



Full wwPDB EM Validation Report ⓘ

Jun 23, 2025 – 12:45 PM JST

PDB ID : 9LWU / pdb_00009lwu
EMDB ID : EMD-63459
Title : Cryo-EM structure of HRD1-SEL1LX3-XTP3B complex in C2 symmetry
Authors : Qian, H.W.; Liu, G.Y.
Deposited on : 2025-02-17
Resolution : 3.50 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.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.44

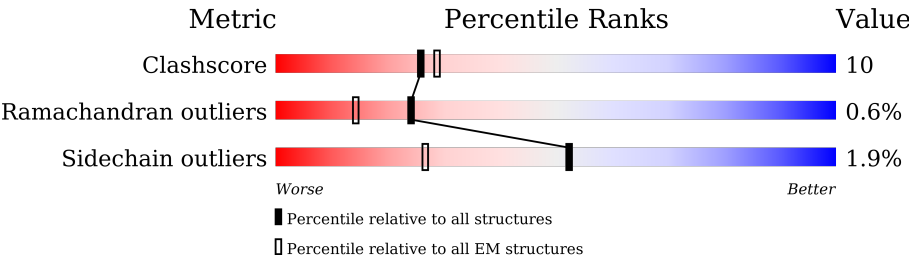
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.




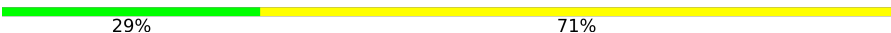
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	617	<div> <div>35%</div> <div>8%</div> <div>57%</div> </div>
1	B	617	<div> <div>35%</div> <div>7%</div> <div>57%</div> </div>
2	C	794	<div> <div>43%</div> <div>8%</div> <div>49%</div> </div>
2	D	794	<div> <div>42%</div> <div>9%</div> <div>49%</div> </div>
3	E	483	<div> <div>6%</div> <div>33%</div> <div>12%</div> <div>52%</div> </div>
3	F	483	<div> <div>6%</div> <div>36%</div> <div>12%</div> <div>52%</div> </div>
4	G	3	<div> <div>100%</div> </div>
4	H	3	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
5	I	7	 14% 86%
5	J	7	 29% 71%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14120 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 E3 ubiquitin-protein ligase synoviolin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	266	Total	C	N	O	S	0	0
			2064	1384	331	332	17		
1	B	266	Total	C	N	O	S	0	0
			2064	1384	331	332	17		

- Molecule 2 is a protein called Protein sel-1 homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	407	Total	C	N	O	S	1	0
			3000	1898	530	560	12		
2	C	407	Total	C	N	O	S	2	0
			3008	1903	533	560	12		

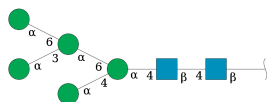
- Molecule 3 is a protein called Endoplasmic reticulum lectin 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	234	Total	C	N	O	S	0	0
			1849	1178	313	345	13		
3	F	234	Total	C	N	O	S	0	0
			1849	1178	313	345	13		

- Molecule 4 is a protein called ALA-ASN-ALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	3	Total	C	N	O	0	0
			18	10	4	4		
4	H	3	Total	C	N	O	0	0
			18	10	4	4		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-4)]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
5	I	7	Total	C	N	O	0	0
			83	46	2	35		
5	J	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

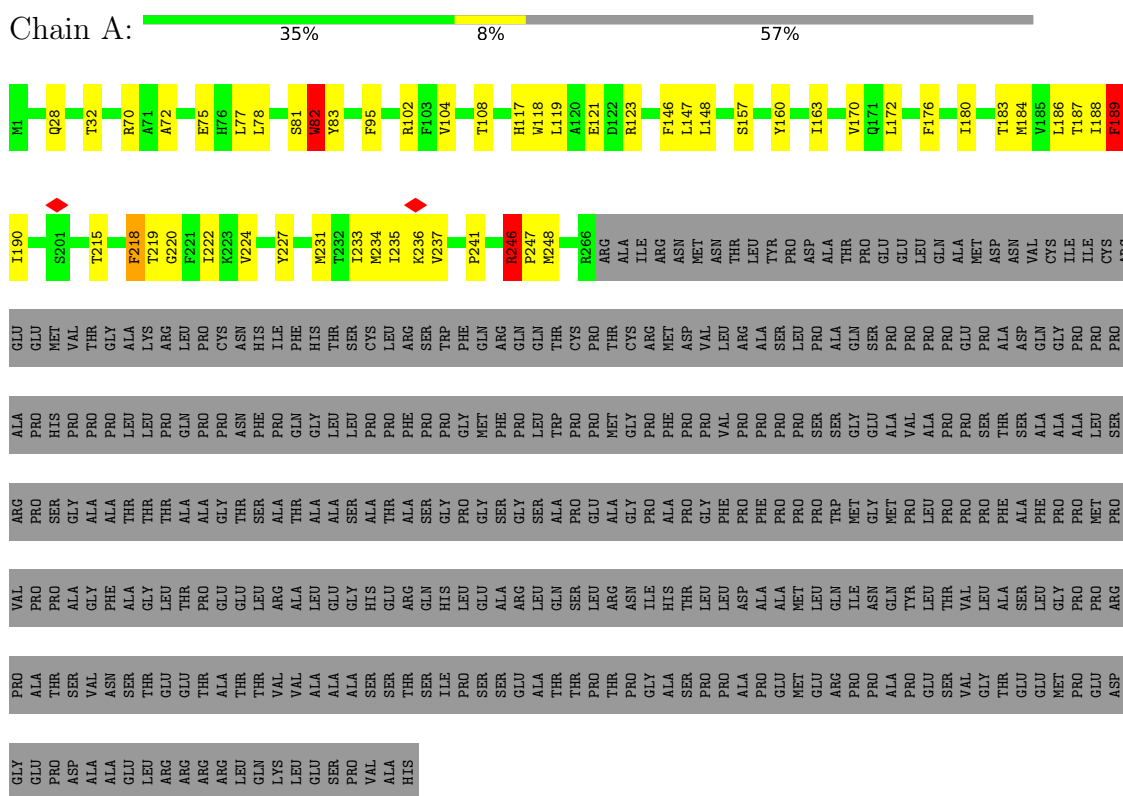


Mol	Chain	Residues	Atoms				AltConf
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	

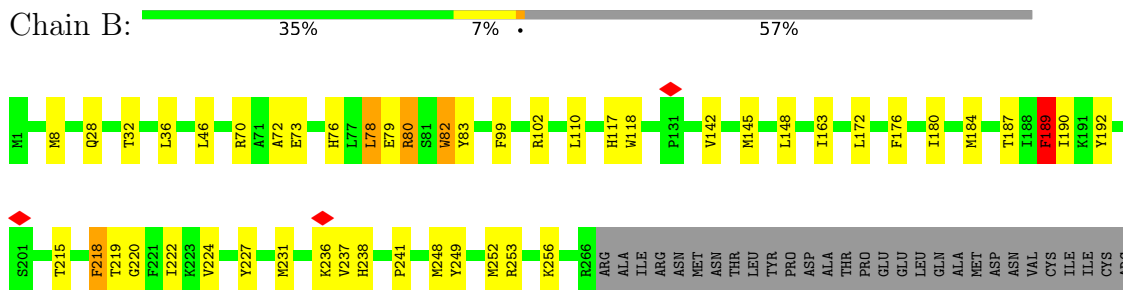
3 Residue-property plots

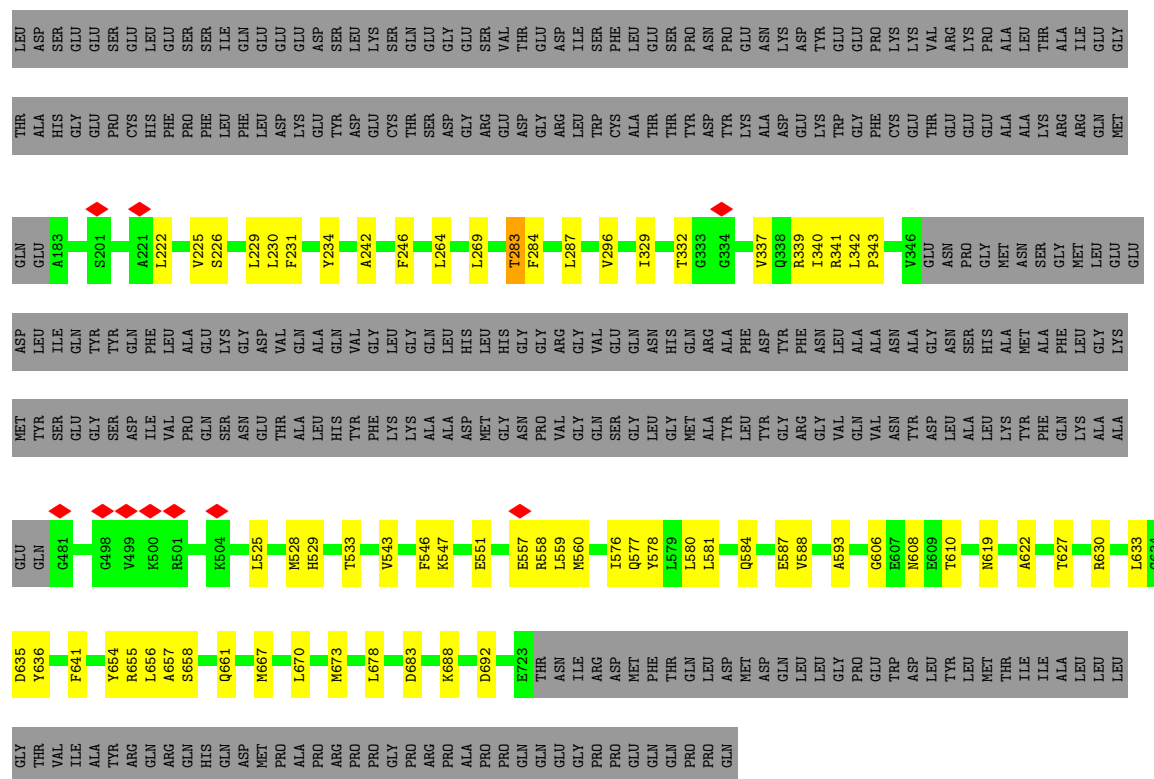
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: E3 ubiquitin-protein ligase synoviolin

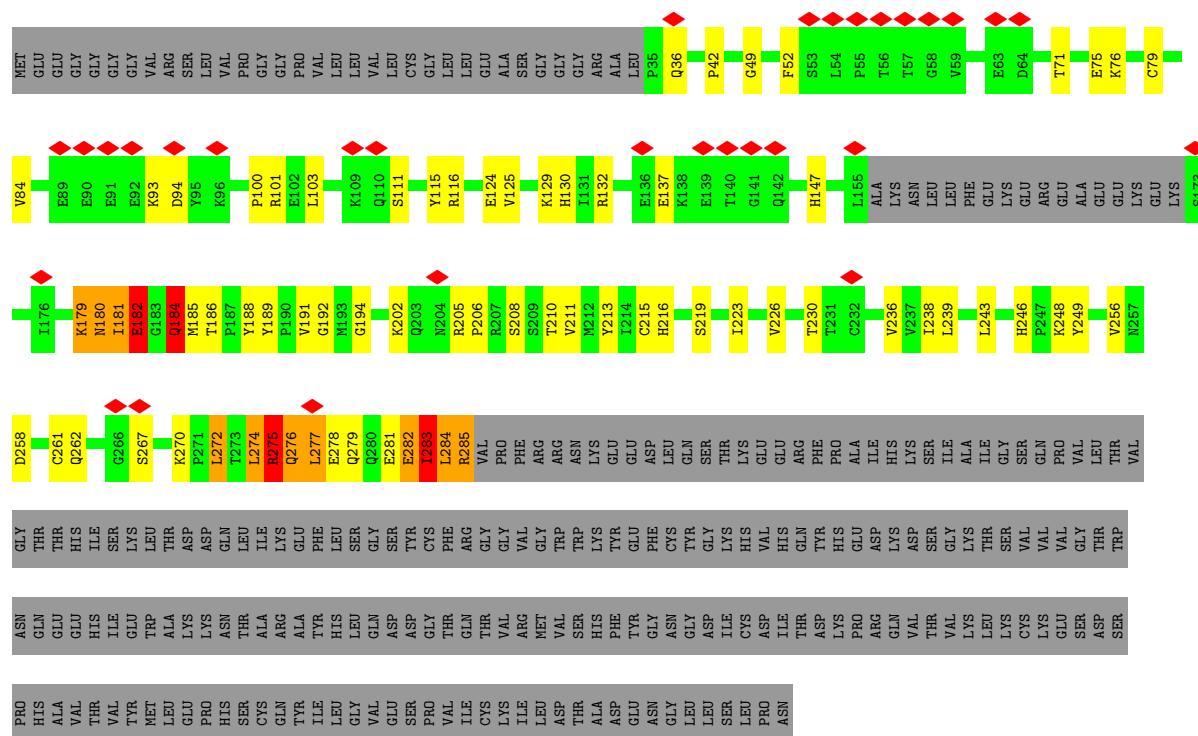
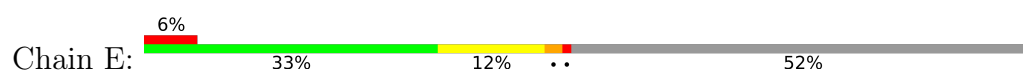


