



## Full wwPDB EM Validation Report ⓘ

Sep 28, 2024 – 05:03 PM EDT

PDB ID : 8GCD  
EMDB ID : EMD-29931  
Title : Full length Integrin AlphaIIbBeta3 in inactive state  
Authors : Huo, T.; Wu, H.; Wang, Z.  
Deposited on : 2023-03-01  
Resolution : 2.97 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

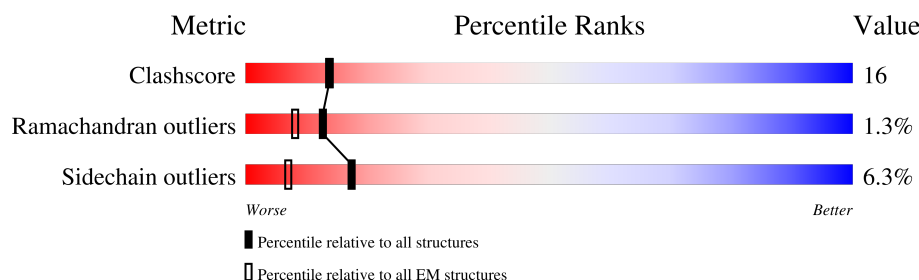
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.97 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  $\geq 3$ , 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	1039	
2	B	788	
3	C	5	
4	D	3	
5	E	2	
5	F	2	

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
3	NAG	C	2	X	-	-	-
5	NAG	E	1	X	-	-	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 13115 atoms, of which 384 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.

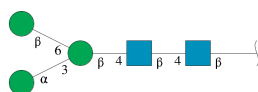
- Molecule 1 is a protein called Integrin alpha-IIb.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	939	Total	C	H	N	O	S	1	0
			7401	4559	212	1246	1355	29		

- Molecule 2 is a protein called Integrin beta-3.

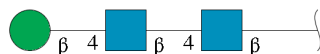
Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	697	Total	C	H	N	O	S	0	0
			5507	3289	172	906	1069	71		

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[beta-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		

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



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

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

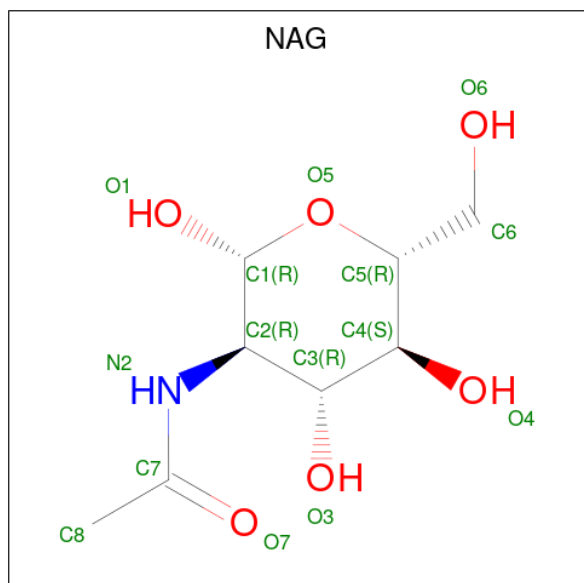


Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	2	Total	C	N	O	0	0
			28	16	2	10		
5	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	A	5	Total	Ca	0
			5	5	
6	B	2	Total	Ca	0
			2	2	

