



Full wwPDB EM Validation Report ⓘ

Jun 29, 2025 – 12:03 am BST

PDB ID : 8PKO / pdb_00008pko
EMDB ID : EMD-17749
Title : The ERAD misfolded glycoprotein checkpoint complex from *Chaetomium thermophilum* (EDEM:PDI heterodimer).
Authors : Roversi, P.; Hitchman, C.J.; Lia, A.; Bayo, Y.
Deposited on : 2023-06-27
Resolution : 2.60 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 : 1.8.4, 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

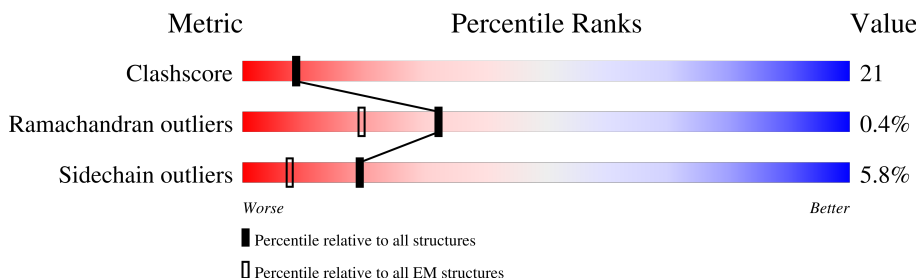
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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	1284	
2	B	507	
3	C	5	
3	E	5	
4	D	2	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11431 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 Green fluorescent protein,alpha-1,2-Mannosidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	972	Total	C	N	O	S	0	0
			7592	4838	1315	1418	21		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-182	MET	-	initiating methionine	UNP P42212
A	-181	VAL	-	expression tag	UNP P42212
A	-180	SER	-	expression tag	UNP P42212
A	-179	LYS	-	expression tag	UNP P42212
A	-178	GLY	-	expression tag	UNP P42212
A	-119	LEU	PHE	conflict	UNP P42212
A	-118	THR	SER	conflict	UNP P42212
A	48	LEU	HIS	conflict	UNP P42212
A	56	LEU	-	linker	UNP P42212
A	57	GLU	-	linker	UNP P42212
A	58	VAL	-	linker	UNP P42212
A	59	LEU	-	linker	UNP P42212
A	60	PHE	-	linker	UNP P42212
A	61	GLN	-	linker	UNP P42212
A	62	GLY	-	linker	UNP P42212
A	1093	GLY	-	expression tag	UNP G0SCX7
A	1094	THR	-	expression tag	UNP G0SCX7
A	1095	LYS	-	expression tag	UNP G0SCX7
A	1096	HIS	-	expression tag	UNP G0SCX7
A	1097	HIS	-	expression tag	UNP G0SCX7
A	1098	HIS	-	expression tag	UNP G0SCX7
A	1099	HIS	-	expression tag	UNP G0SCX7
A	1100	HIS	-	expression tag	UNP G0SCX7
A	1101	HIS	-	expression tag	UNP G0SCX7

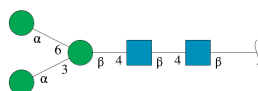
- Molecule 2 is a protein called Protein disulfide-isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	467	Total	C	N	O	S	0	0
			3641	2322	582	726	11		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	18	GLU	-	expression tag	UNP G0SGS2
B	19	THR	-	expression tag	UNP G0SGS2
B	20	GLY	-	expression tag	UNP G0SGS2
B	516	GLY	-	expression tag	UNP G0SGS2
B	517	THR	-	expression tag	UNP G0SGS2
B	518	LYS	-	expression tag	UNP G0SGS2
B	519	HIS	-	expression tag	UNP G0SGS2
B	520	HIS	-	expression tag	UNP G0SGS2
B	521	HIS	-	expression tag	UNP G0SGS2
B	522	HIS	-	expression tag	UNP G0SGS2
B	523	HIS	-	expression tag	UNP G0SGS2
B	524	HIS	-	expression tag	UNP G0SGS2

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	5	Total	C	N	O	0	0
			61	34	2	25		
3	E	5	Total	C	N	O	0	0
			61	34	2	25		

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

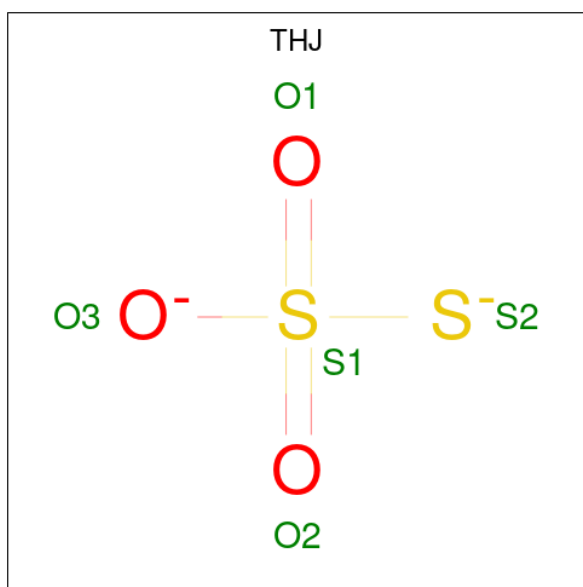


Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	

- Molecule 6 is THIOSULFATE (CCD ID: THJ) (formula: O₃S₂).



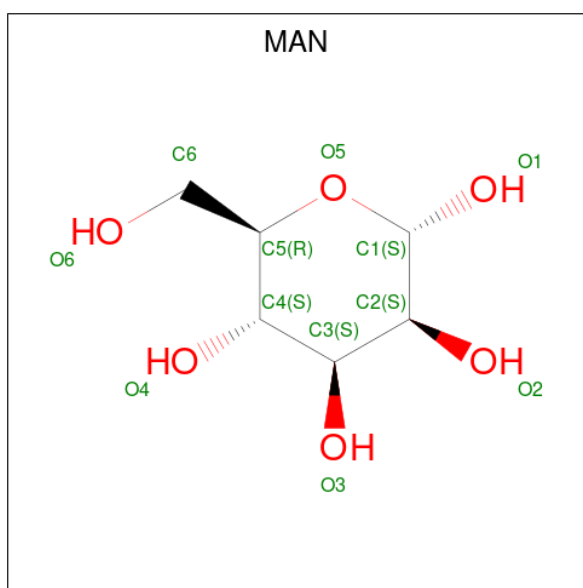
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	O	S	0
			5	3	2	

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 8 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$).



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

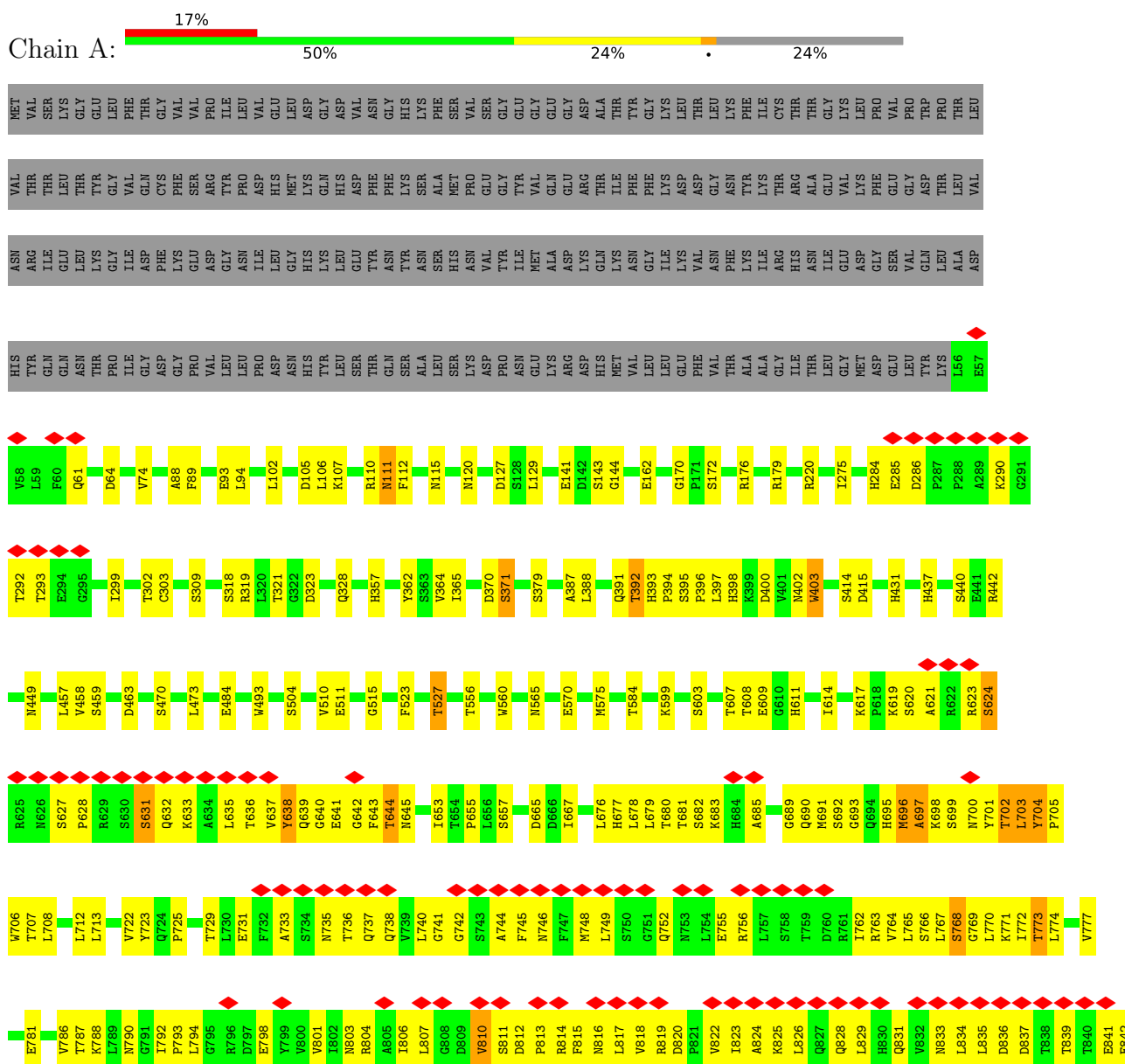
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		AltConf
9	A	3	Total 3	O 3	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: Green fluorescent protein, alpha-1,2-Mannosidase



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1400000	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 ($e^-/\text{\AA}^2$)	1	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.646	Depositor
Minimum map value	-0.310	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	250.5, 250.5, 250.5	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	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, CA, MAN, THJ, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.25	1/7801 (0.0%)	0.74	7/10644 (0.1%)
2	B	1.10	0/3716	0.69	2/5029 (0.0%)
All	All	1.20	1/11517 (0.0%)	0.73	9/15673 (0.1%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275	ILE	C-N	-7.47	1.27	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	ALA	CA-C-N	-7.24	104.13	121.80
1	A	88	ALA	C-N-CA	-7.24	104.13	121.80
1	A	631	SER	CB-CA-C	-5.92	108.75	115.79
2	B	210	THR	CA-C-N	5.86	132.24	121.70
2	B	210	THR	C-N-CA	5.86	132.24	121.70
1	A	685	ALA	CB-CA-C	-5.74	108.97	115.79
1	A	696	MET	CA-CB-CG	5.63	125.37	114.10
1	A	120	ASN	CA-C-N	-5.61	112.33	122.54
1	A	120	ASN	C-N-CA	-5.61	112.33	122.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	703	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	7592	0	7444	325	0
2	B	3641	0	3590	144	0
3	C	61	0	52	0	0
3	E	61	0	52	0	0
4	D	28	0	25	2	0
5	A	1	0	0	0	0
6	A	5	0	0	0	0
7	A	14	0	13	1	0
7	B	14	0	13	0	0
8	A	11	0	7	0	0
9	A	3	0	0	1	0
All	All	11431	0	11196	466	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 21.

