



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 03:07 AM UTC

PDB ID : 8RF0 / pdb_00008rf0
EMDB ID : EMD-19114
Title : WT-CGS sample in nanodisc
Authors : Sedzicki, J.; Ni, D.; Lehmann, F.; Stahlberg, H.; Dehio, C.
Deposited on : 2023-12-12
Resolution : 3.40 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

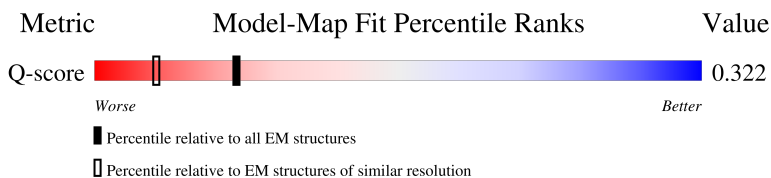
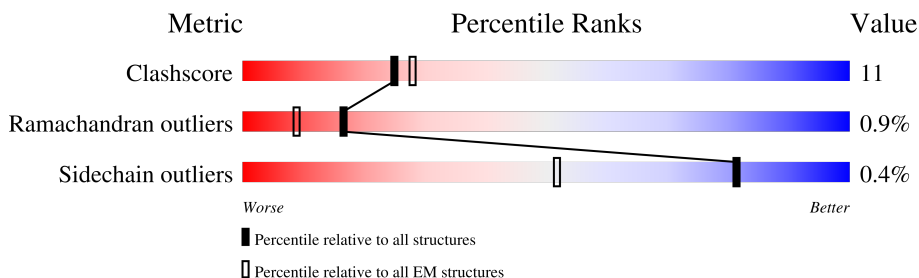
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	2818	 11% 74% 24% ..
2	B	9	 11% 22% 67%
3	C	9	 67% 56% 33% 11%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 21922 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.

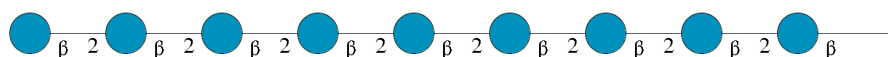
- Molecule 1 is a protein called Cyclic beta-(1,2)-glucan synthase NdvB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2780	Total	C	N	O	S	2	0
			21699	13698	3879	4052	70		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	610	SER	ALA	conflict	UNP A0A6V6ZZ23
A	866	PHE	HIS	conflict	UNP A0A6V6ZZ23

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose.



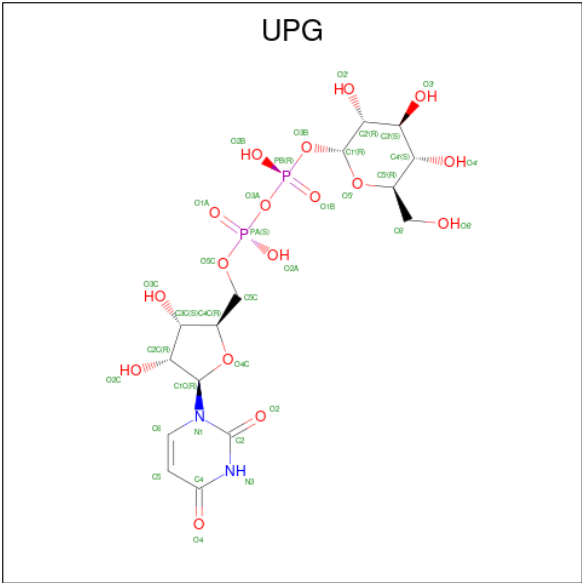
Mol	Chain	Residues	Atoms			AltConf	Trace
2	B	9	Total	C	O	0	0
			99	54	45		

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



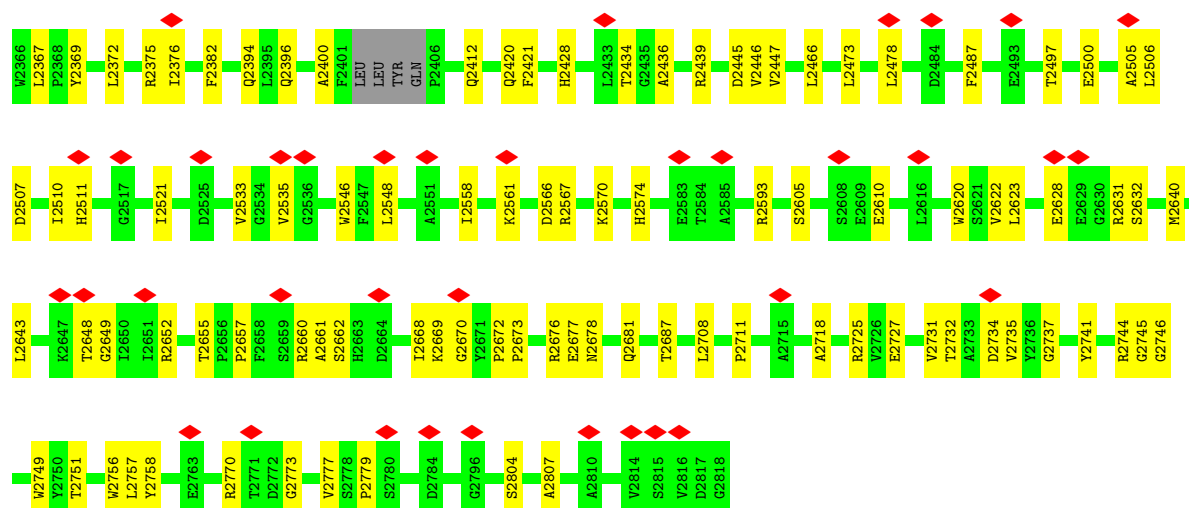
Mol	Chain	Residues	Atoms			AltConf	Trace
3	C	9	Total	C	O	0	0
			99	54	45		

- Molecule 4 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (CCD ID: UPG) (formula: C₁₅H₂₄N₂O₁₇P₂).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			25	9	2	12	2	

G252	A2092	S1988	I1897	G1756	G1662	D1557	K1445	L1322	K1202	H1111	G953	V879
F2253	S2095	L1992	F1898	R1757	R1663	R1558	K1457	Q1325	L1203	L1112	D954	A880
T2254	S2095	H1993	S1899	R1758	I1665	E1559	A1457	V1326	N1206	I1113	N955	L881
S2256	Q2105	V1994	R1759	S1564	T1666	S1564	D1458	V1327	H1209	A1118	A956	I883
R2257	T2106	R1995	R1762	Y1568	L1668	Y1568	F1460	G1330	D1208	W1122	F957	V884
R2263	N2110	V2000	E1763	Y1568	L1668	Y1568	T1461	A1331	H1209	Q1131	L958	F885
P2270	D2111	A2012	A1764	S1574	I1677	S1574	G1468	Q1332	V1211	G1132	I961	A889
Q2271	P2112	ASN	A1765	T1575	E1678	T1575	V1470	S1337	V1210	N1133	P962	A890
G2272	V2113	ARG	F1766	G1576	T1680	G1576	C1471	F1343	K1212	L1134	F963	C891
A2275	T2114	GLY	A1771	W1582	P1685	W1582	A1472	L1346	Q1215	D1135	L965	M893
G2276	G2129	ASP	T1772	M1583	D1692	M1583	A1472	M1347	L1225	G1136	L966	R899
A2277	K2130	GLY	L1773	Q1585	D1693	Q1585	Y1478	P1349	V1140	I1137	V967	S900
T2282	L2131	SER	S1776	A1592	N1694	A1592	H1482	L1350	V1227	D1135	V968	L901
D2288	D2141	P2028	D1782	D1596	P1697	D1596	H1483	V1351	D1236	I1143	L969	Y902
A2292	M2145	V2029	P1783	L1698	L1698	L1698	M1484	M1352	L1240	E1146	S970	R903
L2293	R1936	P2030	L1785	F1699	F1699	R1598	D1495	R1355	I1239	L1151	P971	L904
M2294	A1937	P2033	S1786	M1702	M1702	F1604	D1505	N1364	L1241	P1152	A972	H908
E2303	Q1942	E2036	L1787	F1703	F1703	L1605	I1508	I1367	E1245	D1153	V973	K909
E2304	M1944	P2037	R1788	G1712	G1712	R1606	A1511	I1372	P1246	N1154	E982	L910
R2305	D1949	N2048	K1798	D1713	D1713	W1613	Q1516	M1372	Q1249	K1155	D985	E913
F2309	I1950	G2049	W1718	W1718	W1718	W1614	E1517	H1374	L1250	R1156	R986	W914
L2310	I1951	F2050	R1719	R1719	R1719	T1617	K1518	R1376	L1251	T1157	K999	R915
L2311	S1952	A2054	I1802	I1802	I1802	E1618	R1377	R1377	L1261	L1158	R1002	T916
D2315	E1953	K2055	F1803	F1803	F1803	E1619	P1520	W1382	L1262	P1150	R1003	S919
E2318	Q1955	E2059	T1805	T1805	T1805	P1620	R1521	E1386	A1262	H1162	M920	Q921
E2319	R1956	V2060	P1809	P1809	P1809	V1622	E1522	N1390	D1266	R1163	S922	Q921
A2320	R1957	V2061	K1816	K1816	K1816	T1629	V1523	A1391	D1274	R1164	S923	S923
E2321	I1958	V2062	A1817	A1817	A1817	T1630	P1524	R1392	L1277	L1165	E1029	A924
L2064	N1959	L2064	I1818	I1818	I1818	F1632	V1525	L1396	L1277	E1166	Q925	Q925
N2065	A1960	N2065	A1834	A1834	A1834	F1632	A1528	M1396	L1277	R1168	S1034	G926
S2069	A1961	S2069	L1734	L1734	L1734	E1638	LYS	T1401	K1287	I1169	N1040	D930
T2070	D1962	T2070	A1735	A1735	A1735	F1639	TYR	N1402	A1287	I1170	I1041	Y931
L2075	G1964	L2075	D1736	D1736	D1736	H1640	GLU	L1408	D1290	N1174	G1042	Y932
N2076	R1965	N2076	N1738	N1738	N1738	K1641	PRO	G1413	Y1294	K1180	Q1053	R933
V2077	P1966	V2077	A1739	A1739	A1739	T1642	THR	L1414	E1291	E1182	F1054	Q934
L2078	H1967	L2078	G1740	G1740	G1740	Q1647	PRO	N1417	D1296	H1183	E1067	M935
S2079	V1968	S2079	P1741	P1741	P1741	S1648	G1536	L1417	L1296	E1194	E1077	W936
N2080	F1969	N2080	S1742	S1742	S1742	V1649	A1545	P1422	A1298	F1185	K1076	H937
F2083	R1972	F2083	A1852	A1852	A1852	C1652	E1546	N1417	R1302	E1189	V1073	A938
G2084	R1973	G2084	P1865	P1865	P1865	T1653	V1547	P1422	F1307	L1186	K1078	P939
H2085	L1974	H2085	P1865	P1865	P1865	V1654	E1548	L1427	H1318	A1197	E1077	V940
H2086	L1975	H2086	R1751	R1751	R1751	E1657	S1549	L1427	F1307	L1186	K1078	V941
I2087	L1976	I2087	A1752	A1752	A1752	E1661	A1551	D1441	H1318	L1186	K1078	V941
S2088	S1892	S2088	F1754	F1754	F1754	E1661	V1555	D1441	R1321	L1186	K1078	V941
F2346	W1981	F2346	L1755	L1755	L1755	E1661	V1555	D1441	H1318	L1186	K1078	V941
N2360	L1984	N2360	L1755	L1755	L1755	E1661	V1555	D1441	H1318	L1186	K1078	V941
H2361	L1984	H2361	L1755	L1755	L1755	E1661	V1555	D1441	H1318	L1186	K1078	V941
N2362	L1984	N2362	L1755	L1755	L1755	E1661	V1555	D1441	H1318	L1186	K1078	V941
V2363	L1984	V2363	L1755	L1755	L1755	E1661	V1555	D1441	H1318	L1186	K1078	V941
N2364	L1984	N2364	L1755	L1755	L1755	E1661	V1555	D1441	H1318	L1186	K1078	V941
N2365	L1984	N2365	L1755	L1755	L1755	E1661	V1555	D1441	H1318	L1186	K1078	V941



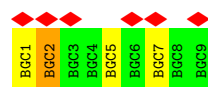
- Molecule 2: beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose

Chain B: 11% 22% 67%



- Molecule 3: beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain C: 67% 56% 33% 11%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50000	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.637	Depositor
Minimum map value	-0.305	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.12	Depositor
Map size ($\text{\AA}$)	394.8, 394.8, 394.8	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.316, 1.316, 1.316	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.18	3/22196 (0.0%)	0.44	13/30155 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1520	PRO	C-N	7.49	1.43	1.33
1	A	1519	ALA	C-N	5.89	1.47	1.33
1	A	1520	PRO	CA-C	5.15	1.59	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1519	ALA	O-C-N	-33.93	82.30	121.32
1	A	2030	PRO	N-CA-CB	10.45	109.81	102.81
1	A	1520	PRO	CA-C-O	-7.41	107.12	120.60
1	A	2037	PRO	N-CA-CB	7.18	110.79	103.25
1	A	2028	PRO	N-CA-CB	7.16	110.77	103.25
1	A	103	ALA	N-CA-C	-7.08	102.98	111.69
1	A	2033	PRO	N-CA-CB	7.01	110.61	103.25
1	A	103	ALA	CA-C-N	-6.64	109.98	120.47
1	A	103	ALA	C-N-CA	-6.64	109.98	120.47
1	A	1888	PRO	N-CA-CB	6.60	110.18	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	692	ASP	CB-CA-C	-6.15	104.08	110.17
1	A	492	PRO	N-CA-C	-5.96	101.84	111.14
1	A	1524	PRO	N-CA-CB	5.50	109.02	103.25

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	ILE	Mainchain
1	A	139	TYR	Peptide
1	A	1519	ALA	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	21699	0	20972	452	0
2	B	99	0	82	8	0
3	C	99	0	82	1	0
4	A	25	0	11	0	0
All	All	21922	0	21147	453	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 11.

