



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 11:12 PM UTC

PDB ID : 6UM1 / pdb_00006um1
EMDB ID : EMD-20815
Title : Structure of M-6-P/IGFII Receptor at pH 4.5
Authors : Wang, R.; Qi, X.; Li, X.
Deposited on : 2019-10-08
Resolution : 3.46 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:

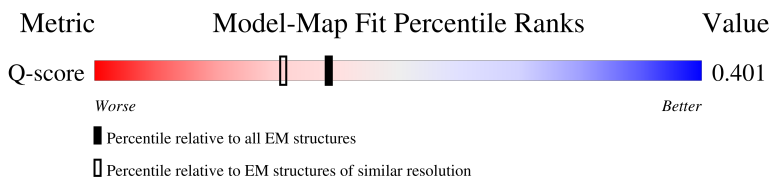
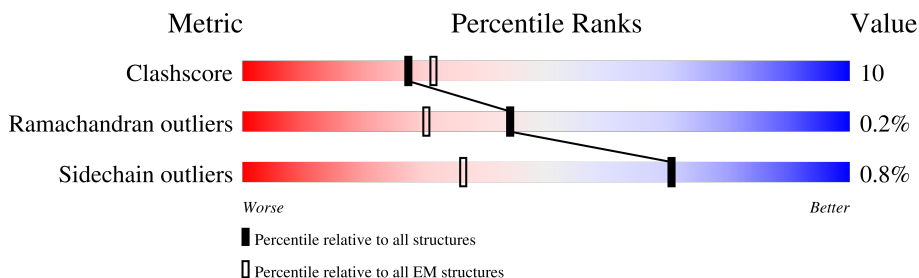
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.46 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	13788 (2.96 - 3.96)

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	2499	14% 71% 16% • 12%
2	B	2	100%
3	C	3	33% 33% 67%

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
4	NAG	A	2508	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 17134 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 Cation-independent mannose-6-phosphate receptor.

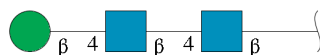
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2208	Total	C	N	O	S	0	0
			17025	10631	2916	3342	136		

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



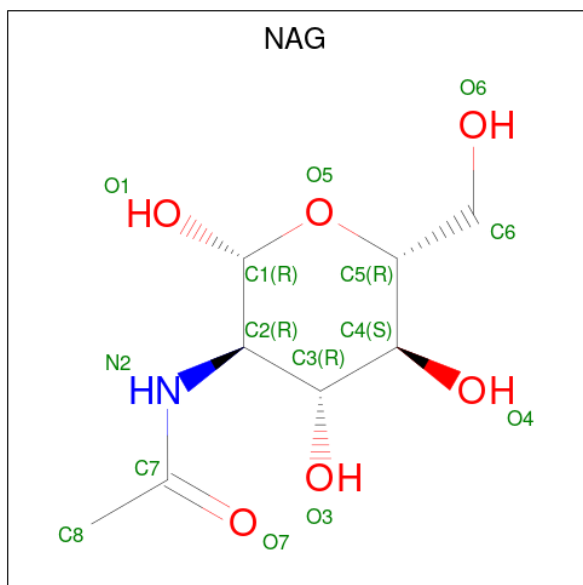
Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	2	Total	C	N	O	0	0
			28	16	2	10		

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



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

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

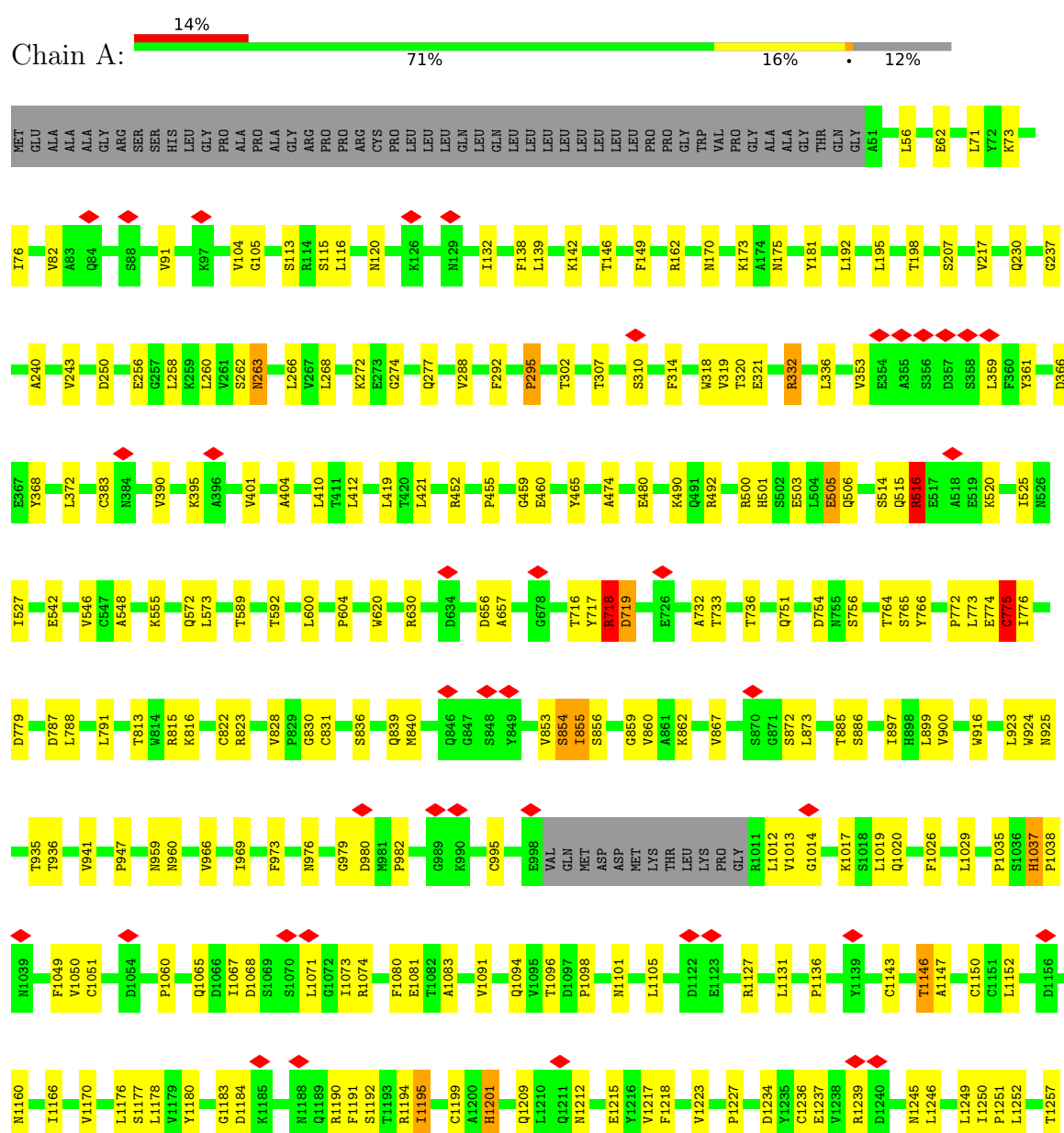


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Cation-independent mannose-6-phosphate receptor





ILE
SER
THR
PHE
HIS
ASP
ASP
SER
ASP
GLU
ASP
LEU
LEU
HIS
VAL

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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	128789	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 ($e^-/\text{\AA}^2$)	80	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	0.137	Depositor
Minimum map value	-0.096	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0145	Depositor
Map size ($\text{\AA}$)	280.0, 280.0, 280.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: BMA, 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	1.06	0/17415	1.38	34/23648 (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	20

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1037	HIS	CA-C-N	11.31	133.98	119.84
1	A	1037	HIS	C-N-CA	11.31	133.98	119.84
1	A	656	ASP	CB-CA-C	-9.91	92.90	109.55
1	A	1425	GLY	N-CA-C	-8.74	92.48	113.18
1	A	1423	GLN	N-CA-C	-7.07	95.00	107.73
1	A	515	GLN	CA-C-N	7.07	130.70	120.38
1	A	515	GLN	C-N-CA	7.07	130.70	120.38
1	A	1914	PHE	CB-CA-C	6.28	122.53	110.17
1	A	1426	SER	N-CA-C	-5.93	98.17	110.80
1	A	1195	ILE	CB-CA-C	5.86	119.34	111.19
1	A	1695	THR	CA-C-N	5.68	128.08	120.58
1	A	1695	THR	C-N-CA	5.68	128.08	120.58
1	A	718	ARG	CA-C-N	5.62	132.27	121.54
1	A	718	ARG	C-N-CA	5.62	132.27	121.54
1	A	718	ARG	O-C-N	5.53	129.34	123.42
1	A	1287	VAL	N-CA-C	-5.43	98.04	109.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	PHE	CB-CA-C	-5.41	102.12	110.78
1	A	1627	VAL	CB-CA-C	5.38	117.07	111.09
1	A	1554	LYS	CA-C-N	5.35	125.29	121.65
1	A	1554	LYS	C-N-CA	5.35	125.29	121.65
1	A	1026	PHE	CB-CA-C	5.32	118.01	110.24
1	A	514	SER	CA-C-N	5.29	129.92	122.46
1	A	514	SER	C-N-CA	5.29	129.92	122.46
1	A	791	LEU	CB-CA-C	-5.29	100.05	110.11
1	A	1234	ASP	N-CA-C	-5.28	99.56	110.80
1	A	716	THR	O-C-N	5.14	129.07	123.27
1	A	366	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	1071	LEU	N-CA-C	-5.11	105.27	112.12
1	A	516	ARG	N-CA-C	5.10	118.28	111.75
1	A	295	PRO	N-CA-CB	5.06	105.75	102.92
1	A	2007	GLN	CA-C-N	5.02	130.06	122.68
1	A	2007	GLN	C-N-CA	5.02	130.06	122.68
1	A	256	GLU	CA-C-N	5.01	125.10	120.34
1	A	256	GLU	C-N-CA	5.01	125.10	120.34

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1035	PRO	Peptide
1	A	1037	HIS	Mainchain
1	A	1051	CYS	Peptide
1	A	1180	TYR	Peptide
1	A	1199	CYS	Peptide
1	A	1201	HIS	Peptide
1	A	1272	GLY	Peptide
1	A	1304	ALA	Peptide
1	A	1576	PHE	Peptide
1	A	1656	GLU	Peptide
1	A	1766	ASN	Peptide
1	A	1914	PHE	Peptide
1	A	2186	LEU	Peptide
1	A	310	SER	Peptide
1	A	505	GLU	Peptide
1	A	813	THR	Peptide
1	A	823	ARG	Peptide
1	A	854	SER	Peptide
1	A	855	ILE	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	995	CYS	Peptide

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	17025	0	16238	328	0
2	B	28	0	25	0	0
3	C	39	0	34	0	0
4	A	42	0	37	9	0
All	All	17134	0	16334	328	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 10.