All (466) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:GLU:HB3	1:A:763:ARG:HB3	1.54	0.89
1:A:700:ASN:ND2	1:A:708:LEU:O	2.06	0.88
1:A:763:ARG:HD3	1:A:804:ARG:HH12	1.38	0.87
1:A:608:THR:OG1	9:A:1301:HOH:O	1.93	0.86
2:B:134:THR:N	2:B:137:THR:OG1	2.08	0.86
1:A:917:ILE:HB	1:A:1046:MET:HB2	1.55	0.85
1:A:823:ILE:HG13	1:A:1068:ARG:HE	1.40	0.83
2:B:362:ALA:H	2:B:421:ASN:HD22	1.22	0.83
1:A:801:VAL:HG22	1:A:1082:ILE:HG12	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:LYS:NZ	2:B:173:ASP:O	2.15	0.79
1:A:623:ARG:NH2	4:D:1:NAG:O6	2.16	0.79
1:A:744:ALA:H	1:A:767:LEU:H	1.29	0.78
1:A:986:SER:O	1:A:990:LYS:NZ	2.19	0.76
1:A:973:ARG:NH2	1:A:998:THR:O	2.20	0.75
1:A:61:GLN:HB3	1:A:64:ASP:HB3	1.69	0.74
1:A:752:GLN:HG2	1:A:764:VAL:HA	1.69	0.74
2:B:375:ASP:N	2:B:375:ASP:OD2	2.16	0.74
1:A:290:LYS:HD2	1:A:292:THR:H	1.53	0.74
1:A:835:LEU:O	1:A:1056:GLN:NE2	2.20	0.74
1:A:972:PRO:HB2	1:A:1004:LEU:HD21	1.68	0.74
1:A:318:SER:OG	1:A:323:ASP:O	2.06	0.73
1:A:771:LYS:HB2	1:A:790:ASN:H	1.53	0.73
1:A:733:ALA:O	1:A:737:GLN:NE2	2.22	0.73
1:A:834:LEU:HB2	1:A:1056:GLN:HG2	1.69	0.73
2:B:472:GLU:HA	2:B:475:GLU:HB3	1.70	0.73
2:B:367:ASP:N	2:B:367:ASP:OD1	2.21	0.73
1:A:644:THR:HG23	1:A:645:ASN:H	1.55	0.71
1:A:819:ARG:HD3	1:A:1069:TYR:HB2	1.72	0.71
1:A:106:LEU:H	1:A:106:LEU:HD12	1.55	0.71
2:B:138:LEU:O	2:B:142:LYS:HB3	1.91	0.71
1:A:828:GLN:HA	1:A:1063:ILE:HA	1.73	0.70
2:B:84:GLU:OE1	2:B:84:GLU:N	2.15	0.70
2:B:139:GLU:OE1	2:B:139:GLU:N	2.21	0.70
1:A:744:ALA:HB3	1:A:766:SER:HA	1.72	0.70
1:A:1016:GLU:HB3	1:A:1021:LEU:HA	1.74	0.69
1:A:770:LEU:HD12	1:A:790:ASN:HD21	1.57	0.69
1:A:667:ILE:O	1:A:704:TYR:OH	2.07	0.68
2:B:127:LEU:O	2:B:172:ARG:NH2	2.26	0.68
1:A:143:SER:OG	1:A:144:GLY:N	2.27	0.67
2:B:311:LYS:HG3	2:B:313:GLN:HE21	1.58	0.67
2:B:92:GLU:N	2:B:92:GLU:OE1	2.27	0.67
2:B:153:VAL:O	2:B:181:SER:OG	2.10	0.67
2:B:131:SER:OG	2:B:132:ASP:N	2.27	0.67
2:B:471:SER:OG	2:B:472:GLU:N	2.24	0.67
1:A:822:VAL:HG13	1:A:823:ILE:HG12	1.77	0.66
1:A:748:MET:HE1	1:A:765:LEU:H	1.59	0.66
2:B:166:LYS:C	2:B:170:LYS:HZ2	2.04	0.66
2:B:167:VAL:HA	2:B:170:LYS:HG2	1.76	0.66
2:B:170:LYS:HB2	2:B:171:LEU:HD22	1.78	0.66
1:A:738:GLN:NE2	1:A:767:LEU:HD21	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:LEU:HB3	1:A:1062:ALA:HB3	1.77	0.66
1:A:956:ILE:HG23	1:A:977:VAL:HB	1.78	0.66
1:A:957:TYR:HA	1:A:975:ASN:HD22	1.61	0.65
2:B:40:LEU:HD21	2:B:72:ILE:HD12	1.79	0.65
1:A:619:LYS:O	1:A:623:ARG:N	2.23	0.65
1:A:925:ALA:HB2	1:A:1041:PRO:HB2	1.78	0.65
2:B:140:GLU:HA	2:B:143:LYS:HG2	1.76	0.65
2:B:196:ILE:HD11	2:B:221:TRP:HE1	1.61	0.65
1:A:763:ARG:HD3	1:A:804:ARG:NH1	2.11	0.65
1:A:1030:GLN:NE2	1:A:1042:ILE:O	2.30	0.64
1:A:689:GLY:HA3	1:A:700:ASN:HB2	1.79	0.64
1:A:999:PRO:HD3	1:A:1040:HIS:HB2	1.79	0.64
2:B:253:ALA:HB3	2:B:259:ARG:HG2	1.79	0.64
1:A:677:HIS:HB2	1:A:696:MET:HB2	1.79	0.64
1:A:1007:VAL:HG21	1:A:1042:ILE:HG23	1.80	0.64
1:A:1046:MET:HE3	1:A:1046:MET:HA	1.80	0.63
1:A:676:LEU:O	1:A:680:THR:OG1	2.09	0.63
1:A:1068:ARG:HB2	1:A:1083:VAL:HG11	1.79	0.63
2:B:294:LEU:HA	2:B:314:LYS:HG2	1.79	0.63
1:A:955:THR:HA	1:A:1061:SER:HA	1.80	0.63
2:B:173:ASP:OD1	2:B:173:ASP:N	2.23	0.63
1:A:738:GLN:HE22	1:A:767:LEU:HD21	1.62	0.62
1:A:640:GLY:O	1:A:644:THR:N	2.27	0.62
1:A:400:ASP:HB3	1:A:402:ASN:OD1	1.99	0.62
1:A:956:ILE:HG21	1:A:1057:LEU:HB3	1.82	0.62
1:A:956:ILE:HB	1:A:1057:LEU:O	2.00	0.61
2:B:101:ARG:HB2	2:B:105:ASN:HB3	1.81	0.61
1:A:292:THR:HG22	1:A:293:THR:HG23	1.80	0.61
1:A:807:LEU:HA	1:A:810:VAL:HG23	1.82	0.61
2:B:310:THR:OG1	2:B:311:LYS:NZ	2.28	0.61
2:B:134:THR:HG22	2:B:135:LYS:H	1.64	0.61
2:B:318:ASP:OD1	2:B:318:ASP:N	2.33	0.61
1:A:633:LYS:NZ	1:A:636:THR:OG1	2.34	0.61
1:A:835:LEU:HG	1:A:836:ASP:H	1.64	0.61
2:B:84:GLU:H	2:B:84:GLU:CD	2.08	0.61
1:A:110:ARG:O	1:A:112:PHE:N	2.34	0.61
1:A:961:GLU:HG2	1:A:981:ARG:HB2	1.83	0.60
1:A:387:ALA:HB1	1:A:627:SER:HB2	1.83	0.60
1:A:655:PRO:O	1:A:657:SER:N	2.34	0.60
2:B:37:SER:OG	2:B:38:ASN:ND2	2.35	0.60
2:B:151:ALA:HA	2:B:196:ILE:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:LEU:HD11	1:A:946:VAL:HG11	1.83	0.60
1:A:61:GLN:HB3	1:A:64:ASP:CB	2.32	0.60
1:A:756:ARG:HA	1:A:762:ILE:HA	1.84	0.60
2:B:211:GLU:CD	2:B:212:LYS:H	2.09	0.60
1:A:624:SER:HB2	2:B:478:ALA:HB1	1.83	0.59
1:A:786:VAL:O	1:A:1080:ASN:ND2	2.30	0.59
1:A:953:TRP:HE1	1:A:1005:GLN:HB3	1.67	0.59
2:B:346:SER:HB2	2:B:362:ALA:HB3	1.83	0.59
1:A:107:LYS:HE2	1:A:107:LYS:HA	1.83	0.59
1:A:633:LYS:HE2	1:A:635:LEU:H	1.67	0.59
1:A:620:SER:O	1:A:624:SER:OG	2.20	0.59
2:B:259:ARG:NH1	2:B:283:ASP:OD1	2.36	0.59
2:B:450:ASN:O	2:B:452:SER:N	2.36	0.59
1:A:395:SER:HA	1:A:398:HIS:CE1	2.38	0.59
2:B:397:GLU:OE2	2:B:400:ARG:NH2	2.23	0.59
2:B:273:THR:HG22	2:B:276:LYS:HB2	1.82	0.59
1:A:309:SER:OG	1:A:371:SER:HB2	2.03	0.59
1:A:638:TYR:HD2	1:A:639:GLN:H	1.51	0.59
1:A:696:MET:SD	2:B:54:LYS:HG3	2.42	0.59
1:A:763:ARG:HD2	1:A:764:VAL:H	1.68	0.58
1:A:94:LEU:HD23	1:A:575:MET:HE2	1.85	0.58
1:A:655:PRO:C	1:A:657:SER:H	2.10	0.58
1:A:1068:ARG:HD2	1:A:1083:VAL:HG21	1.85	0.58
2:B:134:THR:O	2:B:137:THR:OG1	2.22	0.58
2:B:42:LEU:HB3	2:B:74:LEU:HD22	1.85	0.58
2:B:381:TYR:HB2	2:B:388:CYS:SG	2.43	0.58
1:A:745:PHE:HB3	1:A:768:SER:O	2.04	0.58
1:A:973:ARG:HH21	1:A:997:PHE:HD2	1.52	0.57
1:A:744:ALA:O	1:A:768:SER:N	2.37	0.57
2:B:200:LYS:NZ	2:B:225:ALA:O	2.23	0.57
1:A:828:GLN:HE22	1:A:831:GLN:H	1.50	0.57
1:A:696:MET:SD	1:A:696:MET:O	2.62	0.57
1:A:1000:SER:H	1:A:1003:SER:HB3	1.70	0.57
1:A:980:ILE:HB	1:A:1009:VAL:HG13	1.87	0.57
2:B:59:GLU:OE2	2:B:114:LYS:HA	2.05	0.57
2:B:209:PHE:HB2	2:B:221:TRP:CE2	2.40	0.57
1:A:392:THR:O	1:A:392:THR:OG1	2.15	0.57
1:A:834:LEU:HD12	1:A:1056:GLN:HA	1.86	0.57
1:A:1030:GLN:O	1:A:1031:HIS:ND1	2.38	0.57
1:A:955:THR:O	1:A:976:GLN:N	2.34	0.56
1:A:825:LYS:H	1:A:1066:GLN:HE22	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:960:GLY:O	1:A:981:ARG:N	2.34	0.56
1:A:370:ASP:N	1:A:370:ASP:OD1	2.35	0.56
2:B:372:ASP:H	2:B:441:LYS:HE3	1.70	0.56
1:A:756:ARG:HB2	1:A:762:ILE:HG23	1.88	0.56
2:B:346:SER:OG	2:B:347:GLU:O	2.22	0.56
1:A:744:ALA:N	1:A:767:LEU:H	2.01	0.56
1:A:1054:TYR:O	1:A:1058:SER:OG	2.23	0.56
1:A:828:GLN:HE22	1:A:831:GLN:N	2.04	0.56
1:A:609:GLU:O	1:A:609:GLU:HG3	2.06	0.56
1:A:681:THR:OG1	1:A:695:HIS:N	2.40	0.55
2:B:163:VAL:HA	2:B:166:LYS:HE3	1.87	0.55
1:A:639:GLN:HB3	1:A:643:PHE:N	2.21	0.55
2:B:204:GLU:CD	2:B:204:GLU:H	2.15	0.55
1:A:1016:GLU:HG2	1:A:1022:VAL:H	1.71	0.55
2:B:320:ASP:OD1	2:B:320:ASP:N	2.34	0.55
1:A:927:LEU:HD11	1:A:1065:ILE:HG21	1.88	0.55
1:A:979:LEU:HD11	1:A:1054:TYR:HA	1.89	0.55
2:B:166:LYS:NZ	2:B:215:GLU:HB2	2.22	0.55
1:A:934:SER:HB2	1:A:1066:GLN:HB3	1.87	0.55
2:B:65:THR:OG1	2:B:66:ASN:ND2	2.40	0.55
1:A:639:GLN:HB3	1:A:642:GLY:C	2.32	0.55
2:B:191:VAL:HG13	2:B:195:ALA:HB3	1.88	0.55
1:A:825:LYS:H	1:A:1066:GLN:NE2	2.05	0.55
1:A:923:GLY:HA2	1:A:1029:ILE:HG12	1.88	0.55
1:A:811:SER:HB2	1:A:814:ARG:HG3	1.88	0.55
1:A:982:ARG:HB3	1:A:1011:SER:HA	1.89	0.54
1:A:89:PHE:CD1	1:A:89:PHE:C	2.83	0.54
1:A:641:GLU:HA	1:A:644:THR:O	2.07	0.54
1:A:955:THR:O	1:A:975:ASN:HB3	2.07	0.54
2:B:18:GLU:HG2	2:B:20:GLY:H	1.72	0.54
2:B:310:THR:OG1	2:B:311:LYS:N	2.39	0.54
1:A:923:GLY:HA2	1:A:1029:ILE:HA	1.90	0.54
1:A:653:ILE:HD12	1:A:653:ILE:O	2.07	0.54
1:A:803:ASN:O	1:A:807:LEU:HD12	2.07	0.54
1:A:987:PHE:HE1	1:A:1009:VAL:HG11	1.73	0.54
1:A:971:ALA:HA	1:A:974:GLU:HG3	1.90	0.54
1:A:631:SER:OG	1:A:632:GLN:N	2.40	0.53
1:A:700:ASN:O	1:A:703:LEU:HB2	2.07	0.53
1:A:504:SER:HB2	1:A:511:GLU:HG3	1.90	0.53
1:A:744:ALA:HB1	1:A:748:MET:HB3	1.90	0.53
1:A:994:ILE:O	1:A:1038:ARG:NH2	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1003:SER:OG	1:A:1004:LEU:N	2.40	0.53
2:B:351:GLU:OE1	2:B:351:GLU:N	2.34	0.53
1:A:1052:THR:O	1:A:1056:GLN:HG3	2.09	0.53
1:A:110:ARG:O	1:A:111:ASN:C	2.51	0.53
1:A:394:PRO:HB2	1:A:397:LEU:HG	1.91	0.53
1:A:560:TRP:O	1:A:575:MET:HB2	2.08	0.53
1:A:1071:ILE:HD11	1:A:1081:ILE:HG12	1.90	0.52
1:A:463:ASP:OD1	1:A:463:ASP:N	2.34	0.52
1:A:677:HIS:HB2	1:A:696:MET:HA	1.90	0.52
2:B:196:ILE:HD12	2:B:197:VAL:N	2.25	0.52
2:B:216:GLU:O	2:B:220:LYS:HG2	2.10	0.52
2:B:471:SER:O	2:B:473:ASN:N	2.41	0.52
1:A:393:HIS:HD2	1:A:398:HIS:ND1	2.07	0.52
1:A:731:GLU:CD	1:A:771:LYS:HG2	2.34	0.52
1:A:1061:SER:O	1:A:1061:SER:OG	2.26	0.52
1:A:735:ASN:OD1	1:A:736:THR:N	2.43	0.52
1:A:701:TYR:CE1	2:B:55:ALA:HB2	2.45	0.52
1:A:817:LEU:HA	1:A:1069:TYR:HE2	1.74	0.52
2:B:362:ALA:H	2:B:421:ASN:ND2	2.00	0.52
1:A:328:GLN:OE1	1:A:391:GLN:NE2	2.39	0.52
1:A:640:GLY:N	1:A:643:PHE:H	2.07	0.52
1:A:697:ALA:HB2	1:A:702:THR:HB	1.91	0.52
1:A:820:ASP:OD1	1:A:1068:ARG:NE	2.43	0.52
2:B:135:LYS:NZ	2:B:184:GLU:OE1	2.34	0.52
1:A:357:HIS:NE2	1:A:841:GLU:O	2.42	0.52
2:B:67:LEU:HB3	2:B:72:ILE:HB	1.93	0.51
1:A:738:GLN:HB3	1:A:813:PRO:HD3	1.92	0.51
1:A:1069:TYR:O	1:A:1083:VAL:HG22	2.11	0.51
1:A:607:THR:HG23	1:A:611:HIS:O	2.10	0.51
1:A:746:ASN:ND2	1:A:790:ASN:O	2.42	0.51
2:B:24:ILE:HD11	2:B:34:PHE:CZ	2.45	0.51
2:B:147:VAL:O	2:B:175:TYR:HB3	2.11	0.51
1:A:749:LEU:HD12	1:A:752:GLN:HB2	1.92	0.51
1:A:741:GLY:HA2	1:A:765:LEU:HD23	1.93	0.51
1:A:792:ILE:HD12	1:A:793:PRO:HD2	1.93	0.51
2:B:59:GLU:OE2	2:B:115:ALA:N	2.38	0.51
1:A:833:ASN:O	1:A:1056:GLN:NE2	2.43	0.50
1:A:957:TYR:N	1:A:975:ASN:HB2	2.26	0.50
2:B:50:CYS:HB3	2:B:53:CYS:SG	2.51	0.50
2:B:166:LYS:HZ3	2:B:215:GLU:HB2	1.76	0.50
1:A:953:TRP:HB2	1:A:1063:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:GLY:O	1:A:179:ARG:NH2	2.45	0.50
2:B:70:LYS:O	2:B:72:ILE:HG12	2.11	0.50
1:A:842:GLU:HG2	1:A:1015:HIS:N	2.26	0.49
1:A:680:THR:HG22	1:A:693:GLY:O	2.13	0.49
2:B:120:SER:O	2:B:124:LYS:HG3	2.12	0.49
2:B:187:GLU:OE2	2:B:193:ALA:N	2.40	0.49
1:A:733:ALA:HB1	1:A:767:LEU:C	2.38	0.49
1:A:976:GLN:CD	1:A:1002:GLU:HA	2.36	0.49
1:A:400:ASP:O	1:A:402:ASN:N	2.40	0.49
1:A:842:GLU:HB2	1:A:844:PRO:HD2	1.95	0.49
1:A:985:CYS:HB2	1:A:989:ASP:HB2	1.95	0.49
1:A:692:SER:C	1:A:699:SER:HB3	2.37	0.49
1:A:957:TYR:N	1:A:977:VAL:O	2.34	0.49
1:A:1016:GLU:HA	1:A:1022:VAL:HG13	1.93	0.49
2:B:165:LYS:NZ	2:B:169:GLU:HB2	2.27	0.49
2:B:184:GLU:O	2:B:188:ALA:CB	2.61	0.49
1:A:442:ARG:NH2	1:A:777:VAL:HG11	2.28	0.49
2:B:212:LYS:HD2	2:B:212:LYS:O	2.13	0.49
1:A:105:ASP:OD2	1:A:111:ASN:ND2	2.44	0.49
1:A:917:ILE:HG13	1:A:1021:LEU:HB2	1.93	0.49
1:A:798:GLU:N	1:A:798:GLU:OE1	2.45	0.48