All (453) 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:433:ALA:H	1:A:435:MET:HE1	1.33	0.90
1:A:115:PHE:CD1	2:B:9:BGC:O2	2.30	0.83
1:A:619:TYR:HB3	1:A:716:LEU:HD11	1.63	0.81
1:A:682:GLN:HB3	1:A:689:ARG:HH22	1.46	0.79
1:A:423:MET:HG2	1:A:444:LEU:HD22	1.65	0.79
1:A:1748:GLU:HB2	1:A:1773:LEU:HG	1.65	0.76
1:A:963:PHE:HB3	1:A:967:TRP:HZ3	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:TRP:HB2	1:A:529:ARG:HH21	1.52	0.75
1:A:667:ARG:HB3	1:A:752:THR:HA	1.71	0.73
1:A:826:PRO:HD2	1:A:829:ALA:HB2	1.70	0.72
1:A:64:GLU:HG2	1:A:186:ARG:HH12	1.56	0.70
1:A:982:GLU:HA	1:A:986:ARG:HG3	1.73	0.70
1:A:115:PHE:CG	2:B:9:BGC:O2	2.45	0.69
1:A:1668:LEU:HB2	1:A:1798:LYS:HZ2	1.57	0.69
1:A:1976:MET:HE1	1:A:1981:TRP:HB2	1.75	0.68
1:A:2063:ARG:NH2	1:A:2145:MET:SD	2.67	0.68
1:A:1720:ASN:ND2	1:A:2670:GLY:O	2.27	0.68
1:A:690:GLY:HA3	1:A:1518:LYS:HG2	1.75	0.68
1:A:1206:ASN:O	1:A:1209:HIS:ND1	2.28	0.67
1:A:2681:GLN:HB3	1:A:2735:VAL:H	1.58	0.67
1:A:2434:THR:HG23	1:A:2436:ALA:H	1.59	0.67
1:A:2054:ALA:O	1:A:2055:LYS:HG2	1.95	0.67
1:A:1697:PRO:HD2	1:A:2110:ASN:HD21	1.60	0.66
1:A:1905:ASP:HB2	1:A:1944:MET:HE2	1.78	0.66
1:A:2570:LYS:HE3	1:A:2570:LYS:HA	1.78	0.66
1:A:324:ASP:O	1:A:327:SER:N	2.28	0.66
1:A:515:ASN:HD22	1:A:634:VAL:HB	1.60	0.66
1:A:607:LEU:HD12	1:A:608:GLY:H	1.61	0.65
1:A:736:LEU:C	1:A:738:HIS:H	2.03	0.65
1:A:185:LEU:HD12	1:A:288:ILE:HG21	1.78	0.65
1:A:776:ARG:HG3	1:A:900:SER:HB3	1.78	0.65
1:A:780:GLN:HA	1:A:904:LEU:HD11	1.79	0.65
1:A:1604:PHE:HB2	1:A:1680:THR:HB	1.79	0.64
1:A:2770:ARG:HE	1:A:2773:GLY:HA2	1.62	0.64
1:A:170:LEU:HD21	1:A:307:VAL:HG23	1.79	0.64
1:A:2507:ASP:O	1:A:2511:HIS:ND1	2.28	0.64
1:A:481:ILE:HD13	1:A:520:ILE:HD11	1.79	0.64
1:A:963:PHE:HB3	1:A:967:TRP:CZ3	2.32	0.64
1:A:1245:GLU:OE2	1:A:1249:GLN:NE2	2.30	0.64
1:A:2396:GLN:HG2	1:A:2756:TRP:HE1	1.63	0.64
1:A:1936:ARG:HE	1:A:1937:ALA:H	1.44	0.63
1:A:2113:VAL:HG23	1:A:2114:ILE:HG13	1.79	0.63
1:A:2497:THR:HG23	1:A:2500:GLU:H	1.62	0.63
1:A:1003:ARG:NH2	1:A:1146:GLU:OE1	2.31	0.63
1:A:1718:TRP:HB3	1:A:1730:VAL:HG13	1.81	0.63
1:A:2622:VAL:HG22	1:A:2632:SER:HB2	1.79	0.63
1:A:2360:ASN:OD1	1:A:2364:ASN:ND2	2.31	0.63
1:A:2668:ILE:O	1:A:2678:ASN:ND2	2.26	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:GLU:OE2	2:B:4:BGC:H5	1.99	0.63
1:A:61:ARG:O	1:A:65:ASN:ND2	2.30	0.62
1:A:1664:ARG:HG3	1:A:1802:ILE:HG22	1.80	0.62
1:A:1663:ARG:HB2	1:A:1803:PHE:HB2	1.81	0.62
1:A:487:THR:HG22	1:A:619:TYR:HB2	1.82	0.62
1:A:673:THR:HG23	1:A:678:ALA:HB2	1.82	0.62
1:A:1652:CYS:SG	1:A:1663:ARG:NH1	2.73	0.62
1:A:1606:ARG:HG3	1:A:1613:TRP:HB3	1.82	0.61
1:A:2428:HIS:ND1	1:A:2445:ASP:OD2	2.32	0.61
1:A:676:LYS:O	1:A:986:ARG:NH1	2.30	0.61
1:A:1373:ASN:OD1	1:A:1377:ARG:NH2	2.33	0.61
1:A:449:LEU:HD22	1:A:805:ARG:HG3	1.81	0.61
1:A:449:LEU:HB3	1:A:809:THR:HG22	1.82	0.61
1:A:723:GLU:HG2	1:A:727:LYS:HZ3	1.65	0.61
1:A:2075:ILE:O	1:A:2749:TRP:NE1	2.33	0.61
1:A:2372:LEU:HA	1:A:2376:ILE:HD13	1.83	0.61
1:A:862:GLN:NE2	1:A:1524:PRO:HA	2.16	0.61
1:A:171:TRP:CE2	2:B:7:BGC:H6C2	2.35	0.60
1:A:725:ALA:HB1	1:A:745:PHE:HB3	1.83	0.60
1:A:325:PHE:HA	1:A:328:ARG:HD3	1.83	0.60
1:A:811:ILE:HD11	1:A:893:MET:SD	2.41	0.60
1:A:1649:VAL:HG13	1:A:1666:THR:HB	1.85	0.59
1:A:278:LEU:O	1:A:282:ASN:ND2	2.35	0.59
1:A:324:ASP:H	1:A:476:GLU:HG3	1.65	0.59
1:A:2257:ARG:HD3	1:A:2288:ASP:HB3	1.83	0.59
1:A:585:GLU:HB3	1:A:589:GLY:H	1.68	0.59
1:A:2446:VAL:HB	1:A:2505:ALA:HB1	1.85	0.59
1:A:736:LEU:O	1:A:738:HIS:N	2.36	0.59
1:A:1011:PHE:HB3	1:A:1021:PRO:HG3	1.85	0.58
1:A:173:LEU:HA	1:A:176:ILE:HG22	1.86	0.58
1:A:508:ILE:HD11	1:A:524:LEU:HB2	1.85	0.58
1:A:2181:SER:HB2	1:A:2309:PHE:HB2	1.85	0.58
1:A:1002:ARG:HH22	1:A:1225:LEU:HD12	1.68	0.58
1:A:1053:GLN:O	1:A:1133:ASN:ND2	2.36	0.58
1:A:672:LEU:HD11	1:A:690:GLY:HA2	1.86	0.58
1:A:1135:ASP:OD1	1:A:1180:LYS:NZ	2.30	0.58
1:A:1734:LEU:HB3	1:A:1804:TRP:HB2	1.86	0.58
1:A:2439:ARG:HG2	1:A:2478:LEU:HD11	1.86	0.58
1:A:1372:MET:HG2	1:A:1376:ARG:HE	1.69	0.57
1:A:115:PHE:CE1	2:B:9:BGC:H3	2.39	0.57
1:A:199:ARG:NH2	1:A:274:GLU:OE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:LEU:HB2	1:A:53:PHE:HB2	1.85	0.57
1:A:1392:ARG:HB3	1:A:1396:MET:HB2	1.87	0.57
1:A:1003:ARG:HE	1:A:1143:ILE:HG23	1.69	0.57
1:A:1113:ILE:HD11	1:A:1307:PHE:CE1	2.38	0.57
1:A:1122:TRP:HE1	1:A:1251:LEU:HD22	1.69	0.57
1:A:2466:LEU:O	1:A:2497:THR:OG1	2.23	0.57
1:A:98:TYR:OH	1:A:1325:GLN:HB3	2.05	0.57
1:A:648:PRO:HA	1:A:660:GLY:HA3	1.87	0.57
1:A:107:VAL:O	1:A:108:ARG:HB3	2.05	0.57
1:A:489:VAL:HA	1:A:621:MET:HB2	1.87	0.57
1:A:1417:ASN:O	1:A:1461:THR:OG1	2.22	0.56
1:A:2727:GLU:OE1	1:A:2749:TRP:NE1	2.38	0.56
1:A:587:LYS:O	1:A:588:ARG:C	2.46	0.56
1:A:2687:THR:HG21	1:A:2756:TRP:HB3	1.87	0.56
1:A:672:LEU:HD13	1:A:1516:GLN:HE21	1.70	0.56
1:A:796:GLY:O	1:A:799:LYS:HG2	2.05	0.56
1:A:1606:ARG:HH12	1:A:1767:PHE:HA	1.71	0.56
1:A:308:SER:O	1:A:312:LYS:NZ	2.37	0.56
1:A:2506:LEU:O	1:A:2510:ILE:HG12	2.06	0.56
1:A:1067:GLU:HG2	1:A:1254:LEU:HD21	1.86	0.56
1:A:1678:GLU:OE2	1:A:1788:ARG:NE	2.30	0.55
1:A:430:LEU:HD21	1:A:824:MET:HE1	1.88	0.55
1:A:2130:LYS:NZ	1:A:2141:ASP:OD2	2.38	0.55
1:A:21:HIS:HB2	1:A:277:ARG:HE	1.71	0.55
1:A:587:LYS:C	1:A:589:GLY:N	2.64	0.55
1:A:1931:VAL:HG22	1:A:1969:PHE:HB2	1.87	0.55
1:A:2095:SER:HB2	1:A:2105:LEU:HB2	1.87	0.55
1:A:1548:ARG:HG2	1:A:1550:ILE:HD11	1.88	0.55
1:A:2546:TRP:HB3	1:A:2620:TRP:HD1	1.70	0.55
1:A:1020:PRO:HD2	1:A:1041:ILE:HD13	1.88	0.55
1:A:1414:LEU:O	1:A:1417:ASN:ND2	2.39	0.55
1:A:1713:ASP:HB3	1:A:1735:ALA:HB3	1.87	0.55
1:A:1753:LYS:HZ1	1:A:1776:SER:HB3	1.72	0.55
1:A:899:ARG:HB3	1:A:903:ARG:HH12	1.71	0.55
1:A:2255:THR:OG1	1:A:2282:THR:O	2.20	0.55
1:A:2246:LEU:O	1:A:2328:ARG:NH1	2.40	0.55
1:A:736:LEU:C	1:A:738:HIS:N	2.65	0.54
1:A:1693:ASP:OD1	1:A:1694:ASN:N	2.40	0.54
1:A:1702:MET:HE3	1:A:2672:PRO:HG2	1.89	0.54
1:A:1929:ASP:HA	1:A:1967:HIS:HB3	1.89	0.54
1:A:1375:GLY:HA3	1:A:1382:TRP:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:SER:HA	1:A:192:VAL:HG12	1.89	0.54
1:A:696:PHE:HZ	2:B:5:BGC:H6C1	1.72	0.54
1:A:782:LEU:HA	1:A:785:ILE:HD12	1.90	0.54
1:A:1568:TYR:HD2	1:A:1582:TRP:HD1	1.56	0.54
1:A:1576:GLY:HA3	1:A:1617:THR:HG21	1.89	0.54
1:A:1661:GLU:HB3	1:A:1805:THR:HB	1.89	0.54
1:A:2372:LEU:HD12	1:A:2376:ILE:HD13	1.88	0.54
1:A:507:ASN:O	1:A:511:HIS:ND1	2.37	0.54
1:A:630:MET:HB2	1:A:633:ALA:HB2	1.90	0.54
1:A:1631:ILE:HB	1:A:1638:GLU:HB3	1.90	0.54
1:A:1974:ASP:OD1	1:A:1975:LEU:N	2.41	0.54
1:A:2048:ASN:HA	1:A:2718:ALA:HA	1.90	0.54
1:A:1198:ARG:O	1:A:1202:LYS:HG2	2.07	0.53
1:A:1386:GLU:HB2	1:A:1402:ASN:HA	1.90	0.53
1:A:1575:THR:HB	1:A:1619:GLU:HB2	1.90	0.53
1:A:2649:GLY:HA2	1:A:2708:LEU:HD11	1.88	0.53
1:A:734:SER:HB3	1:A:738:HIS:NE2	2.23	0.53
1:A:2734:ASP:O	1:A:2746:GLY:N	2.42	0.53
1:A:796:GLY:HA2	1:A:799:LYS:HD3	1.88	0.53
1:A:1201:GLN:NE2	1:A:1224:GLN:OE1	2.41	0.53
1:A:1348:PRO:HB3	1:A:1352:MET:HE2	1.90	0.53
1:A:1904:ASP:OD2	1:A:1995:ARG:NH2	2.42	0.53
1:A:1629:LYS:HB3	1:A:1640:HIS:HB2	1.91	0.53
1:A:2172:VAL:HG12	1:A:2179:LYS:HA	1.91	0.53
1:A:811:ILE:H	1:A:811:ILE:HD12	1.74	0.53
1:A:999:LYS:HG3	1:A:1143:ILE:HG13	1.90	0.53
1:A:1246:PRO:O	1:A:1250:ARG:HG2	2.09	0.52
1:A:2196:LYS:NZ	1:A:2197:VAL:O	2.42	0.52
1:A:1427:LEU:HD21	1:A:1484:MET:HE2	1.90	0.52
1:A:2660:ARG:HH21	1:A:2662:SER:HA	1.74	0.52
1:A:1559:GLU:HG2	1:A:1574:SER:HB3	1.91	0.52
1:A:1751:ARG:NH2	1:A:2111:ASP:OD1	2.35	0.52
1:A:1734:LEU:HD13	1:A:1818:ILE:HD11	1.92	0.52
1:A:1551:ALA:HA	1:A:1629:LYS:HD2	1.92	0.52
1:A:2050:PHE:HD1	1:A:2064:LEU:HD21	1.75	0.52
1:A:2075:ILE:HG13	1:A:2382:PHE:HB2	1.92	0.52
1:A:2213:ALA:HA	1:A:2216:ILE:HD12	1.91	0.52
1:A:500:SER:O	1:A:504:MET:HG2	2.10	0.51
1:A:1168:ARG:HA	1:A:1168:ARG:NE	2.25	0.51
1:A:848:LEU:HD11	1:A:871:GLU:HG3	1.93	0.51
1:A:2657:PRO:HB3	1:A:2673:PRO:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:ALA:HB1	1:A:754:VAL:HG13	1.93	0.51
1:A:330:THR:HG21	1:A:471:ARG:HD2	1.91	0.51
1:A:607:LEU:HD12	1:A:608:GLY:N	2.25	0.51
1:A:866:PHE:HD2	1:A:868:ILE:HG12	1.75	0.51
1:A:589:GLY:O	1:A:590:LYS:C	2.54	0.51
1:A:621:MET:HE2	1:A:716:LEU:HD13	1.93	0.51
1:A:2079:SER:HA	1:A:2084:GLY:HA2	1.93	0.51
1:A:64:GLU:HG2	1:A:186:ARG:NH1	2.25	0.51
1:A:206:VAL:HG11	1:A:241:ARG:HD3	1.93	0.50
1:A:226:ASP:OD2	1:A:259:ARG:NH2	2.43	0.50
1:A:329:ASN:OD1	1:A:332:ARG:NH2	2.33	0.50
1:A:500:SER:O	1:A:503:GLU:HG2	2.11	0.50
1:A:1073:VAL:O	1:A:1078:LYS:NZ	2.44	0.50
1:A:403:MET:HE2	1:A:705:LEU:HD23	1.93	0.50
1:A:769:SER:HA	1:A:772:HIS:CE1	2.46	0.50
1:A:226:ASP:OD1	1:A:259:ARG:NE	2.41	0.50
1:A:587:LYS:O	1:A:589:GLY:N	2.45	0.50
1:A:889:ALA:O	1:A:893:MET:HG3	2.11	0.50
1:A:1685:PRO:HD3	1:A:1785:LEU:HG	1.93	0.50
1:A:493:CYS:N	1:A:525:VAL:O	2.45	0.50
1:A:1834:ALA:HA	1:A:1837:ARG:HG2	1.93	0.50
1:A:2104:GLN:NE2	1:A:2106:THR:O	2.40	0.50
1:A:1134:LEU:O	1:A:1180:LYS:NZ	2.32	0.50
1:A:2661:ALA:HA	1:A:2669:LYS:HE3	1.94	0.50
1:A:25:ILE:HG22	1:A:141:ALA:HB2	1.93	0.50
1:A:1478:TYR:O	1:A:1482:HIS:ND1	2.43	0.50
1:A:2367:LEU:HD21	1:A:2757:LEU:HD23	1.93	0.50
1:A:543:LEU:HD21	1:A:607:LEU:HD21	1.93	0.50
1:A:1297:LEU:HG	1:A:1322:LEU:HD12	1.93	0.50
1:A:1752:ALA:HA	1:A:2113:VAL:HG11	1.94	0.50
1:A:2240:ARG:HD2	1:A:2315:ASP:HB3	1.94	0.50
1:A:1902:ILE:HG13	1:A:1994:VAL:HG21	1.92	0.50
1:A:2172:VAL:HG23	1:A:2174:ARG:HH21	1.77	0.50
1:A:1972:ARG:HD3	1:A:1975:LEU:HD23	1.93	0.49
1:A:2521:ILE:HG21	1:A:2533:VAL:HB	1.94	0.49
1:A:42:LEU:HD12	1:A:46:GLY:HA3	1.94	0.49
1:A:763:ARG:NH1	1:A:765:GLU:OE1	2.45	0.49
1:A:1374:HIS:HA	1:A:1377:ARG:HG2	1.94	0.49
1:A:1555:VAL:HG23	1:A:1556:ARG:HD2	1.94	0.49
1:A:511:HIS:CD2	1:A:623:LEU:HD21	2.47	0.49
1:A:735:ILE:HG23	1:A:737:SER:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:GLU:OE1	1:A:71:ARG:NH2	2.43	0.49
1:A:585:GLU:HB3	1:A:589:GLY:N	2.28	0.49
1:A:629:LEU:HD21	1:A:634:VAL:HG23	1.94	0.49
1:A:1680:THR:HG23	1:A:1788:ARG:HG3	1.94	0.49
1:A:1902:ILE:HD12	1:A:1994:VAL:HG11	1.93	0.49
1:A:505:MET:HB3	1:A:553:LEU:HD11	1.94	0.49
1:A:2061:VAL:HG22	1:A:2149:ARG:HG3	1.95	0.49
1:A:2152:LEU:HD11	1:A:2365:ASN:HB3	1.94	0.49
1:A:2252:GLY:H	1:A:2294:MET:HB2	1.77	0.49
1:A:862:GLN:O	1:A:864:HIS:ND1	2.44	0.49
1:A:2085:PHE:HZ	1:A:2170:GLN:HB3	1.78	0.49
1:A:105:GLN:C	1:A:107:VAL:H	2.21	0.49
1:A:881:LEU:HA	1:A:884:VAL:HG22	1.93	0.49
1:A:1165:LEU:HD21	1:A:1203:LEU:HB3	1.93	0.49