• Molecule 1: E3 ubiquitin-protein ligase synoviolin

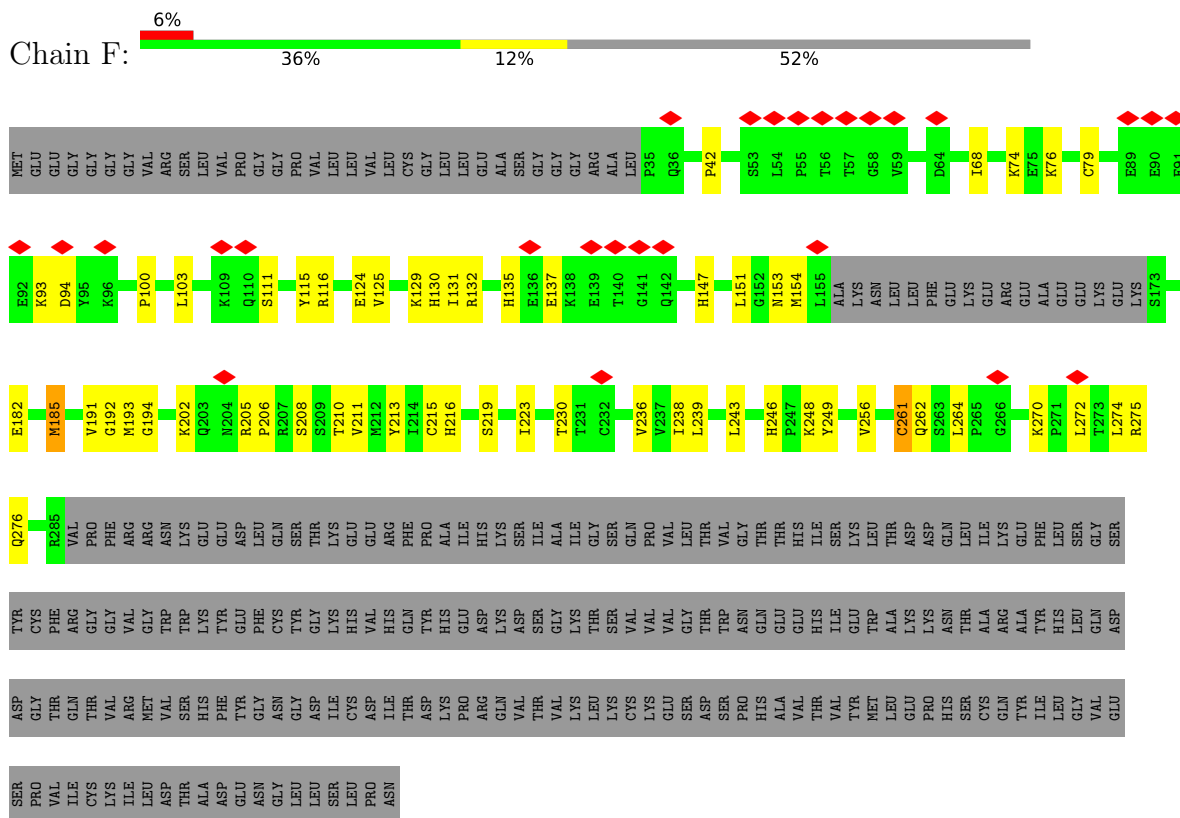




• Molecule 3: Endoplasmic reticulum lectin 1



• Molecule 3: Endoplasmic reticulum lectin 1



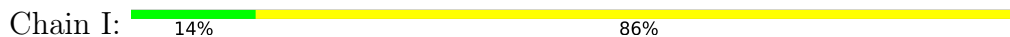
- Molecule 4: ALA-ASN-ALA



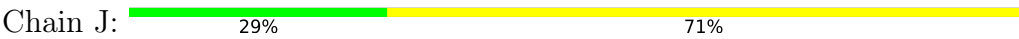
- Molecule 4: ALA-ASN-ALA



- Molecule 5: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-4)] α -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



- Molecule 5: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-4)] α -D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAN1
MAN2
MAN3
MAN4
MAN5
MAN6
MAN7