1:A:794:LEU:HB3	1:A:798:GLU:OE2	2.12	0.48
1:A:807:LEU:HD22	1:A:1083:VAL:HA	1.94	0.48
1:A:1055:GLN:O	1:A:1059:VAL:HG22	2.14	0.48
1:A:957:TYR:CE2	1:A:959:ALA:HB2	2.48	0.48
2:B:159:ALA:O	2:B:162:GLU:HG3	2.13	0.48
1:A:621:ALA:C	2:B:482:SER:HA	2.38	0.48
1:A:676:LEU:HA	1:A:676:LEU:HD23	1.61	0.48
1:A:831:GLN:HB2	1:A:1060:ALA:HA	1.95	0.48
1:A:976:GLN:HA	1:A:1002:GLU:O	2.12	0.48
1:A:843:HIS:N	1:A:844:PRO:HD2	2.29	0.48
2:B:442:ASP:OD1	2:B:442:ASP:N	2.43	0.48
1:A:742:GLY:N	1:A:767:LEU:HD12	2.28	0.48
1:A:1009:VAL:HB	1:A:1046:MET:HE1	1.96	0.48
2:B:323:ILE:HG22	2:B:328:ILE:HD11	1.96	0.48
1:A:755:GLU:CD	1:A:763:ARG:HG3	2.39	0.47
2:B:83:THR:O	2:B:87:GLN:HB2	2.14	0.47
1:A:570:GLU:O	1:A:570:GLU:HG3	2.14	0.47
1:A:655:PRO:C	1:A:657:SER:N	2.73	0.47
2:B:308:GLU:OE2	2:B:335:TYR:OH	2.29	0.47
1:A:997:PHE:O	1:A:1039:ARG:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1071:ILE:HD12	1:A:1078:VAL:HG21	1.96	0.47
2:B:204:GLU:OE1	2:B:204:GLU:N	2.41	0.47
2:B:253:ALA:HB1	2:B:258:GLU:HG2	1.96	0.47
1:A:115:ASN:N	1:A:115:ASN:OD1	2.45	0.47
1:A:918:LEU:O	1:A:920:THR:HG23	2.14	0.47
2:B:26:LEU:HD13	2:B:31:PHE:HA	1.97	0.47
2:B:112:GLN:O	2:B:114:LYS:N	2.45	0.47
2:B:192:LYS:HD2	2:B:192:LYS:HA	1.61	0.47
1:A:812:ASP:HB2	1:A:813:PRO:HD3	1.96	0.47
1:A:955:THR:C	1:A:975:ASN:HB3	2.40	0.47
1:A:826:LEU:HD12	1:A:1065:ILE:HD11	1.95	0.47
1:A:787:THR:O	1:A:794:LEU:N	2.42	0.47
1:A:837:ASP:OD1	1:A:1052:THR:N	2.43	0.47
2:B:400:ARG:NH1	2:B:476:GLU:OE1	2.42	0.47
1:A:807:LEU:HB3	1:A:1069:TYR:HD1	1.80	0.46
2:B:59:GLU:CD	2:B:114:LYS:HA	2.40	0.46
1:A:828:GLN:NE2	1:A:831:GLN:O	2.48	0.46
1:A:831:GLN:C	1:A:907:PRO:HA	2.40	0.46
1:A:908:LEU:HD12	1:A:908:LEU:HA	1.63	0.46
1:A:403:TRP:C	1:A:403:TRP:CD1	2.93	0.46
1:A:1025:LEU:HD22	1:A:1026:LEU:H	1.81	0.46
2:B:198:LEU:O	2:B:200:LYS:N	2.44	0.46
1:A:603:SER:O	1:A:603:SER:OG	2.25	0.46
1:A:680:THR:HG23	1:A:690:GLN:O	2.15	0.46
1:A:774:LEU:HD22	1:A:786:VAL:HG22	1.96	0.46
1:A:823:ILE:HG13	1:A:1068:ARG:NE	2.21	0.46
1:A:983:GLY:O	1:A:985:CYS:N	2.46	0.46
2:B:126:SER:OG	2:B:127:LEU:N	2.48	0.46
1:A:523:PHE:O	1:A:527:THR:HG23	2.16	0.46
2:B:475:GLU:C	2:B:477:ASN:H	2.24	0.46
1:A:987:PHE:HA	1:A:990:LYS:HG2	1.96	0.46
1:A:639:GLN:O	1:A:642:GLY:N	2.48	0.46
1:A:1020:GLY:O	1:A:1021:LEU:HD23	2.16	0.46
2:B:87:GLN:HE21	2:B:87:GLN:HA	1.80	0.46
1:A:679:LEU:O	1:A:683:LYS:HD3	2.16	0.46
1:A:981:ARG:NH1	1:A:1051:GLU:OE2	2.49	0.46
1:A:705:PRO:C	1:A:707:THR:N	2.73	0.45
2:B:18:GLU:HG2	2:B:19:THR:N	2.30	0.45
2:B:28:LYS:NZ	2:B:84:GLU:HG3	2.31	0.45
1:A:918:LEU:HD23	1:A:918:LEU:HA	1.72	0.45
1:A:837:ASP:OD2	1:A:1052:THR:OG1	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1006:LEU:HD23	1:A:1063:ILE:HD13	1.97	0.45
1:A:729:THR:HG23	1:A:773:THR:HG22	1.98	0.45
1:A:953:TRP:HB2	1:A:1063:ILE:CD1	2.47	0.45
1:A:815:PHE:HA	1:A:816:ASN:HA	1.63	0.45
2:B:242:MET:HE3	2:B:242:MET:HB3	1.58	0.45
1:A:302:THR:OG1	1:A:303:CYS:N	2.50	0.45
1:A:362:TYR:N	1:A:362:TYR:CD1	2.84	0.45
1:A:515:GLY:O	1:A:565:ASN:HA	2.17	0.45
1:A:700:ASN:O	1:A:701:TYR:C	2.60	0.45
1:A:733:ALA:HB3	1:A:769:GLY:N	2.32	0.45
1:A:807:LEU:HB3	1:A:1069:TYR:CD1	2.52	0.45
1:A:677:HIS:HB2	1:A:696:MET:CB	2.45	0.45
2:B:137:THR:HA	2:B:140:GLU:OE2	2.17	0.45
1:A:996:ALA:HA	1:A:1038:ARG:HG2	1.98	0.45
1:A:220:ARG:HE	1:A:220:ARG:HB2	1.74	0.45
1:A:627:SER:N	1:A:628:PRO:HD2	2.31	0.45
1:A:665:ASP:N	1:A:665:ASP:OD1	2.49	0.45
1:A:962:ALA:HB3	1:A:990:LYS:HB2	1.99	0.45
1:A:93:GLU:HB2	1:A:102:LEU:HD23	1.97	0.44
1:A:1015:HIS:HD2	1:A:1022:VAL:HG11	1.81	0.44
1:A:639:GLN:C	1:A:643:PHE:H	2.25	0.44
1:A:678:LEU:H	1:A:678:LEU:HD22	1.83	0.44
1:A:829:LEU:HD22	1:A:951:PHE:CD1	2.53	0.44
1:A:831:GLN:CD	1:A:1059:VAL:HG23	2.42	0.44
1:A:925:ALA:N	1:A:1030:GLN:OE1	2.50	0.44
2:B:302:PRO:HB2	2:B:323:ILE:HD11	1.98	0.44
1:A:162:GLU:OE2	1:A:176:ARG:NH1	2.48	0.44
1:A:362:TYR:N	1:A:362:TYR:HD1	2.15	0.44
2:B:314:LYS:H	2:B:314:LYS:HD2	1.82	0.44
1:A:493:TRP:CD1	1:A:493:TRP:C	2.95	0.44
1:A:906:LEU:O	1:A:908:LEU:N	2.45	0.44
1:A:971:ALA:HB3	1:A:972:PRO:HD3	1.99	0.44
2:B:124:LYS:O	2:B:172:ARG:NH1	2.51	0.44
1:A:394:PRO:HD2	1:A:397:LEU:HD12	2.00	0.44
1:A:705:PRO:C	1:A:707:THR:H	2.26	0.44
1:A:762:ILE:O	1:A:801:VAL:N	2.40	0.44
1:A:107:LYS:HE2	1:A:107:LYS:CA	2.48	0.44
1:A:414:SER:OG	1:A:415:ASP:N	2.50	0.44
1:A:458:VAL:HG12	1:A:459:SER:OG	2.17	0.44
1:A:395:SER:N	1:A:396:PRO:HD2	2.33	0.44
1:A:828:GLN:O	1:A:909:ASN:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:LEU:HD23	1:A:473:LEU:HA	1.78	0.44
1:A:825:LYS:N	1:A:1066:GLN:HE22	2.16	0.44
2:B:361:VAL:O	2:B:364:THR:N	2.49	0.44
1:A:819:ARG:HH11	1:A:1069:TYR:N	2.16	0.43
2:B:223:LYS:HD2	2:B:223:LYS:HA	1.68	0.43
2:B:297:LYS:H	2:B:319:GLN:HE22	1.65	0.43
1:A:770:LEU:HD12	1:A:790:ASN:ND2	2.28	0.43
1:A:801:VAL:HG13	1:A:1082:ILE:HD11	2.00	0.43
1:A:365:ILE:HA	1:A:365:ILE:HD12	1.77	0.43
1:A:773:THR:OG1	1:A:788:LYS:HB3	2.17	0.43
1:A:812:ASP:OD2	1:A:812:ASP:N	2.50	0.43
2:B:84:GLU:HG2	2:B:85:LEU:N	2.33	0.43
1:A:387:ALA:HB2	1:A:628:PRO:HD3	2.00	0.43
1:A:741:GLY:H	1:A:767:LEU:HG	1.83	0.43
1:A:804:ARG:H	1:A:804:ARG:HD2	1.83	0.43
1:A:1015:HIS:CD2	1:A:1022:VAL:HG11	2.53	0.43
2:B:61:GLU:O	2:B:65:THR:HG23	2.18	0.43
2:B:65:THR:OG1	2:B:66:ASN:N	2.51	0.43
1:A:129:LEU:HA	1:A:129:LEU:HD23	1.74	0.43
1:A:837:ASP:OD2	1:A:1051:GLU:HB3	2.18	0.43
1:A:962:ALA:HB2	1:A:980:ILE:HG12	2.00	0.43
1:A:61:GLN:HE21	1:A:61:GLN:HB2	1.64	0.43
1:A:704:TYR:O	1:A:706:TRP:N	2.52	0.43
1:A:733:ALA:HB3	1:A:769:GLY:C	2.43	0.43
1:A:953:TRP:O	1:A:954:LYS:HD3	2.19	0.43
1:A:957:TYR:OH	1:A:971:ALA:HB1	2.19	0.43
2:B:362:ALA:HB2	2:B:421:ASN:HB3	1.99	0.43
2:B:409:ASP:OD1	2:B:409:ASP:N	2.25	0.43
1:A:599:LYS:HB2	1:A:599:LYS:HE2	1.58	0.43
1:A:765:LEU:HD23	1:A:765:LEU:HA	1.79	0.43
1:A:980:ILE:HG21	1:A:990:LYS:HB2	2.01	0.43
2:B:465:LYS:O	2:B:465:LYS:HG2	2.19	0.43
1:A:702:THR:O	1:A:703:LEU:C	2.61	0.43
2:B:140:GLU:HG2	2:B:141:PHE:N	2.33	0.43
2:B:374:LYS:HZ3	2:B:374:LYS:HG2	1.63	0.43
1:A:725:PRO:HB3	1:A:777:VAL:HG22	2.00	0.42
1:A:771:LYS:HB2	1:A:790:ASN:N	2.28	0.42
1:A:917:ILE:CG1	1:A:1021:LEU:HB2	2.48	0.42
1:A:692:SER:O	1:A:699:SER:HB3	2.18	0.42
1:A:763:ARG:HD2	1:A:764:VAL:N	2.33	0.42
1:A:913:ASN:CG	7:A:1203:NAG:H83	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1016:GLU:OE1	1:A:1021:LEU:HD22	2.19	0.42
2:B:53:CYS:HB2	2:B:54:LYS:HE2	2.00	0.42
2:B:140:GLU:OE1	2:B:140:GLU:N	2.51	0.42
2:B:168:ALA:HA	2:B:177:PHE:CZ	2.54	0.42
1:A:284:HIS:O	1:A:285:GLU:HB3	2.19	0.42
1:A:457:LEU:HA	1:A:457:LEU:HD12	1.85	0.42
1:A:619:LYS:HA	1:A:619:LYS:HD3	1.74	0.42
1:A:748:MET:CE	1:A:752:GLN:HG3	2.49	0.42
1:A:823:ILE:CG1	1:A:1068:ARG:HE	2.21	0.42
1:A:961:GLU:O	1:A:990:LYS:HE3	2.19	0.42
2:B:25:GLN:C	2:B:26:LEU:HD23	2.44	0.42
2:B:165:LYS:HZ1	2:B:169:GLU:HB2	1.83	0.42
2:B:194:PRO:HG2	2:B:211:GLU:OE2	2.19	0.42
2:B:324:THR:OG1	2:B:326:ASP:N	2.52	0.42
2:B:371:ASP:OD2	2:B:371:ASP:C	2.61	0.42
1:A:703:LEU:HA	1:A:703:LEU:HD23	1.73	0.42
1:A:1030:GLN:HB3	1:A:1038:ARG:NH1	2.34	0.42
2:B:254:GLU:O	2:B:259:ARG:NH1	2.53	0.42
2:B:470:ILE:O	2:B:471:SER:C	2.60	0.42
1:A:740:LEU:O	1:A:806:ILE:HD13	2.19	0.42
2:B:196:ILE:HD12	2:B:197:VAL:CA	2.50	0.42
1:A:286:ASP:OD1	1:A:286:ASP:N	2.48	0.42
1:A:953:TRP:HE1	1:A:1005:GLN:CB	2.31	0.42
2:B:145:ASP:CG	2:B:146:LYS:H	2.27	0.42
2:B:472:GLU:O	2:B:473:ASN:C	2.62	0.42
4:D:1:NAG:H4	4:D:2:NAG:H2	1.50	0.42
1:A:679:LEU:HA	1:A:682:SER:HB3	2.00	0.42
1:A:700:ASN:HD21	1:A:708:LEU:C	2.24	0.42
2:B:42:LEU:HB3	2:B:74:LEU:CD2	2.48	0.42
2:B:114:LYS:HA	2:B:114:LYS:HD2	1.61	0.42
2:B:207:ALA:O	2:B:221:TRP:HZ2	2.02	0.42
1:A:738:GLN:HB2	1:A:812:ASP:OD2	2.20	0.42
1:A:954:LYS:HB2	1:A:976:GLN:NE2	2.34	0.42
2:B:211:GLU:O	2:B:212:LYS:HB3	2.19	0.42
2:B:219:GLN:OE1	2:B:219:GLN:C	2.63	0.42
1:A:820:ASP:OD2	1:A:822:VAL:HG12	2.19	0.42
2:B:273:THR:O	2:B:274:ARG:C	2.63	0.42
2:B:470:ILE:HG13	2:B:471:SER:N	2.34	0.42
1:A:843:HIS:ND1	1:A:1017:GLY:HA2	2.35	0.42
1:A:1016:GLU:HG2	1:A:1021:LEU:HB3	2.02	0.42
2:B:142:LYS:HE3	2:B:142:LYS:HB2	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:GLY:C	1:A:767:LEU:HB2	2.44	0.41
1:A:826:LEU:HA	1:A:1065:ILE:HD13	2.02	0.41
2:B:219:GLN:OE1	2:B:220:LYS:N	2.53	0.41
1:A:364:VAL:HG12	1:A:449:ASN:OD1	2.20	0.41
1:A:723:TYR:CD1	1:A:723:TYR:C	2.98	0.41
1:A:803:ASN:HB3	1:A:806:ILE:CG2	2.50	0.41
1:A:437:HIS:NE2	1:A:781:GLU:OE1	2.53	0.41
1:A:617:LYS:HD2	1:A:617:LYS:HA	1.67	0.41
1:A:697:ALA:HB2	1:A:702:THR:CB	2.49	0.41
1:A:819:ARG:HA	1:A:1069:TYR:HA	2.01	0.41
2:B:229:LEU:HD23	2:B:229:LEU:HA	1.74	0.41
2:B:369:VAL:HG21	2:B:378:ILE:HD12	2.02	0.41
2:B:471:SER:C	2:B:473:ASN:N	2.79	0.41
1:A:842:GLU:H	1:A:842:GLU:HG3	1.67	0.41
2:B:109:TYR:CZ	2:B:111:GLY:HA3	2.55	0.41
1:A:977:VAL:HG11	1:A:1008:VAL:HG23	2.02	0.41
2:B:78:ASP:OD1	2:B:80:THR:OG1	2.37	0.41
2:B:152:TYR:CD1	2:B:186:ALA:HB2	2.56	0.41
1:A:705:PRO:O	1:A:707:THR:N	2.54	0.41
1:A:741:GLY:H	1:A:767:LEU:CD1	2.32	0.41
2:B:137:THR:HA	2:B:140:GLU:CD	2.45	0.41
1:A:641:GLU:HG3	1:A:645:ASN:HB2	2.03	0.41
1:A:820:ASP:HB3	1:A:1068:ARG:HG3	2.02	0.41
1:A:824:ALA:HB3	1:A:918:LEU:HD21	2.03	0.41
2:B:273:THR:CG2	2:B:276:LYS:HB2	2.51	0.41
1:A:704:TYR:O	1:A:705:PRO:C	2.59	0.41
2:B:157:ASP:OD1	2:B:158:LYS:N	2.53	0.41
2:B:475:GLU:OE2	2:B:477:ASN:ND2	2.52	0.41
1:A:803:ASN:O	1:A:806:ILE:HG22	2.21	0.41
1:A:979:LEU:HG	1:A:1057:LEU:HD12	2.03	0.41
1:A:1018:GLN:O	1:A:1020:GLY:N	2.54	0.41
2:B:207:ALA:HB1	2:B:221:TRP:CH2	2.56	0.41
1:A:319:ARG:HD3	1:A:319:ARG:HA	1.81	0.41
1:A:681:THR:C	1:A:683:LYS:H	2.30	0.41
1:A:614:ILE:HG21	1:A:614:ILE:HD13	1.83	0.40
1:A:677:HIS:HA	1:A:680:THR:OG1	2.22	0.40
1:A:683:LYS:CB	1:A:691:MET:HG2	2.50	0.40
1:A:744:ALA:O	1:A:766:SER:OG	2.27	0.40
1:A:763:ARG:HA	1:A:801:VAL:HB	2.03	0.40
1:A:934:SER:OG	1:A:1065:ILE:O	2.28	0.40
1:A:748:MET:HE1	1:A:765:LEU:N	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:ASN:ND2	1:A:951:PHE:HZ	2.20	0.40
2:B:443:LYS:HE2	2:B:443:LYS:HB3	1.84	0.40
1:A:835:LEU:HG	1:A:836:ASP:N	2.32	0.40
1:A:484:GLU:H	1:A:484:GLU:HG2	1.56	0.40
1:A:764:VAL:N	1:A:801:VAL:O	2.54	0.40
2:B:18:GLU:O	2:B:21:SER:N	2.44	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	968/1284 (75%)	827 (85%)	136 (14%)	5 (0%)	25	47
2	B	465/507 (92%)	422 (91%)	42 (9%)	1 (0%)	44	66
All	All	1433/1791 (80%)	1249 (87%)	178 (12%)	6 (0%)	32	52

