



Full wwPDB EM Validation Report ⓘ

May 7, 2026 – 12:32 PM JST

PDB ID : 9VA2 / pdb_00009va2
EMDB ID : EMD-64897
Title : Structure of the ACE2-B0AT1 bound with Phenylalanine
Authors : Yan, R.H.; Zhang, T.
Deposited on : 2025-06-02
Resolution : 2.87 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

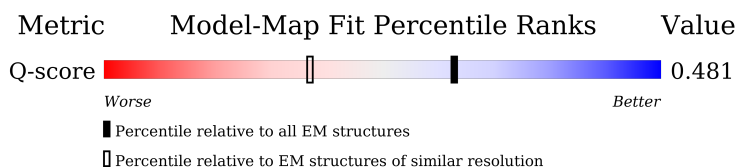
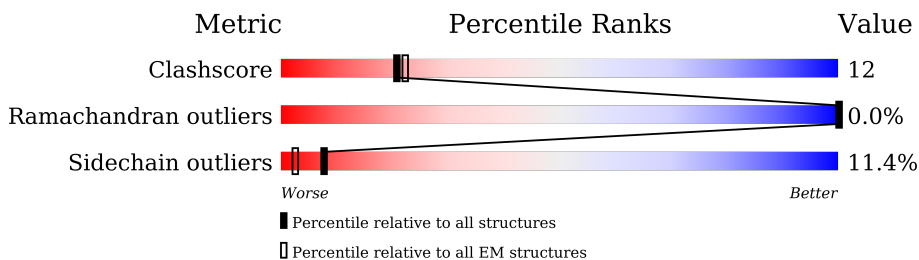
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.87 Å.

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






Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12062 (2.37 - 3.37)

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	808	
1	C	808	
2	B	652	
2	D	652	
3	H	2	

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Mol	Chain	Length	Quality of chain
3	J	2	 50%50%
3	N	2	 50%50%
3	S	2	 50%100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	901	-	-	X	-
5	PHE	B	704	-	-	X	-
5	PHE	D	704	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22094 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 Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	749	Total	C	N	O	S	0	0
			6096	3910	1019	1133	34		
1	C	749	Total	C	N	O	S	0	0
			6096	3910	1019	1133	34		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	TRP	-	expression tag	UNP Q9BYF1
A	11	SER	-	expression tag	UNP Q9BYF1
A	12	HIS	-	expression tag	UNP Q9BYF1
A	13	PRO	-	expression tag	UNP Q9BYF1
A	14	GLN	-	expression tag	UNP Q9BYF1
A	15	PHE	-	expression tag	UNP Q9BYF1
A	16	GLU	-	expression tag	UNP Q9BYF1
A	17	LYS	-	expression tag	UNP Q9BYF1
A	806	LEU	-	expression tag	UNP Q9BYF1
A	807	GLU	-	expression tag	UNP Q9BYF1
A	808	HIS	-	expression tag	UNP Q9BYF1
A	809	HIS	-	expression tag	UNP Q9BYF1
A	810	HIS	-	expression tag	UNP Q9BYF1
A	811	HIS	-	expression tag	UNP Q9BYF1
A	812	HIS	-	expression tag	UNP Q9BYF1
A	813	HIS	-	expression tag	UNP Q9BYF1
A	814	HIS	-	expression tag	UNP Q9BYF1
A	815	HIS	-	expression tag	UNP Q9BYF1
A	816	HIS	-	expression tag	UNP Q9BYF1
A	817	HIS	-	expression tag	UNP Q9BYF1
C	10	TRP	-	expression tag	UNP Q9BYF1
C	11	SER	-	expression tag	UNP Q9BYF1
C	12	HIS	-	expression tag	UNP Q9BYF1
C	13	PRO	-	expression tag	UNP Q9BYF1
C	14	GLN	-	expression tag	UNP Q9BYF1
C	15	PHE	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	16	GLU	-	expression tag	UNP Q9BYF1
C	17	LYS	-	expression tag	UNP Q9BYF1
C	806	LEU	-	expression tag	UNP Q9BYF1
C	807	GLU	-	expression tag	UNP Q9BYF1
C	808	HIS	-	expression tag	UNP Q9BYF1
C	809	HIS	-	expression tag	UNP Q9BYF1
C	810	HIS	-	expression tag	UNP Q9BYF1
C	811	HIS	-	expression tag	UNP Q9BYF1
C	812	HIS	-	expression tag	UNP Q9BYF1
C	813	HIS	-	expression tag	UNP Q9BYF1
C	814	HIS	-	expression tag	UNP Q9BYF1
C	815	HIS	-	expression tag	UNP Q9BYF1
C	816	HIS	-	expression tag	UNP Q9BYF1
C	817	HIS	-	expression tag	UNP Q9BYF1

- Molecule 2 is a protein called Sodium-dependent neutral amino acid transporter B(0)AT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	605	Total	C	N	O	S	0	0
			4799	3171	744	854	30		
2	D	605	Total	C	N	O	S	0	0
			4799	3171	744	854	30		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	ASP	-	expression tag	UNP Q695T7
B	-16	TYR	-	expression tag	UNP Q695T7
B	-15	LYS	-	expression tag	UNP Q695T7
B	-14	ASP	-	expression tag	UNP Q695T7
B	-13	ASP	-	expression tag	UNP Q695T7
B	-12	ASP	-	expression tag	UNP Q695T7
B	-11	ASP	-	expression tag	UNP Q695T7
B	-10	LYS	-	expression tag	UNP Q695T7
B	-9	SER	-	expression tag	UNP Q695T7
B	-8	GLY	-	expression tag	UNP Q695T7
B	-7	PRO	-	expression tag	UNP Q695T7
B	-6	ASP	-	expression tag	UNP Q695T7
B	-5	GLU	-	expression tag	UNP Q695T7
B	-4	VAL	-	expression tag	UNP Q695T7
B	-3	ASP	-	expression tag	UNP Q695T7
B	-2	ALA	-	expression tag	UNP Q695T7

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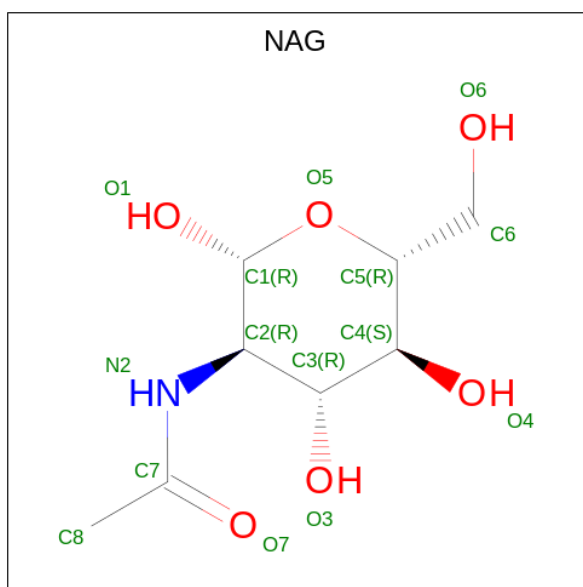
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	SER	-	expression tag	UNP Q695T7
B	0	GLY	-	expression tag	UNP Q695T7
B	1	ARG	-	expression tag	UNP Q695T7
D	-17	ASP	-	expression tag	UNP Q695T7
D	-16	TYR	-	expression tag	UNP Q695T7
D	-15	LYS	-	expression tag	UNP Q695T7
D	-14	ASP	-	expression tag	UNP Q695T7
D	-13	ASP	-	expression tag	UNP Q695T7
D	-12	ASP	-	expression tag	UNP Q695T7
D	-11	ASP	-	expression tag	UNP Q695T7
D	-10	LYS	-	expression tag	UNP Q695T7
D	-9	SER	-	expression tag	UNP Q695T7
D	-8	GLY	-	expression tag	UNP Q695T7
D	-7	PRO	-	expression tag	UNP Q695T7
D	-6	ASP	-	expression tag	UNP Q695T7
D	-5	GLU	-	expression tag	UNP Q695T7
D	-4	VAL	-	expression tag	UNP Q695T7
D	-3	ASP	-	expression tag	UNP Q695T7
D	-2	ALA	-	expression tag	UNP Q695T7
D	-1	SER	-	expression tag	UNP Q695T7
D	0	GLY	-	expression tag	UNP Q695T7
D	1	ARG	-	expression tag	UNP Q695T7

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



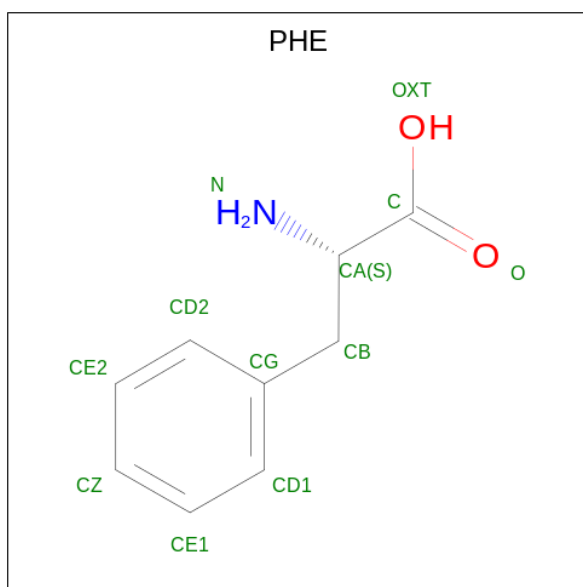
Mol	Chain	Residues	Atoms				AltConf	Trace
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		

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



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

- Molecule 5 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).

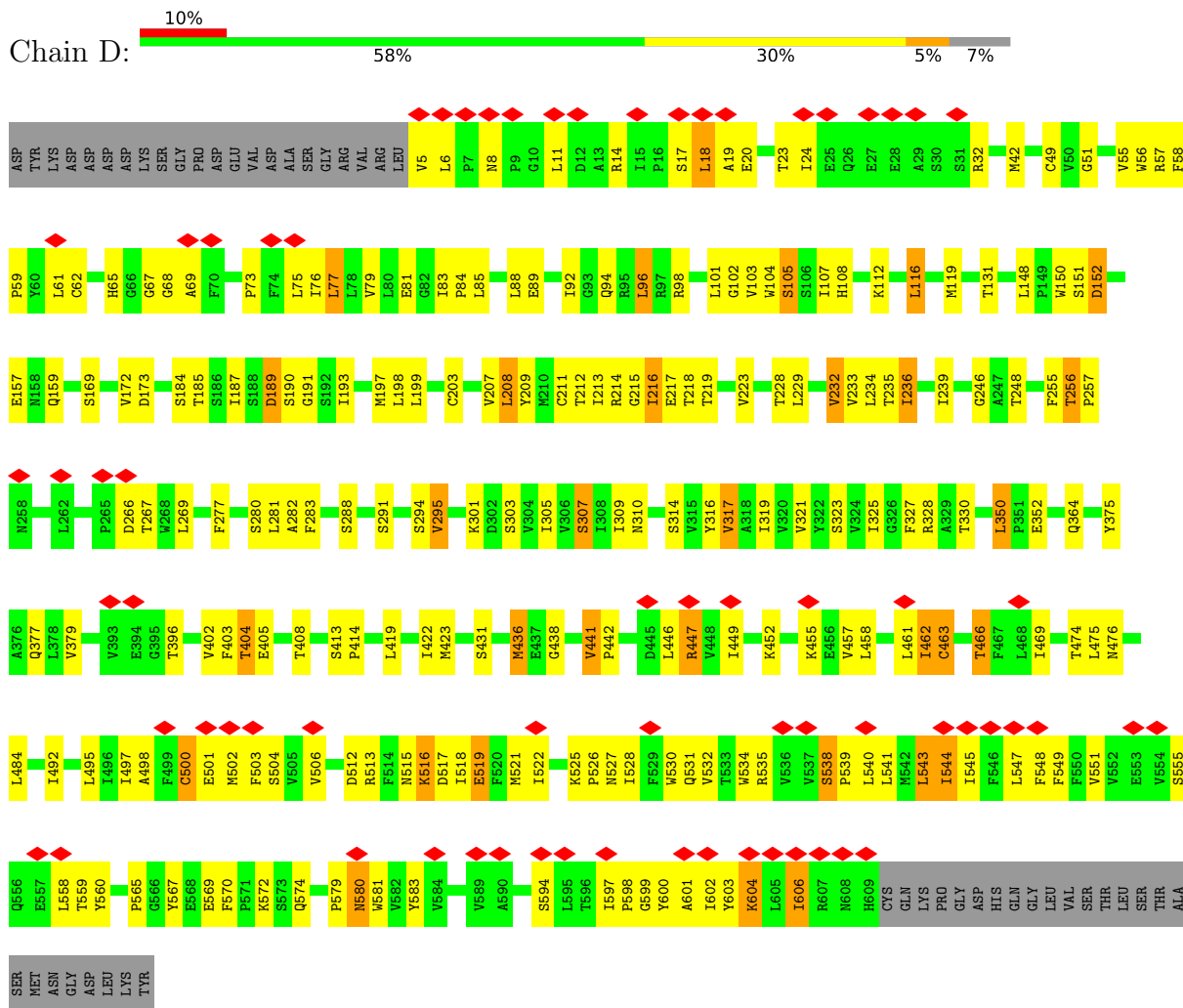


Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			12	9	1	2	
5	D	1	Total	C	N	O	0
			12	9	1	2	



THR
LEU
SER
THR
ALA
ASP
SER
MET
ASN
GLY
ASP
LEU
LYS
TYR

• Molecule 2: Sodium-dependent neutral amino acid transporter B(0)AT1

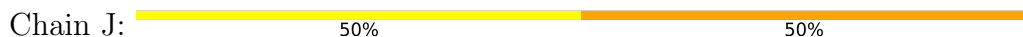


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2

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



MAG1
MAG2

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

Chain N:  50% 50%

MAG1
MAG2

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

Chain S:  50% 100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	361209	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.424	Depositor
Minimum map value	-2.455	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.22	Depositor
Map size (\AA)	307.80002, 307.80002, 307.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8550001, 0.8550001, 0.8550001	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/6259	0.49	0/8498
1	C	0.30	0/6259	0.49	0/8498
2	B	0.22	0/4940	0.49	0/6748
2	D	0.22	0/4940	0.49	0/6748
All	All	0.27	0/22398	0.49	0/30492

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6096	0	5906	126	0
1	C	6096	0	5907	120	0
2	B	4799	0	4763	143	0
2	D	4799	0	4764	141	0
3	H	28	0	25	0	0
3	J	28	0	25	2	0
3	N	28	0	25	3	0
3	S	28	0	25	0	0
4	A	42	0	39	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	42	0	39	2	0
4	C	42	0	39	1	0
4	D	42	0	39	0	0
5	B	12	0	8	6	0
5	D	12	0	8	7	0
All	All	22094	0	21612	524	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 12.