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



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

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

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

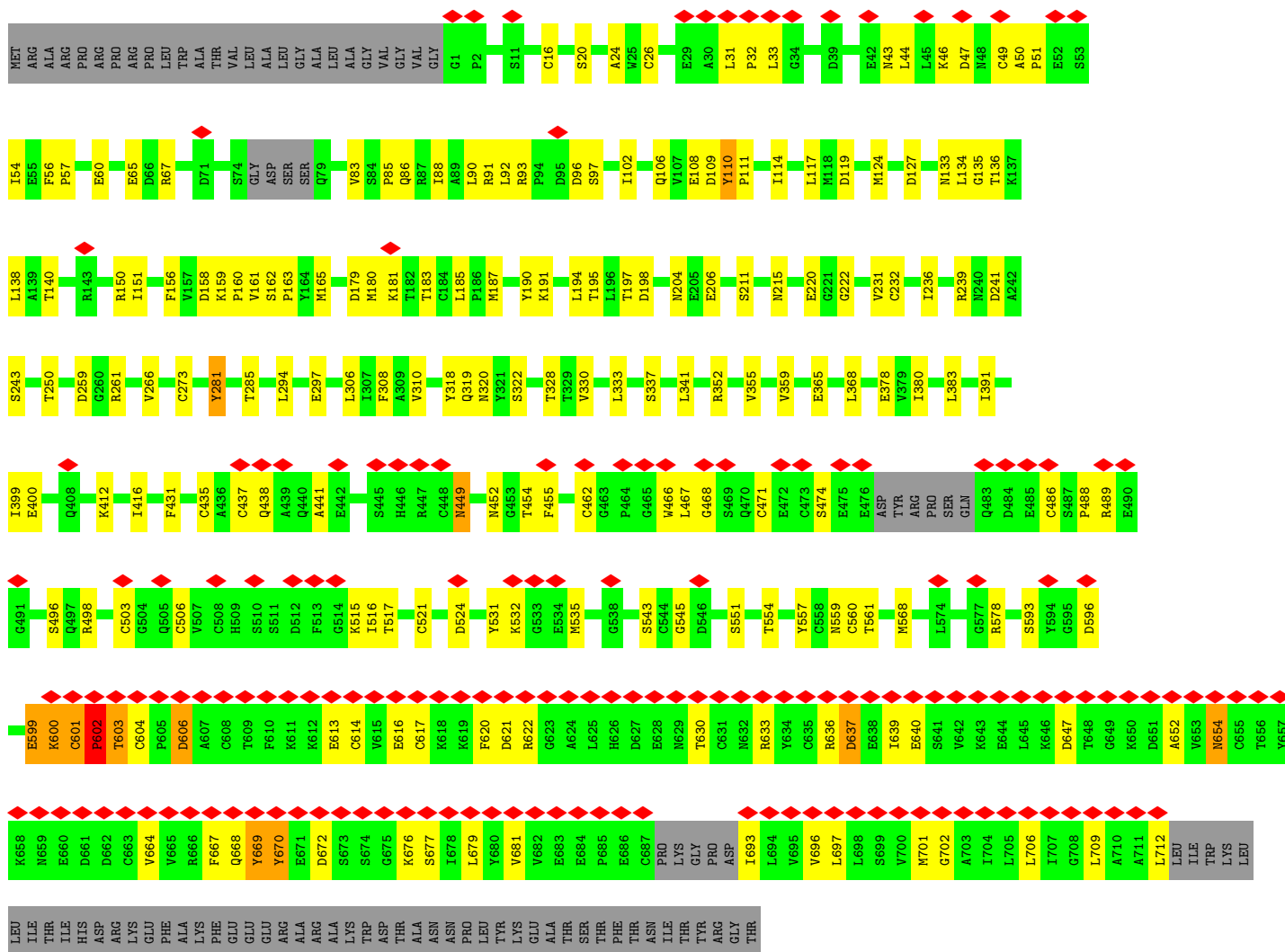
Mol	Chain	Residues	Atoms		AltConf
8	B	1	Total	Mg	0
			1	1	

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total	O	0
			1	1	



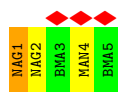
- Molecule 2: Integrin beta-3



- Molecule 3:  $\alpha$ -D-mannopyranose-(1-3)-[ $\beta$ -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