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	644	THR
1	A	111	ASN
2	B	133	VAL
1	A	697	ALA
1	A	818	VAL
1	A	910	VAL

5.3.2 Protein sidechains [i](#)

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	820/1092 (75%)	777 (95%)	43 (5%)	19	41
2	B	389/419 (93%)	362 (93%)	27 (7%)	13	28
All	All	1209/1511 (80%)	1139 (94%)	70 (6%)	19	36

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	VAL
1	A	127	ASP
1	A	141	GLU
1	A	172	SER
1	A	299	ILE
1	A	321	THR
1	A	371	SER
1	A	379	SER
1	A	388	LEU
1	A	392	THR
1	A	403	TRP
1	A	431	HIS
1	A	440	SER
1	A	470	SER
1	A	510	VAL
1	A	527	THR
1	A	556	THR
1	A	584	THR
1	A	624	SER
1	A	637	VAL
1	A	638	TYR
1	A	698	LYS
1	A	702	THR
1	A	704	TYR
1	A	712	LEU
1	A	713	LEU
1	A	722	VAL
1	A	768	SER
1	A	772	ILE
1	A	773	THR
1	A	810	VAL
1	A	839	THR
1	A	927	LEU

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Mol	Chain	Res	Type
1	A	977	VAL
1	A	994	ILE
1	A	1010	VAL
1	A	1025	LEU
1	A	1045	VAL
1	A	1059	VAL
1	A	1070	TYR
1	A	1071	ILE
1	A	1074	SER
1	A	1076	VAL
2	B	23	VAL
2	B	37	SER
2	B	69	ASP
2	B	83	THR
2	B	91	VAL
2	B	103	LEU
2	B	148	VAL
2	B	150	VAL
2	B	156	SER
2	B	171	LEU
2	B	173	ASP
2	B	175	TYR
2	B	197	VAL
2	B	210	THR
2	B	273	THR
2	B	310	THR
2	B	324	THR
2	B	327	SER
2	B	344	ILE
2	B	346	SER
2	B	358	THR
2	B	364	THR
2	B	367	ASP
2	B	374	LYS
2	B	375	ASP
2	B	419	THR
2	B	483	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN

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Mol	Chain	Res	Type
1	A	380	HIS
1	A	393	HIS
1	A	431	HIS
1	A	460	HIS
1	A	645	ASN
1	A	694	GLN
1	A	726	HIS
1	A	828	GLN
1	A	914	GLN
1	A	975	ASN
1	A	1066	GLN
2	B	38	ASN
2	B	52	HIS
2	B	66	ASN
2	B	87	GLN
2	B	290	HIS
2	B	307	GLN
2	B	421	ASN

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 ⓘ

12 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
3	NAG	C	1	1,3	14,14,15	1.37	2 (14%)	17,19,21	1.09	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	2	3	14,14,15	0.71	1 (7%)	17,19,21	0.65	0
3	BMA	C	3	3	11,11,12	1.22	1 (9%)	15,15,17	1.40	3 (20%)
3	MAN	C	4	3	11,11,12	0.82	1 (9%)	15,15,17	1.52	2 (13%)
3	MAN	C	5	3	11,11,12	0.89	1 (9%)	15,15,17	1.51	2 (13%)
4	NAG	D	1	1,4	14,14,15	0.52	0	17,19,21	0.45	0
4	NAG	D	2	4	14,14,15	0.45	0	17,19,21	0.44	0
3	NAG	E	1	1,3	14,14,15	1.25	1 (7%)	17,19,21	0.69	0
3	NAG	E	2	3	14,14,15	0.80	1 (7%)	17,19,21	0.70	0
3	BMA	E	3	3	11,11,12	1.32	2 (18%)	15,15,17	1.37	3 (20%)
3	MAN	E	4	3	11,11,12	0.71	0	15,15,17	1.35	2 (13%)
3	MAN	E	5	3	11,11,12	1.10	2 (18%)	15,15,17	1.11	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
3	NAG	C	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	MAN	C	4	3	-	2/2/19/22	1/1/1/1
3	MAN	C	5	3	-	0/2/19/22	0/1/1/1
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	2/2/19/22	0/1/1/1
3	MAN	E	4	3	-	2/2/19/22	1/1/1/1
3	MAN	E	5	3	-	2/2/19/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	NAG	O5-C1	-4.34	1.36	1.43
3	C	1	NAG	O5-C1	-4.29	1.36	1.43
3	C	3	BMA	O5-C1	-3.22	1.38	1.43
3	E	2	NAG	O5-C1	-2.56	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	5	MAN	C2-C3	-2.26	1.49	1.52
3	E	5	MAN	O5-C1	-2.18	1.40	1.43
3	E	3	BMA	C2-C3	-2.16	1.49	1.52
3	C	1	NAG	C1-C2	-2.12	1.49	1.52
3	C	2	NAG	O5-C1	-2.11	1.40	1.43
3	E	3	BMA	O5-C1	-2.03	1.40	1.43
3	C	5	MAN	C2-C3	-2.02	1.49	1.52
3	C	4	MAN	O5-C5	2.01	1.47	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	MAN	C1-O5-C5	4.42	118.18	112.19
3	E	4	MAN	C1-O5-C5	4.01	117.62	112.19
3	C	5	MAN	C1-O5-C5	3.94	117.53	112.19
3	C	1	NAG	C1-O5-C5	3.44	116.86	112.19
3	E	5	MAN	O2-C2-C3	-3.01	104.11	110.14
3	C	5	MAN	O2-C2-C3	-2.83	104.46	110.14
3	E	3	BMA	O2-C2-C3	-2.70	104.73	110.14
3	C	3	BMA	O2-C2-C3	-2.59	104.94	110.14
3	C	4	MAN	O2-C2-C3	-2.58	104.97	110.14
3	E	3	BMA	O5-C1-C2	-2.58	106.80	110.77
3	E	4	MAN	O2-C2-C3	-2.41	105.31	110.14
3	C	3	BMA	O5-C1-C2	-2.28	107.26	110.77
3	C	3	BMA	C2-C3-C4	2.27	114.82	110.89
3	E	3	BMA	C6-C5-C4	-2.13	108.00	113.00
3	E	5	MAN	C1-O5-C5	2.05	114.96	112.19