All (328) 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:1239:ARG:NH2	1:A:1424:ALA:HB2	1.59	1.17
1:A:718:ARG:HB3	1:A:732:ALA:HB1	1.28	1.13
1:A:1239:ARG:HH22	1:A:1424:ALA:CB	1.71	1.02
1:A:1663:VAL:HG13	1:A:1670:ILE:HG23	1.44	1.00
1:A:718:ARG:HB3	1:A:732:ALA:CB	1.93	0.98
1:A:1663:VAL:CG1	1:A:1670:ILE:HG23	1.95	0.96
1:A:897:ILE:HG12	1:A:924:TRP:CD1	2.02	0.95
1:A:1414:ILE:HD11	1:A:1494:PRO:CG	1.97	0.95
1:A:764:THR:HG22	1:A:766:TYR:H	1.31	0.93
1:A:1257:THR:HG21	1:A:1364:TRP:HZ2	1.33	0.93
1:A:146:THR:HG21	1:A:181:TYR:HB3	1.53	0.90
1:A:295:PRO:HG2	1:A:501:HIS:CE1	2.07	0.90
1:A:1287:VAL:HG13	1:A:1307:PHE:HB3	1.56	0.87
1:A:1323:THR:HB	4:A:2508:NAG:H62	1.57	0.86
1:A:1321:ASN:OD1	4:A:2508:NAG:C1	2.25	0.84
1:A:600:LEU:HB3	1:A:772:PRO:HB3	1.59	0.84
1:A:764:THR:HG22	1:A:766:TYR:N	1.92	0.83
1:A:1414:ILE:HD11	1:A:1494:PRO:HG3	1.61	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:GLY:O	1:A:277:GLN:NE2	2.14	0.81
1:A:1414:ILE:HG22	1:A:1435:VAL:HG23	1.63	0.80
1:A:192:LEU:CD2	1:A:217:VAL:HG11	2.13	0.79
1:A:2053:SER:OG	1:A:2067:GLY:O	2.01	0.78
1:A:718:ARG:CB	1:A:732:ALA:CB	2.61	0.78
1:A:192:LEU:HD22	1:A:217:VAL:HG11	1.65	0.77
1:A:754:ASP:CG	1:A:756:SER:OG	2.29	0.75
1:A:1414:ILE:HD11	1:A:1494:PRO:CB	2.17	0.74
1:A:192:LEU:HD23	1:A:192:LEU:O	1.87	0.72
1:A:1321:ASN:HD21	4:A:2508:NAG:C1	2.02	0.72
1:A:91:VAL:HG13	1:A:104:VAL:HB	1.71	0.71
1:A:897:ILE:CD1	1:A:924:TRP:NE1	2.53	0.71
1:A:1257:THR:HG21	1:A:1364:TRP:CZ2	2.22	0.71
1:A:516:ARG:HB2	1:A:520:LYS:HB3	1.73	0.70
1:A:2272:THR:HB	1:A:2276:GLN:O	1.93	0.67
1:A:1083:ALA:HB1	1:A:1146:THR:HB	1.77	0.67
1:A:1094:GLN:HE22	1:A:1315:ASN:HB2	1.58	0.67
1:A:717:TYR:O	1:A:733:THR:N	2.27	0.67
1:A:1257:THR:CG2	1:A:1364:TRP:HZ2	2.06	0.66
1:A:1195:ILE:HG22	1:A:1218:PHE:HB2	1.77	0.66
1:A:828:VAL:HG23	1:A:831:CYS:SG	2.35	0.66
1:A:1427:ASP:OD1	1:A:1427:ASP:N	2.28	0.66
1:A:2017:LEU:HD22	1:A:2037:LEU:HB2	1.77	0.66
1:A:525:ILE:HD12	1:A:527:ILE:CD1	2.25	0.65
1:A:1287:VAL:CG1	1:A:1307:PHE:HB3	2.27	0.64
1:A:1663:VAL:HG13	1:A:1670:ILE:CG2	2.24	0.64
1:A:2053:SER:CB	1:A:2067:GLY:O	2.46	0.64
1:A:321:GLU:HG3	1:A:501:HIS:CE1	2.33	0.64
1:A:718:ARG:CB	1:A:732:ALA:HB2	2.27	0.64
1:A:1321:ASN:ND2	4:A:2508:NAG:C1	2.60	0.64
1:A:2017:LEU:HD12	1:A:2128:TRP:NE1	2.13	0.63
1:A:899:LEU:HA	1:A:924:TRP:HB2	1.80	0.63
1:A:1495:MET:SD	1:A:1888:GLN:NE2	2.72	0.62
1:A:500:ARG:NH2	1:A:506:GLN:O	2.31	0.62
1:A:1742:LEU:HD12	1:A:1748:GLU:O	1.98	0.62
1:A:899:LEU:HG	1:A:924:TRP:HB2	1.79	0.62
1:A:195:LEU:HD21	1:A:320:THR:HG21	1.82	0.61
1:A:773:LEU:HD11	1:A:822:CYS:HB3	1.83	0.61
1:A:1321:ASN:CG	4:A:2508:NAG:C1	2.73	0.61
1:A:718:ARG:HG2	1:A:718:ARG:HH11	1.64	0.61
1:A:1696:SER:OG	1:A:1697:PRO:HD3	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:VAL:HG22	1:A:314:PHE:HB2	1.82	0.60
1:A:1323:THR:CB	4:A:2508:NAG:H62	2.28	0.60
1:A:1350:VAL:CG2	1:A:1363:GLU:HB3	2.32	0.60
1:A:1250:ILE:N	1:A:1251:PRO:HD2	2.16	0.60
1:A:815:ARG:HD2	1:A:839:GLN:HE21	1.66	0.59
1:A:773:LEU:CD1	1:A:822:CYS:HB3	2.33	0.59
1:A:1291:CYS:SG	1:A:1302:LYS:O	2.61	0.59
1:A:897:ILE:HG12	1:A:924:TRP:NE1	2.16	0.59
1:A:146:THR:HG21	1:A:181:TYR:CB	2.31	0.59
1:A:899:LEU:HG	1:A:924:TRP:CD1	2.38	0.59
1:A:959:ASN:HD21	1:A:980:ASP:HB2	1.68	0.59
1:A:1624:ARG:NH1	1:A:1627:VAL:O	2.35	0.59
1:A:966:VAL:HB	1:A:973:PHE:HB2	1.85	0.58
1:A:897:ILE:CG1	1:A:924:TRP:CD1	2.82	0.58
1:A:2090:TYR:HB3	1:A:2092:GLY:O	2.02	0.58
1:A:718:ARG:HA	1:A:732:ALA:HA	1.85	0.58
1:A:525:ILE:HD12	1:A:527:ILE:HD11	1.83	0.57
1:A:773:LEU:HD11	1:A:822:CYS:CB	2.33	0.57
1:A:116:LEU:HD22	1:A:459:GLY:O	2.04	0.57
1:A:525:ILE:HD13	1:A:604:PRO:HG3	1.85	0.57
1:A:1416:VAL:HG12	1:A:1509:TRP:CZ3	2.40	0.57
1:A:295:PRO:HG2	1:A:501:HIS:ND1	2.19	0.57
1:A:718:ARG:HB2	1:A:732:ALA:HB2	1.86	0.57
1:A:1183:GLY:HA3	1:A:1191:PHE:HB2	1.86	0.57
1:A:1663:VAL:HG12	1:A:1670:ILE:O	2.04	0.57
1:A:91:VAL:HG12	1:A:105:GLY:HA3	1.87	0.57
1:A:717:TYR:O	1:A:733:THR:O	2.23	0.57
1:A:321:GLU:HG3	1:A:501:HIS:HE1	1.68	0.57
1:A:1494:PRO:HB3	1:A:1509:TRP:CE3	2.40	0.57
1:A:899:LEU:HG	1:A:924:TRP:CG	2.41	0.56
1:A:1287:VAL:HG13	1:A:1287:VAL:O	2.04	0.56
1:A:525:ILE:CD1	1:A:527:ILE:HD11	2.35	0.56
1:A:1759:CYS:HB3	1:A:1761:ALA:O	2.05	0.56
1:A:195:LEU:CD2	1:A:320:THR:HG21	2.35	0.56
1:A:1771:ILE:HG22	1:A:1796:PHE:HB2	1.86	0.56
1:A:899:LEU:HG	1:A:924:TRP:CB	2.35	0.55
1:A:1060:PRO:HA	1:A:1080:PHE:HB3	1.88	0.55
1:A:1597:LEU:HB2	1:A:1621:PHE:HB2	1.87	0.55
1:A:260:LEU:HD23	1:A:260:LEU:O	2.06	0.55
1:A:1318:LEU:HB2	1:A:1340:PHE:HB2	1.89	0.55
1:A:764:THR:HG22	1:A:765:SER:N	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1321:ASN:HD21	4:A:2508:NAG:C2	2.19	0.54
1:A:899:LEU:CD1	1:A:924:TRP:CD1	2.91	0.54
1:A:1178:LEU:HB3	1:A:1195:ILE:HG13	1.87	0.54
1:A:2017:LEU:HD12	1:A:2128:TRP:CE2	2.43	0.54
1:A:1425:GLY:C	1:A:1426:SER:O	2.46	0.54
1:A:516:ARG:HB2	1:A:520:LYS:CB	2.38	0.54
1:A:361:TYR:OH	1:A:452:ARG:NH1	2.41	0.54
1:A:1414:ILE:CG2	1:A:1435:VAL:HG23	2.37	0.54
1:A:2268:PHE:HE1	1:A:2277:TYR:HB3	1.73	0.54