1:A:2179:LYS:HB3	1:A:2311:LEU:HB2	1.94	0.49
1:A:650:ILE:HG13	1:A:657:VAL:HG22	1.95	0.48
1:A:2080:ASN:ND2	1:A:2173:ASP:O	2.46	0.48
1:A:1054:PHE:HA	1:A:1133:ASN:HD21	1.78	0.48
1:A:1574:SER:HA	1:A:1632:PHE:HE2	1.78	0.48
1:A:2363:VAL:HA	1:A:2367:LEU:HD12	1.95	0.48
1:A:1296:LEU:HG	1:A:1298:ALA:H	1.78	0.48
1:A:805:ARG:O	1:A:809:THR:HG23	2.14	0.48
1:A:1903:ASN:OD1	1:A:1936:ARG:HD2	2.14	0.48
1:A:2321:GLU:HA	1:A:2324:VAL:HG22	1.96	0.48
1:A:318:THR:C	1:A:370:ARG:HD2	2.38	0.48
1:A:348:GLU:HA	1:A:351:ARG:HB3	1.95	0.48
1:A:520:ILE:O	1:A:564:ARG:NH2	2.47	0.48
1:A:2711:PRO:HG2	1:A:2731:VAL:HA	1.96	0.48
1:A:2640:MET:HA	1:A:2643:LEU:HB2	1.96	0.47
1:A:1848:THR:O	1:A:1852:ALA:N	2.40	0.47
1:A:2063:ARG:NH2	1:A:2065:ASN:OD1	2.47	0.47
1:A:2610:GLU:OE1	1:A:2669:LYS:NZ	2.48	0.47
1:A:2648:THR:HG21	1:A:2737:GLY:HA2	1.97	0.47
1:A:1592:ALA:H	1:A:2210:GLN:HG2	1.80	0.47
1:A:672:LEU:HD13	1:A:1516:GLN:HB3	1.96	0.47
1:A:1224:GLN:HA	1:A:1227:VAL:HG12	1.97	0.47
1:A:66:GLU:OE2	1:A:104:ILE:HG21	2.15	0.47
1:A:1082:HIS:NE2	1:A:1266:ASP:O	2.43	0.47
1:A:1614:TRP:CD1	1:A:1641:LYS:HZ1	2.32	0.47
1:A:1934:ASN:O	1:A:1973:ARG:HB2	2.14	0.47
1:A:2196:LYS:HZ1	1:A:2294:MET:HA	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2676:ARG:NH1	1:A:2734:ASP:OD2	2.47	0.47
1:A:1606:ARG:HA	1:A:1613:TRP:HA	1.96	0.47
1:A:1607:ASP:HA	1:A:1677:ILE:HG22	1.97	0.47
1:A:2088:SER:H	1:A:2092:ALA:HB3	1.79	0.47
1:A:2077:VAL:HG12	1:A:2086:HIS:HB3	1.98	0.46
1:A:1153:ASP:HB3	1:A:1159:ARG:HB3	1.97	0.46
1:A:1748:GLU:O	1:A:1750:ASP:N	2.46	0.46
1:A:2128:THR:HG23	1:A:2130:LYS:H	1.80	0.46
1:A:2593:ARG:NH1	1:A:2605:SER:OG	2.47	0.46
1:A:1296:LEU:HD21	1:A:1337:SER:HA	1.98	0.46
1:A:631:ARG:HH21	1:A:1511:ALA:HB2	1.80	0.46
1:A:1699:PHE:O	1:A:1703:PHE:HD1	1.98	0.46
1:A:299:GLU:OE1	1:A:1321:ARG:NH2	2.48	0.46
1:A:501:VAL:O	1:A:505:MET:HG2	2.15	0.46
1:A:1277:LEU:HA	1:A:1318:HIS:CE1	2.51	0.46
1:A:573:ILE:H	1:A:583:GLY:HA2	1.81	0.46
1:A:913:GLU:OE1	1:A:916:THR:OG1	2.31	0.46
1:A:1327:VAL:HG21	1:A:1408:LEU:CD2	2.46	0.46
1:A:1759:ARG:HB3	1:A:1763:GLU:O	2.15	0.46
1:A:899:ARG:HB3	1:A:903:ARG:NH1	2.31	0.46
1:A:1161:LEU:HD23	1:A:1207:VAL:HG22	1.97	0.45
1:A:1167:GLU:HA	1:A:1170:ILE:HG12	1.97	0.45
1:A:1654:VAL:HA	1:A:1661:GLU:HA	1.98	0.45
1:A:716:LEU:HD12	1:A:717:TYR:H	1.81	0.45
1:A:1020:PRO:HG2	1:A:1040:ASN:HB3	1.98	0.45
1:A:531:ALA:H	1:A:572:ARG:HH12	1.64	0.45
1:A:593:GLU:HA	1:A:596:MET:HE2	1.99	0.45
1:A:1596:ASP:HA	1:A:1598:ARG:HH11	1.81	0.45
1:A:223:LYS:HD2	1:A:223:LYS:C	2.42	0.45
1:A:1505:ASP:HB3	1:A:1508:ILE:HG22	1.98	0.45
1:A:1699:PHE:O	1:A:1702:MET:N	2.50	0.45
3:C:1:BGC:O3	3:C:2:BGC:H6C2	2.16	0.45
1:A:2318:GLU:O	1:A:2321:GLU:HG3	2.17	0.45
1:A:2741:TYR:HB2	1:A:2744:ARG:NH1	2.32	0.45
1:A:1210:GLU:HG3	1:A:1211:VAL:HG23	1.98	0.45
1:A:1364:ASN:HA	1:A:1367:ILE:HG12	1.97	0.45
1:A:1598:ARG:HH21	1:A:1762:ARG:HH12	1.65	0.45
1:A:1722:ARG:HG2	1:A:2670:GLY:HA3	1.99	0.45
1:A:985:ASP:OD1	1:A:985:ASP:N	2.49	0.45
1:A:1302:ARG:NH1	1:A:1348:PRO:HG2	2.32	0.45
1:A:2566:ASP:OD1	1:A:2567:ARG:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2620:TRP:HA	1:A:2623:LEU:HB2	1.98	0.45
1:A:47:ALA:C	1:A:49:SER:H	2.25	0.44
1:A:630:MET:HA	1:A:630:MET:HE2	1.99	0.44
1:A:711:PHE:O	1:A:739:ASP:HB2	2.18	0.44
1:A:1582:TRP:O	1:A:1585:GLN:HG2	2.17	0.44
1:A:1898:PHE:CE2	1:A:1900:LEU:HB2	2.52	0.44
1:A:2315:ASP:OD1	1:A:2315:ASP:N	2.51	0.44
1:A:818:ILE:HA	1:A:821:TRP:CZ2	2.53	0.44
1:A:932:TYR:CE1	1:A:971:PRO:HB2	2.53	0.44
1:A:1157:THR:O	1:A:1160:PRO:HD3	2.17	0.44
1:A:1196:LEU:O	1:A:1200:ILE:HG12	2.17	0.44
1:A:1574:SER:HA	1:A:1632:PHE:CE2	2.53	0.44
1:A:2732:THR:OG1	1:A:2746:GLY:O	2.35	0.44
1:A:268:GLU:HA	1:A:271:MET:HG3	1.98	0.44
1:A:381:ARG:HG2	1:A:384:GLU:HB3	1.99	0.44
1:A:531:ALA:H	1:A:572:ARG:NH1	2.16	0.44
1:A:1459:ASP:HB3	1:A:1472:ALA:HB3	1.99	0.44
1:A:1841:GLN:OE1	1:A:1924:ARG:NH2	2.48	0.44
1:A:2315:ASP:O	1:A:2319:GLU:HB3	2.17	0.44
1:A:102:GLU:HA	1:A:105:GLN:HB2	2.00	0.44
1:A:435:MET:SD	1:A:435:MET:N	2.91	0.44
1:A:1390:ASN:HD22	1:A:1472:ALA:HB1	1.83	0.44
1:A:1665:ILE:HD11	1:A:1801:VAL:HB	1.98	0.44
1:A:1749:THR:OG1	1:A:1776:SER:O	2.34	0.44
1:A:1355[A]:ARG:HG3	1:A:1516:GLN:HE22	1.83	0.44
1:A:1802:ILE:HD12	1:A:1804:TRP:HE1	1.83	0.44
1:A:2510:ILE:HD12	1:A:2574:HIS:ND1	2.32	0.44
1:A:171:TRP:O	2:B:6:BGC:H4	2.18	0.44
1:A:1685:PRO:HD2	1:A:1784:ILE:HA	2.00	0.44
1:A:1694:ASN:HB3	1:A:2208:ASN:HD21	1.82	0.44
1:A:149:ARG:NH2	1:A:299:GLU:O	2.51	0.43
1:A:1642:THR:HA	1:A:1647:GLN:HA	1.99	0.43
1:A:2394:GLN:HG3	1:A:2412:GLN:HE21	1.83	0.43
1:A:2447:VAL:HG21	1:A:2548:LEU:HD11	2.01	0.43
1:A:2652:ARG:HD2	1:A:2655:THR:HA	2.00	0.43
1:A:361:LEU:HG	1:A:362:PRO:HD2	2.00	0.43
1:A:1564:SER:HB3	1:A:1924:ARG:HD3	1.99	0.43
1:A:486:ARG:HD3	1:A:521:TYR:HE2	1.84	0.43
1:A:643:HIS:HB3	1:A:646:ASN:HD22	1.82	0.43
1:A:868:ILE:HA	1:A:871:GLU:OE2	2.18	0.43
1:A:327:SER:O	1:A:331:TYR:HD1	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:VAL:HG22	1:A:621:MET:HG3	2.00	0.43
1:A:592:HIS:O	1:A:595:ASN:N	2.51	0.43
1:A:891:CYS:SG	1:A:937:HIS:ND1	2.83	0.43
1:A:1346:LEU:O	1:A:1350:LEU:HD23	2.17	0.43
1:A:1759:ARG:HD2	1:A:1765:ALA:HB2	1.99	0.43
1:A:2558:ILE:O	1:A:2561:LYS:HG2	2.18	0.43
1:A:2735:VAL:HA	1:A:2745:GLY:HA2	2.00	0.43
1:A:344:ARG:HA	1:A:344:ARG:HD2	1.88	0.43
1:A:1898:PHE:HE2	1:A:1900:LEU:HB2	1.83	0.43
1:A:2628:GLU:HB3	1:A:2631:ARG:HG2	2.01	0.43
1:A:326:GLY:O	1:A:330:THR:HG23	2.19	0.43
1:A:666:PRO:HG2	1:A:756:LEU:HD12	1.99	0.43
1:A:935:MET:O	1:A:937:HIS:N	2.52	0.43
1:A:1592:ALA:HB1	1:A:1865:PRO:HD3	2.01	0.43
1:A:1729:THR:HA	1:A:1809:PRO:HA	1.99	0.43
1:A:2064:LEU:HD13	1:A:2069:SER:HA	2.00	0.43
1:A:32:ILE:H	1:A:32:ILE:HD12	1.83	0.43
1:A:339:ALA:HB2	1:A:349:VAL:HG21	2.01	0.43
1:A:346:GLU:OE1	1:A:346:GLU:N	2.45	0.43
1:A:430:LEU:O	1:A:435:MET:HE3	2.19	0.43
1:A:461:THR:HG21	1:A:846:LEU:HB3	2.01	0.43
1:A:1347:MET:HB2	1:A:1348:PRO:HD3	2.00	0.43
1:A:1559:GLU:H	1:A:1574:SER:HB3	1.81	0.43
1:A:1564:SER:O	1:A:1837:ARG:NH1	2.50	0.43
1:A:637:LEU:HG	1:A:754:VAL:HG21	2.00	0.43
1:A:783:PRO:HA	1:A:786:ILE:HG22	2.01	0.43
1:A:885:PHE:CZ	1:A:973:VAL:HG13	2.54	0.43
1:A:512:TYR:HA	1:A:522:PHE:CZ	2.53	0.42
1:A:797:ARG:O	1:A:801:VAL:HG23	2.19	0.42
1:A:1034:SER:HB3	1:A:1089:THR:HB	2.00	0.42
1:A:2333:LEU:O	1:A:2336:LEU:N	2.52	0.42
1:A:342:SER:HA	1:A:343:PRO:HD3	1.91	0.42
1:A:903:ARG:HH21	1:A:910:LEU:HB3	1.84	0.42
1:A:1422:PRO:HD3	1:A:1457:ALA:HA	2.01	0.42
1:A:2400:ALA:HB1	1:A:2758:TYR:HD2	1.84	0.42
1:A:2676:ARG:NH2	1:A:2677:GLU:OE2	2.52	0.42
1:A:2804:SER:OG	1:A:2807:ALA:O	2.32	0.42
1:A:240:TYR:HE2	1:A:271:MET:HE1	1.84	0.42
1:A:505:MET:N	1:A:505:MET:HE2	2.34	0.42
1:A:1907:ASP:OD1	1:A:1908:MET:N	2.47	0.42
1:A:2303:GLU:OE2	1:A:2305:ARG:NE	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:ARG:HA	1:A:606:PHE:HA	2.01	0.42
1:A:694:TYR:OH	2:B:1:BGC:C1	2.67	0.42
1:A:1076:MET:HE2	1:A:1083:LEU:HD22	2.01	0.42
1:A:1277:LEU:HD21	1:A:1322:LEU:HB3	2.02	0.42
1:A:1984:LEU:O	1:A:1988:SER:OG	2.33	0.42
1:A:2077:VAL:O	1:A:2369:TYR:OH	2.27	0.42
1:A:2334:SER:HA	1:A:2337:GLU:OE2	2.20	0.42
1:A:2725:ARG:NE	1:A:2744:ARG:HH21	2.18	0.42
1:A:194[A]:ARG:HE	1:A:194[A]:ARG:HB2	1.56	0.42
1:A:508:ILE:HD11	1:A:524:LEU:HD12	2.02	0.42
1:A:1137:ILE:HA	1:A:1140:VAL:HG12	2.02	0.42
1:A:2145:MET:HB2	1:A:2160:VAL:HB	2.00	0.42
1:A:2320:ALA:O	1:A:2324:VAL:HG13	2.19	0.42
1:A:452:SER:OG	1:A:805:ARG:NH1	2.52	0.42
1:A:665:GLN:HA	1:A:666:PRO:HD3	1.95	0.42
1:A:809:THR:OG1	1:A:810:PRO:HD3	2.20	0.42
1:A:1598:ARG:HH21	1:A:1762:ARG:NH1	2.18	0.42
1:A:2421:PHE:CE1	1:A:2473:LEU:HB2	2.55	0.42
1:A:562:LYS:HD2	1:A:562:LYS:HA	1.75	0.42
1:A:1898:PHE:HZ	1:A:1992:LEU:HD12	1.84	0.42
1:A:242:LEU:HD23	1:A:242:LEU:HA	1.95	0.42
1:A:684:VAL:HG23	1:A:685:PHE:CD2	2.55	0.42
1:A:1558:ARG:NH1	1:A:1597:ASP:OD1	2.53	0.42
1:A:1078:LYS:HE2	1:A:1261:LEU:HD11	2.02	0.42
1:A:1346:LEU:HA	1:A:1349:PRO:HG2	2.01	0.42
1:A:1520:PRO:O	1:A:1521:ARG:CB	2.68	0.42
1:A:2059:GLU:OE2	1:A:2154:TYR:OH	2.31	0.42
1:A:2083:PHE:HE2	1:A:2179:LYS:HB2	1.85	0.42
1:A:2204:VAL:O	1:A:2204:VAL:HG13	2.20	0.41
1:A:54:MET:SD	1:A:56:PHE:HB3	2.60	0.41
1:A:446:MET:HB3	1:A:816:ALA:HB2	2.02	0.41
1:A:578:GLU:HG3	1:A:579:GLU:CD	2.45	0.41
1:A:621:MET:HE1	1:A:716:LEU:HD22	2.01	0.41
1:A:1042:GLY:HA3	1:A:1111:HIS:HD2	1.85	0.41
1:A:1582:TRP:CE3	1:A:1583:ASN:HB2	2.55	0.41
1:A:414:PRO:O	1:A:418:ILE:HG12	2.20	0.41
1:A:1372:MET:O	1:A:1376:ARG:HG3	2.20	0.41
1:A:594:LEU:O	1:A:598:LEU:HG	2.20	0.41
1:A:1614:TRP:HA	1:A:1621:ARG:HG2	2.02	0.41
1:A:1711:ARG:O	1:A:1713:ASP:N	2.46	0.41
1:A:68:GLU:HG3	1:A:186:ARG:CZ	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1290:ASP:O	1:A:1291:GLU:HB2	2.21	0.41
1:A:2254:THR:HG22	1:A:2292:ALA:HB3	2.03	0.41
1:A:2375:ARG:NH1	1:A:2751:THR:O	2.54	0.41
1:A:825:ASP:N	1:A:826:PRO:HD3	2.35	0.41
1:A:1441:ASP:O	1:A:1445:LYS:HG3	2.20	0.41
1:A:2255:THR:OG1	1:A:2282:THR:OG1	2.34	0.41
1:A:61:ARG:HG3	1:A:65:ASN:HD21	1.86	0.41
1:A:515:ASN:ND2	1:A:634:VAL:HB	2.32	0.41
1:A:813:TRP:HZ3	1:A:967:TRP:HZ2	1.69	0.41
1:A:970:SER:HB3	1:A:971:PRO:HD3	2.02	0.41
1:A:1735:ALA:HB2	1:A:1787:LEU:HD13	2.03	0.41
1:A:255:TRP:O	1:A:259:ARG:HG3	2.21	0.41
1:A:879:VAL:O	1:A:883:ILE:HG23	2.21	0.41
1:A:946:LEU:O	1:A:950:ALA:HB2	2.20	0.41
1:A:1118:ALA:HB1	1:A:1122:TRP:CZ3	2.56	0.41
1:A:2777:VAL:HG12	1:A:2779:PRO:HD3	2.02	0.41
1:A:27:ALA:HB2	1:A:51:PRO:HG3	2.04	0.40
1:A:435:MET:C	1:A:437:TRP:H	2.29	0.40
1:A:739:ASP:OD1	1:A:739:ASP:N	2.54	0.40
1:A:982:GLU:H	1:A:982:GLU:CD	2.29	0.40
1:A:1277:LEU:HD23	1:A:1294:TYR:O	2.21	0.40
1:A:1343:PHE:O	1:A:1347:MET:HE3	2.21	0.40
1:A:1949:ASP:HA	1:A:1952:SER:OG	2.20	0.40
1:A:951:LEU:HB3	1:A:952:PRO:HD3	2.04	0.40
1:A:2037:PRO:O	1:A:2065:ASN:ND2	2.55	0.40
1:A:66:GLU:OE2	1:A:66:GLU:HA	2.21	0.40
1:A:136:GLY:O	1:A:140:VAL:HG23	2.21	0.40
1:A:497:SER:O	1:A:498:ARG:HG2	2.21	0.40
1:A:1355[A]:ARG:HG3	1:A:1516:GLN:NE2	2.36	0.40
1:A:2130:LYS:NZ	1:A:2131:LEU:O	2.55	0.40
1:A:2270:PRO:C	1:A:2272:GLY:H	2.29	0.40
1:A:2420:GLN:HE22	1:A:2505:ALA:HB2	1.86	0.40
1:A:598:LEU:HD22	1:A:617:VAL:HG21	2.03	0.40
1:A:1386:GLU:HB2	1:A:1401:THR:O	2.20	0.40
1:A:1721:ARG:HA	1:A:1721:ARG:HD3	1.82	0.40
1:A:1757:ARG:NE	1:A:2070:THR:O	2.54	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	2772/2818 (98%)	2502 (90%)	245 (9%)	25 (1%)	14	42