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



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	168938	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.028	Depositor
Minimum map value	-2.529	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.091	Depositor
Recommended contour level	0.468	Depositor
Map size (Å)	273.92, 273.92, 273.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.41	7/7363 (0.1%)	0.62	10/10042 (0.1%)
2	B	0.29	2/5425 (0.0%)	0.55	5/7334 (0.1%)
All	All	0.37	9/12788 (0.1%)	0.59	15/17376 (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	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	743	ARG	N-CA	8.84	1.64	1.46
1	A	744	ALA	N-CA	8.53	1.63	1.46
1	A	744	ALA	C-N	8.21	1.52	1.34
1	A	742	VAL	C-N	7.79	1.51	1.34
1	A	743	ARG	C-N	7.57	1.51	1.34
1	A	743	ARG	CA-C	7.00	1.71	1.52
2	B	602	PRO	N-CA	6.35	1.58	1.47
1	A	744	ALA	CA-C	5.59	1.67	1.52
2	B	602	PRO	C-N	5.42	1.46	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	PRO	CA-C-O	-9.34	97.77	120.20
1	A	956	LEU	O-C-N	7.87	135.28	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	PRO	CA-C-N	7.37	133.42	117.20
1	A	743	ARG	C-N-CA	7.25	139.82	121.70
1	A	743	ARG	CA-C-N	7.21	133.05	117.20
1	A	744	ALA	CA-C-N	7.10	132.82	117.20
2	B	601	CYS	CB-CA-C	-6.76	96.88	110.40
1	A	744	ALA	N-CA-C	6.61	128.84	111.00
2	B	601	CYS	N-CA-CB	6.48	122.26	110.60
1	A	956	LEU	CA-C-N	-6.22	103.52	117.20
1	A	743	ARG	N-CA-C	6.05	127.35	111.00
2	B	602	PRO	C-N-CA	5.99	136.68	121.70
1	A	742	VAL	C-N-CA	5.91	136.48	121.70
1	A	742	VAL	O-C-N	-5.46	113.97	122.70
1	A	744	ALA	CA-C-O	-5.25	109.08	120.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	742	VAL	Mainchain
1	A	959	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	7189	212	7055	256	0
2	B	5335	172	5107	148	0
3	C	61	0	52	2	0
4	D	39	0	34	1	0
5	E	28	0	25	6	0
5	F	28	0	25	1	0
6	A	5	0	0	0	0
6	B	2	0	0	0	0
7	A	42	0	39	0	0
8	B	1	0	0	0	0
9	A	1	0	0	0	0
All	All	12731	384	12337	390	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 16.