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	341051	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.305	Depositor
Minimum map value	-2.408	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.104	Depositor
Map size (\AA)	273.92, 273.92, 273.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.34	0/2119	0.70	6/2877 (0.2%)
1	B	0.29	0/2119	0.60	2/2877 (0.1%)
2	C	0.20	0/3075	0.42	0/4171
2	D	0.22	0/3064	0.42	0/4157
3	E	0.37	0/1899	0.58	2/2581 (0.1%)
3	F	0.25	0/1899	0.62	3/2581 (0.1%)
4	G	0.15	0/17	0.46	0/22
4	H	0.14	0/17	0.46	0/22
All	All	0.27	0/14209	0.55	13/19288 (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
3	E	0	1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	261	CYS	CA-CB-SG	11.53	140.93	114.40
1	A	246	ARG	CA-C-N	-6.72	112.88	119.87
1	A	246	ARG	C-N-CA	-6.72	112.88	119.87
1	A	189	PHE	N-CA-C	-6.49	103.83	111.03
1	A	188	ILE	CA-C-N	-5.82	112.72	120.63
1	A	188	ILE	C-N-CA	-5.82	112.72	120.63
1	A	82	TRP	N-CA-C	-5.75	104.92	111.14
1	B	238	HIS	CB-CA-C	-5.53	109.70	117.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	84	VAL	CA-CB-CG1	5.49	119.73	110.40
1	B	189	PHE	N-CA-C	-5.26	104.45	111.24
3	F	185	MET	CB-CG-SD	5.24	128.42	112.70
3	E	283	ILE	N-CA-C	-5.20	105.26	110.30
3	F	262	GLN	CA-CB-CG	5.02	124.14	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	272	LEU	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2064	0	2030	43	0
1	B	2064	0	2030	37	0
2	C	3008	0	2757	45	0
2	D	3000	0	2744	51	0
3	E	1849	0	1751	67	0
3	F	1849	0	1751	40	0
4	G	18	0	14	0	0
4	H	18	0	14	0	0
5	I	83	0	70	0	0
5	J	83	0	70	0	0
6	C	42	0	39	1	0
6	D	42	0	39	1	0
All	All	14120	0	13309	273	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 (273) 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:B:218:PHE:CE1	1:B:222:ILE:HD11	1.70	1.25
1:A:218:PHE:CE1	1:A:222:ILE:HD11	1.77	1.20
3:E:279:GLN:HA	3:E:282:GLU:HB2	1.43	1.01
3:E:270:LYS:HG2	3:E:274:LEU:HD23	1.49	0.94
1:B:218:PHE:HE1	1:B:222:ILE:HD11	1.13	0.92
1:B:218:PHE:CE1	1:B:222:ILE:CD1	2.53	0.90
2:D:283:THR:HG22	2:D:284:PHE:HD1	1.40	0.87
1:A:218:PHE:HE1	1:A:222:ILE:HD11	1.39	0.82
2:C:283:THR:HG22	2:C:284:PHE:HD1	1.43	0.81
3:E:276:GLN:H	3:E:276:GLN:CD	1.96	0.72
2:C:283:THR:CG2	2:C:284:PHE:HD1	2.02	0.72
2:D:283:THR:CG2	2:D:284:PHE:HD1	2.04	0.70
3:E:179:LYS:HG2	3:E:188:TYR:CD2	2.26	0.70
3:F:79:CYS:HA	3:F:261:CYS:HB2	1.74	0.69
1:A:218:PHE:CE1	1:A:222:ILE:CD1	2.67	0.68
3:E:279:GLN:CA	3:E:282:GLU:HB2	2.23	0.66
2:C:619:ASN:HA	2:C:633:LEU:HD11	1.77	0.66
3:E:274:LEU:O	3:E:275:ARG:C	2.39	0.65
3:E:181:ILE:O	3:E:182:GLU:C	2.39	0.65
2:D:226:SER:OG	2:D:245:MET:SD	2.55	0.64
2:D:673:MET:HG3	2:D:678:LEU:HB2	1.79	0.64
3:E:272:LEU:HA	3:E:275:ARG:NH2	2.13	0.63
2:C:673:MET:HG3	2:C:678:LEU:HB2	1.79	0.63
2:C:525:LEU:O	2:C:529:HIS:ND1	2.33	0.62
3:E:79:CYS:HA	3:E:261:CYS:HA	1.83	0.61
2:D:683:ASP:OD2	3:E:230:THR:OG1	2.18	0.60
1:A:215:THR:O	1:A:218:PHE:HB3	2.01	0.60
1:B:163:ILE:HG12	1:B:172:LEU:HD13	1.83	0.60
2:D:339:ARG:HB3	2:D:588:VAL:HG21	1.84	0.59
2:D:525:LEU:O	2:D:529:HIS:ND1	2.34	0.59
3:E:180:ASN:O	3:E:181:ILE:HB	2.02	0.59
3:F:191:VAL:HB	3:F:211:VAL:HB	1.85	0.58
2:C:339:ARG:HB3	2:C:588:VAL:HG21	1.86	0.58
1:A:82:TRP:O	1:A:83:TYR:C	2.44	0.58
2:D:283:THR:CG2	2:D:284:PHE:CD1	2.84	0.58
3:E:284:LEU:O	3:E:285:ARG:C	2.45	0.58
2:D:339:ARG:HH11	2:D:559:LEU:HD11	1.68	0.58
3:E:275:ARG:HH21	3:E:276:GLN:HE22	1.51	0.58
2:C:339:ARG:HH11	2:C:559:LEU:HD11	1.69	0.57
2:C:683:ASP:OD2	3:F:230:THR:OG1	2.18	0.57
3:E:246:HIS:HB3	3:E:249:TYR:HB2	1.86	0.57
2:C:656:LEU:HD21	3:F:182:GLU:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:528:MET:SD	2:D:533:THR:OG1	2.63	0.57
3:F:272:LEU:O	3:F:276:GLN:NE2	2.37	0.56
3:E:274:LEU:O	3:E:276:GLN:N	2.39	0.56
3:E:49:GLY:O	3:E:262:GLN:NE2	2.39	0.56
3:F:205:ARG:HE	3:F:206:PRO:HD2	1.71	0.56
2:C:296:VAL:HG22	2:C:584:GLN:HA	1.86	0.56
3:F:270:LYS:HG2	3:F:274:LEU:HD23	1.87	0.56
2:C:578:TYR:HB3	2:C:593:ALA:HB2	1.88	0.56
2:D:283:THR:HG22	2:D:284:PHE:CD1	2.31	0.55
2:D:656:LEU:HD21	3:E:182:GLU:HG2	1.87	0.55
1:B:231:MET:HE1	1:B:241:PRO:HG2	1.88	0.55
3:E:205:ARG:HE	3:E:206:PRO:HD2	1.71	0.55
2:C:283:THR:HG22	2:C:284:PHE:CD1	2.34	0.55
2:C:528:MET:SD	2:C:533:THR:OG1	2.63	0.55
3:F:246:HIS:HB3	3:F:249:TYR:HB2	1.86	0.55
3:F:93:LYS:HB3	3:F:248:LYS:HE3	1.89	0.55
1:A:75:GLU:O	1:A:78:LEU:N	2.40	0.55
3:E:93:LYS:HB3	3:E:248:LYS:HE3	1.89	0.54
3:E:194:GLY:HA2	3:E:208:SER:HA	1.88	0.54
2:C:688:LYS:NZ	2:C:692:ASP:OD2	2.39	0.54
1:B:82:TRP:O	1:B:83:TYR:C	2.49	0.54
2:C:283:THR:CG2	2:C:284:PHE:CD1	2.86	0.54
1:B:218:PHE:CD1	1:B:222:ILE:CD1	2.91	0.54
3:E:100:PRO:HA	3:E:103:LEU:HD13	1.90	0.54
3:E:276:GLN:O	3:E:279:GLN:HG3	2.08	0.54
1:A:184:MET:O	1:A:187:THR:OG1	2.23	0.54
1:A:163:ILE:HG12	1:A:172:LEU:HD13	1.90	0.54
2:D:578:TYR:HB3	2:D:593:ALA:HB2	1.89	0.54
1:A:219:THR:HA	1:A:222:ILE:HD12	1.90	0.53
1:B:28:GLN:O	1:B:32:THR:OG1	2.24	0.53
2:D:688:LYS:NZ	2:D:692:ASP:OD2	2.39	0.53
2:D:547:LYS:NZ	2:D:551:GLU:OE2	2.36	0.53
3:E:116:ARG:HB2	3:E:223:ILE:HD12	1.90	0.53
1:B:189:PHE:O	1:B:192:TYR:N	2.42	0.53
2:C:222:LEU:O	2:C:226:SER:N	2.36	0.53
3:F:116:ARG:HB2	3:F:223:ILE:HD12	1.90	0.53
3:E:191:VAL:HB	3:E:211:VAL:HB	1.91	0.53
1:B:80:ARG:HD2	1:B:118:TRP:CE2	2.44	0.53
2:C:231:PHE:HZ	2:C:580:LEU:HD22	1.73	0.53
1:A:218:PHE:CD1	1:A:218:PHE:C	2.85	0.52
2:D:319:ARG:HG2	2:D:546:PHE:CZ	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:PHE:CD1	1:B:218:PHE:C	2.86	0.52
2:C:547:LYS:NZ	2:C:551:GLU:OE2	2.37	0.52
3:E:202:LYS:HB3	3:E:205:ARG:HB2	1.92	0.52
2:D:287:LEU:HD11	3:E:274:LEU:HD13	1.90	0.52
3:E:213:TYR:HB3	3:E:243:LEU:HD11	1.92	0.52
3:F:194:GLY:HA2	3:F:208:SER:HA	1.91	0.52
3:F:202:LYS:HB3	3:F:205:ARG:HB2	1.91	0.52
3:E:129:LYS:HB3	3:E:130:HIS:HD2	1.73	0.51
1:A:231:MET:HE1	1:A:241:PRO:HG2	1.93	0.51
2:D:329:ILE:HD13	2:D:519:ILE:HD11	1.91	0.51
2:D:329:ILE:HA	2:D:332:THR:HG22	1.91	0.51
2:C:635:ASP:OD1	2:C:654:TYR:OH	2.21	0.51
2:D:230:LEU:HD11	2:D:264:LEU:HD21	1.92	0.51
2:D:644:ASP:OD1	2:D:644:ASP:N	2.43	0.51
3:F:129:LYS:HB3	3:F:130:HIS:HD2	1.75	0.51
1:B:215:THR:O	1:B:218:PHE:HB3	2.11	0.51
3:F:131:ILE:HD11	3:F:193:MET:HE3	1.93	0.51
3:F:213:TYR:HB3	3:F:243:LEU:HD11	1.92	0.51
2:D:558:ARG:HH22	2:D:577:GLN:HG2	1.75	0.50
3:F:215:CYS:HB3	3:F:243:LEU:HB2	1.93	0.50
3:E:281:GLU:HA	3:E:284:LEU:HD12	1.93	0.50
3:E:281:GLU:C	3:E:283:ILE:N	2.67	0.50
3:F:111:SER:O	3:F:111:SER:OG	2.27	0.50
1:B:218:PHE:C	1:B:218:PHE:HD1	2.19	0.50
3:E:216:HIS:HB2	3:E:239:LEU:HD22	1.93	0.50
2:C:287:LEU:HD11	3:F:274:LEU:HD13	1.94	0.50
1:A:189:PHE:O	1:A:190:ILE:C	2.53	0.49
2:D:630:ARG:HB3	2:D:657:ALA:HB2	1.94	0.49
3:E:216:HIS:HB3	3:E:219:SER:HB3	1.93	0.49
1:B:227:TYR:HB3	1:B:248:MET:HE2	1.93	0.49
3:F:216:HIS:HB3	3:F:219:SER:HB3	1.94	0.49
2:D:296:VAL:HG22	2:D:584:GLN:HA	1.94	0.49
3:E:215:CYS:HB3	3:E:243:LEU:HB2	1.94	0.49
2:C:558:ARG:HH22	2:C:577:GLN:HG2	1.78	0.49
3:F:100:PRO:HA	3:F:103:LEU:HD23	1.94	0.49
3:F:211:VAL:HA	3:F:236:VAL:HG23	1.94	0.49
1:A:246:ARG:HA	1:B:82:TRP:CZ2	2.48	0.49
2:C:581:LEU:HA	2:C:584:GLN:HB2	1.94	0.49
3:E:192:GLY:HA2	3:E:210:THR:HA	1.94	0.49
3:E:272:LEU:HD13	3:E:275:ARG:HH22	1.77	0.49
1:A:218:PHE:CD1	1:A:222:ILE:HD11	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:125:VAL:HG11	3:E:238:ILE:HD11	1.93	0.49
2:C:230:LEU:HD11	2:C:264:LEU:HD21	1.93	0.48
2:C:329:ILE:HA	2:C:332:THR:HG22	1.95	0.48
2:C:630:ARG:HB3	2:C:657:ALA:HB2	1.95	0.48
3:E:211:VAL:HA	3:E:236:VAL:HG23	1.95	0.48
2:C:543:VAL:HA	2:C:546:PHE:HB2	1.96	0.48
2:D:342:LEU:N	2:D:343:PRO:HD2	2.28	0.48
3:F:216:HIS:HB2	3:F:239:LEU:HD22	1.96	0.48
3:E:76:LYS:N	3:E:267:SER:OG	2.43	0.48
2:C:230:LEU:HD13	2:C:246:PHE:HE2	1.78	0.48
3:F:125:VAL:HG11	3:F:238:ILE:HD11	1.96	0.48
2:D:222:LEU:O	2:D:226:SER:N	2.38	0.48
1:A:172:LEU:HD21	1:A:233:ILE:HG21	1.96	0.47
1:B:219:THR:HA	1:B:222:ILE:HD12	1.95	0.47
2:C:667:MET:HA	2:C:670:LEU:HB2	1.96	0.47
3:E:71:THR:OG1	3:E:75:GLU:OE1	2.32	0.47
1:B:248:MET:O	1:B:252:MET:HG2	2.15	0.47
2:D:269:LEU:HD21	2:D:576:ILE:HD12	1.96	0.47
2:C:608:ASN:HB3	6:C:803:NAG:N2	2.30	0.47
1:A:82:TRP:CH2	1:B:249:TYR:CD2	3.03	0.47
2:D:667:MET:HA	2:D:670:LEU:HB2	1.96	0.47
3:E:282:GLU:OE2	3:E:285:ARG:HB3	2.15	0.47
2:C:283:THR:CG2	2:C:284:PHE:N	2.78	0.47
1:A:218:PHE:C	1:A:218:PHE:HD1	2.22	0.47
2:D:283:THR:CG2	2:D:284:PHE:N	2.77	0.47
2:D:608:ASN:HB3	6:D:803:NAG:N2	2.30	0.47
3:E:111:SER:O	3:E:111:SER:OG	2.27	0.47
3:E:179:LYS:CG	3:E:180:ASN:H	2.27	0.47
2:C:269:LEU:HD21	2:C:576:ILE:HD12	1.97	0.47
2:C:341:ARG:NH2	2:C:587:GLU:OE2	2.48	0.47
2:D:230:LEU:HD13	2:D:246:PHE:HE2	1.79	0.47
1:A:28:GLN:O	1:A:32:THR:OG1	2.26	0.47
2:D:581:LEU:HA	2:D:584:GLN:HB2	1.98	0.47
3:E:42:PRO:HB2	3:E:256:VAL:HG22	1.97	0.46
2:D:231:PHE:HZ	2:D:580:LEU:HD22	1.80	0.46
2:D:635:ASP:OD1	2:D:654:TYR:OH	2.21	0.46
1:B:80:ARG:O	1:B:83:TYR:HB2	2.15	0.46
1:A:83:TYR:HD2	1:A:246:ARG:HD2	1.81	0.46
2:D:229:LEU:HB3	2:D:242:ALA:HB2	1.97	0.46
2:D:319:ARG:NE	3:E:281:GLU:OE2	2.49	0.46
1:A:236:LYS:HG2	1:A:237:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:627:THR:HG22	2:D:661:GLN:HB3	1.97	0.46
2:D:339:ARG:NH2	2:D:551:GLU:O	2.49	0.46
1:B:142:VAL:HA	1:B:145:MET:HG2	1.97	0.46
2:C:627:THR:HG22	2:C:661:GLN:HB3	1.96	0.46
1:B:189:PHE:O	1:B:190:ILE:C	2.59	0.46
3:F:131:ILE:HB	3:F:151:LEU:HB2	1.98	0.45
2:D:319:ARG:HD2	3:E:281:GLU:OE1	2.16	0.45
2:D:340:ILE:O	2:D:592:ASN:ND2	2.49	0.45
1:A:160:TYR:HA	1:A:163:ILE:HG22	1.98	0.45
1:B:252:MET:O	1:B:256:LYS:N	2.45	0.45
3:F:115:TYR:HB3	3:F:124:GLU:HG3	1.99	0.45
3:F:153:ASN:N	3:F:153:ASN:OD1	2.47	0.45
3:E:52:PHE:HB3	3:E:262:GLN:HE22	1.80	0.45
1:A:215:THR:O	1:A:219:THR:HG23	2.17	0.45
2:D:315:LEU:HD21	2:D:542:ALA:HB1	1.99	0.45
3:E:185:MET:C	3:E:186:THR:CG2	2.89	0.45
1:A:77:LEU:O	1:A:81:SER:HB2	2.16	0.45
2:D:341:ARG:NH2	2:D:587:GLU:OE2	2.50	0.45
1:A:70:ARG:HG3	1:A:72:ALA:H	1.82	0.45
3:E:115:TYR:HB3	3:E:124:GLU:HG3	1.98	0.44
2:D:543:VAL:HA	2:D:546:PHE:HB2	1.98	0.44
3:E:275:ARG:HE	3:E:276:GLN:HE22	1.65	0.44
3:F:76:LYS:HB3	3:F:264:LEU:HD12	1.99	0.44
3:E:179:LYS:HD3	3:E:181:ILE:HG12	2.00	0.44
3:E:277:LEU:HA	3:E:277:LEU:HD13	1.63	0.44
1:A:104:VAL:O	1:A:108:THR:HG23	2.17	0.44
1:A:117:HIS:CD2	1:A:148:LEU:HD13	2.53	0.44
3:E:179:LYS:HZ2	3:E:181:ILE:N	2.15	0.44
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.75	0.44
2:D:606:GLY:O	2:D:610:THR:OG1	2.36	0.44
1:B:73:GLU:HA	1:B:76:HIS:HB3	1.99	0.44
3:E:129:LYS:HB3	3:E:130:HIS:CD2	2.52	0.44
3:E:184:GLN:H	3:E:184:GLN:HG2	1.54	0.44
2:C:337:VAL:HG21	2:C:557:GLU:HA	2.00	0.44
3:F:185:MET:HE3	3:F:185:MET:HA	2.00	0.44
3:F:272:LEU:HA	3:F:275:ARG:HH22	1.82	0.44
1:A:220:GLY:O	1:A:224:VAL:HG12	2.17	0.43
2:C:606:GLY:O	2:C:610:THR:OG1	2.35	0.43
1:A:231:MET:O	1:A:235:ILE:HD12	2.17	0.43
1:B:36:LEU:HD13	1:B:46:LEU:HD11	1.98	0.43
3:F:193:MET:HE2	3:F:211:VAL:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:PHE:CD1	1:A:222:ILE:CD1	3.01	0.43
3:E:276:GLN:O	3:E:277:LEU:C	2.61	0.43
1:B:236:LYS:HG2	1:B:237:VAL:HG13	2.00	0.43
1:B:253:ARG:HA	1:B:256:LYS:HB2	2.00	0.43
1:A:123:ARG:HA	1:A:123:ARG:HD2	1.76	0.43
3:F:42:PRO:HB2	3:F:256:VAL:HG22	1.99	0.43
3:F:154:MET:SD	3:F:154:MET:N	2.92	0.43
1:B:102:ARG:HD2	1:B:102:ARG:HA	1.85	0.43
2:C:229:LEU:HB3	2:C:242:ALA:HB2	2.00	0.43
2:C:340:ILE:HD11	2:C:560:MET:HE1	1.99	0.43
2:D:222:LEU:HA	2:D:225:VAL:HG22	2.00	0.43
3:F:137:GLU:HB2	3:F:147:HIS:CE1	2.54	0.43
3:F:129:LYS:HB3	3:F:130:HIS:CD2	2.54	0.43
3:F:94:ASP:OD1	3:F:94:ASP:N	2.52	0.43
1:A:227:TYR:HB3	1:A:248:MET:HE2	2.01	0.43
2:C:339:ARG:NH2	2:C:551:GLU:O	2.52	0.43
1:B:70:ARG:HG3	1:B:72:ALA:H	1.83	0.42
1:A:234:MET:SD	1:A:241:PRO:HG3	2.60	0.42
3:E:36:GLN:H	3:E:36:GLN:HG2	1.61	0.42
3:E:185:MET:HE3	3:E:185:MET:HA	2.01	0.42
2:C:342:LEU:N	2:C:343:PRO:HD2	2.34	0.42
3:F:100:PRO:HG3	3:F:246:HIS:CD2	2.54	0.42
1:A:157:SER:HA	1:A:160:TYR:CD2	2.54	0.42
1:A:231:MET:SD	1:A:248:MET:HE1	2.59	0.42
1:B:231:MET:SD	1:B:248:MET:HE1	2.59	0.42
2:D:658:SER:HB2	2:D:667:MET:HG3	2.00	0.42
1:A:95:PHE:HD2	1:A:170:VAL:HG12	1.84	0.42
1:A:186:LEU:O	1:A:190:ILE:HG12	2.19	0.42
2:D:319:ARG:O	2:D:320:LEU:C	2.63	0.42
3:E:94:ASP:OD1	3:E:94:ASP:N	2.52	0.42
2:C:658:SER:HB2	2:C:667:MET:HG3	2.00	0.42
3:F:74:LYS:HD2	3:F:74:LYS:HA	1.79	0.42
2:D:598:ASP:OD1	2:D:636:TYR:OH	2.33	0.42
3:F:192:GLY:HA2	3:F:210:THR:HA	2.02	0.42
1:B:8:MET:HE2	1:B:8:MET:HB3	1.95	0.42
1:B:184:MET:O	1:B:187:THR:OG1	2.37	0.42
3:E:130:HIS:CE1	3:E:132:ARG:HB2	2.54	0.42
3:E:270:LYS:O	3:E:275:ARG:NH1	2.53	0.42
3:E:272:LEU:HD22	3:E:275:ARG:HH22	1.84	0.42
2:D:636:TYR:HA	2:D:641:PHE:HB2	2.03	0.41
3:E:275:ARG:NH2	3:E:276:GLN:HE22	2.15	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:MET:HB3	1:B:189:PHE:CE2	2.55	0.41
3:E:76:LYS:H	3:E:267:SER:HG	1.65	0.41
1:A:176:PHE:O	1:A:180:ILE:HG13	2.21	0.41
2:C:222:LEU:HA	2:C:225:VAL:HG22	2.01	0.41
2:C:622:ALA:HB1	2:C:630:ARG:HD2	2.02	0.41
1:A:180:ILE:O	1:A:183:THR:OG1	2.30	0.41
3:F:130:HIS:CE1	3:F:132:ARG:HB2	2.55	0.41
1:A:246:ARG:HB3	1:A:247:PRO:HD3	2.03	0.41
1:B:78:LEU:HD13	1:B:78:LEU:HA	1.94	0.41
3:F:68:ILE:HD13	3:F:68:ILE:HA	1.87	0.41
1:A:118:TRP:HA	1:A:121:GLU:HG2	2.03	0.41
1:A:146:PHE:O	1:A:147:LEU:C	2.63	0.41
3:E:101:ARG:NH1	3:E:189:TYR:OH	2.54	0.41
3:E:226:VAL:HG23	3:E:236:VAL:HG12	2.03	0.41
3:E:281:GLU:O	3:E:284:LEU:N	2.54	0.41
1:B:176:PHE:O	1:B:180:ILE:HG13	2.21	0.41
2:D:522:PHE:HB3	2:D:549:VAL:HG23	2.01	0.40
1:B:79:GLU:O	1:B:80:ARG:C	2.63	0.40
2:C:283:THR:HG22	2:C:284:PHE:N	2.37	0.40
1:A:102:ARG:HD2	1:A:102:ARG:HA	1.84	0.40
2:D:341:ARG:HA	2:D:592:ASN:HD21	1.87	0.40
3:E:137:GLU:HB2	3:E:147:HIS:CE1	2.56	0.40
2:C:525:LEU:HA	2:C:528:MET:HB2	2.04	0.40
2:C:636:TYR:HA	2:C:641:PHE:HB2	2.03	0.40
1:B:117:HIS:CE1	1:B:148:LEU:HD13	2.56	0.40
1:B:220:GLY:O	1:B:224:VAL:HG12	2.21	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	264/617 (43%)	248 (94%)	15 (6%)	1 (0%)	30	64
1	B	264/617 (43%)	252 (96%)	11 (4%)	1 (0%)	30	64
2	C	405/794 (51%)	391 (96%)	13 (3%)	1 (0%)	44	75
2	D	404/794 (51%)	390 (96%)	13 (3%)	1 (0%)	44	75
3	E	230/483 (48%)	209 (91%)	15 (6%)	6 (3%)	4	28
3	F	230/483 (48%)	219 (95%)	11 (5%)	0	100	100
4	G	1/3 (33%)	1 (100%)	0	0	100	100
4	H	1/3 (33%)	1 (100%)	0	0	100	100
All	All	1799/3794 (47%)	1711 (95%)	78 (4%)	10 (1%)	24	56