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	TYR
1	A	246	SER
1	A	407	ASN
1	A	498	ARG
1	A	737	SER
1	A	1291	GLU
1	A	1519	ALA
1	A	1520	PRO
1	A	1897	ILE
1	A	2028	PRO
1	A	2037	PRO
1	A	108	ARG
1	A	588	ARG
1	A	2000	VAL
1	A	617	VAL
1	A	650	ILE
1	A	2487	PHE
1	A	1517	GLU
1	A	2055	LYS
1	A	1525	VAL
1	A	1622	VAL
1	A	579	GLU
1	A	2535	VAL
1	A	657	VAL
1	A	2036	GLU

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	2222/2333 (95%)	2212 (100%)	10 (0%)	81	81

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ARG
1	A	194[A]	ARG
1	A	194[B]	ARG
1	A	493	CYS
1	A	494	MET
1	A	586	ARG
1	A	1326	VAL
1	A	1327	VAL
1	A	1355[A]	ARG
1	A	1355[B]	ARG

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	369	HIS
1	A	515	ASN
1	A	1015	GLN
1	A	1111	HIS
1	A	1162	HIS
1	A	1430	GLN
1	A	1516	GLN
1	A	1850	GLN
1	A	1851	GLN
1	A	1955	GLN
1	A	1967	HIS
1	A	2068	GLN
1	A	2370	GLN
1	A	2412	GLN
1	A	2663	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 ⓘ

