



Full wwPDB EM Validation Report ⓘ

Oct 15, 2024 – 12:47 AM JST

PDB ID : 8J0N
EMDB ID : EMD-35906
Title : cryo-EM structure of human EMC
Authors : Li, M.; Zhang, C.; Wu, J.; Lei, M.
Deposited on : 2023-04-11
Resolution : 3.47 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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

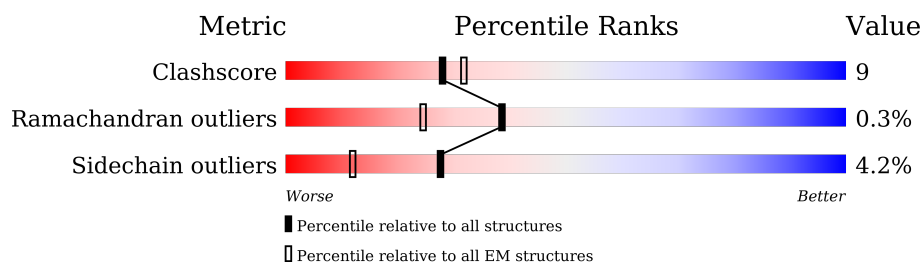
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.47 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	993	<div> <div>17%</div> <div>71%</div> <div>23%</div> <div>• •</div> </div>
2	B	297	<div> <div>27%</div> <div>76%</div> <div>22%</div> <div>•</div> </div>
3	C	261	<div> <div>22%</div> <div>68%</div> <div>25%</div> <div>• 7%</div> </div>
4	D	183	<div> <div>13%</div> <div>64%</div> <div>20%</div> <div>• 15%</div> </div>
5	E	131	<div> <div>26%</div> <div>61%</div> <div>13%</div> <div>5%</div> <div>21%</div> </div>
6	F	110	<div> <div>26%</div> <div>74%</div> <div>17%</div> <div>9%</div> </div>
7	G	242	<div> <div>16%</div> <div>34%</div> <div>11%</div> <div>•</div> <div>55%</div> </div>
8	H	210	<div> <div>14%</div> <div>64%</div> <div>28%</div> <div>• 7%</div> </div>

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Mol	Chain	Length	Quality of chain
9	J	207	<div><div></div><div>10%</div><div>55%</div><div>17%</div><div>28%</div></div>
10	L	3	<div><div></div><div>100%</div></div>
10	M	3	<div><div></div><div>33%</div><div>67%</div><div>33%</div></div>
10	N	3	<div><div></div><div>33%</div><div>67%</div><div>33%</div><div>33%</div></div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 18475 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 ER membrane protein complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	949	Total	C	N	O	S	0	0
			7544	4839	1290	1390	25		

- Molecule 2 is a protein called ER membrane protein complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	296	Total	C	N	O	S	0	0
			2438	1530	431	463	14		

- Molecule 3 is a protein called ER membrane protein complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	243	Total	C	N	O	S	0	0
			1976	1284	325	355	12		

- Molecule 4 is a protein called ER membrane protein complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	156	Total	C	N	O	S	0	0
			1222	798	197	212	15		

- Molecule 5 is a protein called ER membrane protein complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	103	Total	C	N	O	S	0	0
			817	528	142	144	3		

- Molecule 6 is a protein called ER membrane protein complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	100	Total	C	N	O	S	0	0
			781	526	127	126	2		

- | Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7 | G | 110 | Total | C | N | O | S | 0 | 0 |
| | | | 875 | 564 | 153 | 156 | 2 | | |

- | Mol | Chain | Residues | Atoms | | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|---|
| 8 | H | 195 | Total | C | N | O | S | 0 | 0 |
| | | | 1559 | 984 | 272 | 291 | 12 | | |

- | Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|-------|
| 9 | J | 149 | Total
1146 | C
710 | N
209 | O
224 | S
3 | 0 | 0 |

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- A diagram of a 1D chain. It starts with a green circle, followed by a horizontal line. Below the line are the labels β , 4, β , 4, β . Above the line are two blue squares. The chain ends with a vertical line and a curly brace.

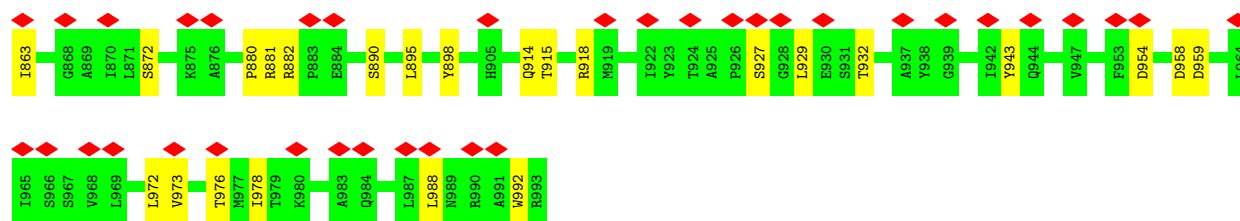
Mol	Chain	Residues	Atoms				AltConf	Trace
10	L	3	Total 39	C 22	N 2	O 15	0	0
10	M	3	Total 39	C 22	N 2	O 15	0	0
10	N	3	Total 39	C 22	N 2	O 15	0	0

3 Residue-property plots

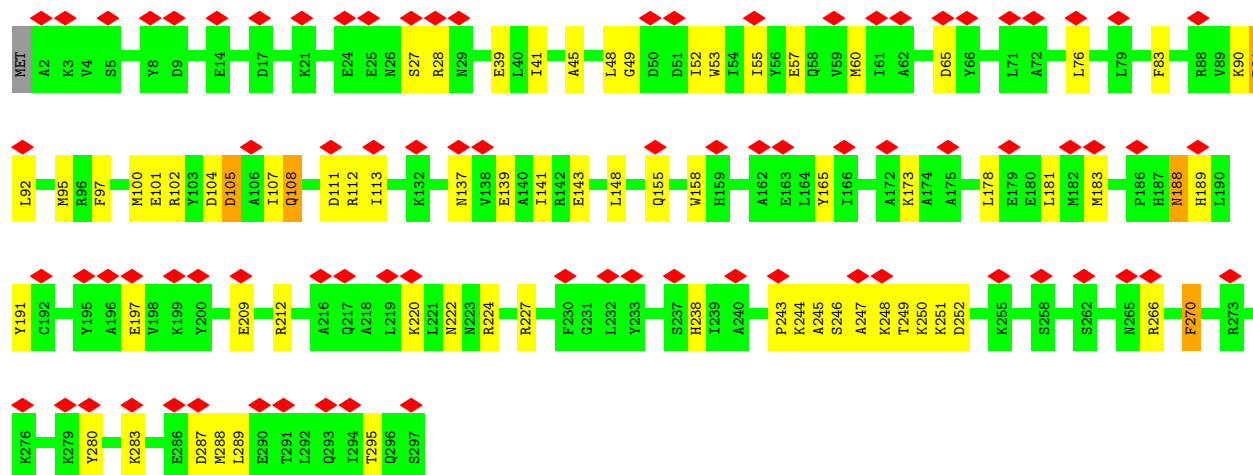
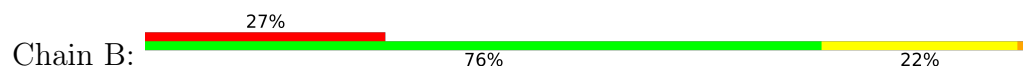
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: ER membrane protein complex subunit 1

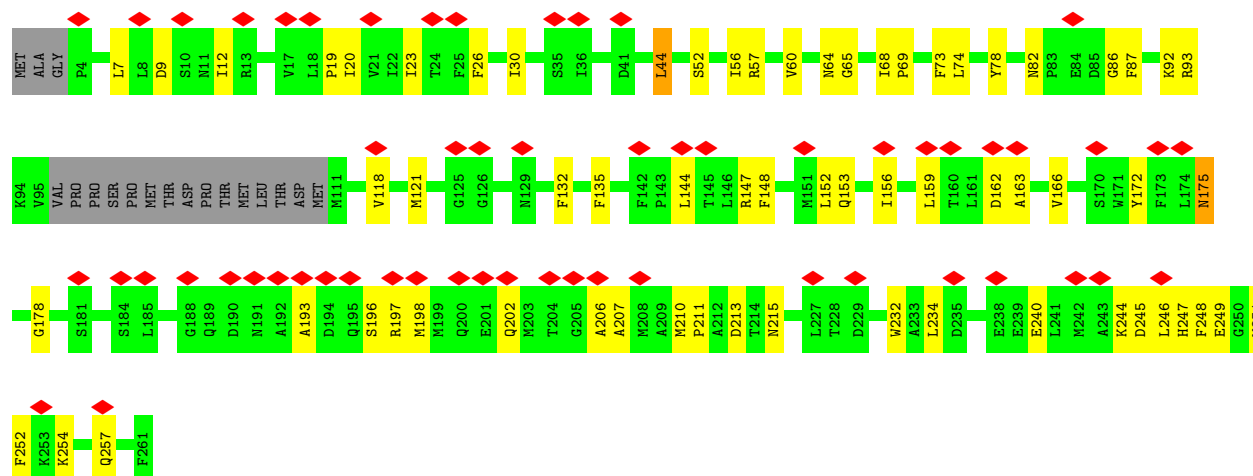




• Molecule 2: ER membrane protein complex subunit 2



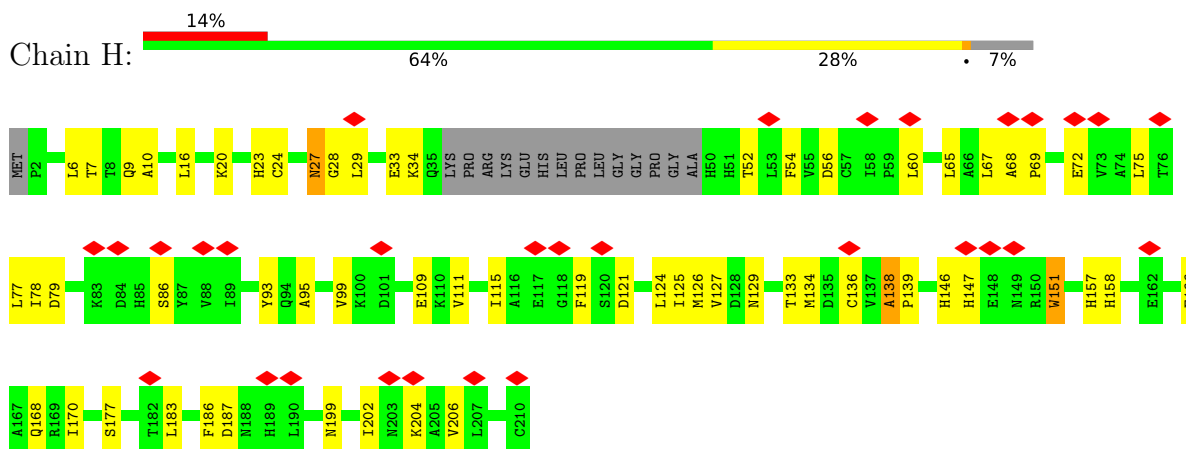
• Molecule 3: ER membrane protein complex subunit 3



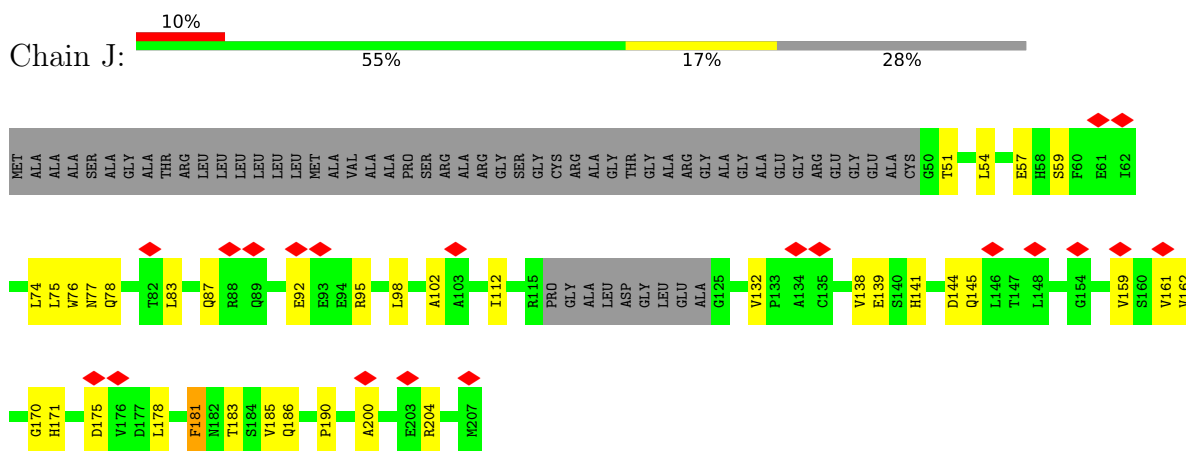
• Molecule 4: ER membrane protein complex subunit 4