All (524) 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:81:GLN:NE2	4:A:901:NAG:H82	1.71	1.04
1:A:620:VAL:O	1:A:680:SER:HA	1.69	0.93
1:C:620:VAL:O	1:C:680:SER:HA	1.69	0.92
2:B:212:THR:HG21	2:B:436:MET:HG3	1.56	0.88
2:D:212:THR:HG21	2:D:436:MET:HG3	1.56	0.86
1:A:295:ASP:OD1	1:A:295:ASP:N	2.17	0.78
1:A:81:GLN:NE2	4:A:901:NAG:C8	2.48	0.76
2:B:198:LEU:HG	2:B:474:THR:HG21	1.67	0.75
2:D:198:LEU:HG	2:D:474:THR:HG21	1.67	0.74
1:C:53:ASN:OD1	1:C:340:GLN:NE2	2.21	0.74
1:A:53:ASN:OD1	1:A:340:GLN:NE2	2.21	0.73
1:C:295:ASP:OD1	1:C:295:ASP:N	2.17	0.71
2:B:11:LEU:HA	2:B:14:ARG:HH21	1.56	0.71
2:D:11:LEU:HA	2:D:14:ARG:HH21	1.56	0.71
1:A:99:ALA:O	1:A:102:GLN:NE2	2.24	0.71
2:B:49:CYS:HB3	2:B:310:ASN:HD21	1.55	0.71
2:D:213:ILE:HG23	2:D:214:ARG:HG3	1.72	0.70
2:D:69:ALA:HB2	2:D:257:PRO:HA	1.74	0.70
1:A:81:GLN:HE22	4:A:901:NAG:C8	2.05	0.70
2:D:98:ARG:HE	2:D:102:GLY:HA3	1.56	0.70
2:B:213:ILE:HG23	2:B:214:ARG:HG3	1.72	0.70
2:B:69:ALA:HB2	2:B:257:PRO:HA	1.74	0.70
2:D:49:CYS:HB3	2:D:310:ASN:HD21	1.55	0.70
1:A:22:GLU:HG2	1:A:26:LYS:HE2	1.73	0.70
1:A:644:ARG:NH1	1:A:667:GLU:OE1	2.25	0.70
2:B:354:ASN:OD1	4:B:703:NAG:N2	2.25	0.70
1:C:22:GLU:HG2	1:C:26:LYS:HE2	1.73	0.69
2:D:6:LEU:HD23	2:D:8:ASN:H	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:519:GLU:HG3	2:D:525:LYS:HD3	1.74	0.69
2:B:519:GLU:HG3	2:B:525:LYS:HD3	1.74	0.69
2:B:6:LEU:HD23	2:B:8:ASN:H	1.57	0.69
1:A:111:ASP:OD1	1:A:111:ASP:N	2.27	0.68
1:C:644:ARG:NH1	1:C:667:GLU:OE1	2.25	0.68
2:B:98:ARG:HE	2:B:102:GLY:HA3	1.56	0.68
2:D:116:LEU:HA	2:D:119:MET:HE3	1.75	0.68
2:D:513:ARG:HA	2:D:516:LYS:HE2	1.76	0.68
1:C:420:SER:OG	4:C:902:NAG:H83	1.94	0.67
2:D:191:GLY:HA3	2:D:476:ASN:HD22	1.59	0.67
1:A:757:ILE:O	1:A:761:ILE:HG23	1.95	0.67
1:C:757:ILE:O	1:C:761:ILE:HG23	1.95	0.67
2:B:513:ARG:HA	2:B:516:LYS:HE2	1.76	0.67
2:D:189:ASP:N	2:D:189:ASP:OD2	2.28	0.67
2:B:189:ASP:OD2	2:B:189:ASP:N	2.28	0.67
1:C:111:ASP:N	1:C:111:ASP:OD1	2.27	0.67
2:B:116:LEU:HA	2:B:119:MET:HE3	1.75	0.66
1:C:325:GLN:HE21	1:C:325:GLN:HA	1.60	0.66
1:A:325:GLN:HA	1:A:325:GLN:HE21	1.60	0.66
2:B:458:LEU:O	2:B:462:ILE:HG23	1.97	0.65
1:A:245:ARG:NH2	1:A:260:GLY:O	2.28	0.65
1:A:68:LYS:NZ	1:A:68:LYS:HB3	2.12	0.65
2:D:502:MET:HE2	2:D:538:SER:HB3	1.78	0.65
2:B:598:PRO:O	2:B:601:ALA:HB3	1.97	0.65
2:B:191:GLY:HA3	2:B:476:ASN:HD22	1.59	0.64
1:C:99:ALA:O	1:C:102:GLN:NE2	2.24	0.64
2:D:598:PRO:O	2:D:601:ALA:HB3	1.97	0.64
2:D:458:LEU:O	2:D:462:ILE:HG23	1.97	0.64
2:B:502:MET:HE2	2:B:538:SER:HB3	1.78	0.64
1:C:68:LYS:NZ	1:C:68:LYS:HB3	2.12	0.64
1:A:308:PHE:HE1	1:A:358:ILE:HD13	1.63	0.64
1:C:308:PHE:HE1	1:C:358:ILE:HD13	1.63	0.64
1:A:420:SER:OG	4:A:902:NAG:H83	1.97	0.63
1:C:24:GLN:HA	1:C:27:THR:HG22	1.79	0.63
1:C:245:ARG:NH2	1:C:260:GLY:O	2.28	0.63
1:A:23:GLU:HG3	1:A:24:GLN:HG3	1.81	0.63
2:B:213:ILE:HG22	2:B:218:THR:HG21	1.81	0.63
2:D:62:CYS:O	2:D:67:GLY:N	2.31	0.63
2:B:62:CYS:O	2:B:67:GLY:N	2.31	0.63
1:C:88:ILE:HG22	1:C:94:LYS:H	1.63	0.63
1:A:88:ILE:HG22	1:A:94:LYS:H	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:208:LEU:HD11	2:D:436:MET:HG2	1.81	0.62
1:A:95:LEU:HA	1:A:98:GLN:HB2	1.81	0.62
2:D:213:ILE:HG22	2:D:218:THR:HG21	1.81	0.62
1:A:24:GLN:HA	1:A:27:THR:HG22	1.79	0.62
2:B:208:LEU:HD11	2:B:436:MET:HG2	1.80	0.62
1:C:95:LEU:HA	1:C:98:GLN:HB2	1.81	0.62
2:B:190:SER:OG	2:B:191:GLY:N	2.33	0.61
1:C:580:ASN:HD21	1:C:582:ARG:HB2	1.66	0.61
1:C:23:GLU:HG3	1:C:24:GLN:HG3	1.81	0.61
1:A:580:ASN:HD21	1:A:582:ARG:HB2	1.66	0.60
2:D:567:TYR:HE2	2:D:574:GLN:HE21	1.47	0.60
2:D:283:PHE:CE2	5:D:704:PHE:HE2	2.19	0.60
2:B:233:VAL:HG21	2:B:423:MET:HB2	1.84	0.60
2:B:567:TYR:HE2	2:B:574:GLN:HE21	1.47	0.60
1:A:465:LYS:HG3	1:A:467:GLU:HG3	1.83	0.60
2:D:190:SER:OG	2:D:191:GLY:N	2.33	0.60
1:C:293:VAL:HG13	1:C:366:MET:HE3	1.83	0.60
2:B:512:ASP:O	2:B:516:LYS:HG2	2.02	0.59
1:C:465:LYS:HG3	1:C:467:GLU:HG3	1.84	0.59
2:D:233:VAL:HG21	2:D:423:MET:HB2	1.84	0.59
1:A:293:VAL:HG13	1:A:366:MET:HE3	1.83	0.59
1:C:739:VAL:HG23	1:C:741:ILE:HG13	1.85	0.59
2:D:185:THR:OG1	2:D:189:ASP:OD1	2.21	0.59
2:B:551:VAL:O	2:B:555:SER:OG	2.21	0.59
1:C:678:ARG:HB2	2:D:350:LEU:O	2.03	0.58
2:D:512:ASP:O	2:D:516:LYS:HG2	2.02	0.58
2:B:185:THR:OG1	2:B:189:ASP:OD1	2.21	0.58
2:D:116:LEU:O	2:D:119:MET:HG2	2.04	0.58
2:B:431:SER:HB3	5:B:704:PHE:HD1	1.69	0.57
2:D:551:VAL:O	2:D:555:SER:OG	2.21	0.57
2:B:540:LEU:O	2:B:544:ILE:HG23	2.05	0.57
1:C:25:ALA:HB1	1:C:97:LEU:HD21	1.87	0.57
2:B:20:GLU:O	2:B:24:ILE:HG12	2.05	0.57
2:B:599:GLY:O	2:B:602:ILE:HG13	2.05	0.57
1:C:212:VAL:HG11	1:C:565:PRO:HG2	1.87	0.57
1:C:292:ASP:OD1	1:C:294:THR:HG23	2.05	0.57
1:A:212:VAL:HG11	1:A:565:PRO:HG2	1.87	0.57
1:C:457:GLU:HG2	1:C:512:PHE:HB3	1.87	0.56
2:D:20:GLU:O	2:D:24:ILE:HG12	2.05	0.56
1:A:292:ASP:OD1	1:A:294:THR:HG23	2.05	0.56
1:C:136:ASP:OD2	3:N:1:NAG:C8	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:753:ILE:HD11	2:D:207:VAL:HG23	1.87	0.56
2:D:540:LEU:O	2:D:544:ILE:HG23	2.05	0.56
2:D:599:GLY:O	2:D:602:ILE:HG13	2.05	0.56
1:A:56:GLU:OE2	1:A:56:GLU:HA	2.06	0.56
1:A:93:VAL:O	1:A:94:LYS:NZ	2.36	0.56
2:B:116:LEU:O	2:B:119:MET:HG2	2.04	0.56
1:C:750:MET:O	1:C:754:VAL:HG23	2.06	0.56
1:A:457:GLU:HG2	1:A:512:PHE:HB3	1.87	0.56
1:A:25:ALA:HB1	1:A:97:LEU:HD21	1.87	0.56
1:A:750:MET:O	1:A:754:VAL:HG23	2.06	0.56
1:C:543:ASP:OD1	1:C:544:ILE:N	2.39	0.55
2:B:73:PRO:HA	2:B:76:ILE:HG22	1.89	0.55
2:B:283:PHE:CE2	5:B:704:PHE:HE2	2.23	0.55
1:A:346:PRO:HA	1:A:359:LEU:O	2.07	0.55
2:B:68:GLY:HA3	2:B:256:THR:H	1.71	0.55
2:D:527:ASN:H	2:D:530:TRP:HD1	1.55	0.55
1:C:68:LYS:HB3	1:C:68:LYS:HZ2	1.69	0.55
1:C:313:LYS:O	1:C:317:SER:OG	2.24	0.55
2:B:527:ASN:H	2:B:530:TRP:HD1	1.55	0.55
2:D:539:PRO:O	2:D:543:LEU:HG	2.06	0.55
2:D:68:GLY:HA3	2:D:256:THR:H	1.71	0.55
2:D:73:PRO:HA	2:D:76:ILE:HG22	1.89	0.55
1:A:543:ASP:OD1	1:A:544:ILE:N	2.39	0.55
1:A:313:LYS:O	1:A:317:SER:OG	2.24	0.54
1:C:93:VAL:O	1:C:94:LYS:NZ	2.35	0.54
1:A:68:LYS:HB3	1:A:68:LYS:HZ2	1.70	0.54
2:B:56:TRP:CZ3	2:B:396:THR:HG22	2.42	0.54
2:B:539:PRO:O	2:B:543:LEU:HG	2.06	0.54
1:A:85:LEU:HD13	1:A:85:LEU:H	1.73	0.54
1:C:332:MET:HE2	1:C:336:PRO:HD3	1.90	0.54
1:A:209:VAL:HG11	1:A:565:PRO:HB3	1.90	0.54
2:D:56:TRP:CZ3	2:D:396:THR:HG22	2.42	0.54
2:B:462:ILE:O	2:B:466:THR:OG1	2.25	0.54
1:A:332:MET:HE2	1:A:336:PRO:HD3	1.90	0.54
1:C:56:GLU:OE2	1:C:56:GLU:HA	2.06	0.54
1:C:617:SER:O	1:C:697:ARG:NH1	2.40	0.54
2:D:462:ILE:O	2:D:466:THR:OG1	2.25	0.54
2:D:236:ILE:O	2:D:239:ILE:HG13	2.08	0.54
2:B:20:GLU:O	2:B:23:THR:OG1	2.21	0.54
1:C:346:PRO:HA	1:C:359:LEU:O	2.07	0.54
2:D:431:SER:HB3	5:D:704:PHE:HD1	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:SER:O	1:A:697:ARG:NH1	2.40	0.53
2:B:236:ILE:O	2:B:239:ILE:HG13	2.07	0.53
1:C:71:ALA:HA	1:C:74:LYS:HE3	1.90	0.53
2:B:528:ILE:HA	2:B:531:GLN:HG2	1.90	0.53
1:C:136:ASP:OD2	3:N:1:NAG:H81	2.08	0.53
1:C:623:SER:HB3	2:D:352:GLU:OE2	2.08	0.53
2:D:528:ILE:HA	2:D:531:GLN:HG2	1.90	0.53
1:C:209:VAL:HG11	1:C:565:PRO:HB3	1.90	0.53
2:D:11:LEU:HD11	2:D:108:HIS:H	1.74	0.53
1:A:325:GLN:HE21	1:A:325:GLN:CA	2.22	0.53
2:B:518:ILE:O	2:B:522:ILE:HG12	2.09	0.53
2:B:558:LEU:HD11	2:B:583:TYR:HE1	1.74	0.53
1:C:740:SER:HB3	1:C:743:LEU:HB3	1.90	0.53
1:A:71:ALA:HA	1:A:74:LYS:HE3	1.90	0.52
1:C:85:LEU:HD13	1:C:85:LEU:H	1.73	0.52
2:D:518:ILE:O	2:D:522:ILE:HG12	2.09	0.52
2:D:558:LEU:HD11	2:D:583:TYR:HE1	1.74	0.52
2:D:602:ILE:O	2:D:606:ILE:HG23	2.10	0.52
2:B:11:LEU:HD11	2:B:108:HIS:H	1.74	0.52
2:D:105:SER:HB3	2:D:112:LYS:HG3	1.91	0.52
1:A:81:GLN:CD	4:A:901:NAG:H82	2.33	0.52
2:B:565:PRO:HA	2:B:570:PHE:CD1	2.45	0.52
1:C:325:GLN:HE21	1:C:325:GLN:CA	2.22	0.52
2:D:565:PRO:HA	2:D:570:PHE:CD1	2.45	0.52
2:B:602:ILE:O	2:B:606:ILE:HG23	2.10	0.52
1:A:733:PRO:HA	2:B:159:GLN:HE22	1.75	0.52
1:C:750:MET:HE1	2:D:203:CYS:HA	1.91	0.52
2:D:531:GLN:OE1	2:D:535:ARG:NH2	2.38	0.51
2:B:303:SER:O	2:B:307:SER:OG	2.28	0.51
2:D:301:LYS:O	2:D:305:ILE:HG13	2.10	0.51
2:B:150:TRP:HB2	2:B:172:VAL:HG12	1.92	0.51
2:B:105:SER:HB3	2:B:112:LYS:HG3	1.91	0.51
1:C:94:LYS:N	1:C:94:LYS:HD2	2.26	0.51
1:C:81:GLN:OE1	1:C:81:GLN:HA	2.11	0.51
2:D:446:LEU:HD23	2:D:446:LEU:O	2.11	0.51
2:B:446:LEU:HD23	2:B:446:LEU:O	2.11	0.51
2:D:283:PHE:CE2	5:D:704:PHE:CE2	2.99	0.51
1:A:225:ASP:OD2	1:A:578:ASN:ND2	2.43	0.51
2:B:32:ARG:NH1	2:B:291:SER:OG	2.44	0.51
1:C:87:GLU:OE2	1:C:87:GLU:HA	2.11	0.51
2:D:11:LEU:HD12	2:D:107:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:GLU:HA	2:B:92:ILE:HG22	1.93	0.51
2:B:152:ASP:OD1	2:B:152:ASP:N	2.44	0.51
2:D:303:SER:O	2:D:307:SER:OG	2.28	0.51
2:B:294:SER:OG	2:B:295:VAL:N	2.44	0.51
2:B:301:LYS:O	2:B:305:ILE:HG13	2.10	0.50
2:B:531:GLN:O	2:B:535:ARG:HG2	2.11	0.50
1:C:27:THR:O	1:C:31:LYS:HG2	2.12	0.50
2:D:32:ARG:NH1	2:D:291:SER:OG	2.44	0.50
2:B:404:THR:O	2:B:408:THR:HG23	2.11	0.50
2:D:150:TRP:HB2	2:D:172:VAL:HG12	1.92	0.50
2:D:404:THR:O	2:D:408:THR:HG23	2.11	0.50
2:D:531:GLN:O	2:D:535:ARG:HG2	2.11	0.50
1:A:94:LYS:HD2	1:A:94:LYS:N	2.26	0.50
2:B:11:LEU:HD12	2:B:107:ILE:HD12	1.92	0.50
2:B:295:VAL:HG12	2:B:521:MET:HE3	1.94	0.50
2:D:89:GLU:HA	2:D:92:ILE:HG22	1.93	0.50
1:A:87:GLU:OE2	1:A:87:GLU:HA	2.11	0.50
2:B:234:LEU:HD21	2:B:317:VAL:HG23	1.94	0.50
2:D:75:LEU:O	2:D:79:VAL:HG23	2.11	0.50
3:N:1:NAG:H62	3:N:2:NAG:HN2	1.76	0.50
1:A:81:GLN:NE2	4:A:901:NAG:C7	2.75	0.50
1:A:81:GLN:HE22	4:A:901:NAG:C7	2.24	0.50
1:A:81:GLN:OE1	1:A:81:GLN:HA	2.11	0.50
2:B:282:ALA:HB1	2:B:497:ILE:HD11	1.94	0.50
2:B:458:LEU:HA	2:B:461:LEU:HD12	1.94	0.50
2:D:277:PHE:CZ	5:D:704:PHE:HB2	2.46	0.50
1:A:53:ASN:HA	1:A:340:GLN:NE2	2.27	0.50
2:D:20:GLU:O	2:D:23:THR:OG1	2.21	0.50
1:A:86:GLN:HG3	1:A:87:GLU:H	1.77	0.50
1:C:53:ASN:HA	1:C:340:GLN:NE2	2.27	0.50
1:C:493:HIS:HD2	1:C:499:ASP:OD2	1.95	0.50
2:D:458:LEU:HA	2:D:461:LEU:HD12	1.94	0.50
2:B:232:VAL:O	2:B:235:THR:OG1	2.27	0.49
2:D:282:ALA:HB1	2:D:497:ILE:HD11	1.94	0.49
3:J:1:NAG:H62	3:J:2:NAG:HN2	1.76	0.49
2:B:75:LEU:O	2:B:79:VAL:HG23	2.12	0.49
2:D:56:TRP:HZ3	2:D:396:THR:HG22	1.77	0.49
2:D:216:ILE:O	2:D:217:GLU:HB3	2.13	0.49
1:A:294:THR:O	1:A:298:VAL:HG23	2.13	0.49
1:C:86:GLN:HG3	1:C:87:GLU:H	1.77	0.49
2:D:294:SER:OG	2:D:295:VAL:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:VAL:C	1:A:94:LYS:HZ2	2.20	0.49
2:D:526:PRO:HB2	2:D:531:GLN:HE22	1.78	0.49
1:A:27:THR:O	1:A:31:LYS:HG2	2.12	0.49
1:C:471:ASP:OD1	1:C:471:ASP:N	2.46	0.49
2:B:184:SER:OG	2:B:476:ASN:HB3	2.13	0.48
2:B:413:SER:N	2:B:414:PRO:HD2	2.28	0.48
1:C:41:TYR:OH	1:C:355:ASP:OD1	2.24	0.48
2:D:184:SER:OG	2:D:476:ASN:HB3	2.13	0.48
1:A:493:HIS:HD2	1:A:499:ASP:OD2	1.95	0.48
1:C:225:ASP:OD2	1:C:578:ASN:ND2	2.43	0.48
1:C:294:THR:O	1:C:298:VAL:HG23	2.13	0.48
2:D:94:GLN:HG2	2:D:521:MET:HE1	1.96	0.48
2:B:235:THR:HG22	2:B:316:TYR:OH	2.13	0.48
2:D:234:LEU:HD21	2:D:317:VAL:HG23	1.94	0.48
2:B:56:TRP:HZ3	2:B:396:THR:HG22	1.77	0.48
2:B:526:PRO:HB2	2:B:531:GLN:HE22	1.78	0.48
1:C:733:PRO:HB3	2:D:159:GLN:HE22	1.78	0.48
2:D:235:THR:HG22	2:D:316:TYR:OH	2.13	0.48
2:D:295:VAL:HG12	2:D:521:MET:HE3	1.94	0.48
2:B:216:ILE:O	2:B:217:GLU:HB3	2.13	0.48
2:B:232:VAL:O	2:B:236:ILE:HG23	2.14	0.48
2:D:232:VAL:O	2:D:236:ILE:HG23	2.14	0.48
1:A:471:ASP:OD1	1:A:471:ASP:N	2.46	0.48
2:B:515:ASN:ND2	2:B:525:LYS:HE3	2.29	0.48
2:B:277:PHE:CZ	5:B:704:PHE:HB2	2.48	0.48
1:C:65:ALA:O	1:C:68:LYS:NZ	2.46	0.48
1:A:57:GLU:HA	1:A:60:GLN:NE2	2.29	0.48
2:D:515:ASN:ND2	2:D:525:LYS:HE3	2.29	0.48
2:B:148:LEU:O	2:B:151:SER:OG	2.22	0.47
2:D:413:SER:N	2:D:414:PRO:HD2	2.28	0.47
1:A:136:ASP:OD2	3:J:1:NAG:C8	2.63	0.47
2:D:58:PHE:HB3	2:D:59:PRO:HD3	1.96	0.47
2:D:232:VAL:O	2:D:235:THR:OG1	2.27	0.47