18 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	BGC	B	1	2	11,11,12	0.72	0	15,15,17	1.49	2 (13%)
2	BGC	B	2	2	11,11,12	0.41	0	15,15,17	1.43	3 (20%)
2	BGC	B	3	2	11,11,12	0.61	0	15,15,17	1.92	2 (13%)
2	BGC	B	4	2	11,11,12	0.49	0	15,15,17	1.20	2 (13%)
2	BGC	B	5	2	11,11,12	0.52	0	15,15,17	1.12	2 (13%)
2	BGC	B	6	2	11,11,12	0.49	0	15,15,17	0.99	1 (6%)
2	BGC	B	7	2	11,11,12	0.59	0	15,15,17	1.79	3 (20%)
2	BGC	B	8	2	11,11,12	0.26	0	15,15,17	0.73	0
2	BGC	B	9	2	11,11,12	0.47	0	15,15,17	1.42	2 (13%)
3	BGC	C	1	3	11,11,12	0.21	0	15,15,17	0.37	0
3	BGC	C	2	3	11,11,12	0.73	1 (9%)	15,15,17	1.08	1 (6%)
3	BGC	C	3	3	11,11,12	0.33	0	15,15,17	0.68	0
3	BGC	C	4	3	11,11,12	0.33	0	15,15,17	0.45	0
3	BGC	C	5	3	11,11,12	0.70	1 (9%)	15,15,17	0.87	1 (6%)
3	BGC	C	6	3	11,11,12	0.21	0	15,15,17	0.40	0
3	BGC	C	7	3	11,11,12	0.67	0	15,15,17	0.87	1 (6%)
3	BGC	C	8	3	11,11,12	0.18	0	15,15,17	0.43	0
3	BGC	C	9	3	11,11,12	0.18	0	15,15,17	0.37	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	BGC	B	1	2	-	0/2/19/22	0/1/1/1
2	BGC	B	2	2	-	2/2/19/22	0/1/1/1
2	BGC	B	3	2	-	2/2/19/22	0/1/1/1
2	BGC	B	4	2	-	1/2/19/22	0/1/1/1
2	BGC	B	5	2	-	2/2/19/22	0/1/1/1
2	BGC	B	6	2	-	2/2/19/22	0/1/1/1
2	BGC	B	7	2	-	0/2/19/22	0/1/1/1
2	BGC	B	8	2	-	2/2/19/22	0/1/1/1
2	BGC	B	9	2	-	2/2/19/22	0/1/1/1
3	BGC	C	1	3	-	2/2/19/22	0/1/1/1
3	BGC	C	2	3	-	2/2/19/22	0/1/1/1
3	BGC	C	3	3	-	0/2/19/22	0/1/1/1
3	BGC	C	4	3	-	2/2/19/22	0/1/1/1
3	BGC	C	5	3	-	2/2/19/22	0/1/1/1
3	BGC	C	6	3	-	2/2/19/22	0/1/1/1
3	BGC	C	7	3	-	2/2/19/22	0/1/1/1
3	BGC	C	8	3	-	0/2/19/22	0/1/1/1
3	BGC	C	9	3	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	BGC	O5-C1	2.22	1.47	1.43
3	C	5	BGC	O5-C1	2.06	1.47	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	BGC	C1-C2-C3	6.02	118.40	109.64
2	B	7	BGC	C1-C2-C3	5.09	117.05	109.64
3	C	2	BGC	C1-O5-C5	3.84	117.33	112.19
2	B	9	BGC	C1-C2-C3	3.83	115.22	109.64
2	B	1	BGC	C1-C2-C3	3.19	114.29	109.64
3	C	7	BGC	C1-O5-C5	3.00	116.20	112.19
3	C	5	BGC	C1-O5-C5	2.85	116.00	112.19
2	B	2	BGC	C3-C4-C5	2.80	115.31	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7	BGC	O5-C5-C4	-2.57	104.58	110.83
2	B	1	BGC	C2-C3-C4	2.26	114.84	110.86
2	B	4	BGC	C1-C2-C3	-2.20	106.45	109.64
2	B	5	BGC	C1-O5-C5	-2.18	109.26	112.19
2	B	2	BGC	O5-C1-C2	-2.17	105.61	110.79
2	B	4	BGC	O5-C5-C6	2.15	111.84	107.66
2	B	7	BGC	O5-C1-C2	2.14	115.89	110.79
2	B	9	BGC	C3-C4-C5	-2.12	106.38	110.23
2	B	5	BGC	C1-C2-C3	2.12	112.74	109.64
2	B	3	BGC	C2-C3-C4	2.11	114.58	110.86
2	B	2	BGC	C1-C2-C3	-2.07	106.62	109.64
2	B	6	BGC	C3-C4-C5	2.06	113.97	110.23

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	7	BGC	O5-C5-C6-O6
2	B	5	BGC	O5-C5-C6-O6
2	B	2	BGC	O5-C5-C6-O6
2	B	9	BGC	O5-C5-C6-O6
3	C	7	BGC	C4-C5-C6-O6
3	C	9	BGC	C4-C5-C6-O6
3	C	2	BGC	O5-C5-C6-O6
2	B	3	BGC	O5-C5-C6-O6
3	C	5	BGC	O5-C5-C6-O6
3	C	9	BGC	O5-C5-C6-O6
2	B	9	BGC	C4-C5-C6-O6
3	C	4	BGC	O5-C5-C6-O6
3	C	6	BGC	O5-C5-C6-O6
3	C	4	BGC	C4-C5-C6-O6
3	C	6	BGC	C4-C5-C6-O6
2	B	5	BGC	C4-C5-C6-O6
2	B	2	BGC	C4-C5-C6-O6
2	B	3	BGC	C4-C5-C6-O6
2	B	8	BGC	C4-C5-C6-O6
2	B	6	BGC	C4-C5-C6-O6
3	C	2	BGC	C4-C5-C6-O6
2	B	8	BGC	O5-C5-C6-O6
2	B	6	BGC	O5-C5-C6-O6
3	C	5	BGC	C4-C5-C6-O6
2	B	4	BGC	C4-C5-C6-O6

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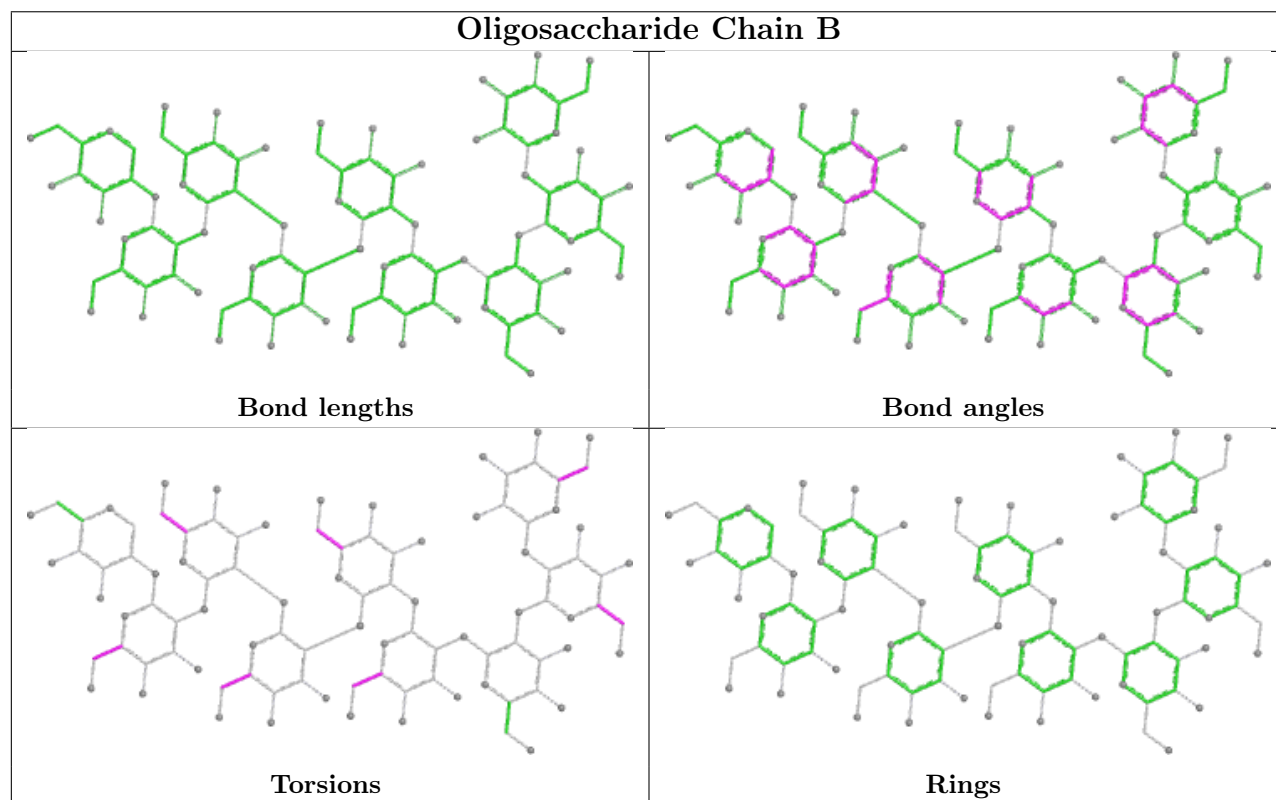
Mol	Chain	Res	Type	Atoms
3	C	1	BGC	C4-C5-C6-O6
3	C	1	BGC	O5-C5-C6-O6

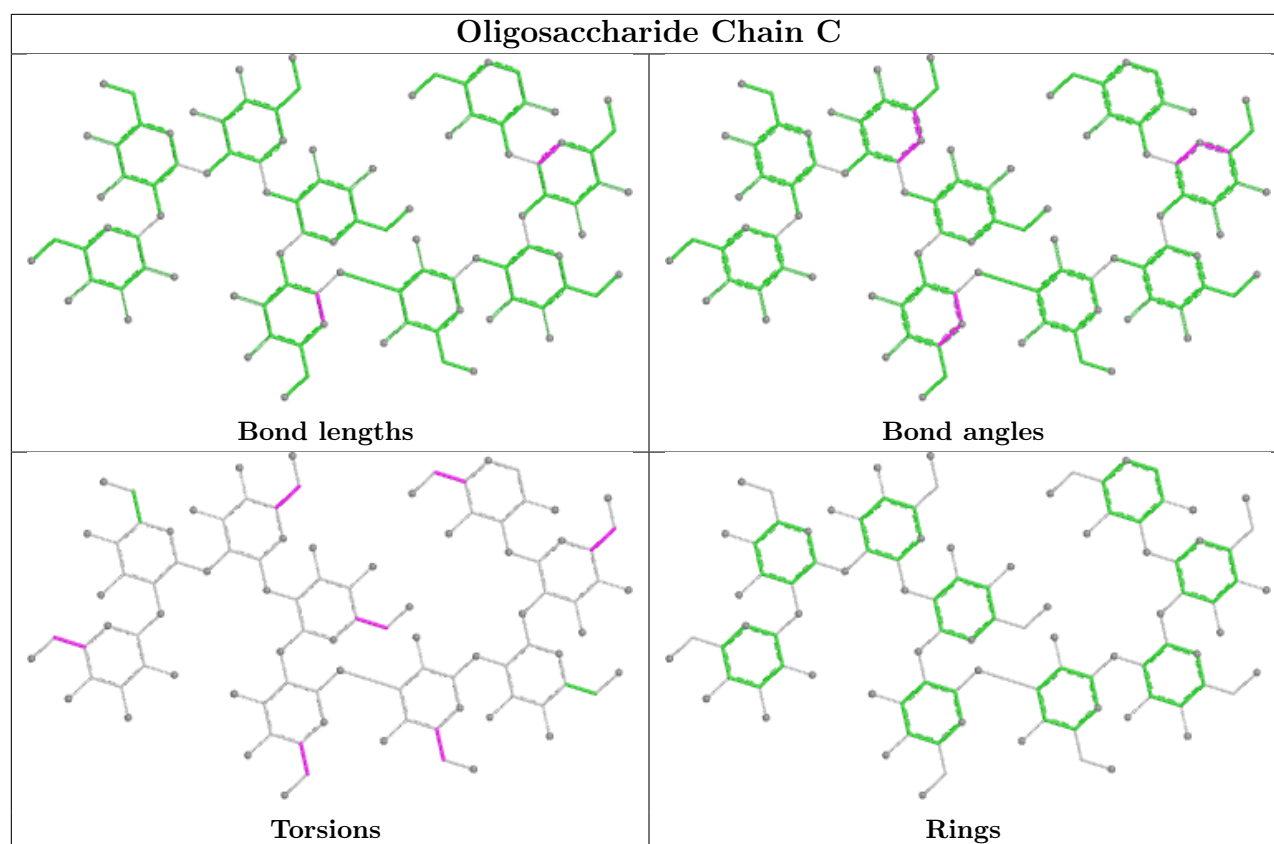
There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	BGC	1	0
2	B	9	BGC	3	0
2	B	4	BGC	1	0
3	C	2	BGC	1	0
2	B	7	BGC	1	0
2	B	6	BGC	1	0
2	B	5	BGC	1	0
2	B	1	BGC	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](#)

1 ligand is 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	UPG	A	2901	-	25,26,38	0.84	1 (4%)	38,40,58	0.75	1 (2%)

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	UPG	A	2901	-	-	3/16/32/59	0/2/2/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2901	UPG	PB-O1B	3.20	1.60	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2901	UPG	O3B-PB-O2B	2.69	117.90	107.80

There are no chirality outliers.

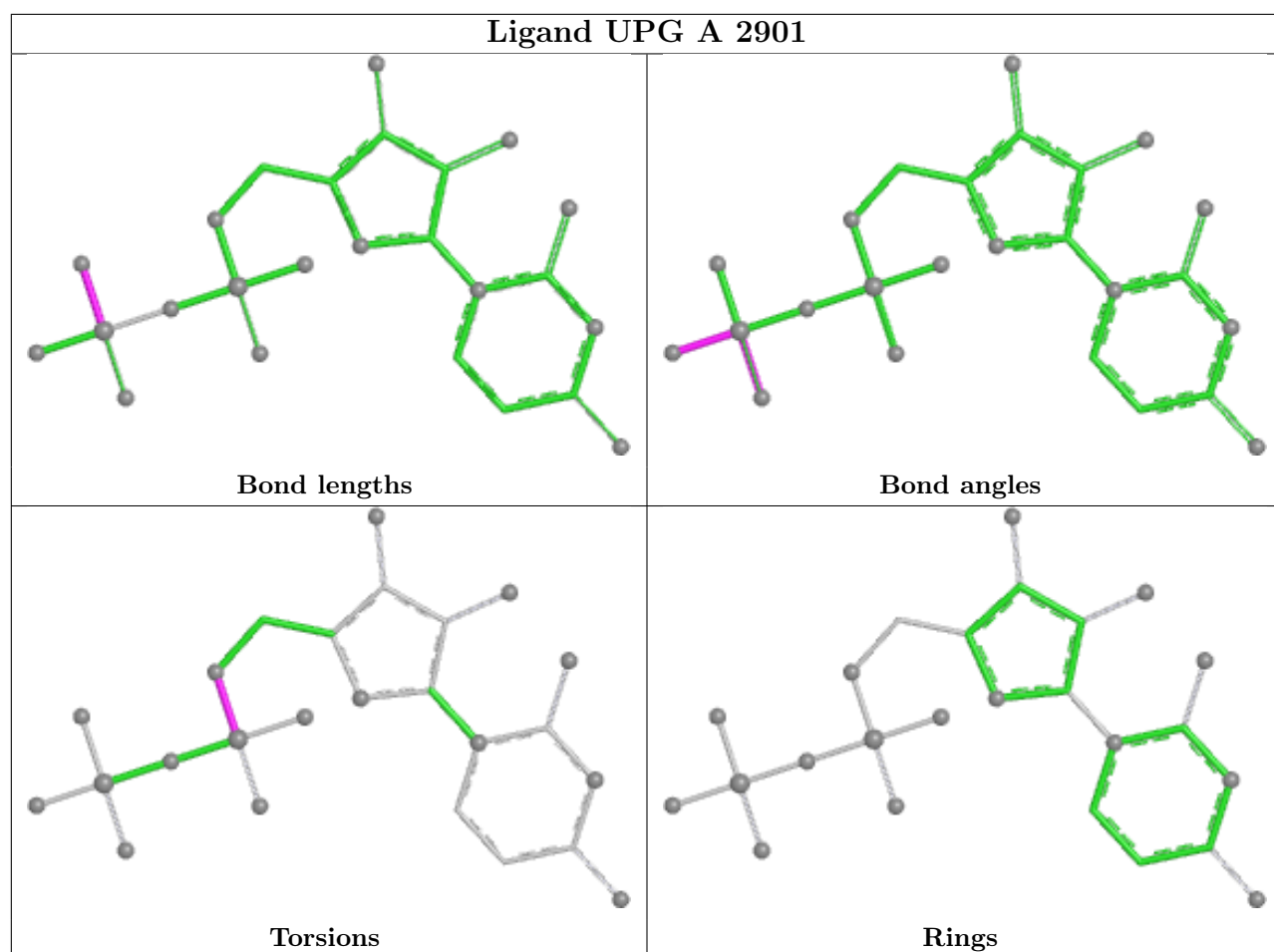
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2901	UPG	C5C-O5C-PA-O1A
4	A	2901	UPG	C5C-O5C-PA-O2A
4	A	2901	UPG	C5C-O5C-PA-O3A

There are no ring outliers.