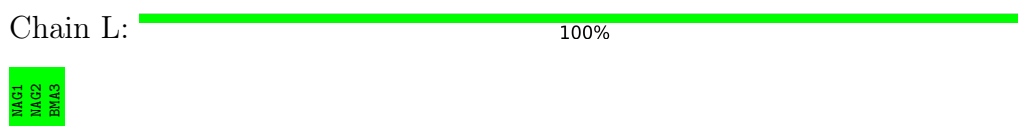
- Molecule 8: ER membrane protein complex subunit 8



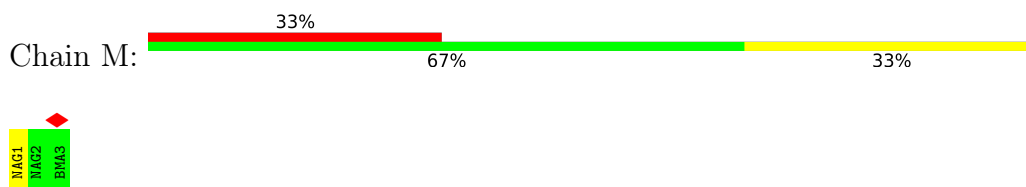
- Molecule 9: ER membrane protein complex subunit 10



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: 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	693381	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.374	Depositor
Minimum map value	-0.543	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.159	Depositor
Map size (\AA)	383.68002, 383.68002, 383.68002	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.09, 1.09, 1.09	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.36	3/7716 (0.0%)	0.58	5/10479 (0.0%)
2	B	0.25	0/2482	0.51	1/3336 (0.0%)
3	C	0.26	0/2020	0.54	1/2727 (0.0%)
4	D	0.29	0/1251	0.60	1/1691 (0.1%)
5	E	0.29	0/838	0.62	1/1134 (0.1%)
6	F	0.25	0/803	0.46	0/1089
7	G	0.26	0/898	0.55	0/1217
8	H	0.26	0/1600	0.48	0/2179
9	J	0.25	0/1165	0.57	1/1580 (0.1%)
All	All	0.31	3/18773 (0.0%)	0.56	10/25432 (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	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	582	PRO	CG-CD	-20.04	0.84	1.50
1	A	582	PRO	N-CD	8.44	1.59	1.47
1	A	582	PRO	CB-CG	6.04	1.80	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	582	PRO	N-CD-CG	-17.64	76.74	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	69	PRO	CA-N-CD	-11.31	95.66	111.50
5	E	103	PRO	CA-N-CD	-10.11	97.35	111.50
1	A	582	PRO	CA-N-CD	-9.81	97.77	111.50
1	A	582	PRO	CA-CB-CG	-8.78	87.32	104.00
1	A	582	PRO	N-CA-CB	-7.43	94.38	103.30
9	J	98	LEU	CA-CB-CG	6.70	130.72	115.30
1	A	690	LEU	CA-CB-CG	6.66	130.62	115.30
2	B	48	LEU	CA-CB-CG	6.46	130.15	115.30
4	D	175	GLU	CA-CB-CG	5.11	124.64	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	929	LEU	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	7544	0	7597	145	0
2	B	2438	0	2391	51	0
3	C	1976	0	2005	50	0
4	D	1222	0	1254	29	0
5	E	817	0	812	20	0
6	F	781	0	810	13	0
7	G	875	0	887	17	0
8	H	1559	0	1493	41	0
9	J	1146	0	1121	22	0
10	L	39	0	34	0	0
10	M	39	0	34	0	0
10	N	39	0	34	2	0
All	All	18475	0	18472	346	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 9.