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	NAG	O5-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6
3	E	3	BMA	C4-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
3	C	4	MAN	O5-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
3	E	4	MAN	O5-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
3	C	4	MAN	C4-C5-C6-O6
3	E	5	MAN	O5-C5-C6-O6
3	E	5	MAN	C4-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6

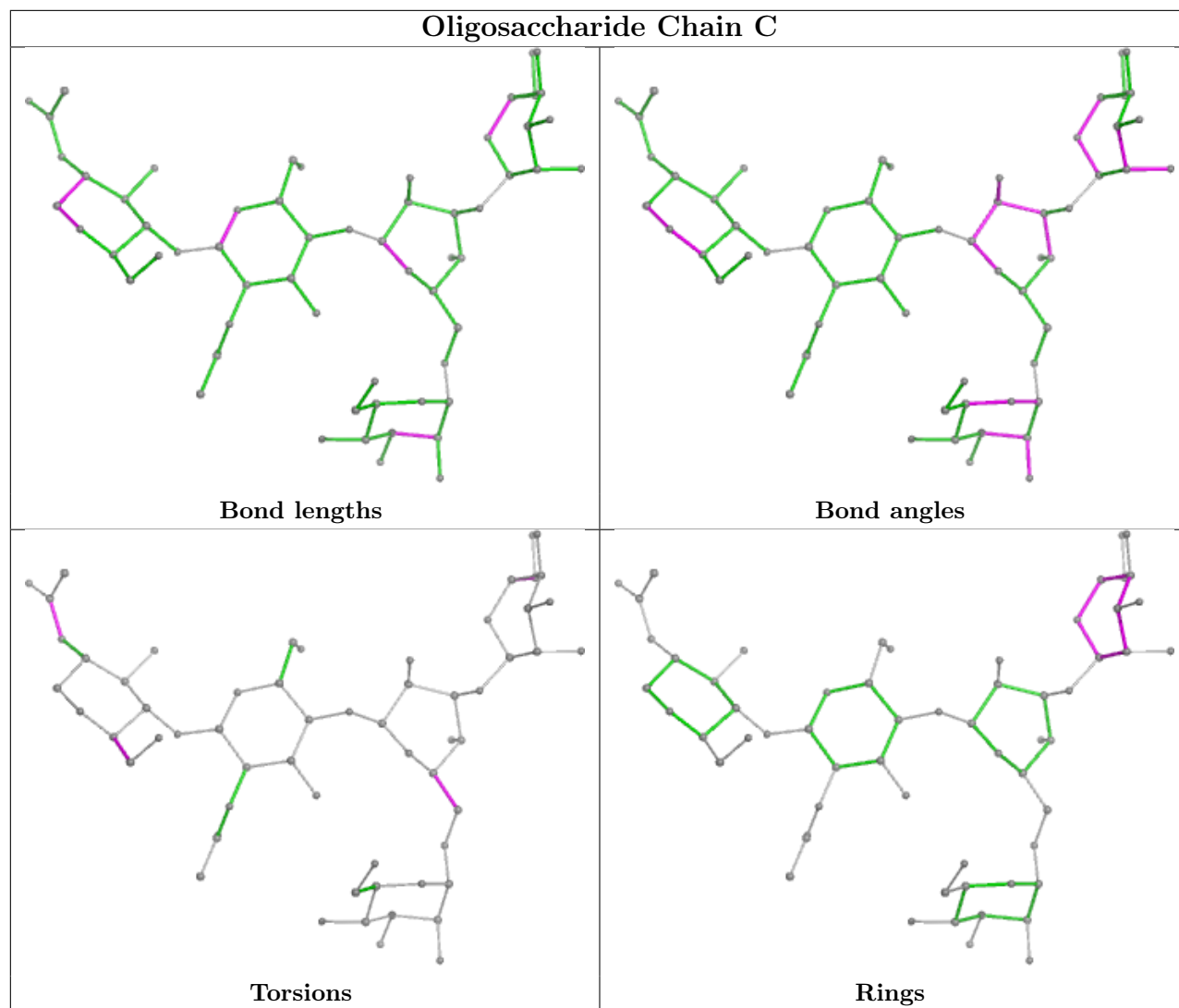
All (2) ring outliers are listed below:

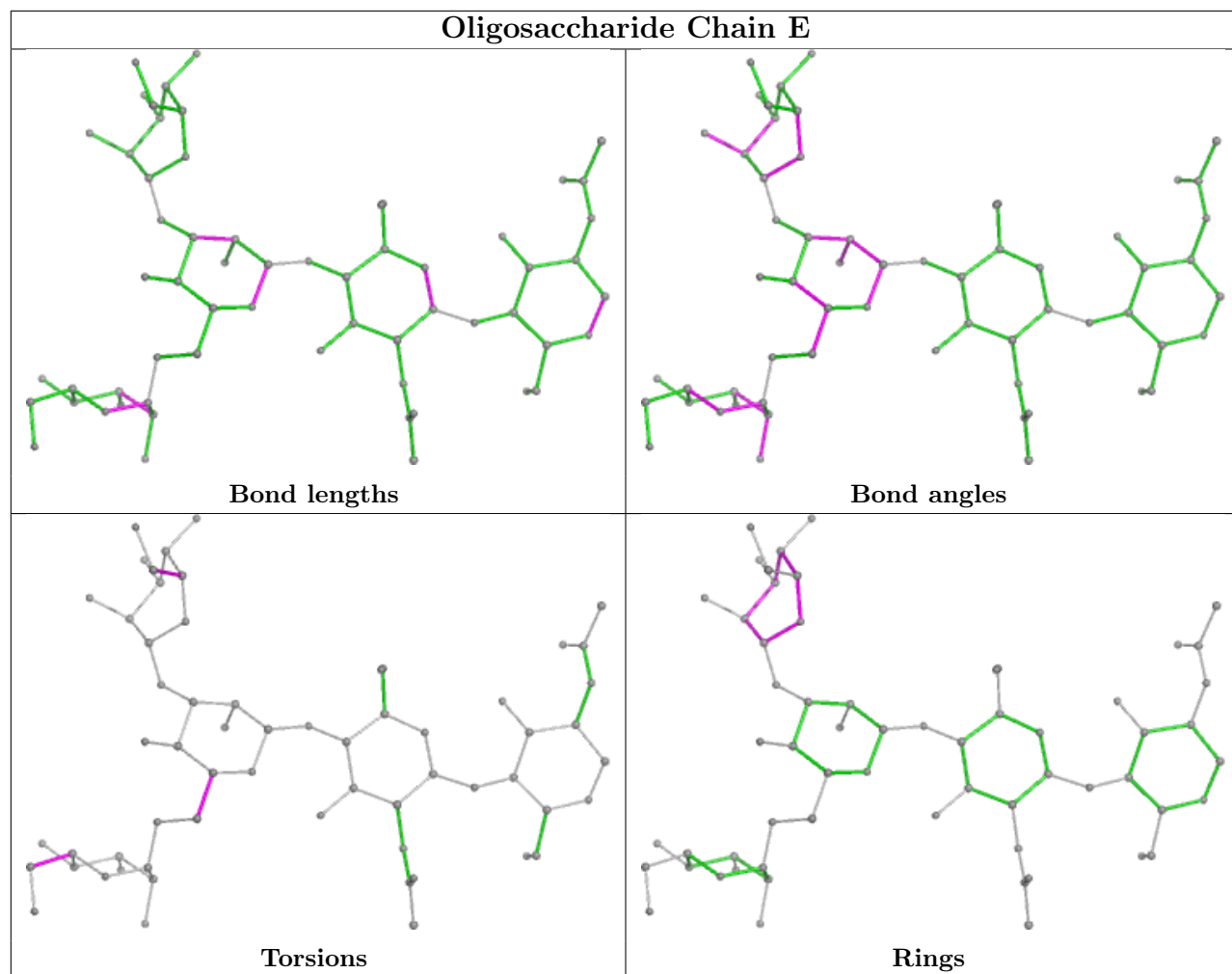
Mol	Chain	Res	Type	Atoms
3	C	4	MAN	C1-C2-C3-C4-C5-O5
3	E	4	MAN	C1-C2-C3-C4-C5-O5

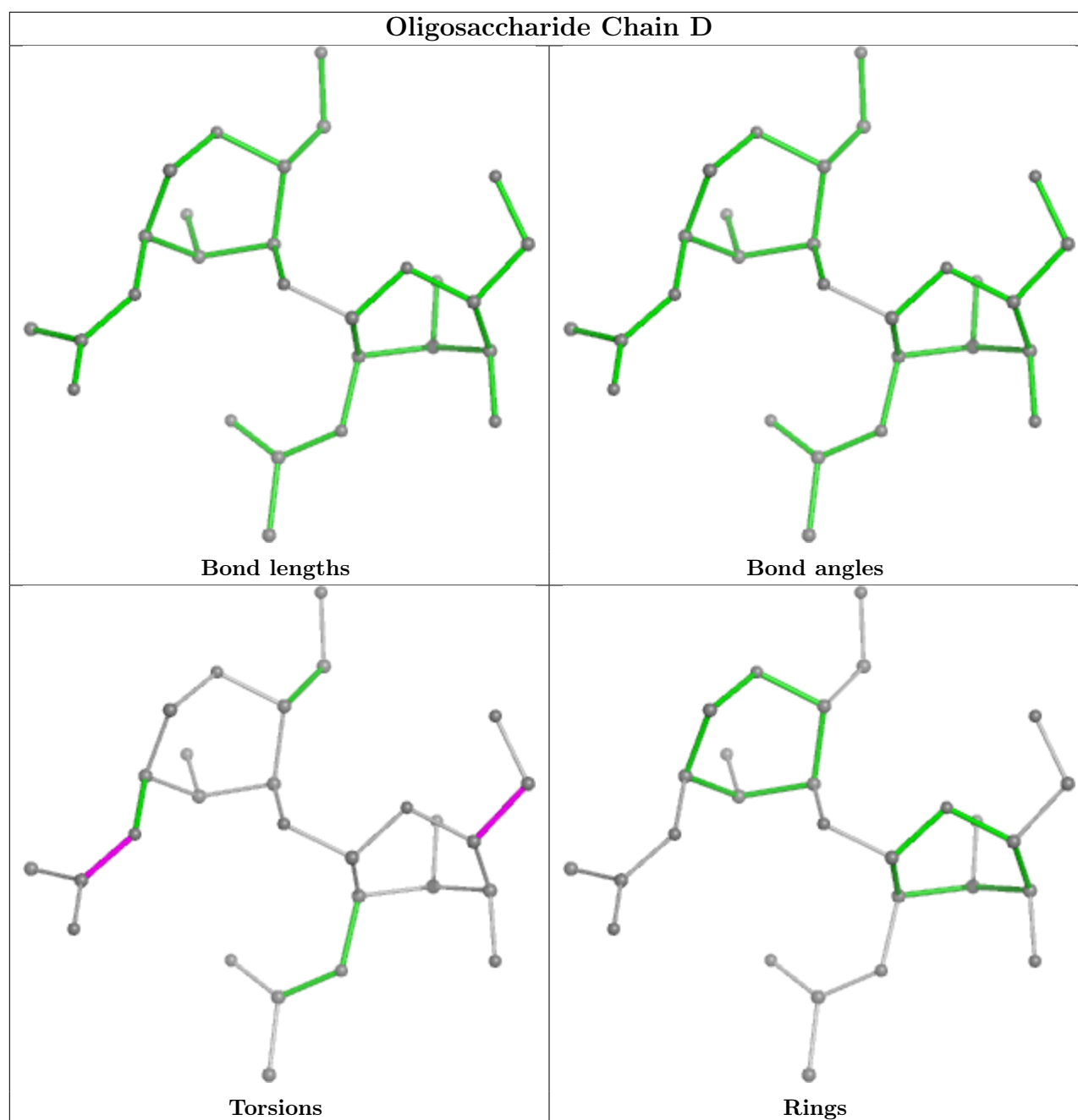
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2	NAG	1	0
4	D	1	NAG	2	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](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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
8	MAN	A	1204	5	11,11,12	3.73	8 (72%)	15,15,17	1.86	4 (26%)
6	THJ	A	1202	-	2,4,4	0.86	0	2,6,6	0.22	0
7	NAG	A	1203	1	14,14,15	0.25	0	17,19,21	0.40	0
7	NAG	B	601	2	14,14,15	0.20	0	17,19,21	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
8	MAN	A	1204	5	-	0/2/19/22	0/1/1/1
7	NAG	A	1203	1	-	4/6/23/26	0/1/1/1
7	NAG	B	601	2	-	3/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1204	MAN	O5-C1	-6.05	1.34	1.43
8	A	1204	MAN	C4-C5	-5.70	1.41	1.53
8	A	1204	MAN	O2-C2	-5.26	1.32	1.43
8	A	1204	MAN	C4-C3	-3.98	1.42	1.52
8	A	1204	MAN	C1-C2	-3.73	1.43	1.52
8	A	1204	MAN	O4-C4	-3.24	1.35	1.43
8	A	1204	MAN	C6-C5	-2.83	1.42	1.51
8	A	1204	MAN	O3-C3	-2.38	1.37	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1204	MAN	C1-O5-C5	3.37	116.75	112.19
8	A	1204	MAN	C6-C5-C4	-3.33	105.21	113.00
8	A	1204	MAN	O2-C2-C3	-3.14	103.84	110.14
8	A	1204	MAN	O3-C3-C4	-2.24	105.17	110.35

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1203	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	1203	NAG	O7-C7-N2-C2
7	A	1203	NAG	C4-C5-C6-O6
7	B	601	NAG	C1-C2-N2-C7
7	A	1203	NAG	O5-C5-C6-O6
7	B	601	NAG	C3-C2-N2-C7
7	B	601	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1203	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.