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	275	ARG
2	D	234	TYR
3	E	274	LEU
1	B	218	PHE
2	C	234	TYR
3	E	180	ASN
3	E	181	ILE
3	E	182	GLU
1	A	218	PHE
3	E	184	GLN

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	202/519 (39%)	199 (98%)	3 (2%)	60	77
1	B	202/519 (39%)	196 (97%)	6 (3%)	36	63
2	C	270/649 (42%)	267 (99%)	3 (1%)	70	83
2	D	269/649 (41%)	267 (99%)	2 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	201/433 (46%)	189 (94%)	12 (6%)	16	43
3	F	201/433 (46%)	200 (100%)	1 (0%)	86	93
4	G	1/1 (100%)	1 (100%)	0	100	100
4	H	1/1 (100%)	1 (100%)	0	100	100
All	All	1347/3204 (42%)	1320 (98%)	27 (2%)	52	72

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	TRP
1	A	189	PHE
1	A	246	ARG
2	D	245	MET
2	D	283	THR
3	E	179	LYS
3	E	182	GLU
3	E	184	GLN
3	E	258	ASP
3	E	275	ARG
3	E	276	GLN
3	E	277	LEU
3	E	278	GLU
3	E	282	GLU
3	E	283	ILE
3	E	284	LEU
3	E	285	ARG
1	B	78	LEU
1	B	80	ARG
1	B	82	TRP
1	B	99	PHE
1	B	110	LEU
1	B	189	PHE
2	C	283	THR
2	C	655[A]	ARG
2	C	655[B]	ARG
3	F	135	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	E	130	HIS
3	E	221	HIS
3	E	262	GLN
1	B	238	HIS
2	C	237	GLN
3	F	130	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 ⓘ

14 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	$\# Z > 2$
5	NAG	I	1	4,5	14,14,15	0.40	0	17,19,21	0.67	0
5	NAG	I	2	5	14,14,15	0.66	1 (7%)	17,19,21	0.82	0
5	MAN	I	3	5	11,11,12	1.17	1 (9%)	15,15,17	1.25	2 (13%)
5	MAN	I	4	5	11,11,12	0.82	1 (9%)	15,15,17	1.45	3 (20%)
5	MAN	I	5	5	11,11,12	1.41	3 (27%)	15,15,17	1.20	2 (13%)
5	MAN	I	6	5	11,11,12	0.92	0	15,15,17	1.30	2 (13%)
5	MAN	I	7	5	11,11,12	0.79	0	15,15,17	1.08	2 (13%)
5	NAG	J	1	4,5	14,14,15	0.38	0	17,19,21	0.66	0
5	NAG	J	2	5	14,14,15	0.60	0	17,19,21	0.81	0
5	MAN	J	3	5	11,11,12	1.15	2 (18%)	15,15,17	1.20	2 (13%)
5	MAN	J	4	5	11,11,12	0.82	1 (9%)	15,15,17	1.46	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	J	5	5	11,11,12	1.43	3 (27%)	15,15,17	1.18	2 (13%)
5	MAN	J	6	5	11,11,12	0.92	0	15,15,17	1.28	2 (13%)
5	MAN	J	7	5	11,11,12	0.74	0	15,15,17	1.07	2 (13%)

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	NAG	I	1	4,5	-	4/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
5	MAN	I	3	5	-	0/2/19/22	1/1/1/1
5	MAN	I	4	5	-	2/2/19/22	0/1/1/1
5	MAN	I	5	5	-	2/2/19/22	0/1/1/1
5	MAN	I	6	5	-	2/2/19/22	1/1/1/1
5	MAN	I	7	5	-	1/2/19/22	0/1/1/1
5	NAG	J	1	4,5	-	4/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
5	MAN	J	3	5	-	0/2/19/22	1/1/1/1
5	MAN	J	4	5	-	2/2/19/22	0/1/1/1
5	MAN	J	5	5	-	2/2/19/22	0/1/1/1
5	MAN	J	6	5	-	2/2/19/22	1/1/1/1
5	MAN	J	7	5	-	1/2/19/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	3	MAN	O5-C5	3.02	1.49	1.43
5	J	3	MAN	O5-C5	2.95	1.49	1.43
5	J	5	MAN	C2-C3	2.50	1.56	1.52
5	I	5	MAN	C2-C3	2.46	1.56	1.52
5	J	5	MAN	C1-C2	2.40	1.57	1.52
5	I	5	MAN	C1-C2	2.32	1.57	1.52
5	J	5	MAN	O5-C5	2.29	1.48	1.43
5	I	5	MAN	O5-C5	2.24	1.48	1.43
5	I	2	NAG	C1-C2	2.15	1.55	1.52
5	I	4	MAN	C1-C2	2.07	1.56	1.52
5	J	3	MAN	C1-C2	2.02	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	4	MAN	C1-C2	2.01	1.56	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	6	MAN	C1-O5-C5	3.80	117.33	112.19
5	J	6	MAN	C1-O5-C5	3.79	117.33	112.19
5	I	3	MAN	C1-O5-C5	3.28	116.64	112.19
5	J	4	MAN	C1-C2-C3	3.26	113.68	109.67
5	I	4	MAN	C1-C2-C3	3.23	113.64	109.67
5	I	5	MAN	C1-O5-C5	3.14	116.44	112.19
5	J	3	MAN	C1-O5-C5	3.13	116.43	112.19
5	J	5	MAN	C1-O5-C5	3.05	116.32	112.19
5	I	7	MAN	C1-O5-C5	2.65	115.78	112.19
5	J	7	MAN	C1-O5-C5	2.61	115.73	112.19
5	I	4	MAN	O2-C2-C3	-2.56	105.00	110.14
5	J	4	MAN	O2-C2-C3	-2.54	105.05	110.14
5	J	4	MAN	C1-O5-C5	2.38	115.42	112.19
5	J	3	MAN	O2-C2-C3	-2.35	105.42	110.14
5	I	4	MAN	C1-O5-C5	2.34	115.36	112.19
5	I	3	MAN	O2-C2-C3	-2.32	105.50	110.14
5	I	6	MAN	O2-C2-C3	-2.24	105.64	110.14
5	J	6	MAN	O2-C2-C3	-2.23	105.68	110.14
5	I	7	MAN	O2-C2-C3	-2.17	105.78	110.14
5	J	7	MAN	O2-C2-C3	-2.12	105.89	110.14
5	J	5	MAN	O2-C2-C3	-2.04	106.05	110.14
5	I	5	MAN	O2-C2-C3	-2.03	106.07	110.14

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	5	MAN	O5-C5-C6-O6
5	I	5	MAN	O5-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
5	J	5	MAN	C4-C5-C6-O6
5	I	4	MAN	O5-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
5	J	4	MAN	O5-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
5	I	5	MAN	C4-C5-C6-O6

