



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 04:57 AM UTC

PDB ID : 6CMX / pdb_00006cmx
EMDB ID : EMD-7526
Title : Human Teneurin 2 extra-cellular region
Authors : Shalev-Benami, M.; Li, J.; Sudhof, T.; Skiniotis, G.; Arac, D.
Deposited on : 2018-03-06
Resolution : 3.10 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

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:

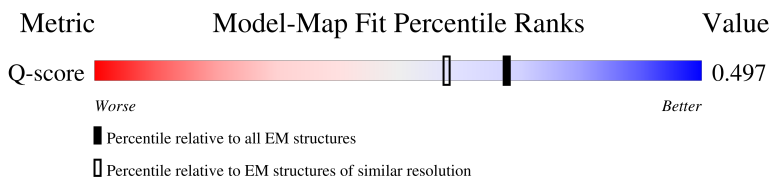
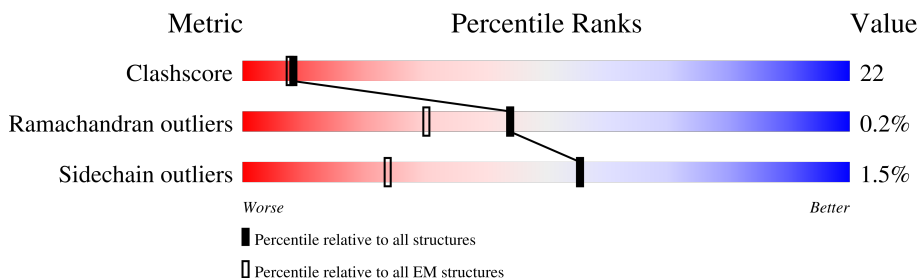
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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

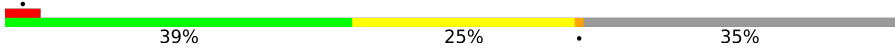
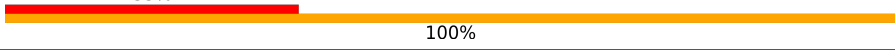
The reported resolution of this entry is 3.10 Å.

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	1999	
2	B	3	
3	C	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	1	X	-	-	-
4	NAG	A	2704	X	-	-	-
4	NAG	A	2708	X	-	-	-

2 Entry composition [i](#)

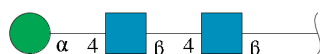
There are 5 unique types of molecules in this entry. The entry contains 10139 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Teneurin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1300	9919	6354	1729	1803	33	0	0

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



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

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
3	C	2	22	12	10	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

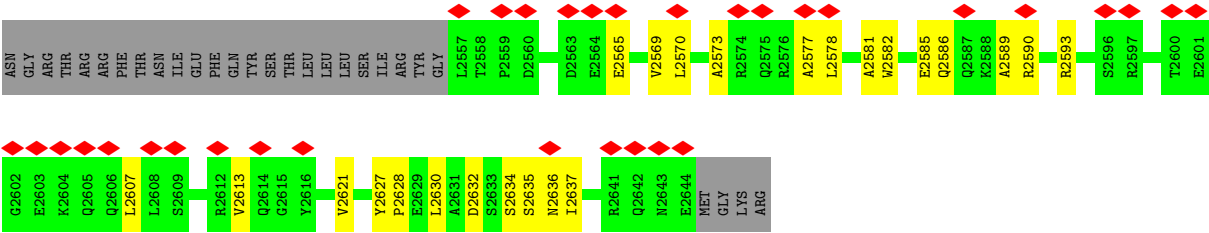
- Molecule 5 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			11	6	5	
5	A	1	Total	C	O	0
			11	6	5	
5	A	1	Total	C	O	0
			11	6	5	



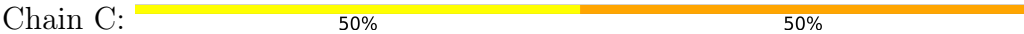




• Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	426107	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	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	0.373	Depositor
Minimum map value	-0.250	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	260.0, 260.0, 260.0	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.36	8/10159 (0.1%)	0.56	18/13820 (0.1%)

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	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2424	HIS	ND1-CE1	5.27	1.37	1.32
1	A	2493	HIS	ND1-CE1	5.25	1.37	1.32
1	A	2208	HIS	ND1-CE1	5.17	1.37	1.32
1	A	989	HIS	ND1-CE1	5.15	1.37	1.32
1	A	1851	HIS	ND1-CE1	5.14	1.37	1.32
1	A	2227	HIS	ND1-CE1	5.13	1.37	1.32
1	A	2014	ASN	CG-OD1	5.13	1.33	1.23
1	A	1643	GLN	CD-OE1	5.07	1.33	1.23

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	989	HIS	CB-CG-CD2	-6.75	122.42	131.20
1	A	2424	HIS	CB-CG-CD2	-6.59	122.63	131.20
1	A	2227	HIS	CB-CG-CD2	-6.59	122.64	131.20
1	A	2208	HIS	CB-CG-CD2	-6.55	122.69	131.20
1	A	2137	LYS	CA-C-N	6.53	130.65	120.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2137	LYS	C-N-CA	6.53	130.65	120.34
1	A	2493	HIS	CB-CG-CD2	-6.52	122.72	131.20
1	A	906	VAL	N-CA-C	6.43	117.18	110.62
1	A	1851	HIS	CB-CG-CD2	-6.42	122.85	131.20
1	A	989	HIS	CB-CG-ND1	5.81	131.41	122.70
1	A	2424	HIS	CB-CG-ND1	5.70	131.26	122.70
1	A	2208	HIS	CB-CG-ND1	5.70	131.25	122.70
1	A	2493	HIS	CB-CG-ND1	5.68	131.22	122.70
1	A	2227	HIS	CB-CG-ND1	5.64	131.16	122.70
1	A	1851	HIS	CB-CG-ND1	5.52	130.98	122.70
1	A	1662	PHE	O-C-N	-5.47	116.40	122.86
1	A	986	VAL	CG1-CB-CG2	5.43	122.75	110.80
1	A	2053	TYR	CA-CB-CG	5.11	123.09	113.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1907	TYR	Peptide
1	A	2012	ASP	Peptide
1	A	2137	LYS	Peptide
1	A	2432	GLY	Peptide

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	9919	0	9403	416	0
2	B	39	0	34	2	0
3	C	22	0	19	1	0
4	A	126	0	115	15	0
5	A	33	0	30	2	0
All	All	10139	0	9601	427	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 22.