1:A:1535:LEU:HD23	1:A:1708:ASN:HD22	1.73	0.53
1:A:1355:THR:HG23	1:A:1356:SER:N	2.24	0.53
1:A:2065:VAL:O	1:A:2089:HIS:HB2	2.09	0.53
1:A:2173:VAL:HG21	1:A:2266:PRO:HG2	1.90	0.53
1:A:935:THR:HG21	1:A:947:PRO:HG3	1.91	0.53
1:A:1019:LEU:HB3	1:A:1029:LEU:HG	1.91	0.53
1:A:885:THR:HG23	1:A:886:SER:O	2.09	0.52
1:A:2053:SER:HB3	1:A:2067:GLY:O	2.09	0.52
1:A:897:ILE:HD13	1:A:924:TRP:NE1	2.25	0.52
1:A:1236:CYS:O	1:A:1311:LEU:HD21	2.09	0.52
1:A:1338:ILE:HG21	1:A:1340:PHE:CZ	2.44	0.52
1:A:872:SER:HB3	1:A:900:VAL:HG12	1.91	0.52
1:A:1029:LEU:HD13	1:A:1049:PHE:HE1	1.74	0.52
1:A:1875:PHE:HA	1:A:1958:ARG:HB3	1.92	0.51
1:A:525:ILE:HD12	1:A:527:ILE:HD13	1.91	0.51
1:A:969:ILE:HD11	1:A:1065:GLN:HE21	1.75	0.51
1:A:1393:LEU:HD11	1:A:1511:THR:HG21	1.92	0.51
1:A:2017:LEU:CD2	1:A:2037:LEU:HB2	2.40	0.51
1:A:1143:CYS:SG	1:A:1160:ASN:ND2	2.83	0.51
1:A:1695:THR:O	1:A:1698:ASP:HB2	2.11	0.51
1:A:1883:LEU:HB3	1:A:1894:LEU:HA	1.93	0.51
1:A:1955:THR:HG22	1:A:1955:THR:O	2.11	0.50
1:A:525:ILE:CD1	1:A:604:PRO:HG3	2.41	0.50
1:A:840:MET:HB3	1:A:853:VAL:HB	1.92	0.50
1:A:460:GLU:HG3	1:A:465:TYR:CE1	2.45	0.50
1:A:816:LYS:HZ2	1:A:1096:THR:HG21	1.76	0.50
1:A:1288:ILE:HG23	1:A:1304:ALA:HB2	1.94	0.50
1:A:1416:VAL:CG1	1:A:1509:TRP:CH2	2.95	0.50
1:A:774:GLU:O	1:A:776:ILE:N	2.44	0.50
1:A:542:GLU:OE1	1:A:542:GLU:N	2.39	0.50
1:A:1239:ARG:HH22	1:A:1424:ALA:HB2	0.74	0.50
1:A:1387:THR:HG23	1:A:1517:VAL:HG22	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:VAL:HG13	1:A:82:VAL:O	2.12	0.49
1:A:302:THR:HA	1:A:319:VAL:O	2.11	0.49
1:A:897:ILE:CG1	1:A:924:TRP:NE1	2.76	0.49
1:A:1973:GLY:O	1:A:1974:ARG:NH1	2.45	0.49
1:A:1098:PRO:HD2	1:A:1170:VAL:HG21	1.94	0.49
1:A:1201:HIS:CD2	1:A:1223:VAL:HG21	2.47	0.49
1:A:1201:HIS:CD2	1:A:1396:TYR:CD2	3.01	0.49
1:A:91:VAL:HG13	1:A:104:VAL:CB	2.41	0.49
1:A:1314:GLU:O	1:A:1317:VAL:HG12	2.13	0.49
1:A:1416:VAL:HG13	1:A:1509:TRP:CH2	2.48	0.49
1:A:2216:VAL:HG23	1:A:2275:CYS:O	2.13	0.49
1:A:113:SER:HB2	1:A:116:LEU:HB3	1.95	0.49
1:A:1423:GLN:NE2	1:A:1429:CYS:H	2.11	0.49
1:A:460:GLU:HG3	1:A:465:TYR:HE1	1.77	0.48
1:A:1271:CYS:N	1:A:1322:TYR:OH	2.44	0.48
1:A:751:GLN:OE1	1:A:751:GLN:N	2.46	0.48
1:A:923:LEU:HD22	1:A:1352:LEU:HD11	1.96	0.48
1:A:1252:LEU:HD22	1:A:1364:TRP:HZ3	1.78	0.48
1:A:1416:VAL:CG1	1:A:1509:TRP:CZ3	2.96	0.48
1:A:1657:GLN:HG3	1:A:1706:PRO:HD3	1.96	0.48
1:A:2115:THR:HB	1:A:2125:HIS:C	2.39	0.48
1:A:775:CYS:O	1:A:776:ILE:HG12	2.14	0.48
1:A:2083:VAL:HG23	1:A:2101:ILE:HB	1.95	0.48
1:A:1387:THR:HG23	1:A:1517:VAL:CG2	2.44	0.48
1:A:2110:GLY:HA3	1:A:2129:ASP:HB3	1.96	0.47
1:A:839:GLN:HB3	1:A:856:SER:HB3	1.95	0.47
1:A:1732:ASP:OD1	1:A:1734:GLY:O	2.33	0.47
1:A:266:LEU:HB2	1:A:292:PHE:HB2	1.96	0.47
1:A:1904:PRO:HG2	1:A:1953:HIS:HA	1.95	0.47
1:A:2101:ILE:HG23	1:A:2126:PHE:HB3	1.96	0.47
1:A:836:SER:N	1:A:859:GLY:O	2.44	0.47
1:A:1426:SER:O	1:A:1427:ASP:C	2.57	0.47
1:A:1201:HIS:NE2	1:A:1396:TYR:HD2	2.12	0.47
1:A:1670:ILE:HD11	1:A:1803:VAL:HA	1.97	0.47
1:A:1131:LEU:HD12	1:A:1150:CYS:HB3	1.96	0.47
1:A:1184:ASP:N	1:A:1190:ARG:O	2.48	0.47
1:A:1830:SER:HB2	1:A:1849:THR:HG23	1.96	0.47
1:A:368:TYR:HA	1:A:395:LYS:HG2	1.97	0.47
1:A:779:ASP:HA	1:A:867:VAL:HG11	1.96	0.47
1:A:1013:VAL:HG22	1:A:1014:GLY:O	2.15	0.47
1:A:1201:HIS:CD2	1:A:1223:VAL:CG2	2.98	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:TRP:NE1	1:A:320:THR:HG22	2.30	0.46
1:A:490:LYS:O	1:A:492:ARG:NH2	2.46	0.46
1:A:1194:ARG:HB2	1:A:1217:VAL:HG23	1.97	0.46
1:A:1672:LEU:HD12	1:A:1675:LEU:HD12	1.96	0.46
1:A:62:GLU:HG2	1:A:73:LYS:HG2	1.97	0.46
1:A:336:LEU:HD23	1:A:412:LEU:HG	1.98	0.46
1:A:1029:LEU:HD13	1:A:1049:PHE:CE1	2.50	0.46
1:A:1509:TRP:CD1	1:A:1511:THR:HB	2.50	0.46
1:A:1551:TYR:HB3	1:A:1635:LEU:HD23	1.97	0.46
1:A:1569:ALA:O	1:A:1572:VAL:HG12	2.15	0.46
1:A:170:ASN:HB2	1:A:173:LYS:HB2	1.97	0.46
1:A:2266:PRO:HB3	1:A:2281:TRP:CG	2.51	0.46
1:A:372:LEU:HB2	1:A:390:VAL:HG12	1.97	0.46
1:A:1127:ARG:HD2	1:A:1152:LEU:HD21	1.97	0.46
1:A:1067:ILE:HG22	1:A:1074:ARG:HB2	1.97	0.46
1:A:230:GLN:HB2	1:A:243:VAL:HG11	1.96	0.46
1:A:1177:SER:OG	1:A:1194:ARG:NH1	2.48	0.46
1:A:332:ARG:HA	1:A:332:ARG:HD3	1.51	0.46
1:A:1019:LEU:HD22	1:A:1029:LEU:HD11	1.98	0.46
1:A:1091:VAL:HG13	1:A:1166:ILE:HG23	1.98	0.46
1:A:1406:THR:HG23	1:A:1806:ASP:HB2	1.98	0.46
1:A:1689:GLU:HB2	1:A:2225:TYR:HD2	1.82	0.46
1:A:873:LEU:HD12	1:A:873:LEU:O	2.16	0.45
1:A:115:SER:O	1:A:138:PHE:HB2	2.16	0.45
1:A:383:CYS:HA	1:A:401:VAL:HG11	1.99	0.45
1:A:1355:THR:HG21	1:A:1361:LEU:CD2	2.45	0.45
1:A:1624:ARG:HE	1:A:1650:HIS:HB3	1.80	0.45
1:A:258:LEU:HB3	1:A:268:LEU:HB2	1.98	0.45
1:A:1600:VAL:HA	1:A:1618:VAL:HG12	1.98	0.45
1:A:104:VAL:HG13	1:A:132:ILE:HG22	1.98	0.45
1:A:410:LEU:HD23	1:A:421:LEU:HD11	1.98	0.45
1:A:546:VAL:HG21	1:A:589:THR:HG21	1.97	0.45
1:A:941:VAL:O	1:A:1019:LEU:HD21	2.16	0.45
1:A:1735:ARG:N	1:A:1754:GLU:O	2.46	0.45
1:A:1068:ASP:O	1:A:1073:ILE:O	2.34	0.45
1:A:1268:PHE:HA	1:A:1290:SER:HA	1.99	0.45
1:A:372:LEU:HD11	1:A:455:PRO:HG3	1.98	0.44
1:A:548:ALA:O	1:A:555:LYS:N	2.51	0.44