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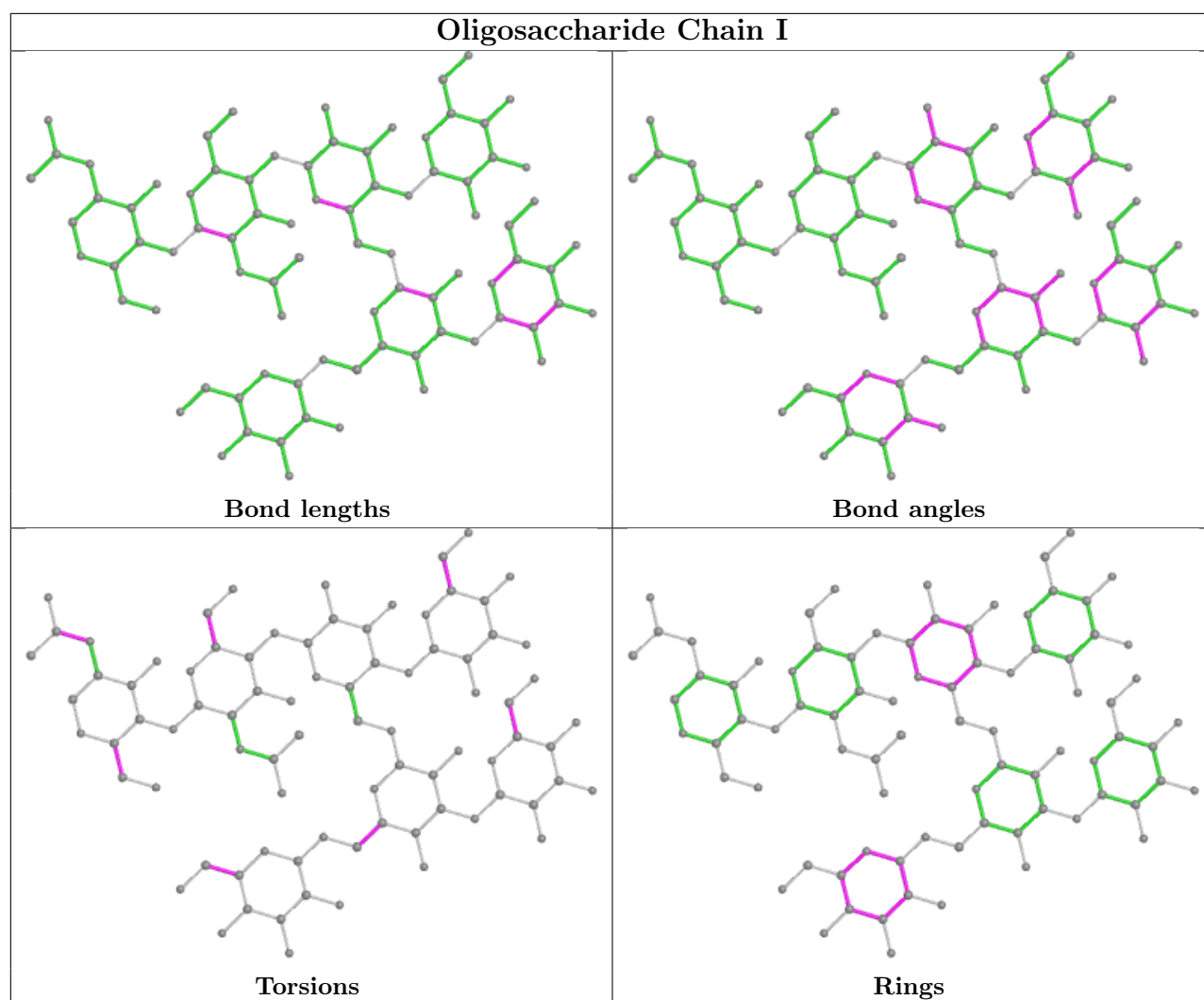
Mol	Chain	Res	Type	Atoms
5	I	1	NAG	C4-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
5	J	2	NAG	C4-C5-C6-O6
5	I	1	NAG	C8-C7-N2-C2
5	I	1	NAG	O7-C7-N2-C2
5	J	1	NAG	C8-C7-N2-C2
5	J	1	NAG	O7-C7-N2-C2
5	I	2	NAG	C4-C5-C6-O6
5	J	6	MAN	O5-C5-C6-O6
5	I	6	MAN	O5-C5-C6-O6
5	I	7	MAN	O5-C5-C6-O6
5	J	7	MAN	O5-C5-C6-O6
5	I	4	MAN	C4-C5-C6-O6
5	J	4	MAN	C4-C5-C6-O6
5	J	6	MAN	C4-C5-C6-O6
5	I	6	MAN	C4-C5-C6-O6

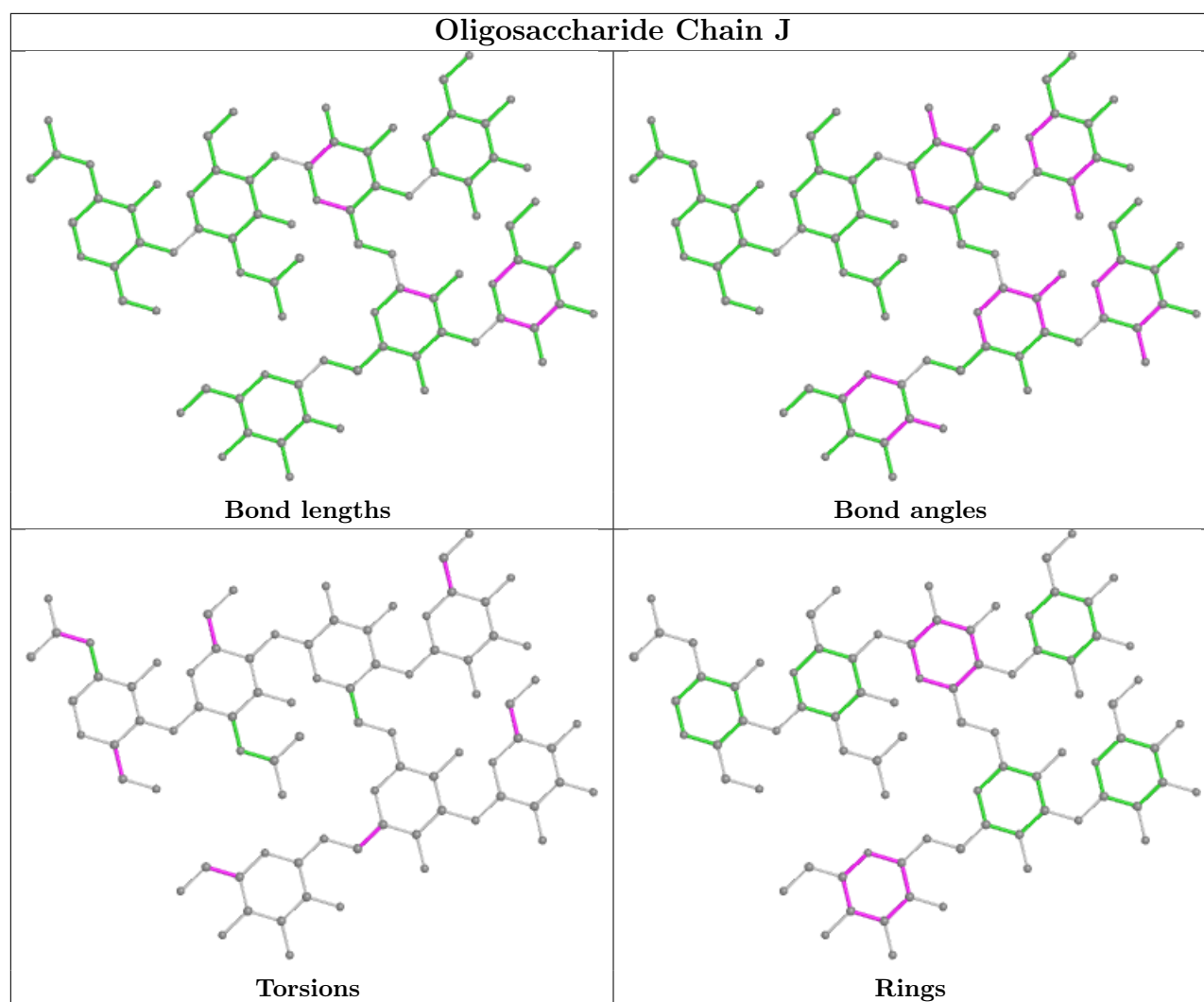
All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	6	MAN	C1-C2-C3-C4-C5-O5
5	I	6	MAN	C1-C2-C3-C4-C5-O5
5	I	3	MAN	C1-C2-C3-C4-C5-O5
5	J	3	MAN	C1-C2-C3-C4-C5-O5

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](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	C	801	2	14,14,15	0.48	0	17,19,21	0.47	0
6	NAG	D	803	2	14,14,15	0.86	1 (7%)	17,19,21	1.12	2 (11%)
6	NAG	C	802	2	14,14,15	0.31	0	17,19,21	0.49	0
6	NAG	D	802	2	14,14,15	0.30	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	C	803	2	14,14,15	0.89	1 (7%)	17,19,21	1.11	2 (11%)
6	NAG	D	801	2	14,14,15	0.46	0	17,19,21	0.39	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
6	NAG	C	801	2	-	2/6/23/26	0/1/1/1
6	NAG	D	803	2	-	3/6/23/26	0/1/1/1
6	NAG	C	802	2	-	2/6/23/26	0/1/1/1
6	NAG	D	802	2	-	2/6/23/26	0/1/1/1
6	NAG	C	803	2	-	3/6/23/26	0/1/1/1
6	NAG	D	801	2	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	803	NAG	C1-C2	2.74	1.56	1.52
6	D	803	NAG	C1-C2	2.67	1.56	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	803	NAG	C1-O5-C5	3.47	116.90	112.19
6	C	803	NAG	C1-O5-C5	3.40	116.80	112.19
6	C	803	NAG	C2-N2-C7	2.31	126.20	122.90
6	D	803	NAG	C2-N2-C7	2.27	126.14	122.90

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	801	NAG	C4-C5-C6-O6
6	D	801	NAG	C4-C5-C6-O6
6	D	803	NAG	C4-C5-C6-O6
6	C	803	NAG	C4-C5-C6-O6
6	C	801	NAG	O5-C5-C6-O6
6	D	803	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	C	803	NAG	O5-C5-C6-O6
6	D	801	NAG	O5-C5-C6-O6
6	C	802	NAG	C4-C5-C6-O6
6	D	802	NAG	C4-C5-C6-O6
6	D	802	NAG	O5-C5-C6-O6
6	C	802	NAG	O5-C5-C6-O6
6	D	803	NAG	C3-C2-N2-C7
6	C	803	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	803	NAG	1	0
6	C	803	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.

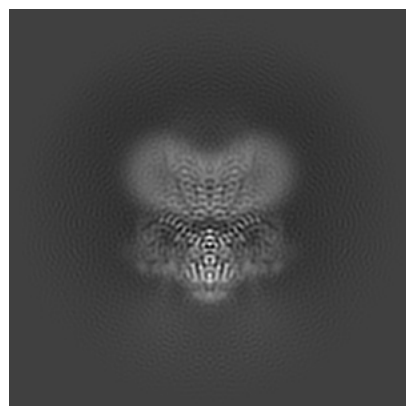
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63459. These allow visual inspection of the internal detail of the map and identification of artifacts.

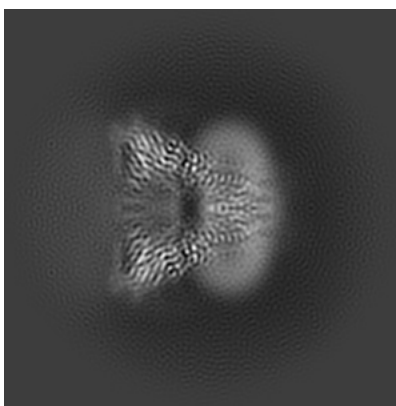
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

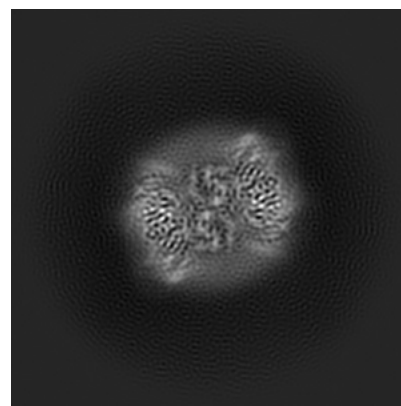
6.1.1 Primary map



X

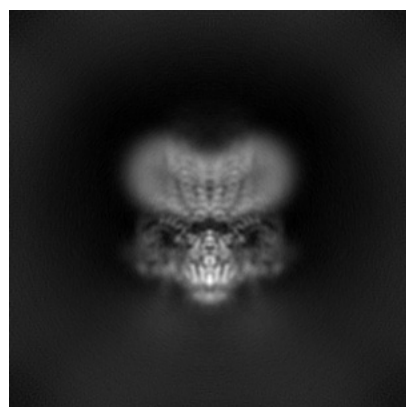


Y

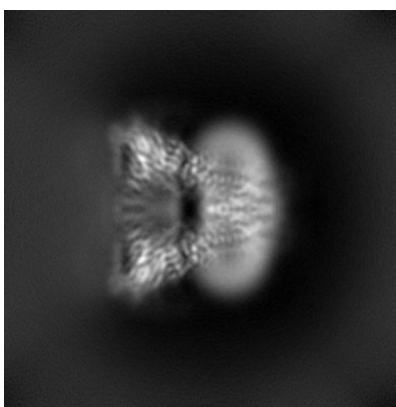


Z

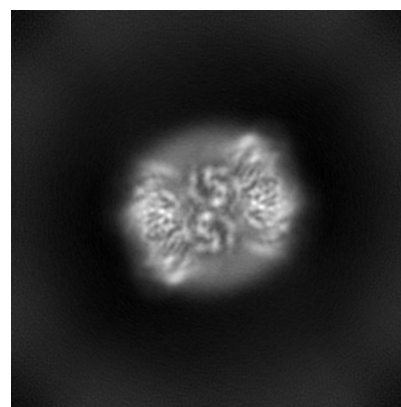
6.1.2 Raw map



X



Y

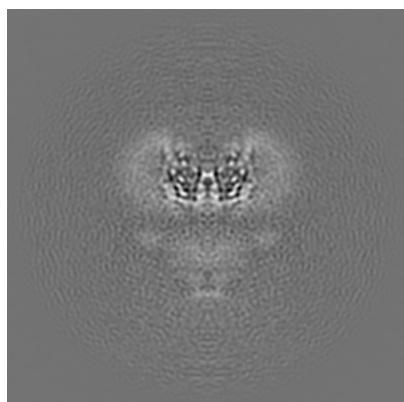


Z

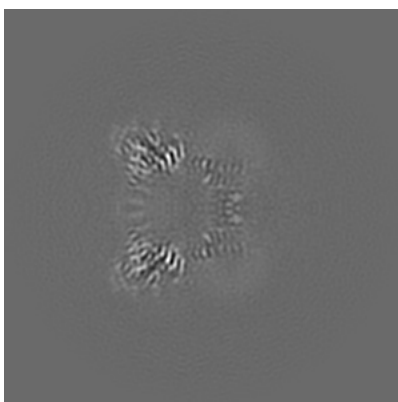
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