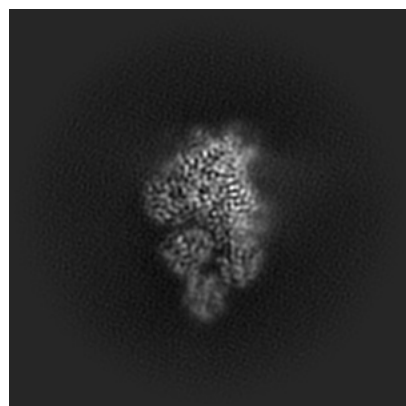
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17749. These allow visual inspection of the internal detail of the map and identification of artifacts.

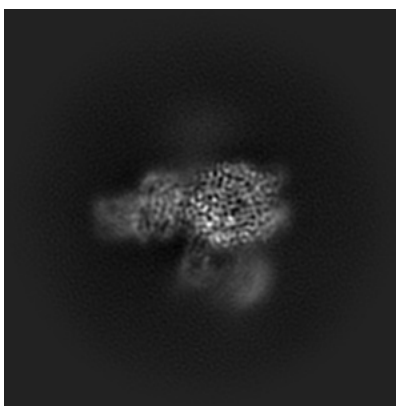
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

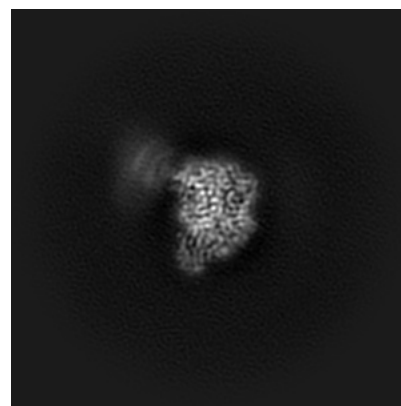
6.1.1 Primary map



X

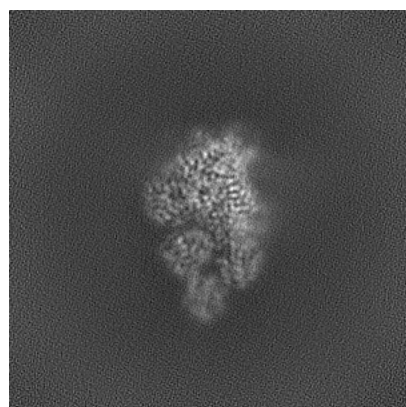


Y

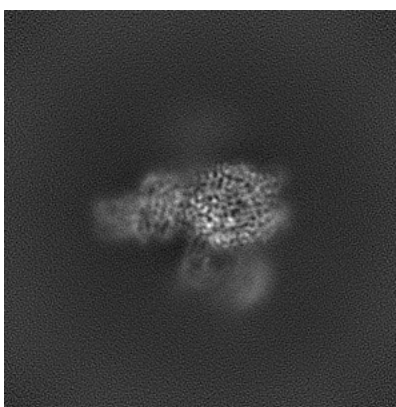


Z

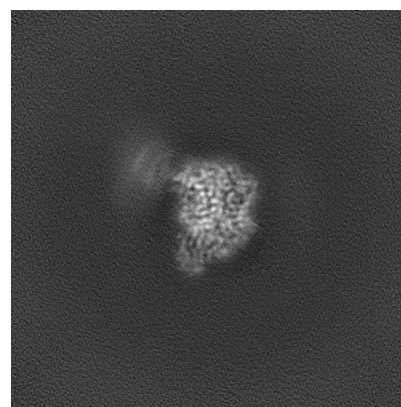
6.1.2 Raw map



X



Y

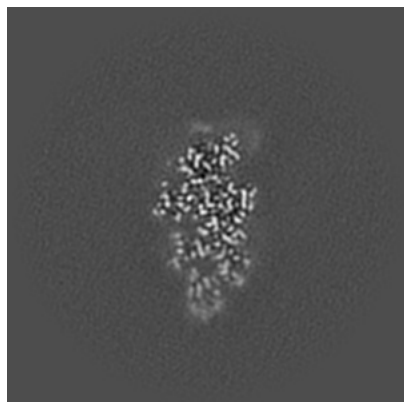


Z

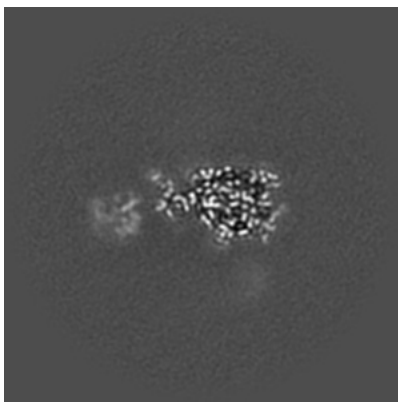
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

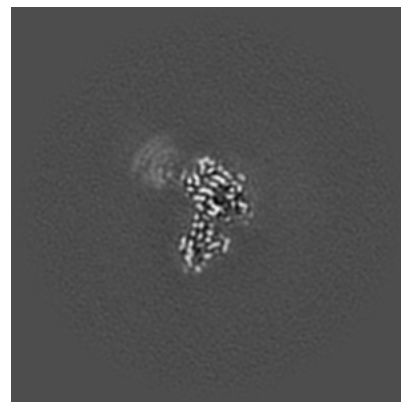
6.2.1 Primary map



X Index: 150

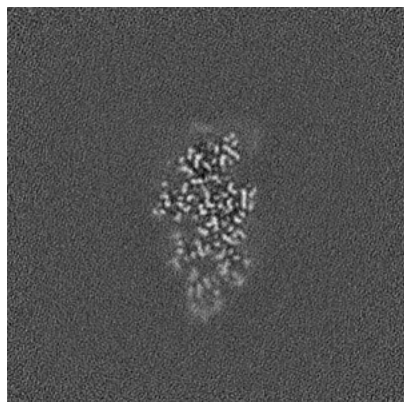


Y Index: 150

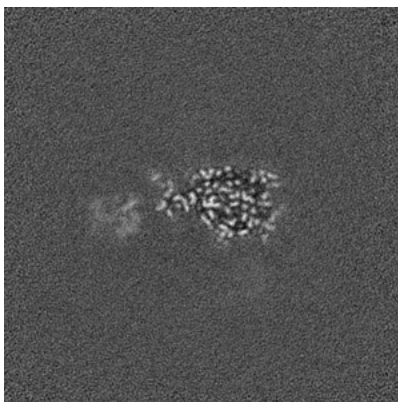


Z Index: 150

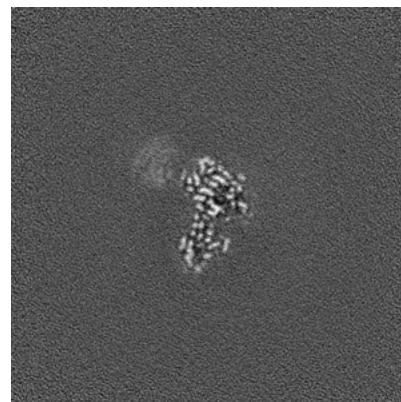
6.2.2 Raw map



X Index: 150



Y Index: 150

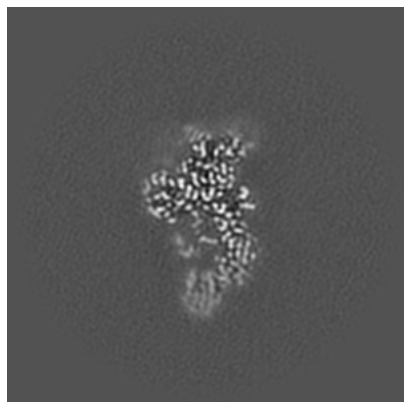


Z Index: 150

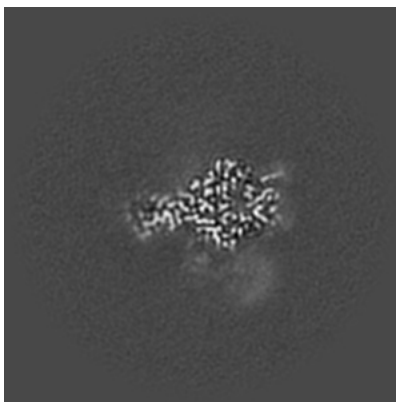
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

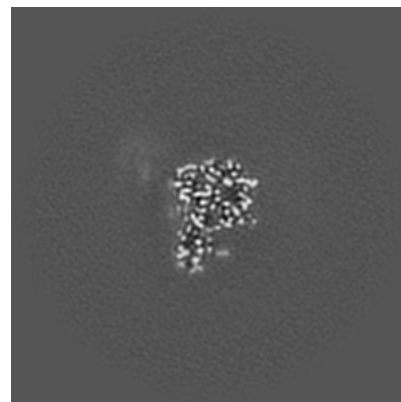
6.3.1 Primary map



X Index: 143

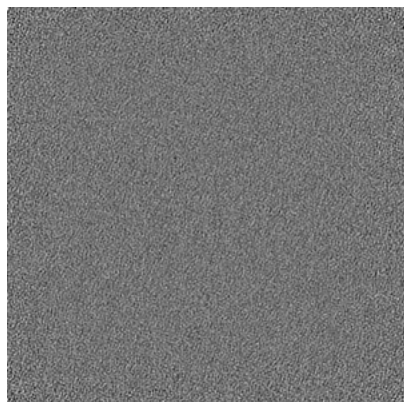


Y Index: 167

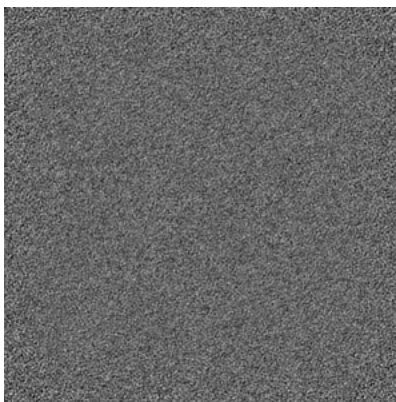


Z Index: 160

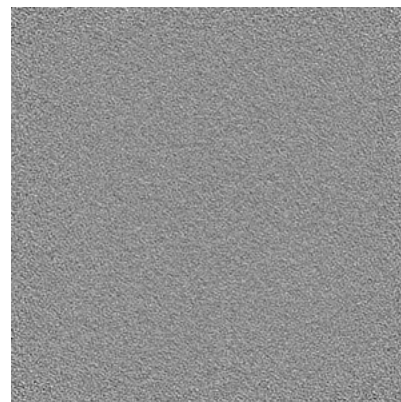
6.3.2 Raw map



X Index: 0



Y Index: 0

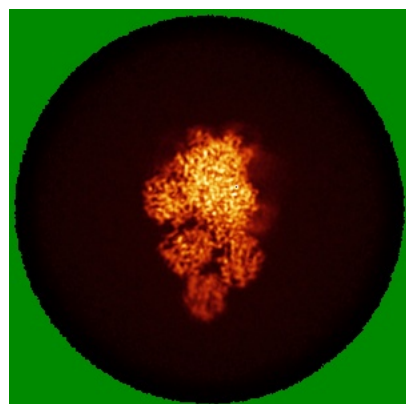


Z Index: 299

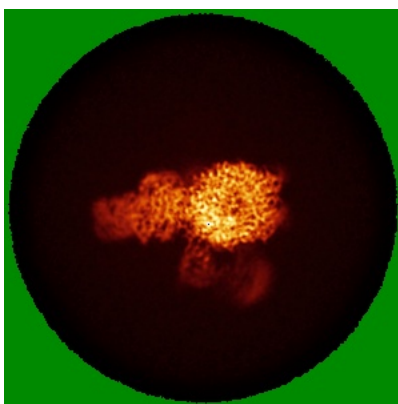
The images above show the largest variance slices of the map in three orthogonal directions.