1:A:2268:PHE:HA	1:A:2279:PHE:CB	2.47	0.44
1:A:1450:ARG:HB2	1:A:1465:VAL:HG22	1.99	0.44
1:A:175:ASN:HD21	1:A:237:GLY:HA2	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1402:ALA:HB3	1:A:1412:TYR:HB2	2.00	0.44
1:A:548:ALA:HB3	1:A:555:LYS:HB2	1.99	0.44
1:A:1105:LEU:HD11	1:A:1176:LEU:HD13	1.99	0.44
1:A:1265:THR:OG1	1:A:1295:ARG:NH2	2.50	0.44
1:A:307:THR:HB	1:A:736:THR:HG21	1.99	0.44
1:A:830:GLY:C	1:A:855:ILE:HG12	2.43	0.44
1:A:1212:ASN:O	1:A:1215:GLU:HG2	2.18	0.44
1:A:1245:ASN:HD22	1:A:1372:PRO:HD2	1.81	0.44
1:A:764:THR:CG2	1:A:766:TYR:H	2.17	0.44
1:A:1261:ALA:HB3	1:A:1264:TYR:HB2	1.99	0.44
1:A:1696:SER:OG	1:A:2009:HIS:N	2.31	0.44
1:A:1786:LEU:HA	1:A:1796:PHE:HA	1.99	0.44
1:A:1866:LEU:HB3	1:A:1873:ALA:HB3	1.99	0.44
1:A:1773:PHE:HB3	1:A:1803:VAL:HG21	2.00	0.43
1:A:2035:ILE:HA	1:A:2054:VAL:HG22	2.00	0.43
1:A:527:ILE:HD11	1:A:620:TRP:CZ3	2.53	0.43
1:A:1321:ASN:HD21	4:A:2508:NAG:H2	1.81	0.43
1:A:816:LYS:HE3	1:A:1096:THR:HG21	2.00	0.43
1:A:1019:LEU:C	1:A:1019:LEU:HD12	2.43	0.43
1:A:2120:ASP:OD1	1:A:2121:SER:N	2.52	0.43
1:A:1252:LEU:HD21	1:A:1368:TYR:HE2	1.83	0.43
1:A:1423:GLN:NE2	1:A:1429:CYS:SG	2.87	0.43
1:A:2259:PRO:HA	1:A:2284:SER:HA	2.01	0.43
1:A:916:TRP:CG	1:A:1356:SER:HB3	2.54	0.43
1:A:1271:CYS:H	1:A:1322:TYR:HH	1.63	0.43
1:A:1292:GLN:HE21	1:A:1302:LYS:HB2	1.83	0.43
1:A:718:ARG:HH11	1:A:718:ARG:CG	2.30	0.43
1:A:899:LEU:HD11	1:A:924:TRP:CD1	2.54	0.43
1:A:1414:ILE:CD1	1:A:1494:PRO:HG3	2.42	0.43
1:A:2081:VAL:HG12	1:A:2103:LEU:HB3	2.00	0.43
1:A:2254:PHE:HE2	1:A:2278:LEU:HD21	1.84	0.43
1:A:207:SER:OG	1:A:630:ARG:NH1	2.51	0.43
1:A:1192:SER:O	1:A:1215:GLU:HA	2.19	0.43
1:A:527:ILE:HD11	1:A:620:TRP:HZ3	1.83	0.43
1:A:776:ILE:HD13	1:A:787:ASP:HA	2.01	0.43
1:A:1314:GLU:HB2	1:A:1317:VAL:HG13	2.01	0.43
1:A:56:LEU:HB3	1:A:76:ILE:HD13	2.00	0.42
1:A:897:ILE:HD11	1:A:924:TRP:CE2	2.54	0.42
1:A:1536:PHE:HB3	1:A:1597:LEU:HD11	2.02	0.42
1:A:1981:VAL:HG22	1:A:1982:ARG:HD2	2.01	0.42
1:A:62:GLU:HB3	1:A:71:LEU:HD11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:LEU:HD23	1:A:474:ALA:HB1	2.01	0.42
1:A:1209:GLN:HB3	1:A:1217:VAL:HG13	1.99	0.42
1:A:718:ARG:CG	1:A:718:ARG:NH1	2.81	0.42
1:A:897:ILE:CD1	1:A:924:TRP:CE2	3.02	0.42
1:A:1201:HIS:CD2	1:A:1396:TYR:HD2	2.37	0.42
1:A:1411:HIS:O	1:A:1438:LEU:N	2.44	0.42
1:A:120:ASN:CG	4:A:2501:NAG:O7	2.62	0.42
1:A:1877:ARG:HB3	1:A:1880:SER:HB3	2.01	0.42
1:A:353:VAL:HG21	1:A:359:LEU:O	2.20	0.42
1:A:1517:VAL:HG23	1:A:1517:VAL:O	2.19	0.42
1:A:2241:CYS:HB2	1:A:2275:CYS:HB2	1.89	0.42
1:A:788:LEU:HD11	1:A:873:LEU:CD1	2.50	0.42
1:A:250:ASP:O	1:A:272:LYS:HD3	2.20	0.42
1:A:390:VAL:HG23	1:A:404:ALA:HB3	2.01	0.41
1:A:840:MET:HA	1:A:854:SER:O	2.21	0.41
1:A:979:GLY:HA3	1:A:1017:LYS:HE2	2.01	0.41
1:A:1050:VAL:HG23	1:A:1081:GLU:HG2	2.01	0.41
1:A:1788:ARG:NH2	1:A:1789:THR:O	2.53	0.41
1:A:1284:LYS:HB2	1:A:1286:LYS:HG2	2.02	0.41
1:A:1338:ILE:HG21	1:A:1340:PHE:CE1	2.55	0.41
1:A:1338:ILE:CG2	1:A:1340:PHE:CZ	3.02	0.41
1:A:936:THR:HG22	1:A:1020:GLN:HB3	2.02	0.41
1:A:1012:LEU:HD22	1:A:1013:VAL:HG12	2.01	0.41
1:A:2057:LYS:HA	1:A:2063:VAL:HG13	2.02	0.41
1:A:2214:ARG:HD2	1:A:2214:ARG:HA	1.85	0.41
1:A:503:GLU:HG3	1:A:505:GLU:H	1.86	0.41
1:A:2159:LEU:HG	1:A:2163:TYR:HB2	2.02	0.41
1:A:240:ALA:HB1	1:A:288:VAL:HG21	2.02	0.41
1:A:718:ARG:HD2	1:A:718:ARG:C	2.45	0.41
1:A:2075:ASP:HB3	1:A:2082:ILE:HD12	2.02	0.41
1:A:925:ASN:ND2	1:A:1363:GLU:OE2	2.39	0.41
1:A:1583:VAL:HG21	1:A:1645:LEU:HD12	2.03	0.41
1:A:262:SER:O	1:A:263:ASN:C	2.64	0.41
1:A:572:GLN:HG2	1:A:592:THR:HG22	2.01	0.41
1:A:718:ARG:HG2	1:A:718:ARG:NH1	2.33	0.41
1:A:860:VAL:HG13	1:A:862:LYS:HE2	2.03	0.41
1:A:872:SER:CB	1:A:900:VAL:HG12	2.51	0.41
1:A:1136:PRO:HB3	1:A:1147:ALA:HA	2.01	0.41
1:A:1435:VAL:HG21	1:A:1479:THR:HG21	2.02	0.41
1:A:1623:CYS:SG	1:A:1624:ARG:N	2.93	0.41
1:A:1201:HIS:CD2	1:A:1396:TYR:CE2	3.09	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1686:ASP:HA	1:A:1786:LEU:HB3	2.04	0.40
1:A:1743:ASN:HB2	1:A:1750:TYR:HE2	1.86	0.40
1:A:1067:ILE:HG13	1:A:1067:ILE:O	2.21	0.40
1:A:1249:LEU:C	1:A:1251:PRO:HD2	2.46	0.40
1:A:2185:GLN:NE2	1:A:2188:SER:OG	2.54	0.40
1:A:139:LEU:HB2	1:A:162:ARG:HB3	2.03	0.40
1:A:941:VAL:O	1:A:1019:LEU:CD2	2.70	0.40
1:A:1414:ILE:HD11	1:A:1494:PRO:HB2	2.00	0.40
1:A:1757:THR:HA	1:A:1758:PRO:HD3	1.97	0.40
1:A:1787:LEU:HD13	1:A:2278:LEU:HD21	2.04	0.40
1:A:2103:LEU:HD13	1:A:2128:TRP:HD1	1.87	0.40
1:A:527:ILE:O	1:A:573:LEU:HD21	2.21	0.40
1:A:717:TYR:HD1	1:A:717:TYR:HA	1.65	0.40
1:A:900:VAL:HG11	1:A:1350:VAL:HG21	2.03	0.40
1:A:923:LEU:HD13	1:A:1352:LEU:HD11	2.03	0.40
1:A:1101:ASN:HB3	1:A:1227:PRO:HB3	2.03	0.40
1:A:1237:GLU:HB3	1:A:1246:LEU:HD12	2.03	0.40
1:A:2000:LYS:HD2	1:A:2039:GLN:HA	2.02	0.40
1:A:2010:ARG:HD2	1:A:2134:CYS:HA	2.03	0.40
1:A:142:LYS:HB3	1:A:198:THR:HG21	2.04	0.40
1:A:960:ASN:O	1:A:976:ASN:ND2	2.55	0.40
1:A:980:ASP:O	1:A:982:PRO:HD3	2.21	0.40
1:A:1845:VAL:HG12	1:A:1864:VAL:HG13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	2200/2499 (88%)	2044 (93%)	151 (7%)	5 (0%)	43 74