No monomer is involved in short contacts.

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.

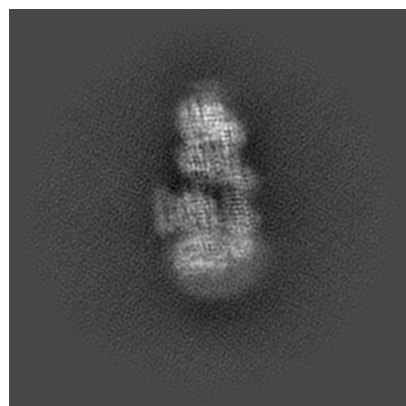
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19114. These allow visual inspection of the internal detail of the map and identification of artifacts.

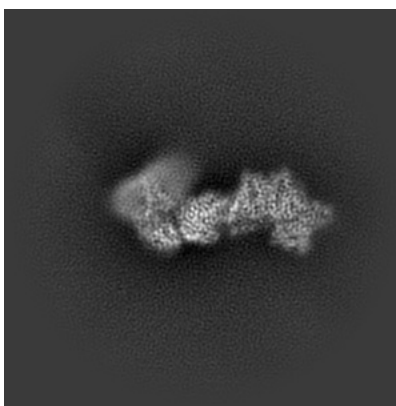
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

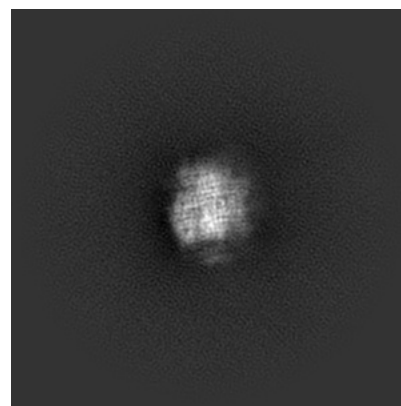
6.1.1 Primary map



X

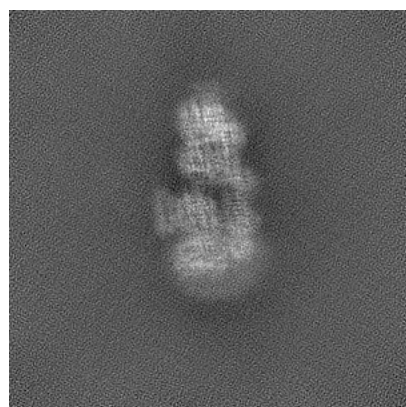


Y

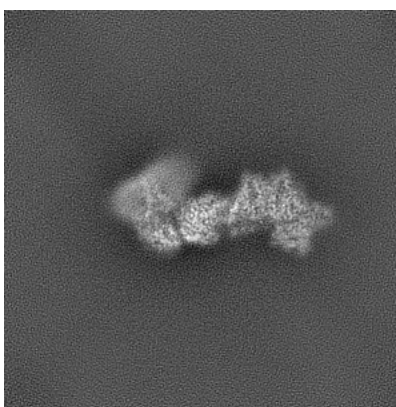


Z

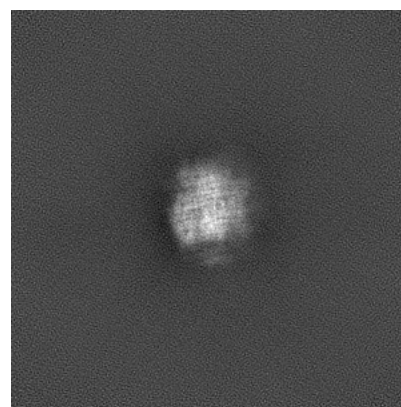
6.1.2 Raw map



X



Y

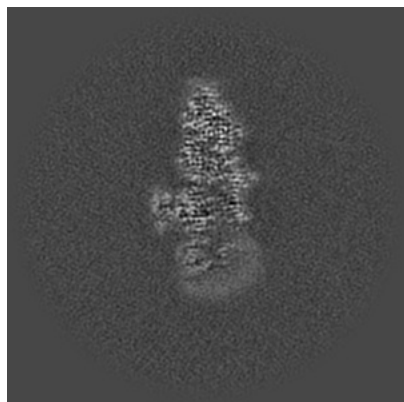


Z

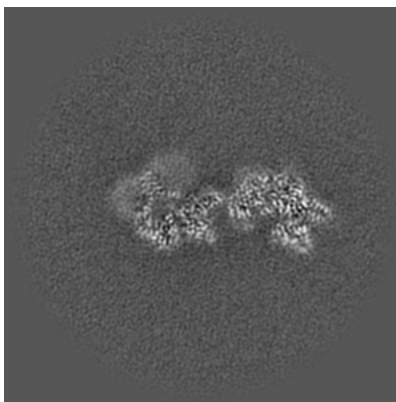
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

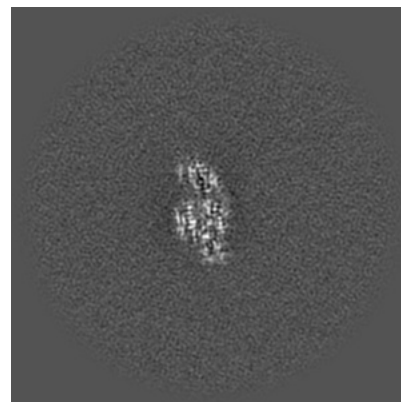
6.2.1 Primary map



X Index: 150

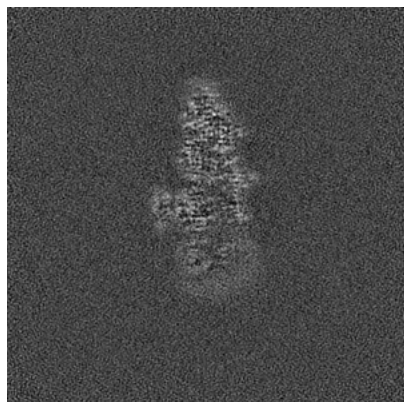


Y Index: 150

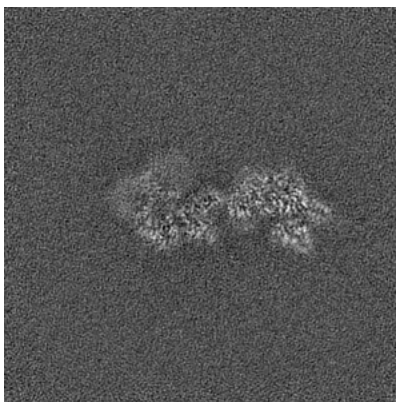


Z Index: 150

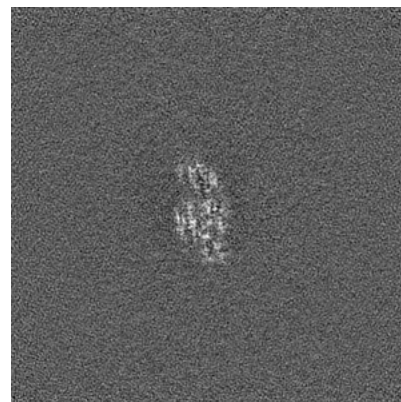
6.2.2 Raw map



X Index: 150



Y Index: 150

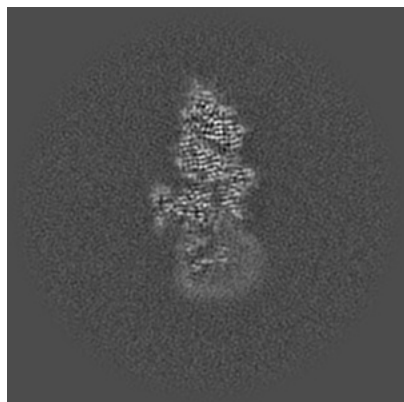


Z Index: 150

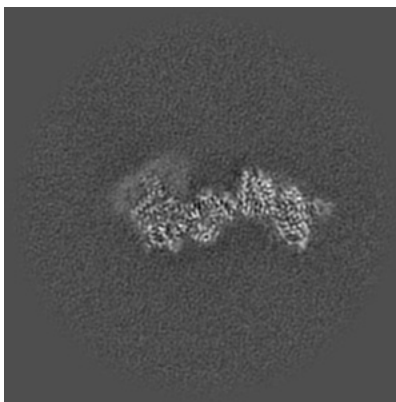
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

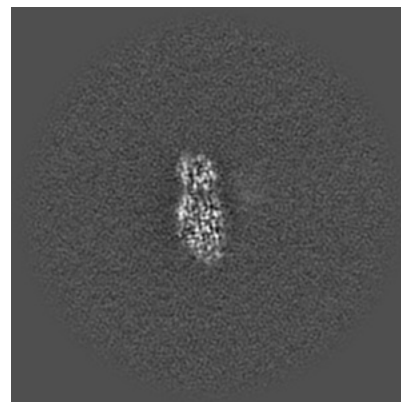
6.3.1 Primary map



X Index: 152

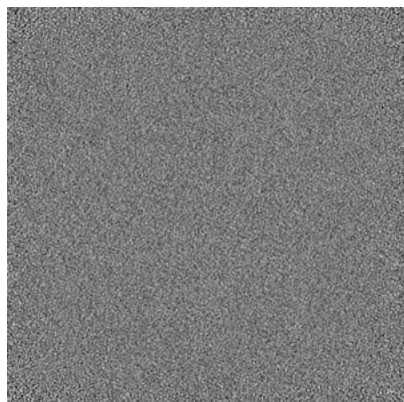


Y Index: 141

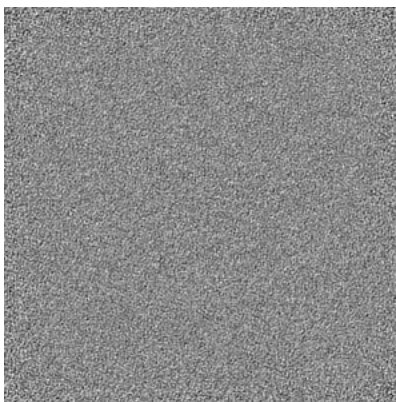


Z Index: 144

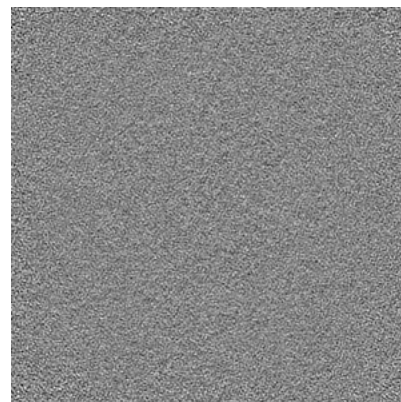
6.3.2 Raw map



X Index: 0



Y Index: 0

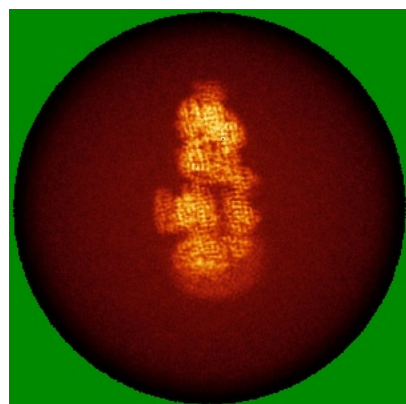


Z Index: 0

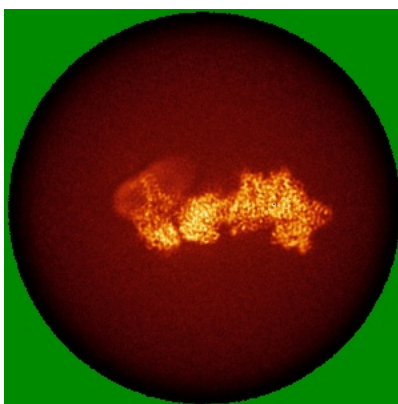
The images above show the largest variance slices of the map in three orthogonal directions.