All (390) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:378:GLU:OE1	2:B:633:ARG:NE	1.80	1.15
1:A:826:CYS:HB3	1:A:889:GLN:O	1.45	1.15
2:B:378:GLU:OE1	2:B:633:ARG:CZ	1.97	1.12
1:A:964:ILE:HA	2:B:693:ILE:HD11	1.31	1.07
1:A:602:CYS:O	1:A:642:GLU:OE2	1.74	1.05
1:A:786:LEU:O	1:A:900:ARG:HA	1.61	1.01
1:A:761:VAL:CG2	1:A:957:ARG:HH22	1.74	0.99
1:A:921:GLN:HE21	1:A:957:ARG:HB2	1.27	0.98
2:B:578:ARG:NH1	2:B:601:CYS:H	1.59	0.98
1:A:785:GLU:HA	1:A:902:MET:HB3	1.46	0.97
1:A:761:VAL:HG21	1:A:957:ARG:HH22	1.32	0.94
1:A:799:LEU:HD12	1:A:930:PHE:HB2	1.53	0.90
1:A:826:CYS:CB	1:A:889:GLN:O	2.20	0.90
2:B:67:ARG:H	2:B:86:GLN:HE22	1.24	0.83
2:B:378:GLU:CD	2:B:633:ARG:NH2	2.33	0.82
2:B:557:TYR:HB2	2:B:559:ASN:OD1	1.79	0.82
1:A:876:VAL:HG21	1:A:917:ARG:HD3	1.63	0.80
1:A:793:THR:HG22	1:A:896:ALA:HA	1.65	0.79
2:B:578:ARG:NH1	2:B:601:CYS:N	2.30	0.78
1:A:785:GLU:HA	1:A:902:MET:CB	2.12	0.78
1:A:761:VAL:HG23	1:A:957:ARG:NH1	1.99	0.77
1:A:18:GLN:HB3	1:A:440:TYR:HB2	1.65	0.76
1:A:761:VAL:HG23	1:A:957:ARG:HH12	1.50	0.76
1:A:921:GLN:HE21	1:A:957:ARG:CB	1.97	0.76
1:A:761:VAL:CG2	1:A:957:ARG:NH2	2.49	0.75
1:A:794:VAL:HG22	1:A:895:MET:HB3	1.67	0.75
1:A:900:ARG:HH11	1:A:900:ARG:H	1.35	0.75
2:B:672:ASP:HB3	2:B:676:LYS:HG3	1.69	0.75
1:A:826:CYS:HB3	1:A:889:GLN:C	2.06	0.74
1:A:837:VAL:HG11	1:A:908:PHE:CE1	2.23	0.73
1:A:143:TYR:HB2	1:A:203:ILE:HG12	1.71	0.73
1:A:761:VAL:HG23	1:A:957:ARG:NH2	2.04	0.73
1:A:964:ILE:CA	2:B:693:ILE:HD11	2.15	0.72
2:B:150:ARG:HD2	2:B:239:ARG:HD2	1.70	0.72
1:A:794:VAL:CG2	1:A:895:MET:HB3	2.19	0.72
1:A:958:ALA:C	1:A:959:LEU:HD12	2.10	0.71
2:B:516:ILE:HG22	2:B:521:CYS:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:378:GLU:CD	2:B:633:ARG:CZ	2.59	0.70
1:A:421:LEU:HD23	1:A:435:LEU:HD11	1.73	0.69
1:A:451:GLN:NE2	1:A:582:PRO:O	2.25	0.69
2:B:454:THR:HG22	2:B:455:PHE:H	1.57	0.69
1:A:648:GLU:OE1	1:A:649:LEU:N	2.26	0.69
1:A:663:LEU:HA	1:A:670:GLU:O	1.93	0.69
2:B:400:GLU:HB2	4:D:1:NAG:H83	1.75	0.68
2:B:578:ARG:HH11	2:B:601:CYS:N	1.91	0.68
1:A:761:VAL:HG23	1:A:957:ARG:HH22	1.56	0.68
1:A:816:LEU:HD11	1:A:908:PHE:HD1	1.58	0.68
2:B:602:PRO:O	2:B:604:CYS:N	2.25	0.67
1:A:519:ARG:O	1:A:553:ARG:NH1	2.28	0.67
2:B:114:ILE:HB	2:B:151:ILE:HG22	1.77	0.67
1:A:761:VAL:HG23	1:A:957:ARG:CZ	2.24	0.66
1:A:964:ILE:HG23	1:A:966:ILE:HG22	1.76	0.66
1:A:900:ARG:HG2	1:A:901:ALA:H	1.60	0.66
2:B:602:PRO:C	2:B:604:CYS:H	1.99	0.66