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	ASN
1	A	657	ALA
1	A	719	ASP
1	A	1038	PRO
1	A	775	CYS

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	1904/2142 (89%)	1888 (99%)	16 (1%)	73 77

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	332	ARG
1	A	480	GLU
1	A	516	ARG
1	A	718	ARG
1	A	719	ASP
1	A	775	CYS
1	A	1146	THR
1	A	1279	CYS
1	A	1423	GLN
1	A	1426	SER
1	A	1427	ASP
1	A	1435	VAL
1	A	1902	CYS
1	A	2083	VAL
1	A	2241	CYS
1	A	2249	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	127	GLN
1	A	311	ASN
1	A	325	HIS
1	A	348	GLN
1	A	379	GLN
1	A	477	HIS
1	A	501	HIS
1	A	533	GLN
1	A	570	ASN
1	A	688	GLN
1	A	839	GLN
1	A	959	ASN
1	A	1039	ASN
1	A	1065	GLN
1	A	1094	GLN
1	A	1201	HIS
1	A	1292	GLN
1	A	1399	ASN
1	A	1567	ASN
1	A	1631	ASN
1	A	1705	GLN
1	A	1708	ASN
1	A	1764	HIS
1	A	1887	HIS
1	A	2089	HIS
1	A	2145	ASN
1	A	2153	ASN
1	A	2185	GLN
1	A	2211	HIS
1	A	2227	GLN
1	A	2276	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	0.37	0	17,19,21	0.70	0
2	NAG	B	2	2	14,14,15	0.36	0	17,19,21	0.74	0
3	NAG	C	1	3,1	14,14,15	0.29	0	17,19,21	1.03	2 (11%)
3	NAG	C	2	3	14,14,15	0.31	0	17,19,21	1.05	2 (11%)
3	BMA	C	3	3	11,11,12	0.39	0	15,15,17	0.65	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
3	NAG	C	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	C2-N2-C7	2.37	126.08	122.90
3	C	2	NAG	C8-C7-N2	2.31	119.95	116.12
3	C	1	NAG	C8-C7-N2	2.28	119.90	116.12
3	C	1	NAG	C2-N2-C7	2.04	125.63	122.90

There are no chirality outliers.

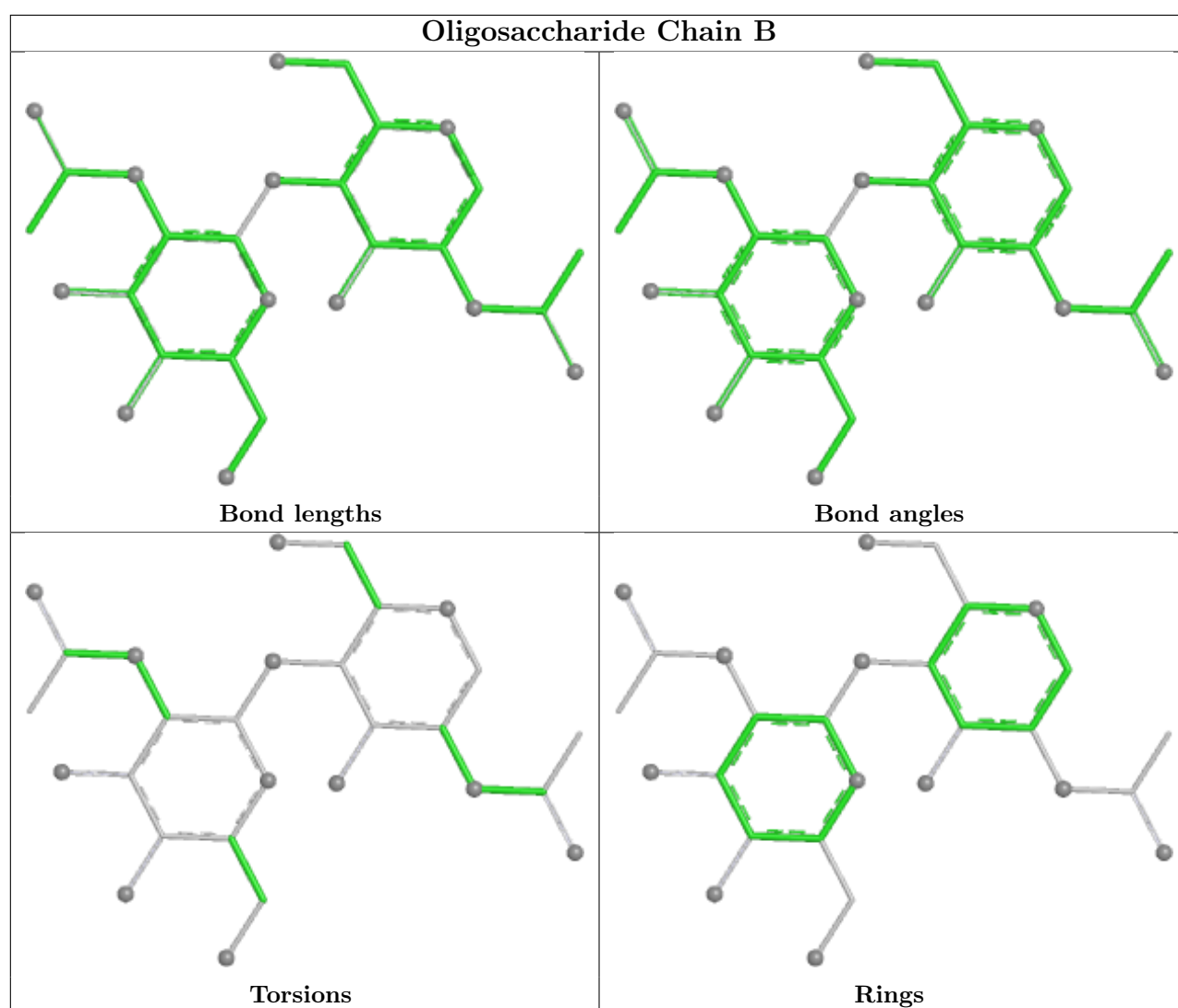
All (6) torsion outliers are listed below:

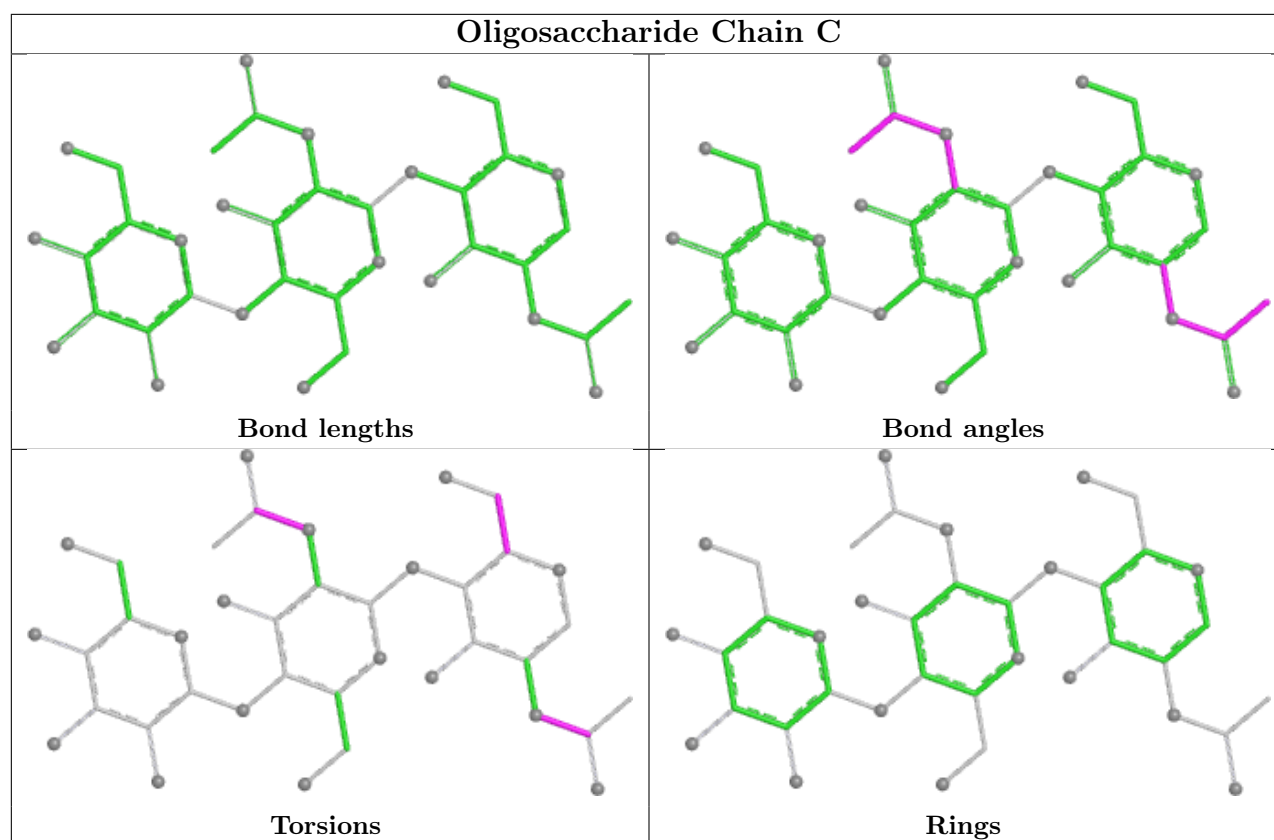
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2

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 oligosaccharide.





