



## Full wwPDB EM Validation Report ⓘ

May 17, 2025 – 11:12 PM EDT

PDB ID : 7ROQ / pdb\_00007roq  
EMDB ID : EMD-6724  
Title : Alternative Structure of Human ABCA1  
Authors : Aller, S.G.  
Deposited on : 2021-08-01  
Resolution : 4.10 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](mailto: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.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

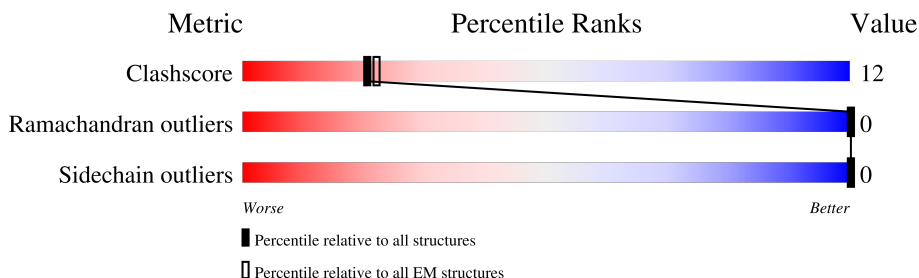
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.10 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	2305	<div> <div>24%</div> <div>59%</div> <div>20%</div> <div>21%</div> </div>
2	B	5	<div> <div>40%</div> <div>20%</div> <div>80%</div> </div>
3	C	2	<div> <div>50%</div> <div>50%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13971 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 ABCA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1831	Total	C	N	O	S	0	0
			13787	8878	2338	2494	77		

There are 44 discrepancies between the modelled and reference sequences:

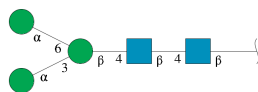
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP O95477
A	-19	ALA	-	expression tag	UNP O95477
A	-18	ASP	-	expression tag	UNP O95477
A	-17	TYR	-	expression tag	UNP O95477
A	-16	LYS	-	expression tag	UNP O95477
A	-15	ASP	-	expression tag	UNP O95477
A	-14	ASP	-	expression tag	UNP O95477
A	-13	ASP	-	expression tag	UNP O95477
A	-12	ASP	-	expression tag	UNP O95477
A	-11	LYS	-	expression tag	UNP O95477
A	-10	SER	-	expression tag	UNP O95477
A	-9	GLY	-	expression tag	UNP O95477
A	-8	PRO	-	expression tag	UNP O95477
A	-7	ASP	-	expression tag	UNP O95477
A	-6	GLU	-	expression tag	UNP O95477
A	-5	VAL	-	expression tag	UNP O95477
A	-4	ASP	-	expression tag	UNP O95477
A	-3	ALA	-	expression tag	UNP O95477
A	-2	SER	-	expression tag	UNP O95477
A	-1	GLY	-	expression tag	UNP O95477
A	0	ARG	-	expression tag	UNP O95477
A	2262	LEU	-	expression tag	UNP O95477
A	2263	GLU	-	expression tag	UNP O95477
A	2264	GLY	-	expression tag	UNP O95477
A	2265	SER	-	expression tag	UNP O95477
A	2266	ASP	-	expression tag	UNP O95477
A	2267	GLU	-	expression tag	UNP O95477
A	2268	VAL	-	expression tag	UNP O95477

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	2269	ASP	-	expression tag	UNP O95477
A	2270	ALA	-	expression tag	UNP O95477
A	2271	VAL	-	expression tag	UNP O95477
A	2272	GLU	-	expression tag	UNP O95477
A	2273	GLY	-	expression tag	UNP O95477
A	2274	SER	-	expression tag	UNP O95477
A	2275	HIS	-	expression tag	UNP O95477
A	2276	HIS	-	expression tag	UNP O95477
A	2277	HIS	-	expression tag	UNP O95477
A	2278	HIS	-	expression tag	UNP O95477
A	2279	HIS	-	expression tag	UNP O95477
A	2280	HIS	-	expression tag	UNP O95477
A	2281	HIS	-	expression tag	UNP O95477
A	2282	HIS	-	expression tag	UNP O95477
A	2283	HIS	-	expression tag	UNP O95477
A	2284	HIS	-	expression tag	UNP O95477

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



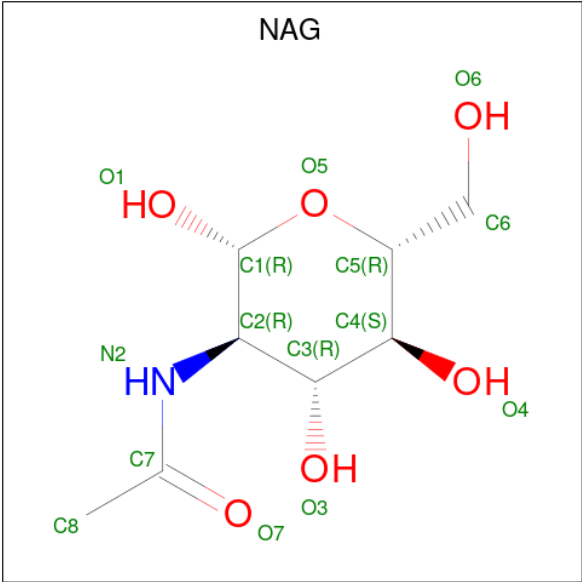
Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	5	Total	C	N	O	0	0
			61	34	2	25		

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



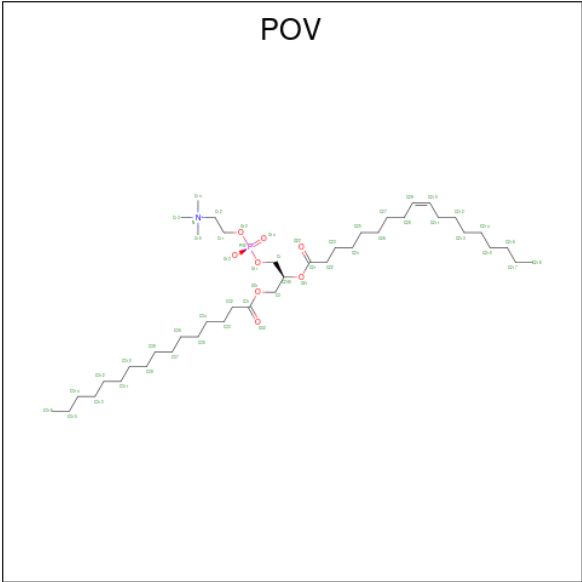
Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



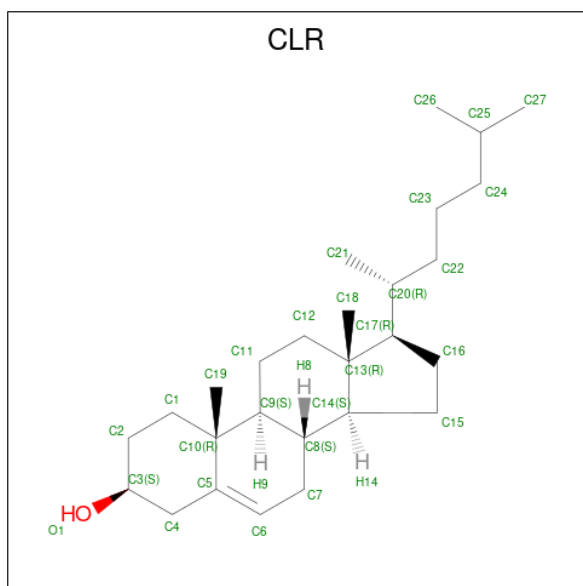
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	14	8	1	5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0

- Molecule 5 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (CCD ID: POV) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	C	0
			11	11	

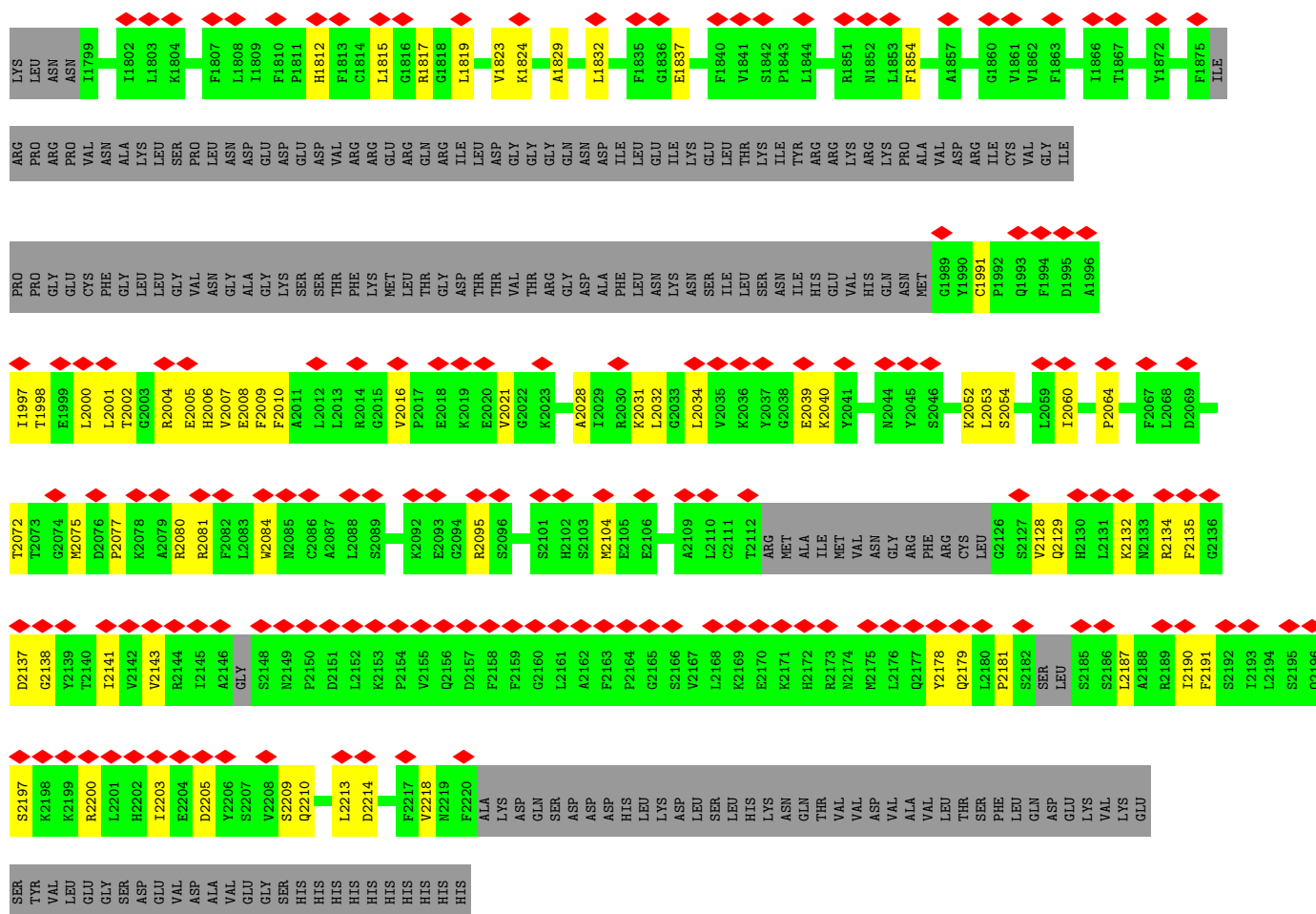
- Molecule 6 is CHOLESTEROL (CCD ID: CLR) (formula:  $C_{27}H_{46}O$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			21	20	1	
6	A	1	Total	C	O	0
			21	20	1	