All (427) 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:1646:ASN:O	4:A:2705:NAG:C1	1.97	1.11
1:A:2128:ILE:HD11	1:A:2310:ARG:HD2	1.50	0.91
1:A:1888:THR:OG1	1:A:2141:ASP:OD2	1.89	0.88
1:A:1577:ASP:HB2	1:A:1586:ASN:OD1	1.74	0.88
1:A:933:GLU:HG2	1:A:1620:VAL:HG11	1.57	0.85
1:A:1573:THR:OG1	1:A:2444:LYS:O	1.94	0.84
1:A:960:TYR:O	1:A:1009:LYS:NZ	2.11	0.83
4:A:2706:NAG:H3	4:A:2706:NAG:H82	1.61	0.83
1:A:2126:ASP:O	1:A:2310:ARG:NH2	2.11	0.82
1:A:1732:GLU:OE2	1:A:1747:TYR:OH	1.98	0.81
1:A:1917:ASP:OD2	1:A:1920:THR:OG1	1.98	0.81
1:A:2012:ASP:O	1:A:2014:ASN:N	2.12	0.79
1:A:2284:GLY:N	1:A:2288:GLY:O	2.16	0.78
1:A:1835:LEU:HD11	1:A:2323:GLY:HA3	1.68	0.76
1:A:1491:PHE:CE1	1:A:1502:LEU:HD13	2.21	0.76
1:A:933:GLU:OE2	1:A:2400:VAL:HG12	1.86	0.75
1:A:2349:TYR:O	1:A:2422:LYS:NZ	2.20	0.75
1:A:1555:THR:OG1	1:A:1565:THR:OG1	2.03	0.75
1:A:1886:LEU:N	1:A:1886:LEU:HD23	2.01	0.74
1:A:1756:TRP:NE1	1:A:2351:THR:O	2.22	0.73
1:A:1904:GLU:OE1	1:A:2627:TYR:OH	2.07	0.73
1:A:1585:THR:HB	4:A:2704:NAG:H82	1.72	0.71
1:A:952:TYR:OH	1:A:1561:GLY:O	2.07	0.71
1:A:1476:HIS:NE2	1:A:1479:THR:OG1	2.24	0.71
1:A:2573:ALA:HB1	1:A:2632:ASP:CB	2.20	0.71
1:A:2245:ASN:ND2	1:A:2340:LEU:O	2.24	0.70
1:A:1799:MET:HB3	1:A:1805:VAL:HG23	1.72	0.70
1:A:2261:LYS:NZ	1:A:2279:PHE:O	2.24	0.70
1:A:1481:SER:HG	1:A:1484:THR:HG1	1.38	0.70
4:A:2705:NAG:O7	4:A:2705:NAG:O3	2.05	0.69
1:A:2062:ARG:HH22	1:A:2340:LEU:HD22	1.58	0.69
1:A:2172:VAL:HG22	1:A:2187:THR:HG22	1.74	0.69
1:A:1596:SER:HB2	4:A:2704:NAG:H83	1.75	0.68
1:A:2223:ASP:OD1	1:A:2224:LEU:N	2.26	0.68
5:A:2717:MAN:H3	3:C:2:MAN:O3	1.94	0.68
2:B:1:NAG:O3	2:B:1:NAG:H82	1.93	0.68
1:A:2228:LEU:HD22	1:A:2283:ILE:HD12	1.76	0.68
1:A:2310:ARG:NH2	1:A:2332:TYR:CD2	2.62	0.67
1:A:1568:ASP:OD1	1:A:1569:GLU:N	2.26	0.67
1:A:934:THR:O	1:A:936:VAL:N	2.27	0.67
1:A:1645:CYS:SG	1:A:1646:ASN:N	2.67	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2248:THR:HB	1:A:2285:PHE:O	1.94	0.66
1:A:1775:LEU:HD21	1:A:2422:LYS:HA	1.77	0.66
1:A:1856:TYR:HB3	1:A:1881:LEU:HD12	1.77	0.66
1:A:2128:ILE:HD11	1:A:2310:ARG:CD	2.25	0.65
1:A:1762:LEU:HD11	1:A:2360:PHE:HE1	1.59	0.65
1:A:1531:ILE:HG12	1:A:1546:THR:HG22	1.78	0.65
1:A:2203:PRO:O	1:A:2204:THR:OG1	2.15	0.65
1:A:2001:GLU:HA	1:A:2008:VAL:HG22	1.79	0.65
1:A:1614:ARG:HH12	1:A:1881:LEU:HD21	1.62	0.64
1:A:1846:HIS:ND1	1:A:1861:TYR:OH	2.28	0.64
4:A:2706:NAG:H82	4:A:2706:NAG:C3	2.24	0.64
1:A:2565:GLU:O	1:A:2569:VAL:N	2.30	0.63
1:A:1780:ARG:NH2	1:A:2348:ASN:O	2.32	0.62
1:A:1886:LEU:CD1	1:A:2489:GLY:HA2	2.29	0.62
1:A:2304:TYR:CE1	1:A:2309:GLY:O	2.52	0.62
1:A:2077:TYR:HD1	1:A:2088:VAL:HG22	1.64	0.62
1:A:1693:ILE:HG22	1:A:1715:VAL:HG13	1.81	0.62
1:A:1505:ASN:OD1	1:A:1506:ASN:N	2.32	0.62
1:A:1525:MET:HE3	1:A:1531:ILE:HD12	1.81	0.62
1:A:1646:ASN:O	1:A:1647:ASN:HB2	1.99	0.62
1:A:932:PRO:O	1:A:1607:ILE:HD13	2.00	0.61
1:A:1953:PHE:N	1:A:1960:ASN:OD1	2.31	0.61
1:A:2014:ASN:HD22	1:A:2014:ASN:C	2.08	0.61
1:A:1734:ILE:HG22	1:A:1741:PHE:HE2	1.65	0.61
1:A:2011:TYR:O	1:A:2012:ASP:O	2.19	0.61
4:A:2702:NAG:HO3	4:A:2702:NAG:HO6	1.47	0.61
1:A:1553:LEU:O	1:A:1567:SER:N	2.32	0.61
1:A:1679:ARG:NH1	1:A:1679:ARG:HG2	2.15	0.61
1:A:1020:LEU:HG	1:A:1046:LEU:HD11	1.82	0.60
1:A:1787:THR:HB	1:A:1795:ILE:HD11	1.83	0.60
1:A:949:LYS:O	1:A:1063:ASP:N	2.32	0.60
1:A:1609:ILE:O	1:A:1609:ILE:HG22	2.00	0.60
1:A:1776:ALA:HB1	1:A:1787:THR:OG1	2.02	0.60
1:A:1020:LEU:HB2	1:A:1074:ILE:HD11	1.84	0.60
1:A:1679:ARG:HH11	1:A:1679:ARG:CG	2.14	0.60
1:A:965:LYS:HD2	1:A:1004:THR:HG22	1.82	0.60
1:A:1471:ASN:O	1:A:1472:ALA:HB3	2.02	0.60
1:A:1784:SER:OG	1:A:1801:ALA:HB2	2.02	0.60
1:A:1948:LYS:HE2	1:A:1950:ILE:HD11	1.84	0.60
1:A:1535:VAL:HA	1:A:1541:LEU:HA	1.84	0.59
1:A:1756:TRP:HZ3	1:A:1767:VAL:CG2	2.15	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1906:VAL:HG12	1:A:2630:LEU:HD21	1.85	0.59
1:A:2119:PRO:C	1:A:2120:LEU:HD12	2.28	0.59
1:A:2244:ASP:OD1	1:A:2246:THR:OG1	2.15	0.59
1:A:2080:ASP:OD1	1:A:2081:GLY:N	2.34	0.58
1:A:1074:ILE:HG21	1:A:1076:HIS:CE1	2.39	0.58
1:A:1555:THR:O	1:A:1565:THR:OG1	2.21	0.58
1:A:1756:TRP:CZ3	1:A:1767:VAL:CG2	2.87	0.58
1:A:2206:ILE:HD13	1:A:2289:LEU:HD21	1.85	0.58
1:A:1846:HIS:HD1	1:A:1861:TYR:HH	1.47	0.58
1:A:1958:MET:SD	1:A:2194:GLN:OE1	2.62	0.58
1:A:2015:GLN:OE1	1:A:2225:GLN:NE2	2.37	0.58
1:A:923:ALA:HB2	1:A:2406:ARG:HH21	1.69	0.58
1:A:1958:MET:SD	1:A:2184:SER:OG	2.62	0.57
1:A:1720:LEU:HD21	1:A:2367:ILE:HG21	1.84	0.57
1:A:2634:SER:O	1:A:2637:ILE:HG22	2.04	0.57
1:A:2011:TYR:O	1:A:2014:ASN:ND2	2.37	0.57
1:A:2245:ASN:OD1	1:A:2246:THR:N	2.37	0.57
1:A:2066:LEU:HD13	1:A:2262:GLN:OE1	2.05	0.56
1:A:1480:VAL:HG22	1:A:1487:TYR:CD1	2.40	0.56
1:A:2088:VAL:HB	1:A:2096:TRP:HB2	1.87	0.56
1:A:1575:PHE:HE2	1:A:2459:VAL:H	1.53	0.56
1:A:1638:VAL:HG21	1:A:1899:LEU:HD21	1.86	0.56
1:A:2390:ALA:O	1:A:2393:ASN:ND2	2.39	0.56
1:A:2485:TYR:OH	1:A:2628:PRO:O	2.24	0.56
1:A:965:LYS:CD	1:A:1004:THR:HG22	2.36	0.56
1:A:1679:ARG:HD3	1:A:1679:ARG:H	1.70	0.56
1:A:1756:TRP:CZ3	1:A:1767:VAL:HG21	2.40	0.56
1:A:2101:ASP:OD1	1:A:2102:LEU:N	2.38	0.56
1:A:2491:ASP:OD1	1:A:2491:ASP:N	2.27	0.56
1:A:1899:LEU:O	1:A:2395:GLN:NE2	2.38	0.55
1:A:917:LEU:HD13	1:A:1084:PHE:CE2	2.41	0.55
1:A:2304:TYR:CZ	1:A:2309:GLY:O	2.59	0.55
1:A:2364:LEU:O	1:A:2368:ILE:N	2.38	0.55
1:A:1730:ARG:NH2	1:A:1748:ASP:O	2.40	0.55
1:A:2179:VAL:HG12	1:A:2179:VAL:O	2.06	0.55
1:A:1039:LEU:HG	1:A:1039:LEU:O	2.07	0.54
1:A:1906:VAL:HG21	1:A:2627:TYR:CE1	2.43	0.54
1:A:1996:ILE:O	1:A:1997:SER:OG	2.17	0.54
1:A:1664:SER:OG	1:A:1677:ILE:O	2.26	0.54
1:A:1679:ARG:HG2	1:A:1679:ARG:HH11	1.72	0.54
1:A:2266:THR:OG1	1:A:2269:GLY:O	2.17	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1893:PHE:CE2	1:A:2630:LEU:HD23	2.42	0.54
1:A:2077:TYR:CD1	1:A:2088:VAL:HG22	2.42	0.54
1:A:1770:PHE:CE2	1:A:1789:ILE:HD12	2.42	0.54
1:A:2014:ASN:ND2	1:A:2014:ASN:O	2.26	0.54
1:A:1854:ILE:HD12	1:A:2493:HIS:CB	2.38	0.54
1:A:2222:TYR:OH	1:A:2283:ILE:HD11	2.07	0.53
1:A:1787:THR:CB	1:A:1795:ILE:HD11	2.38	0.53
1:A:1487:TYR:HB3	1:A:1490:ASN:HD21	1.73	0.53
1:A:1588:THR:HG22	1:A:1594:VAL:HG13	1.91	0.53
1:A:1789:ILE:HG22	1:A:1791:LYS:H	1.74	0.53
1:A:1912:VAL:HG22	1:A:1928:LEU:HD12	1.91	0.53
1:A:1690:LEU:HD12	1:A:1970:ASN:OD1	2.08	0.53
1:A:1584:LEU:HD11	1:A:1587:VAL:HG22	1.90	0.53
1:A:1679:ARG:HA	1:A:1694:GLU:HB3	1.91	0.53
1:A:1755:LEU:CD1	1:A:1757:LEU:HB2	2.39	0.53
1:A:2120:LEU:HG	1:A:2131:LEU:HD12	1.90	0.52
1:A:2138:ILE:HG23	1:A:2143:TYR:O	2.09	0.52
1:A:1875:SER:HB3	1:A:1881:LEU:HD21	1.91	0.52
1:A:1936:THR:O	1:A:1951:TYR:HA	2.09	0.52
1:A:1838:VAL:HG11	1:A:2329:PHE:HZ	1.74	0.52