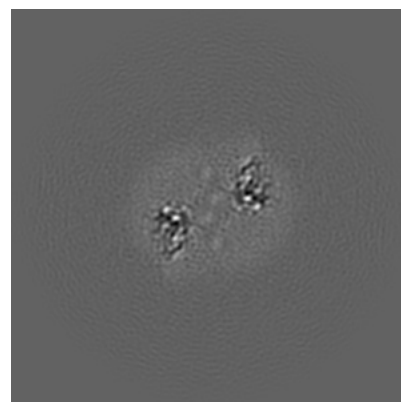
6.2.1 Primary map



X Index: 128

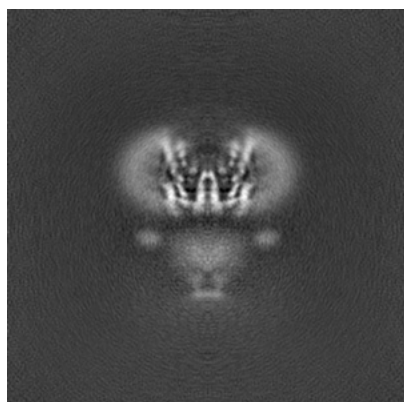


Y Index: 128

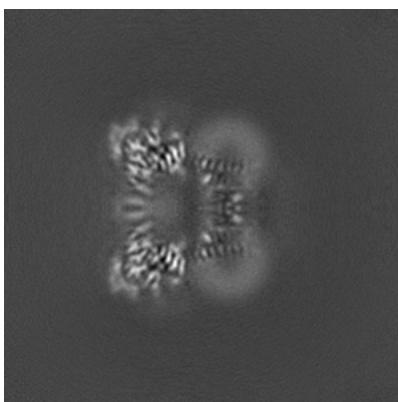


Z Index: 128

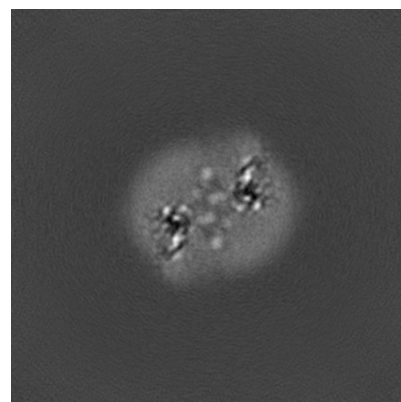
6.2.2 Raw map



X Index: 128



Y Index: 128

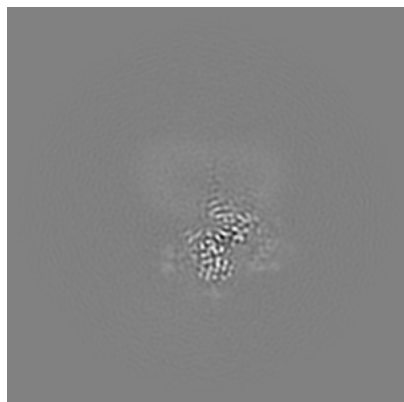


Z Index: 128

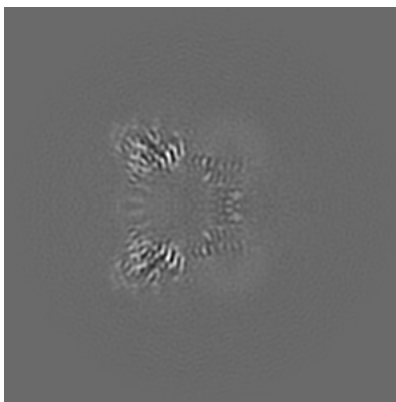
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

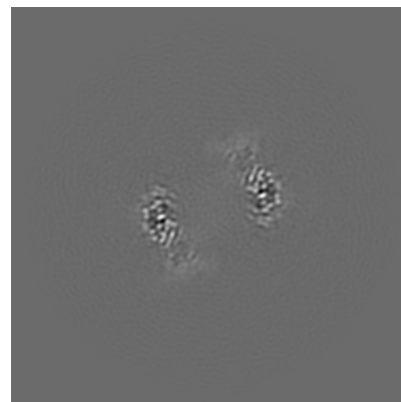
6.3.1 Primary map



X Index: 159

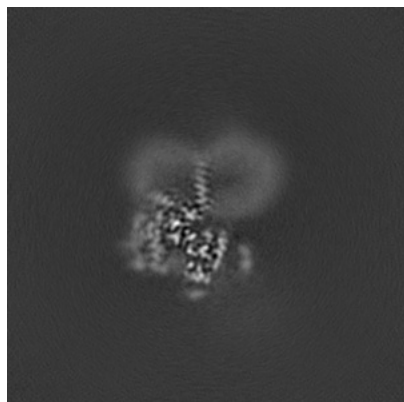


Y Index: 128

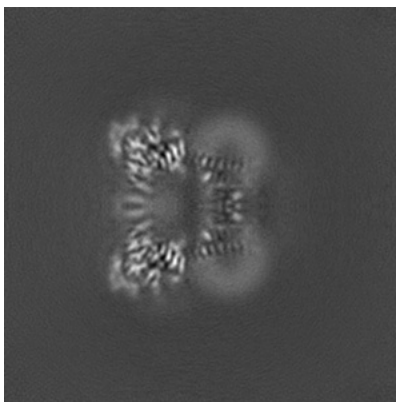


Z Index: 108

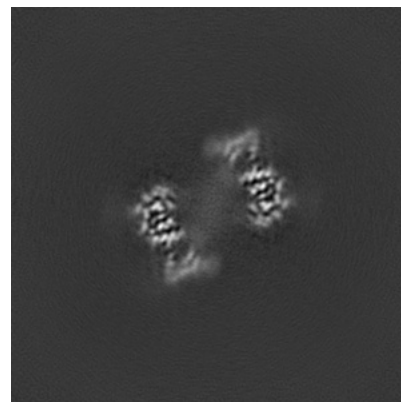
6.3.2 Raw map



X Index: 101



Y Index: 128

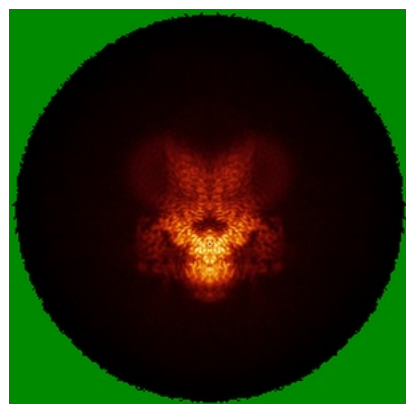


Z Index: 109

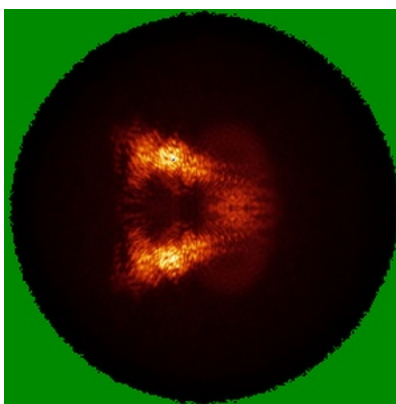
The images above show the largest variance slices of the map in three orthogonal directions.

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

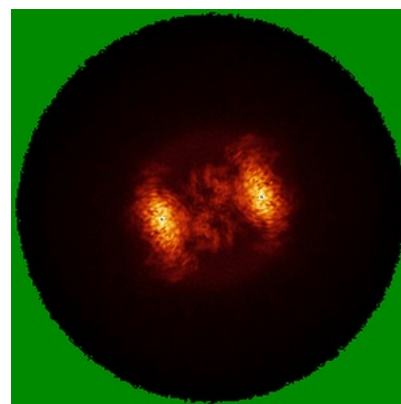
6.4.1 Primary map



X

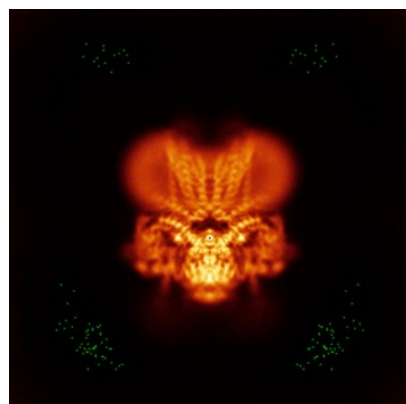


Y

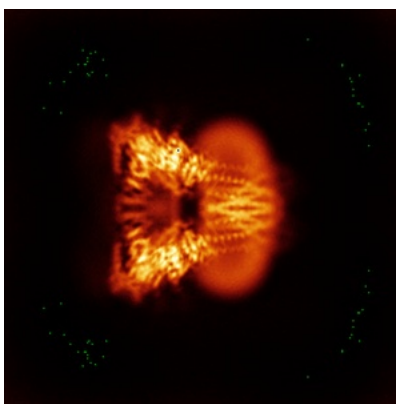


Z

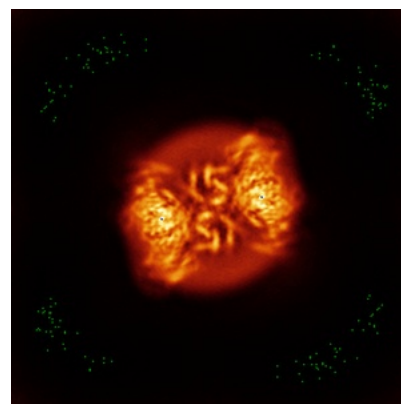
6.4.2 Raw map



X



Y

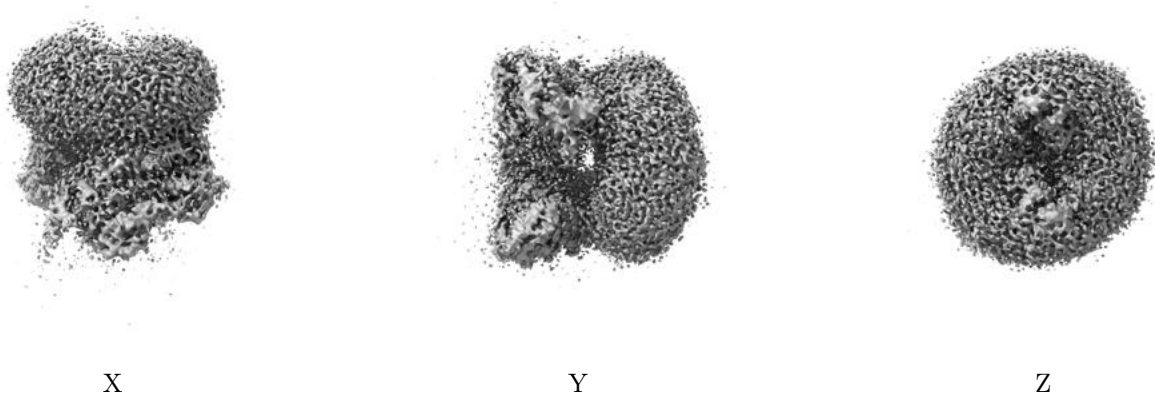


Z

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.

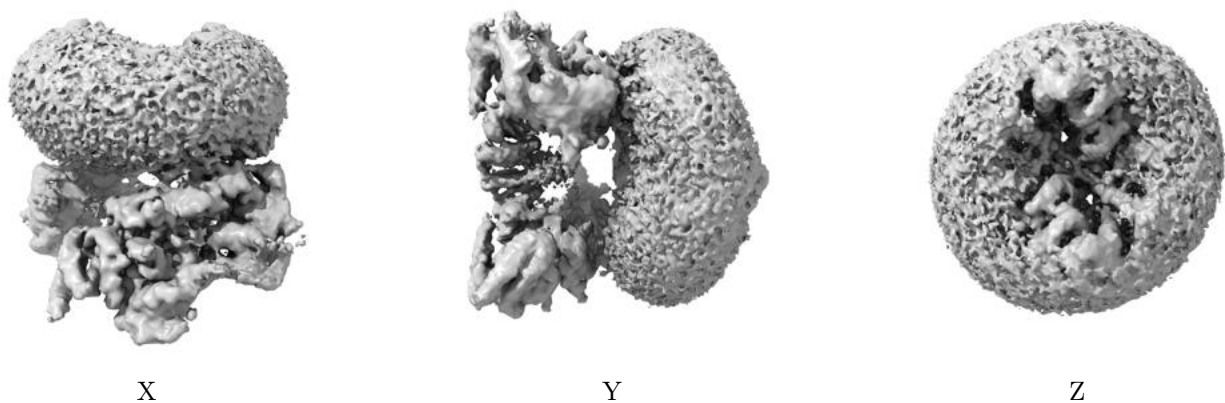
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.104. 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.