5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	2508	-	14,14,15	0.40	0	17,19,21	1.17	1 (5%)
4	NAG	A	2501	1	14,14,15	0.59	0	17,19,21	0.94	1 (5%)
4	NAG	A	2507	1	14,14,15	0.44	0	17,19,21	1.31	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	2508	-	-	3/6/23/26	0/1/1/1
4	NAG	A	2501	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2507	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2507	NAG	C1-O5-C5	3.07	116.30	112.19
4	A	2507	NAG	C2-N2-C7	2.50	126.25	122.90
4	A	2508	NAG	C4-C3-C2	-2.44	107.44	111.02
4	A	2507	NAG	O5-C1-C2	-2.43	107.53	111.29
4	A	2501	NAG	O5-C1-C2	2.05	114.46	111.29

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2508	NAG	C1-C2-N2-C7
4	A	2507	NAG	O5-C5-C6-O6
4	A	2507	NAG	C4-C5-C6-O6
4	A	2508	NAG	O5-C5-C6-O6
4	A	2508	NAG	C4-C5-C6-O6
4	A	2507	NAG	C1-C2-N2-C7
4	A	2507	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2508	NAG	8	0
4	A	2501	NAG	1	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.

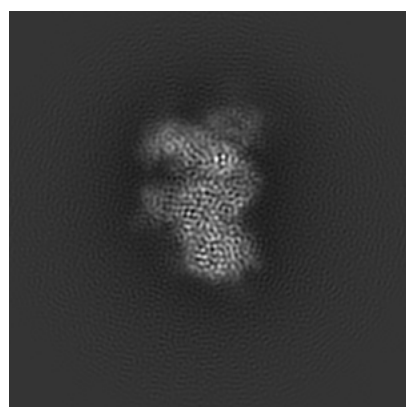
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20815. These allow visual inspection of the internal detail of the map and identification of artifacts.

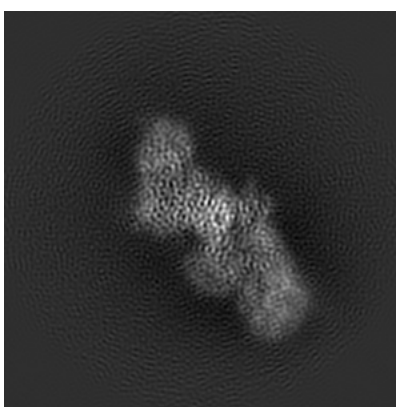
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

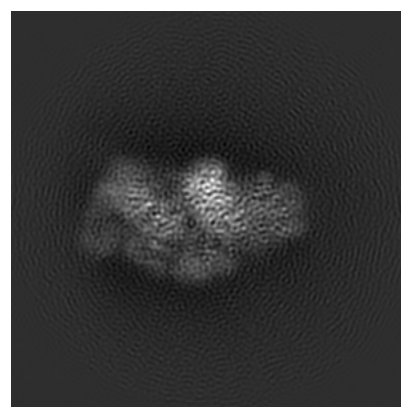
6.1.1 Primary map



X



Y

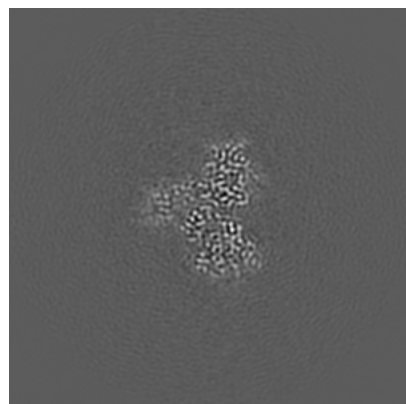


Z

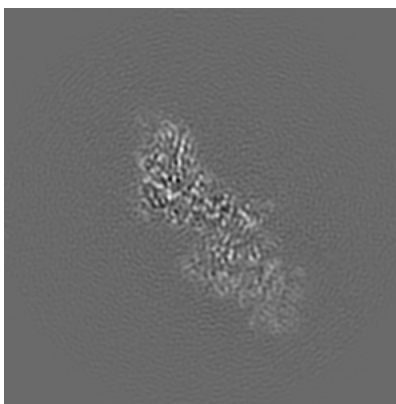
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

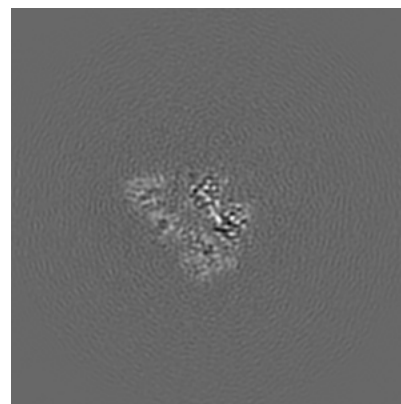
6.2.1 Primary map



X Index: 140



Y Index: 140

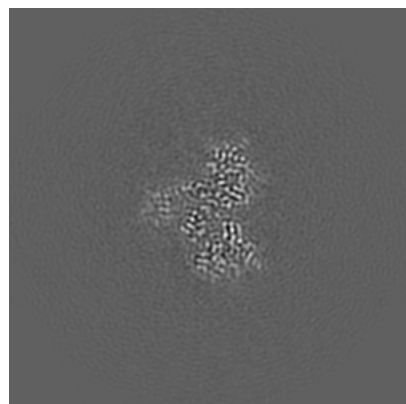


Z Index: 140

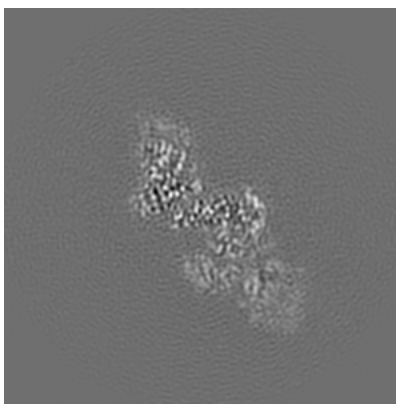
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

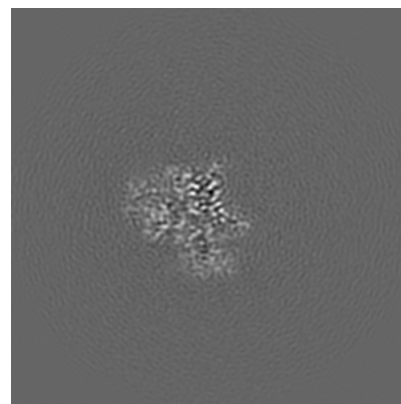
6.3.1 Primary map



X Index: 141



Y Index: 145

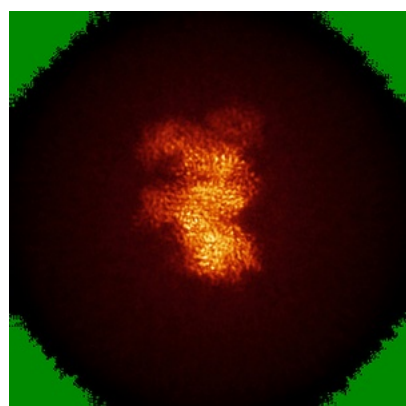


Z Index: 149

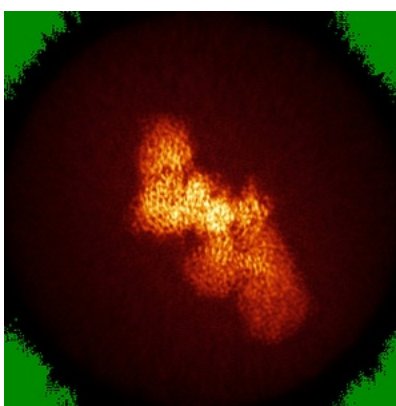
The images above show the largest variance slices of the map in three orthogonal directions.

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

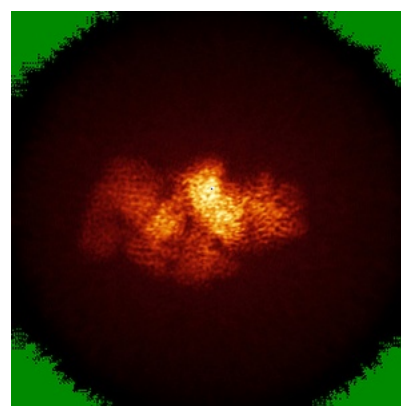
6.4.1 Primary map



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 0.0145. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