1:A:964:ILE:HG13	1:A:966:ILE:CG2	2.26	0.66
1:A:693:MET:SD	1:A:693:MET:N	2.69	0.65
2:B:110:TYR:HD1	2:B:111:PRO:HD2	1.61	0.65
1:A:794:VAL:O	1:A:894:GLU:HA	1.96	0.65
1:A:785:GLU:CA	1:A:902:MET:HB3	2.24	0.65
2:B:320:ASN:ND2	3:C:1:NAG:H62	2.12	0.65
2:B:320:ASN:HD21	3:C:1:NAG:H62	1.60	0.65
1:A:900:ARG:HH11	1:A:900:ARG:N	1.95	0.65
2:B:134:LEU:O	2:B:204:ASN:ND2	2.29	0.64
1:A:653:LEU:HD11	1:A:705:VAL:HG21	1.79	0.64
1:A:917:ARG:HB3	1:A:920:ASP:HB2	1.79	0.64
2:B:667:PHE:HB2	2:B:681:VAL:HG22	1.79	0.63
1:A:2:ASN:OD1	1:A:2:ASN:N	2.30	0.63
1:A:921:GLN:NE2	1:A:957:ARG:HB2	2.09	0.63
1:A:828:PRO:HG2	1:A:832:VAL:H	1.63	0.63
1:A:125:THR:HG21	1:A:165:ARG:HB3	1.81	0.63
2:B:441:ALA:HB1	2:B:455:PHE:HB3	1.81	0.63
1:A:964:ILE:HG13	1:A:966:ILE:HG22	1.80	0.62
1:A:565:ILE:N	1:A:596:THR:O	2.32	0.62
2:B:86:GLN:N	2:B:86:GLN:OE1	2.32	0.62
1:A:2:ASN:O	1:A:3:LEU:C	2.35	0.62
1:A:958:ALA:C	1:A:959:LEU:CD1	2.69	0.61
1:A:288:TYR:OH	2:B:259:ASP:OD1	2.15	0.61
1:A:795:ASN:H	1:A:936:PRO:HD3	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLU:HG2	1:A:151:LEU:HD13	1.82	0.60
1:A:812:LEU:HD11	1:A:878:VAL:HG21	1.83	0.60
1:A:317:ARG:NH2	1:A:350:THR:O	2.32	0.60
1:A:801:ILE:HG23	1:A:928:ALA:HA	1.82	0.60
1:A:54:PHE:HA	1:A:67:SER:HA	1.83	0.60
1:A:964:ILE:HG13	1:A:966:ILE:HB	1.84	0.60
1:A:277:LEU:O	1:A:278:HIS:ND1	2.32	0.60
1:A:939:VAL:O	1:A:941:PRO:HD3	2.01	0.60
2:B:49:CYS:SG	2:B:50:ALA:N	2.75	0.60
1:A:511:ASP:HB3	1:A:519:ARG:HD2	1.84	0.59
2:B:462:CYS:SG	2:B:471:CYS:N	2.74	0.59
5:E:1:NAG:H4	5:E:2:NAG:N2	2.16	0.59
1:A:795:ASN:HA	1:A:893:GLN:O	2.02	0.59
2:B:559:ASN:OD1	2:B:559:ASN:N	2.29	0.59
1:A:636:ASP:OD1	1:A:698:GLN:NE2	2.35	0.59
2:B:498:ARG:NH2	2:B:524:ASP:OD1	2.35	0.59
5:F:1:NAG:H3	5:F:2:NAG:O5	2.03	0.59
1:A:805:GLY:O	1:A:886:THR:OG1	2.20	0.58
1:A:902:MET:SD	1:A:904:THR:HG23	2.44	0.58
2:B:679:LEU:HB3	2:B:681:VAL:HG23	1.84	0.58
1:A:249:ASN:OD1	1:A:249:ASN:N	2.35	0.58
1:A:761:VAL:CG2	1:A:957:ARG:HH12	2.17	0.58
1:A:879:SER:HB3	1:A:925:GLN:HB3	1.85	0.58
2:B:306:LEU:HB3	2:B:328:THR:HG22	1.85	0.58
2:B:319:GLN:HA	2:B:330:VAL:HG21	1.86	0.58
2:B:161:VAL:HG13	2:B:163:PRO:HD2	1.85	0.58
1:A:137:SER:OG	1:A:138:GLY:N	2.35	0.58
1:A:667:GLU:O	1:A:668:GLY:C	2.43	0.57
1:A:963:ALA:HB1	2:B:693:ILE:HD13	1.87	0.57
2:B:709:LEU:HA	2:B:712:LEU:HD12	1.87	0.57
1:A:760:VAL:HG12	1:A:956:LEU:HB2	1.86	0.57
2:B:652:ALA:HB3	2:B:668:GLN:HE21	1.69	0.57