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

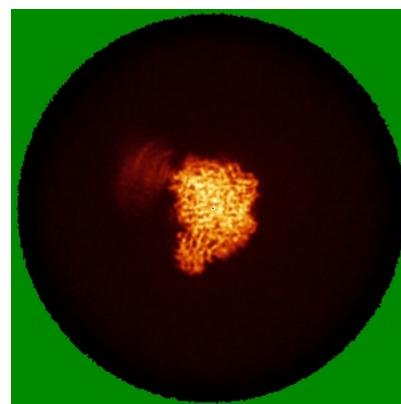
6.4.1 Primary map



X

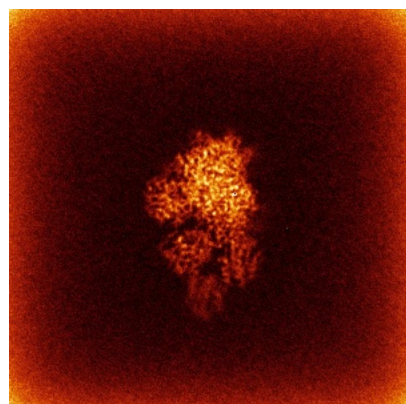


Y

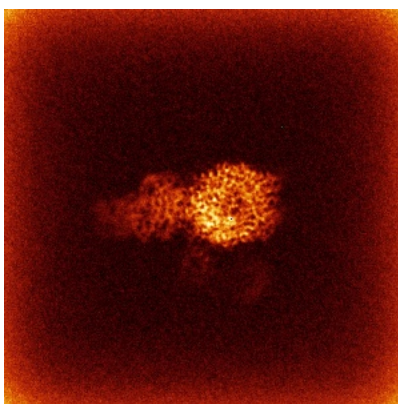


Z

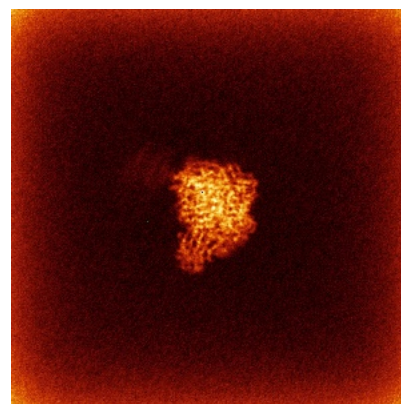
6.4.2 Raw map



X



Y



Z

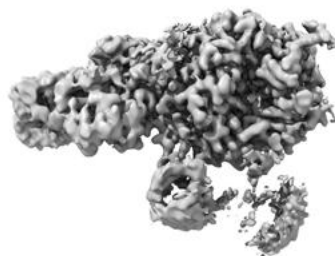
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

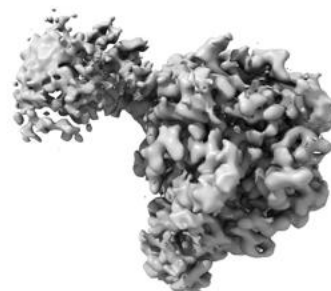
6.5.1 Primary map



X



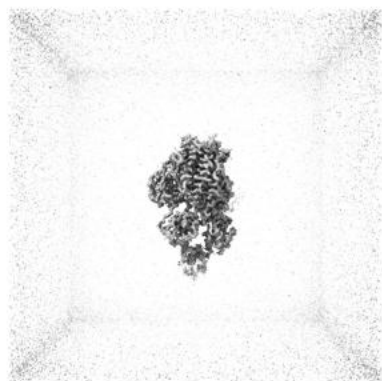
Y



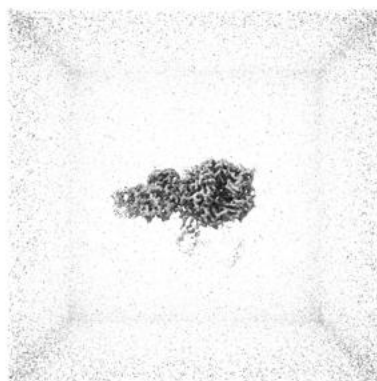
Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

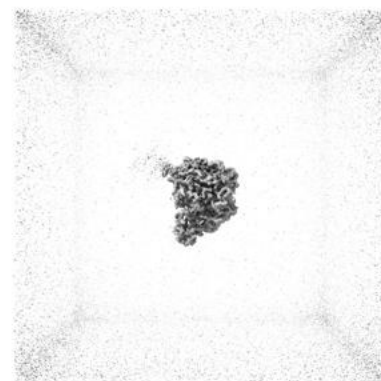
6.5.2 Raw map



X



Y



Z

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.

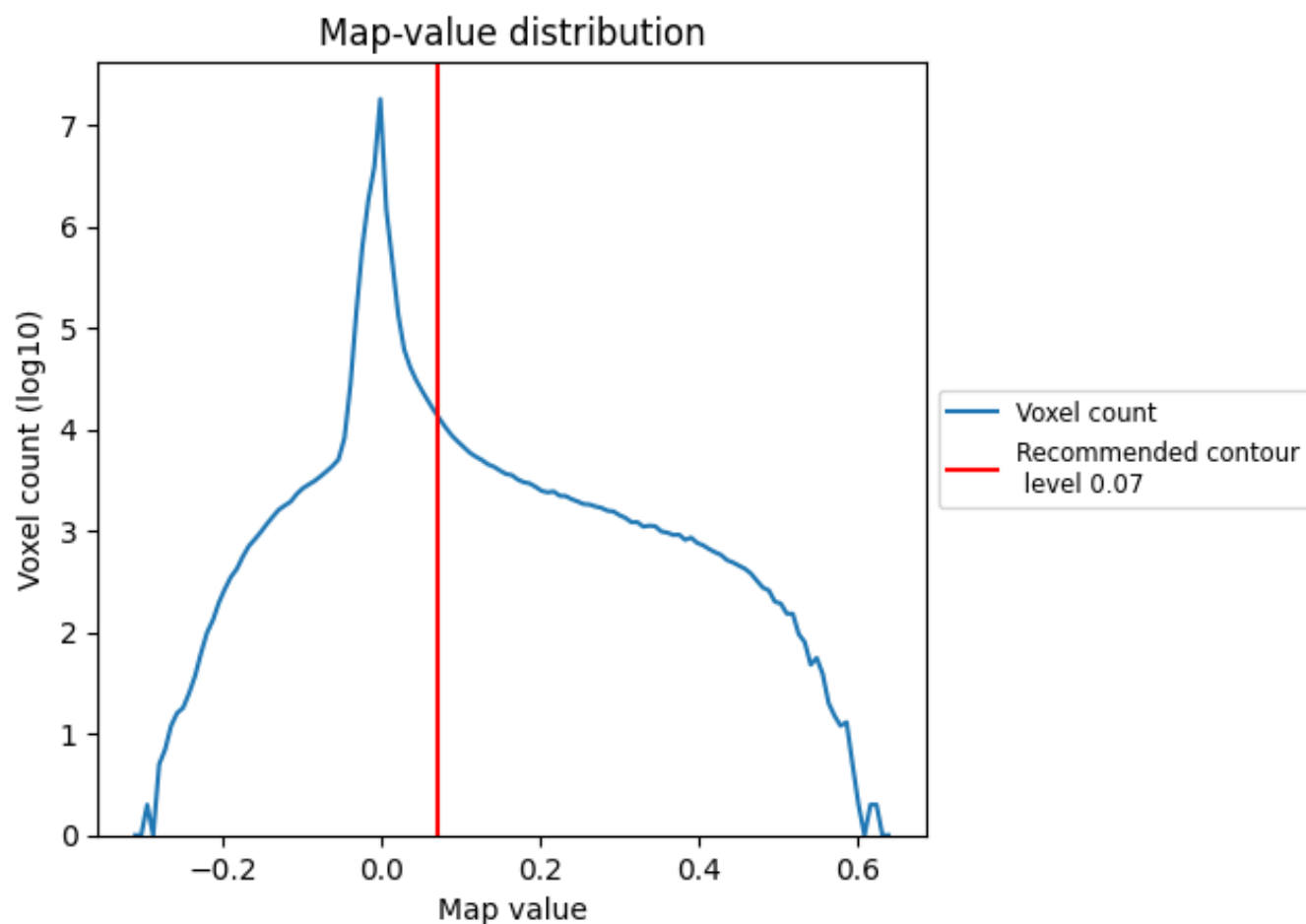
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

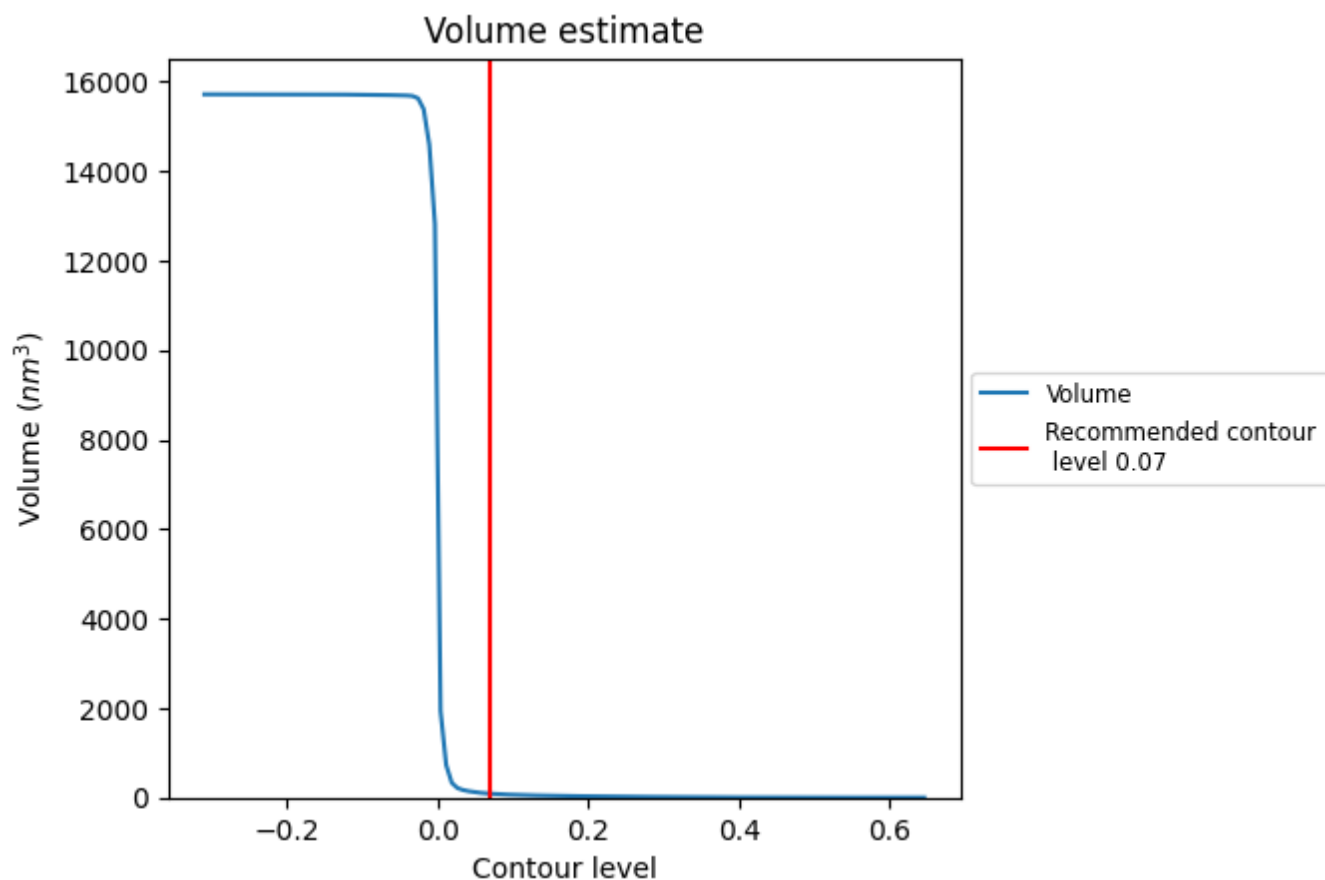
This section contains the results of statistical analysis of the map.

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.

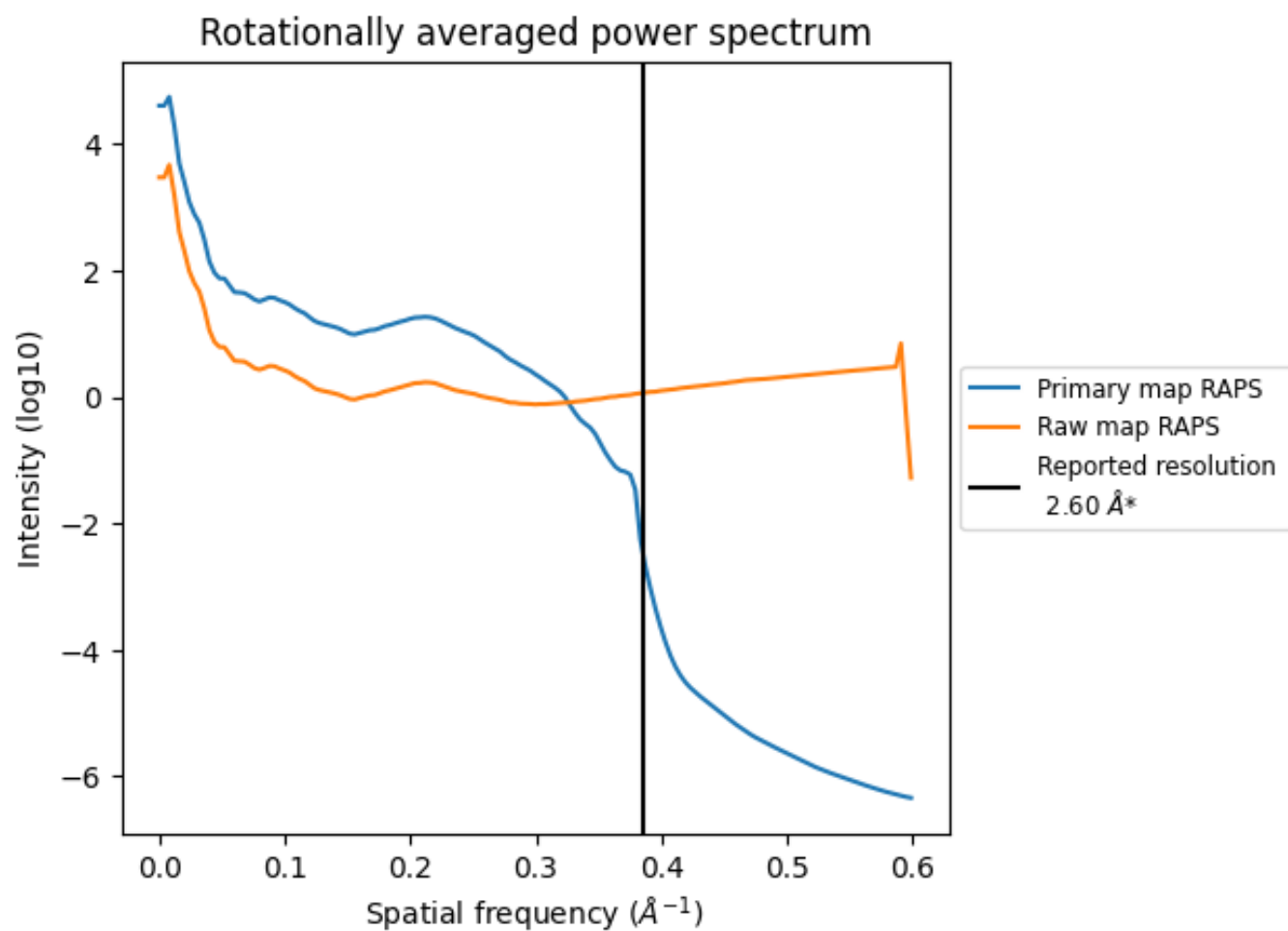
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 87 nm^3 ; this corresponds to an approximate mass of 78 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 ⓘ