1:A:474:MET:HE1	1:A:499:ASP:HB2	1.97	0.47
2:B:94:GLN:HG2	2:B:521:MET:HE1	1.96	0.47
1:C:57:GLU:HA	1:C:60:GLN:NE2	2.29	0.47
1:C:733:PRO:HB3	2:D:159:GLN:NE2	2.30	0.47
2:B:530:TRP:HB3	2:B:534:TRP:CZ3	2.49	0.47
1:C:474:MET:HE1	1:C:499:ASP:HB2	1.97	0.47
1:A:455:MET:HB3	1:A:455:MET:HE3	1.80	0.47
2:B:58:PHE:HB3	2:B:59:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:604:LYS:HD2	2:B:604:LYS:HA	1.38	0.47
1:C:740:SER:O	1:C:742:TRP:N	2.47	0.47
1:C:761:ILE:HG13	1:C:762:PHE:N	2.29	0.47
2:D:548:PHE:O	2:D:551:VAL:HG22	2.15	0.47
1:A:419:LYS:NZ	1:A:428:PHE:O	2.48	0.47
1:A:65:ALA:O	1:A:68:LYS:NZ	2.46	0.47
2:D:101:LEU:O	2:D:105:SER:OG	2.30	0.47
2:D:530:TRP:HB3	2:D:534:TRP:CZ3	2.49	0.47
1:A:761:ILE:HG13	1:A:762:PHE:N	2.29	0.47
2:D:148:LEU:O	2:D:151:SER:OG	2.22	0.47
2:B:283:PHE:CE2	5:B:704:PHE:CE2	3.02	0.46
2:B:85:LEU:HD21	2:B:498:ALA:HB1	1.97	0.46
2:B:462:ILE:HG13	2:B:463:CYS:N	2.30	0.46
2:D:604:LYS:HA	2:D:604:LYS:HD2	1.38	0.46
1:A:524:GLN:OE1	1:A:580:ASN:N	2.41	0.46
1:A:547:SER:O	1:A:547:SER:OG	2.32	0.46
2:B:525:LYS:HA	2:B:525:LYS:HD2	1.73	0.46
2:B:548:PHE:O	2:B:551:VAL:HG22	2.15	0.46
1:A:125:THR:O	1:A:129:THR:OG1	2.33	0.46
1:A:309:LYS:HA	1:A:309:LYS:HD3	1.67	0.46
2:B:286:LEU:HD12	2:B:286:LEU:HA	1.82	0.46
1:C:105:SER:HB2	1:C:190:MET:HE2	1.98	0.46
1:C:589:GLU:HB3	1:C:590:PRO:HD3	1.98	0.46
2:D:152:ASP:OD1	2:D:152:ASP:N	2.44	0.46
2:B:365:GLN:NE2	4:B:702:NAG:O7	2.35	0.46
1:C:57:GLU:HA	1:C:60:GLN:CD	2.41	0.46
1:C:309:LYS:HA	1:C:309:LYS:HD3	1.67	0.46
2:B:503:PHE:HA	2:B:506:VAL:HG12	1.97	0.46
2:B:531:GLN:OE1	2:B:535:ARG:NH2	2.38	0.46
1:C:93:VAL:C	1:C:94:LYS:HZ2	2.20	0.46
1:C:125:THR:O	1:C:129:THR:OG1	2.33	0.46
1:C:360:MET:HE2	1:C:362:THR:HB	1.98	0.46
1:A:360:MET:HE2	1:A:362:THR:HB	1.98	0.46
2:B:81:GLU:OE2	2:B:538:SER:OG	2.33	0.46
2:B:104:TRP:CZ2	2:B:501:GLU:HB2	2.51	0.46
1:C:107:VAL:HG21	1:C:193:ALA:HB3	1.98	0.46
1:A:57:GLU:HA	1:A:60:GLN:CD	2.41	0.45
1:A:589:GLU:HB3	1:A:590:PRO:HD3	1.98	0.45
2:B:96:LEU:HD22	2:B:103:VAL:HA	1.98	0.45
2:B:209:TYR:HB2	2:B:463:CYS:SG	2.56	0.45
1:C:404:VAL:O	1:C:407:ILE:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:85:LEU:HD21	2:D:498:ALA:HB1	1.98	0.45
2:D:526:PRO:HB2	2:D:531:GLN:NE2	2.31	0.45
1:A:32:PHE:HE1	1:A:391:LEU:HD11	1.81	0.45
1:A:349:TRP:HB2	1:A:357:ARG:HG3	1.98	0.45
2:B:500:CYS:SG	2:B:501:GLU:N	2.90	0.45
2:D:104:TRP:CZ2	2:D:501:GLU:HB2	2.51	0.45
1:A:108:LEU:HD11	1:A:190:MET:HB2	1.99	0.45
2:D:503:PHE:HA	2:D:506:VAL:HG12	1.97	0.45
2:D:558:LEU:HD11	2:D:583:TYR:CE1	2.52	0.45
2:B:101:LEU:O	2:B:105:SER:OG	2.30	0.45
1:C:499:ASP:N	1:C:500:PRO:HD2	2.32	0.45
2:D:569:GLU:OE2	2:D:572:LYS:HG2	2.17	0.45
1:A:107:VAL:HG21	1:A:193:ALA:HB3	1.98	0.45
2:B:447:ARG:HE	2:B:447:ARG:HB2	1.61	0.45
1:A:64:ASN:HA	1:A:67:ASP:OD2	2.17	0.45
2:B:197:MET:HB2	2:B:474:THR:HG23	1.98	0.45
2:D:500:CYS:SG	2:D:501:GLU:N	2.90	0.45
1:A:105:SER:HB2	1:A:190:MET:HE2	1.98	0.45
1:A:404:VAL:O	1:A:407:ILE:HG12	2.16	0.45
2:B:526:PRO:HB2	2:B:531:GLN:NE2	2.31	0.45
1:C:32:PHE:HE1	1:C:391:LEU:HD11	1.81	0.45
1:C:524:GLN:OE1	1:C:580:ASN:N	2.41	0.45
2:D:96:LEU:HD22	2:D:103:VAL:HA	1.98	0.45
1:A:247:LYS:HD3	1:A:247:LYS:HA	1.75	0.44
1:A:499:ASP:N	1:A:500:PRO:HD2	2.32	0.44
1:C:64:ASN:HA	1:C:67:ASP:OD2	2.17	0.44
1:C:349:TRP:HB2	1:C:357:ARG:HG3	1.98	0.44
2:D:518:ILE:HA	2:D:521:MET:HG3	1.99	0.44
2:B:502:MET:CE	2:B:538:SER:HB3	2.47	0.44
1:C:404:VAL:O	1:C:408:MET:HG2	2.17	0.44
2:D:209:TYR:HB2	2:D:463:CYS:SG	2.57	0.44
1:A:403:ALA:O	1:A:407:ILE:HG23	2.17	0.44
2:D:55:VAL:HG12	2:D:56:TRP:HD1	1.82	0.44
2:D:208:LEU:O	2:D:212:THR:HG22	2.17	0.44
2:D:600:TYR:O	2:D:603:TYR:HB3	2.18	0.44
2:B:65:HIS:NE2	2:B:267:THR:HA	2.33	0.44
1:A:404:VAL:O	1:A:408:MET:HG2	2.17	0.44
1:A:740:SER:O	1:A:741:ILE:C	2.61	0.44
2:B:569:GLU:OE2	2:B:572:LYS:HG2	2.17	0.44
1:C:574:VAL:HG23	1:C:576:ALA:H	1.83	0.44
1:C:754:VAL:HA	1:C:757:ILE:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:17:SER:C	2:D:19:ALA:H	2.26	0.44
2:D:197:MET:HB2	2:D:474:THR:HG23	1.98	0.44
2:D:236:ILE:HD11	2:D:419:LEU:HD23	2.00	0.44
2:D:502:MET:CE	2:D:538:SER:HB3	2.47	0.44
1:A:574:VAL:HG23	1:A:576:ALA:H	1.83	0.44
2:B:441:VAL:HG22	2:B:442:PRO:HD3	2.00	0.44
2:B:208:LEU:O	2:B:212:THR:HG22	2.17	0.44
1:C:108:LEU:HD11	1:C:190:MET:HB2	1.99	0.44
1:C:247:LYS:HA	1:C:247:LYS:HD3	1.75	0.44
1:C:325:GLN:O	1:C:329:GLU:HG2	2.18	0.44
1:C:622:ILE:HB	1:C:679:ILE:HB	1.99	0.44
2:D:217:GLU:O	2:D:217:GLU:HG2	2.18	0.44
2:B:169:SER:HB3	2:B:570:PHE:CE2	2.53	0.43
2:B:236:ILE:HD11	2:B:419:LEU:HD23	2.00	0.43
1:C:535:HIS:CD2	1:C:542:CYS:HB2	2.53	0.43
1:C:715:PHE:O	1:C:716:ARG:HB2	2.18	0.43
2:D:441:VAL:HG22	2:D:442:PRO:HD3	2.00	0.43
2:D:525:LYS:HA	2:D:525:LYS:HD2	1.73	0.43
1:A:325:GLN:O	1:A:329:GLU:HG2	2.18	0.43
1:A:619:LYS:NZ	1:A:680:SER:HB2	2.33	0.43
2:B:55:VAL:HG12	2:B:56:TRP:HD1	1.82	0.43
2:B:452:LYS:H	2:B:452:LYS:HG3	1.59	0.43
2:B:466:THR:HA	2:B:469:ILE:HG22	2.01	0.43
2:D:81:GLU:OE2	2:D:538:SER:OG	2.33	0.43
2:D:462:ILE:HG13	2:D:463:CYS:N	2.30	0.43
2:B:558:LEU:HD11	2:B:583:TYR:CE1	2.52	0.43
2:B:600:TYR:O	2:B:603:TYR:HB3	2.18	0.43
2:D:215:GLY:O	2:D:219:THR:HG23	2.17	0.43
1:A:225:ASP:O	1:A:229:THR:HG23	2.19	0.43
1:A:622:ILE:HB	1:A:679:ILE:HB	1.99	0.43
2:D:277:PHE:O	5:D:704:PHE:N	2.52	0.43
2:D:283:PHE:CZ	5:D:704:PHE:HE2	2.35	0.43
1:A:513:ILE:HD12	1:A:513:ILE:HA	1.87	0.43
1:C:287:GLN:OE1	1:C:287:GLN:HA	2.19	0.43
1:C:403:ALA:O	1:C:407:ILE:HG23	2.17	0.43
1:C:455:MET:HE3	1:C:455:MET:HB3	1.80	0.43
1:A:535:HIS:CD2	1:A:542:CYS:HB2	2.53	0.43
2:B:269:LEU:HD13	2:B:549:PHE:HA	2.00	0.43
1:A:363:LYS:HE2	1:A:363:LYS:HB2	1.29	0.43
2:B:17:SER:C	2:B:19:ALA:H	2.26	0.43
2:D:65:HIS:NE2	2:D:267:THR:HA	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ASN:HB3	1:A:58:ASN:ND2	2.34	0.43
1:A:611:SER:OG	1:A:614:ALA:HB2	2.19	0.43
1:A:715:PHE:O	1:A:716:ARG:HB2	2.18	0.43
2:B:528:ILE:O	2:B:532:VAL:HG22	2.19	0.43
2:D:269:LEU:HD13	2:D:549:PHE:HA	2.01	0.43
2:D:364:GLN:HG2	2:D:375:TYR:CE1	2.54	0.43
1:A:227:GLU:HG2	1:A:454:TYR:OH	2.18	0.43
1:A:754:VAL:HA	1:A:757:ILE:HG22	2.00	0.43
1:A:710:ARG:HH21	1:C:715:PHE:HA	1.83	0.42
2:B:215:GLY:O	2:B:219:THR:HG23	2.17	0.42
1:C:225:ASP:O	1:C:229:THR:HG23	2.19	0.42
2:D:169:SER:HB3	2:D:570:PHE:CE2	2.53	0.42
1:A:740:SER:HG	1:A:742:TRP:CD1	2.37	0.42
2:B:364:GLN:HG2	2:B:375:TYR:CE1	2.54	0.42
2:B:518:ILE:HA	2:B:521:MET:HG3	1.99	0.42
1:C:334:THR:OG1	1:C:335:ASP:N	2.52	0.42
1:C:619:LYS:NZ	1:C:680:SER:HB2	2.33	0.42
2:D:20:GLU:N	2:D:20:GLU:OE2	2.53	0.42
2:D:545:ILE:HA	2:D:548:PHE:HB2	2.01	0.42
2:B:83:ILE:HD11	2:B:303:SER:HB3	2.01	0.42
2:B:173:ASP:OD1	2:B:173:ASP:N	2.53	0.42
2:B:431:SER:O	5:B:704:PHE:CE1	2.72	0.42
1:C:144:LEU:HA	1:C:148:LEU:HB2	2.02	0.42
1:A:755:VAL:HA	1:A:758:VAL:HG12	2.02	0.42
1:C:227:GLU:HG2	1:C:454:TYR:OH	2.18	0.42
1:A:144:LEU:HA	1:A:148:LEU:HB2	2.02	0.42
1:A:305:GLN:O	1:A:309:LYS:HG2	2.20	0.42
1:A:418:LEU:HB2	1:A:424:LEU:HD11	2.02	0.42
1:A:423:LEU:HD23	1:A:423:LEU:HA	1.91	0.42
2:B:217:GLU:O	2:B:217:GLU:HG2	2.18	0.42
2:D:528:ILE:O	2:D:532:VAL:HG22	2.19	0.42
2:D:580:ASN:N	2:D:580:ASN:HD22	2.18	0.42
1:A:223:ILE:HG22	1:A:227:GLU:OE2	2.20	0.42
1:A:633:TYR:OH	1:A:715:PHE:O	2.25	0.42
2:B:545:ILE:HA	2:B:548:PHE:HB2	2.01	0.42
1:C:418:LEU:HB2	1:C:424:LEU:HD11	2.02	0.42
1:C:53:ASN:HB3	1:C:58:ASN:ND2	2.34	0.42
2:B:356:THR:OG1	2:B:359:ASN:OD1	2.31	0.42
2:D:17:SER:O	2:D:18:LEU:HG	2.20	0.42
2:B:17:SER:O	2:B:18:LEU:HG	2.20	0.42
1:C:46:ALA:HB1	1:C:62:MET:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:547:SER:O	1:C:547:SER:OG	2.32	0.42
1:C:611:SER:OG	1:C:614:ALA:HB2	2.19	0.42
2:D:466:THR:HA	2:D:469:ILE:HG22	2.01	0.42
2:B:20:GLU:N	2:B:20:GLU:OE2	2.52	0.42
1:C:56:GLU:O	1:C:59:VAL:HG13	2.20	0.42
2:D:77:LEU:HD13	2:D:77:LEU:HA	1.85	0.42
2:B:580:ASN:N	2:B:580:ASN:HD22	2.18	0.41
1:C:513:ILE:HD12	1:C:513:ILE:HA	1.87	0.41
1:A:215:TYR:CD2	1:A:577:LYS:HE3	2.55	0.41
2:B:80:LEU:HD12	2:B:80:LEU:HA	1.91	0.41
2:B:438:GLY:O	2:B:442:PRO:HG2	2.20	0.41
2:D:447:ARG:HE	2:D:447:ARG:HB2	1.61	0.41
1:C:216:ASP:N	1:C:216:ASP:OD1	2.53	0.41
1:A:35:GLU:H	1:A:35:GLU:HG2	1.67	0.41
1:A:287:GLN:HA	1:A:287:GLN:OE1	2.19	0.41
1:C:223:ILE:HG22	1:C:227:GLU:OE2	2.20	0.41
1:C:257:SER:HB3	1:C:610:TRP:CE2	2.56	0.41
1:C:743:LEU:HD12	1:C:743:LEU:HA	1.89	0.41
2:D:187:ILE:HG22	2:D:560:TYR:OH	2.20	0.41
1:A:56:GLU:O	1:A:59:VAL:HG13	2.20	0.41
1:A:216:ASP:OD1	1:A:216:ASP:N	2.53	0.41
1:A:315:PHE:CD1	1:A:380:GLN:HG3	2.56	0.41
1:A:743:LEU:HD12	1:A:743:LEU:HA	1.89	0.41
2:B:11:LEU:HD13	2:B:14:ARG:NH2	2.35	0.41
2:B:101:LEU:HD22	2:B:112:LYS:HE2	2.02	0.41
1:C:215:TYR:CD2	1:C:577:LYS:HE3	2.55	0.41
1:C:315:PHE:CD1	1:C:380:GLN:HG3	2.55	0.41
2:D:83:ILE:HD11	2:D:303:SER:HB3	2.01	0.41
2:D:173:ASP:OD1	2:D:173:ASP:N	2.53	0.41
1:A:35:GLU:HG3	1:A:72:PHE:CZ	2.56	0.41
1:A:46:ALA:HB1	1:A:62:MET:HA	2.01	0.41
1:A:81:GLN:HE22	4:A:901:NAG:H82	1.56	0.41
1:C:102:GLN:OE1	1:C:102:GLN:N	2.42	0.41
1:C:419:LYS:NZ	1:C:428:PHE:O	2.48	0.41
1:C:633:TYR:OH	1:C:715:PHE:O	2.25	0.41
1:A:435:GLU:OE2	1:A:540:HIS:NE2	2.51	0.41
2:B:308:ILE:HD12	2:B:308:ILE:HA	1.90	0.41
1:C:92:THR:HG22	1:C:93:VAL:N	2.36	0.41
1:C:378:HIS:NE2	1:C:402:GLU:OE2	2.53	0.41
1:A:741:ILE:HD13	1:A:744:ILE:HD12	2.03	0.41
2:B:187:ILE:HG22	2:B:560:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:283:PHE:CZ	5:B:704:PHE:HE2	2.39	0.41
1:C:755:VAL:HA	1:C:758:VAL:HG12	2.02	0.41
2:D:51:GLY:O	5:D:704:PHE:OXT	2.39	0.41
1:A:297:MET:HG3	1:A:423:LEU:HD21	2.03	0.41
1:A:619:LYS:HD3	1:A:725:LEU:HD22	2.03	0.41
1:C:305:GLN:O	1:C:309:LYS:HG2	2.20	0.41
1:C:371:THR:O	1:C:375:GLU:HG2	2.21	0.41
2:D:83:ILE:CG2	2:D:84:PRO:HD3	2.51	0.41
2:D:101:LEU:HD22	2:D:112:LYS:HE2	2.02	0.41
2:D:492:ILE:HD12	2:D:492:ILE:HA	1.84	0.41
1:A:257:SER:HB3	1:A:610:TRP:CE2	2.56	0.41
2:B:246:GLY:HA3	2:B:327:PHE:HA	2.03	0.41
2:D:81:GLU:C	2:D:84:PRO:HD2	2.46	0.41
1:A:378:HIS:NE2	1:A:402:GLU:OE2	2.53	0.40
1:A:419:LYS:HE3	1:A:426:PRO:HA	2.02	0.40
2:B:155:LEU:HD23	2:B:162:TYR:HA	2.04	0.40
2:B:229:LEU:O	2:B:233:VAL:HG22	2.21	0.40
1:A:92:THR:HG22	1:A:93:VAL:N	2.36	0.40
2:B:543:LEU:HG	2:B:543:LEU:H	1.70	0.40
1:C:92:THR:HG22	1:C:93:VAL:HG12	2.03	0.40
2:D:229:LEU:O	2:D:233:VAL:HG22	2.21	0.40
2:D:541:LEU:O	2:D:545:ILE:HG23	2.22	0.40
1:A:92:THR:HG22	1:A:93:VAL:HG12	2.03	0.40
1:A:334:THR:OG1	1:A:335:ASP:N	2.52	0.40
2:B:51:GLY:HA2	2:B:427:LEU:HB3	2.03	0.40
2:B:57:ARG:C	2:B:61:LEU:HD13	2.47	0.40
2:B:81:GLU:C	2:B:84:PRO:HD2	2.46	0.40
2:B:452:LYS:HE3	2:B:452:LYS:HB2	1.91	0.40
1:C:619:LYS:HZ2	1:C:680:SER:HB2	1.87	0.40
2:D:246:GLY:HA3	2:D:327:PHE:HA	2.03	0.40
2:D:438:GLY:O	2:D:442:PRO:HG2	2.20	0.40
2:D:579:PRO:HB2	2:D:581:TRP:CD1	2.56	0.40
2:B:279:PHE:HB3	2:B:281:LEU:HG	2.04	0.40
2:B:517:ASP:O	2:B:521:MET:HG3	2.22	0.40
1:C:110:GLU:OE1	1:C:110:GLU:HA	2.21	0.40
1:C:578:ASN:OD1	1:C:579:MET:N	2.55	0.40
2:D:57:ARG:C	2:D:61:LEU:HD13	2.46	0.40
1:A:22:GLU:O	1:A:26:LYS:HG3	2.21	0.40
1:A:184:VAL:HG22	1:A:464:PHE:HE1	1.86	0.40
1:A:578:ASN:OD1	1:A:579:MET:N	2.55	0.40
2:B:83:ILE:HG23	2:B:84:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:266:ASP:OD2	2:B:267:THR:N	2.55	0.40
2:D:266:ASP:OD2	2:D:267:THR:N	2.55	0.40
2:D:328:ARG:HE	2:D:405:GLU:CD	2.30	0.40
2:D:517:ASP:O	2:D:521:MET:HG3	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	747/808 (92%)	687 (92%)	60 (8%)	0	100	100
1	C	747/808 (92%)	687 (92%)	59 (8%)	1 (0%)	48	74
2	B	603/652 (92%)	562 (93%)	41 (7%)	0	100	100
2	D	603/652 (92%)	561 (93%)	42 (7%)	0	100	100
All	All	2700/2920 (92%)	2497 (92%)	202 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	741	ILE