1:A:897:ARG:HH11	1:A:898:GLY:N	2.03	0.56
1:A:959:LEU:CD1	1:A:959:LEU:N	2.68	0.56
2:B:51:PRO:HA	2:B:54:ILE:HD12	1.87	0.56
1:A:651:VAL:HB	1:A:685:VAL:HG12	1.85	0.56
1:A:791:PRO:O	1:A:897:ARG:HB2	2.05	0.56
1:A:608:CYS:O	1:A:727:ASN:ND2	2.39	0.56
1:A:812:LEU:HB2	1:A:914:LEU:HB3	1.88	0.56
2:B:616:GLU:O	2:B:622:ARG:N	2.38	0.56
5:E:1:NAG:H4	5:E:2:NAG:HN2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:PRO:O	1:A:67:SER:HB3	2.05	0.55
1:A:666:VAL:O	1:A:667:GLU:C	2.43	0.55
2:B:667:PHE:HE2	2:B:669:TYR:HD1	1.55	0.55
2:B:449:ASN:HB3	2:B:452:ASN:HB2	1.89	0.55
1:A:335:ARG:O	1:A:338:HIS:ND1	2.39	0.55
1:A:921:GLN:HB3	1:A:957:ARG:HB2	1.89	0.55
1:A:113:TRP:NE1	1:A:148:GLY:O	2.39	0.55
1:A:963:ALA:C	2:B:693:ILE:HG12	2.27	0.55
1:A:795:ASN:HB2	1:A:936:PRO:HG3	1.88	0.55
1:A:664:SER:H	1:A:670:GLU:HA	1.71	0.54
1:A:966:ILE:HG23	1:A:967:TRP:N	2.22	0.54
1:A:763:ALA:HB1	1:A:959:LEU:CD2	2.37	0.54
1:A:763:ALA:HB2	1:A:959:LEU:HG	1.88	0.54
1:A:82:GLN:HE22	1:A:149:ASN:HD22	1.53	0.54
1:A:661:ARG:HG3	1:A:662:ALA:N	2.20	0.54
1:A:458:VAL:HG11	1:A:569:LEU:HD22	1.89	0.54
1:A:652:HIS:HB2	1:A:720:GLN:HB3	1.88	0.54
1:A:912:PRO:O	1:A:915:TYR:HB2	2.08	0.54
1:A:793:THR:HG22	1:A:896:ALA:CA	2.36	0.54
1:A:77:ARG:NH1	1:A:211:ILE:HA	2.22	0.54
1:A:964:ILE:HG13	1:A:966:ILE:CB	2.38	0.54
2:B:43:ASN:O	2:B:47:ASP:N	2.41	0.53
1:A:415:SER:HA	1:A:441:GLY:HA3	1.91	0.53
1:A:323:ALA:HB1	1:A:352:LEU:HD11	1.90	0.53
1:A:965:PRO:HG2	2:B:697:LEU:CA	2.39	0.53
1:A:84:LEU:HB3	1:A:113:TRP:CH2	2.44	0.53
1:A:937:TYR:HD2	1:A:940:PRO:HB3	1.74	0.53
1:A:874:ASP:N	1:A:921:GLN:OE1	2.42	0.52
2:B:613:GLU:O	2:B:617:CYS:N	2.34	0.52
2:B:106:GLN:HE22	2:B:355:VAL:HG22	1.74	0.52
1:A:965:PRO:HG2	2:B:697:LEU:HA	1.91	0.52
1:A:812:LEU:HB3	1:A:914:LEU:N	2.25	0.52
2:B:412:LYS:HG3	2:B:431:PHE:HE2	1.74	0.52
2:B:593:SER:HA	2:B:601:CYS:HA	1.92	0.52
1:A:197:GLN:OE1	1:A:253:TYR:OH	2.18	0.52
1:A:836:LYS:HD3	1:A:837:VAL:H	1.75	0.52
2:B:160:PRO:HD2	2:B:285:THR:HG22	1.91	0.52
1:A:780:VAL:H	1:A:907:ALA:HB3	1.75	0.52
1:A:902:MET:SD	1:A:903:VAL:N	2.83	0.52
2:B:156:PHE:CE2	2:B:222:GLY:HA2	2.45	0.51
1:A:187:GLY:HA2	1:A:191:PHE:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:498:ARG:HH12	2:B:524:ASP:HB2	1.75	0.51
1:A:829:GLN:O	1:A:886:THR:HG23	2.11	0.51
2:B:20:SER:O	2:B:93:ARG:NH2	2.44	0.51
1:A:803:LEU:HD12	1:A:888:VAL:HG21	1.91	0.51