All (346) 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)
2:B:60:MET:HE3	2:B:92:LEU:HD23	1.58	0.82
2:B:104:ASP:OD2	2:B:108:GLN:NE2	2.14	0.81
1:A:836:GLN:HG3	1:A:880:PRO:HA	1.68	0.76
3:C:57:ARG:HH12	4:D:45:VAL:HG11	1.49	0.75
1:A:243:ARG:HB3	1:A:266:LEU:HD11	1.68	0.74
1:A:487:ARG:HH22	5:E:42:PRO:HG2	1.54	0.72
1:A:228:GLY:HA3	1:A:278:PRO:HG3	1.73	0.71
9:J:145:GLN:HB3	9:J:162:VAL:HG13	1.74	0.70
1:A:461:PRO:HA	1:A:578:THR:HB	1.73	0.69
5:E:103:PRO:HD2	5:E:104:SER:H	1.56	0.69
2:B:224:ARG:HA	3:C:251:MET:HE1	1.72	0.69
2:B:57:GLU:HG3	2:B:92:LEU:HD21	1.75	0.69
2:B:28:ARG:HE	5:E:91:TYR:HE1	1.39	0.69
9:J:51:THR:HB	9:J:75:LEU:HD11	1.73	0.68
3:C:148:PHE:HZ	4:D:156:LEU:HD13	1.59	0.68
1:A:319:THR:HG23	1:A:335:VAL:HG13	1.76	0.67
1:A:62:VAL:HG23	1:A:78:VAL:HG22	1.75	0.67
2:B:90:LYS:HB3	2:B:113:ILE:HD11	1.77	0.67
9:J:132:VAL:HG21	9:J:161:VAL:HB	1.78	0.66
1:A:192:VAL:HG21	1:A:195:SER:HB2	1.78	0.66
5:E:103:PRO:HD2	5:E:104:SER:N	2.11	0.66
1:A:261:LEU:HB2	1:A:266:LEU:HD13	1.79	0.65
5:E:85:ARG:NH1	8:H:24:CYS:SG	2.70	0.65
8:H:7:THR:HG22	8:H:9:GLN:H	1.59	0.65
1:A:787:SER:OG	1:A:788:GLU:N	2.29	0.65
2:B:108:GLN:O	2:B:112:ARG:HG3	1.96	0.65
1:A:428:HIS:HB2	1:A:448:SER:HB2	1.79	0.65
9:J:112:ILE:HD12	9:J:159:VAL:HG11	1.79	0.64
1:A:633:ASP:CG	1:A:634:GLN:H	2.01	0.64
8:H:166:GLU:O	8:H:170:ILE:HG13	1.97	0.64
5:E:100:LEU:HA	8:H:133:THR:HA	1.79	0.63
8:H:93:TYR:HB2	8:H:125:ILE:HB	1.81	0.63
3:C:52:SER:O	3:C:56:ILE:HG12	1.98	0.62
1:A:295:LEU:HB2	1:A:299:HIS:HB3	1.81	0.62
1:A:747:SER:OG	1:A:749:ASP:OD1	2.18	0.62
1:A:316:PHE:HB3	1:A:319:THR:OG1	2.00	0.62
1:A:92:LEU:HD13	1:A:97:VAL:HG22	1.82	0.61
1:A:203:ASN:OD1	1:A:204:VAL:N	2.32	0.61
1:A:191:VAL:HG21	1:A:223:LEU:HD13	1.81	0.61
4:D:126:SER:HB2	4:D:129:LYS:HE3	1.82	0.61
9:J:145:GLN:OE1	9:J:186:GLN:NE2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:248:PHE:HA	3:C:251:MET:SD	2.41	0.61
1:A:91:LEU:HD11	1:A:131:LEU:HD13	1.81	0.61
2:B:220:LYS:HB3	3:C:240:GLU:HG3	1.81	0.61
2:B:197:GLU:HG3	8:H:67:LEU:HD22	1.83	0.61
6:F:33:VAL:HG21	6:F:62:LEU:HD13	1.81	0.60
1:A:113:ASN:OD1	1:A:114:ILE:N	2.32	0.60
1:A:128:PHE:HZ	1:A:131:LEU:HD23	1.66	0.60
5:E:10:VAL:HG13	5:E:56:THR:HG23	1.83	0.60
9:J:139:GLU:HB2	9:J:170:GLY:HA2	1.83	0.60
5:E:70:MET:HG2	6:F:14:ILE:HG23	1.84	0.60
1:A:33:ARG:HG3	1:A:943:TYR:HB2	1.83	0.59
1:A:619:LEU:HG	1:A:620:LYS:H	1.67	0.59
1:A:792:VAL:HG22	1:A:807:VAL:HG22	1.83	0.59
3:C:210:MET:HG3	3:C:211:PRO:HD3	1.83	0.59
1:A:33:ARG:HD3	1:A:914:GLN:HB3	1.83	0.59
2:B:52:ILE:HA	2:B:55:ILE:HB	1.84	0.59
3:C:254:LYS:HA	3:C:257:GLN:HE22	1.67	0.59
1:A:958:ASP:OD2	1:A:959:ASP:N	2.36	0.58
3:C:147:ARG:NH1	4:D:163:ASP:OD2	2.36	0.58
1:A:844:ILE:HG23	1:A:863:ILE:HG23	1.85	0.58
4:D:73:ALA:HB1	4:D:136:TYR:HB2	1.85	0.58
10:N:2:NAG:H83	10:N:2:NAG:H3	1.85	0.58
5:E:72:ALA:HB2	6:F:15:SER:HB3	1.84	0.58
9:J:92:GLU:HA	9:J:95:ARG:HE	1.69	0.58
9:J:144:ASP:HB2	9:J:183:THR:HG22	1.86	0.58
2:B:139:GLU:O	2:B:143:GLU:HG3	2.04	0.58
1:A:80:LYS:O	1:A:918:ARG:NH2	2.37	0.57
5:E:88:PRO:HA	5:E:91:TYR:CE2	2.39	0.57
8:H:52:THR:OG1	8:H:121:ASP:OD2	2.14	0.57
1:A:744:VAL:HG22	1:A:759:ILE:HG22	1.86	0.57
2:B:105:ASP:HA	2:B:108:GLN:OE1	2.05	0.57
1:A:616:PRO:HG3	1:A:652:PHE:HD1	1.69	0.57
1:A:533:GLN:OE1	1:A:533:GLN:N	2.38	0.56
2:B:209:GLU:HG2	2:B:212:ARG:HH21	1.68	0.56
1:A:723:GLY:HA3	4:D:165:LEU:HD11	1.88	0.56
3:C:20:ILE:HD11	3:C:172:TYR:HB2	1.88	0.56
7:G:135:PRO:HB2	7:G:137:PRO:HD2	1.87	0.56
1:A:106:ILE:HD11	1:A:120:GLU:HG2	1.87	0.56
2:B:227:ARG:NH2	8:H:187:ASP:OD1	2.39	0.56
2:B:102:ARG:HB3	2:B:105:ASP:OD1	2.05	0.56
8:H:157:HIS:O	8:H:158:HIS:ND1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:28:GLY:HA3	8:H:93:TYR:CE2	2.42	0.55
2:B:224:ARG:NH2	5:E:77:LYS:HD3	2.22	0.55
3:C:244:LYS:HD2	3:C:246:LEU:HD12	1.88	0.55
1:A:587:CYS:HB2	1:A:606:PRO:HD3	1.89	0.55
7:G:48:GLU:OE2	7:G:48:GLU:N	2.40	0.55
1:A:731:VAL:HG21	4:D:165:LEU:HD13	1.89	0.55
5:E:88:PRO:HA	5:E:91:TYR:HE2	1.71	0.54
3:C:193:ALA:HB1	3:C:196:SER:HB3	1.88	0.54
1:A:460:LEU:HB2	1:A:527:ARG:HG3	1.88	0.54
8:H:20:LYS:NZ	8:H:183:LEU:O	2.28	0.54
8:H:95:ALA:HB2	8:H:127:VAL:HB	1.89	0.54
7:G:104:ARG:HH12	7:G:143:SER:HB3	1.72	0.54
2:B:91:ARG:HD3	2:B:92:LEU:HD12	1.89	0.54
3:C:153:GLN:HG3	3:C:156:ILE:HD12	1.90	0.54
5:E:41:LEU:HD23	5:E:41:LEU:H	1.73	0.54
8:H:147:HIS:HD2	8:H:151:TRP:HB3	1.72	0.54
1:A:539:VAL:HG22	1:A:545:LEU:HD23	1.90	0.53
1:A:777:LYS:HD2	1:A:799:LYS:HB2	1.90	0.53
1:A:253:GLU:HG3	1:A:254:TRP:H	1.73	0.53
9:J:139:GLU:OE2	9:J:170:GLY:N	2.41	0.53
1:A:108:ARG:HB3	1:A:120:GLU:HG3	1.90	0.53
1:A:146:LEU:HD11	1:A:175:TYR:HB3	1.89	0.53
1:A:501:HIS:O	1:A:505:MET:HG2	2.08	0.53
3:C:56:ILE:O	3:C:60:VAL:HG22	2.08	0.53
1:A:449:LEU:HD21	1:A:548:ILE:HD11	1.90	0.53
1:A:256:LEU:HD23	1:A:256:LEU:H	1.74	0.53
7:G:49:GLY:HA3	7:G:84:PHE:CZ	2.44	0.53
8:H:133:THR:OG1	8:H:134:MET:N	2.41	0.53
3:C:78:TYR:O	3:C:82:ASN:N	2.42	0.53
1:A:239:ASP:O	1:A:243:ARG:HA	2.09	0.52
1:A:890:SER:HB3	1:A:895:LEU:HD12	1.91	0.52
1:A:882:ARG:HB3	1:A:898:TYR:HB2	1.92	0.52
1:A:735:SER:HB3	1:A:812:GLU:HG3	1.90	0.52
9:J:83:LEU:HD13	9:J:185:VAL:HG12	1.92	0.52
2:B:165:TYR:HE2	2:B:173:LYS:HD3	1.75	0.52
7:G:151:LYS:HE2	7:G:151:LYS:HA	1.92	0.52
1:A:619:LEU:HG	1:A:620:LYS:N	2.24	0.52
5:E:68:LYS:HZ3	6:F:18:ALA:HA	1.74	0.52
2:B:92:LEU:HA	2:B:95:MET:HE2	1.91	0.51
4:D:165:LEU:HA	4:D:168:ILE:HG22	1.91	0.51
8:H:69:PRO:O	8:H:72:GLU:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:VAL:HG11	1:A:377:LEU:HD13	1.92	0.51
3:C:82:ASN:HB3	3:C:86:GLY:HA2	1.92	0.51
1:A:708:VAL:HG12	1:A:709:LYS:HG3	1.92	0.51
3:C:207:ALA:O	3:C:210:MET:HG2	2.11	0.50
1:A:181:TYR:HB2	1:A:187:TRP:HZ3	1.77	0.50
2:B:249:THR:HA	2:B:252:ASP:OD2	2.11	0.50
9:J:178:LEU:H	9:J:178:LEU:HD23	1.75	0.50
2:B:28:ARG:HH12	8:H:23:HIS:HB3	1.76	0.50
2:B:245:ALA:HB3	2:B:250:LYS:HE3	1.92	0.50
3:C:249:GLU:HA	3:C:252:PHE:HB3	1.94	0.50
1:A:206:ASP:OD1	1:A:206:ASP:N	2.45	0.49
3:C:162:ASP:OD2	3:C:163:ALA:N	2.45	0.49
1:A:141:ARG:HG3	1:A:142:TYR:CD2	2.47	0.49
9:J:87:GLN:N	9:J:87:GLN:OE1	2.45	0.49
1:A:60:LYS:O	1:A:918:ARG:NH2	2.45	0.49
2:B:266:ARG:NH2	3:C:245:ASP:O	2.45	0.49
1:A:23:TYR:HB3	7:G:149:PHE:HD2	1.77	0.49
1:A:666:ALA:CB	1:A:667:PRO:HD3	2.43	0.49
8:H:199:ASN:HB3	8:H:202:ILE:HB	1.93	0.49
1:A:52:LYS:O	1:A:67:ASN:HA	2.12	0.49
1:A:739:ASN:OD1	4:D:173:ARG:NH2	2.45	0.49
7:G:105:PHE:HD2	7:G:140:MET:HB3	1.78	0.49
1:A:141:ARG:HA	1:A:156:LEU:HD22	1.95	0.49
6:F:18:ALA:O	6:F:22:ASN:ND2	2.45	0.49
1:A:285:ASP:OD1	1:A:285:ASP:N	2.46	0.49
2:B:266:ARG:HB2	2:B:270:PHE:CZ	2.47	0.49
3:C:178:GLY:HA3	6:F:98:LEU:HD13	1.95	0.49
1:A:24:GLU:OE2	1:A:24:GLU:N	2.44	0.49
7:G:56:VAL:HG13	7:G:57:LYS:H	1.77	0.49
2:B:148:LEU:HD21	2:B:158:TRP:CH2	2.48	0.48
7:G:53:VAL:CG1	7:G:54:PRO:HD2	2.43	0.48
1:A:261:LEU:HD22	1:A:264:LEU:HD21	1.94	0.48
1:A:448:SER:O	1:A:448:SER:OG	2.32	0.48
8:H:6:LEU:HB3	8:H:54:PHE:HD2	1.79	0.48
1:A:53:LYS:HD3	1:A:112:THR:HB	1.94	0.48
1:A:245:LEU:HG	1:A:261:LEU:HD21	1.96	0.48
3:C:247:HIS:O	3:C:251:MET:HB3	2.14	0.48
6:F:52:PHE:HE1	6:F:93:LEU:HD11	1.78	0.48
8:H:29:LEU:HD13	8:H:60:LEU:HD11	1.94	0.48
4:D:52:VAL:HG23	4:D:52:VAL:O	2.14	0.48
8:H:138:ALA:HB3	8:H:139:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:92:LYS:HD2	3:C:93:ARG:H	1.79	0.47
1:A:635:ASP:O	1:A:636:TYR:HD1	1.98	0.47
1:A:247:THR:HG23	1:A:257:ARG:HG2	1.97	0.47
8:H:99:VAL:HA	8:H:129:ASN:HB2	1.96	0.47
1:A:217:THR:HG21	1:A:246:GLN:HE22	1.80	0.47
1:A:531:ASN:OD1	1:A:531:ASN:N	2.48	0.47
4:D:120:PHE:O	4:D:124:GLU:HG2	2.14	0.47
2:B:65:ASP:OD2	5:E:95:HIS:NE2	2.48	0.47
3:C:92:LYS:HZ3	3:C:215:ASN:HB2	1.79	0.47
3:C:144:LEU:HD23	3:C:152:LEU:HD11	1.97	0.47
1:A:377:LEU:HG	1:A:389:THR:HG21	1.97	0.47
3:C:198:MET:O	3:C:202:GLN:HG3	2.15	0.47
1:A:551:SER:OG	1:A:552:SER:N	2.48	0.46
4:D:78:LYS:O	4:D:81:PRO:HD2	2.14	0.46
2:B:178:LEU:HD23	2:B:178:LEU:HA	1.76	0.46
3:C:26:PHE:O	3:C:30:ILE:HG12	2.15	0.46
8:H:124:LEU:HD22	8:H:126:MET:HE3	1.96	0.46
4:D:17:TRP:CD1	8:H:75:LEU:HD13	2.50	0.46
1:A:89:ALA:HB3	1:A:131:LEU:HD21	1.97	0.46
2:B:280:TYR:HA	2:B:283:LYS:HG2	1.97	0.46
4:D:68:ARG:HA	4:D:68:ARG:NE	2.31	0.46
1:A:133:LEU:HD23	1:A:140:VAL:HG21	1.97	0.46
3:C:118:VAL:O	3:C:121:MET:HG3	2.16	0.46
8:H:77:LEU:HD12	8:H:186:PHE:HZ	1.79	0.46
1:A:156:LEU:HD23	1:A:157:SER:H	1.81	0.46
1:A:442:LEU:HD22	1:A:443:TRP:HD1	1.81	0.46
1:A:672:TYR:HB3	1:A:696:TRP:HZ2	1.79	0.46
1:A:576:ARG:NH2	1:A:586:GLN:OE1	2.49	0.46
1:A:733:TYR:CG	1:A:816:GLN:HG3	2.51	0.46
2:B:155:GLN:HB3	2:B:181:LEU:HD11	1.98	0.46
3:C:132:PHE:HB3	3:C:135:PHE:CD2	2.51	0.46
4:D:82:MET:SD	4:D:82:MET:N	2.80	0.46
8:H:93:TYR:CB	8:H:125:ILE:HB	2.45	0.46
2:B:41:ILE:O	2:B:45:ALA:HB2	2.16	0.46
2:B:247:ALA:O	2:B:251:LYS:HG2	2.16	0.46
1:A:127:SER:HB2	1:A:148:LYS:HB2	1.98	0.46
1:A:39:LYS:HD2	1:A:428:HIS:CE1	2.51	0.45
1:A:159:GLY:O	1:A:160:HIS:ND1	2.49	0.45
1:A:633:ASP:CG	1:A:634:GLN:N	2.70	0.45
1:A:783:HIS:O	1:A:793:TYR:HA	2.17	0.45
3:C:92:LYS:NZ	3:C:215:ASN:HB2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:11:PRO:HG2	6:F:12:PRO:HD3	1.98	0.45
9:J:54:LEU:HB2	9:J:74:LEU:HD22	1.98	0.45
1:A:540:THR:HG22	1:A:542:SER:H	1.82	0.45
1:A:731:VAL:CG2	4:D:165:LEU:HD13	2.47	0.45
2:B:247:ALA:HB1	2:B:251:LYS:NZ	2.32	0.45
7:G:58:PRO:O	7:G:62:ILE:HG12	2.16	0.45
1:A:187:TRP:CD1	1:A:201:LYS:HB2	2.52	0.45
1:A:992:TRP:HZ2	2:B:53:TRP:HB3	1.81	0.45
3:C:65:GLY:HA2	3:C:68:ILE:HD12	1.99	0.45
4:D:61:ASP:OD2	4:D:64:LEU:HB2	2.16	0.45
9:J:200:ALA:HB1	9:J:204:ARG:HH11	1.82	0.45
9:J:51:THR:HG22	9:J:77:ASN:HB2	1.99	0.44
1:A:167:LEU:HB3	1:A:168:PRO:HD2	2.00	0.44
1:A:734:LYS:HE2	1:A:789:ASN:ND2	2.33	0.44
8:H:202:ILE:O	8:H:206:VAL:HG12	2.17	0.44
1:A:153:LEU:HD13	1:A:163:TRP:CE3	2.52	0.44
2:B:295:THR:HG23	4:D:14:ARG:HB2	1.98	0.44
7:G:53:VAL:HG13	7:G:54:PRO:HD2	1.99	0.44
1:A:338:CYS:SG	1:A:363:LYS:HG2	2.58	0.44
2:B:288:MET:HG3	2:B:289:LEU:HD22	2.00	0.44
1:A:371:GLN:HE22	1:A:398:SER:HA	1.83	0.44
1:A:621:ARG:NH2	1:A:646:GLU:HB2	2.33	0.44
1:A:765:VAL:HG11	1:A:824:SER:HB3	1.99	0.44
1:A:318:GLN:HG3	1:A:358:GLU:OE2	2.18	0.44
1:A:972:LEU:HB3	3:C:26:PHE:HB3	1.98	0.44
9:J:102:ALA:HB2	9:J:138:VAL:HG21	1.99	0.44
1:A:525:LEU:HD23	1:A:525:LEU:HA	1.83	0.44
1:A:604:PHE:HA	1:A:611:TRP:HA	1.99	0.43
1:A:988:LEU:HD21	2:B:83:PHE:HE2	1.82	0.43
1:A:157:SER:OG	1:A:158:SER:N	2.51	0.43
1:A:927:SER:OG	1:A:932:THR:HB	2.19	0.43
3:C:254:LYS:HA	3:C:257:GLN:NE2	2.33	0.43
1:A:567:ASP:HB2	1:A:594:LYS:HE3	2.01	0.43
2:B:28:ARG:HH12	8:H:23:HIS:CB	2.30	0.43
3:C:44:LEU:HD23	3:C:44:LEU:HA	1.75	0.43
3:C:211:PRO:HB2	3:C:213:ASP:OD1	2.19	0.43
9:J:92:GLU:OE2	9:J:92:GLU:N	2.39	0.43
2:B:100:MET:O	2:B:101:GLU:HG3	2.19	0.43
3:C:92:LYS:HD2	3:C:93:ARG:N	2.34	0.43
8:H:16:LEU:HD23	8:H:16:LEU:HA	1.80	0.43
1:A:734:LYS:HE2	1:A:789:ASN:HD21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:110:ILE:HG13	4:D:111:GLN:N	2.34	0.43
1:A:156:LEU:HD23	1:A:157:SER:N	2.34	0.43
1:A:520:ILE:HG22	1:A:522:ILE:H	1.83	0.43
1:A:643:ILE:HD11	1:A:671:PHE:CZ	2.53	0.43
1:A:151:LEU:HG	1:A:163:TRP:HZ3	1.83	0.43
1:A:689:ASP:OD1	1:A:689:ASP:N	2.39	0.43
2:B:224:ARG:HH22	5:E:77:LYS:HD3	1.83	0.43
2:B:243:PRO:HG2	2:B:244:LYS:HD3	2.00	0.43
3:C:44:LEU:HD21	3:C:206:ALA:HB1	2.00	0.43
3:C:73:PHE:HD1	3:C:74:LEU:HD22	1.84	0.43
8:H:27:ASN:ND2	8:H:65:LEU:HD11	2.33	0.43
1:A:261:LEU:HD13	1:A:264:LEU:HD11	2.01	0.43
1:A:689:ASP:C	1:A:690:LEU:HD12	2.39	0.43
1:A:710:VAL:HG22	1:A:743:VAL:HG12	2.01	0.43
1:A:729:ARG:HD3	3:C:147:ARG:NH2	2.34	0.43
7:G:49:GLY:O	7:G:83:SER:HA	2.19	0.43
1:A:167:LEU:HD22	1:A:175:TYR:CE1	2.54	0.42
3:C:7:LEU:HD12	5:E:32:ARG:HD3	2.01	0.42
3:C:232:TRP:CE2	3:C:234:LEU:HB2	2.54	0.42
9:J:57:GLU:N	9:J:57:GLU:OE2	2.52	0.42
1:A:52:LYS:HG2	1:A:69:ARG:HG2	2.01	0.42
6:F:49:LEU:O	6:F:53:ILE:HG12	2.18	0.42
6:F:82:ARG:HB2	6:F:83:PRO:HD3	2.00	0.42
8:H:33:GLU:OE1	8:H:34:LYS:N	2.52	0.42
1:A:757:ILE:HB	1:A:778:ALA:HB3	2.02	0.42
7:G:68:LEU:HD12	7:G:99:VAL:HG21	2.00	0.42
8:H:109:GLU:OE2	8:H:146:HIS:ND1	2.52	0.42
1:A:146:LEU:HB2	1:A:151:LEU:HD13	2.01	0.42
1:A:724:ARG:HH21	1:A:881:ARG:HE	1.66	0.42
3:C:152:LEU:HD22	3:C:166:VAL:HG12	2.02	0.42
3:C:193:ALA:O	3:C:197:ARG:N	2.53	0.42
4:D:116:ILE:O	4:D:120:PHE:HB2	2.18	0.42
9:J:87:GLN:HE21	9:J:181:PHE:HB3	1.85	0.42
1:A:134:VAL:HG22	1:A:142:TYR:HB2	2.01	0.42
1:A:426:GLU:OE1	1:A:427:ASP:N	2.53	0.42
1:A:973:VAL:O	1:A:976:THR:HG22	2.20	0.42
3:C:19:PRO:O	3:C:23:ILE:HG12	2.19	0.42
4:D:19:ILE:HB	8:H:68:ALA:HB1	2.01	0.42
5:E:96:ARG:NH2	8:H:24:CYS:O	2.52	0.42
7:G:56:VAL:HG13	7:G:57:LYS:N	2.35	0.42
8:H:111:VAL:O	8:H:115:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:76:TRP:CZ2	9:J:78:GLN:HG2	2.55	0.42
2:B:141:ILE:HD13	2:B:165:TYR:CE1	2.54	0.42
8:H:10:ALA:HB2	8:H:56:ASP:HA	2.02	0.42
8:H:136:CYS:O	8:H:168:GLN:NE2	2.46	0.42
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.82	0.42
1:A:290:GLN:NE2	1:A:381:GLU:OE1	2.52	0.42
1:A:719:VAL:HG21	1:A:736:LEU:HD13	2.02	0.42
2:B:188:ASN:HB3	2:B:191:TYR:HD2	1.85	0.42
4:D:84:LEU:HD12	4:D:146:LEU:HD11	2.02	0.42
8:H:86:SER:O	8:H:86:SER:OG	2.33	0.42
1:A:33:ARG:NH1	1:A:915:THR:O	2.50	0.41
1:A:689:ASP:O	1:A:690:LEU:HD12	2.20	0.41
2:B:270:PHE:HB2	3:C:249:GLU:OE2	2.20	0.41
4:D:18:ALA:HA	8:H:72:GLU:OE1	2.20	0.41
4:D:107:TRP:HA	4:D:110:ILE:HG12	2.02	0.41
1:A:279:THR:HG21	1:A:324:PHE:CD1	2.55	0.41
1:A:615:ALA:HA	1:A:616:PRO:HD3	1.92	0.41
2:B:49:GLY:HA2	2:B:52:ILE:HG22	2.02	0.41
4:D:17:TRP:HZ3	8:H:79:ASP:OD2	2.02	0.41
2:B:183:MET:CG	3:C:68:ILE:HD11	2.50	0.41
1:A:153:LEU:HB2	1:A:163:TRP:HB3	2.03	0.41
1:A:862:LEU:HD23	1:A:872:SER:HB3	2.02	0.41
5:E:59:GLY:O	5:E:63:ILE:HG12	2.21	0.41
1:A:251:GLU:HG3	1:A:252:THR:HG23	2.02	0.41
1:A:741:LEU:HD23	1:A:762:ILE:O	2.21	0.41
1:A:973:VAL:HG22	3:C:26:PHE:CE2	2.55	0.41
1:A:978:ILE:HD13	1:A:978:ILE:HA	1.94	0.41
4:D:108:ARG:O	4:D:111:GLN:HG3	2.20	0.41
7:G:46:LYS:HE2	7:G:87:HIS:CD2	2.55	0.41
1:A:616:PRO:HG3	1:A:652:PHE:CD1	2.52	0.41
1:A:743:VAL:HG22	1:A:760:PHE:HB2	2.01	0.41
1:A:992:TRP:CZ2	2:B:53:TRP:HB3	2.55	0.41
8:H:34:LYS:HE2	8:H:34:LYS:HA	2.03	0.41
8:H:78:ILE:HD13	8:H:78:ILE:HA	1.86	0.41
1:A:105:ARG:HE	1:A:105:ARG:HB3	1.66	0.41
3:C:12:ILE:HG23	6:F:110:TYR:HE2	1.85	0.41
3:C:175:ASN:ND2	6:F:98:LEU:HD11	2.34	0.41
9:J:112:ILE:HD12	9:J:159:VAL:HG21	2.02	0.41
2:B:189:HIS:CE1	2:B:222:ASN:HD22	2.39	0.41
4:D:48:LEU:HD23	4:D:48:LEU:HA	1.87	0.41
4:D:163:ASP:OD1	4:D:163:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:89:LEU:HD23	6:F:89:LEU:HA	1.90	0.41
7:G:62:ILE:HD13	7:G:62:ILE:HA	1.85	0.41
7:G:117:LYS:HD3	7:G:117:LYS:HA	1.57	0.41
2:B:76:LEU:HD12	2:B:76:LEU:HA	1.95	0.41
5:E:2:ALA:HB3	5:E:3:PRO:HD3	2.03	0.41
1:A:726:MET:HG3	1:A:881:ARG:HH22	1.87	0.40
1:A:743:VAL:CG2	1:A:760:PHE:HB2	2.51	0.40
1:A:806:THR:HA	1:A:836:GLN:O	2.21	0.40
3:C:213:ASP:OD1	3:C:213:ASP:N	2.54	0.40
1:A:191:VAL:HG22	1:A:197:VAL:HG22	2.02	0.40
1:A:331:THR:HB	1:A:380:VAL:HB	2.03	0.40
2:B:105:ASP:OD1	2:B:105:ASP:N	2.53	0.40
2:B:137:ASN:O	2:B:141:ILE:HG13	2.21	0.40
1:A:279:THR:HG21	1:A:324:PHE:CG	2.56	0.40
4:D:76:PRO:HG2	4:D:136:TYR:CE1	2.57	0.40
9:J:141:HIS:CD2	10:N:1:NAG:H81	2.56	0.40
1:A:565:LYS:O	1:A:568:SER:OG	2.38	0.40
2:B:104:ASP:O	2:B:107:ILE:HB	2.22	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	943/993 (95%)	837 (89%)	102 (11%)	4 (0%)	30	64
2	B	294/297 (99%)	283 (96%)	11 (4%)	0	100	100
3	C	239/261 (92%)	221 (92%)	18 (8%)	0	100	100
4	D	152/183 (83%)	144 (95%)	8 (5%)	0	100	100
5	E	101/131 (77%)	93 (92%)	8 (8%)	0	100	100
6	F	98/110 (89%)	96 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	108/242 (45%)	95 (88%)	12 (11%)	1 (1%)	14	48
8	H	191/210 (91%)	172 (90%)	18 (9%)	1 (0%)	25	59
9	J	145/207 (70%)	137 (94%)	8 (6%)	0	100	100
All	All	2271/2634 (86%)	2078 (92%)	187 (8%)	6 (0%)	38	69