1:A:2582:TRP:CH2	1:A:2613:VAL:HG12	2.44	0.52
1:A:952:TYR:HB2	1:A:1060:TRP:CD2	2.44	0.52
1:A:1886:LEU:N	1:A:1886:LEU:CD2	2.73	0.52
1:A:1476:HIS:HD2	1:A:1491:PHE:CE2	2.27	0.52
1:A:1491:PHE:CZ	1:A:1502:LEU:HD13	2.44	0.52
1:A:2630:LEU:HB3	1:A:2636:ASN:HD22	1.75	0.52
1:A:1565:THR:HA	1:A:1575:PHE:CD1	2.45	0.51
1:A:2135:GLN:OE1	1:A:2136:TYR:O	2.26	0.51
1:A:2154:TYR:OH	1:A:2312:THR:HG21	2.10	0.51
1:A:1711:ARG:NH1	1:A:2415:GLU:O	2.37	0.51
1:A:1720:LEU:HD11	1:A:2367:ILE:HG21	1.90	0.51
1:A:1780:ARG:HH12	1:A:2359:MET:HE3	1.75	0.51
1:A:984:VAL:HG22	1:A:1025:VAL:HG22	1.93	0.51
1:A:2346:LEU:HB3	1:A:2422:LYS:HD3	1.92	0.51
1:A:2483:MET:SD	1:A:2570:LEU:HD11	2.51	0.51
4:A:2702:NAG:O4	5:A:2703:MAN:O5	2.29	0.51
1:A:1534:THR:HB	1:A:1543:VAL:HB	1.93	0.51
1:A:1006:ILE:HG13	1:A:1006:ILE:O	2.11	0.51
1:A:1775:LEU:HD12	1:A:1776:ALA:N	2.26	0.51
1:A:1979:PRO:HG2	1:A:1986:LEU:HB2	1.93	0.51
1:A:906:VAL:N	1:A:1031:TYR:OH	2.38	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2194:GLN:HG2	1:A:2212:HIS:NE2	2.25	0.51
1:A:1775:LEU:HD12	1:A:1776:ALA:H	1.75	0.51
1:A:1977:ILE:HG22	1:A:1979:PRO:HD3	1.92	0.51
1:A:2049:MET:SD	1:A:2244:ASP:HA	2.51	0.51
1:A:2211:ASN:N	1:A:2216:GLU:O	2.44	0.50
1:A:2197:TYR:CE1	1:A:2206:ILE:HG12	2.47	0.50
1:A:2462:ILE:HG22	1:A:2462:ILE:O	2.12	0.50
1:A:1576:TYR:HD1	1:A:1587:VAL:HG22	1.77	0.50
1:A:1935:CYS:SG	1:A:1936:THR:N	2.85	0.50
1:A:1566:LYS:O	1:A:1573:THR:O	2.30	0.50
1:A:2054:ASP:HB3	1:A:2060:ILE:HD12	1.94	0.50
1:A:1756:TRP:HZ3	1:A:1767:VAL:HG23	1.77	0.49
1:A:2136:TYR:CE1	1:A:2147:ARG:HG3	2.47	0.49
1:A:1778:LEU:HD12	1:A:1778:LEU:H	1.77	0.49
1:A:2210:TYR:HD1	1:A:2217:ILE:HD13	1.77	0.49
1:A:1069:ASN:OD1	1:A:1076:HIS:NE2	2.44	0.49
1:A:2105:ASN:ND2	1:A:2126:ASP:OD1	2.44	0.49
1:A:1756:TRP:CZ3	1:A:1767:VAL:HG23	2.48	0.49
1:A:2045:LEU:HD11	1:A:2048:TRP:HB2	1.94	0.49
1:A:2214:ASN:O	1:A:2216:GLU:N	2.43	0.49
1:A:1787:THR:HG22	1:A:1798:ARG:HG3	1.95	0.49
1:A:1730:ARG:HH22	1:A:1749:GLN:HA	1.77	0.49
1:A:1578:TYR:HB3	1:A:1582:GLY:HA2	1.94	0.49
1:A:2014:ASN:HB2	1:A:2027:HIS:HA	1.95	0.49
1:A:1686:MET:HB3	1:A:1942:ILE:HD11	1.95	0.48
1:A:2410:ALA:HA	1:A:2414:LEU:HD12	1.94	0.48
1:A:1652:VAL:N	1:A:1660:ILE:O	2.42	0.48
1:A:958:ALA:HB2	1:A:1050:PHE:HE1	1.78	0.48
1:A:1594:VAL:CG2	1:A:2449:ALA:HB1	2.43	0.48
1:A:1630:SER:HA	1:A:1643:GLN:HA	1.94	0.48
1:A:1826:ILE:HB	1:A:1839:THR:HB	1.96	0.48
4:A:2706:NAG:C3	4:A:2706:NAG:C8	2.90	0.48
1:A:2175:ARG:HB2	1:A:2184:SER:HB2	1.95	0.48
1:A:2586:GLN:HE21	1:A:2590:ARG:HE	1.61	0.48
1:A:1503:ILE:HG21	4:A:2701:NAG:H83	1.94	0.48
1:A:1799:MET:O	1:A:1799:MET:HG2	2.13	0.48
1:A:1908:ASP:CB	1:A:2635:SER:HB3	2.43	0.48
1:A:2151:ILE:HG23	1:A:2593:ARG:NH2	2.28	0.48
1:A:922:SER:OG	1:A:928:ASN:O	2.26	0.48
1:A:906:VAL:CB	1:A:974:PRO:HG2	2.44	0.48
1:A:2047:TYR:CD2	1:A:2242:ALA:HB1	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1456:GLN:HB2	1:A:1470:PHE:O	2.14	0.48
1:A:1808:TYR:CE1	1:A:1817:LEU:HD13	2.49	0.48
1:A:2480:LEU:N	1:A:2480:LEU:HD23	2.29	0.48
1:A:2630:LEU:O	1:A:2636:ASN:ND2	2.47	0.48
1:A:1695:TRP:HD1	1:A:2411:PHE:CE1	2.32	0.48
1:A:1716:HIS:O	1:A:1716:HIS:ND1	2.47	0.48
1:A:1591:THR:O	1:A:1854:ILE:O	2.31	0.47
1:A:912:ILE:HG22	1:A:966:ILE:HG12	1.96	0.47
1:A:2395:GLN:O	1:A:2401:GLN:HB3	2.14	0.47
1:A:2110:ASN:HB3	1:A:2117:LEU:HD23	1.95	0.47
1:A:2297:VAL:HG23	1:A:2306:VAL:HG23	1.97	0.47
1:A:1066:HIS:ND1	1:A:1077:LYS:HA	2.30	0.47
1:A:1686:MET:HE1	1:A:1967:TYR:HB2	1.95	0.47
1:A:1756:TRP:O	1:A:1758:PRO:HD3	2.14	0.47
1:A:1770:PHE:CE2	1:A:1776:ALA:CB	2.97	0.47
1:A:2585:GLU:O	1:A:2589:ALA:N	2.45	0.47
1:A:1608:ASP:OD1	1:A:1619:THR:HG23	2.13	0.47
1:A:1750:VAL:HG12	1:A:1751:GLY:N	2.30	0.47
1:A:1789:ILE:HG23	1:A:1793:GLY:O	2.14	0.47
1:A:1720:LEU:HD11	1:A:2367:ILE:CG2	2.45	0.47
1:A:1777:GLY:HA2	1:A:1786:ARG:HA	1.96	0.47
1:A:1928:LEU:HD13	1:A:2178:GLY:HA2	1.96	0.47
1:A:2127:ARG:HB3	1:A:2138:ILE:HB	1.96	0.47
1:A:1514:ARG:NH2	1:A:1518:GLY:O	2.44	0.47
1:A:1553:LEU:HB3	1:A:1567:SER:HB3	1.96	0.47
1:A:2053:TYR:HD2	1:A:2057:GLY:C	2.22	0.47
1:A:2350:VAL:HG12	1:A:2356:TRP:CD1	2.49	0.47
4:A:2706:NAG:H3	4:A:2706:NAG:C8	2.32	0.46
1:A:1906:VAL:CG1	1:A:2630:LEU:HD11	2.46	0.46
1:A:2112:GLY:O	1:A:2113:ASN:OD1	2.32	0.46
1:A:1585:THR:HB	4:A:2704:NAG:C8	2.44	0.46
1:A:2098:TYR:HD1	1:A:2106:LEU:HD11	1.81	0.46
1:A:1905:ILE:HB	1:A:1912:VAL:HB	1.97	0.46
1:A:1907:TYR:HB2	1:A:2156:SER:HB2	1.98	0.46
1:A:2265:TYR:CE1	1:A:2271:ILE:HG22	2.50	0.46
1:A:1057:LEU:O	1:A:1541:LEU:HD23	2.16	0.46
1:A:1796:VAL:O	1:A:1808:TYR:N	2.42	0.46
1:A:1066:HIS:CD2	1:A:1468:TYR:CE1	3.02	0.46
1:A:1575:PHE:CZ	1:A:2445:GLY:O	2.68	0.46
4:A:2701:NAG:O4	4:A:2702:NAG:C1	2.64	0.46
1:A:1800:PHE:HB3	1:A:2056:MET:SD	2.56	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1864:PRO:CG	1:A:2125:ARG:HG2	2.46	0.46
1:A:2585:GLU:HB3	1:A:2607:LEU:HD21	1.97	0.46
1:A:1508:ASN:OD1	1:A:1526:PRO:CB	2.64	0.46
1:A:2033:ARG:HH21	1:A:2057:GLY:HA2	1.81	0.46
1:A:2286:HIS:HB3	1:A:2299:PHE:CZ	2.51	0.46
1:A:2636:ASN:OD1	1:A:2636:ASN:C	2.59	0.46
1:A:1576:TYR:CE1	1:A:1587:VAL:HG13	2.51	0.45
1:A:2041:MET:HE1	1:A:2240:TYR:CD2	2.51	0.45
1:A:2181:ARG:HE	1:A:2197:TYR:HD2	1.64	0.45
1:A:1874:TYR:CE1	1:A:1880:ILE:HG12	2.52	0.45
1:A:1951:TYR:O	1:A:1952:ARG:C	2.59	0.45
1:A:2181:ARG:NH1	1:A:2385:LEU:HD13	2.32	0.45
1:A:2261:LYS:CE	1:A:2279:PHE:O	2.65	0.45
1:A:1655:ALA:HB1	1:A:1920:THR:HA	1.99	0.45
1:A:1986:LEU:HD11	1:A:2217:ILE:HG21	1.97	0.45
1:A:2249:PRO:HD3	1:A:2283:ILE:HG22	1.98	0.45
1:A:2297:VAL:HG23	1:A:2306:VAL:CG2	2.46	0.45
1:A:2059:VAL:O	1:A:2077:TYR:HB2	2.15	0.45
1:A:2058:ARG:O	1:A:2059:VAL:C	2.60	0.45
1:A:2270:GLU:H	1:A:2306:VAL:CG1	2.30	0.45
1:A:1060:TRP:NE1	1:A:1554:MET:SD	2.82	0.45
1:A:1605:ILE:HG22	1:A:1607:ILE:HG13	1.99	0.45
1:A:1633:VAL:HG11	1:A:2401:GLN:NE2	2.31	0.45
1:A:1657:GLY:HA3	1:A:1685:PRO:HG3	1.98	0.45
1:A:1680:CYS:HB2	1:A:2411:PHE:CZ	2.51	0.45
1:A:1950:ILE:HG22	1:A:1952:ARG:HG2	1.97	0.45
1:A:2184:SER:OG	1:A:2194:GLN:OE1	2.32	0.45
1:A:1065:HIS:CE1	1:A:1499:VAL:HG21	2.52	0.45
1:A:1871:ILE:HD12	1:A:1886:LEU:HD21	1.98	0.45
1:A:2126:ASP:OD2	1:A:2330:ASN:CG	2.60	0.45
1:A:906:VAL:CB	1:A:974:PRO:CG	2.95	0.45
1:A:1468:TYR:HB3	1:A:1476:HIS:CE1	2.52	0.45
1:A:1471:ASN:O	1:A:1472:ALA:CB	2.65	0.45
1:A:1543:VAL:HG22	1:A:1553:LEU:HD13	1.97	0.45
1:A:1886:LEU:HD13	1:A:2489:GLY:HA2	1.99	0.45
1:A:2096:TRP:HA	1:A:2110:ASN:HD21	1.82	0.45
1:A:2377:TYR:CD2	1:A:2381:PRO:HD3	2.52	0.45
1:A:2181:ARG:HB3	1:A:2197:TYR:HE2	1.82	0.44
1:A:2205:ARG:HG3	1:A:2222:TYR:CE2	2.52	0.44
1:A:2482:LYS:O	1:A:2482:LYS:HG3	2.16	0.44