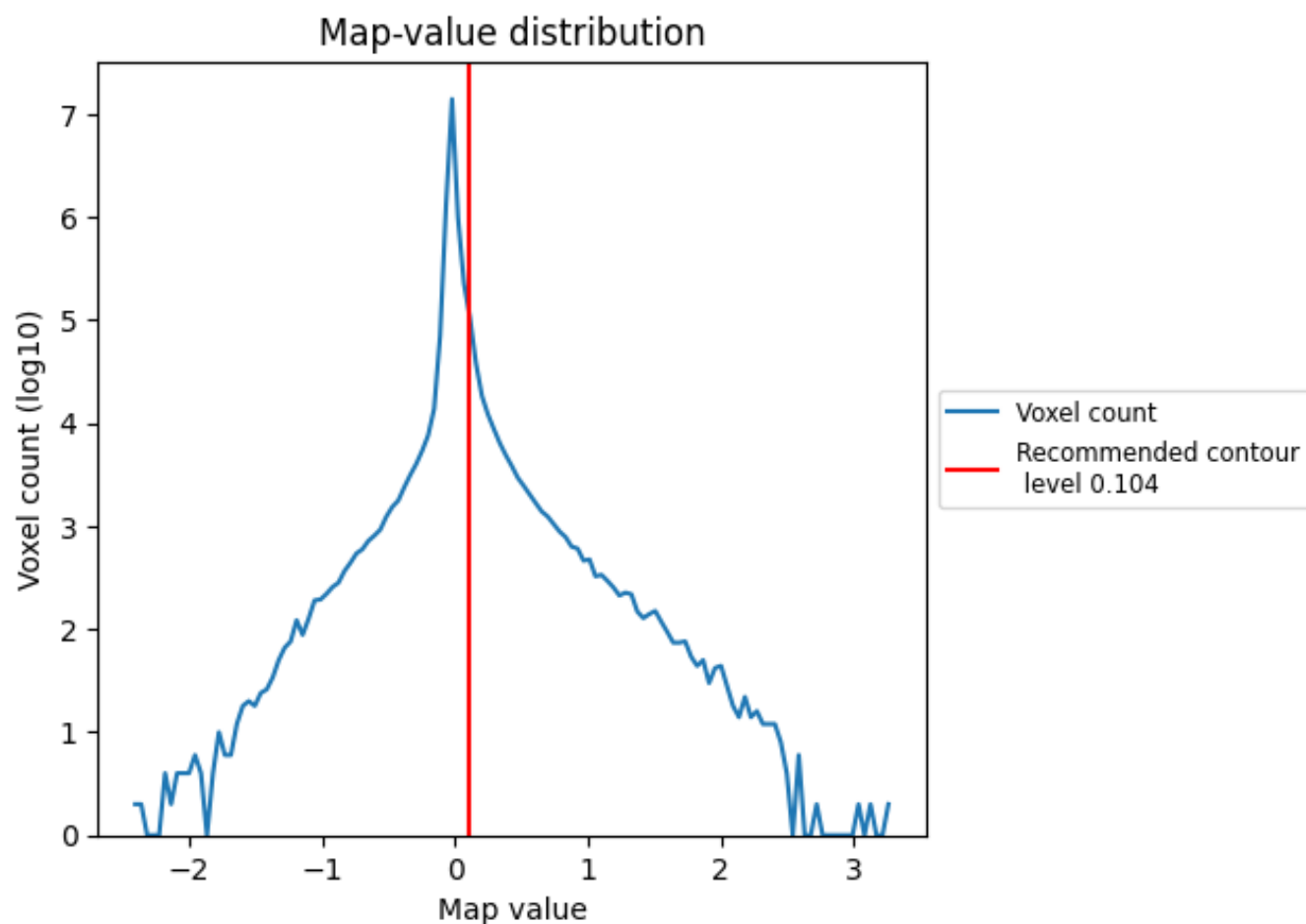
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

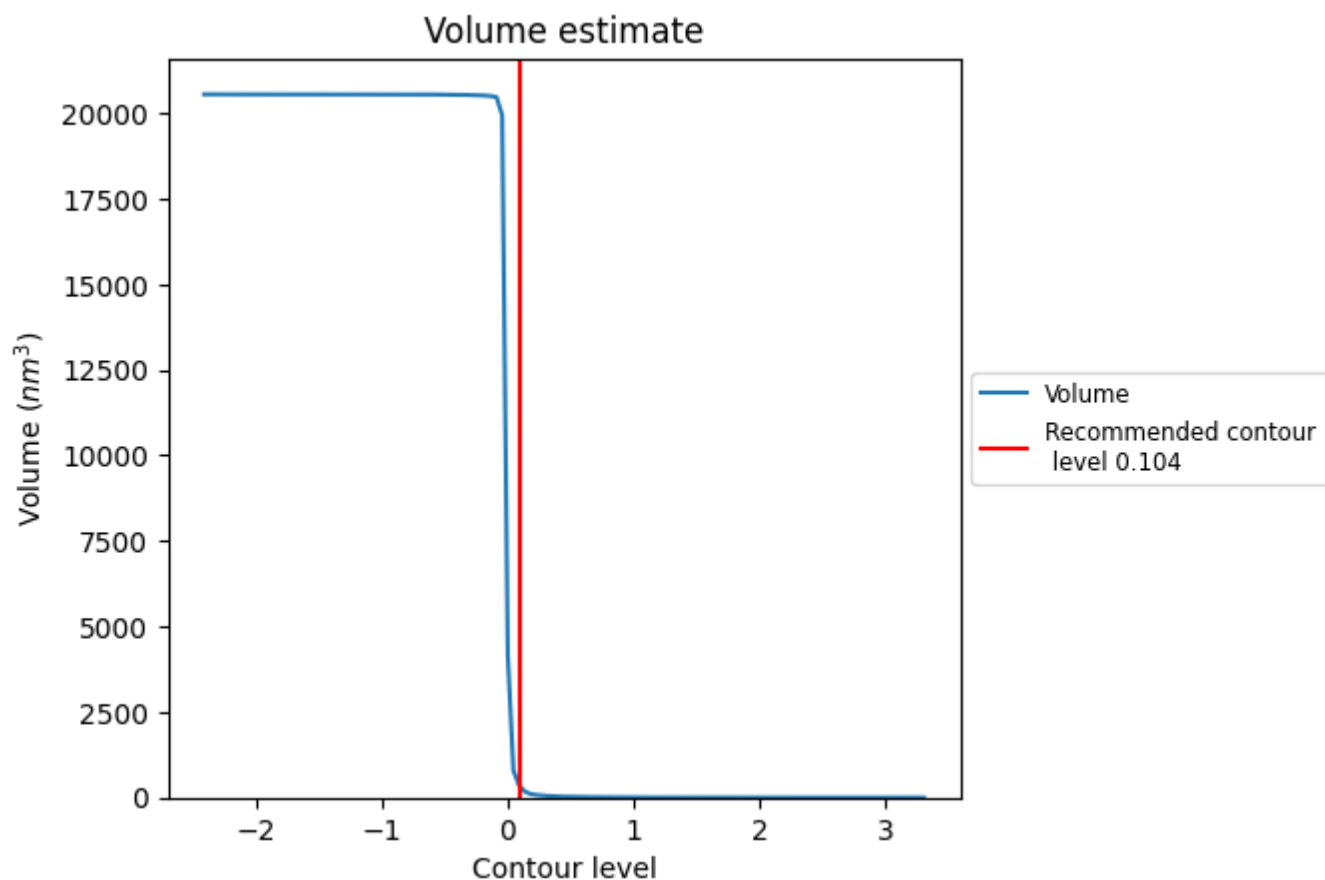
This section contains the results of statistical analysis of the map.

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.

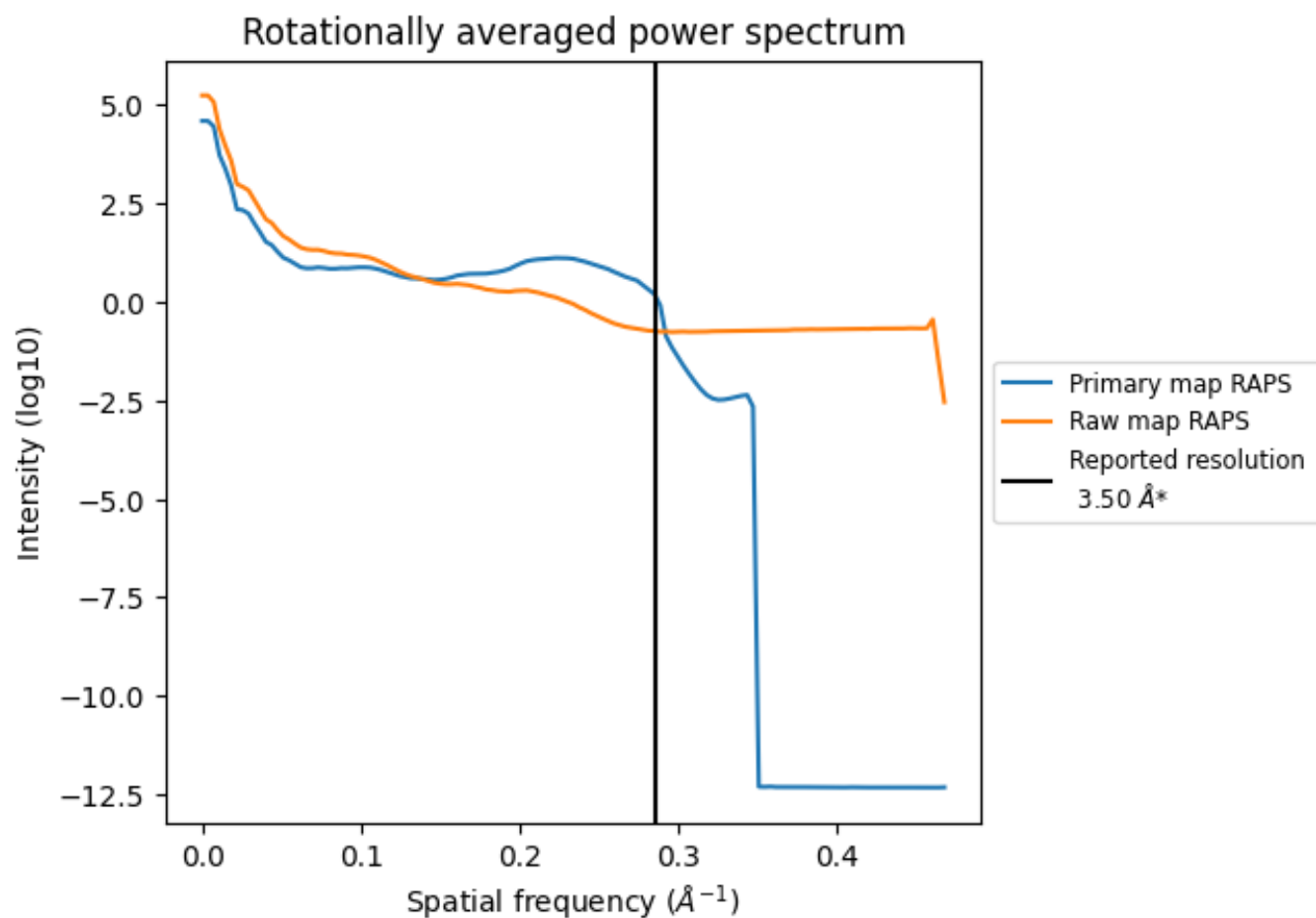
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 312 nm^3 ; this corresponds to an approximate mass of 282 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 ⓘ