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	ALA
1	A	666	ALA
8	H	138	ALA
1	A	195	SER
1	A	296	SER
7	G	56	VAL

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	837/872 (96%)	804 (96%)	33 (4%)	27	57
2	B	254/255 (100%)	241 (95%)	13 (5%)	20	49
3	C	219/235 (93%)	213 (97%)	6 (3%)	40	65
4	D	133/149 (89%)	126 (95%)	7 (5%)	19	47
5	E	86/112 (77%)	79 (92%)	7 (8%)	9	34
6	F	79/85 (93%)	77 (98%)	2 (2%)	42	68
7	G	97/207 (47%)	91 (94%)	6 (6%)	15	43
8	H	171/182 (94%)	166 (97%)	5 (3%)	37	64
9	J	127/158 (80%)	122 (96%)	5 (4%)	27	57
All	All	2003/2255 (89%)	1919 (96%)	84 (4%)	27	54

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	PHE
1	A	93	HIS
1	A	124	ASP
1	A	156	LEU
1	A	162	LYS
1	A	181	TYR
1	A	219	TRP
1	A	246	GLN
1	A	272	PHE
1	A	305	TYR
1	A	338	CYS
1	A	363	LYS
1	A	364	ASP
1	A	381	GLU
1	A	396	GLU
1	A	530	PHE
1	A	551	SER
1	A	572	LEU
1	A	598	MET
1	A	605	ASN
1	A	621	ARG
1	A	625	GLN
1	A	644	ASP
1	A	660	ARG
1	A	682	CYS
1	A	685	ARG
1	A	728	ASP
1	A	779	LYS
1	A	803	ASN
1	A	817	TYR
1	A	847	MET
1	A	860	HIS
1	A	954	ASP
2	B	27	SER
2	B	39	GLU
2	B	91	ARG
2	B	97	PHE
2	B	105	ASP
2	B	108	GLN
2	B	111	ASP
2	B	188	ASN
2	B	238	HIS
2	B	246	SER

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Mol	Chain	Res	Type
2	B	248	LYS
2	B	270	PHE
2	B	287	ASP
3	C	9	ASP
3	C	44	LEU
3	C	64	ASN
3	C	87	PHE
3	C	159	LEU
3	C	175	ASN
4	D	43	TYR
4	D	82	MET
4	D	88	TYR
4	D	89	MET
4	D	100	MET
4	D	120	PHE
4	D	122	MET
5	E	69	ASP
5	E	77	LYS
5	E	85	ARG
5	E	87	HIS
5	E	91	TYR
5	E	95	HIS
5	E	96	ARG
6	F	29	CYS
6	F	94	PHE
7	G	43	ASP
7	G	66	ARG
7	G	70	ASP
7	G	142	SER
7	G	147	SER
7	G	149	PHE
8	H	27	ASN
8	H	119	PHE
8	H	151	TRP
8	H	177	SER
8	H	204	LYS
9	J	59	SER
9	J	171	HIS
9	J	175	ASP
9	J	181	PHE
9	J	190	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	371	GLN
8	H	27	ASN
8	H	147	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 ⓘ

9 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	$\# Z > 2$
10	NAG	L	1	1,10	14,14,15	0.24	0	17,19,21	0.39	0
10	NAG	L	2	10	14,14,15	0.22	0	17,19,21	0.37	0
10	BMA	L	3	10	11,11,12	0.56	0	15,15,17	0.75	0
10	NAG	M	1	1,10	14,14,15	0.53	0	17,19,21	0.79	1 (5%)
10	NAG	M	2	10	14,14,15	0.20	0	17,19,21	0.38	0
10	BMA	M	3	10	11,11,12	0.59	0	15,15,17	0.77	0
10	NAG	N	1	10,9	14,14,15	0.37	0	17,19,21	0.61	0
10	NAG	N	2	10	14,14,15	0.42	0	17,19,21	1.25	1 (5%)
10	BMA	N	3	10	11,11,12	0.59	0	15,15,17	0.75	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
10	NAG	L	1	1,10	-	0/6/23/26	0/1/1/1
10	NAG	L	2	10	-	0/6/23/26	0/1/1/1
10	BMA	L	3	10	-	0/2/19/22	0/1/1/1
10	NAG	M	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	M	2	10	-	1/6/23/26	0/1/1/1
10	BMA	M	3	10	-	0/2/19/22	0/1/1/1
10	NAG	N	1	10,9	-	2/6/23/26	0/1/1/1
10	NAG	N	2	10	-	5/6/23/26	0/1/1/1
10	BMA	N	3	10	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	N	2	NAG	C2-N2-C7	4.29	129.01	122.90
10	M	1	NAG	C1-O5-C5	2.47	115.54	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