1:A:912:PRO:HA	1:A:915:TYR:HB2	1.93	0.51
2:B:606:ASP:N	2:B:606:ASP:OD1	2.43	0.51
1:A:353:TYR:OH	2:B:297:GLU:OE1	2.23	0.51
2:B:416:ILE:HD12	2:B:416:ILE:H	1.76	0.51
1:A:153:ARG:HG2	1:A:154:ILE:HD12	1.92	0.51
1:A:368:ARG:NH1	1:A:431:GLY:O	2.43	0.51
1:A:965:PRO:HD2	2:B:696:VAL:HG23	1.91	0.51
2:B:96:ASP:OD1	2:B:97:SER:N	2.42	0.51
2:B:640:GLU:H	2:B:679:LEU:HB2	1.76	0.51
1:A:153:ARG:HA	1:A:156:VAL:HG12	1.93	0.51
1:A:648:GLU:OE2	1:A:686:LEU:HG	2.11	0.51
1:A:763:ALA:HB1	1:A:959:LEU:HD21	1.93	0.51
2:B:83:VAL:HG13	2:B:102:ILE:HG23	1.93	0.51
1:A:227:ASN:HB3	1:A:230:TYR:HD2	1.76	0.50
1:A:657:ALA:HA	1:A:708:GLY:H	1.75	0.50
1:A:669:PHE:N	1:A:669:PHE:CD1	2.78	0.50
1:A:807:SER:O	1:A:834:PRO:HG3	2.11	0.50
2:B:333:LEU:HD11	2:B:337:SER:HA	1.93	0.50
1:A:230:TYR:OH	1:A:279:ARG:NH2	2.40	0.50
1:A:812:LEU:HB2	1:A:914:LEU:CB	2.40	0.50
1:A:959:LEU:N	1:A:959:LEU:HD13	2.26	0.50
2:B:194:LEU:HB2	2:B:206:GLU:OE2	2.12	0.50
1:A:819:GLN:O	1:A:902:MET:CE	2.59	0.50
1:A:663:LEU:HD22	1:A:670:GLU:HB3	1.93	0.50
2:B:232:CYS:O	2:B:236:ILE:HG12	2.12	0.50
1:A:25:PHE:HE2	1:A:427:ILE:HD12	1.77	0.50
1:A:661:ARG:NH2	5:E:2:NAG:H61	2.26	0.50
1:A:688:GLU:OE1	1:A:690:GLY:N	2.45	0.50
1:A:795:ASN:N	1:A:936:PRO:HD3	2.26	0.50
2:B:60:GLU:OE2	2:B:91:ARG:NH2	2.38	0.50
1:A:651:VAL:HG22	1:A:721:LEU:HD22	1.94	0.50
1:A:653:LEU:HG	1:A:657:ALA:HB3	1.94	0.49
1:A:777:GLY:N	1:A:908:PHE:HB2	2.27	0.49
1:A:460:LEU:HB3	1:A:594:GLU:HG3	1.94	0.49
1:A:803:LEU:O	1:A:886:THR:N	2.37	0.49
1:A:144:SER:CB	1:A:147:ARG:HE	2.25	0.49
1:A:436:ILE:HG22	1:A:447:VAL:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:LEU:O	1:A:519:ARG:NH1	2.45	0.49
1:A:967:TRP:CG	1:A:967:TRP:O	2.65	0.49
2:B:179:ASP:OD1	2:B:180:MET:HG3	2.12	0.49
2:B:709:LEU:HD12	2:B:712:LEU:HD12	1.95	0.49
1:A:897:ARG:HG3	1:A:897:ARG:O	2.11	0.49
1:A:965:PRO:HD3	2:B:693:ILE:CG1	2.43	0.49
2:B:158:ASP:HB3	2:B:187:MET:HE3	1.95	0.49
1:A:208:ARG:HG3	1:A:209:PRO:HD3	1.94	0.49
1:A:225:SER:OG	1:A:226:SER:N	2.43	0.49
1:A:836:LYS:CD	1:A:837:VAL:H	2.25	0.49
1:A:602:CYS:C	1:A:642:GLU:OE2	2.49	0.49
1:A:87:PHE:CD2	1:A:124:LYS:HD3	2.47	0.49
1:A:812:LEU:CB	1:A:914:LEU:CB	2.91	0.48
1:A:837:VAL:HG12	1:A:838:ASP:H	1.76	0.48
1:A:462:VAL:HG21	1:A:567:LEU:HD12	1.96	0.48
1:A:812:LEU:HA	1:A:910:TRP:HB3	1.96	0.48
1:A:245:ASP:OD1	1:A:247:ASP:N	2.45	0.48
2:B:108:GLU:HG3	2:B:391:ILE:HG22	1.95	0.48
1:A:22:SER:OG	1:A:95:ALA:O	2.25	0.48