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	663/717 (92%)	598 (90%)	65 (10%)	7	22
1	C	663/717 (92%)	598 (90%)	65 (10%)	7	22
2	B	531/571 (93%)	460 (87%)	71 (13%)	4	11
2	D	531/571 (93%)	460 (87%)	71 (13%)	4	11
All	All	2388/2576 (93%)	2116 (89%)	272 (11%)	8	16

All (272) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	30	ASP
1	A	35	GLU
1	A	37	GLU
1	A	39	LEU
1	A	42	GLN
1	A	56	GLU
1	A	59	VAL
1	A	68	LYS
1	A	73	LEU
1	A	75	GLU
1	A	76	GLN
1	A	77	SER
1	A	78	THR
1	A	81	GLN
1	A	85	LEU
1	A	87	GLU
1	A	92	THR
1	A	94	LYS
1	A	96	GLN
1	A	100	LEU
1	A	106	SER
1	A	111	ASP
1	A	124	SER
1	A	183	TYR
1	A	209	VAL
1	A	257	SER
1	A	259	ILE
1	A	287	GLN
1	A	291	ILE
1	A	293	VAL
1	A	294	THR
1	A	295	ASP

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Mol	Chain	Res	Type
1	A	297	MET
1	A	299	ASP
1	A	317	SER
1	A	325	GLN
1	A	343	VAL
1	A	356	PHE
1	A	362	THR
1	A	363	LYS
1	A	365	THR
1	A	392	LEU
1	A	400	PHE
1	A	411	SER
1	A	414	THR
1	A	416	LYS
1	A	429	GLN
1	A	430	GLU
1	A	463	VAL
1	A	471	ASP
1	A	491	VAL
1	A	517	THR
1	A	542	CYS
1	A	581	VAL
1	A	602	SER
1	A	609	ASP
1	A	623	SER
1	A	626	SER
1	A	692	SER
1	A	721	SER
1	A	723	GLU
1	A	745	VAL
1	A	753	ILE
1	A	761	ILE
2	B	5	VAL
2	B	18	LEU
2	B	42	MET
2	B	77	LEU
2	B	88	LEU
2	B	96	LEU
2	B	105	SER
2	B	116	LEU
2	B	131	THR
2	B	152	ASP

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Mol	Chain	Res	Type
2	B	159	GLN
2	B	189	ASP
2	B	193	ILE
2	B	199	LEU
2	B	208	LEU
2	B	211	CYS
2	B	216	ILE
2	B	223	VAL
2	B	228	THR
2	B	232	VAL
2	B	236	ILE
2	B	248	THR
2	B	255	PHE
2	B	256	THR
2	B	280	SER
2	B	281	LEU
2	B	288	SER
2	B	295	VAL
2	B	307	SER
2	B	309	ILE
2	B	314	SER
2	B	317	VAL
2	B	319	ILE
2	B	321	VAL
2	B	323	SER
2	B	325	ILE
2	B	330	THR
2	B	350	LEU
2	B	377	GLN
2	B	379	VAL
2	B	402	VAL
2	B	403	PHE
2	B	404	THR
2	B	422	ILE
2	B	436	MET
2	B	441	VAL
2	B	447	ARG
2	B	449	ILE
2	B	452	LYS
2	B	455	LYS
2	B	457	VAL
2	B	462	ILE

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Mol	Chain	Res	Type
2	B	463	CYS
2	B	466	THR
2	B	475	LEU
2	B	484	LEU
2	B	495	LEU
2	B	500	CYS
2	B	504	SER
2	B	516	LYS
2	B	519	GLU
2	B	538	SER
2	B	543	LEU
2	B	544	ILE
2	B	547	LEU
2	B	559	THR
2	B	580	ASN
2	B	594	SER
2	B	597	ILE
2	B	604	LYS
2	B	606	ILE
1	C	24	GLN
1	C	30	ASP
1	C	35	GLU
1	C	37	GLU
1	C	39	LEU
1	C	42	GLN
1	C	56	GLU
1	C	59	VAL
1	C	68	LYS
1	C	73	LEU
1	C	75	GLU
1	C	76	GLN
1	C	77	SER
1	C	78	THR
1	C	81	GLN
1	C	85	LEU
1	C	87	GLU
1	C	92	THR
1	C	94	LYS
1	C	96	GLN
1	C	100	LEU
1	C	106	SER
1	C	111	ASP

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Mol	Chain	Res	Type
1	C	124	SER
1	C	183	TYR
1	C	209	VAL
1	C	257	SER
1	C	259	ILE
1	C	287	GLN
1	C	291	ILE
1	C	293	VAL
1	C	294	THR
1	C	295	ASP
1	C	297	MET
1	C	299	ASP
1	C	317	SER
1	C	325	GLN
1	C	343	VAL
1	C	356	PHE
1	C	362	THR
1	C	363	LYS
1	C	365	THR
1	C	392	LEU
1	C	400	PHE
1	C	411	SER
1	C	414	THR
1	C	416	LYS
1	C	429	GLN
1	C	430	GLU
1	C	463	VAL
1	C	471	ASP
1	C	491	VAL
1	C	517	THR
1	C	542	CYS
1	C	581	VAL
1	C	602	SER
1	C	609	ASP
1	C	623	SER
1	C	626	SER
1	C	692	SER
1	C	721	SER
1	C	723	GLU
1	C	745	VAL
1	C	753	ILE
1	C	761	ILE

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Mol	Chain	Res	Type
2	D	5	VAL
2	D	18	LEU
2	D	42	MET
2	D	77	LEU
2	D	88	LEU
2	D	96	LEU
2	D	105	SER
2	D	116	LEU
2	D	131	THR
2	D	152	ASP
2	D	157	GLU
2	D	189	ASP
2	D	193	ILE
2	D	199	LEU
2	D	208	LEU
2	D	211	CYS
2	D	216	ILE
2	D	223	VAL
2	D	228	THR
2	D	232	VAL
2	D	236	ILE
2	D	248	THR
2	D	255	PHE
2	D	256	THR
2	D	280	SER
2	D	281	LEU
2	D	288	SER
2	D	295	VAL
2	D	307	SER
2	D	309	ILE
2	D	314	SER
2	D	317	VAL
2	D	319	ILE
2	D	321	VAL
2	D	323	SER
2	D	325	ILE
2	D	330	THR
2	D	350	LEU
2	D	377	GLN
2	D	379	VAL
2	D	402	VAL
2	D	403	PHE