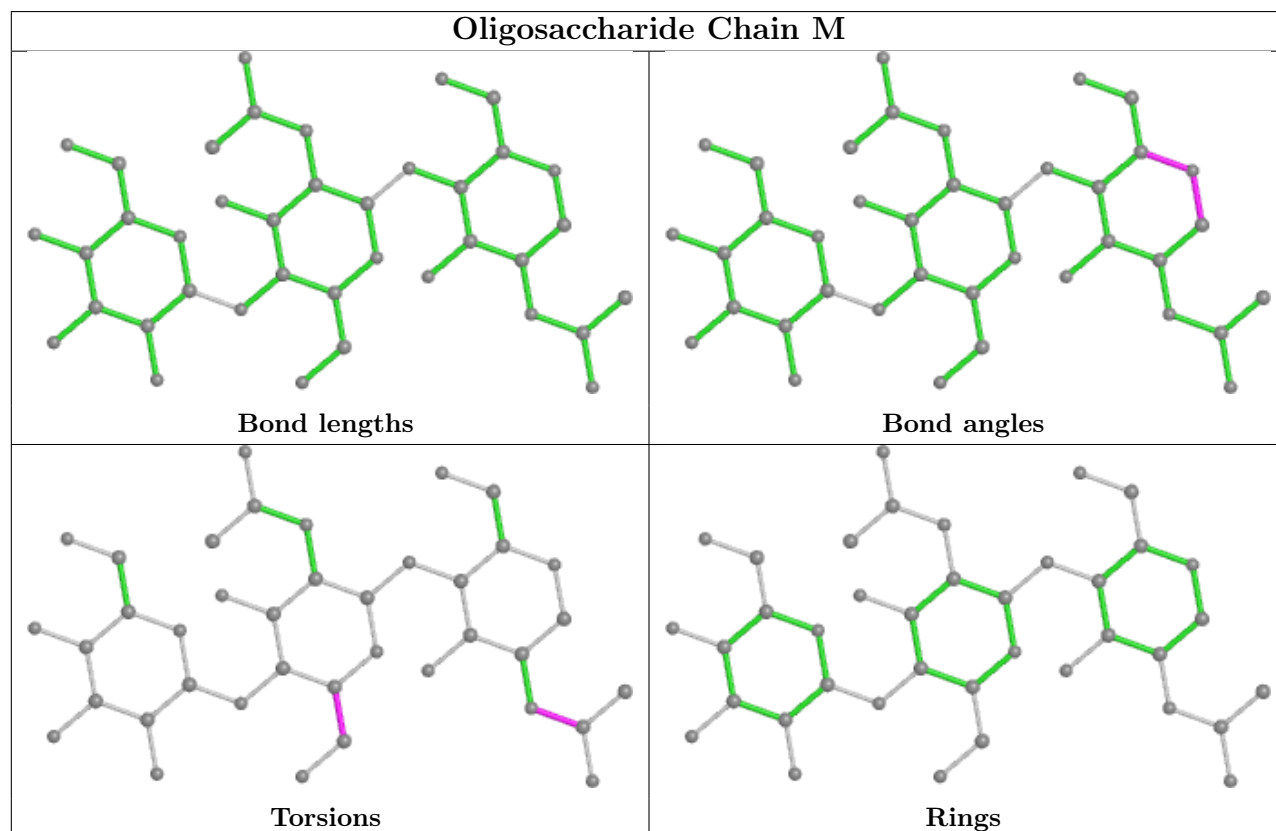
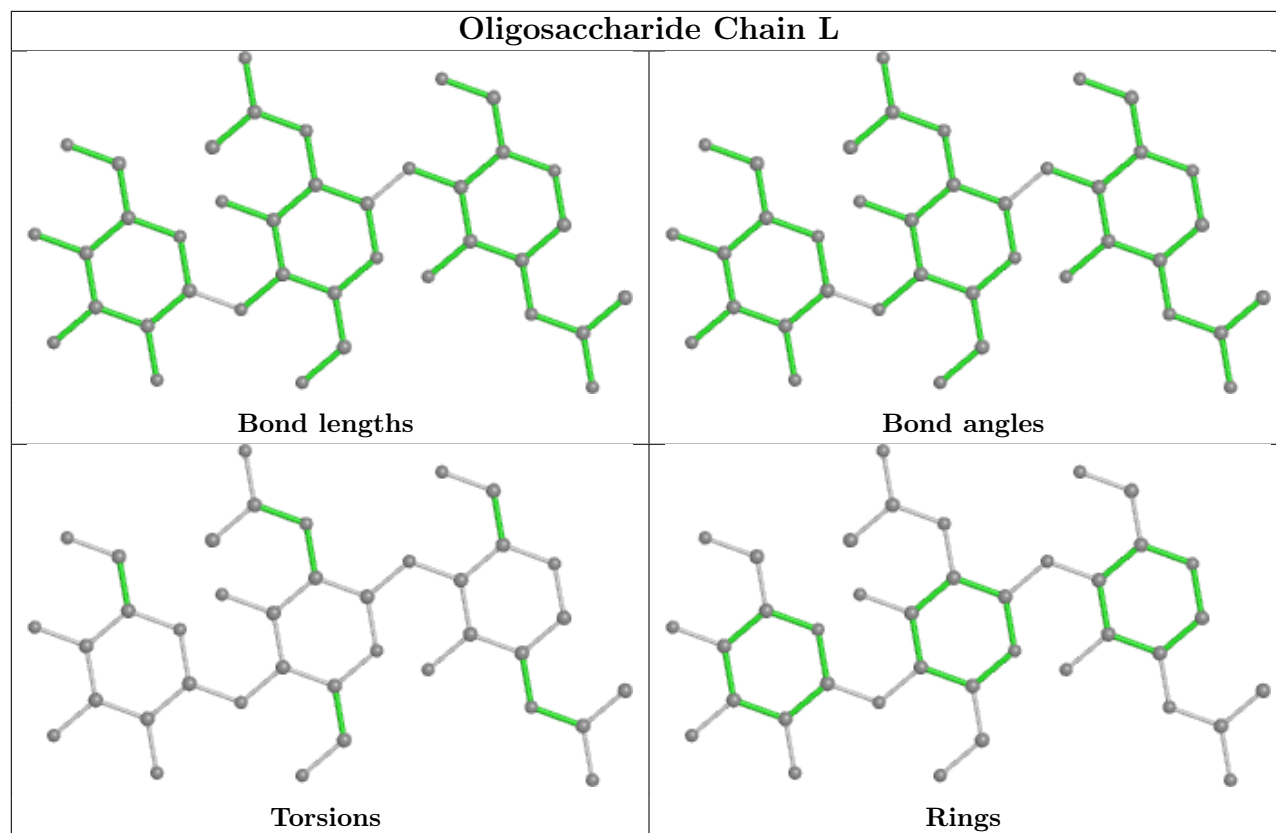
Mol	Chain	Res	Type	Atoms
10	N	2	NAG	O5-C5-C6-O6
10	N	2	NAG	C4-C5-C6-O6
10	M	1	NAG	C8-C7-N2-C2
10	M	1	NAG	O7-C7-N2-C2
10	N	2	NAG	C8-C7-N2-C2
10	N	2	NAG	O7-C7-N2-C2
10	N	1	NAG	O5-C5-C6-O6
10	N	1	NAG	C4-C5-C6-O6
10	N	2	NAG	C3-C2-N2-C7
10	M	2	NAG	O5-C5-C6-O6

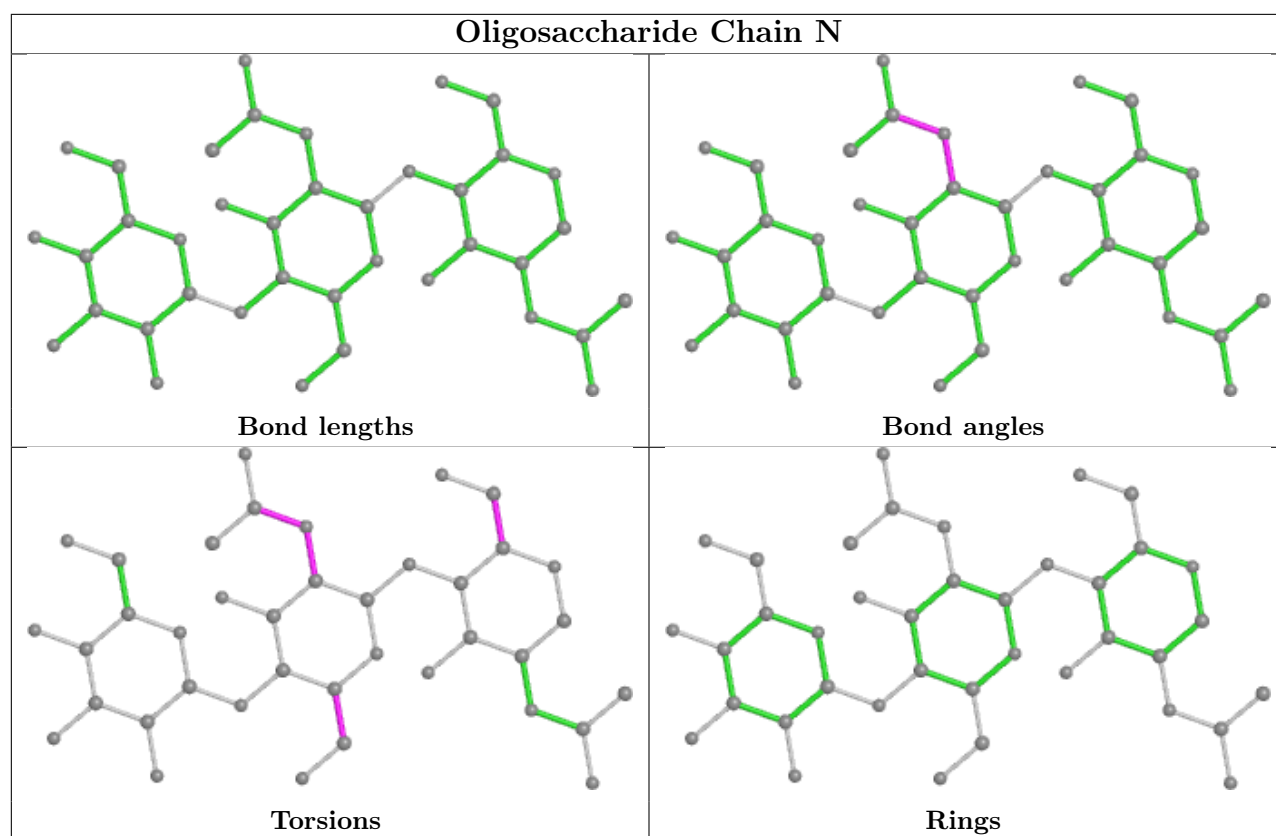
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	N	2	NAG	1	0
10	N	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](#)

There are no ligands in this entry.

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.

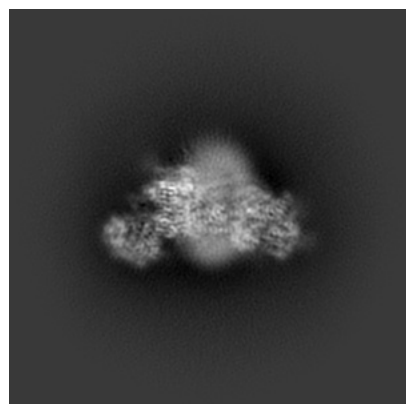
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35906. These allow visual inspection of the internal detail of the map and identification of artifacts.

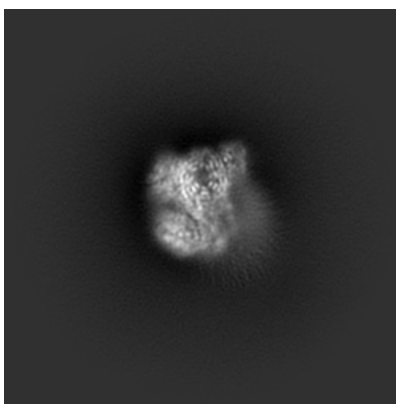
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