L1636	M1637	L1638	T1639	K1640	L1641	Q1642	M1649	T1650	T1651	S1652	V1653	D1654	V1655	L1656	I1659	I1662	F1663	A1664	M1665	S1666	A1670	V1673	V1674	I1677	Q1678	E1679	R1680	K1683	H1686	F1689	I1690	S1691	G1692	V1693	K1694	P1695	V1696	I1697	L1700	S1701	M1702	W1705	D1706	M1707	C1708	A1714	T1715												
Q1543	A1544	L1545	P1546	P1547	S1548	Q1549	I1555	K1556	K1559	L1562	K1563	L1564	A1565	K1566	D1571	R1572	F1573	L1574	T1586	K1587	V1590	K1591	V1592	W1593	F1594	M1595	N1596	K1597	I1602	S1603	S1604	F1605	L1606	M1607	V1608	M1609	M1610	M1611	A1612	I1613	L1614	R1615	A1616	N1617	E1622	I1629	T1630	A1631	F1632										
T1455	M1456	Q1457	N1458	P1459	C1463	Q1464	C1465	D1468	K1469	I1470	K1471	K1472	M1473	L1474	P1475	V1476	C1477	A1481	L1484	P1485	K1490	Q1491	N1492	T1493	I1496	L1497	Q1498	D1499	S1506	D1507	V1510	A1511	T1512	I1516	K1522	W1526	V1527	M1528	E1529	F1530	R1531	F1535	S1536	L1537	M1541	T1542													
C1359	I1360	A1361	L1362	V1363	F1364	V1368	K1373	Y1374	L1377	E1378	L1379	Q1380	P1381	W1382	M1383	Y1388	E1397	D1398	T1401	L1404	L1405	N1406	K1410	D1411	G1415	T1416	R1417	P1423	I1424	P1425	D1426	Q1430	A1431	E1434	E1435	W1436	A1439	M1446	L1448	F1449	Q1450	N1451	W1454																
THR	GLU	ASP	ALA	ALA	ASP	PRO	ASN	ASP	SER	ILE	PRO	GLU	SER	ARG	GLU	THR	ASP	LEU	LEU	SER	GLY	MET	ASP	GLY	GLY	GLY	VAL	GLY	VAL	ASP	ALA	GLU	THR	SER	THR	ASP	GLY	THR	LEU	PRO	ALA	ARG	ASN	ARG	ALA	PHE	GLY	ASP	LYS	GLN	SER	CYS	LEU	ARG	PRO	PHE			
E1224	I1225	D1226	D1227	R1228	L1229	S1230	D1231	L1232	G1233	I1234	S1235	S1236	Y1237	G1238	I1239	S1240	E1241	T1242	E1246	I1247	F1248	L1249	K1250	V1251	A1252	GLU	GLU	SER	GLY	VAL	ASP	ALA	GLU	THR	SER	THR	ASP	GLY	THR	LEU	PRO	ALA	ARG	ASN	ARG	ALA	PHE	GLY	ASP	LYS	GLN	SER	CYS	LEU	ARG	PRO	PHE		
ASP	ALA	GLY	LEU	GLY	SER	ASP	HIS	GLU	SER	ASP	THR	L1176	T1177	I1178	D1179	V1180	S1181	A1182	I1183	S1184	N1185	L1186	I1187	R1188	K1189	H1190	V1191	S1192	E1193	A1194	R1195	L1196	V1197	E1198	D1199	I1200	G1201	H1202	E1203	L1204	T1205	Y1206	V1207	L1208	P1209	V1210	E1211	A1212	A1213	K1214	E1215	G1216	A1217	F1218	V1219	E1220	L1221	F1222	H1223
I1101	A1102	I1103	I1104	S1105	H1106	G1107	K1108	L1109	C1110	G1113	F1117	L1118	K1119	M1120	Q1121	L1122	G1123	T1124	G1125	Y1126	Y1127	L1128	T1129	L1130	V1131	K1132	K1133	ASP	VAL	GLU	SER	SER	LEU	SER	SER	CYS	ARG	ASN	SER	SER	THR	VAL	SER	TYR	LEU	LYS	LYS	GLU	ASP	SER	VAL	SER	GLN	SER	SER	SER	SER		
S1023	S1024	K1025	L1026	K1027	S1028	K1029	Q1032	L1033	S1034	G1035	G1036	M1037	Q1038	R1039	K1040	L1041	L1045	A1046	F1047	V1048	G1049	G1050	V1054	I1055	L1056	D1057	P1058	T1060	V1063	D1069	K1077	Y1078	R1079	T1082	T1083	I1084	L1085	L1086	T1087	H1089	D1092	E1093	A1094	V1095	L1097	D1099	R1100												
P951	P952	T953	S954	G955	T956	A957	Y958	L959	L960	G961	K962	D963	T964	R965	S966	E967	M968	S969	T970	I971	R972	Q973	C978	P979	N982	V983	L984	F985	D986	N987	L988	T989	E992	H993	I994	W995	R999	L1000	K1001	S1004	E1005	K1006	E1011	M1012	E1013	Q1014	M1015	A1016	L1017	D1018	L1021	PRO							
C887	M888	E889	E890	E891	T892	T893	H894	L895	K896	S900	I901	Q902	N903	L904	V905	K906	V907	TYR	ARG	GLY	ASP	MET	LYS	VAL	ALA	VAL	D917	G918	L919	A920	L921	N922	F923	Y924	E925	G926	Q927	I928	T929	S930	F931	L932	G933	H934	N935	G936	A937	G938	K939	T940	T941	S944	I945	L946	L949	F950			
PHE	GLU	SER	PRO	VAL	GLU	GLU	ASP	GLY	F819	T823	S826	Y835	H838	F846	PRO	GLY	GLN	TRP	GLY	ILE	PRO	ARG	PRO	TRP	THR	PHE	PRO	CYS	THR	LYS	SER	TYR	TRP	PHE	GLY	GLU	GLU	SER	ASP	GLU	LYS	SER	SER	HIS	PRO	GLY	SER	ASN	GLN	LYS	ARG	ILE	SER	SER	GLU	I886			



• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	790156	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.485	Depositor
Minimum map value	-0.354	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	261.308, 261.308, 261.308	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.30654, 1.30654, 1.30654	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: CLR, BMA, NAG, MAN, POV

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	0.14	0/14084	0.37	0/19149

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13787	0	13251	325	0
2	B	61	0	52	1	0
3	C	28	0	25	1	0
4	A	42	0	39	2	0
5	A	11	0	16	0	0
6	A	42	0	54	1	0
All	All	13971	0	13437	326	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 12.

All (326) 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:1424:ILE:HG13	1:A:1425:PRO:HD3	1.56	0.88
1:A:1465:CYS:SG	1:A:1477:CYS:N	2.50	0.85
1:A:1614:LEU:HD13	1:A:1629:ILE:HD11	1.62	0.80
1:A:995:TRP:HE1	1:A:999:ARG:HE	1.32	0.75
1:A:1451:ASN:O	1:A:1455:THR:OG1	2.07	0.73
1:A:2075:MET:O	1:A:2080:ARG:NH2	2.22	0.71
1:A:520:ILE:HG22	1:A:524:MET:HE1	1.73	0.70
1:A:625:PRO:HB3	1:A:1510:VAL:HG13	1.73	0.70
1:A:1336:ARG:HG2	1:A:1705:TRP:CD1	2.27	0.70
1:A:2016:VAL:HG13	1:A:2021:VAL:HG12	1.72	0.70
1:A:2010:PHE:HB3	1:A:2060:ILE:HG21	1.72	0.70
1:A:930:SER:HB2	1:A:1101:ILE:HG22	1.73	0.70
1:A:1663:PHE:HD1	1:A:1775:LEU:HD21	1.56	0.70
1:A:49:TYR:HB3	1:A:629:ASP:HB2	1.73	0.69
1:A:2004:ARG:NH1	1:A:2008:GLU:OE2	2.26	0.69
1:A:533:TRP:NE1	1:A:596:LEU:HD21	2.08	0.68
1:A:1607:ASN:OD1	1:A:1611:ASN:ND2	2.26	0.67
1:A:579:ARG:O	1:A:1596:ASN:ND2	2.28	0.67
1:A:1680:ARG:NH2	1:A:1760:PHE:O	2.28	0.67
1:A:1096:VAL:HG13	1:A:1097:LEU:HD12	1.76	0.66
1:A:78:ASN:HA	1:A:582:PRO:HB3	1.78	0.65
1:A:383:ILE:HD11	1:A:510:LEU:HD13	1.78	0.65
1:A:1448:LEU:HB2	1:A:1484:LEU:HD11	1.78	0.65
1:A:552:VAL:HG11	1:A:604:ILE:HD13	1.79	0.65
1:A:383:ILE:HG22	1:A:533:TRP:HD1	1.62	0.64
1:A:557:ARG:HG2	1:A:1636:LEU:HD22	1.78	0.64
1:A:1339:ILE:HG23	1:A:2000:LEU:HD21	1.79	0.64
1:A:1638:LEU:HD23	1:A:1642:GLN:HB3	1.78	0.64
1:A:1362:LEU:HD21	1:A:1721:PHE:HB3	1.81	0.63
1:A:534:ALA:HB2	1:A:558:MET:HE2	1.79	0.63
1:A:1689:PHE:HE1	1:A:1695:PRO:HB3	1.63	0.63
1:A:1039:ARG:HH11	1:A:1039:ARG:HA	1.65	0.62
1:A:742:ARG:HB3	1:A:745:LEU:HB3	1.82	0.62
1:A:1991:CYS:HG	1:A:2054:SER:HG	1.48	0.61
1:A:1686:HIS:O	1:A:1690:ILE:HD12	2.00	0.61
1:A:1417:ARG:NH2	1:A:1426:ASP:OD2	2.32	0.61
1:A:989:THR:O	1:A:993:HIS:ND1	2.31	0.60
1:A:1766:ALA:HA	1:A:1769:VAL:HG12	1.83	0.60
1:A:547:GLU:HG2	1:A:548:LEU:H	1.66	0.60
1:A:597:GLN:O	1:A:601:GLU:HG2	2.01	0.60
1:A:1610:ASN:HA	1:A:1613:ILE:HD12	1.83	0.60
1:A:386:THR:HG21	1:A:538:PHE:H	1.67	0.59