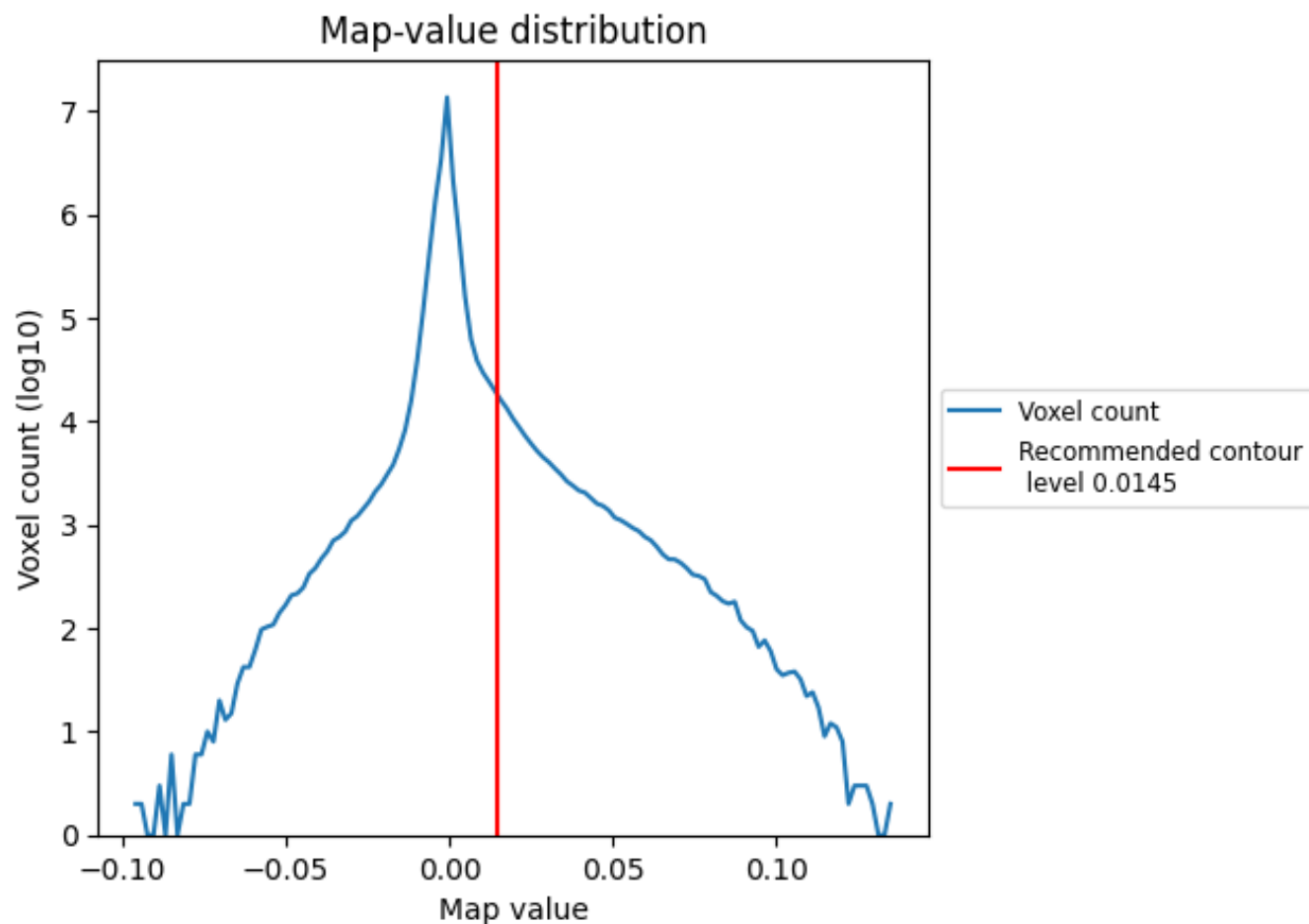
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

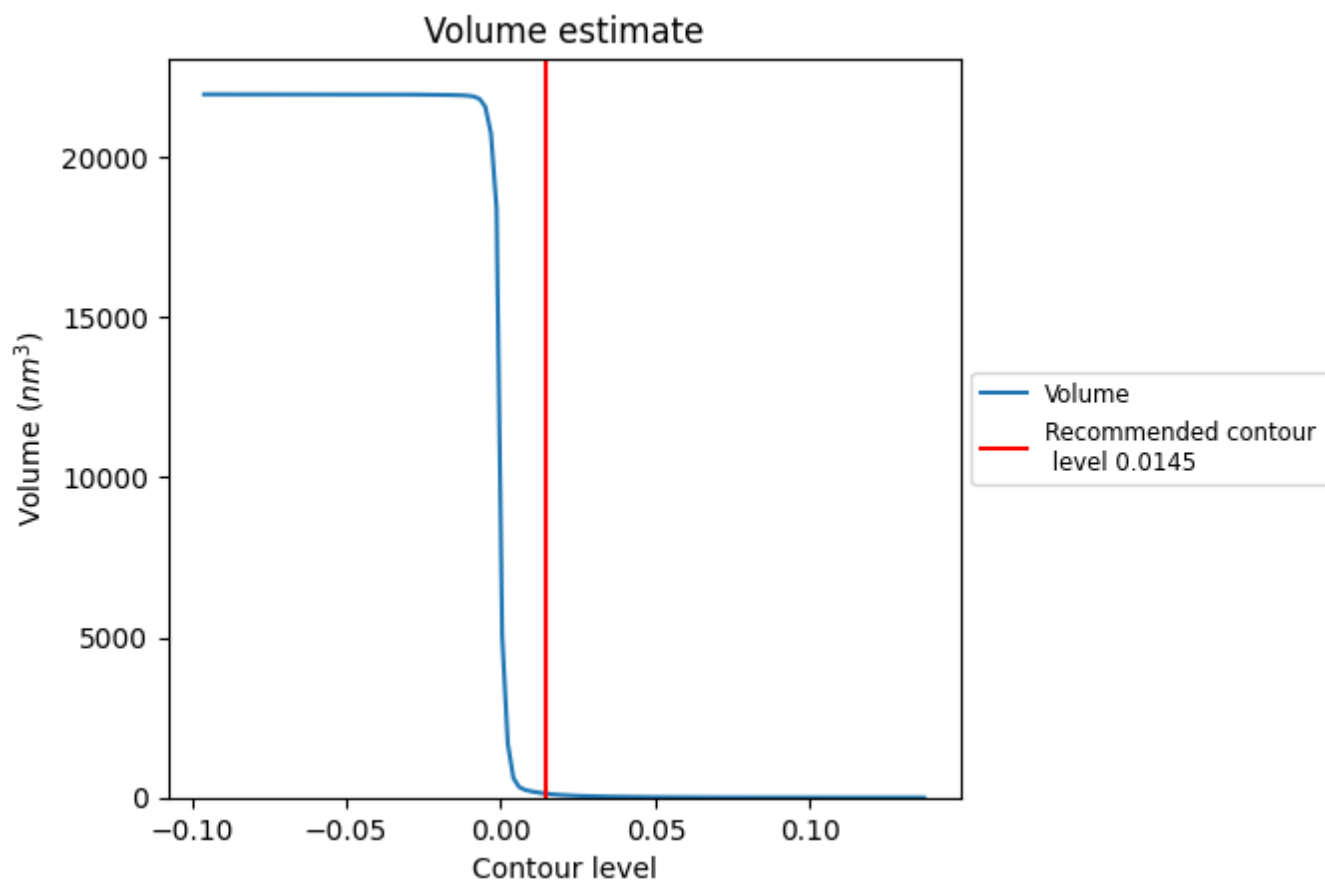
This section contains the results of statistical analysis of the map.

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.

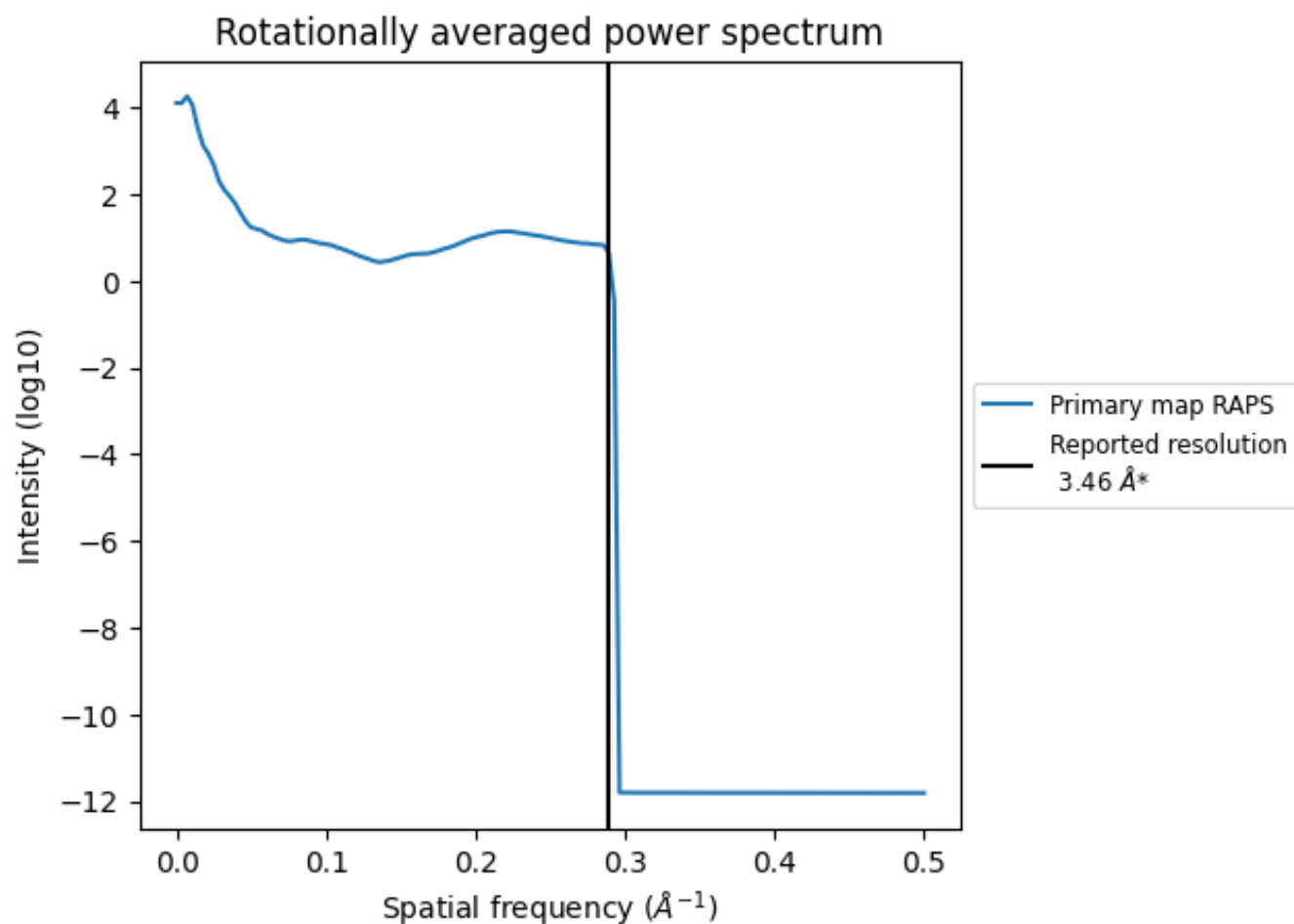
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 124 nm³; this corresponds to an approximate mass of 112 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 0.289 $\text{\AA}^{-1}$