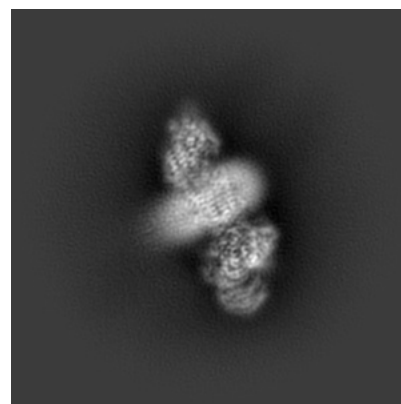
6.1.1 Primary map



X

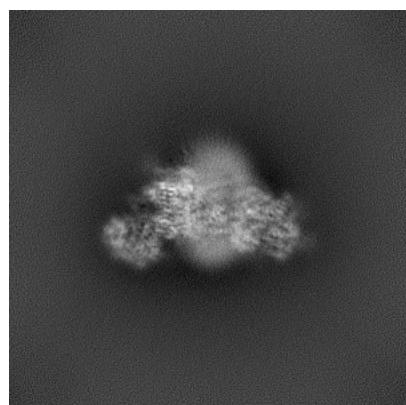


Y

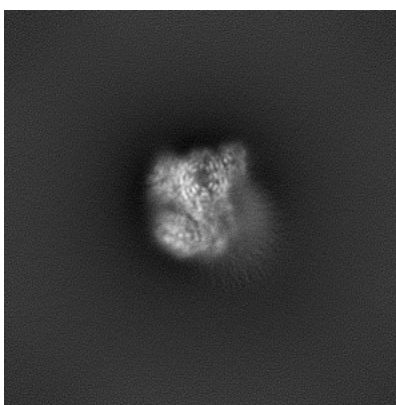


Z

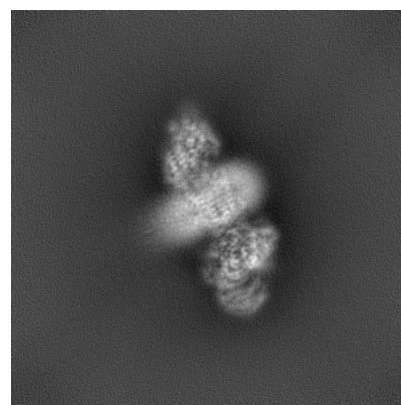
6.1.2 Raw map



X



Y

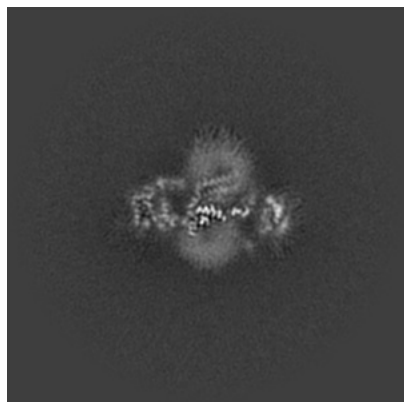


Z

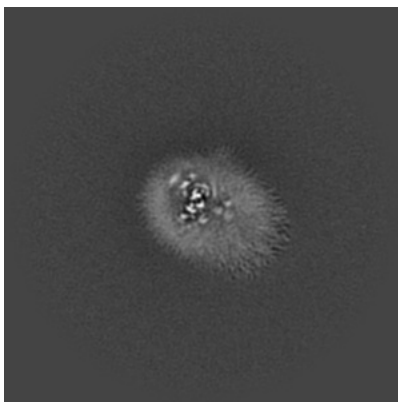
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

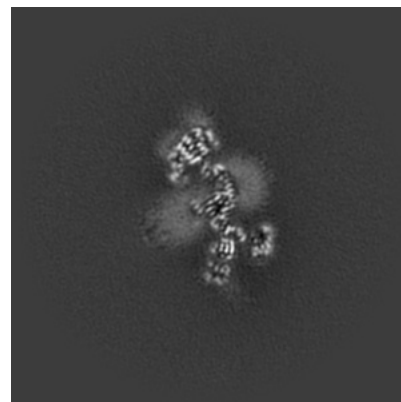
6.2.1 Primary map



X Index: 176

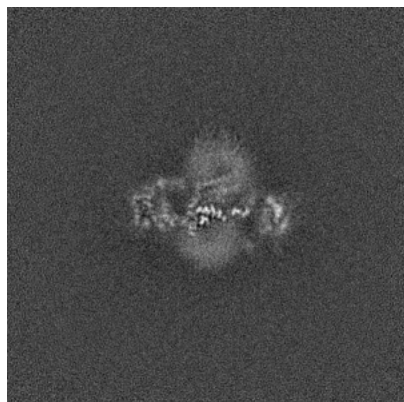


Y Index: 176

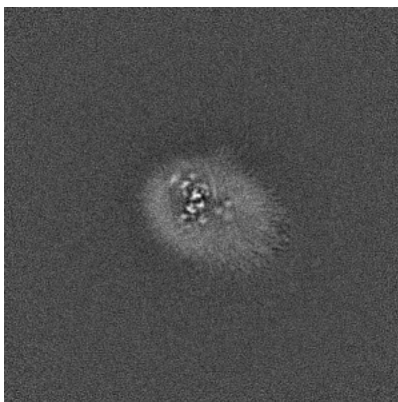


Z Index: 176

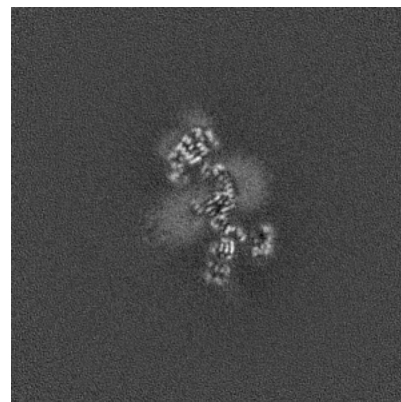
6.2.2 Raw map



X Index: 176



Y Index: 176

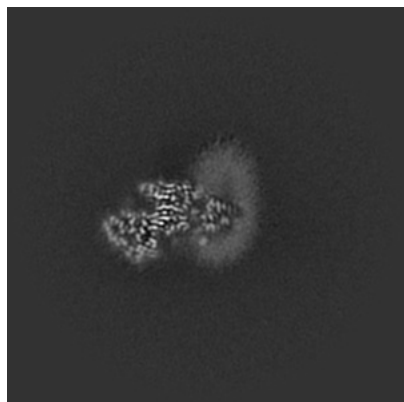


Z Index: 176

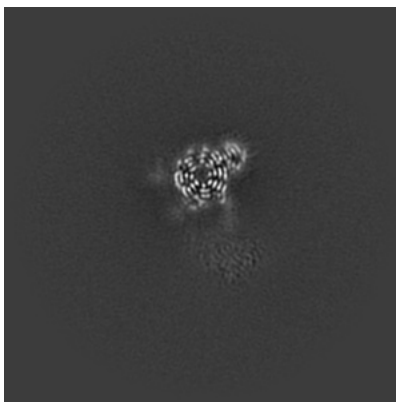
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

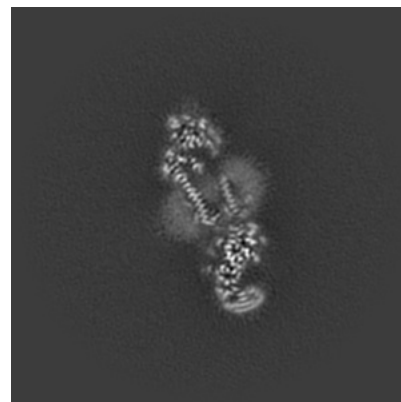
6.3.1 Primary map



X Index: 194

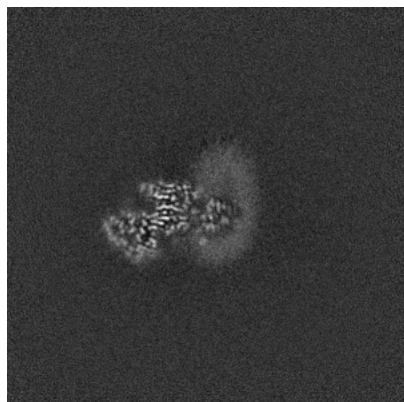


Y Index: 141

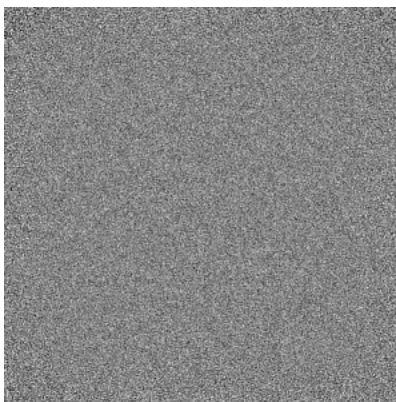


Z Index: 157

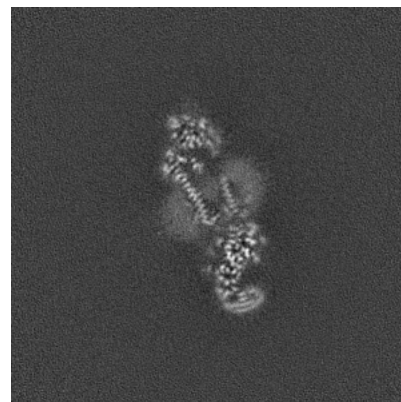
6.3.2 Raw map



X Index: 194



Y Index: 0

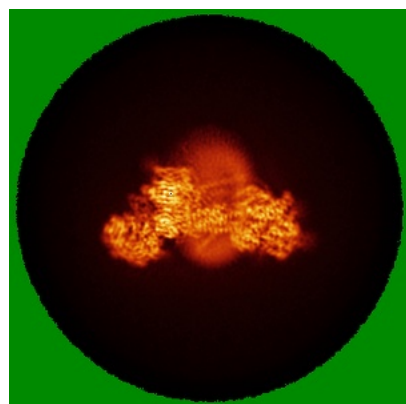


Z Index: 157

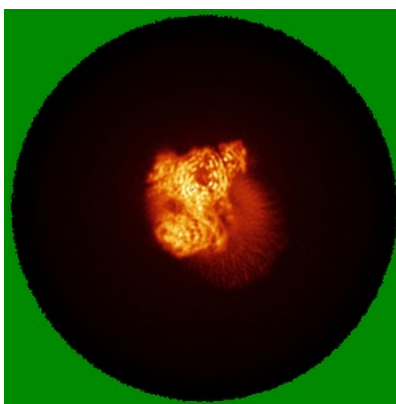
The images above show the largest variance slices of the map in three orthogonal directions.

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

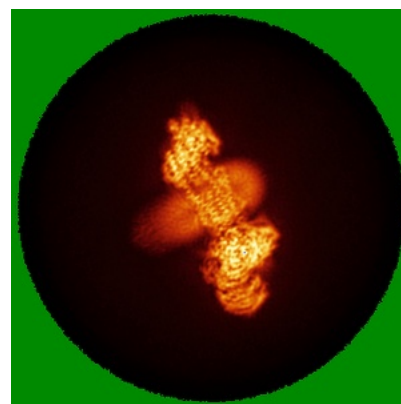
6.4.1 Primary map



X

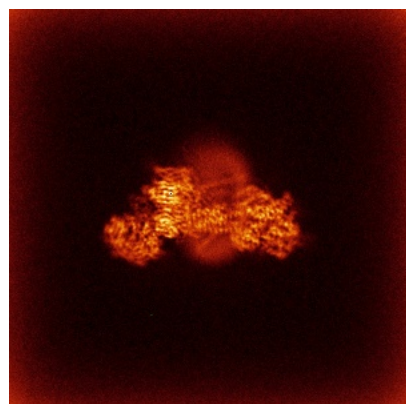


Y

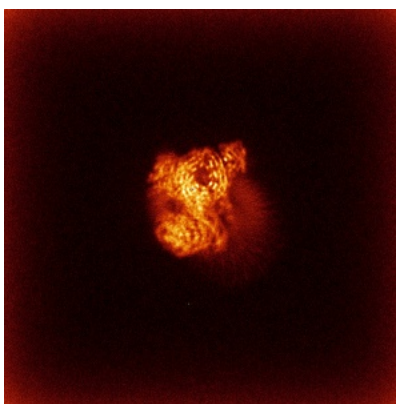


Z

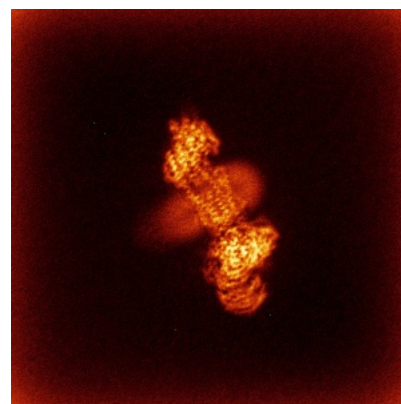
6.4.2 Raw map



X



Y

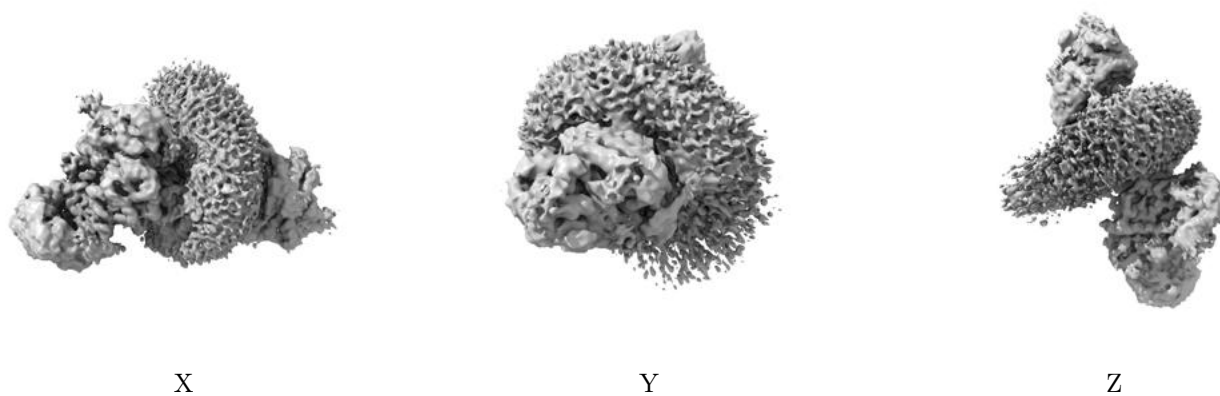


Z

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.