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Mol	Chain	Res	Type
2	D	404	THR
2	D	422	ILE
2	D	436	MET
2	D	441	VAL
2	D	447	ARG
2	D	449	ILE
2	D	452	LYS
2	D	455	LYS
2	D	457	VAL
2	D	462	ILE
2	D	463	CYS
2	D	466	THR
2	D	475	LEU
2	D	484	LEU
2	D	495	LEU
2	D	500	CYS
2	D	504	SER
2	D	516	LYS
2	D	519	GLU
2	D	538	SER
2	D	543	LEU
2	D	544	ILE
2	D	547	LEU
2	D	559	THR
2	D	580	ASN
2	D	594	SER
2	D	597	ILE
2	D	604	LYS
2	D	606	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	42	GLN
1	A	53	ASN
1	A	81	GLN
1	A	117	ASN
1	A	139	GLN
1	A	154	ASN
1	A	250	ASN
1	A	277	ASN

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Mol	Chain	Res	Type
1	A	340	GLN
1	A	345	HIS
1	A	378	HIS
1	A	493	HIS
1	A	552	GLN
1	A	599	ASN
2	B	40	GLN
2	B	142	ASN
2	B	145	GLN
2	B	159	GLN
2	B	194	GLN
2	B	310	ASN
2	B	386	ASN
2	B	435	ASN
2	B	444	GLN
2	B	476	ASN
2	B	580	ASN
1	C	34	HIS
1	C	42	GLN
1	C	53	ASN
1	C	117	ASN
1	C	154	ASN
1	C	250	ASN
1	C	277	ASN
1	C	340	GLN
1	C	345	HIS
1	C	378	HIS
1	C	417	HIS
1	C	493	HIS
1	C	552	GLN
1	C	599	ASN
1	C	638	ASN
2	D	40	GLN
2	D	142	ASN
2	D	145	GLN
2	D	159	GLN
2	D	194	GLN
2	D	310	ASN
2	D	377	GLN
2	D	386	ASN
2	D	435	ASN
2	D	476	ASN

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Mol	Chain	Res	Type
2	D	580	ASN
2	D	609	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 ⓘ

8 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	H	1	3,1	14,14,15	0.38	0	17,19,21	0.53	0
3	NAG	H	2	3	14,14,15	0.39	0	17,19,21	0.50	0
3	NAG	J	1	3,1	14,14,15	1.00	1 (7%)	17,19,21	0.56	0
3	NAG	J	2	3	14,14,15	0.55	0	17,19,21	0.40	0
3	NAG	N	1	3,1	14,14,15	1.00	1 (7%)	17,19,21	0.55	0
3	NAG	N	2	3	14,14,15	0.54	0	17,19,21	0.40	0
3	NAG	S	1	3,1	14,14,15	0.39	0	17,19,21	0.53	0
3	NAG	S	2	3	14,14,15	0.37	0	17,19,21	0.49	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
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	J	2	3	-	3/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	N	2	3	-	3/6/23/26	0/1/1/1
3	NAG	S	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	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)
3	N	1	NAG	O5-C1	-3.47	1.38	1.43
3	J	1	NAG	O5-C1	-3.46	1.38	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

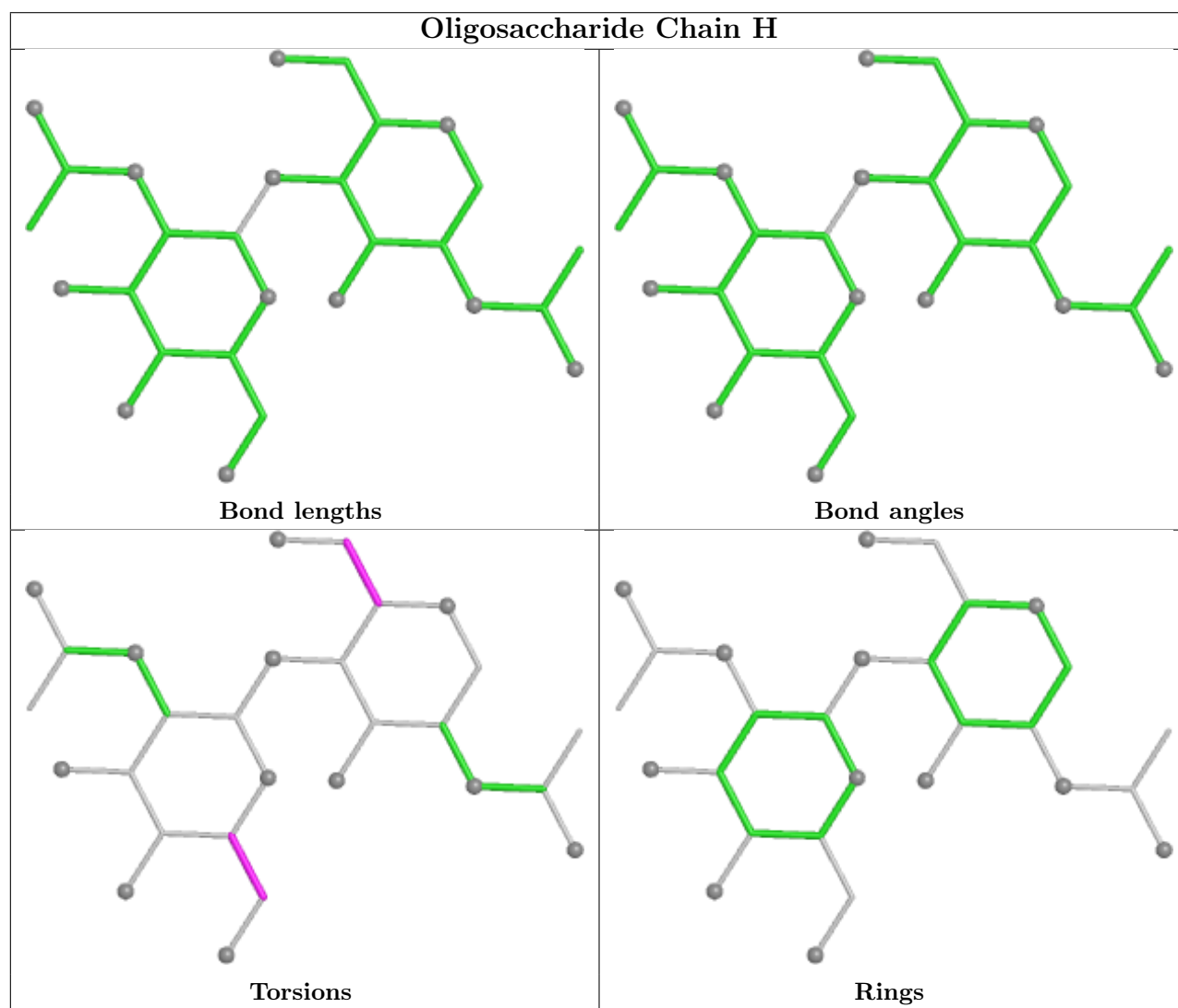
Mol	Chain	Res	Type	Atoms
3	H	1	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	S	2	NAG	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	J	2	NAG	C1-C2-N2-C7
3	N	2	NAG	C1-C2-N2-C7

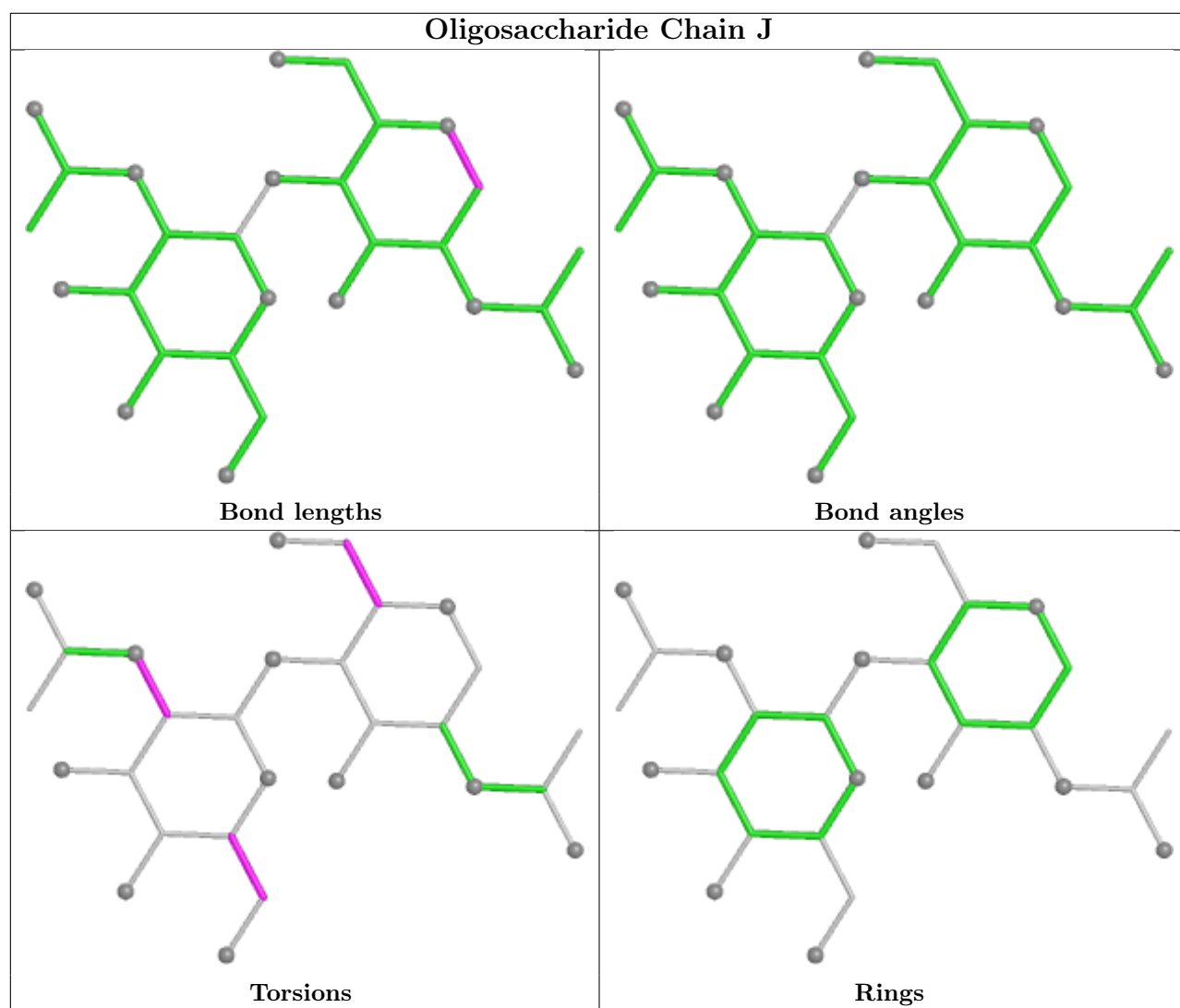
There are no ring outliers.

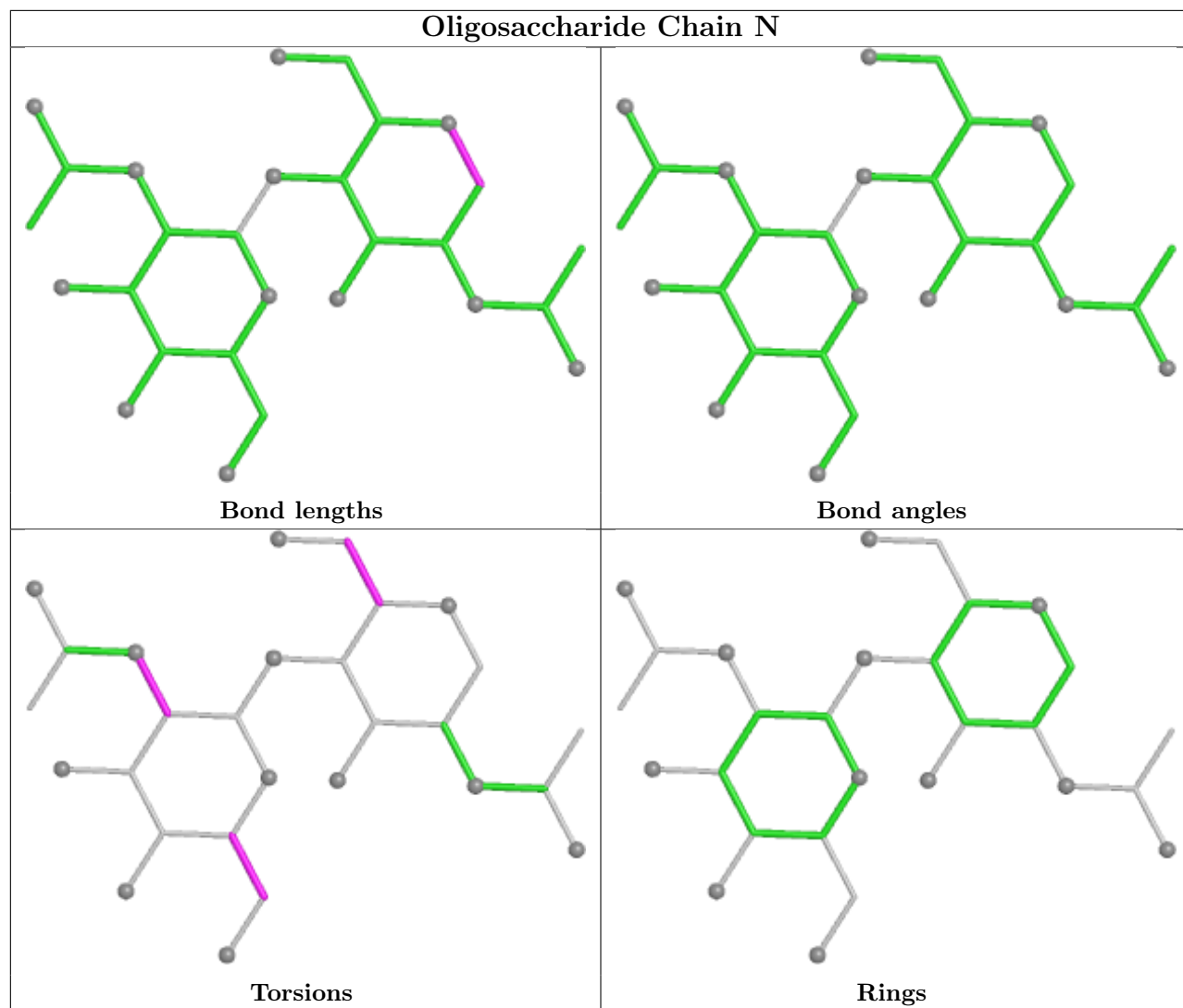
4 monomers are involved in 5 short contacts:

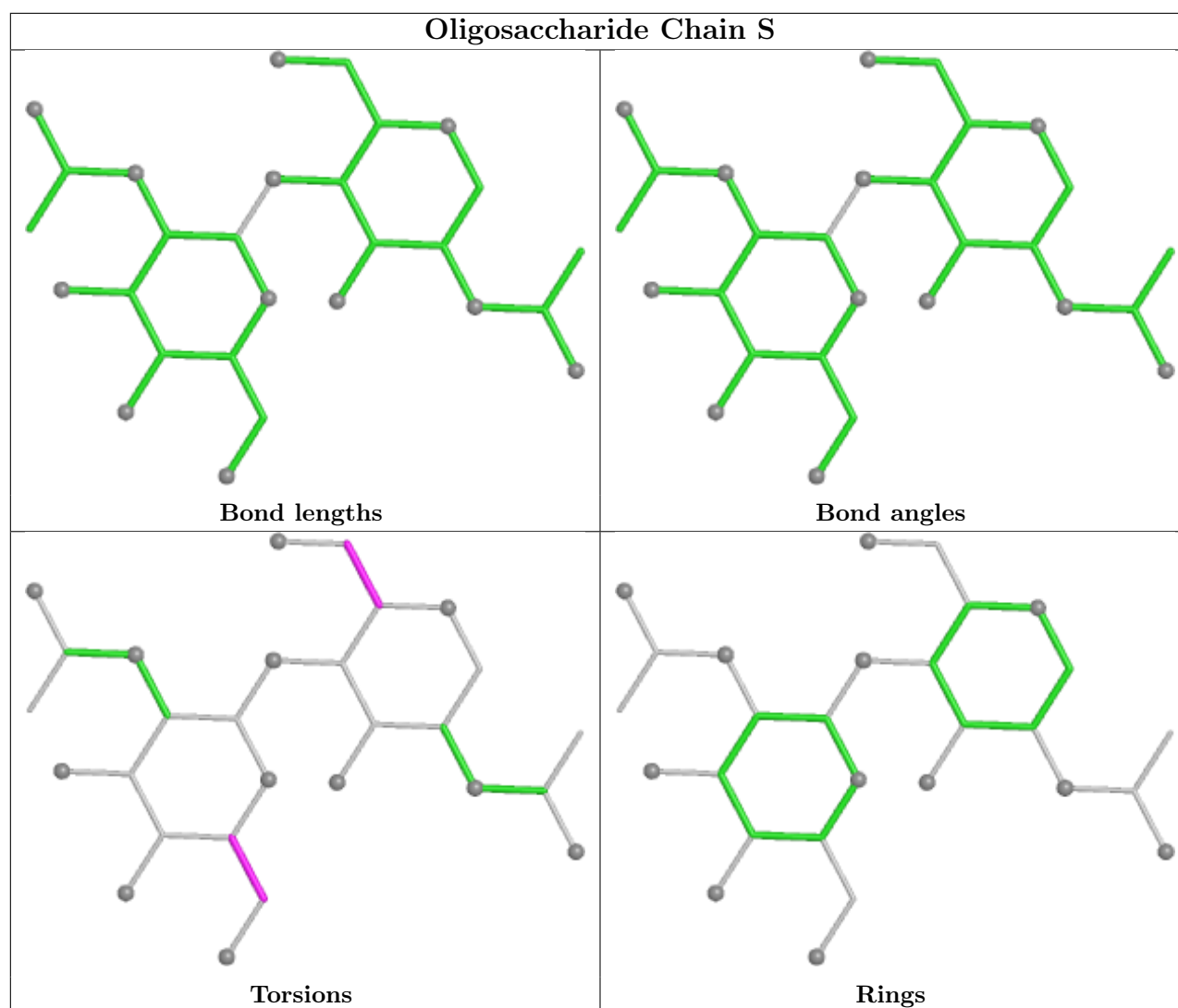
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	2	NAG	1	0
3	N	2	NAG	1	0
3	N	1	NAG	3	0
3	J	1	NAG	2	0

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](#)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	902	1	14,14,15	0.33	0	17,19,21	0.48	0
4	NAG	B	702	2	14,14,15	0.48	0	17,19,21	0.66	1 (5%)
4	NAG	D	703	2	14,14,15	0.47	0	17,19,21	0.66	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	701	2	14,14,15	0.24	0	17,19,21	0.48	0
4	NAG	A	901	1	14,14,15	0.36	0	17,19,21	1.07	1 (5%)
4	NAG	D	702	2	14,14,15	0.35	0	17,19,21	0.46	0
5	PHE	B	704	-	11,12,12	0.71	1 (9%)	14,15,15	0.96	2 (14%)
4	NAG	C	901	1	14,14,15	0.36	0	17,19,21	1.08	1 (5%)
4	NAG	C	902	1	14,14,15	0.33	0	17,19,21	0.48	0
4	NAG	A	903	1	14,14,15	0.36	0	17,19,21	0.52	0
4	NAG	B	703	2	14,14,15	0.35	0	17,19,21	0.45	0
5	PHE	D	704	-	11,12,12	0.71	1 (9%)	14,15,15	0.95	2 (14%)
4	NAG	C	903	1	14,14,15	0.37	0	17,19,21	0.52	0
4	NAG	D	701	2	14,14,15	0.24	0	17,19,21	0.46	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
4	NAG	A	902	1	-	2/6/23/26	0/1/1/1
4	NAG	B	702	2	-	2/6/23/26	0/1/1/1
4	NAG	D	703	2	-	2/6/23/26	0/1/1/1
4	NAG	B	701	2	-	2/6/23/26	0/1/1/1
4	NAG	A	901	1	-	1/6/23/26	0/1/1/1
4	NAG	D	702	2	-	2/6/23/26	0/1/1/1
5	PHE	B	704	-	-	0/8/8/8	0/1/1/1
4	NAG	C	901	1	-	1/6/23/26	0/1/1/1
4	NAG	C	902	1	-	2/6/23/26	0/1/1/1
4	NAG	A	903	1	-	2/6/23/26	0/1/1/1
4	NAG	B	703	2	-	2/6/23/26	0/1/1/1
5	PHE	D	704	-	-	0/8/8/8	0/1/1/1
4	NAG	C	903	1	-	2/6/23/26	0/1/1/1
4	NAG	D	701	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)
5	D	704	PHE	OXT-C	-2.15	1.23	1.30
5	B	704	PHE	OXT-C	-2.14	1.23	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	901	NAG	C1-O5-C5	2.98	116.23	112.19
4	A	901	NAG	C1-O5-C5	2.95	116.19	112.19
5	B	704	PHE	OXT-C-O	-2.71	117.94	124.09
5	D	704	PHE	OXT-C-O	-2.69	117.98	124.09
5	B	704	PHE	OXT-C-CA	2.20	120.89	113.38
4	D	703	NAG	C1-O5-C5	2.20	115.17	112.19
5	D	704	PHE	OXT-C-CA	2.19	120.86	113.38
4	B	702	NAG	C1-O5-C5	2.17	115.13	112.19

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	702	NAG	O5-C5-C6-O6
4	D	703	NAG	O5-C5-C6-O6
4	B	703	NAG	O5-C5-C6-O6
4	D	702	NAG	O5-C5-C6-O6
4	A	902	NAG	O5-C5-C6-O6
4	B	701	NAG	O5-C5-C6-O6
4	C	902	NAG	O5-C5-C6-O6
4	D	701	NAG	O5-C5-C6-O6
4	A	903	NAG	O5-C5-C6-O6
4	C	903	NAG	O5-C5-C6-O6
4	A	902	NAG	C4-C5-C6-O6
4	B	701	NAG	C4-C5-C6-O6
4	C	902	NAG	C4-C5-C6-O6
4	D	701	NAG	C4-C5-C6-O6
4	A	903	NAG	C4-C5-C6-O6
4	C	903	NAG	C4-C5-C6-O6
4	D	703	NAG	C4-C5-C6-O6
4	B	702	NAG	C4-C5-C6-O6
4	B	703	NAG	C4-C5-C6-O6
4	D	702	NAG	C4-C5-C6-O6
4	C	901	NAG	C4-C5-C6-O6
4	A	901	NAG	C4-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	902	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	702	NAG	1	0
4	A	901	NAG	7	0
5	B	704	PHE	6	0
4	C	902	NAG	1	0
4	B	703	NAG	1	0
5	D	704	PHE	7	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.

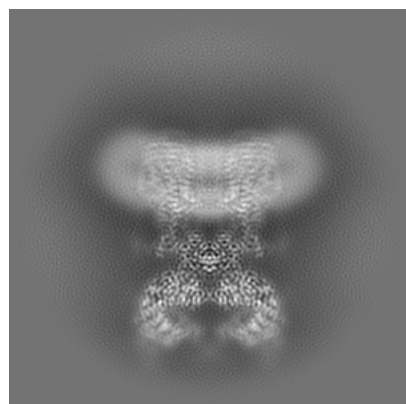
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64897. These allow visual inspection of the internal detail of the map and identification of artifacts.

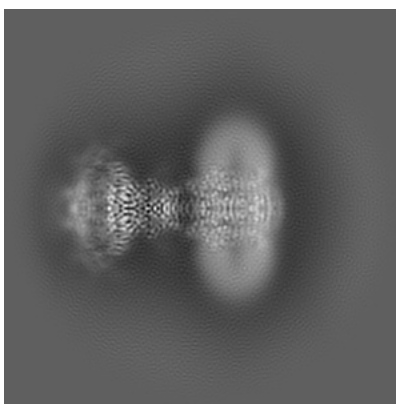
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

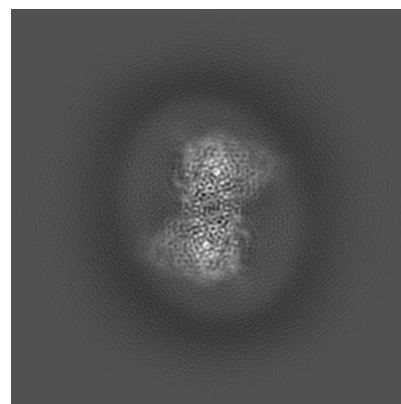
6.1.1 Primary map



X

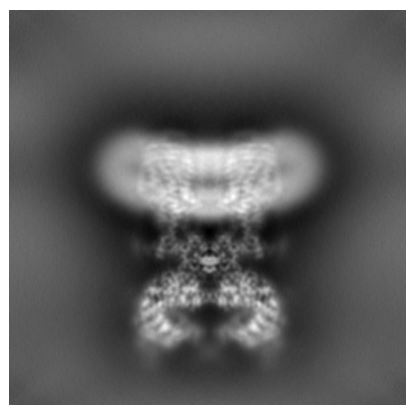


Y

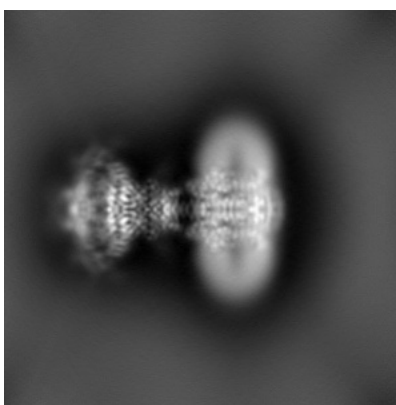


Z

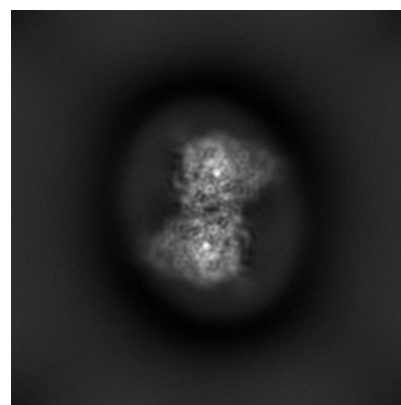
6.1.2 Raw map



X



Y

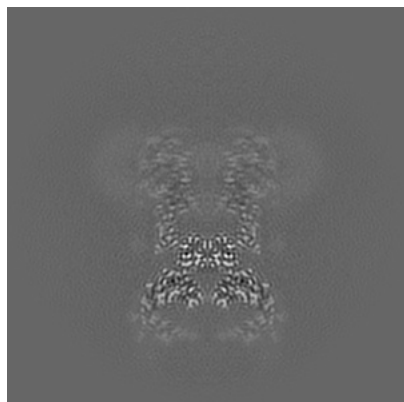


Z

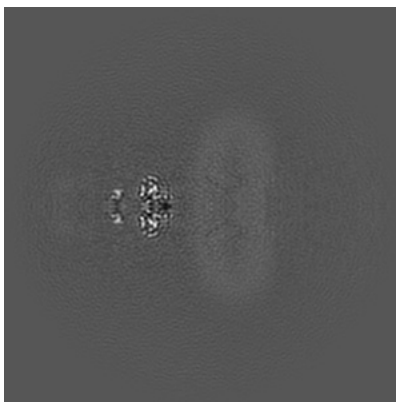
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

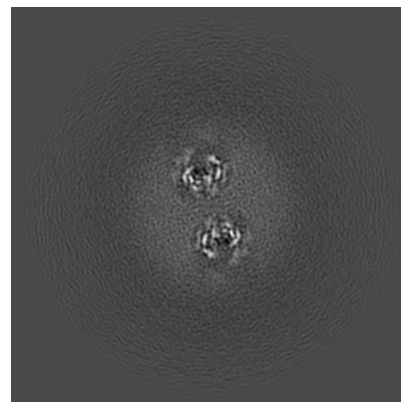
6.2.1 Primary map



X Index: 180

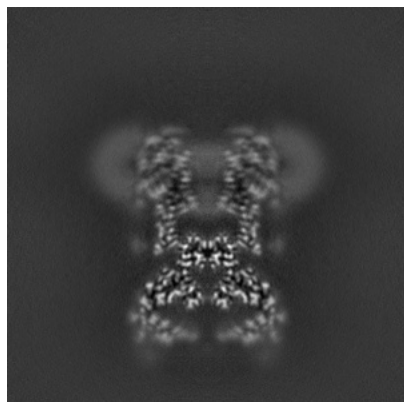


Y Index: 180

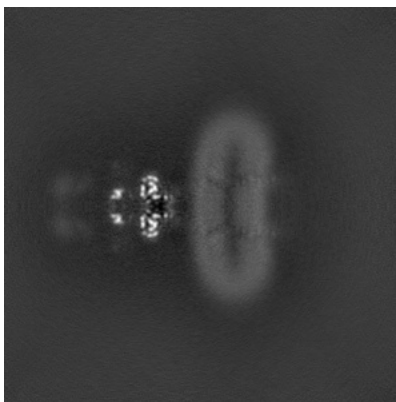


Z Index: 180

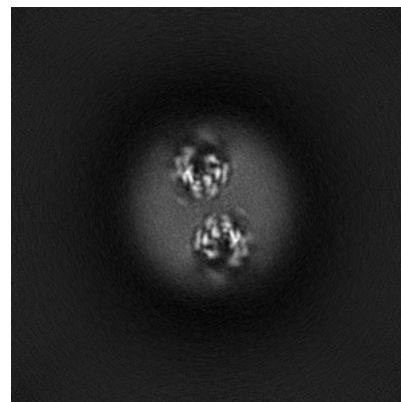
6.2.2 Raw map



X Index: 180



Y Index: 180

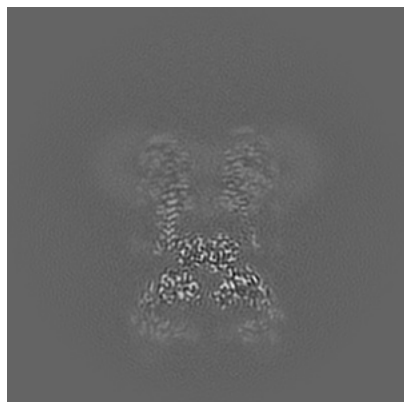


Z Index: 180

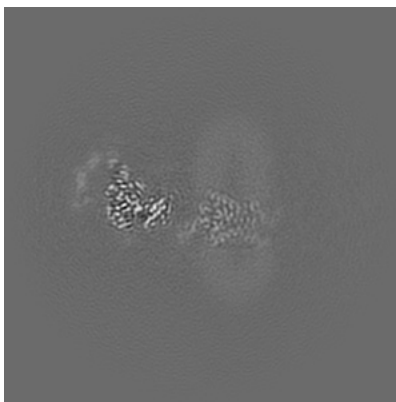
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

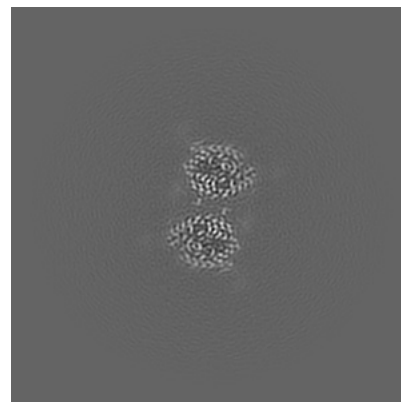
6.3.1 Primary map



X Index: 177

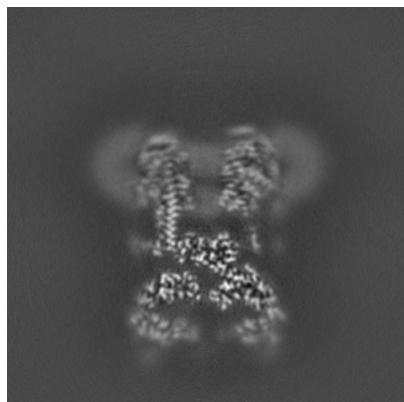


Y Index: 201

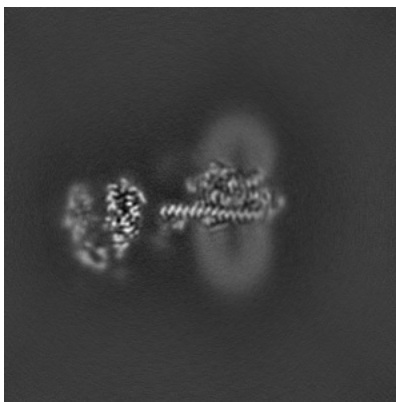


Z Index: 108

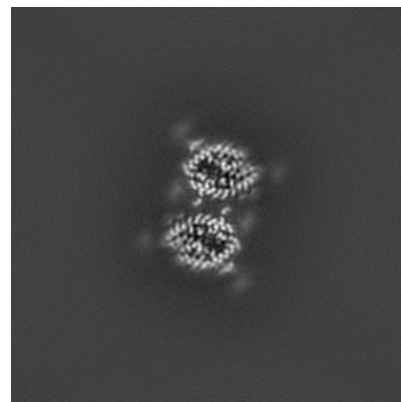
6.3.2 Raw map



X Index: 176



Y Index: 146

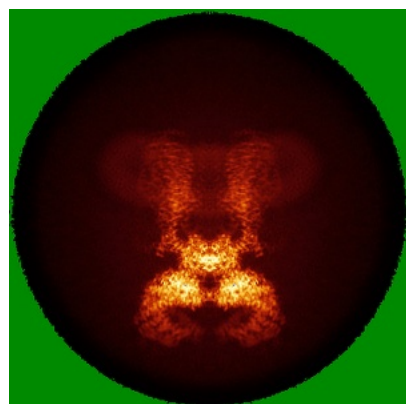


Z Index: 107

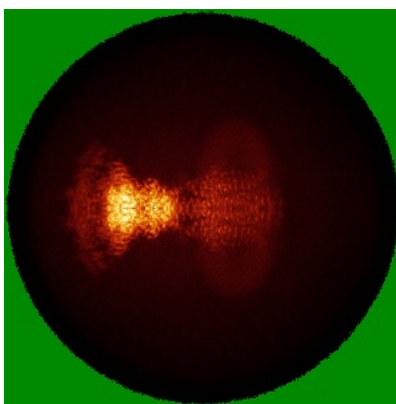
The images above show the largest variance slices of the map in three orthogonal directions.