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1680:ARG:NH1	1:A:1757:SER:O	2.35	0.59
1:A:1490:LYS:NZ	1:A:1492:ASN:OD1	2.36	0.59
1:A:554:TYR:OH	1:A:601:GLU:OE2	2.19	0.59
1:A:775:LEU:HD11	1:A:789:PHE:CE2	2.38	0.59
1:A:988:LEU:HD23	1:A:992:GLU:HG3	1.83	0.58
1:A:547:GLU:HG2	1:A:548:LEU:N	2.18	0.58
1:A:712:TYR:HB3	1:A:801:GLY:HA3	1.85	0.58
1:A:928:ILE:HG23	1:A:1099:ASP:H	1.68	0.58
1:A:1415:GLY:O	1:A:1615:ARG:NH2	2.36	0.58
1:A:613:LYS:HZ1	1:A:1586:THR:HA	1.69	0.58
1:A:636:MET:HE3	1:A:709:LEU:HD11	1.85	0.58
1:A:984:LEU:HD21	1:A:1041:LEU:HD22	1.84	0.58
1:A:1036:GLY:HA2	1:A:1063:VAL:HG23	1.84	0.58
1:A:1381:PRO:HD2	1:A:1383:MET:HE2	1.84	0.58
1:A:1458:ASN:HB3	1:A:1459:PRO:HD3	1.86	0.57
1:A:1060:THR:HB	1:A:1063:VAL:HG11	1.86	0.57
1:A:1423:PRO:HB2	1:A:1426:ASP:HB2	1.85	0.57
1:A:59:LYS:NZ	1:A:621:GLN:OE1	2.38	0.57
1:A:2081:ARG:HA	1:A:2084:TRP:HE3	1.69	0.57
1:A:613:LYS:HD2	1:A:615:THR:H	1.70	0.57
1:A:1474:LEU:HB3	1:A:1475:PRO:HD2	1.86	0.57
1:A:366:PRO:HA	1:A:369:ARG:HH12	1.70	0.56
1:A:612:GLU:OE1	1:A:614:LYS:NZ	2.37	0.56
1:A:1673:VAL:O	1:A:1677:ILE:HD12	2.06	0.56
1:A:633:LEU:HD21	1:A:798:GLU:HG2	1.88	0.56
1:A:937:ALA:HB1	1:A:1107:GLY:H	1.71	0.56
1:A:86:THR:HG22	1:A:88:GLY:H	1.71	0.56
1:A:282:ARG:HA	1:A:285:VAL:HG12	1.88	0.56
1:A:509:LYS:O	1:A:510:LEU:HD22	2.06	0.56
1:A:533:TRP:HE1	1:A:596:LEU:HD21	1.71	0.56
1:A:96:ASN:H	4:A:2301:NAG:H81	1.70	0.55
1:A:1222:PHE:HA	1:A:1225:ILE:HG12	1.88	0.55
1:A:931:PHE:CE2	1:A:939:LYS:HG2	2.42	0.55
1:A:1343:SER:HB2	1:A:1346:GLY:HA3	1.88	0.55
1:A:712:TYR:HH	1:A:1472:LYS:H	1.52	0.55
1:A:2072:THR:HG23	1:A:2075:MET:HG3	1.88	0.55
1:A:1555:ILE:HG23	1:A:1574:LEU:HD12	1.89	0.55
1:A:1746:GLY:HA2	1:A:1749:ILE:HG22	1.89	0.55
1:A:744:ASN:HD22	1:A:1762:ILE:HD11	1.70	0.54
1:A:1430:GLN:NE2	1:A:1492:ASN:O	2.39	0.54
1:A:2187:LEU:HD12	1:A:2191:PHE:HE2	1.72	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1339:ILE:HA	1:A:2000:LEU:HD11	1.88	0.54
1:A:57:PRO:HB2	1:A:76:ASN:HD22	1.71	0.54
1:A:385:TYR:CE2	1:A:396:MET:HE3	2.42	0.54
1:A:1119:LYS:HE3	1:A:1242:THR:HB	1.91	0.53
1:A:770:TYR:O	1:A:775:LEU:HB2	2.07	0.53
1:A:2007:VAL:HB	1:A:2060:ILE:HD13	1.89	0.53
1:A:271:GLU:O	1:A:275:MET:HE3	2.09	0.53
1:A:1336:ARG:NH2	1:A:1702:ASN:OD1	2.41	0.53
1:A:2197:SER:HB2	1:A:2200:ARG:HG2	1.90	0.53
1:A:651:SER:O	1:A:655:ILE:HG12	2.09	0.52
1:A:931:PHE:N	1:A:1086:LEU:O	2.43	0.52
1:A:71:GLN:HA	1:A:74:ILE:HG22	1.91	0.52
1:A:605:ILE:HG12	1:A:1614:LEU:HB2	1.91	0.52
1:A:1047:PHE:CE1	1:A:1054:VAL:HG11	2.45	0.52
1:A:767:TRP:O	1:A:768:GLN:HG3	2.09	0.52
1:A:601:GLU:OE1	1:A:1629:ILE:HG21	2.09	0.52
1:A:669:GLU:O	1:A:673:ILE:HG12	2.09	0.52
1:A:385:TYR:HB3	1:A:512:PRO:HA	1.91	0.52
1:A:598:ASP:HB2	1:A:1606:LEU:HD21	1.91	0.52
1:A:661:TYR:OH	1:A:986:ASP:OD2	2.26	0.52
1:A:889:GLU:HG2	1:A:1113:GLY:HA2	1.92	0.52
1:A:1607:ASN:O	1:A:1611:ASN:ND2	2.42	0.52
1:A:1680:ARG:NH1	1:A:1758:PHE:O	2.42	0.51
1:A:1706:ASP:OD2	1:A:1754:TYR:OH	2.17	0.51
1:A:994:ILE:HD12	1:A:1012:MET:HG2	1.91	0.51
1:A:1001:LYS:HD3	1:A:1049:GLY:HA3	1.91	0.51
1:A:1592:VAL:HG22	1:A:1609:ILE:HD12	1.93	0.51
1:A:1997:ILE:HG12	1:A:2053:LEU:HD22	1.93	0.51
1:A:55:HIS:NE2	1:A:1506:SER:OG	2.43	0.51
1:A:927:GLN:HA	1:A:1079:ARG:HH21	1.76	0.51
1:A:1382:TRP:HH2	1:A:1417:ARG:HH21	1.58	0.51
1:A:1406:ASN:O	1:A:1410:LYS:HG2	2.10	0.51
1:A:1237:TYR:O	1:A:2129:GLN:NE2	2.44	0.51
1:A:782:LEU:HD23	1:A:784:PRO:HD2	1.93	0.51
1:A:578:PRO:HB3	1:A:624:TYR:HB2	1.93	0.50
1:A:1516:ILE:HG13	1:A:1530:PHE:CE2	2.46	0.50
1:A:978:CYS:HB2	1:A:1046:ALA:HB2	1.94	0.50
1:A:1196:LEU:HD12	1:A:1206:TYR:HE1	1.76	0.50
1:A:1812:HIS:CE1	1:A:1815:LEU:H	2.30	0.50
1:A:576:PRO:HG3	1:A:1474:LEU:HD11	1.94	0.50
1:A:31:TRP:HD1	1:A:647:ALA:HA	1.76	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:MET:HA	1:A:643:PHE:CZ	2.47	0.49
1:A:640:MET:HE2	1:A:791:CYS:SG	2.52	0.49
1:A:377:PRO:HB2	1:A:533:TRP:CZ3	2.47	0.49
1:A:1025:LYS:HZ2	1:A:1037:MET:HG2	1.77	0.49
1:A:641:PRO:O	1:A:645:THR:OG1	2.20	0.49
1:A:1611:ASN:OD1	1:A:1629:ILE:N	2.37	0.49
1:A:1093:GLU:HG3	1:A:1097:LEU:HD13	1.94	0.49
1:A:1717:VAL:O	1:A:1720:ILE:HG22	2.13	0.49
1:A:396:MET:HG2	1:A:510:LEU:HD12	1.95	0.49
1:A:1335:LYS:HB2	1:A:2009:PHE:CE1	2.48	0.49
1:A:534:ALA:HB3	1:A:596:LEU:HG	1.95	0.48
1:A:1507:ASP:OD1	2:B:1:NAG:H61	2.12	0.48
1:A:2143:VAL:HG21	1:A:2203:ILE:HD12	1.94	0.48
1:A:619:MET:HB3	1:A:1594:PHE:HE1	1.79	0.48
1:A:1379:LEU:HD23	1:A:1381:PRO:HG3	1.96	0.48
1:A:1359:CYS:SG	1:A:1720:ILE:HD11	2.53	0.48
1:A:1436:TRP:CZ3	1:A:1499:ASP:HB2	2.49	0.48
1:A:1663:PHE:CD1	1:A:1775:LEU:HD21	2.42	0.48
1:A:536:ILE:HD11	1:A:596:LEU:HD12	1.95	0.48
1:A:940:THR:O	1:A:944:SER:OG	2.23	0.48
1:A:1190:HIS:HB2	1:A:1221:LEU:HD12	1.95	0.48
1:A:1556:LYS:HD3	1:A:1559:LYS:HD3	1.94	0.48
1:A:1674:VAL:HG11	1:A:1767:TYR:HB2	1.96	0.48
1:A:391:ALA:HB2	1:A:547:GLU:HA	1.96	0.48
1:A:50:GLU:HG3	1:A:628:VAL:HG23	1.96	0.48
1:A:944:SER:HB3	1:A:949:LEU:HB2	1.95	0.48
1:A:378:LEU:O	1:A:509:LYS:NZ	2.47	0.48
1:A:385:TYR:CE1	1:A:392:THR:HG22	2.49	0.48
1:A:646:LEU:HA	1:A:649:ILE:HD12	1.95	0.48
1:A:553:LYS:HG2	1:A:1630:THR:OG1	2.14	0.48
1:A:609:THR:HG21	1:A:1617:ASN:HB3	1.96	0.48
1:A:640:MET:N	1:A:641:PRO:HD2	2.29	0.48
1:A:2138:GLY:HA3	1:A:2181:PRO:HA	1.95	0.48
1:A:1001:LYS:NZ	1:A:1048:VAL:O	2.33	0.47
1:A:1013:GLU:O	1:A:1017:LEU:HG	2.15	0.47
1:A:1592:VAL:HG22	1:A:1609:ILE:CD1	2.45	0.47
1:A:1656:LEU:O	1:A:1659:ILE:HG22	2.14	0.47
1:A:372:TRP:CH2	1:A:376:LYS:HD3	2.50	0.47
1:A:1607:ASN:HD21	1:A:1630:THR:HA	1.78	0.47
1:A:376:LYS:HB3	1:A:377:PRO:HD3	1.97	0.47
1:A:938:GLY:C	1:A:940:THR:H	2.23	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2129:GLN:HG2	1:A:2132:LYS:HE3	1.96	0.47
3:C:2:NAG:O7	3:C:2:NAG:O4	2.20	0.47
1:A:1055:ILE:HA	1:A:1085:ILE:HB	1.96	0.47
1:A:579:ARG:NH2	1:A:585:ASP:OD1	2.48	0.47
1:A:1590:VAL:HG21	1:A:1609:ILE:HG21	1.96	0.47
1:A:1670:ALA:HA	1:A:1673:VAL:HG12	1.97	0.47
1:A:1200:ILE:HG22	1:A:1203:GLU:HB2	1.96	0.47
1:A:1474:LEU:HB3	1:A:1475:PRO:CD	2.45	0.47
1:A:53:GLU:HG3	1:A:625:PRO:HA	1.96	0.46
1:A:1058:GLU:HB3	1:A:1088:THR:HA	1.97	0.46
1:A:141:ASN:HA	1:A:146:ASP:HA	1.97	0.46
1:A:620:GLN:OE1	1:A:621:GLN:N	2.48	0.46
1:A:1484:LEU:HG	1:A:1485:PRO:HD3	1.97	0.46
1:A:297:SER:OG	1:A:298:THR:N	2.48	0.46
1:A:752:ILE:HD12	6:A:2305:CLR:H122	1.70	0.46
1:A:1037:MET:HE2	1:A:1037:MET:HA	1.97	0.46
1:A:1058:GLU:N	1:A:1087:SER:O	2.45	0.46
1:A:1673:VAL:HG11	1:A:1770:LEU:HD12	1.98	0.46
1:A:1119:LYS:NZ	1:A:1241:GLU:HB3	2.30	0.46
1:A:1512:THR:HG23	1:A:1531:ARG:HH12	1.81	0.46
1:A:1824:LYS:HD3	1:A:1824:LYS:C	2.40	0.46