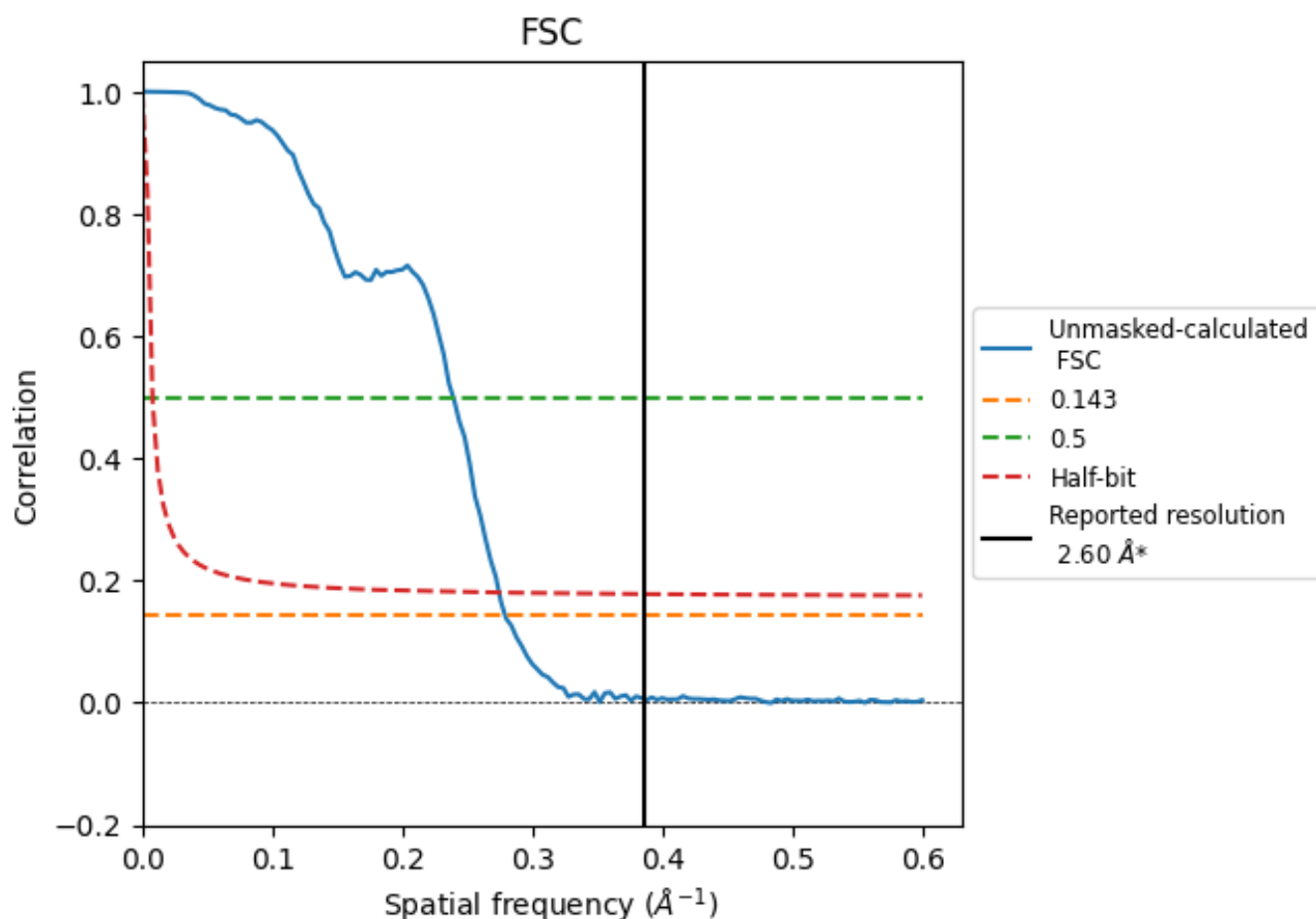


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 \AA^{-1}

8.2 Resolution estimates [i](#)

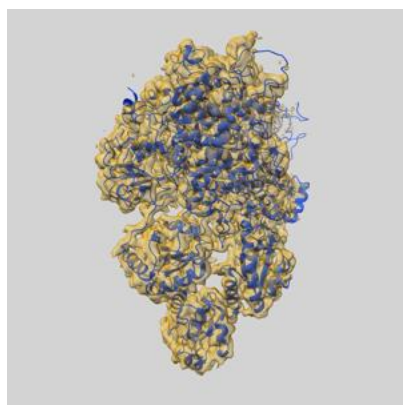
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.59	4.19	3.65

*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 3.59 differs from the reported value 2.6 by more than 10 %

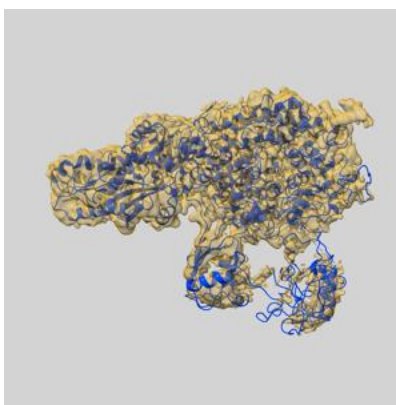
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17749 and PDB model 8PKO. Per-residue inclusion information can be found in section [3](#) on page [8](#).

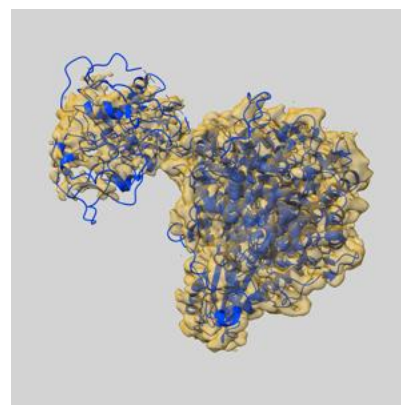
9.1 Map-model overlay [i](#)



X



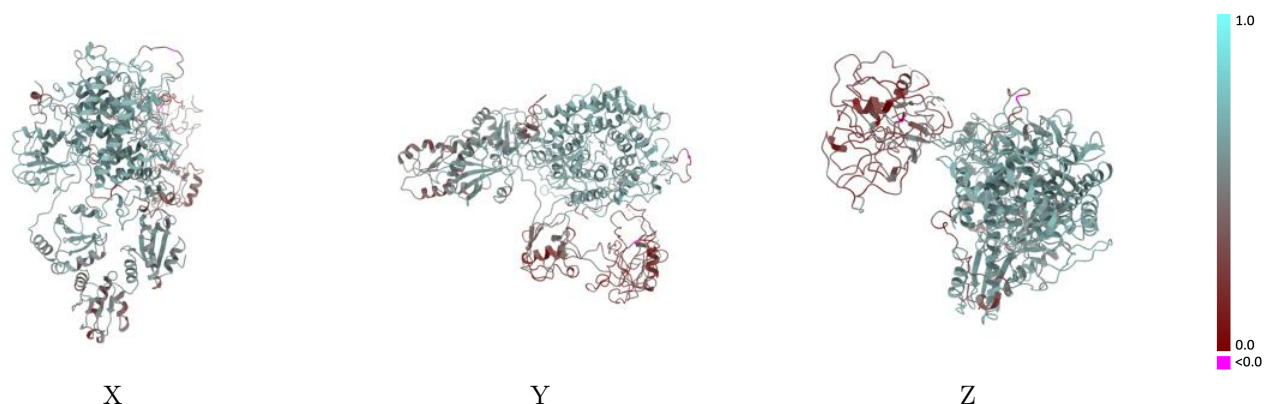
Y



Z

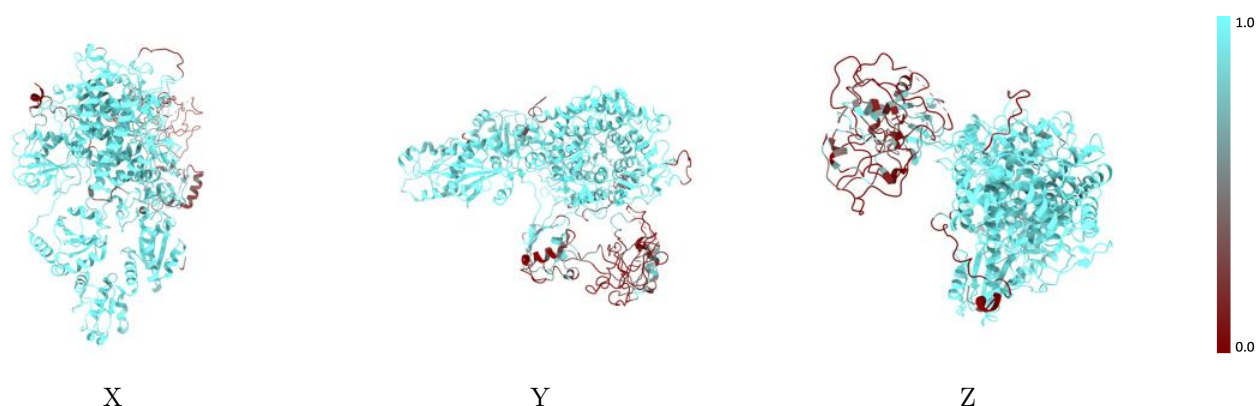
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



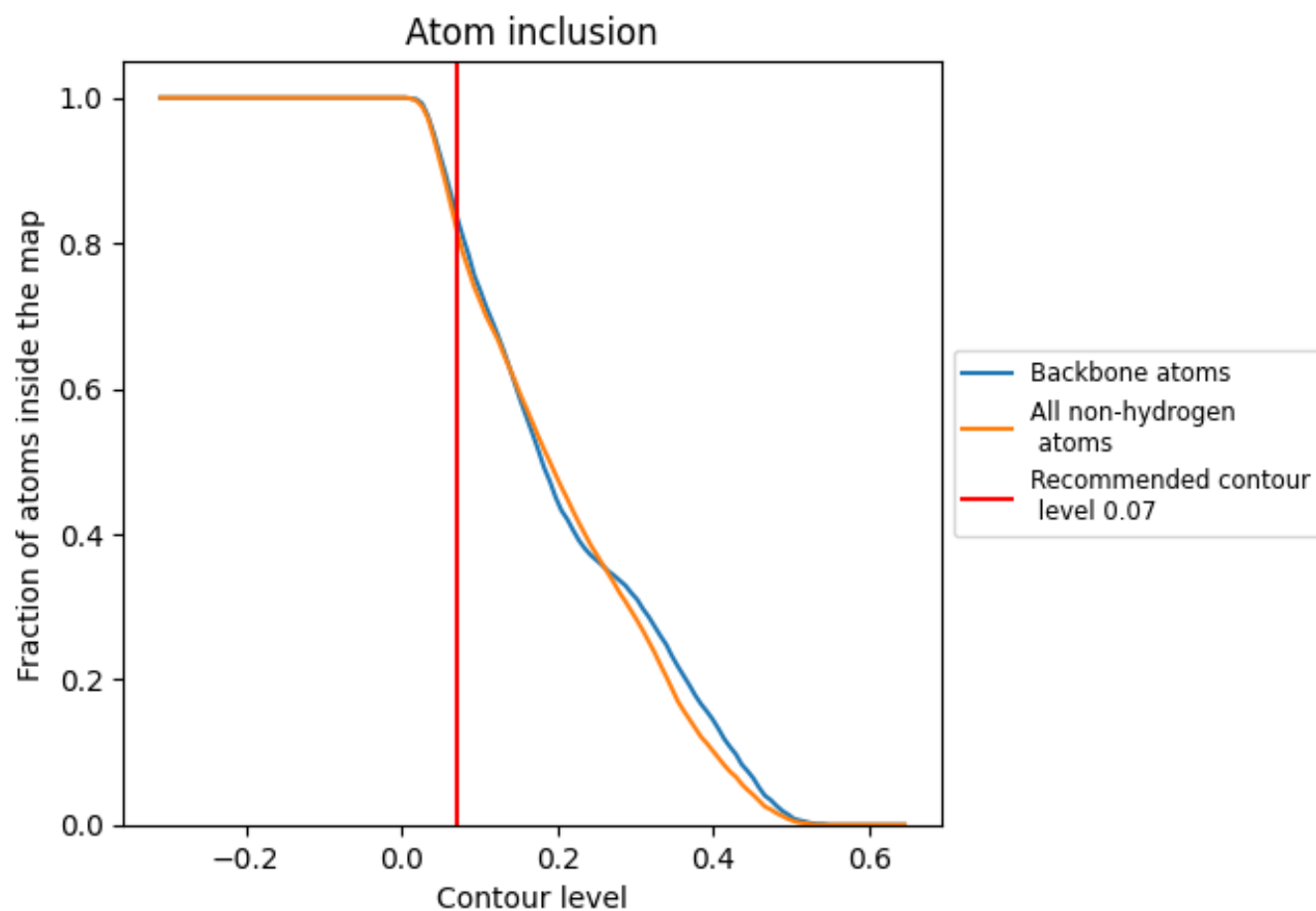
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 82% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8200	<div></div> 0.5200
A	<div></div> 0.7580	<div></div> 0.5100
B	<div></div> 0.9460	<div></div> 0.5390
C	<div></div> 0.9020	<div></div> 0.5670
D	<div></div> 0.7860	<div></div> 0.4760
E	<div></div> 0.8360	<div></div> 0.5250