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

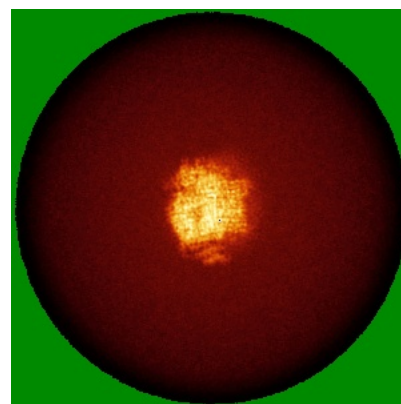
6.4.1 Primary map



X

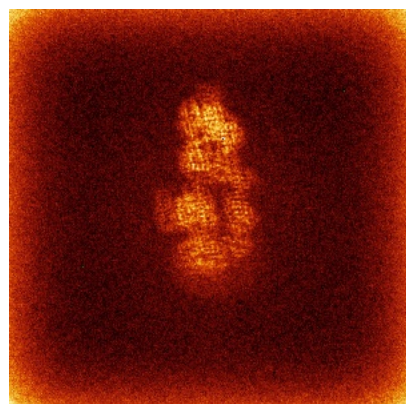


Y

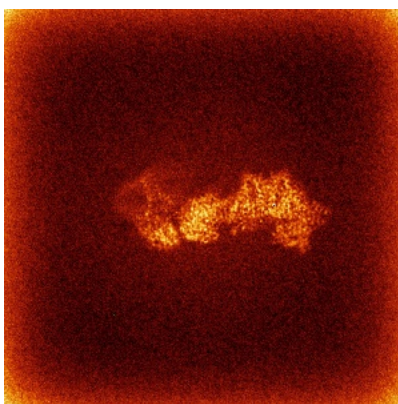


Z

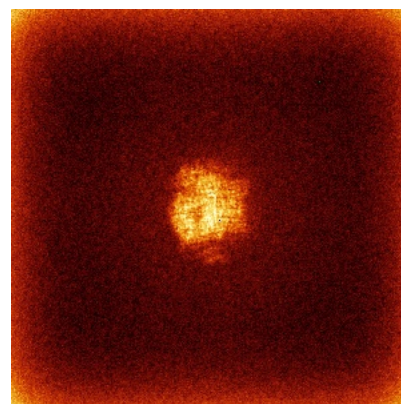
6.4.2 Raw map



X



Y

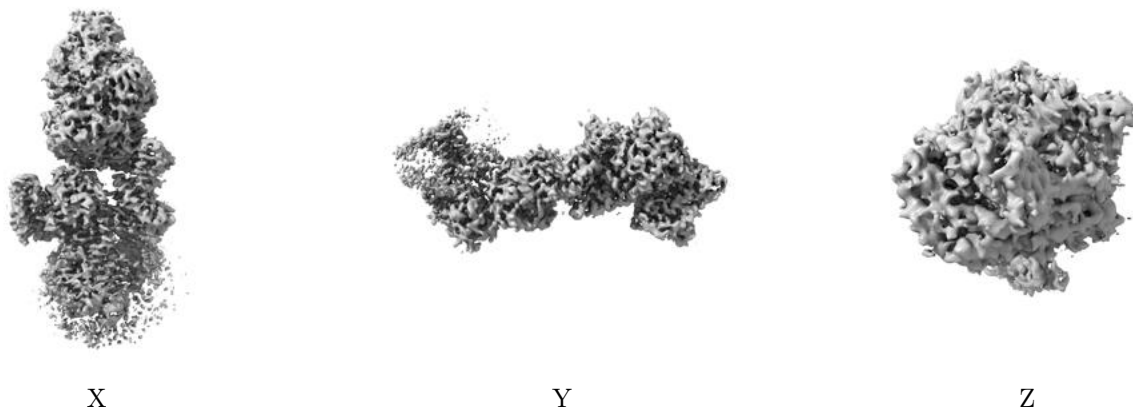


Z

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.

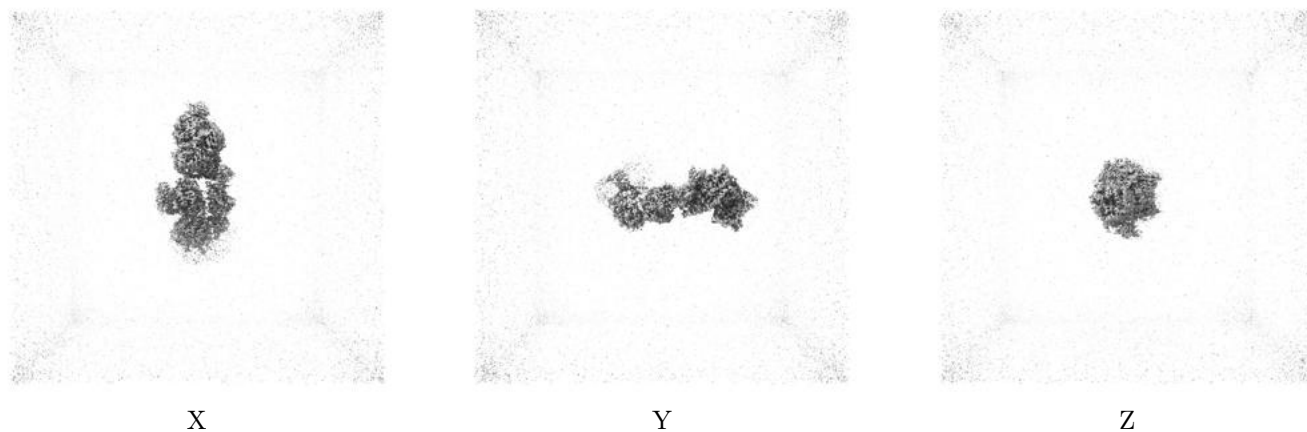
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

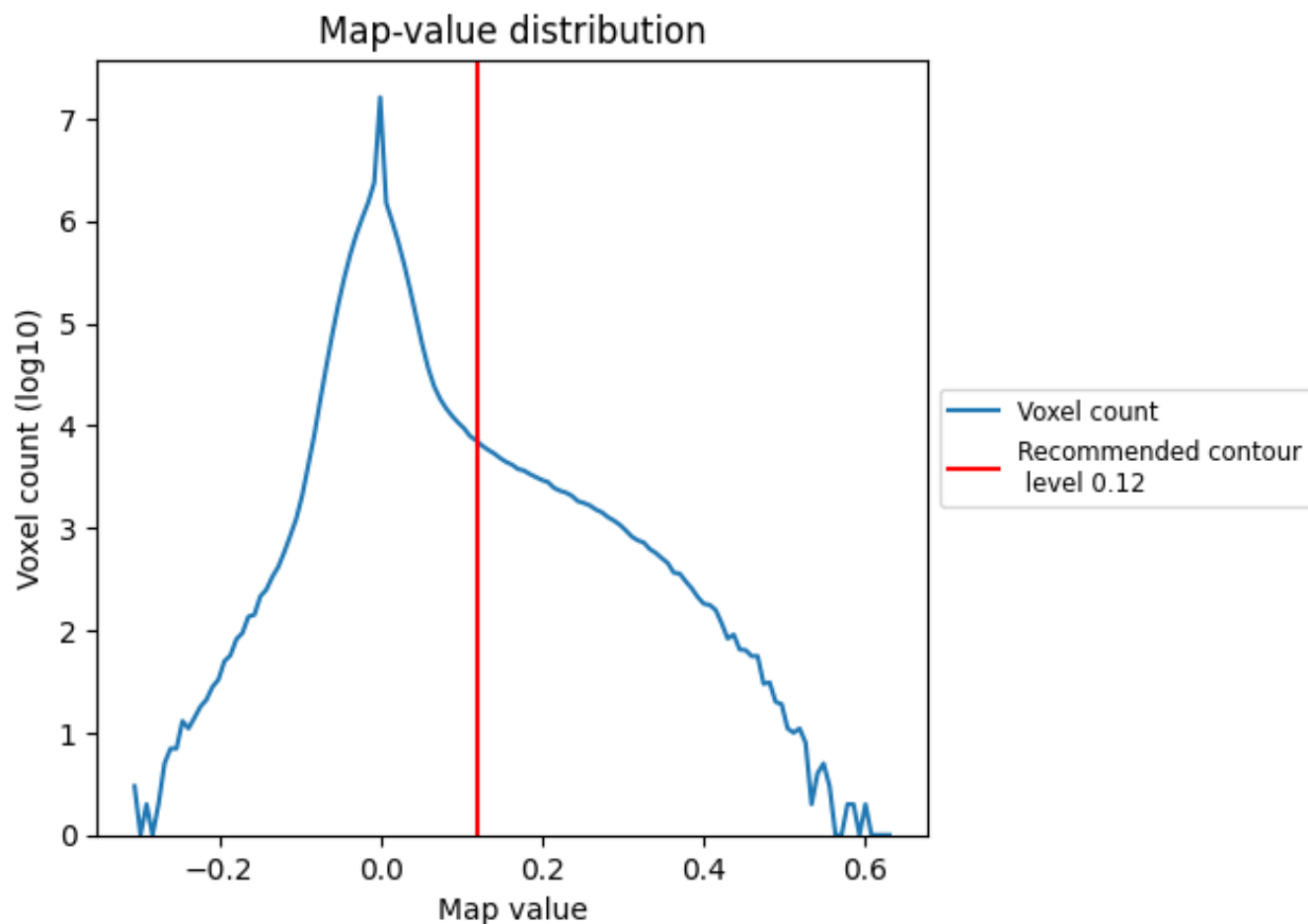
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

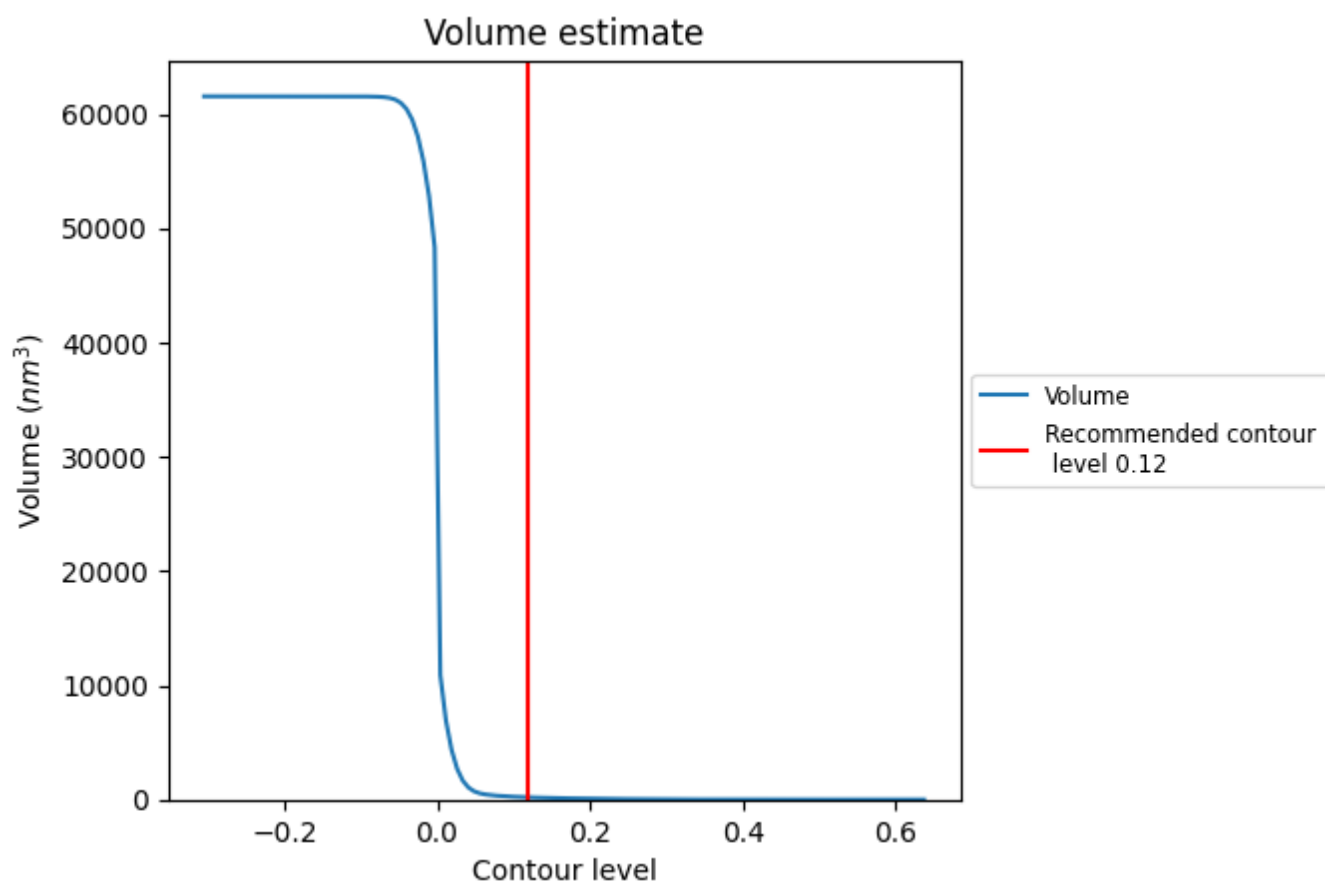
This section contains the results of statistical analysis of the map.

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.

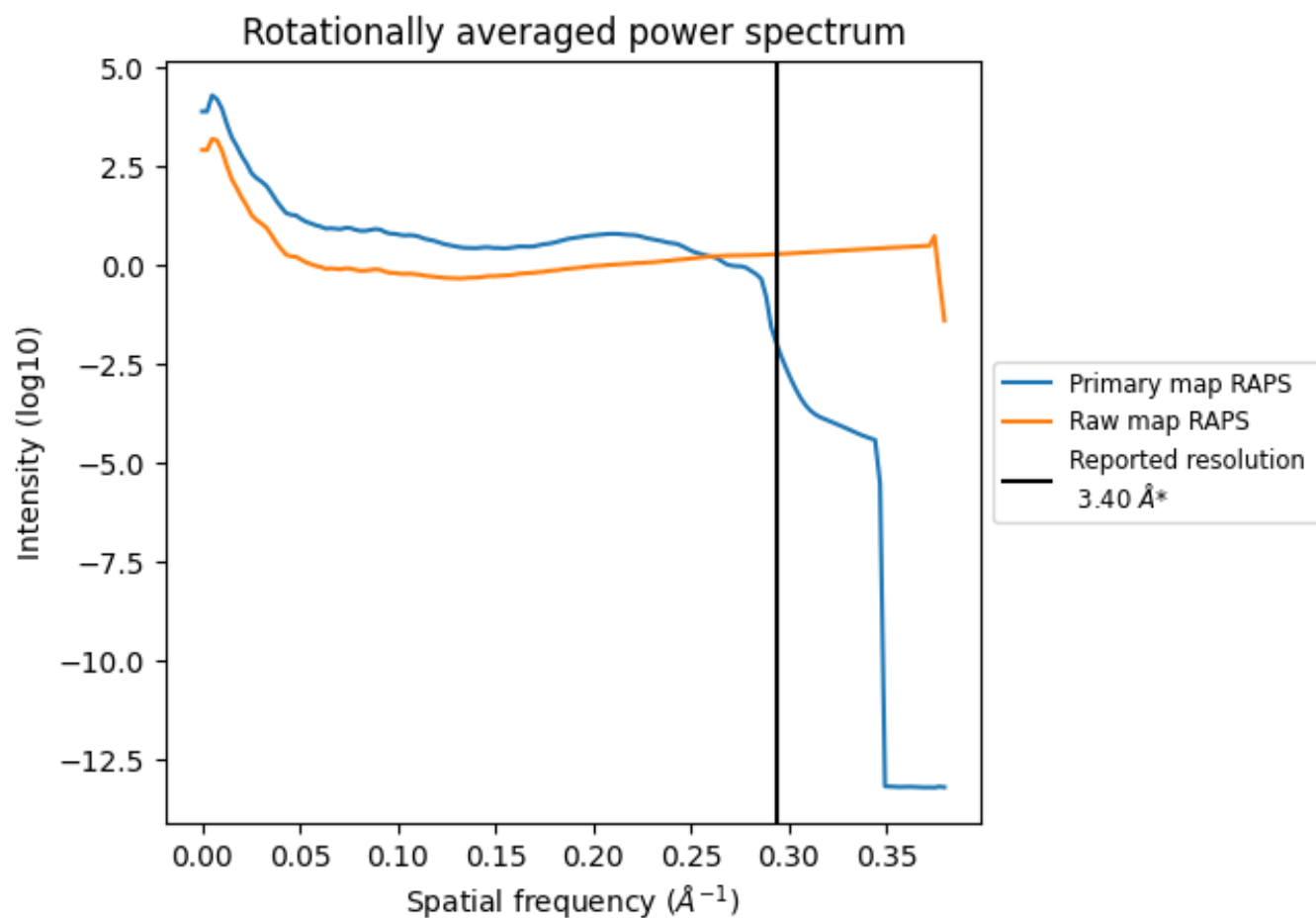
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 193 nm³; this corresponds to an approximate mass of 174 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 ⓘ