1:A:628:VAL:HG12	1:A:1474:LEU:HA	1.98	0.46
1:A:516:GLU:O	1:A:520:ILE:HG12	2.16	0.46
1:A:383:ILE:HG12	1:A:509:LYS:O	2.16	0.46
1:A:492:ASN:OD1	1:A:496:ARG:NH2	2.49	0.46
1:A:740:PHE:HE2	1:A:749:CYS:HB3	1.81	0.46
1:A:1529:GLU:HG3	1:A:1597:LYS:HG2	1.97	0.46
1:A:534:ALA:HA	1:A:558:MET:HG3	1.99	0.45
1:A:1819:LEU:O	1:A:1823:VAL:HG23	2.17	0.45
1:A:43:ARG:NH1	1:A:633:LEU:HB2	2.31	0.45
1:A:379:LEU:HB2	1:A:505:VAL:HG13	1.98	0.45
1:A:1077:LYS:HA	1:A:1077:LYS:HD2	1.88	0.45
1:A:1191:VAL:HG22	1:A:1193:GLU:H	1.81	0.45
1:A:1659:ILE:HA	1:A:1662:ILE:HG22	1.99	0.45
1:A:999:ARG:HH12	1:A:1005:GLU:HG3	1.81	0.45
1:A:282:ARG:HE	1:A:286:MET:HE1	1.81	0.45
1:A:611:THR:HB	1:A:614:LYS:HD3	1.98	0.45
1:A:922:ASN:O	1:A:1100:ARG:NH2	2.50	0.45
1:A:385:TYR:CZ	1:A:396:MET:HE3	2.51	0.45
1:A:928:ILE:HD11	1:A:1086:LEU:HD23	1.99	0.45
1:A:774:THR:HA	1:A:777:ILE:HD12	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1528:ASN:OD1	1:A:1528:ASN:N	2.50	0.45
1:A:388:ASP:OD1	1:A:388:ASP:N	2.50	0.44
1:A:1120:ASN:ND2	1:A:2205:ASP:OD1	2.50	0.44
1:A:2080:ARG:HG3	1:A:2084:TRP:CZ3	2.52	0.44
1:A:1338:LEU:HD13	1:A:2005:GLU:HG2	1.99	0.44
1:A:1380:GLN:HB3	1:A:1604:SER:HA	1.99	0.44
1:A:386:THR:HG21	1:A:538:PHE:N	2.32	0.44
1:A:541:ILE:HG23	1:A:542:THR:H	1.80	0.44
1:A:932:LEU:HB3	1:A:1248:PHE:HE2	1.83	0.44
1:A:636:MET:O	1:A:640:MET:N	2.50	0.44
1:A:727:VAL:O	1:A:730:ILE:HG22	2.18	0.44
1:A:1335:LYS:NZ	1:A:1998:THR:HG21	2.33	0.44
1:A:1130:LEU:HD13	1:A:1237:TYR:HB3	1.98	0.44
1:A:2002:THR:O	1:A:2006:HIS:ND1	2.43	0.44
1:A:1037:MET:HE1	1:A:1040:LYS:HD3	1.98	0.44
1:A:2187:LEU:HA	1:A:2190:ILE:HD13	2.00	0.44
1:A:2077:PRO:HB3	1:A:2080:ARG:NH1	2.33	0.44
1:A:96:ASN:N	4:A:2301:NAG:H81	2.33	0.43
1:A:377:PRO:HB2	1:A:533:TRP:HZ3	1.84	0.43
1:A:409:PHE:HB2	1:A:502:MET:HE3	2.00	0.43
1:A:1045:LEU:O	1:A:1048:VAL:HG22	2.18	0.43
1:A:1456:MET:SD	1:A:1456:MET:N	2.90	0.43
1:A:2141:ILE:CG1	1:A:2178:TYR:HB2	2.48	0.43
1:A:13:LYS:HG3	1:A:14:ASN:N	2.33	0.43
1:A:566:THR:OG1	1:A:1374:TYR:O	2.36	0.43
1:A:1124:THR:HG22	1:A:1125:GLY:H	1.83	0.43
1:A:1362:LEU:HD23	1:A:1724:PHE:HD2	1.84	0.43
1:A:2002:THR:HG23	1:A:2005:GLU:H	1.82	0.43
1:A:426:PHE:O	1:A:430:SER:HB3	2.18	0.43
1:A:619:MET:HB3	1:A:1594:PHE:CE1	2.53	0.43
1:A:1430:GLN:OE1	1:A:1493:THR:OG1	2.37	0.43
1:A:1434:GLU:HA	1:A:1490:LYS:HE2	2.00	0.43
1:A:2034:LEU:HD11	1:A:2052:LYS:HB3	2.01	0.43
1:A:43:ARG:HH12	1:A:633:LEU:HB2	1.84	0.43
1:A:575:ASP:OD1	1:A:576:PRO:HD2	2.19	0.43
1:A:762:VAL:O	1:A:765:VAL:HG12	2.19	0.43
1:A:1218:PHE:CZ	1:A:1222:PHE:HE1	2.37	0.43
1:A:2132:LYS:HZ3	1:A:2210:GLN:HG3	1.84	0.43
1:A:2137:ASP:HB3	1:A:2179:GLN:NE2	2.34	0.43
1:A:613:LYS:NZ	1:A:1586:THR:HA	2.34	0.43
1:A:906:LYS:HD3	1:A:945:ILE:HD11	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1388:TYR:HE2	1:A:1498:GLN:NE2	2.16	0.43
1:A:2187:LEU:HD23	1:A:2187:LEU:H	1.84	0.43
1:A:656:ILE:O	1:A:660:VAL:HG22	2.19	0.43
1:A:755:PHE:O	1:A:759:LEU:HG	2.18	0.43
1:A:1388:TYR:HB3	1:A:1496:ILE:H	1.84	0.43
1:A:1594:PHE:CD2	1:A:1602:ILE:HG12	2.53	0.43
1:A:2128:VAL:HG23	1:A:2213:LEU:HD13	2.00	0.43
1:A:671:MET:HE1	1:A:676:LEU:HD12	2.00	0.43
1:A:906:LYS:O	1:A:917:ASP:N	2.52	0.42
1:A:1829:ALA:O	1:A:1832:LEU:HG	2.18	0.42
1:A:689:SER:O	1:A:693:LEU:HD23	2.19	0.42
1:A:2075:MET:SD	1:A:2080:ARG:HB3	2.59	0.42
1:A:560:ILE:HD13	1:A:560:ILE:HA	1.92	0.42
1:A:659:ILE:O	1:A:662:GLU:HG3	2.19	0.42
1:A:1127:TYR:HB2	1:A:1240:SER:O	2.20	0.42
1:A:384:LEU:HD13	1:A:519:LEU:HD11	2.00	0.42
1:A:674:MET:HE2	1:A:674:MET:HB3	1.98	0.42
1:A:759:LEU:N	1:A:760:PRO:HD2	2.35	0.42
1:A:1750:THR:OG1	1:A:1751:PRO:HD3	2.19	0.42
1:A:134:GLN:NE2	1:A:135:ILE:HG13	2.34	0.42
1:A:2104:MET:HG3	1:A:2214:ASP:HA	2.01	0.42
1:A:1025:LYS:HB2	1:A:1028:SER:HB2	2.02	0.42
1:A:1069:ARG:HG3	1:A:2218:VAL:HG11	2.01	0.42
1:A:27:LEU:HD22	1:A:650:TYR:CZ	2.54	0.42
1:A:634:ARG:O	1:A:638:ARG:HG2	2.19	0.42
1:A:671:MET:HE3	1:A:671:MET:HB3	1.90	0.42
1:A:782:LEU:HD22	1:A:785:VAL:HG13	2.01	0.42
1:A:989:THR:HG22	1:A:1029:LYS:HD3	2.01	0.42
1:A:381:GLY:HA3	1:A:533:TRP:HB2	2.02	0.42
1:A:520:ILE:O	1:A:523:SER:OG	2.20	0.42
1:A:40:ILE:HD11	1:A:709:LEU:HD22	2.02	0.42
1:A:108:ASP:OD1	1:A:111:ARG:NH2	2.48	0.42
1:A:917:ASP:N	1:A:917:ASP:OD1	2.50	0.42
1:A:1241:GLU:CD	1:A:2209:SER:HB3	2.45	0.42
1:A:396:MET:HA	1:A:399:VAL:HG12	2.02	0.41
1:A:664:GLU:HA	1:A:664:GLU:OE1	2.20	0.41
1:A:670:THR:HG22	1:A:979:PRO:HG3	2.02	0.41
1:A:56:PHE:O	1:A:620:GLN:NE2	2.53	0.41
1:A:362:LEU:HD22	1:A:372:TRP:CE3	2.55	0.41
1:A:592:GLY:O	1:A:596:LEU:HD23	2.21	0.41
1:A:59:LYS:HB2	1:A:619:MET:HB2	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1651:THR:O	1:A:1655:VAL:HG23	2.21	0.41
1:A:2000:LEU:HD12	1:A:2001:LEU:HD12	2.03	0.41
1:A:2032:LEU:HD12	1:A:2052:LYS:HG2	2.01	0.41
1:A:712:TYR:HE2	1:A:1471:LYS:HE2	1.85	0.41
1:A:1404:LEU:HD22	1:A:1537:LEU:HD21	2.02	0.41
1:A:2028:ALA:HA	1:A:2031:LYS:HZ3	1.85	0.41
1:A:125:MET:HE1	1:A:261:LEU:CB	2.51	0.41
1:A:522:LYS:HD3	1:A:522:LYS:HA	1.96	0.41
1:A:1611:ASN:O	1:A:1615:ARG:HG3	2.21	0.41
1:A:2064:PRO:HA	1:A:2095:ARG:HD2	2.02	0.41
1:A:2134:ARG:HG3	1:A:2135:PHE:N	2.34	0.41
1:A:652:VAL:HG23	1:A:733:CYS:HB2	2.02	0.41
1:A:712:TYR:HH	1:A:1472:LYS:N	2.19	0.41
1:A:69:TRP:O	1:A:73:ILE:HG12	2.20	0.41
1:A:279:SER:HA	1:A:282:ARG:HG2	2.03	0.41
1:A:692:PRO:HA	1:A:695:VAL:HG12	2.03	0.41
1:A:1338:LEU:CD1	1:A:2005:GLU:HG2	2.51	0.41
1:A:1339:ILE:HD12	1:A:1339:ILE:H	1.85	0.41
1:A:731:LEU:HA	1:A:731:LEU:HD23	1.80	0.41
1:A:1082:ARG:HB2	1:A:1084:ILE:HD11	2.03	0.41
1:A:1092:ASP:OD1	1:A:1092:ASP:N	2.54	0.41
1:A:1388:TYR:CB	1:A:1496:ILE:H	2.34	0.41
1:A:1401:THR:HG23	1:A:1537:LEU:HD23	2.03	0.41
1:A:1640:LYS:NZ	1:A:1837:GLU:OE2	2.41	0.41
1:A:1817:ARG:NH2	1:A:1854:PHE:HA	2.36	0.41
1:A:580:ALA:HA	1:A:586:MET:HE3	2.03	0.40
1:A:1379:LEU:HD13	1:A:1632:PHE:HE1	1.86	0.40
1:A:1694:LYS:O	1:A:1697:ILE:HG22	2.21	0.40
1:A:110:ARG:HD2	1:A:1545:LEU:HD12	2.03	0.40
1:A:379:LEU:HD12	1:A:505:VAL:HG22	2.02	0.40
1:A:619:MET:SD	1:A:1592:VAL:HB	2.62	0.40
1:A:1204:LEU:HD21	1:A:1206:TYR:CZ	2.56	0.40
1:A:2039:GLU:O	1:A:2040:LYS:HD3	2.21	0.40
1:A:352:THR:N	1:A:353:PRO:HD2	2.36	0.40
1:A:1535:PHE:CG	1:A:1609:ILE:HD11	2.55	0.40
1:A:59:LYS:N	1:A:619:MET:O	2.47	0.40
1:A:574:TRP:NE1	1:A:1529:GLU:OE2	2.55	0.40
1:A:1222:PHE:HD2	1:A:1225:ILE:HD11	1.87	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	1807/2305 (78%)	1692 (94%)	115 (6%)	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	1390/2027 (69%)	1390 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	361	ASN
1	A	1406	ASN
1	A	1686	HIS
1	A	1734	ASN
1	A	2129	GLN
1	A	2179	GLN
1	A	2202	HIS