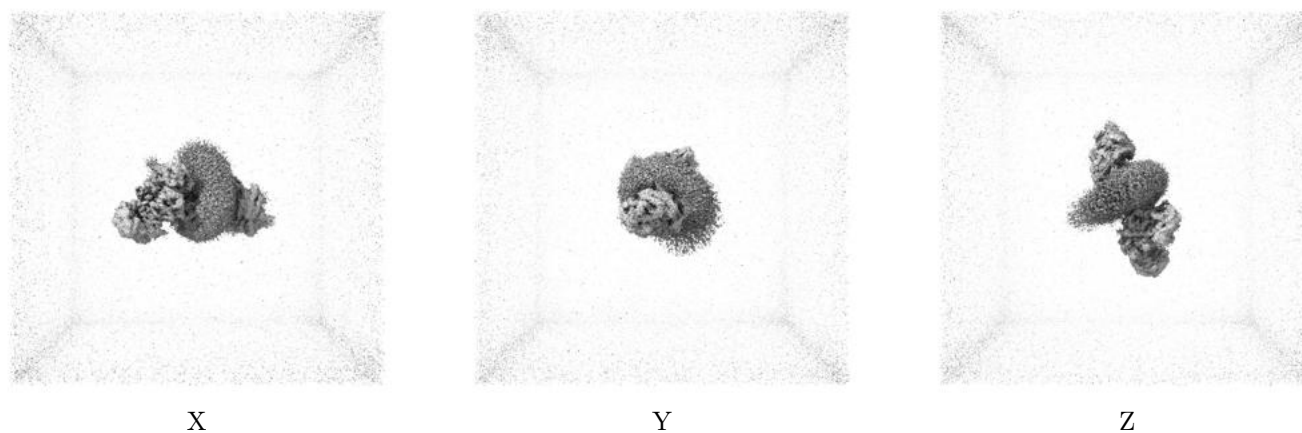
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.159. 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.

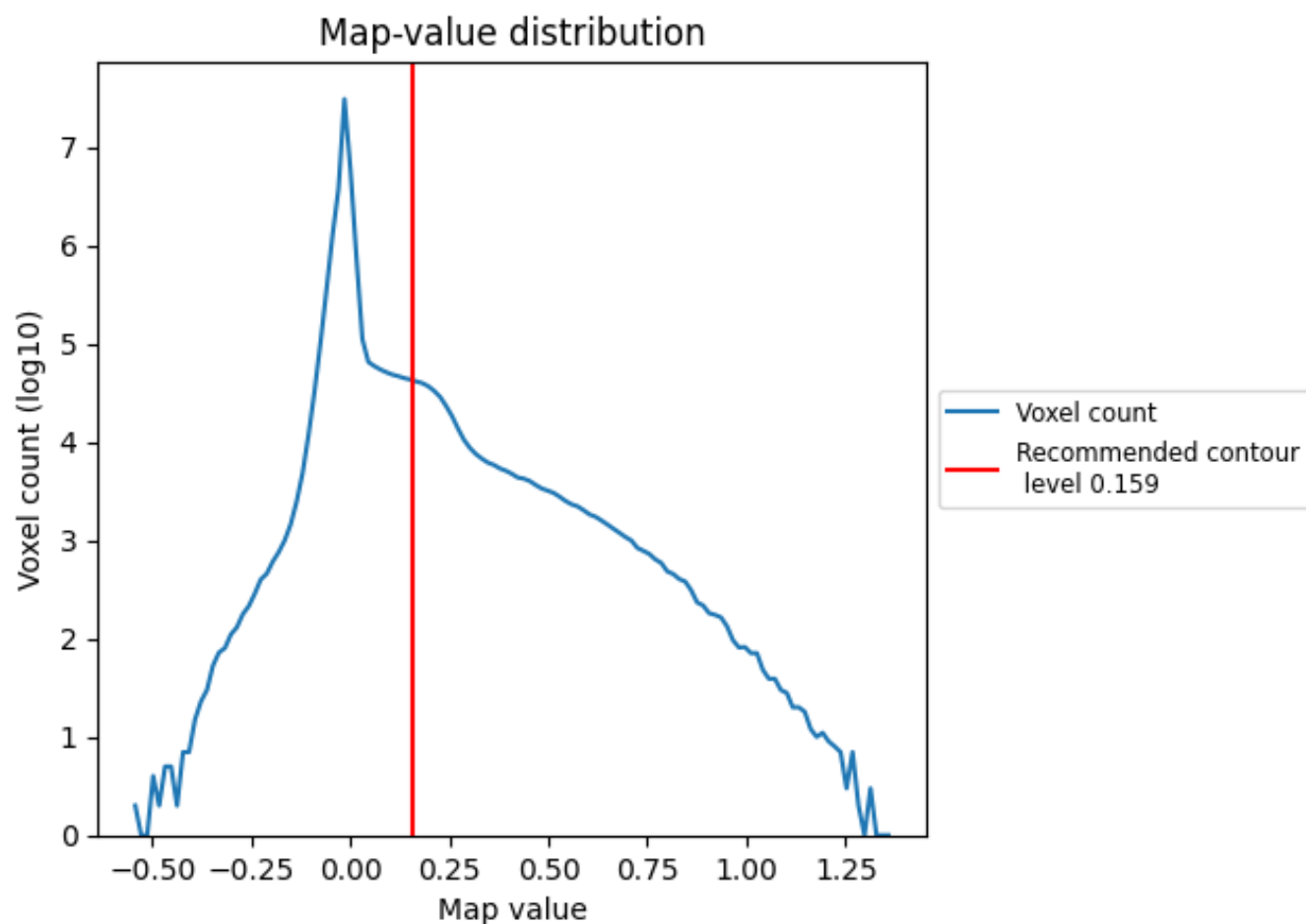
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

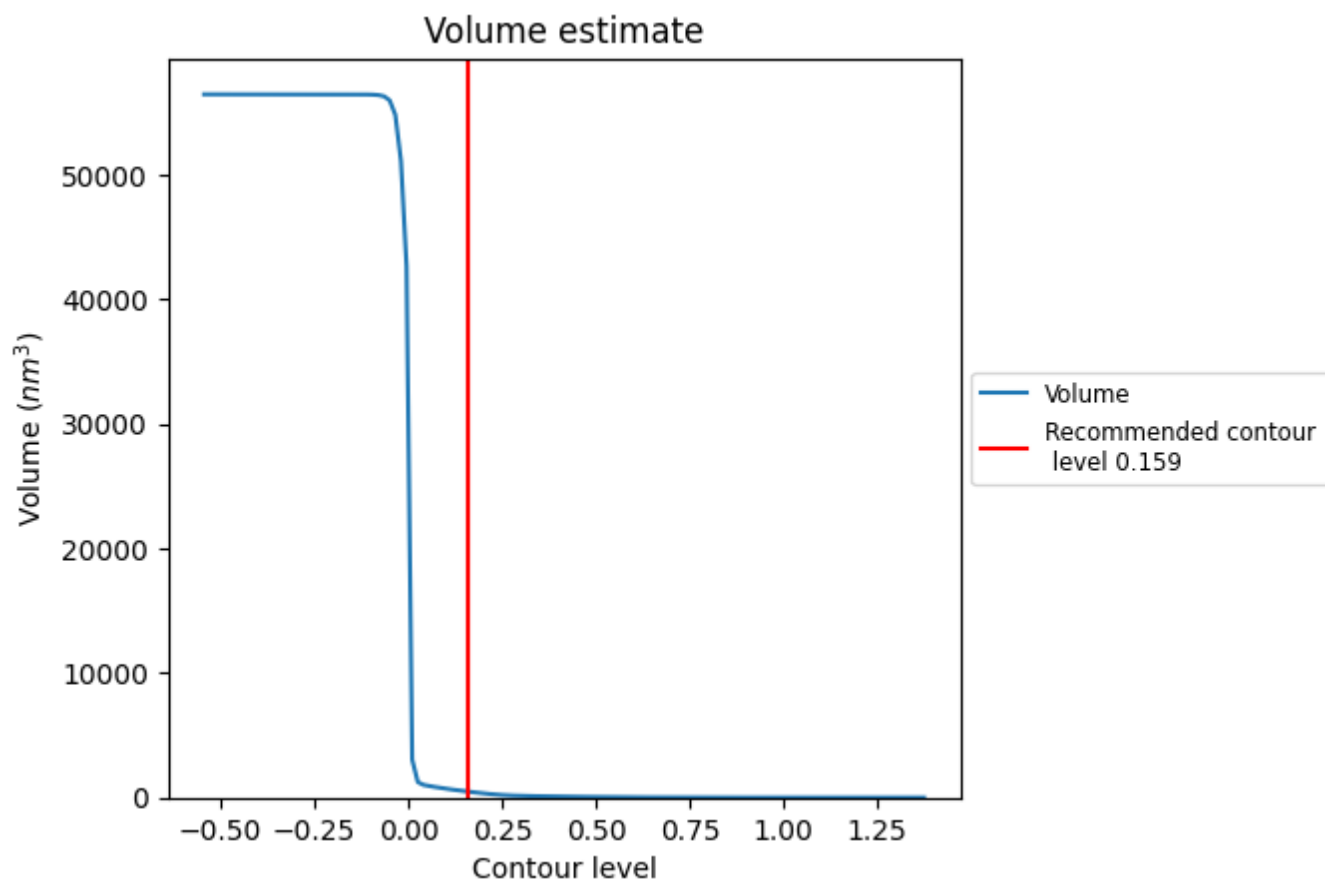
This section contains the results of statistical analysis of the map.

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.

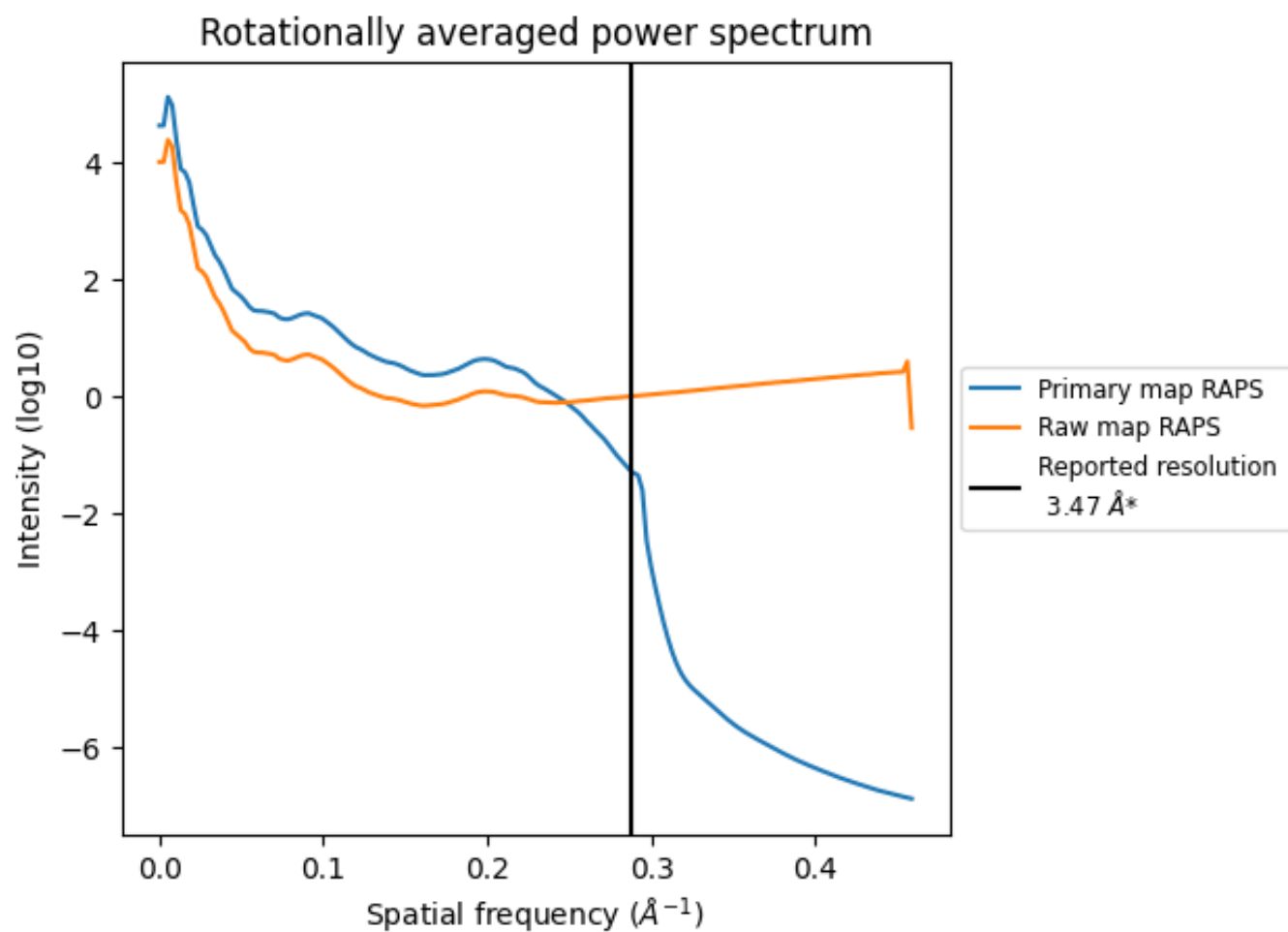
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 481 nm³; this corresponds to an approximate mass of 435 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 ⓘ

