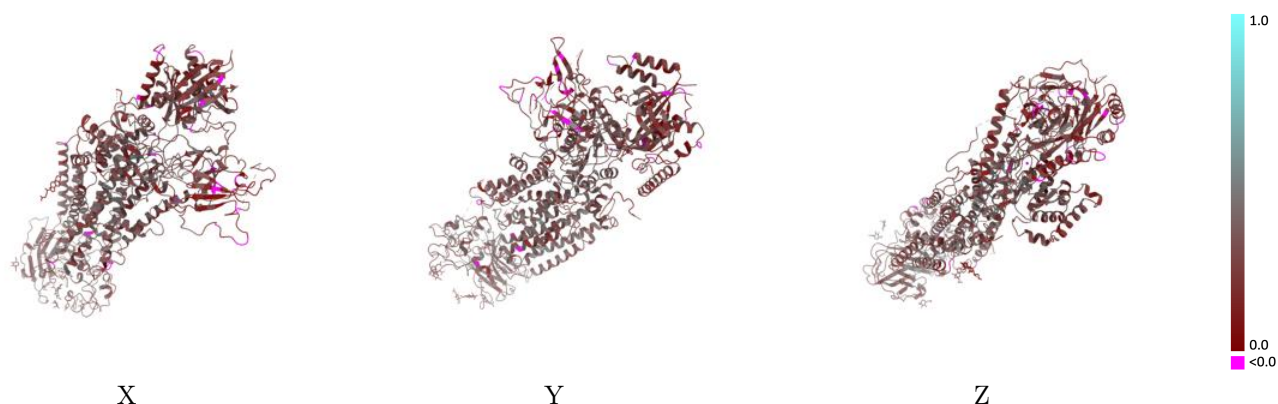
Y



Z

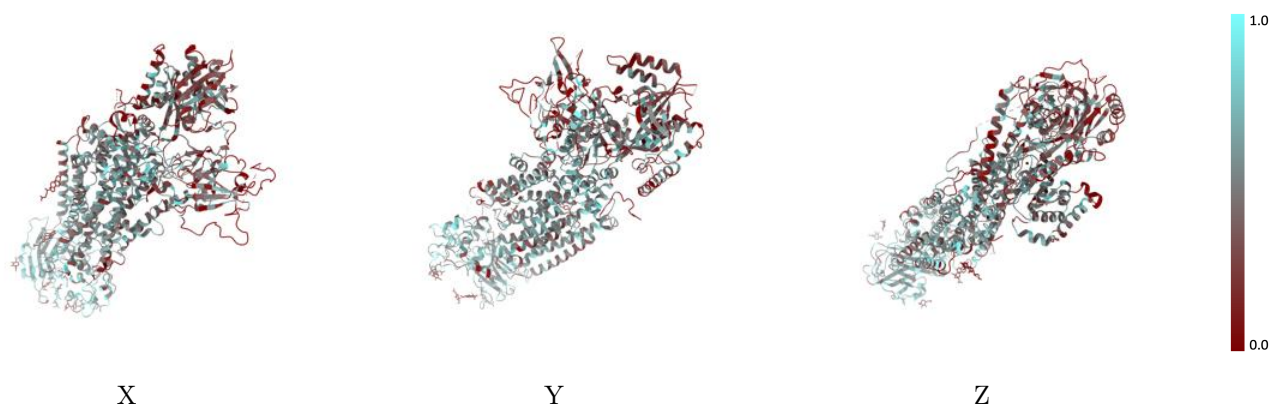
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



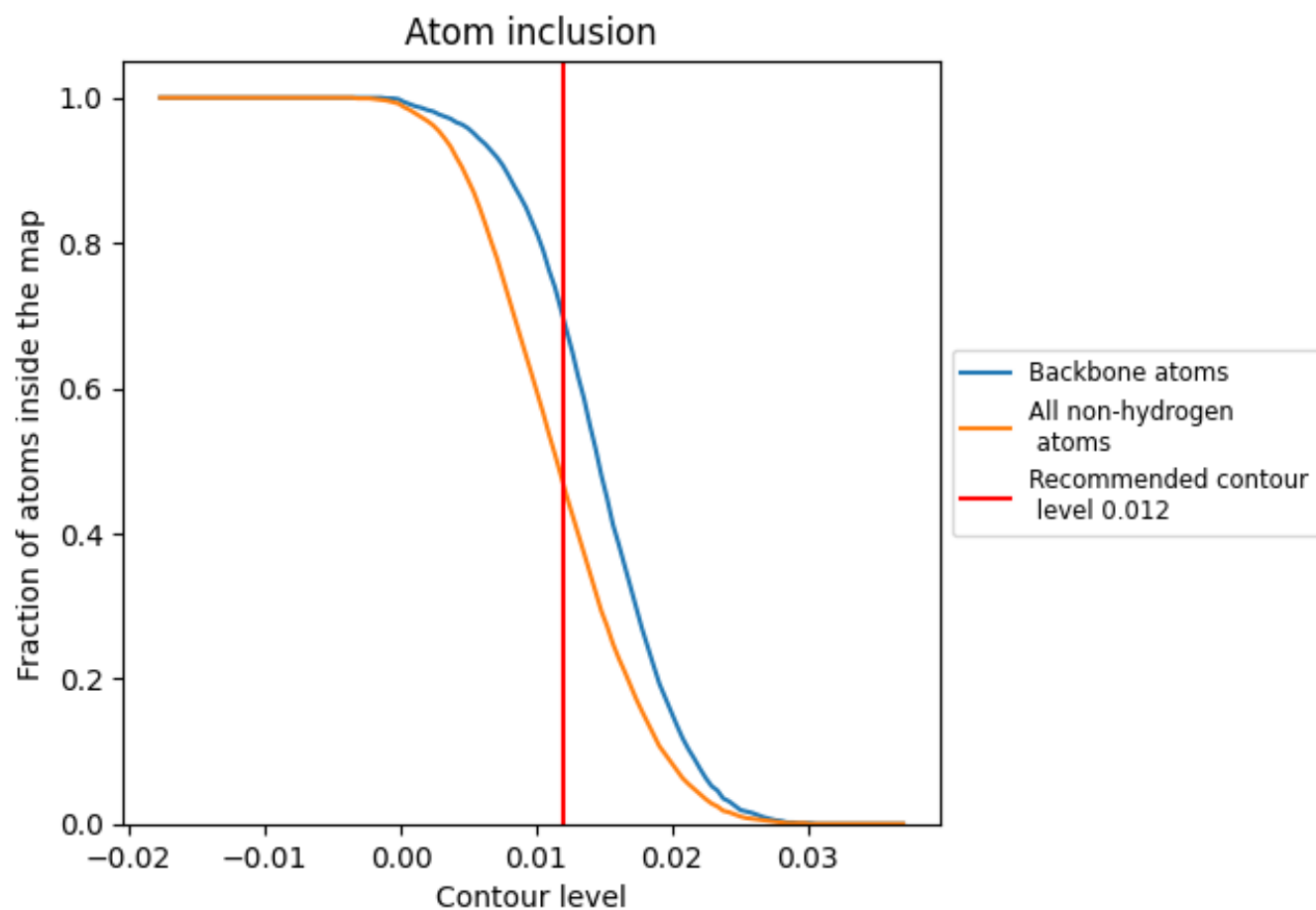
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