2:B:2:NAG:H4	2:B:3:MAN:H2	1.43	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1574:THR:O	1:A:1574:THR:HG23	2.17	0.44
1:A:1902:LEU:HD21	1:A:1905:ILE:HD11	1.98	0.44
1:A:1946:VAL:HB	1:A:2200:LEU:HD11	1.99	0.44
1:A:1620:VAL:CG2	1:A:2398:THR:HG21	2.47	0.44
1:A:1656:ASN:HB3	1:A:1943:GLY:HA2	2.00	0.44
1:A:1697:LEU:HD11	1:A:1709:PHE:CE1	2.53	0.44
1:A:1864:PRO:HG2	1:A:2125:ARG:HG2	1.99	0.44
1:A:2581:ALA:HB2	1:A:2637:ILE:HG21	1.99	0.44
1:A:1683:SER:HA	1:A:1689:GLY:O	2.17	0.44
1:A:1904:GLU:CD	1:A:1913:THR:HG22	2.43	0.44
1:A:1928:LEU:O	1:A:1934:SER:HA	2.18	0.44
1:A:1018:TYR:CG	1:A:1052:LEU:HD21	2.53	0.44
1:A:1594:VAL:HG21	1:A:2449:ALA:HB1	1.99	0.44
1:A:1766:ASN:HB2	1:A:1779:GLN:HG2	2.00	0.44
1:A:2211:ASN:OD1	4:A:2712:NAG:H2	2.18	0.44
1:A:2263:LEU:HD22	1:A:2265:TYR:HE1	1.82	0.44
1:A:983:MET:H	1:A:992:GLN:HA	1.83	0.44
1:A:2261:LYS:HD3	1:A:2263:LEU:HG	1.99	0.44
1:A:1965:TYR:CD1	1:A:1977:ILE:HG12	2.53	0.44
1:A:2192:HIS:ND1	1:A:2212:HIS:CD2	2.86	0.44
1:A:2447:MET:H	1:A:2458:GLY:HA3	1.83	0.44
1:A:912:ILE:O	1:A:912:ILE:HG13	2.18	0.44
1:A:1658:MET:HA	1:A:1683:SER:O	2.18	0.44
1:A:917:LEU:HD13	1:A:1084:PHE:HE2	1.83	0.43
1:A:950:LEU:HG	1:A:1060:TRP:HB3	2.00	0.43
1:A:2219:SER:N	1:A:2232:GLU:O	2.50	0.43
1:A:1489:TYR:HA	1:A:1503:ILE:O	2.18	0.43
1:A:1856:TYR:HB2	1:A:1874:TYR:O	2.18	0.43
1:A:1787:THR:HG22	1:A:1798:ARG:CB	2.49	0.43
1:A:2105:ASN:OD1	1:A:2126:ASP:OD1	2.37	0.43
1:A:2314:PRO:HG3	1:A:2332:TYR:CE1	2.54	0.43
1:A:1056:ASN:O	1:A:1514:ARG:NH2	2.38	0.43
1:A:1653:MET:HE1	1:A:1657:GLY:O	2.18	0.43
1:A:1682:ILE:HD12	1:A:2369:PRO:CG	2.49	0.43
1:A:1726:ASP:O	1:A:1730:ARG:N	2.49	0.43
1:A:1909:SER:HB2	1:A:2621:VAL:HG11	2.01	0.43
1:A:2217:ILE:O	1:A:2218:THR:OG1	2.24	0.43
1:A:2314:PRO:HG2	1:A:2316:TYR:CZ	2.53	0.43
1:A:2442:ILE:O	1:A:2446:ILE:HG12	2.18	0.43
1:A:915:SER:N	1:A:963:LEU:O	2.48	0.43
1:A:2248:THR:HG23	1:A:2250:LEU:CD1	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1596:SER:HB2	4:A:2704:NAG:C8	2.47	0.43
1:A:1599:ARG:HG2	1:A:1607:ILE:HG12	2.00	0.43
1:A:2146:GLN:O	1:A:2146:GLN:HG2	2.18	0.43
1:A:2318:MET:O	1:A:2322:VAL:HG13	2.18	0.43
1:A:957:THR:OG1	1:A:1561:GLY:O	2.33	0.43
1:A:1825:TYR:CE1	1:A:1841:PRO:HD3	2.54	0.43
1:A:2008:VAL:HG12	1:A:2017:ILE:HG12	1.99	0.43
1:A:2478:TYR:O	1:A:2495:PHE:CD2	2.72	0.43
1:A:1747:TYR:CE1	1:A:1753:PRO:HB3	2.54	0.43
1:A:1817:LEU:HB3	1:A:1825:TYR:HB2	2.00	0.43
1:A:2170:TRP:HB2	1:A:2293:LEU:HD21	2.01	0.43
1:A:913:ILE:HG13	1:A:913:ILE:O	2.18	0.43
1:A:1009:LYS:HD2	1:A:1049:GLY:HA2	2.01	0.43
1:A:1860:ILE:HG12	1:A:1871:ILE:HG12	2.00	0.43
1:A:2147:ARG:O	1:A:2150:ASP:N	2.48	0.43
1:A:2270:GLU:OE1	1:A:2307:LEU:HD23	2.18	0.43
1:A:2578:LEU:HD12	1:A:2582:TRP:HE1	1.83	0.43
1:A:1659:GLY:O	1:A:1682:ILE:HA	2.19	0.42
1:A:956:ARG:NH2	1:A:1077:LYS:O	2.42	0.42
1:A:1618:VAL:HG21	1:A:2397:ILE:HD13	2.01	0.42
1:A:1974:ILE:HD11	1:A:2200:LEU:HD23	2.00	0.42
1:A:2365:SER:HA	1:A:2371:PHE:HB3	2.01	0.42
1:A:1942:ILE:HB	1:A:1947:ASP:OD2	2.18	0.42
1:A:1477:GLN:O	1:A:1478:TYR:HB3	2.19	0.42
1:A:2105:ASN:O	1:A:2122:TYR:CZ	2.73	0.42
1:A:995:PHE:HE1	1:A:1001:LEU:HD21	1.84	0.42
1:A:1620:VAL:HG12	1:A:1620:VAL:O	2.19	0.42
1:A:1622:THR:HB	1:A:1631:TYR:CD1	2.54	0.42
1:A:1794:ARG:HG2	1:A:1810:TYR:CE1	2.54	0.42
1:A:2144:LEU:HD21	1:A:2147:ARG:HB2	2.01	0.42
1:A:2179:VAL:HG11	1:A:2385:LEU:HD13	2.01	0.42
1:A:2317:THR:O	1:A:2320:LYS:HG2	2.20	0.42
1:A:951:ARG:NH2	1:A:1079:THR:HG22	2.34	0.42
1:A:1020:LEU:CG	1:A:1046:LEU:HD11	2.49	0.42
1:A:1697:LEU:HD12	1:A:1698:ARG:N	2.35	0.42
1:A:1768:SER:O	1:A:1768:SER:OG	2.30	0.42
1:A:2118:MET:HE3	1:A:2132:GLY:HA3	2.01	0.42
1:A:2157:LYS:O	1:A:2157:LYS:HG2	2.19	0.42
1:A:1577:ASP:CB	1:A:1586:ASN:OD1	2.57	0.42
1:A:1499:VAL:O	1:A:1514:ARG:NE	2.47	0.42
1:A:1644:LEU:HD23	1:A:1650:LEU:HA	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1873:ASP:O	1:A:1881:LEU:N	2.38	0.42
1:A:2188:ASN:OD1	1:A:2189:LEU:HD12	2.20	0.42
1:A:2286:HIS:O	1:A:2286:HIS:CD2	2.73	0.42
1:A:2396:LEU:HD21	1:A:2405:GLU:HG2	2.01	0.42
1:A:2577:ALA:O	1:A:2581:ALA:N	2.50	0.42
1:A:1508:ASN:OD1	1:A:1526:PRO:HG3	2.20	0.42
1:A:1584:LEU:HD11	1:A:1587:VAL:CG2	2.50	0.42
1:A:2131:LEU:HD22	1:A:2136:TYR:OH	2.19	0.42
1:A:1636:ASP:CB	1:A:1898:LYS:HD2	2.49	0.42
1:A:2185:TYR:O	1:A:2192:HIS:HA	2.19	0.42
1:A:2267:ALA:O	1:A:2268:TYR:HB2	2.20	0.42
1:A:1988:VAL:HG12	1:A:1990:LEU:HG	2.01	0.41
1:A:2286:HIS:O	1:A:2286:HIS:CG	2.73	0.41
1:A:995:PHE:CE1	1:A:1001:LEU:HD21	2.55	0.41
1:A:1769:TYR:HA	1:A:1775:LEU:HA	2.02	0.41
1:A:1835:LEU:HD12	1:A:1835:LEU:H	1.85	0.41
1:A:2304:TYR:OH	1:A:2309:GLY:O	2.38	0.41
1:A:1500:THR:O	1:A:1511:LYS:HA	2.21	0.41
1:A:2105:ASN:O	1:A:2122:TYR:OH	2.16	0.41
1:A:1512:ILE:HG12	1:A:1523:LEU:HD13	2.02	0.41
1:A:1846:HIS:HB3	1:A:1861:TYR:HE1	1.86	0.41
1:A:2036:GLU:OE2	1:A:2048:TRP:NE1	2.50	0.41
1:A:1773:GLY:O	1:A:1774:ARG:C	2.63	0.41
1:A:2363:GLN:OE1	1:A:2373:ARG:NH1	2.53	0.41
1:A:2479:TYR:HE1	1:A:2493:HIS:HB3	1.86	0.41
1:A:935:GLN:NE2	1:A:1599:ARG:HG3	2.35	0.41
1:A:1541:LEU:HD12	1:A:1541:LEU:C	2.46	0.41
1:A:1574:THR:HA	1:A:1589:ARG:HA	2.02	0.41
1:A:1756:TRP:HH2	1:A:2420:THR:HG21	1.86	0.41
1:A:2012:ASP:C	1:A:2014:ASN:N	2.79	0.41
1:A:2204:THR:HG22	1:A:2300:THR:HG21	2.03	0.41
1:A:1020:LEU:HD21	1:A:1046:LEU:HD21	2.03	0.41
1:A:1770:PHE:CE2	1:A:1776:ALA:HB2	2.55	0.41
1:A:1808:TYR:CD1	1:A:1815:MET:HE2	2.56	0.41
1:A:2039:TYR:OH	1:A:2240:TYR:HB3	2.21	0.41
1:A:1917:ASP:OD1	1:A:1921:GLY:N	2.54	0.41
1:A:2017:ILE:HD11	1:A:2223:ASP:OD1	2.20	0.41
1:A:2137:LYS:HB2	1:A:2138:ILE:HA	2.03	0.41
1:A:912:ILE:HD12	1:A:1045:ALA:HB2	2.02	0.40
1:A:1055:SER:HB3	1:A:1065:HIS:ND1	2.36	0.40
1:A:1750:VAL:HG12	1:A:1751:GLY:H	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1779:GLN:HB2	1:A:1784:SER:HB3	2.03	0.40
1:A:1800:PHE:CB	1:A:2056:MET:SD	3.10	0.40
1:A:1821:SER:O	1:A:1823:ARG:N	2.54	0.40
1:A:1907:TYR:O	1:A:1908:ASP:C	2.64	0.40
1:A:2061:LYS:HZ3	1:A:2063:GLU:HG3	1.85	0.40
1:A:2305:ASP:O	1:A:2308:ALA:O	2.38	0.40
1:A:2327:ALA:HB1	1:A:2328:PRO:HD2	2.03	0.40
1:A:1966:THR:HG1	1:A:1976:SER:HG	1.63	0.40
1:A:2062:ARG:NH2	1:A:2340:LEU:HD13	2.36	0.40
1:A:1634:VAL:HG13	1:A:1639:ARG:NH1	2.37	0.40
1:A:1793:GLY:O	1:A:1794:ARG:C	2.64	0.40
1:A:2105:ASN:CG	1:A:2126:ASP:OD1	2.64	0.40
1:A:2128:ILE:CD1	1:A:2310:ARG:HD2	2.36	0.40
1:A:1568:ASP:HB3	1:A:1572:TRP:HB3	2.03	0.40
1:A:1575:PHE:CD2	1:A:2447:MET:CB	3.04	0.40
1:A:2315:ASP:C	1:A:2317:THR:H	2.29	0.40
1:A:2354:LYS:HA	1:A:2357:LEU:HD12	2.04	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	1292/1999 (65%)	1165 (90%)	124 (10%)	3 (0%)	43	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2012	ASP
1	A	2013	ILE
1	A	1868	ALA