### 5.3.3 RNA

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

7 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	$\# Z  > 2$
2	NAG	B	1	1,2	14,14,15	0.35	0	17,19,21	0.42	0
2	NAG	B	2	2	14,14,15	0.32	0	17,19,21	0.61	0
2	BMA	B	3	2	11,11,12	1.65	3 (27%)	15,15,17	1.81	2 (13%)
2	MAN	B	4	2	11,11,12	0.60	0	15,15,17	1.08	2 (13%)
2	MAN	B	5	2	11,11,12	0.65	0	15,15,17	0.97	2 (13%)
3	NAG	C	1	1,3	14,14,15	0.19	0	17,19,21	0.46	0
3	NAG	C	2	3	14,14,15	0.58	0	17,19,21	0.79	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
2	NAG	B	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1
2	MAN	B	5	2	-	0/2/19/22	0/1/1/1
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	BMA	C4-C3	2.96	1.60	1.52
2	B	3	BMA	O2-C2	2.66	1.48	1.43
2	B	3	BMA	C6-C5	2.55	1.60	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	BMA	C3-C4-C5	4.63	118.62	110.23
2	B	4	MAN	C1-O5-C5	2.94	116.12	112.19
2	B	3	BMA	O5-C5-C6	-2.66	102.49	107.66
2	B	5	MAN	C1-O5-C5	2.38	115.37	112.19
2	B	4	MAN	O2-C2-C3	-2.23	105.54	110.15
2	B	5	MAN	O2-C2-C3	-2.11	105.78	110.15

There are no chirality outliers.

All (14) torsion outliers are listed below:

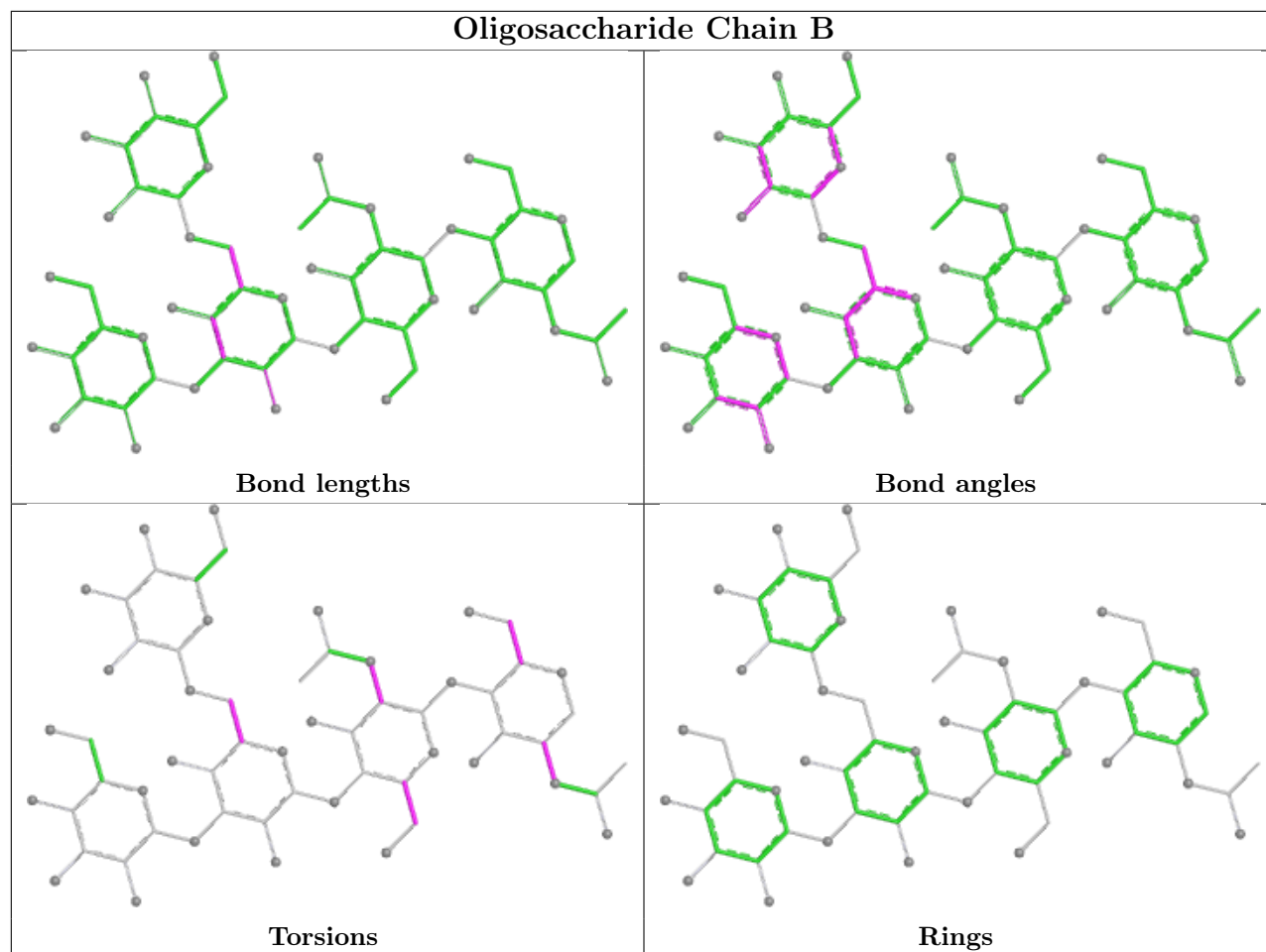
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
3	C	2	NAG	C1-C2-N2-C7
2	B	2	NAG	C3-C2-N2-C7
3	C	2	NAG	C3-C2-N2-C7
3	C	2	NAG	C4-C5-C6-O6
2	B	2	NAG	C1-C2-N2-C7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

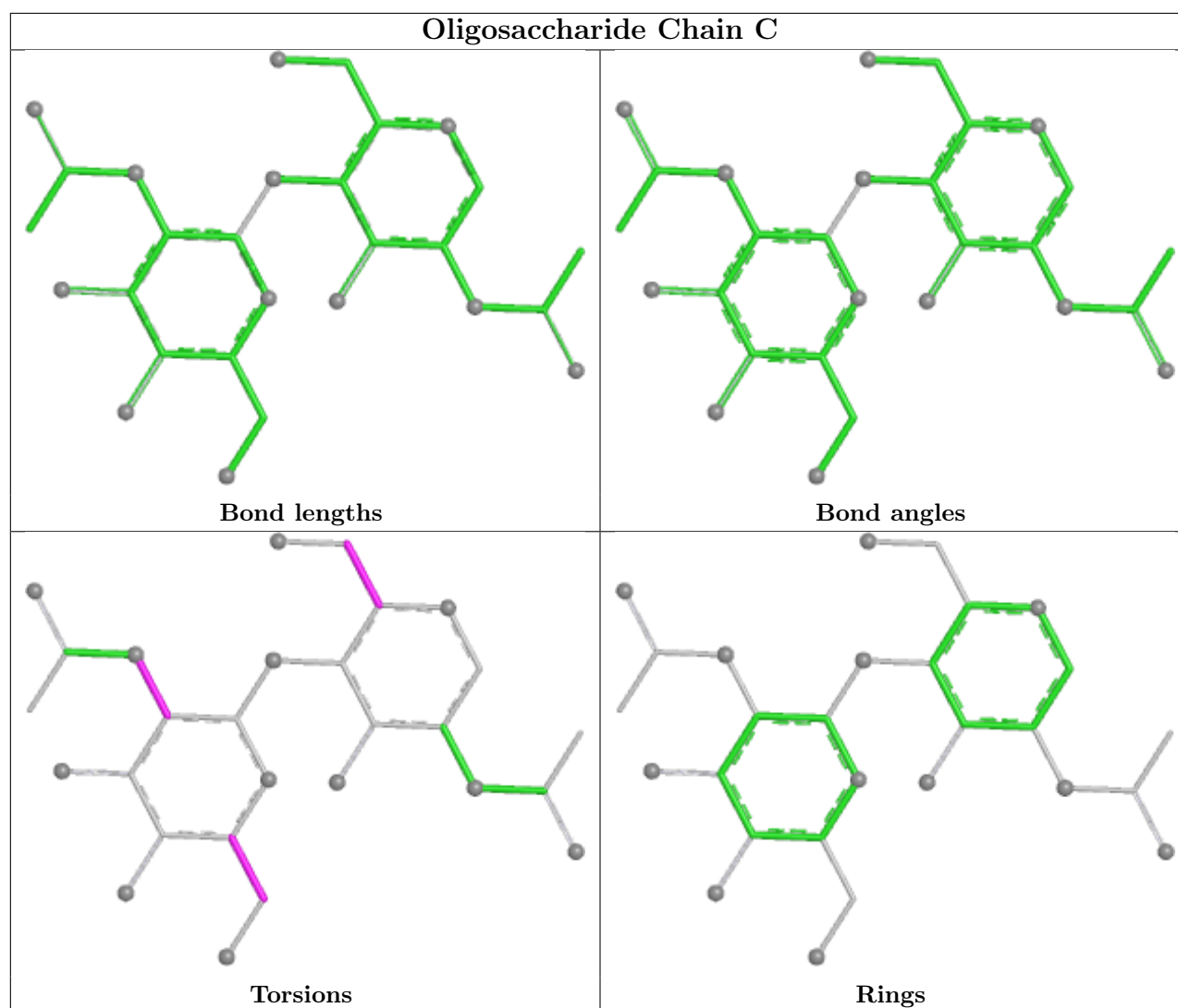
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	1	0
3	C	2	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 [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	A	2302	1	14,14,15	0.93	1 (7%)	17,19,21	1.09	1 (5%)
5	POV	A	2304	-	10,10,51	0.37	0	9,9,59	0.45	0
4	NAG	A	2303	1	14,14,15	0.82	1 (7%)	17,19,21	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	CLR	A	2306	-	24,24,31	1.17	2 (8%)	38,39,48	1.21	4 (10%)
4	NAG	A	2301	1	14,14,15	0.26	0	17,19,21	0.46	0
6	CLR	A	2305	-	24,24,31	1.16	3 (12%)	38,39,48	1.17	2 (5%)

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
4	NAG	A	2302	1	-	4/6/23/26	0/1/1/1
5	POV	A	2304	-	-	3/8/8/55	-
4	NAG	A	2303	1	-	1/6/23/26	0/1/1/1
6	CLR	A	2306	-	-	-	0/4/4/4
4	NAG	A	2301	1	-	2/6/23/26	0/1/1/1
6	CLR	A	2305	-	-	-	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2302	NAG	O5-C1	3.02	1.48	1.43
4	A	2303	NAG	O5-C1	-2.89	1.38	1.43
6	A	2305	CLR	C16-C17	2.29	1.58	1.53
6	A	2306	CLR	C16-C17	2.27	1.58	1.53
6	A	2305	CLR	C18-C13	-2.26	1.50	1.54
6	A	2306	CLR	C18-C13	-2.24	1.50	1.54
6	A	2305	CLR	C7-C6	2.09	1.54	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2302	NAG	C1-O5-C5	3.89	117.40	112.19
6	A	2305	CLR	C18-C13-C12	2.44	114.20	110.61
6	A	2306	CLR	C18-C13-C12	2.40	114.14	110.61
6	A	2306	CLR	C10-C5-C6	2.20	126.14	122.93
6	A	2305	CLR	C19-C10-C9	-2.15	109.25	111.66
6	A	2306	CLR	C12-C13-C14	-2.06	104.16	107.25
6	A	2306	CLR	C20-C17-C16	-2.01	109.23	113.75

There are no chirality outliers.