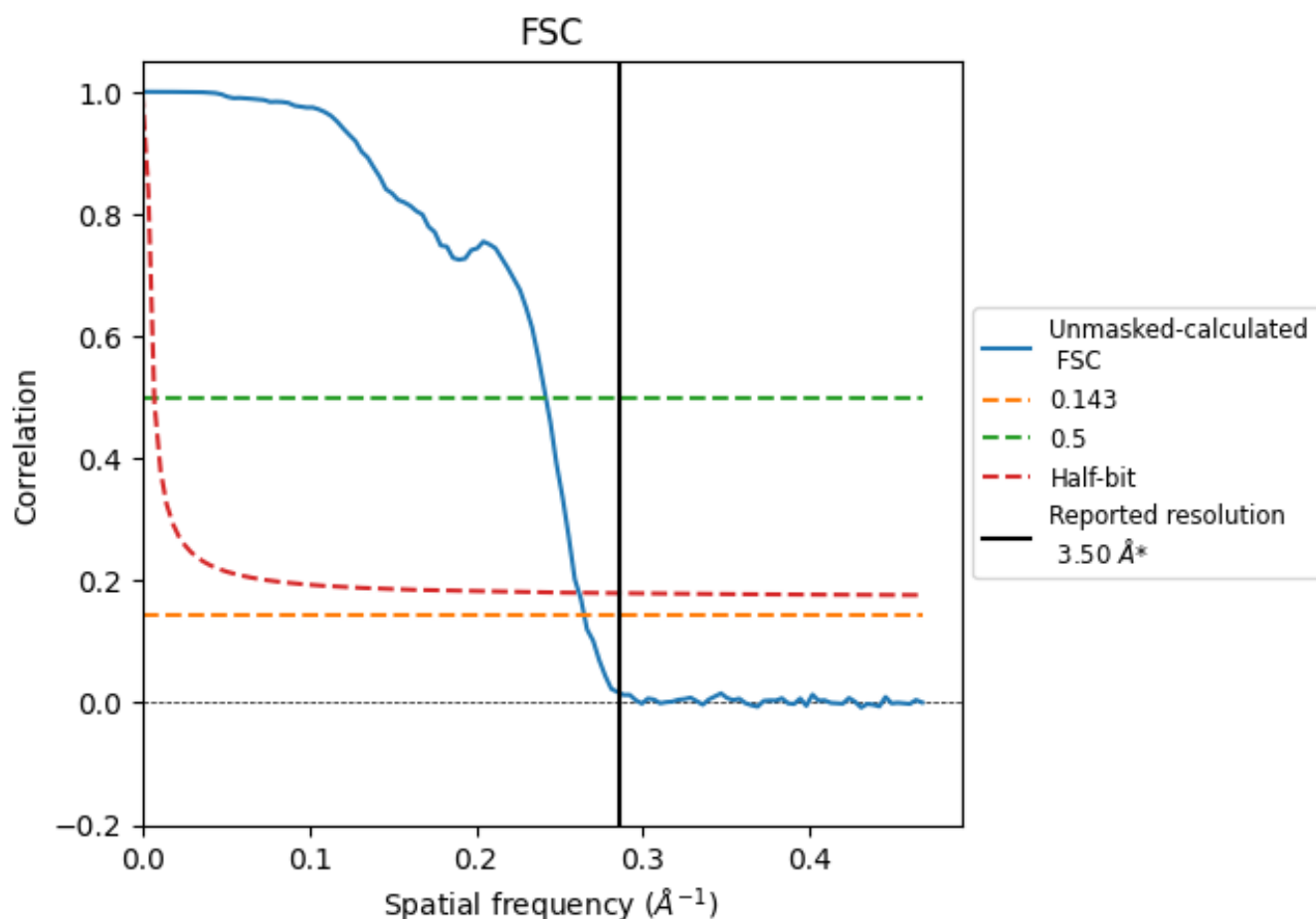


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 \AA^{-1}

8.2 Resolution estimates [i](#)

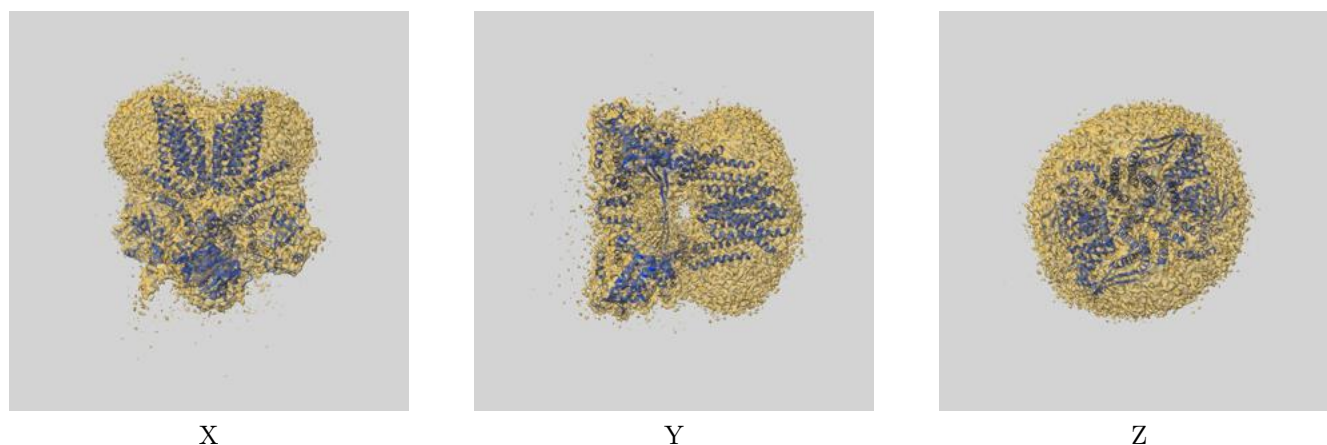
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.78	4.14	3.82

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

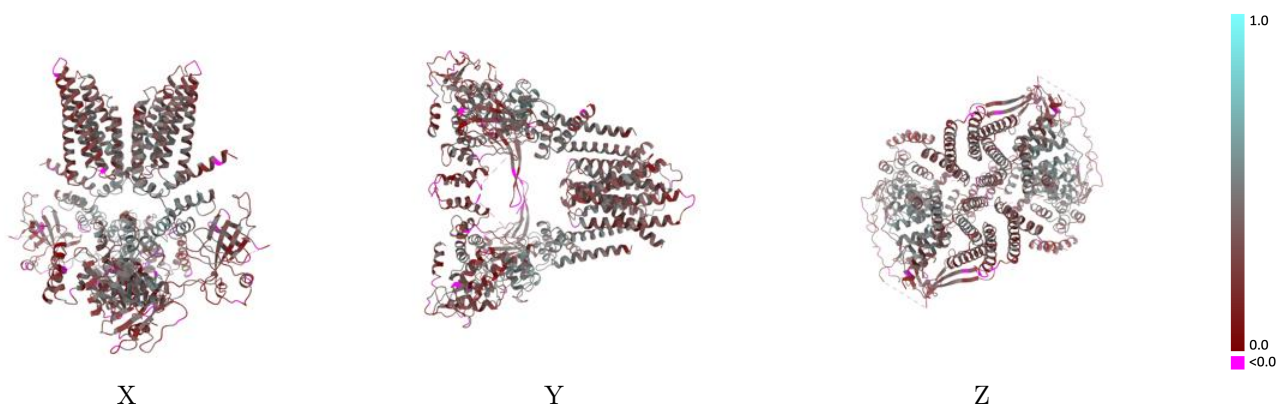
This section contains information regarding the fit between EMDB map EMD-63459 and PDB model 9LWU. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



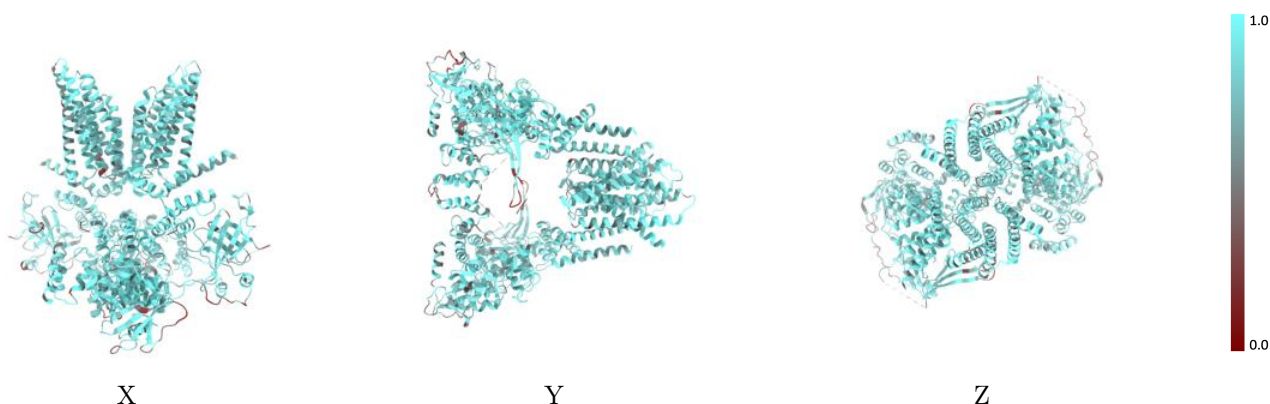
The images above show the 3D surface view of the map at the recommended contour level 0.104 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



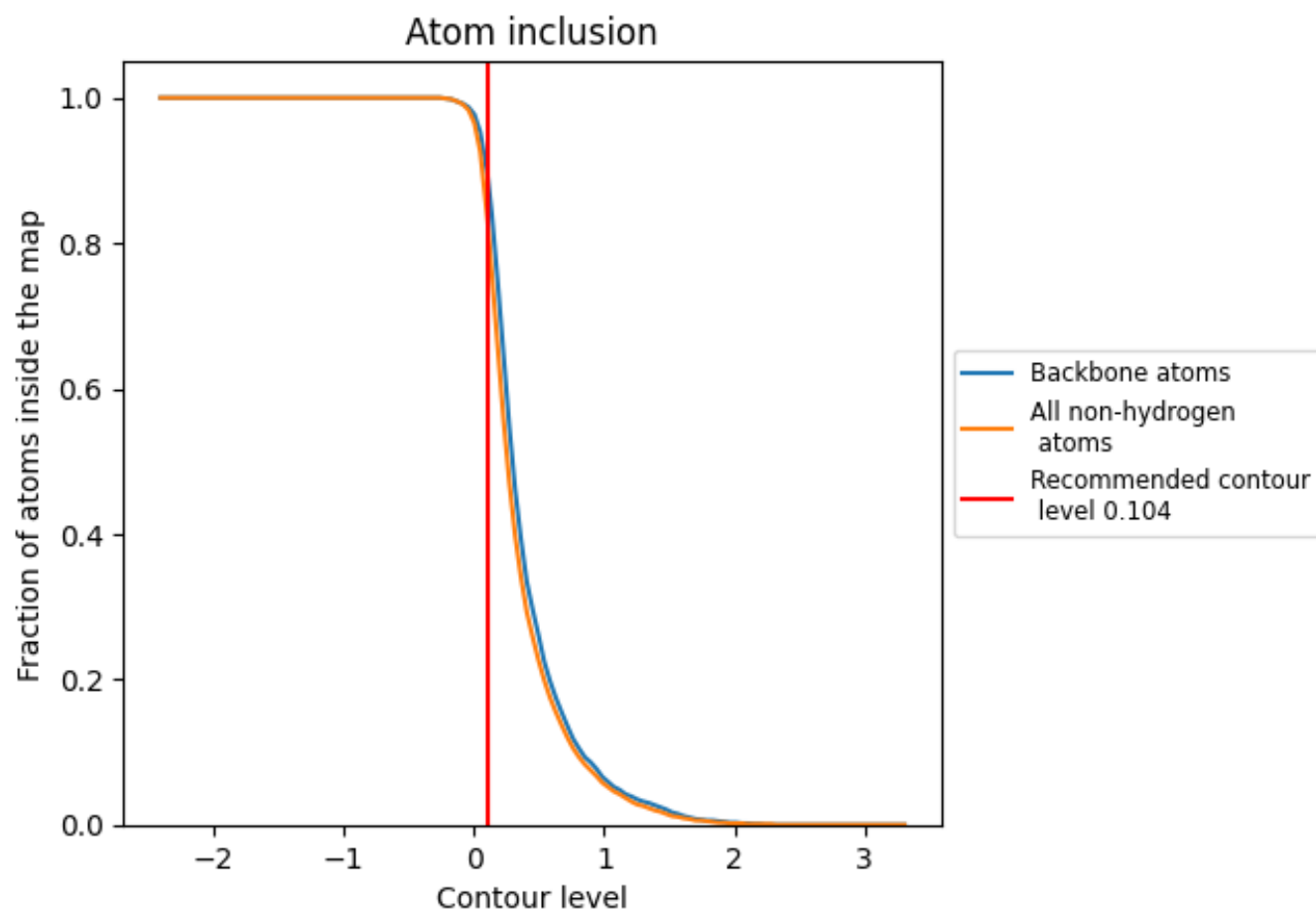
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.104).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 83% 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 (0.104) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8300	<div></div> 0.3380
A	<div></div> 0.8450	<div></div> 0.3500
B	<div></div> 0.8430	<div></div> 0.3480
C	<div></div> 0.8680	<div></div> 0.3840
D	<div></div> 0.8690	<div></div> 0.3860
E	<div></div> 0.7620	<div></div> 0.2550
F	<div></div> 0.7570	<div></div> 0.2530
G	<div></div> 0.1110	<div></div> -0.2130
H	<div></div> 0.1110	<div></div> -0.2380
I	<div></div> 0.7950	<div></div> 0.3200
J	<div></div> 0.7830	<div></div> 0.3030

1.0
0.0
<0.0