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	991/1735 (57%)	976 (98%)	15 (2%)	57 75

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1031	TYR
1	A	1477	GLN
1	A	1500	THR
1	A	1679	ARG
1	A	1694	GLU
1	A	1767	VAL
1	A	1778	LEU
1	A	1779	GLN
1	A	1786	ARG
1	A	1886	LEU
1	A	2014	ASN
1	A	2060	ILE
1	A	2310	ARG
1	A	2480	LEU
1	A	2491	ASP

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	928	ASN
1	A	938	HIS
1	A	2173	GLN
1	A	2298	HIS
1	A	2401	GLN
1	A	2586	GLN
1	A	2638	GLN

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 ⓘ

5 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	2,1	14,14,15	2.46	1 (7%)	17,19,21	2.16	6 (35%)
2	NAG	B	2	2	14,14,15	0.90	1 (7%)	17,19,21	2.09	5 (29%)
2	MAN	B	3	2	11,11,12	2.00	3 (27%)	15,15,17	1.08	1 (6%)
3	MAN	C	1	3	11,11,12	1.87	3 (27%)	15,15,17	1.58	3 (20%)
3	MAN	C	2	3	11,11,12	1.73	3 (27%)	15,15,17	0.87	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	2,1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	MAN	B	3	2	-	2/2/19/22	0/1/1/1
3	MAN	C	1	3	-	2/2/19/22	0/1/1/1
3	MAN	C	2	3	-	0/2/19/22	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	C1-C2	8.91	1.64	1.52
2	B	3	MAN	O5-C1	4.41	1.51	1.43
3	C	1	MAN	O5-C1	4.19	1.50	1.43
3	C	2	MAN	O5-C1	3.75	1.50	1.43
2	B	3	MAN	C2-C3	-3.27	1.47	1.52
3	C	1	MAN	C2-C3	-2.88	1.48	1.52
3	C	2	MAN	C2-C3	-2.86	1.48	1.52
2	B	3	MAN	O5-C5	2.76	1.48	1.43
3	C	1	MAN	O5-C5	2.53	1.48	1.43
2	B	2	NAG	O4-C4	2.37	1.48	1.43
3	C	2	MAN	O5-C5	2.21	1.47	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C4-C3-C2	6.12	119.98	111.02
2	B	1	NAG	O5-C1-C2	-5.60	102.62	111.29
2	B	1	NAG	C1-O5-C5	4.07	117.65	112.19
2	B	1	NAG	C4-C3-C2	-3.28	106.21	111.02
2	B	2	NAG	C2-N2-C7	-3.18	118.63	122.90
3	C	1	MAN	C3-C4-C5	3.16	115.95	110.23
3	C	1	MAN	C2-C3-C4	2.95	116.04	110.86
2	B	2	NAG	O5-C1-C2	-2.85	106.89	111.29
2	B	1	NAG	O4-C4-C5	2.39	115.21	109.32
2	B	2	NAG	O4-C4-C3	2.37	115.97	110.38
2	B	1	NAG	O5-C5-C4	2.18	116.13	110.83
2	B	3	MAN	C1-O5-C5	2.11	115.02	112.19
3	C	2	MAN	C1-O5-C5	-2.10	109.37	112.19
2	B	2	NAG	O3-C3-C2	-2.06	105.11	109.40
2	B	1	NAG	C2-N2-C7	-2.02	120.19	122.90
3	C	1	MAN	C1-C2-C3	2.01	112.56	109.64

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1	NAG	C1

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	B	1	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

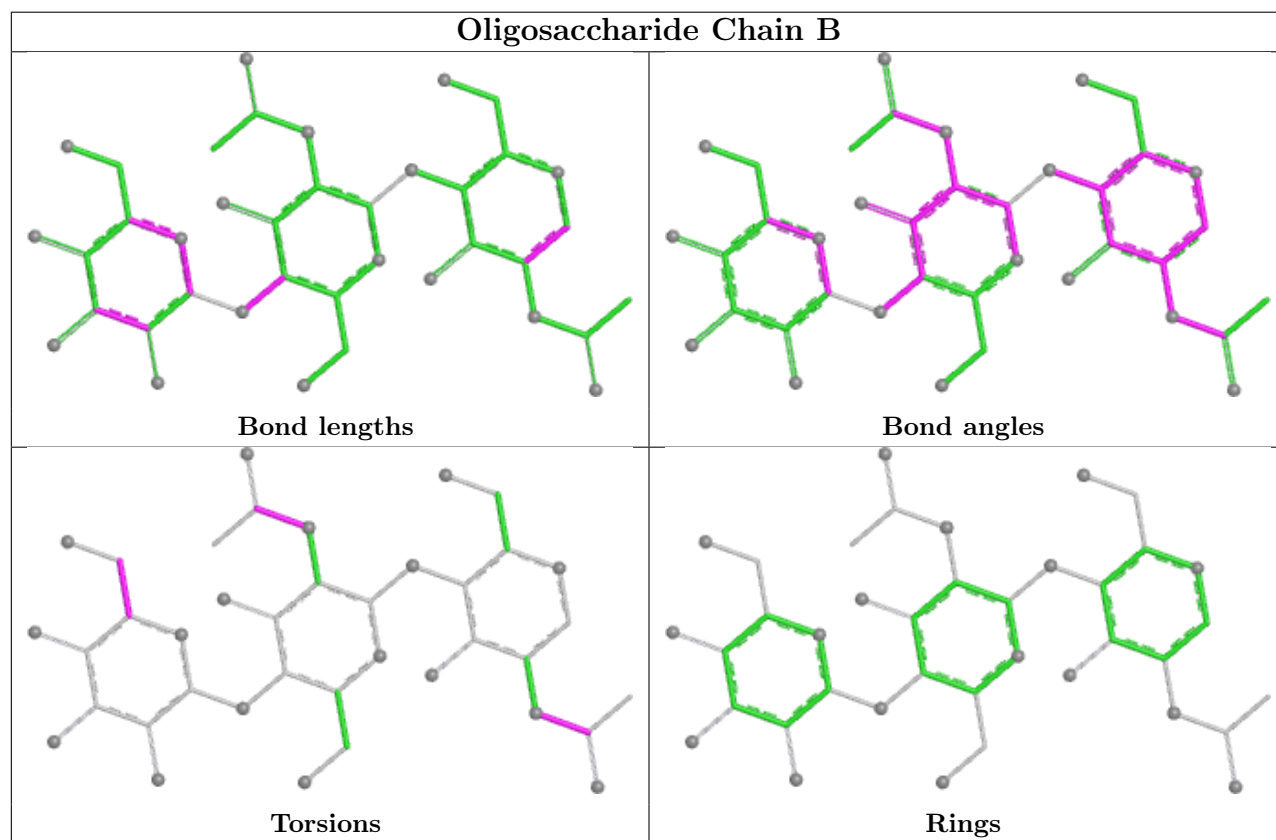
Mol	Chain	Res	Type	Atoms
3	C	1	MAN	C4-C5-C6-O6
2	B	3	MAN	O5-C5-C6-O6
2	B	1	NAG	O7-C7-N2-C2
3	C	1	MAN	O5-C5-C6-O6
2	B	3	MAN	C4-C5-C6-O6

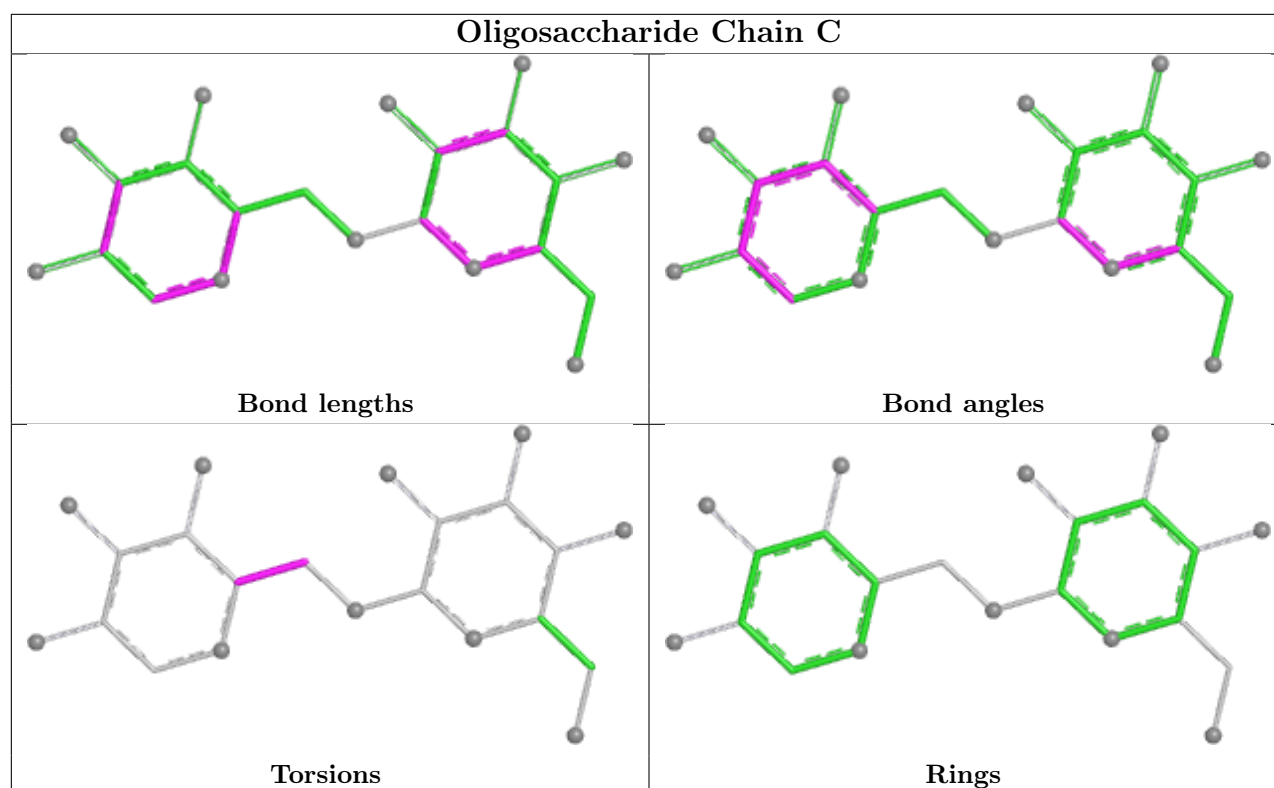
There are no ring outliers.

4 monomers are involved in 3 short contacts:

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

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





5.6 Ligand geometry [i](#)

12 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$
5	MAN	A	2716	-	11,11,12	1.93	3 (27%)	15,15,17	1.08	1 (6%)
5	MAN	A	2717	-	11,11,12	0.25	0	15,15,17	0.73	0
4	NAG	A	2702	-	14,14,15	1.83	3 (21%)	17,19,21	1.56	3 (17%)
4	NAG	A	2704	1	14,14,15	2.15	1 (7%)	17,19,21	3.01	3 (17%)
4	NAG	A	2707	-	14,14,15	0.33	0	17,19,21	0.83	1 (5%)
4	NAG	A	2706	-	14,14,15	0.41	0	17,19,21	0.98	1 (5%)
5	MAN	A	2703	-	11,11,12	1.97	3 (27%)	15,15,17	1.05	0
4	NAG	A	2712	-	14,14,15	1.99	5 (35%)	17,19,21	1.87	5 (29%)
4	NAG	A	2713	-	14,14,15	1.80	3 (21%)	17,19,21	1.57	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	2701	1	14,14,15	1.91	4 (28%)	17,19,21	1.79	3 (17%)
4	NAG	A	2705	-	14,14,15	0.35	0	17,19,21	0.63	0
4	NAG	A	2708	1	14,14,15	2.28	1 (7%)	17,19,21	2.03	1 (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
5	MAN	A	2716	-	-	2/2/19/22	1/1/1/1
5	MAN	A	2717	-	-	0/2/19/22	1/1/1/1
4	NAG	A	2702	-	-	0/6/23/26	0/1/1/1
4	NAG	A	2704	1	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	A	2707	-	-	4/6/23/26	0/1/1/1
4	NAG	A	2706	-	-	6/6/23/26	0/1/1/1
5	MAN	A	2703	-	-	0/2/19/22	1/1/1/1
4	NAG	A	2712	-	-	1/6/23/26	0/1/1/1
4	NAG	A	2713	-	-	3/6/23/26	0/1/1/1
4	NAG	A	2701	1	-	4/6/23/26	0/1/1/1
4	NAG	A	2705	-	-	4/6/23/26	0/1/1/1
4	NAG	A	2708	1	1/1/5/7	5/6/23/26	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2708	NAG	C1-C2	8.48	1.63	1.52
4	A	2704	NAG	C1-C2	7.74	1.62	1.52
5	A	2703	MAN	O5-C1	4.58	1.51	1.43
5	A	2716	MAN	O5-C1	4.30	1.50	1.43
4	A	2712	NAG	O5-C1	3.99	1.50	1.43
4	A	2701	NAG	O5-C1	3.95	1.50	1.43
4	A	2702	NAG	O5-C1	3.83	1.50	1.43
4	A	2713	NAG	O5-C1	3.66	1.49	1.43
4	A	2702	NAG	C7-N2	3.56	1.45	1.34
4	A	2701	NAG	C7-N2	3.54	1.45	1.34
4	A	2712	NAG	C7-N2	3.49	1.45	1.34
4	A	2713	NAG	C7-N2	3.43	1.45	1.34
5	A	2716	MAN	C2-C3	-3.10	1.47	1.52
5	A	2703	MAN	C2-C3	-2.86	1.48	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2712	NAG	O5-C5	2.78	1.48	1.43
5	A	2703	MAN	O5-C5	2.62	1.48	1.43
4	A	2701	NAG	O5-C5	2.61	1.48	1.43
5	A	2716	MAN	O5-C5	2.60	1.48	1.43
4	A	2712	NAG	C3-C2	-2.41	1.47	1.52
4	A	2702	NAG	C2-N2	2.23	1.49	1.46
4	A	2712	NAG	C2-N2	2.22	1.49	1.46
4	A	2701	NAG	C2-N2	2.19	1.49	1.46
4	A	2713	NAG	O5-C5	2.11	1.47	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2704	NAG	O5-C1-C2	-11.11	94.10	111.29
4	A	2708	NAG	O5-C1-C2	-7.76	99.29	111.29
4	A	2701	NAG	C1-O5-C5	-4.57	106.07	112.19
4	A	2704	NAG	C1-O5-C5	-4.46	106.21	112.19
4	A	2712	NAG	C3-C4-C5	3.98	117.44	110.23
4	A	2701	NAG	C3-C4-C5	3.40	116.40	110.23
4	A	2702	NAG	C2-N2-C7	-3.14	118.69	122.90
4	A	2712	NAG	C1-O5-C5	2.91	116.09	112.19
4	A	2713	NAG	C3-C4-C5	2.90	115.50	110.23
4	A	2702	NAG	C8-C7-N2	2.90	120.93	116.12
4	A	2712	NAG	C2-N2-C7	-2.78	119.17	122.90
4	A	2701	NAG	C8-C7-N2	2.76	120.70	116.12
4	A	2712	NAG	O5-C5-C4	2.76	117.55	110.83
4	A	2704	NAG	C2-N2-C7	-2.72	119.25	122.90
4	A	2702	NAG	C3-C4-C5	2.72	115.17	110.23
4	A	2712	NAG	C8-C7-N2	2.66	120.52	116.12
4	A	2707	NAG	C2-N2-C7	-2.51	119.53	122.90
4	A	2713	NAG	C2-N2-C7	-2.49	119.56	122.90
4	A	2706	NAG	C4-C3-C2	2.45	114.61	111.02
4	A	2713	NAG	C8-C7-N2	2.21	119.79	116.12
5	A	2716	MAN	C6-C5-C4	-2.01	108.08	113.02

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	2704	NAG	C1
4	A	2708	NAG	C1

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2704	NAG	C8-C7-N2-C2
4	A	2704	NAG	O7-C7-N2-C2
4	A	2705	NAG	C3-C2-N2-C7
4	A	2706	NAG	C8-C7-N2-C2
4	A	2707	NAG	C1-C2-N2-C7
4	A	2708	NAG	C1-C2-N2-C7
4	A	2708	NAG	C8-C7-N2-C2
4	A	2708	NAG	O7-C7-N2-C2
4	A	2713	NAG	O5-C5-C6-O6
4	A	2706	NAG	O7-C7-N2-C2
4	A	2713	NAG	C4-C5-C6-O6
4	A	2708	NAG	O5-C5-C6-O6
4	A	2701	NAG	C4-C5-C6-O6
4	A	2706	NAG	C4-C5-C6-O6
5	A	2716	MAN	O5-C5-C6-O6
4	A	2701	NAG	O5-C5-C6-O6
4	A	2706	NAG	O5-C5-C6-O6
4	A	2701	NAG	C8-C7-N2-C2
4	A	2701	NAG	O7-C7-N2-C2
4	A	2705	NAG	C8-C7-N2-C2
4	A	2708	NAG	C4-C5-C6-O6
4	A	2705	NAG	O5-C5-C6-O6
4	A	2705	NAG	O7-C7-N2-C2
5	A	2716	MAN	C4-C5-C6-O6
4	A	2707	NAG	C4-C5-C6-O6
4	A	2707	NAG	O5-C5-C6-O6
4	A	2712	NAG	C4-C5-C6-O6
4	A	2706	NAG	C3-C2-N2-C7
4	A	2706	NAG	C1-C2-N2-C7
4	A	2713	NAG	C1-C2-N2-C7
4	A	2707	NAG	C3-C2-N2-C7

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2716	MAN	C1-C2-C3-C4-C5-O5
5	A	2717	MAN	C1-C2-C3-C4-C5-O5
5	A	2703	MAN	C1-C2-C3-C4-C5-O5

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2717	MAN	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2702	NAG	3	0
4	A	2704	NAG	4	0
4	A	2706	NAG	4	0
5	A	2703	MAN	1	0
4	A	2712	NAG	1	0
4	A	2701	NAG	2	0
4	A	2705	NAG	2	0

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.

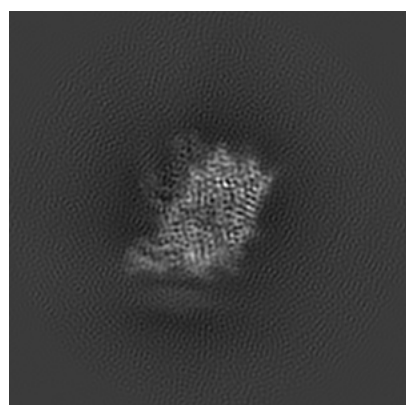
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7526. These allow visual inspection of the internal detail of the map and identification of artifacts.

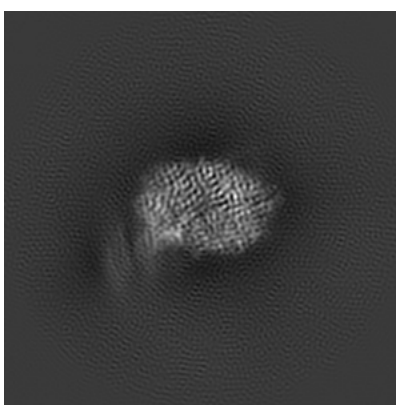
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

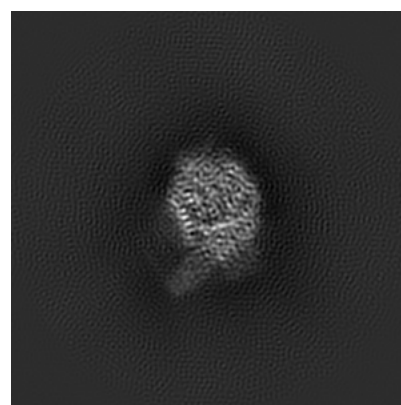
6.1.1 Primary map



X



Y

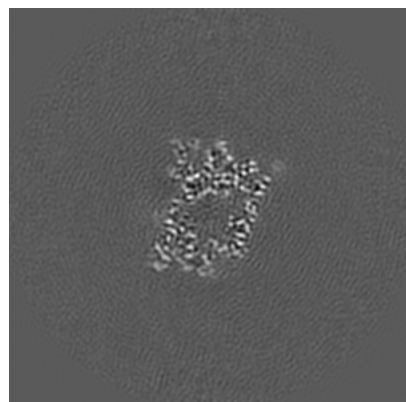


Z

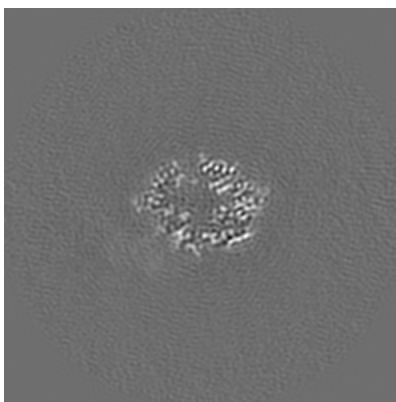
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

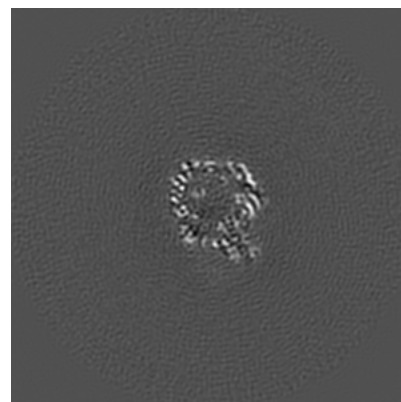
6.2.1 Primary map



X Index: 130



Y Index: 130

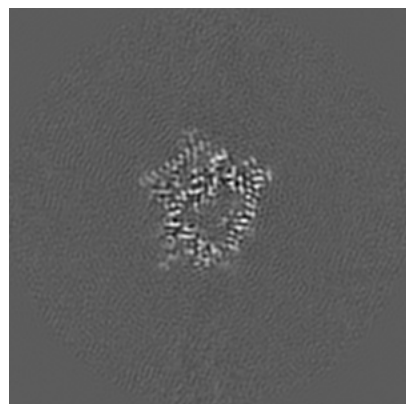


Z Index: 130

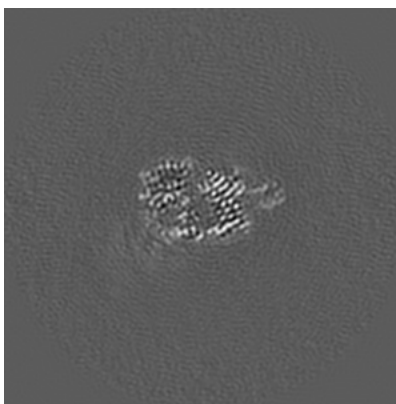
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

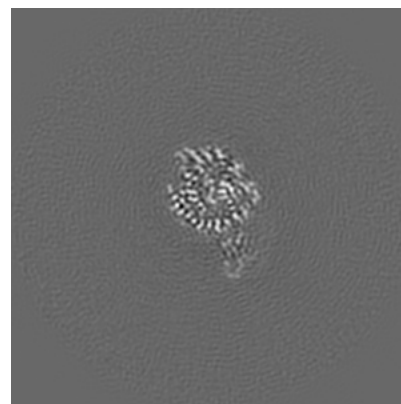
6.3.1 Primary map



X Index: 141



Y Index: 121

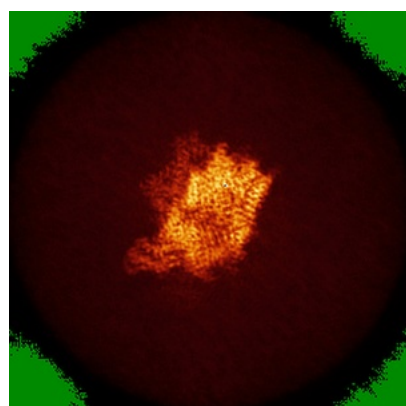


Z Index: 146

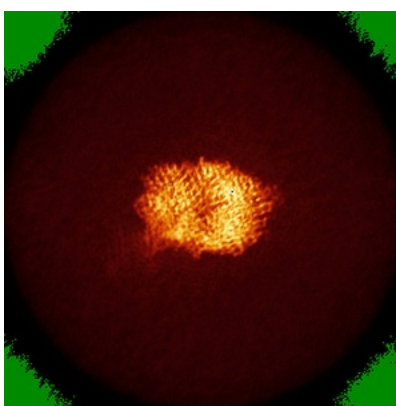
The images above show the largest variance slices of the map in three orthogonal directions.