All (10) torsion outliers are listed below:

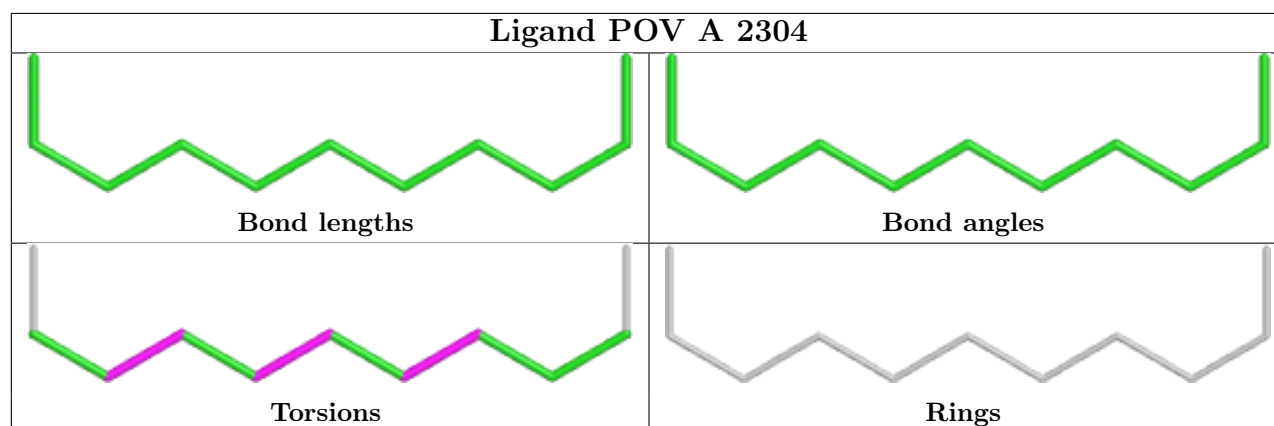
Mol	Chain	Res	Type	Atoms
4	A	2301	NAG	O5-C5-C6-O6
4	A	2301	NAG	C4-C5-C6-O6
4	A	2302	NAG	C4-C5-C6-O6
4	A	2303	NAG	O5-C5-C6-O6
4	A	2302	NAG	O5-C5-C6-O6
5	A	2304	POV	C27-C28-C29-C210
4	A	2302	NAG	C1-C2-N2-C7
5	A	2304	POV	C25-C26-C27-C28
4	A	2302	NAG	C3-C2-N2-C7
5	A	2304	POV	C23-C24-C25-C26

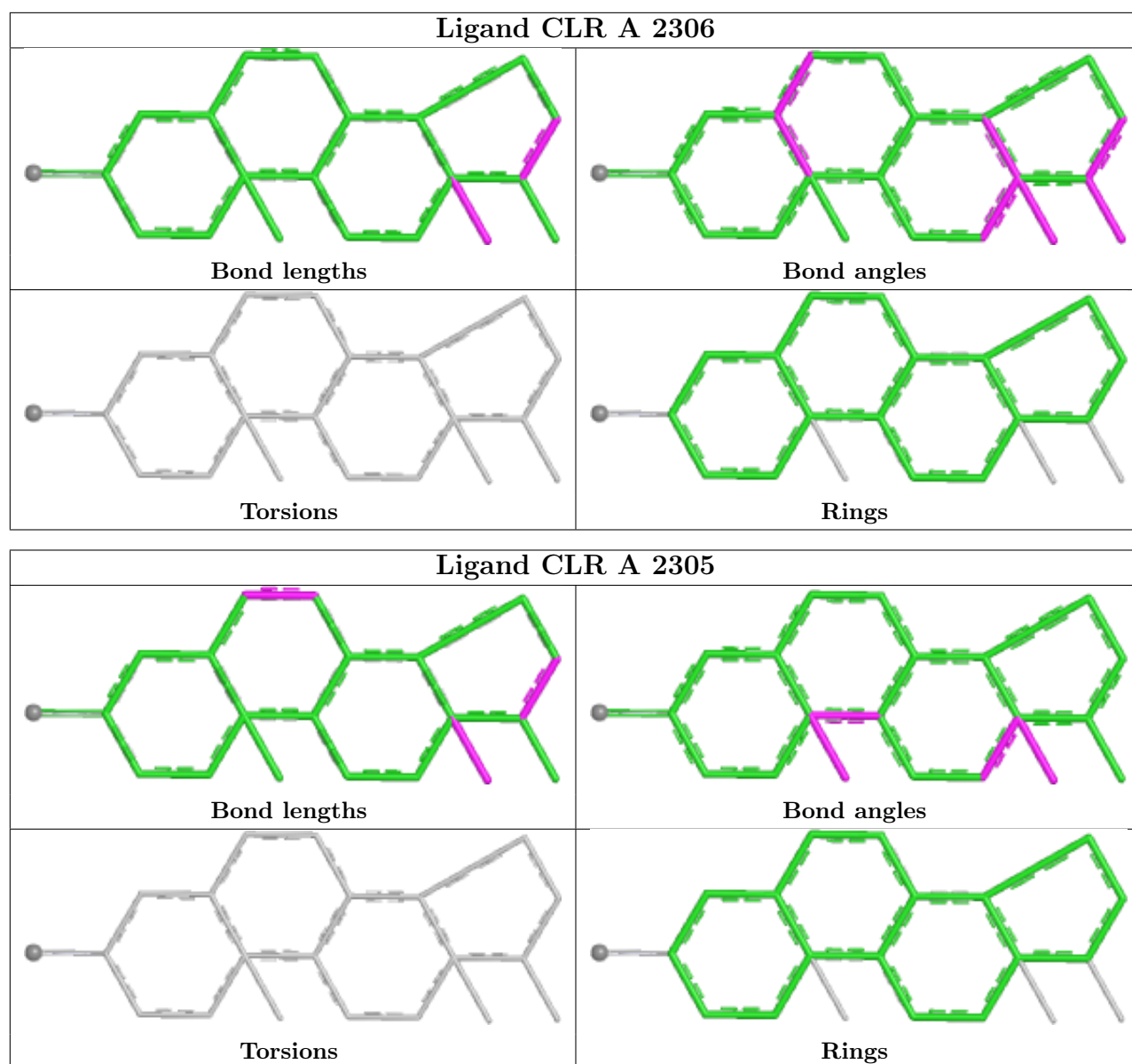
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2301	NAG	2	0
6	A	2305	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.

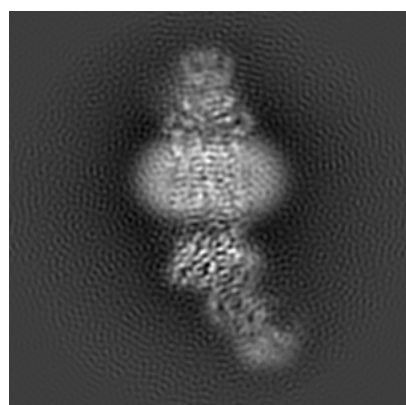
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6724. These allow visual inspection of the internal detail of the map and identification of artifacts.

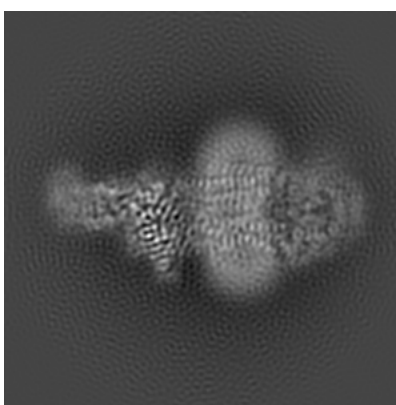
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

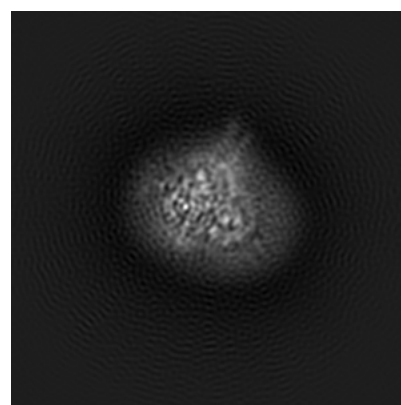
#### 6.1.1 Primary map



X



Y

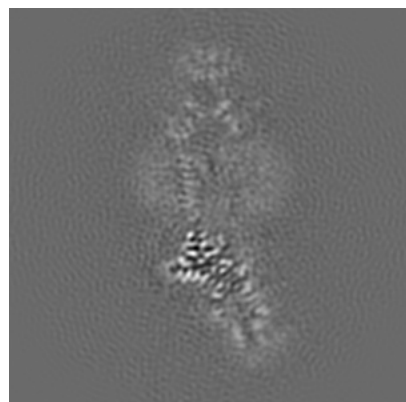


Z

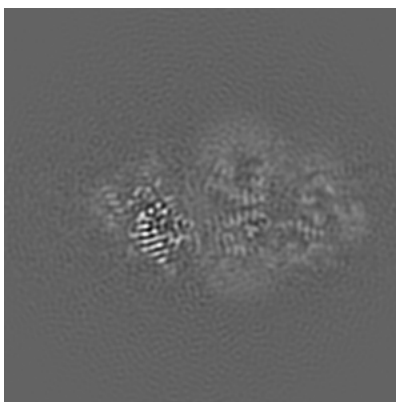
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

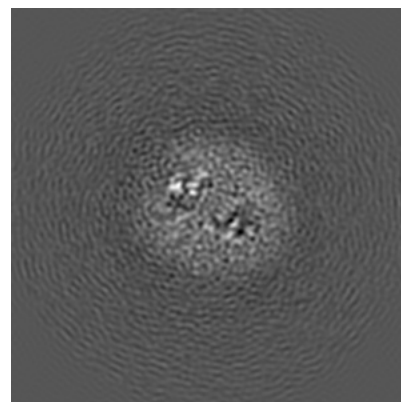
#### 6.2.1 Primary map



X Index: 100



Y Index: 100

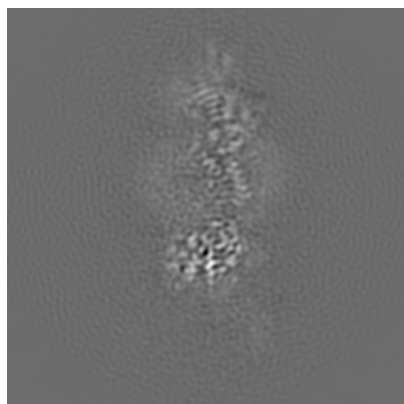


Z Index: 100

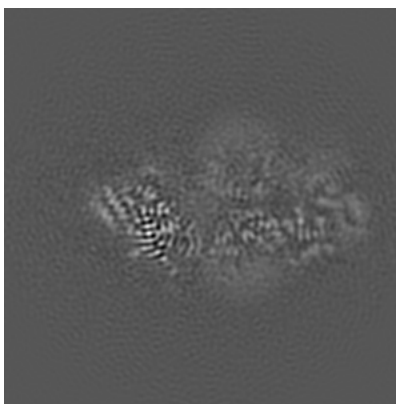
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

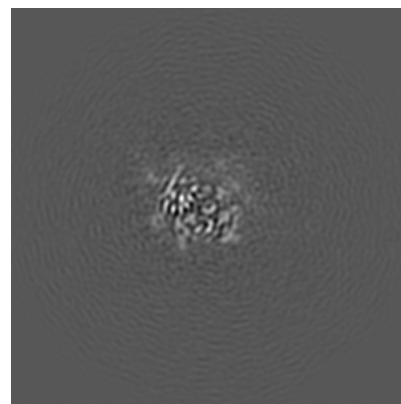
### 6.3.1 Primary map



X Index: 87



Y Index: 102

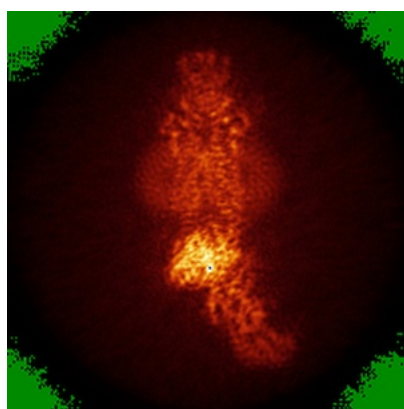


Z Index: 76

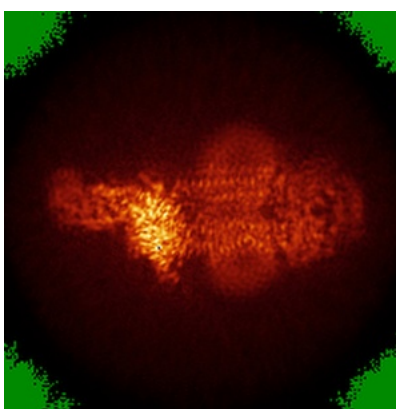
The images above show the largest variance slices of the map in three orthogonal directions.