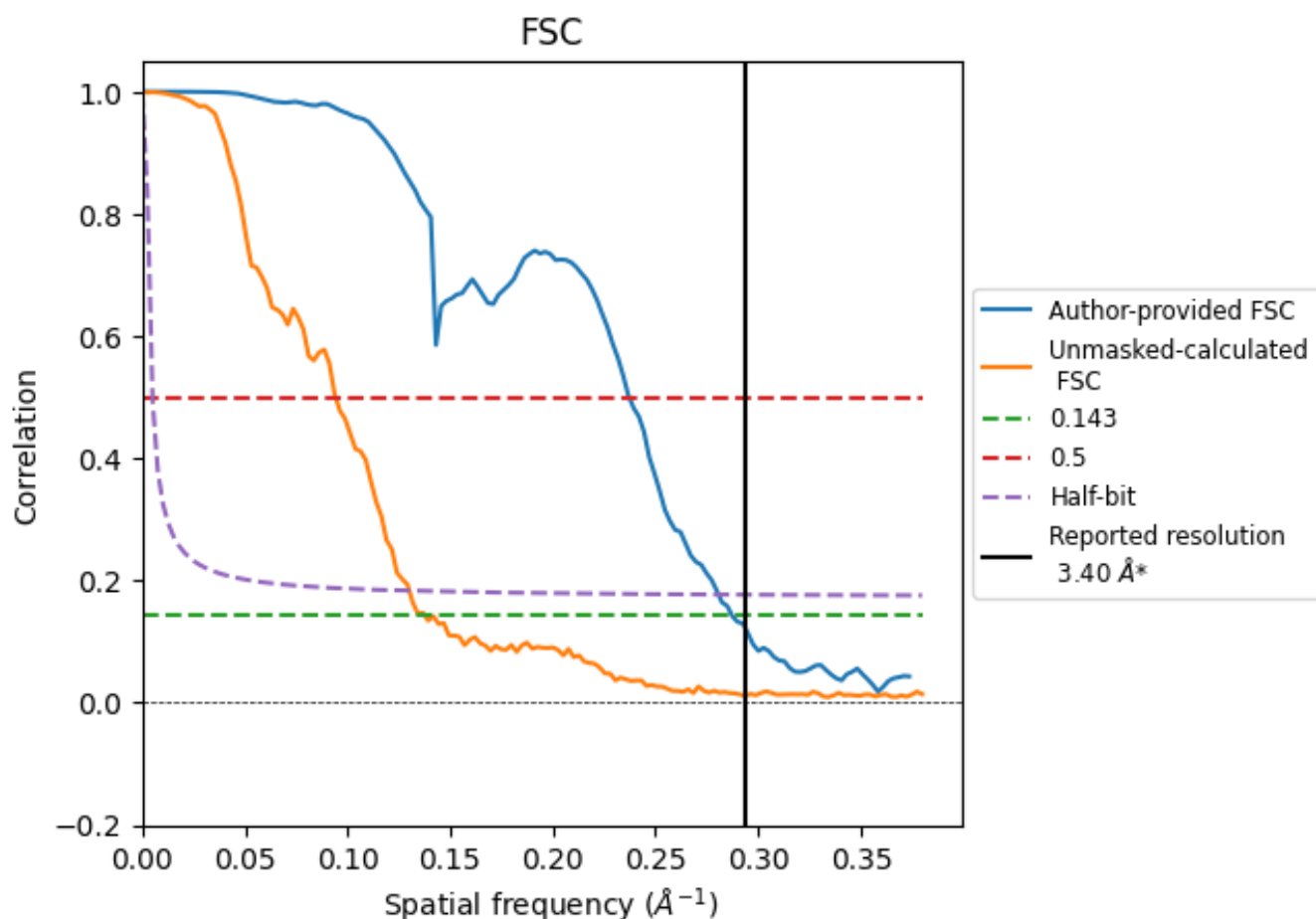


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

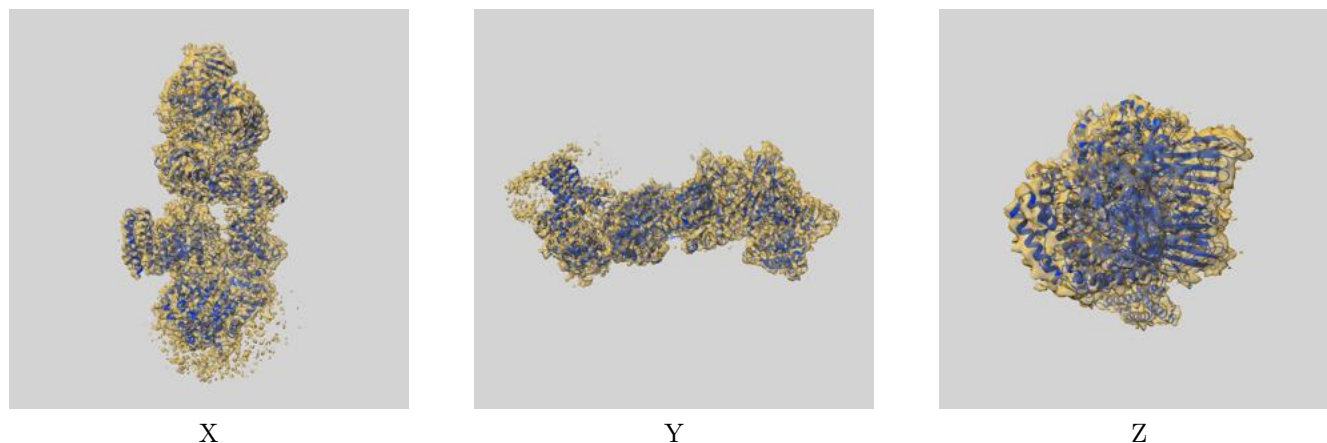
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.48	4.22	3.56
Unmasked-calculated*	7.27	10.62	7.69

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.27 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

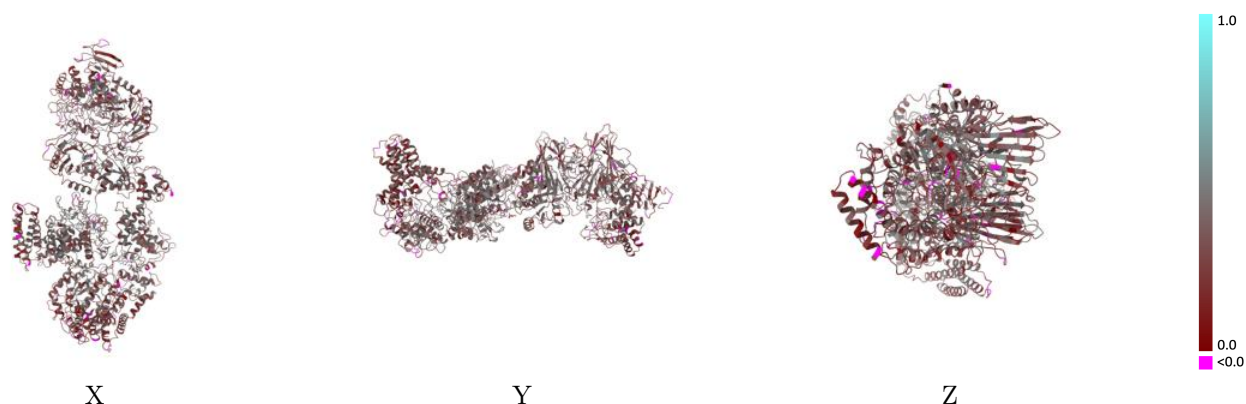
This section contains information regarding the fit between EMDB map EMD-19114 and PDB model 8RF0. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



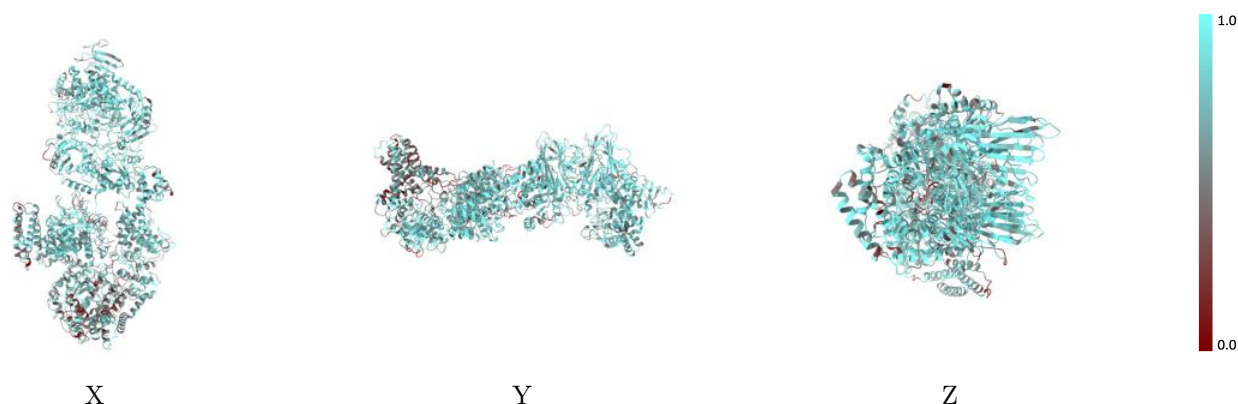
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



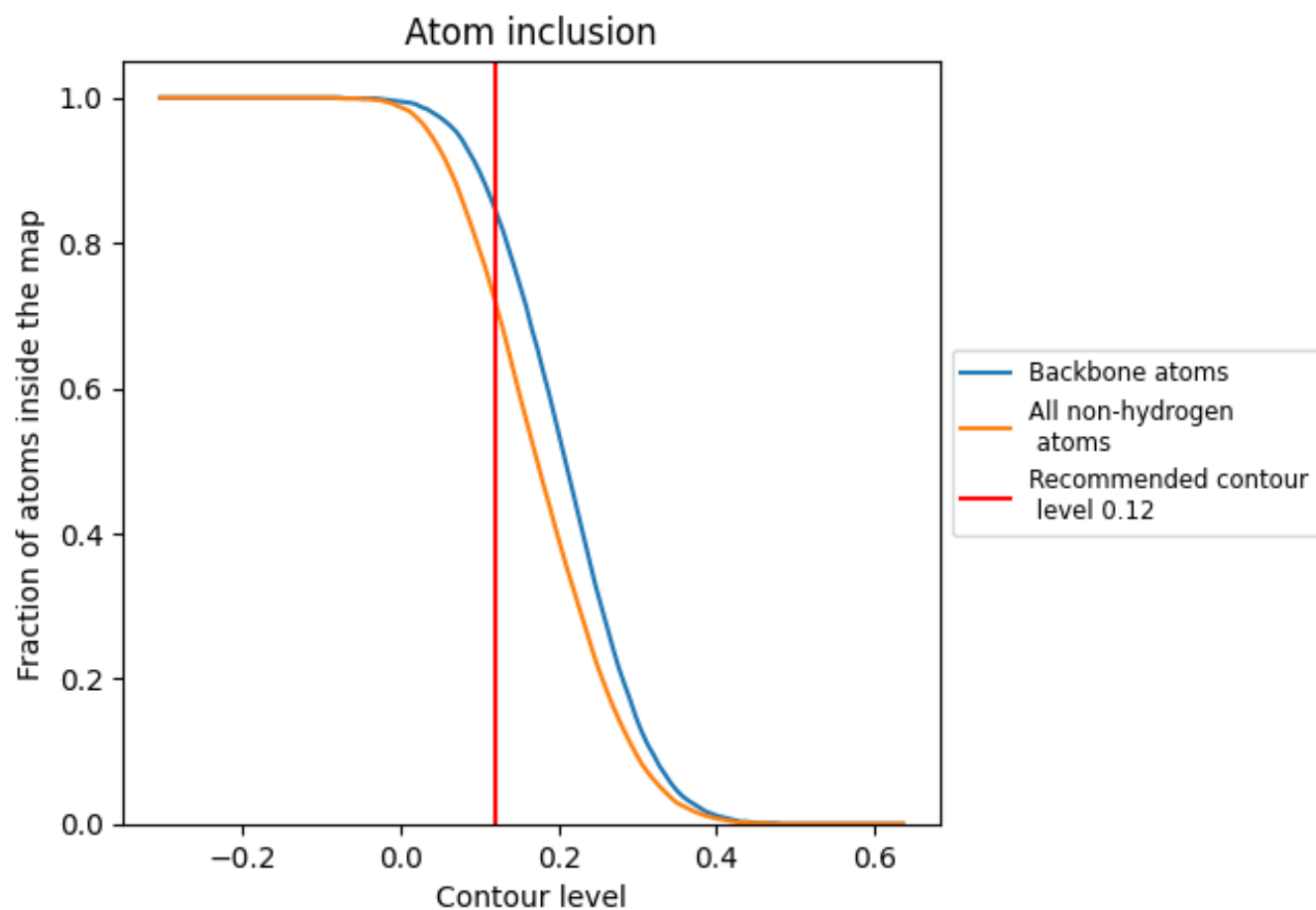
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 72% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7190	0.3220
A	0.7210	0.3210
B	0.8280	0.4980
C	0.2930	0.2020