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

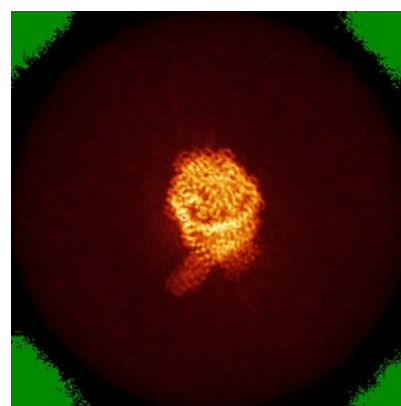
6.4.1 Primary map



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.

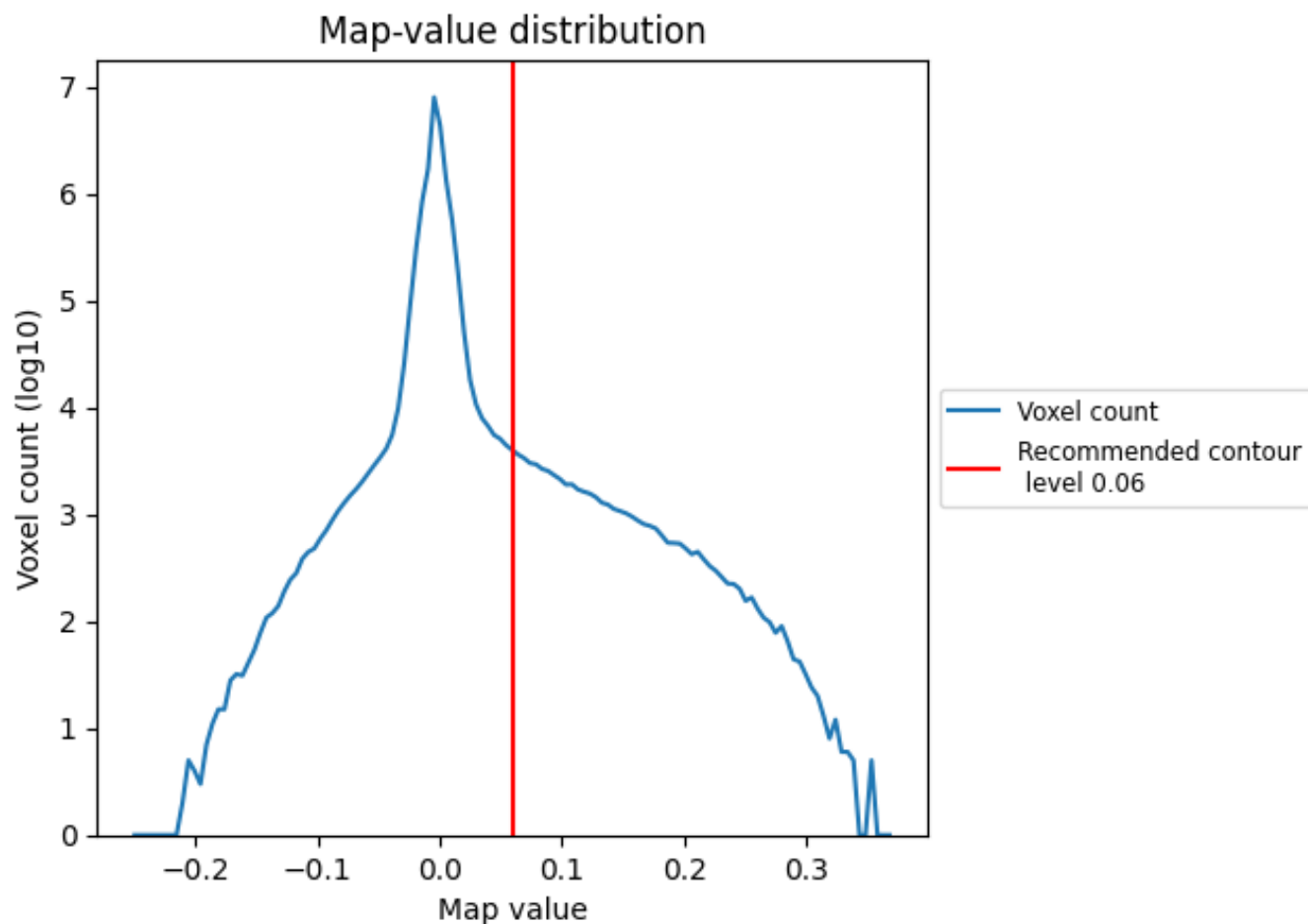
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

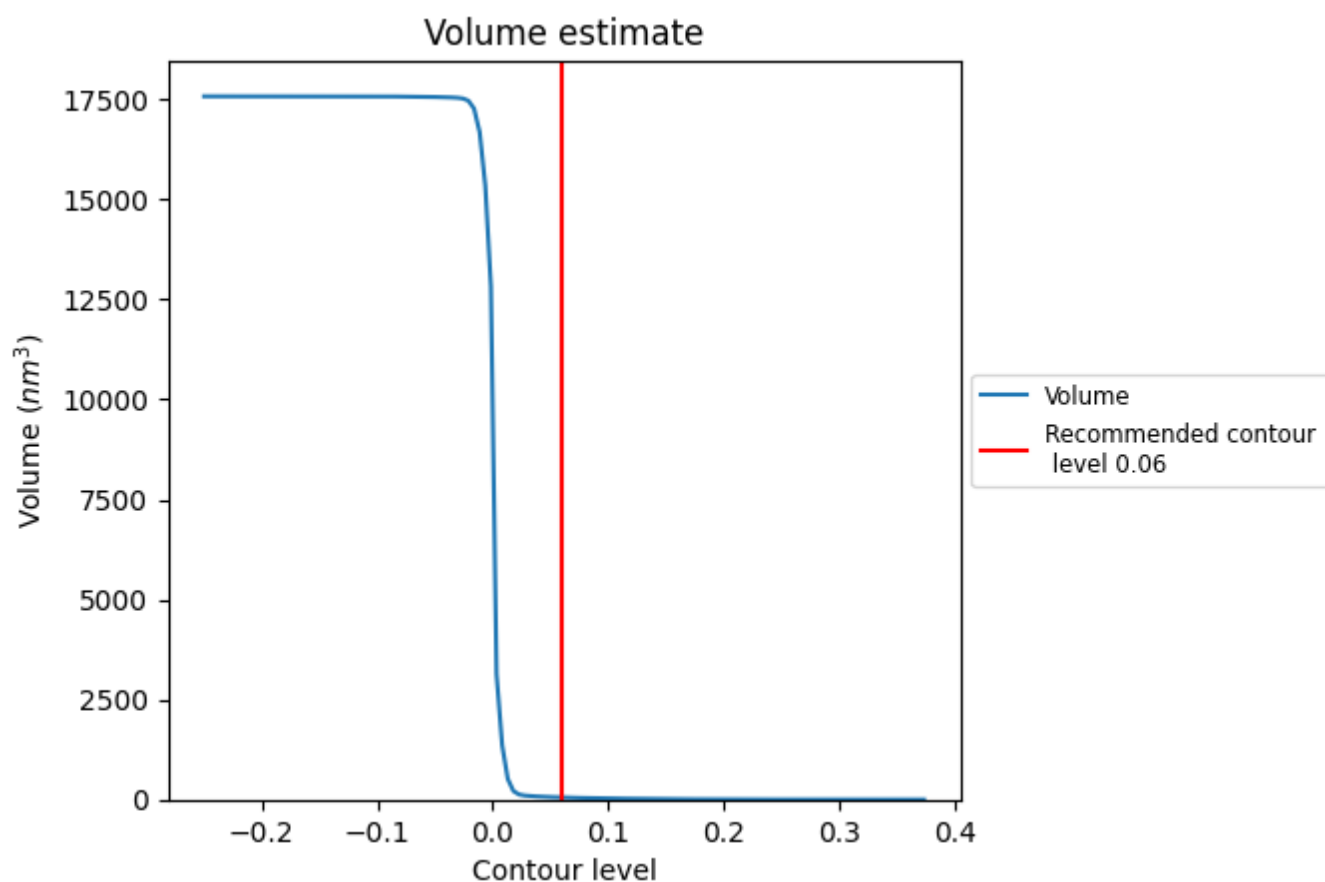
This section contains the results of statistical analysis of the map.

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.

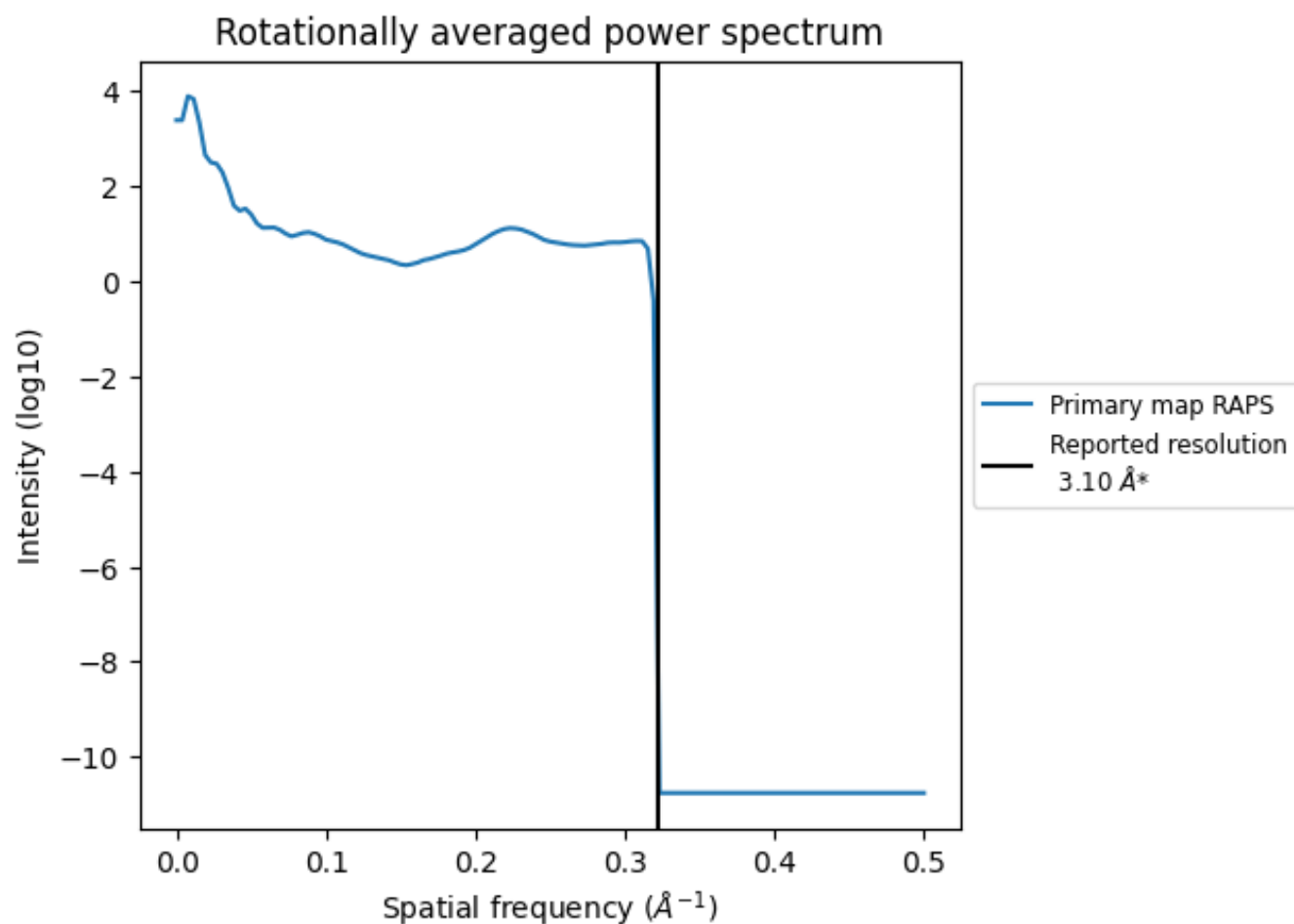
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 53 nm^3 ; this corresponds to an approximate mass of 48 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 0.323 $\text{\AA}^{-1}$