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

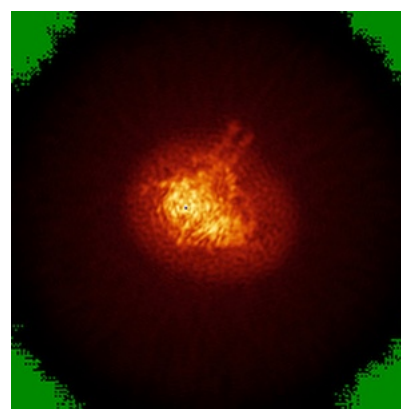
### 6.4.1 Primary map



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 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

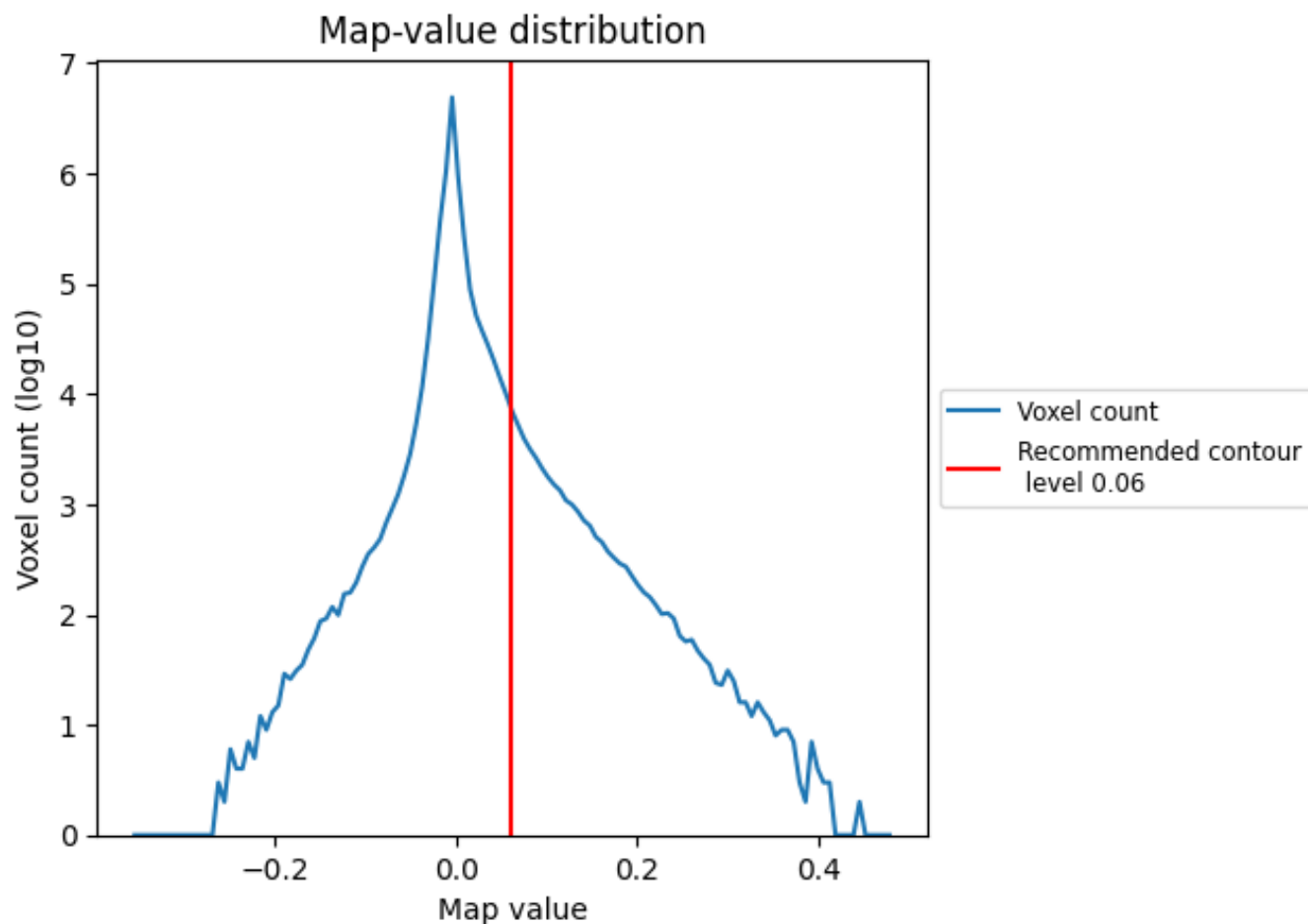
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

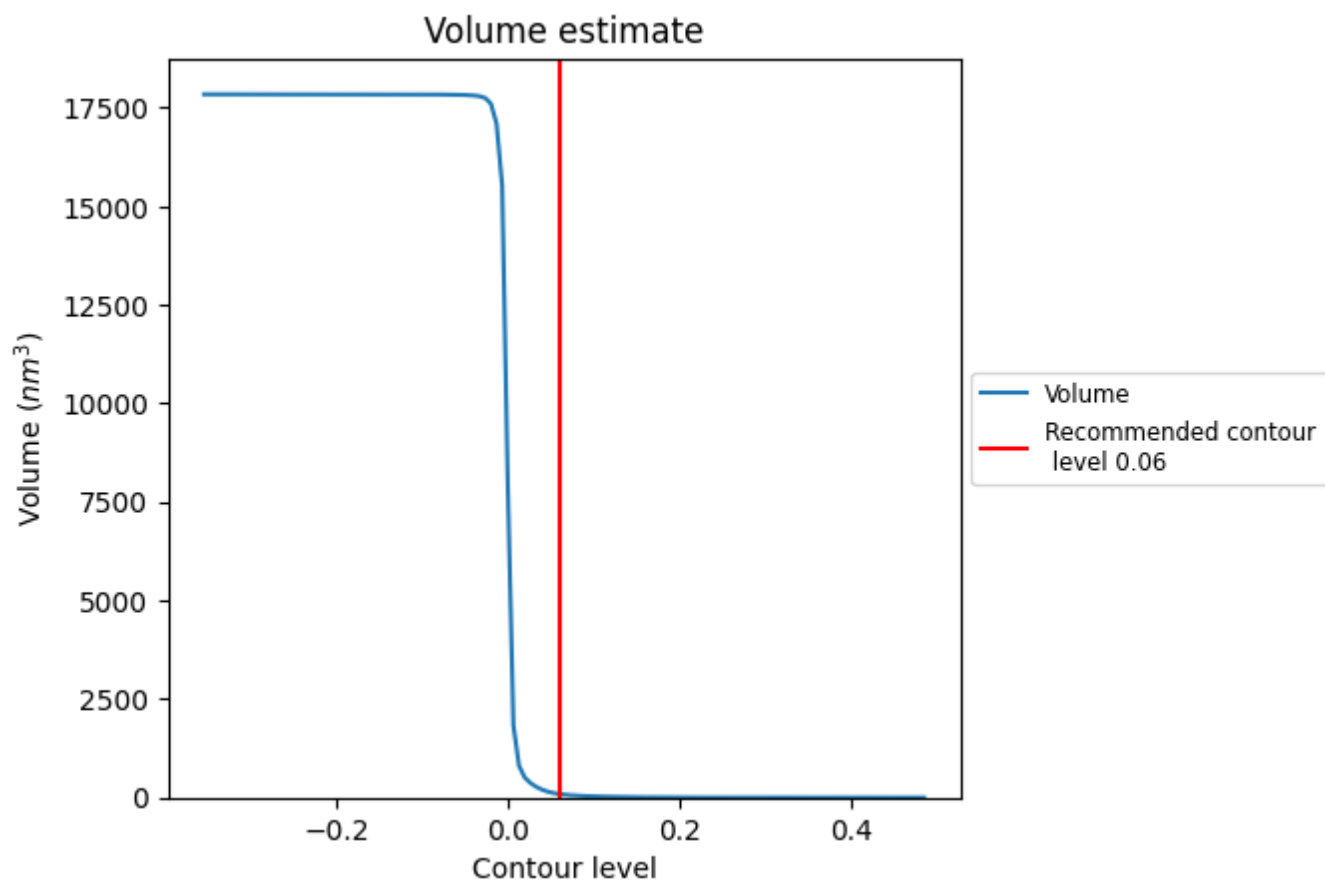
This section contains the results of statistical analysis of the map.