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

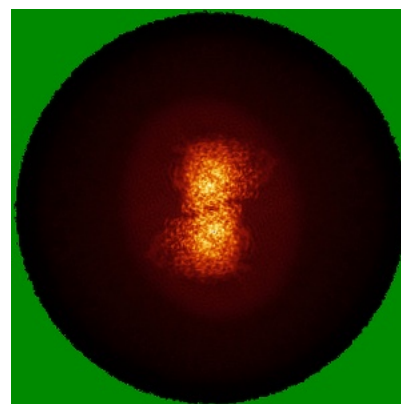
6.4.1 Primary map



X

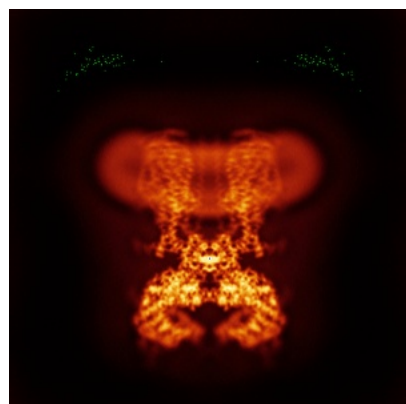


Y

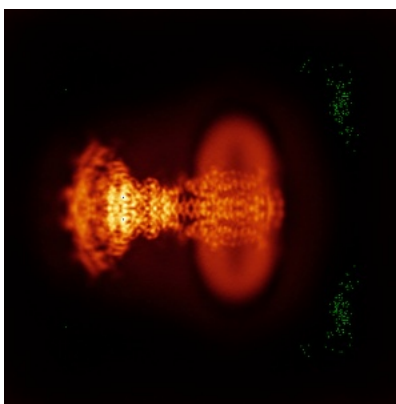


Z

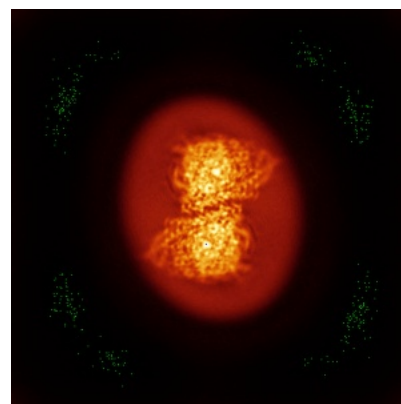
6.4.2 Raw map



X



Y

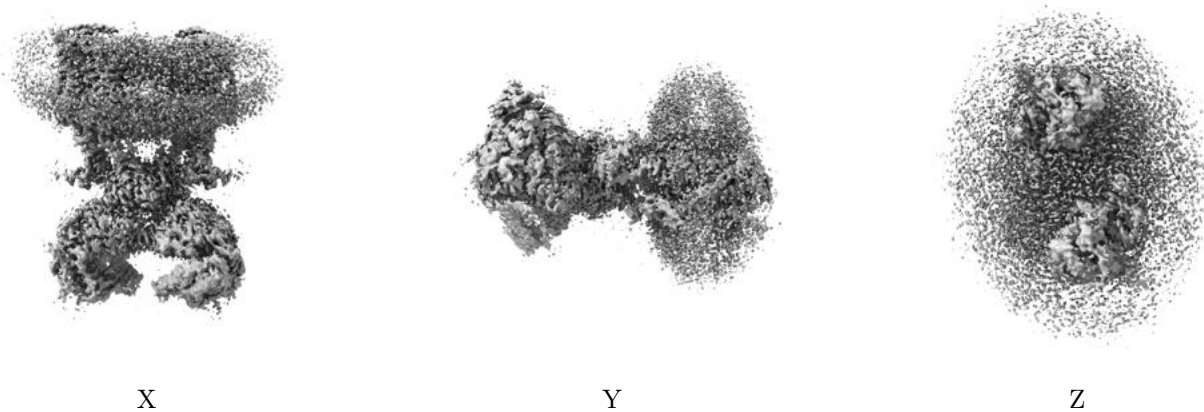


Z

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.

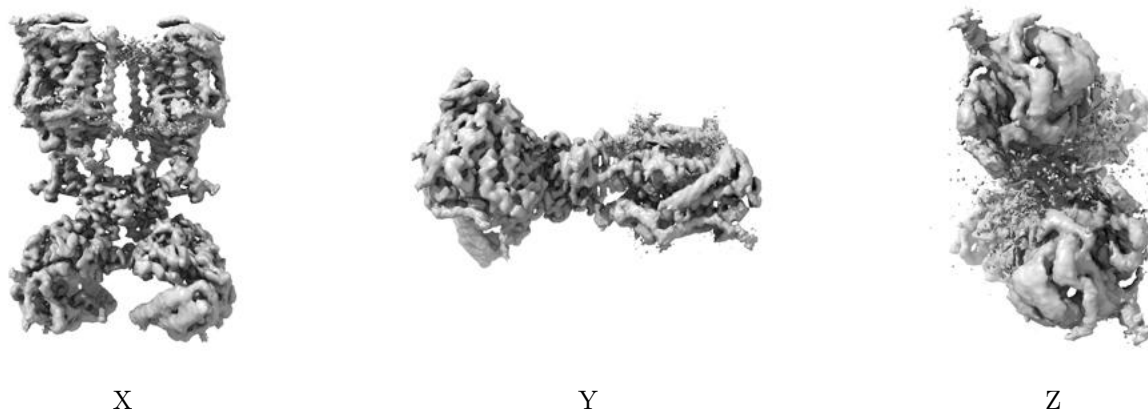
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.22. 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.

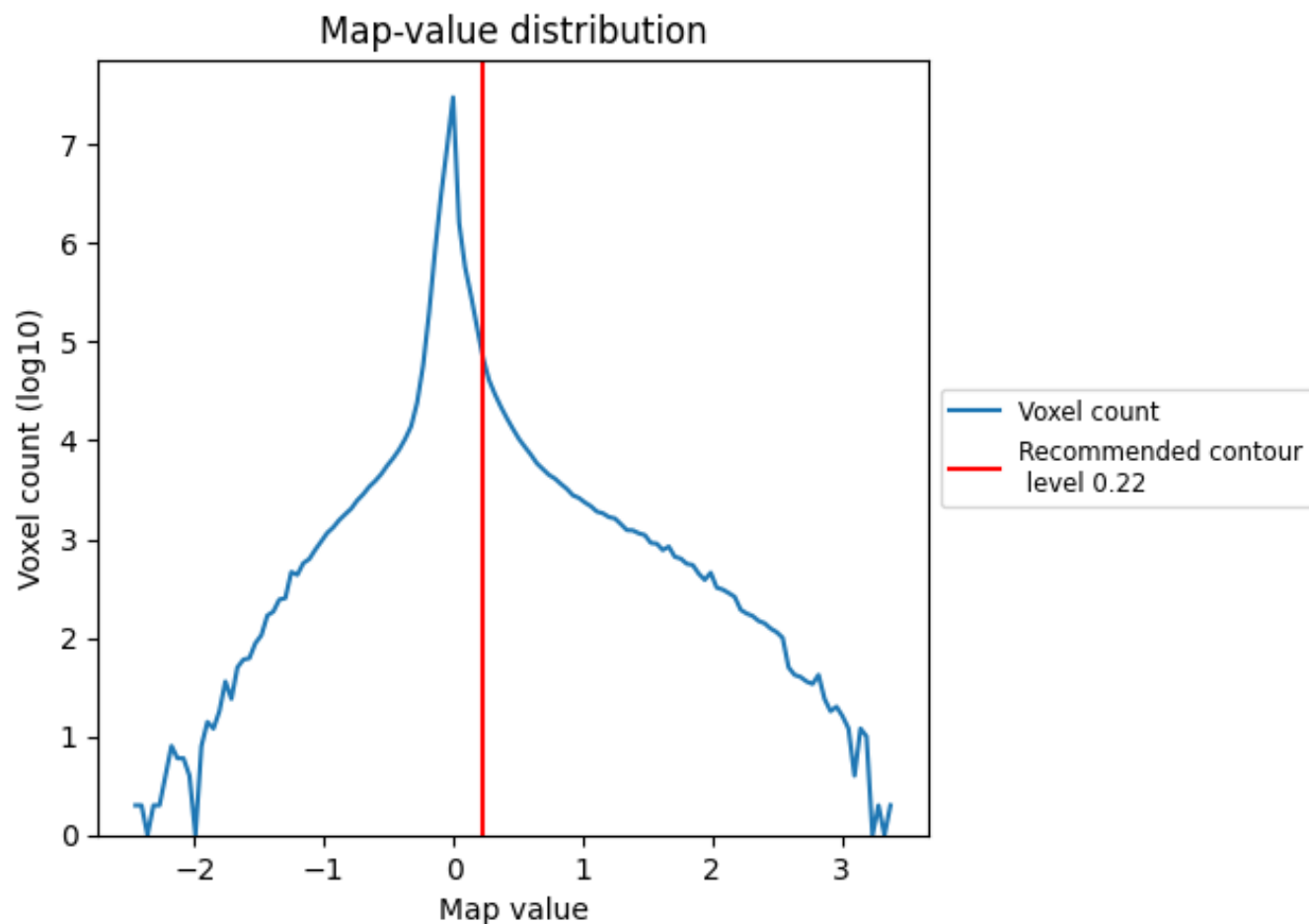
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

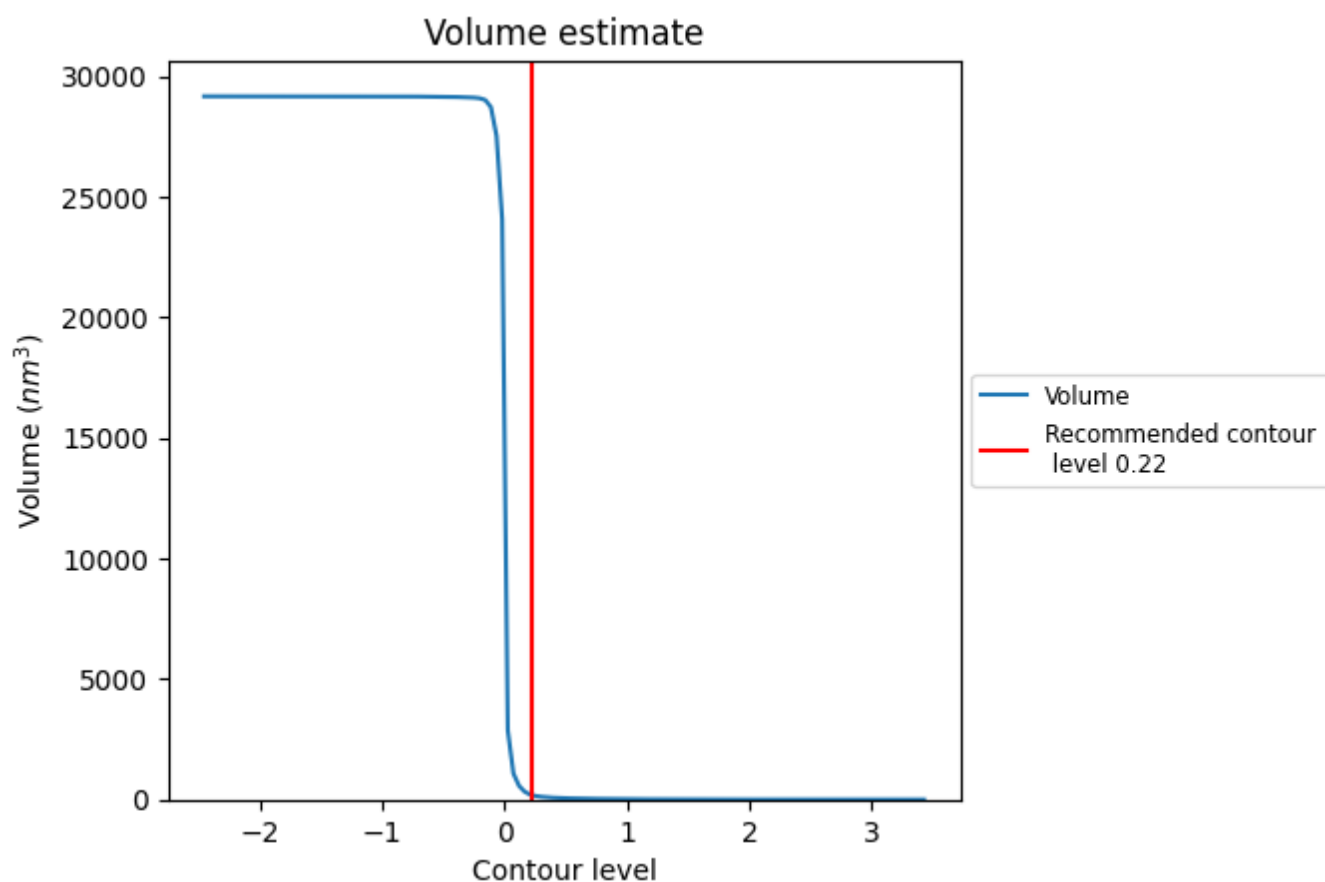
This section contains the results of statistical analysis of the map.

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.