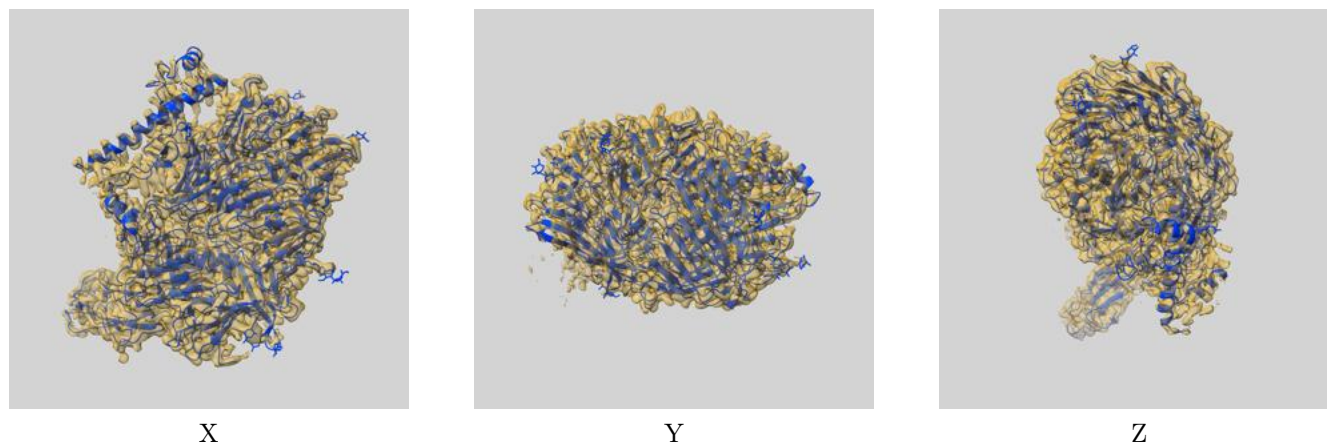
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

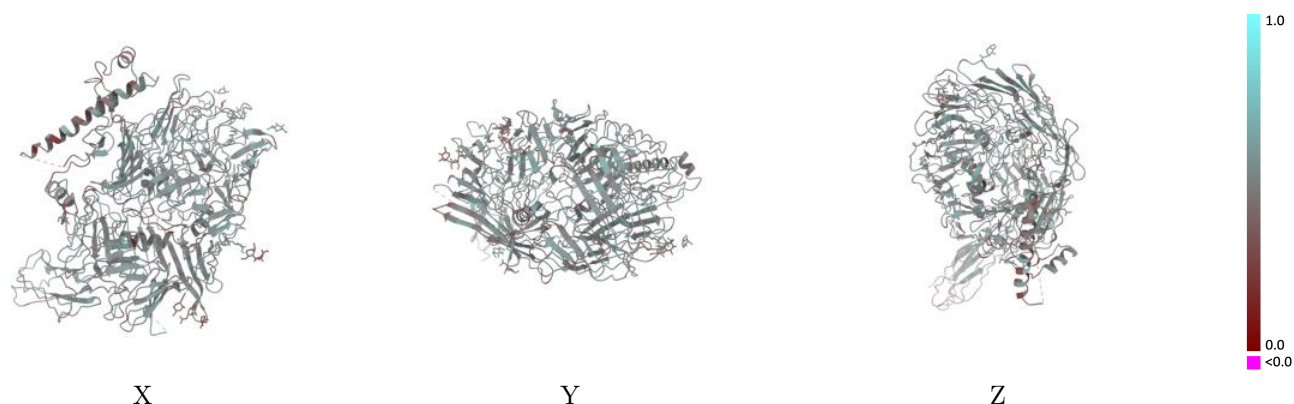
This section contains information regarding the fit between EMDB map EMD-7526 and PDB model 6CMX. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



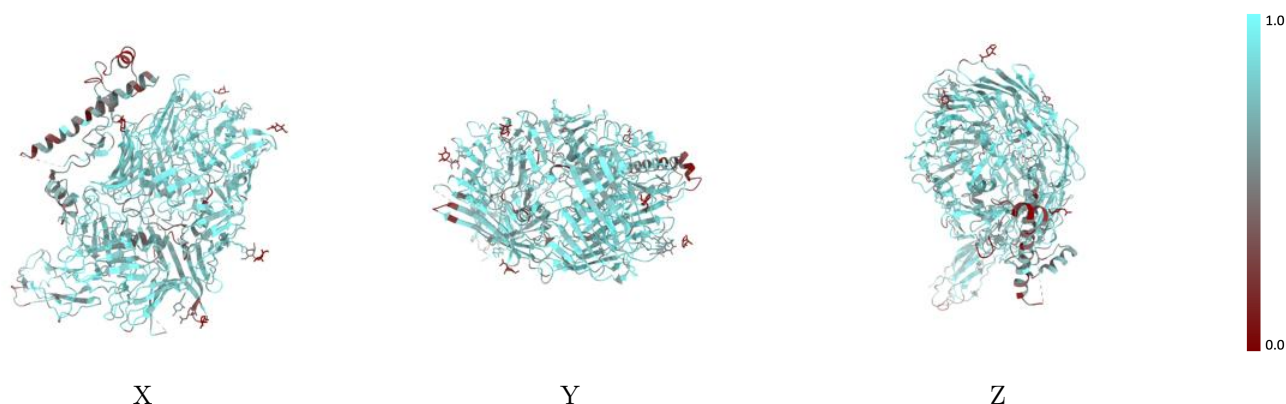
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



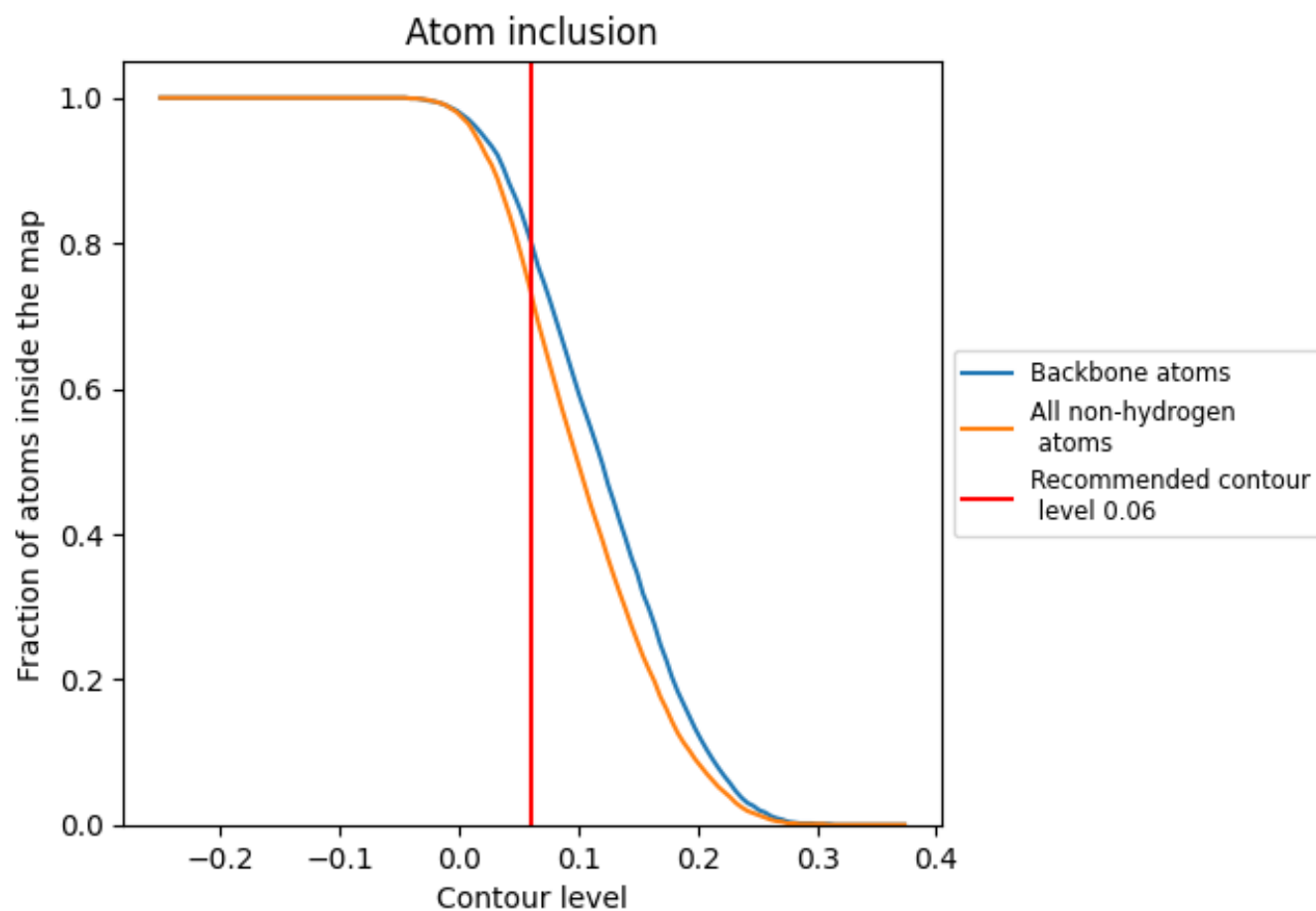
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 80% of all backbone atoms, 74% 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	0.7350	0.4970
A	0.7360	0.4980
B	0.4360	0.4000
C	0.5000	0.3700