### 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.

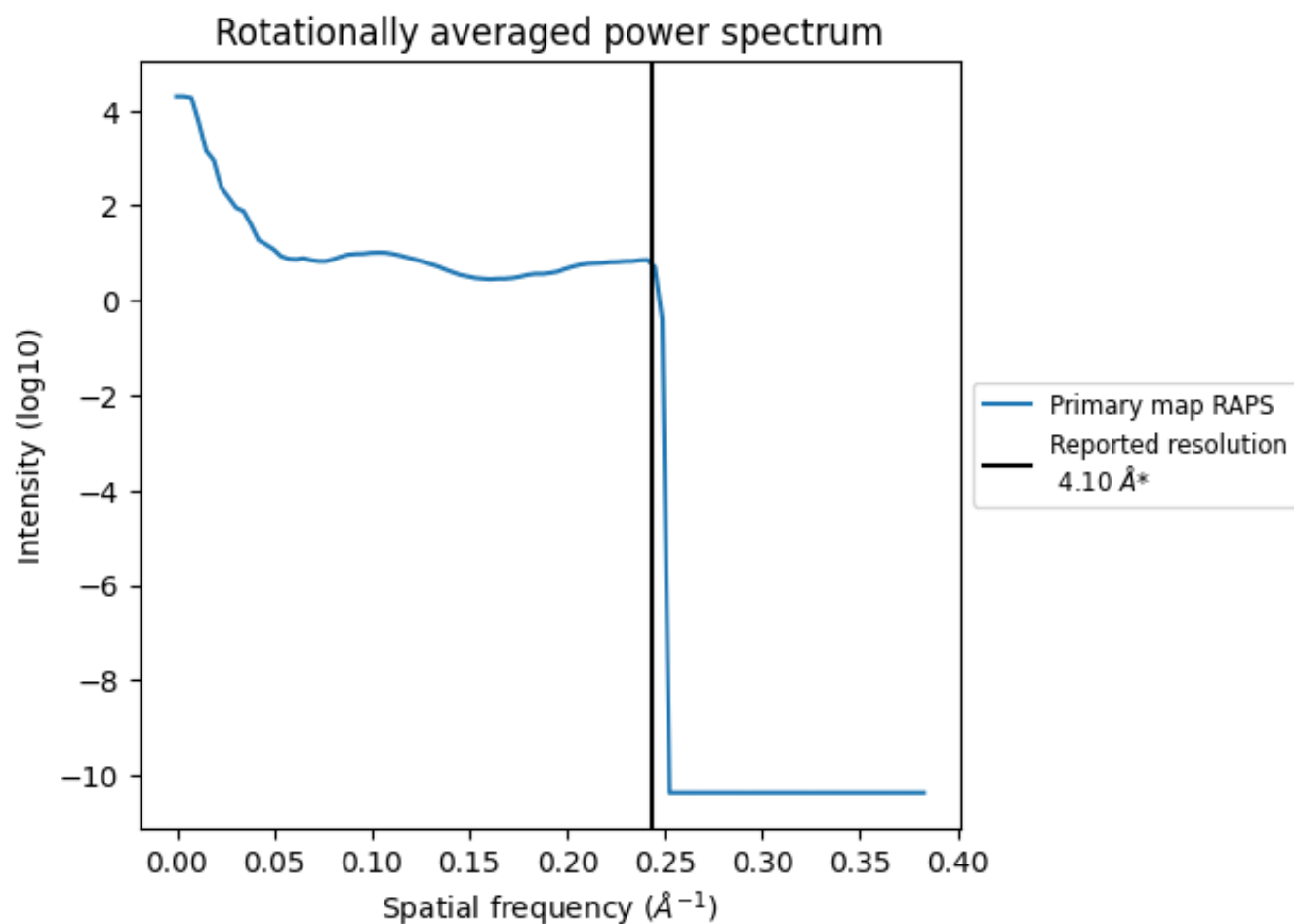
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 89 nm<sup>3</sup>; this corresponds to an approximate mass of 81 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 0.244 Å<sup>-1</sup>

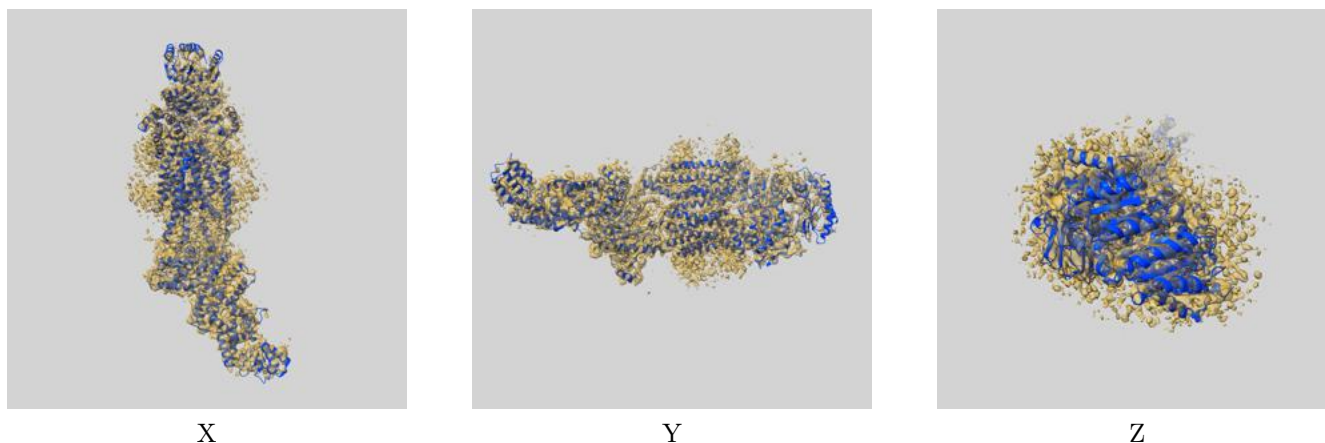
## 8 Fourier-Shell correlation ⓘ

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

## 9 Map-model fit [i](#)

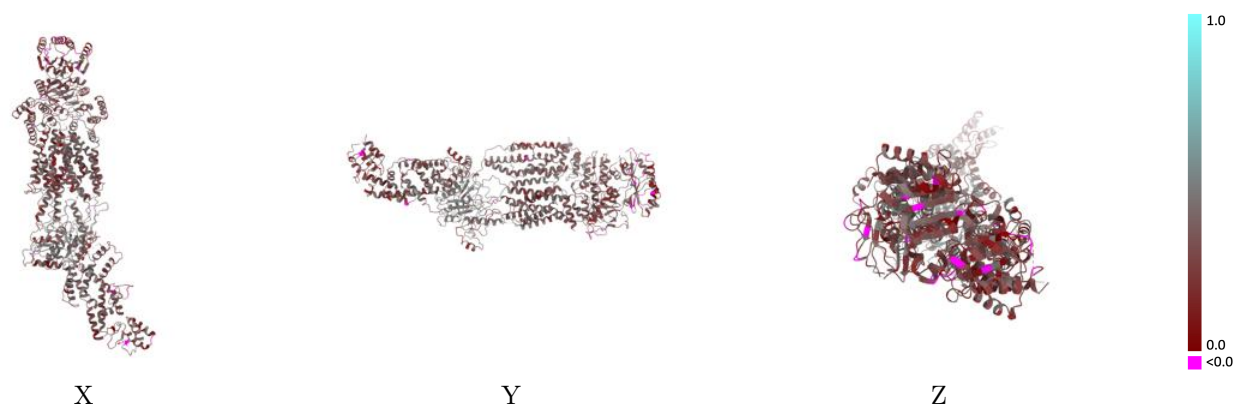
This section contains information regarding the fit between EMDB map EMD-6724 and PDB model 7ROQ. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

### 9.1 Map-model overlay [i](#)



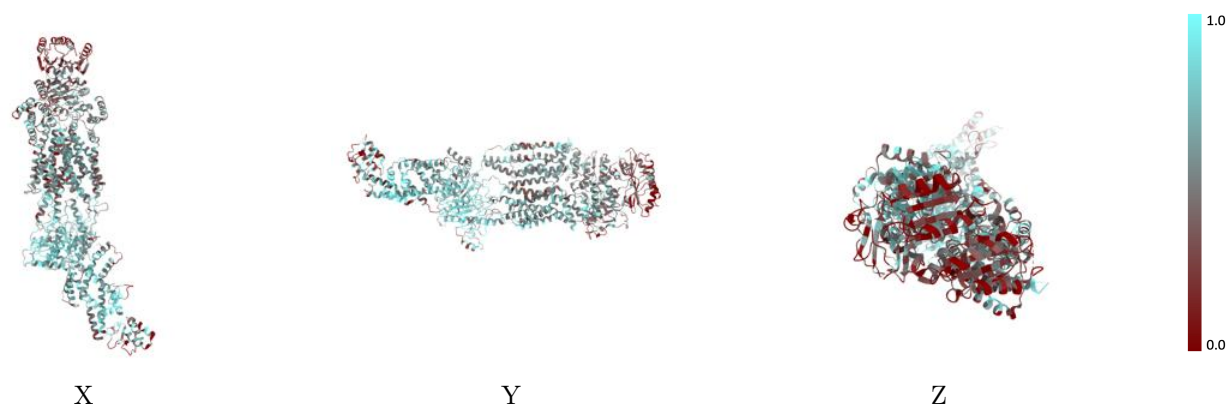
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



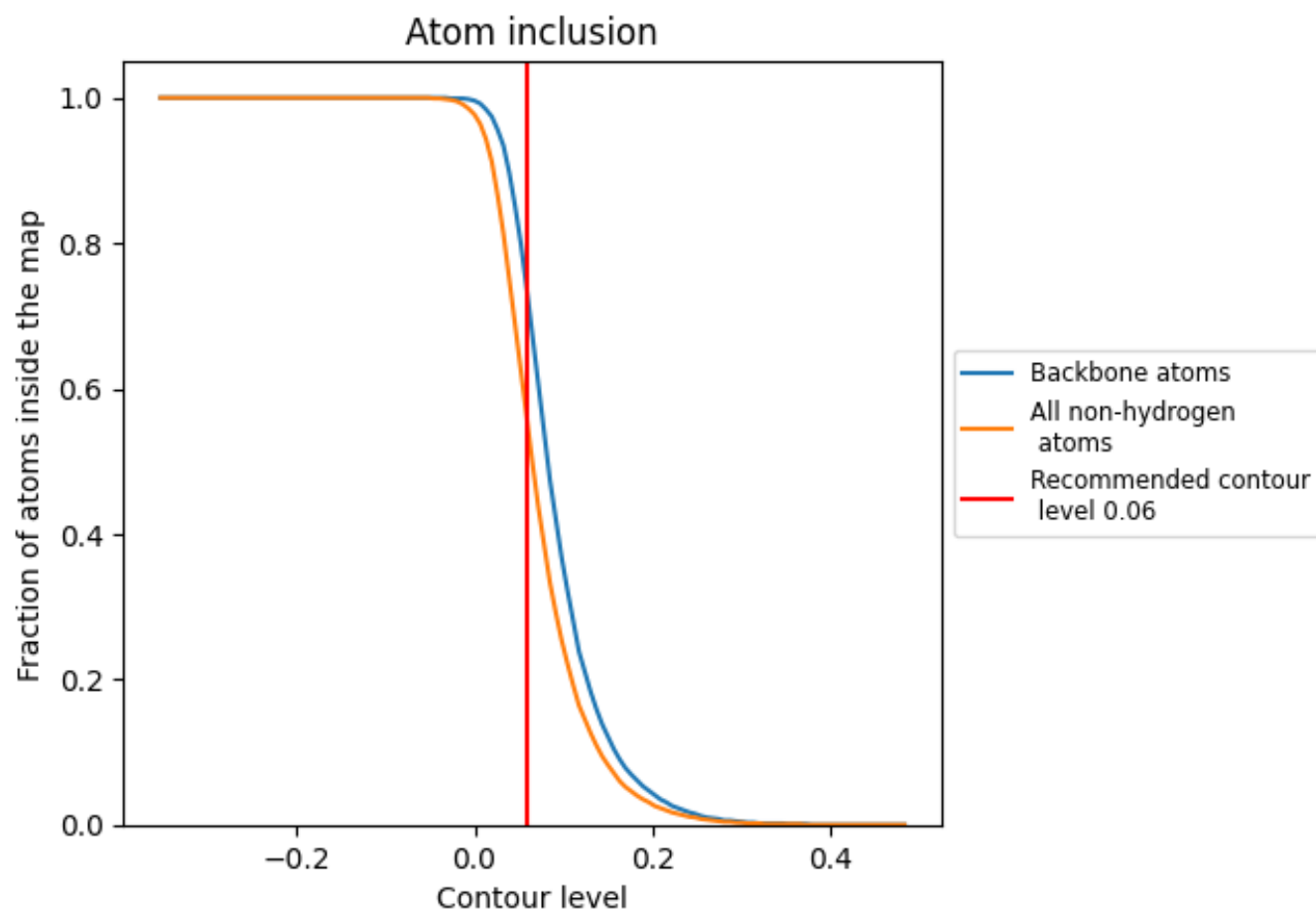
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 55% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5490	<div></div> 0.3380
A	<div></div> 0.5480	<div></div> 0.3370
B	<div></div> 0.6390	<div></div> 0.4220
C	<div></div> 0.6070	<div></div> 0.4270