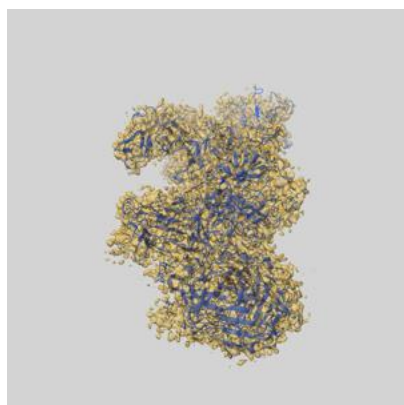
8 Fourier-Shell correlation

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

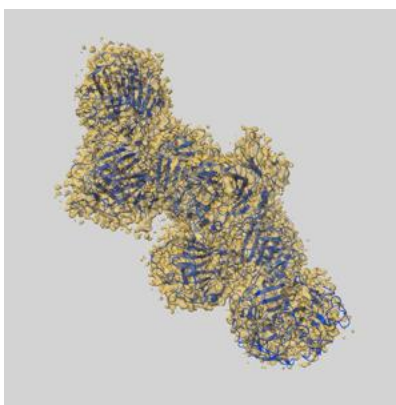
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20815 and PDB model 6UM1. Per-residue inclusion information can be found in section 3 on page 6.

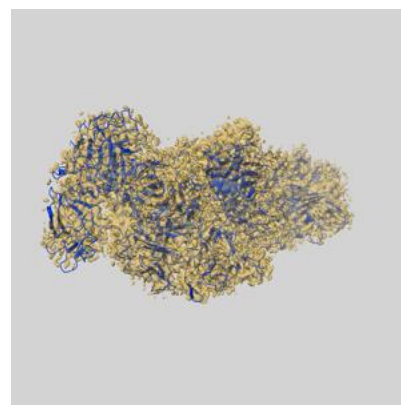
9.1 Map-model overlay [i](#)



X



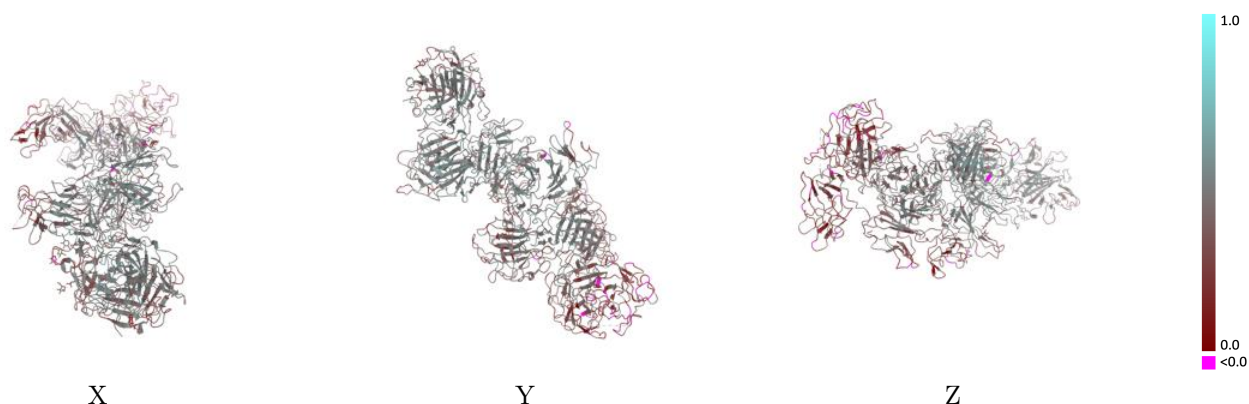
Y



Z

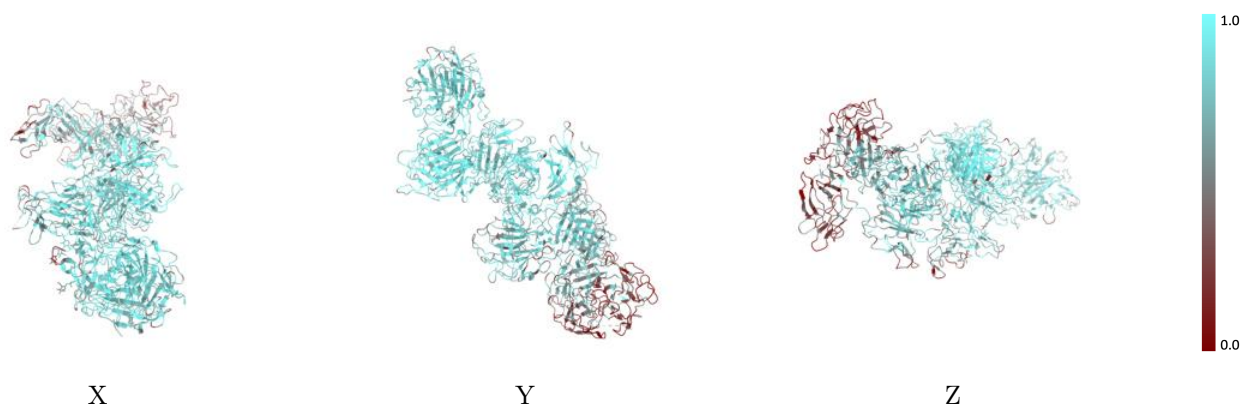
The images above show the 3D surface view of the map at the recommended contour level 0.0145 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



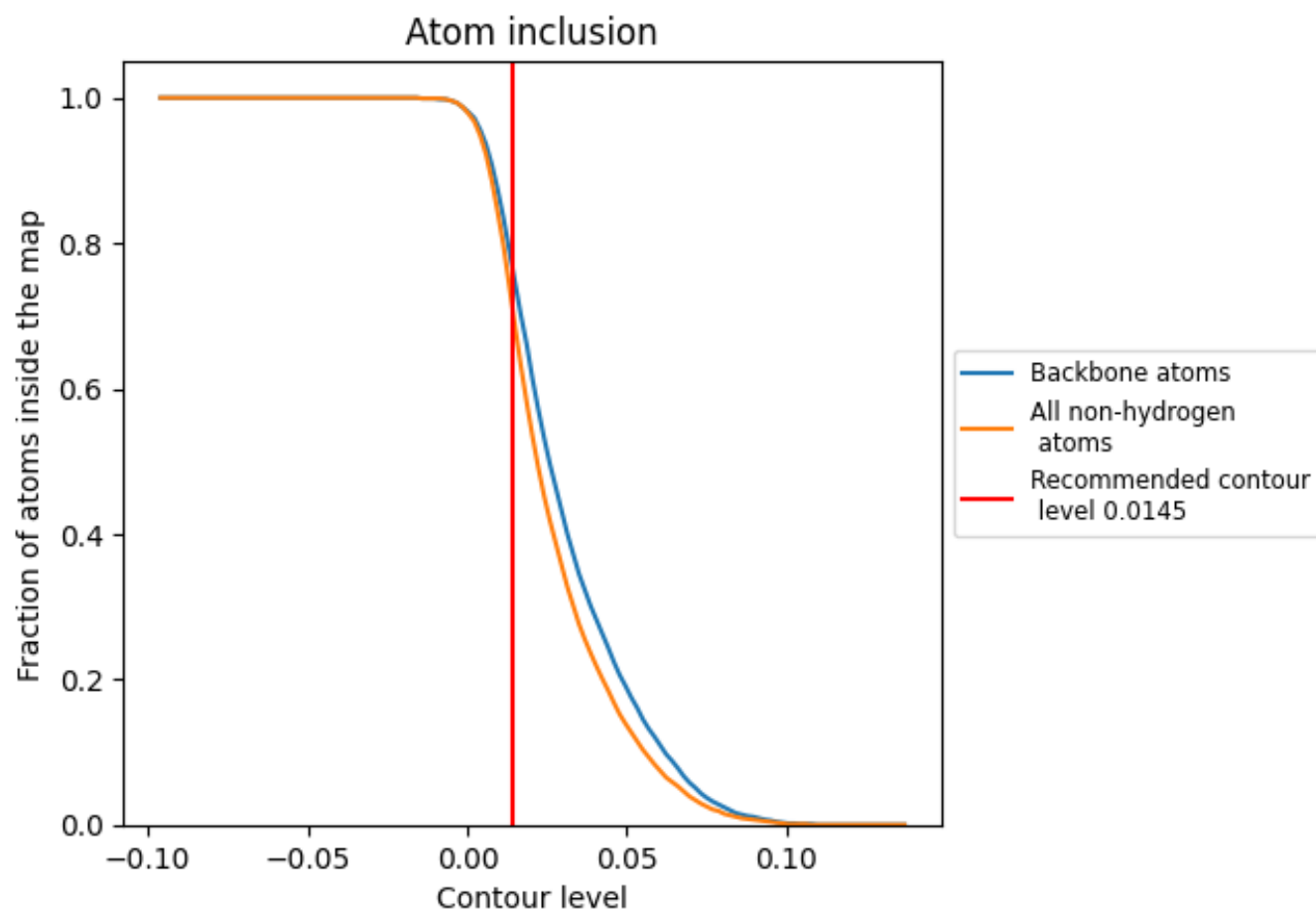
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0145).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 70% 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 (0.0145) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6990	0.4010
A	0.7000	0.4010
B	0.5710	0.3220
C	0.5900	0.3430