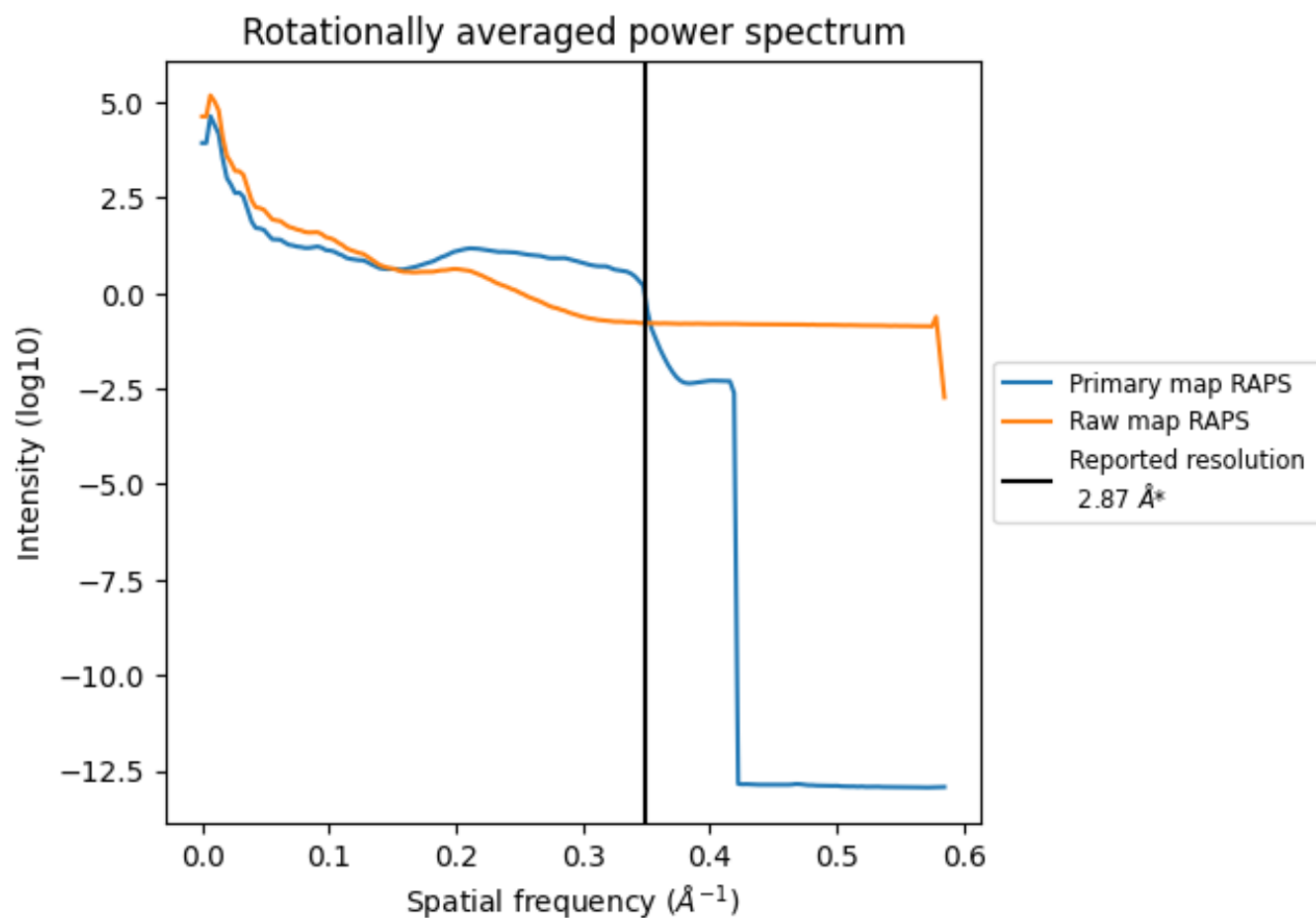
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 190 nm³; this corresponds to an approximate mass of 172 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 ⓘ

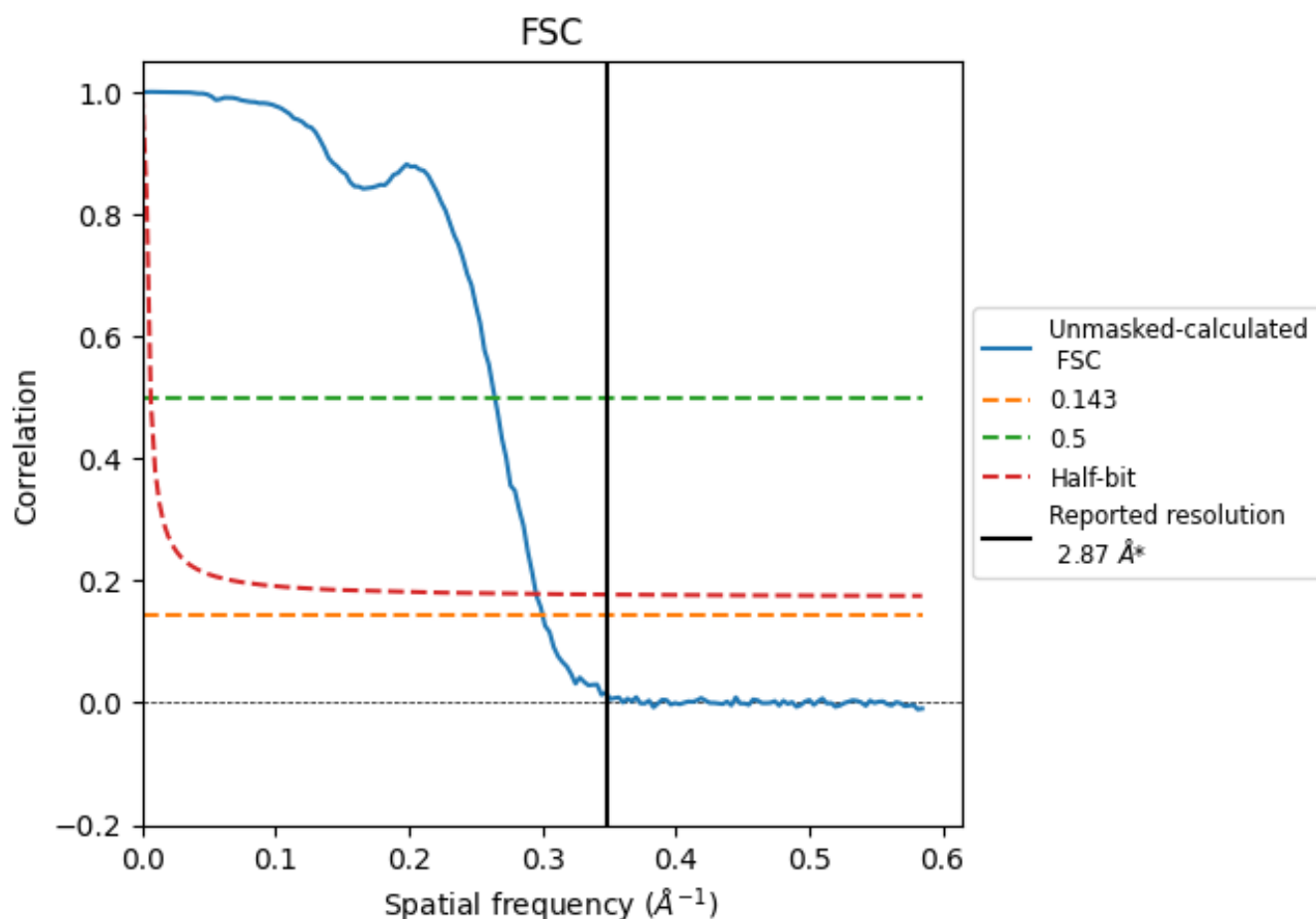


*Reported resolution corresponds to spatial frequency of 0.348 Å⁻¹

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 0.348 \AA^{-1}

8.2 Resolution estimates [i](#)

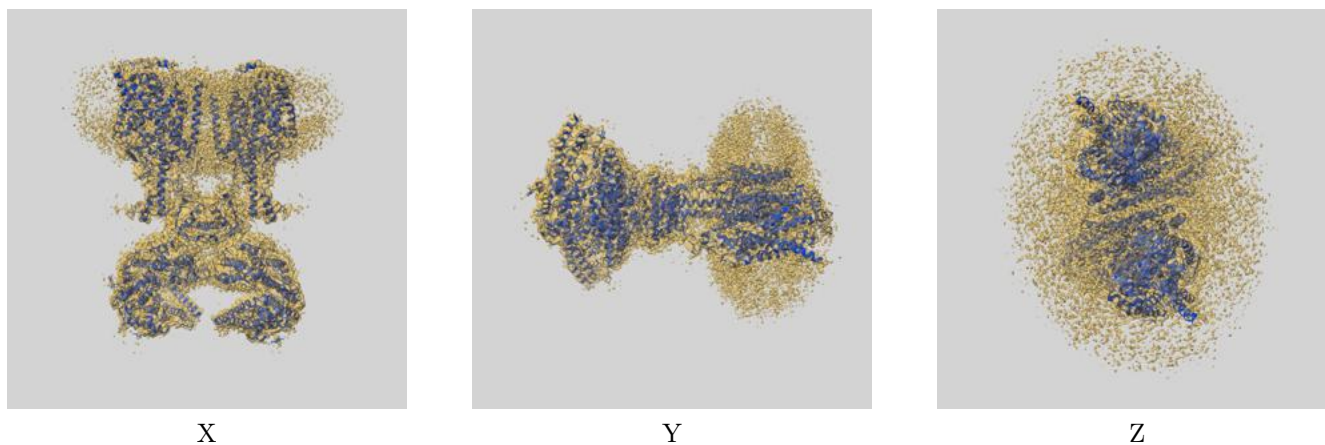
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.87	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.33	3.78	3.39

*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 3.33 differs from the reported value 2.87 by more than 10 %

9 Map-model fit [i](#)

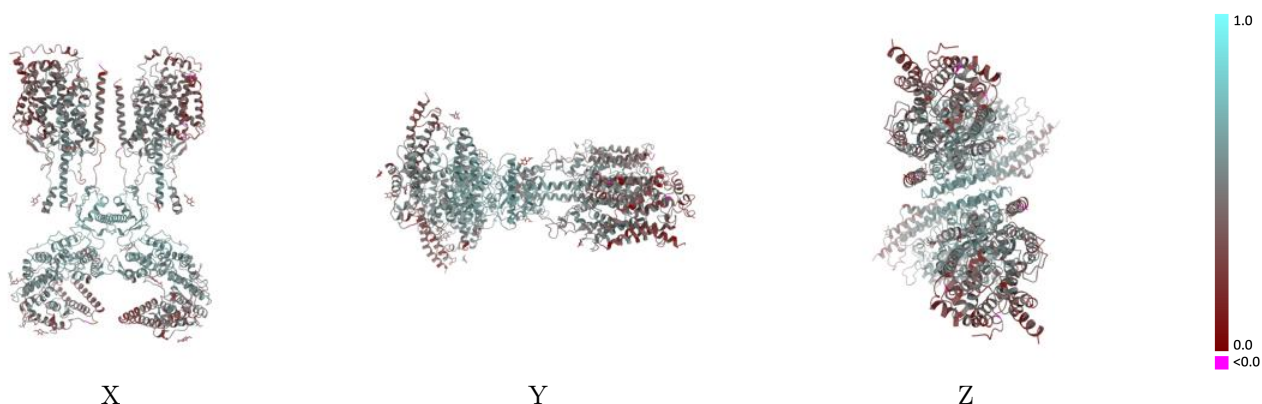
This section contains information regarding the fit between EMDB map EMD-64897 and PDB model 9VA2. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



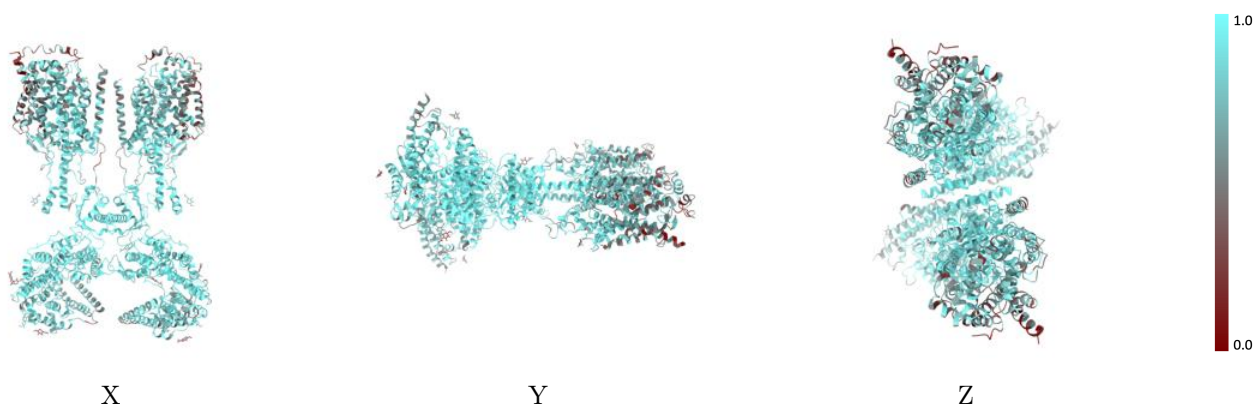
The images above show the 3D surface view of the map at the recommended contour level 0.22 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



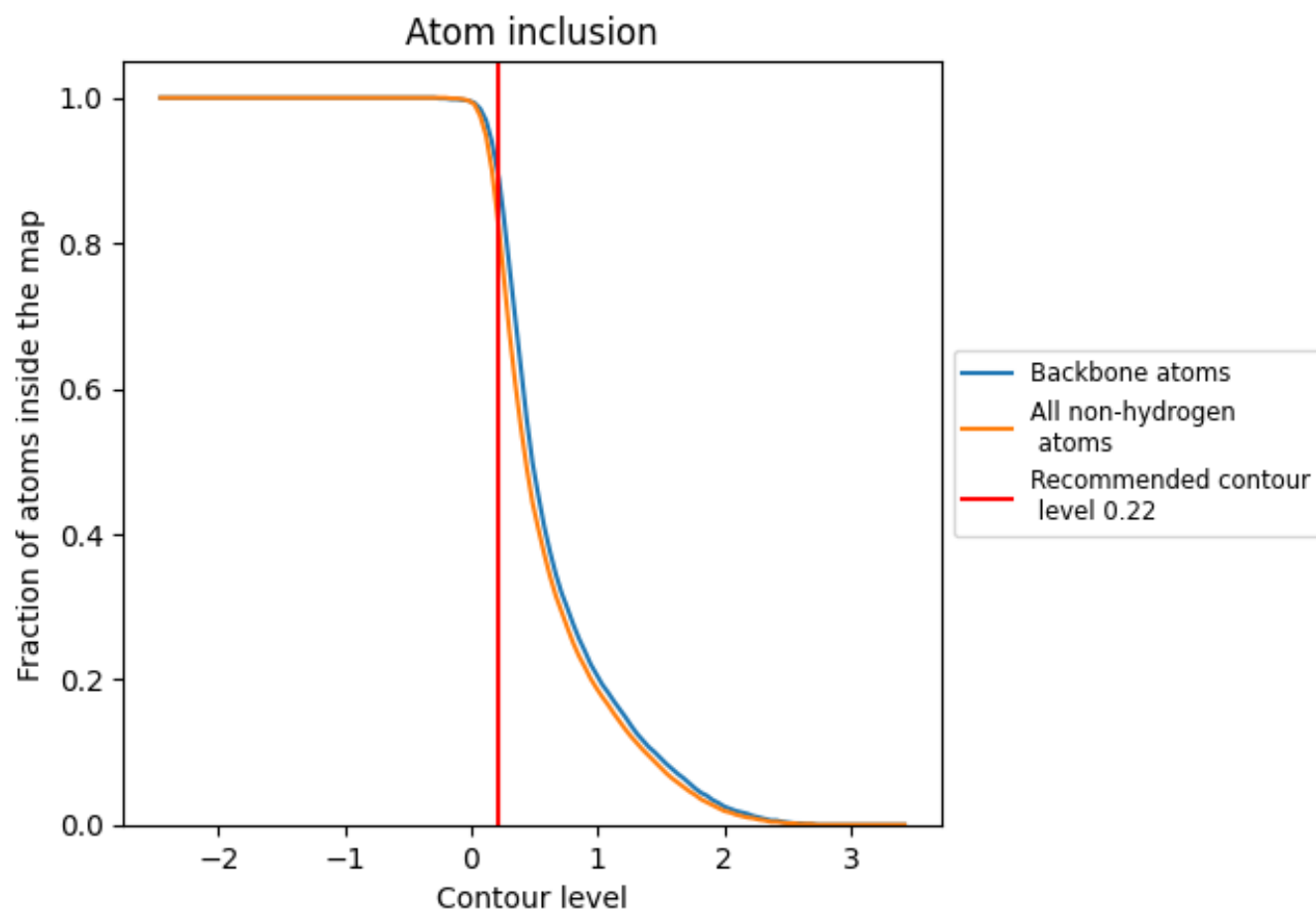
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.22).

9.4 Atom inclusion ⓘ



At the recommended contour level, 89% 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 (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8190	<div></div> 0.4810
A	<div></div> 0.8820	<div></div> 0.5230
B	<div></div> 0.7440	<div></div> 0.4300
C	<div></div> 0.8790	<div></div> 0.5180
D	<div></div> 0.7430	<div></div> 0.4340
H	<div></div> 0.3570	<div></div> 0.3730
J	<div></div> 0.7500	<div></div> 0.3190
N	<div></div> 0.8210	<div></div> 0.3760
S	<div></div> 0.3930	<div></div> 0.3590

1.0

0.0

<0.0