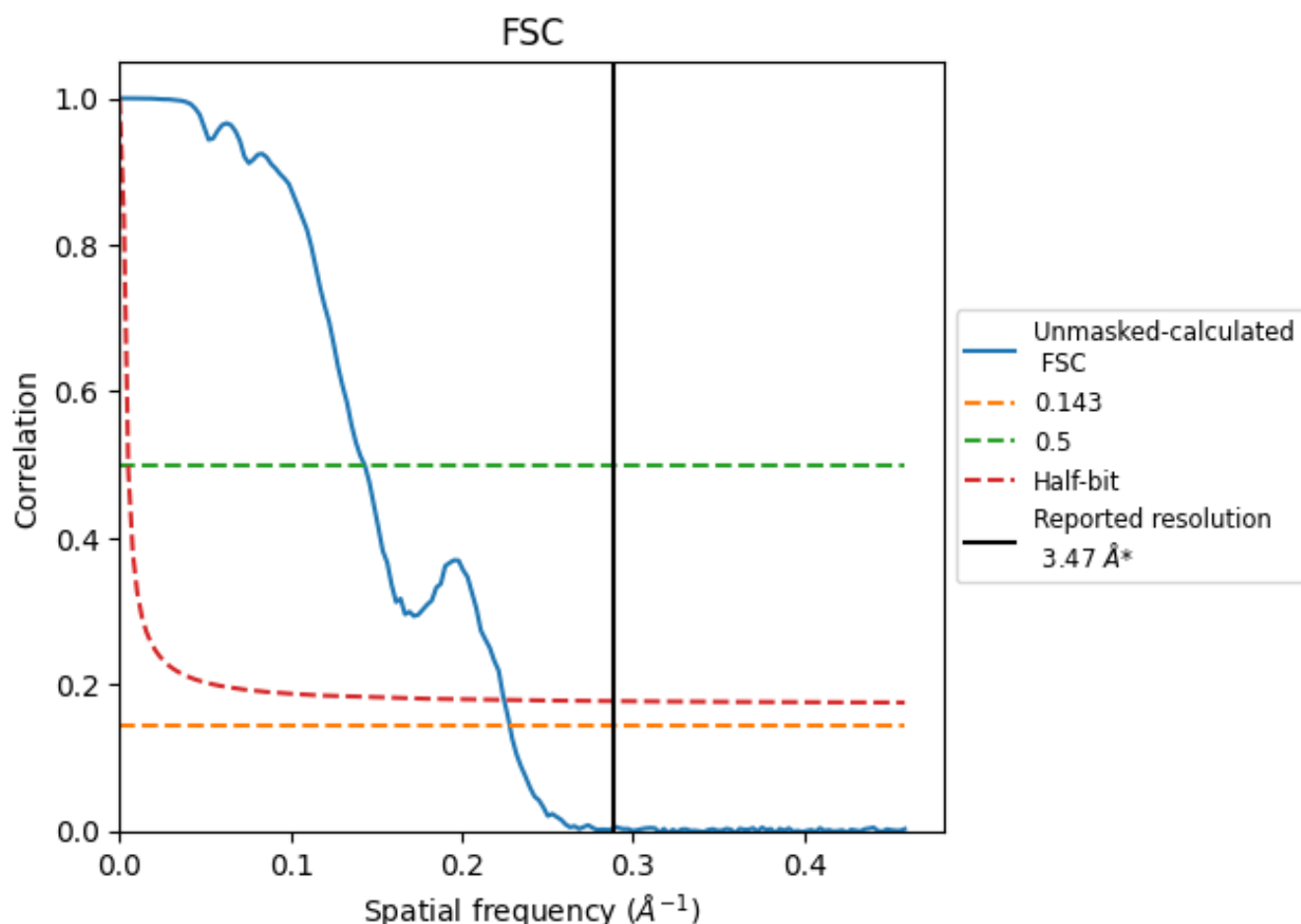


*Reported resolution corresponds to spatial frequency of 0.288 Å⁻¹

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 0.288 Å⁻¹

8.2 Resolution estimates [i](#)

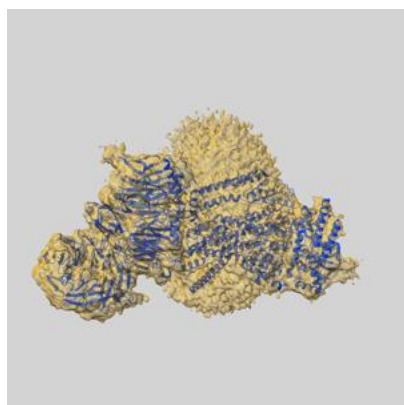
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.47	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.39	6.99	4.45

*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 4.39 differs from the reported value 3.47 by more than 10 %

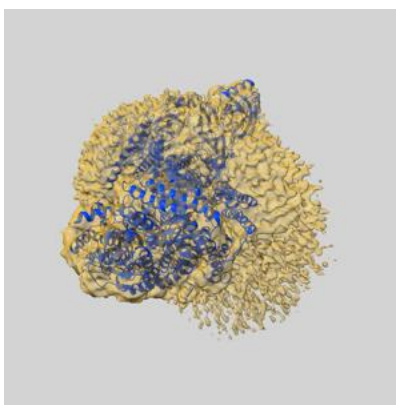
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35906 and PDB model 8J0N. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

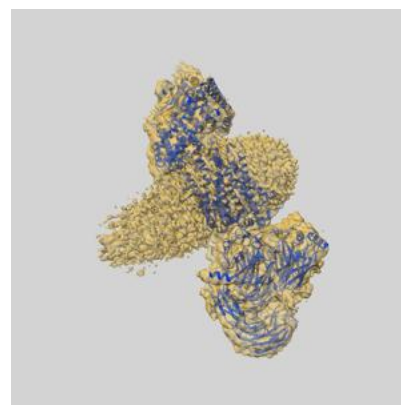
9.1 Map-model overlay [i](#)



X



Y



Z

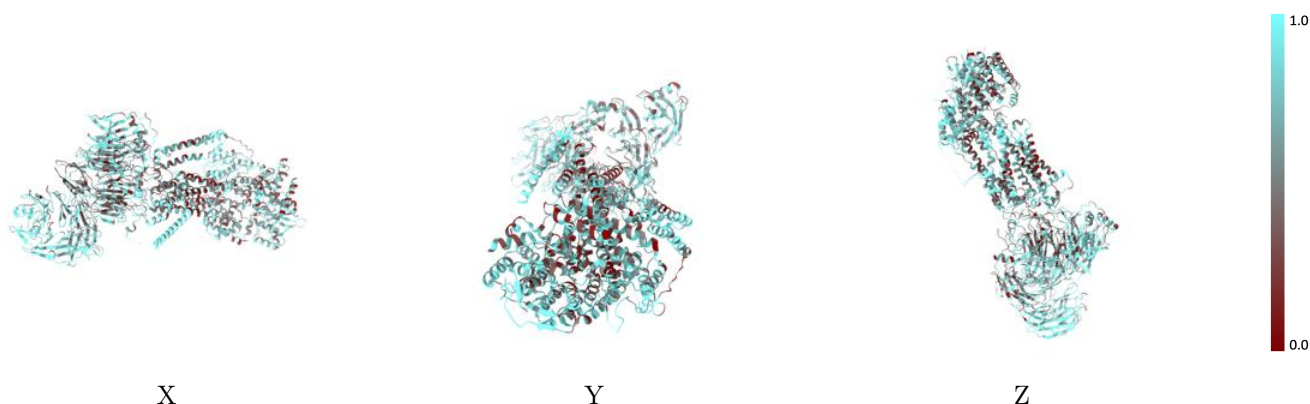
The images above show the 3D surface view of the map at the recommended contour level 0.159 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



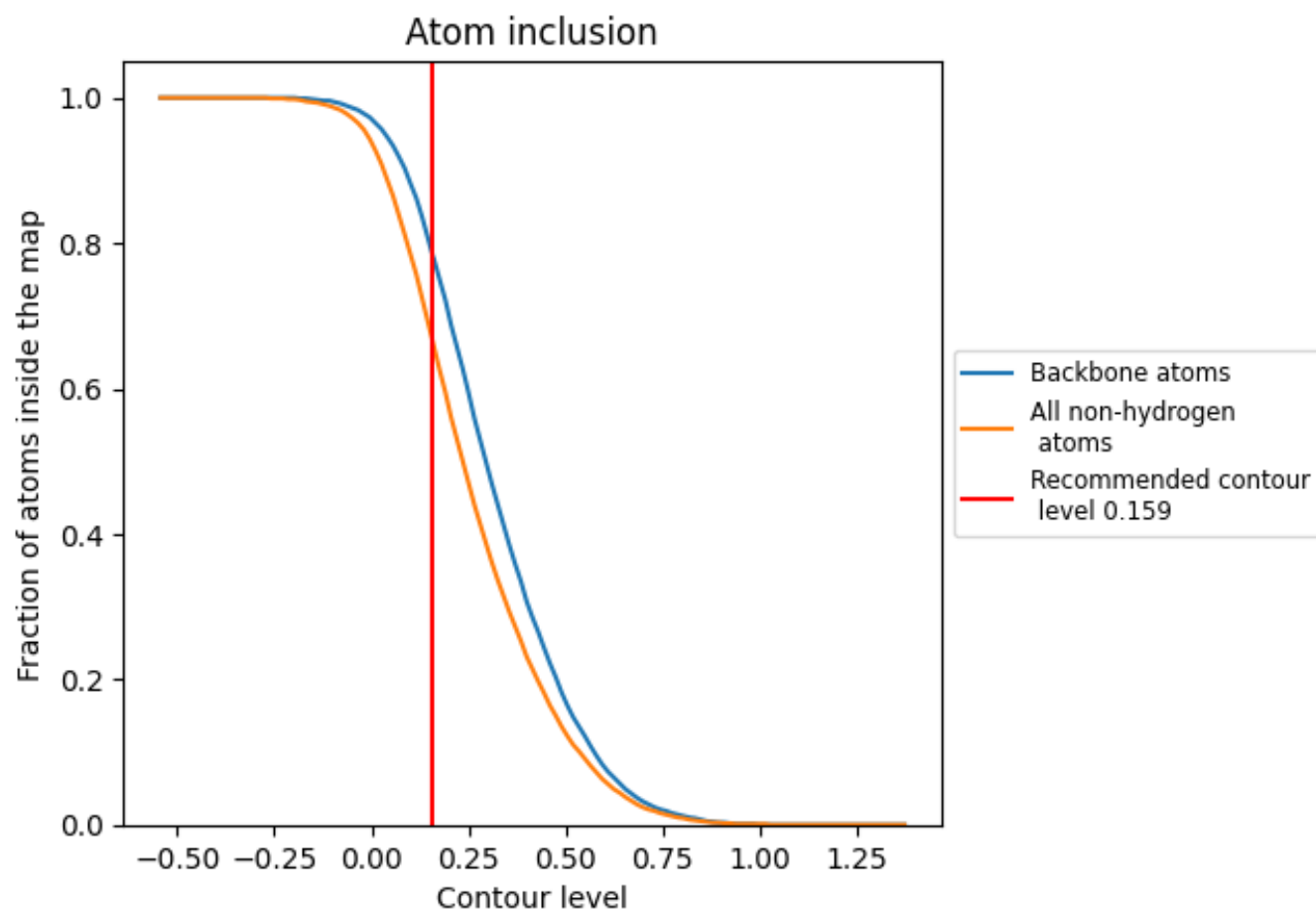
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.159).

9.4 Atom inclusion ⓘ



At the recommended contour level, 78% of all backbone atoms, 66% 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 (0.159) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6620	<div></div> 0.0310
A	<div></div> 0.6840	<div></div> 0.0300
B	<div></div> 0.6310	<div></div> 0.0190
C	<div></div> 0.6370	<div></div> 0.0540
D	<div></div> 0.7230	<div></div> 0.0560
E	<div></div> 0.5840	<div></div> 0.0010
F	<div></div> 0.5780	<div></div> -0.0060
G	<div></div> 0.5080	<div></div> 0.0710
H	<div></div> 0.7200	<div></div> 0.0280
J	<div></div> 0.7190	<div></div> 0.0140
L	<div></div> 0.6670	<div></div> 0.0340
M	<div></div> 0.5380	<div></div> 0.0610
N	<div></div> 0.3850	<div></div> 0.0810