1:A:365:ASP:OD2	1:A:370:GLY:N	2.39	0.48
2:B:161:VAL:O	2:B:165:MET:HG2	2.13	0.48
2:B:596:ASP:N	2:B:599:GLU:OE2	2.46	0.48
2:B:600:LYS:HA	2:B:600:LYS:HD3	1.55	0.48
2:B:359:VAL:HG11	2:B:368:LEU:HD12	1.94	0.48
1:A:763:ALA:HA	1:A:959:LEU:HD11	1.95	0.48
2:B:359:VAL:HG12	2:B:416:ILE:HG13	1.94	0.48
1:A:356:PHE:HE1	1:A:390:LEU:HD13	1.78	0.48
2:B:119:ASP:HB3	2:B:124:MET:SD	2.54	0.48
1:A:671:ARG:NH2	2:B:545:GLY:O	2.47	0.47
2:B:435:CYS:O	2:B:438:GLN:NE2	2.45	0.47
1:A:511:ASP:OD1	1:A:520:ARG:NH2	2.47	0.47
1:A:263:THR:O	1:A:263:THR:HG22	2.15	0.47
2:B:639:ILE:HG23	2:B:679:LEU:HD12	1.97	0.47
1:A:548:THR:OG1	1:A:549:MET:N	2.47	0.47
1:A:784:TYR:HE2	1:A:949:ALA:HB3	1.80	0.47
1:A:819:GLN:O	1:A:902:MET:HE3	2.14	0.47
2:B:557:TYR:HD2	5:E:1:NAG:H5	1.80	0.47
2:B:639:ILE:HA	2:B:679:LEU:HD12	1.97	0.47
1:A:761:VAL:CB	1:A:957:ARG:HH12	2.27	0.47
1:A:959:LEU:HA	1:A:960:GLU:OE2	2.15	0.47
1:A:965:PRO:HG2	2:B:697:LEU:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:PRO:HG2	2:B:93:ARG:HD2	1.96	0.47
2:B:462:CYS:HB3	2:B:466:TRP:HD1	1.80	0.47
1:A:664:SER:OG	1:A:665:ASN:N	2.46	0.46
2:B:637:ASP:OD1	2:B:637:ASP:N	2.48	0.46
2:B:468:GLY:HA2	2:B:503:CYS:SG	2.55	0.46
1:A:669:PHE:O	1:A:670:GLU:C	2.53	0.46
1:A:914:LEU:HD12	1:A:922:PHE:CD2	2.50	0.46
1:A:925:GLN:NE2	1:A:950:GLN:OE1	2.49	0.46
1:A:74:ASP:H	1:A:88:LYS:HD2	1.80	0.46
2:B:578:ARG:HH12	2:B:601:CYS:H	1.54	0.46
1:A:790:GLY:O	1:A:897:ARG:CZ	2.64	0.46
1:A:917:ARG:HG2	1:A:920:ASP:HB2	1.97	0.46
1:A:958:ALA:N	1:A:959:LEU:CD1	2.78	0.46
1:A:42:THR:H	1:A:51:GLY:HA2	1.81	0.46
2:B:310:VAL:HG11	2:B:318:TYR:CD2	2.50	0.46
1:A:801:ILE:O	1:A:888:VAL:N	2.47	0.46
1:A:965:PRO:CG	2:B:697:LEU:HA	2.46	0.46
2:B:435:CYS:H	2:B:438:GLN:HE21	1.62	0.46
1:A:27:LYS:HE3	1:A:27:LYS:HB3	1.70	0.45
2:B:365:GLU:OE1	2:B:365:GLU:N	2.46	0.45
2:B:515:LYS:HE3	2:B:517:THR:HG22	1.98	0.45
2:B:652:ALA:HB1	2:B:670:TYR:HB3	1.97	0.45
1:A:70:PHE:CE2	1:A:133:ALA:HB2	2.52	0.45
1:A:807:SER:HB2	1:A:832:VAL:HA	1.98	0.45
1:A:931:ASN:HA	1:A:945:PRO:O	2.16	0.45
1:A:965:PRO:HD2	2:B:696:VAL:CG2	2.47	0.45
1:A:464:ASP:OD2	1:A:728:SER:OG	2.30	0.45
1:A:914:LEU:C	1:A:916:GLN:N	2.70	0.45
2:B:531:TYR:HE2	5:E:1:NAG:O5	2.00	0.45
2:B:601:CYS:O	2:B:601:CYS:SG	2.73	0.45
2:B:183:THR:O	2:B:183:THR:OG1	2.32	0.45
1:A:900:ARG:HG2	1:A:901:ALA:N	2.29	0.45
2:B:231:VAL:HG12	2:B:273:CYS:HB2	1.98	0.45
1:A:1:LEU:H2	1:A:366:LEU:HD23	1.82	0.45
2:B:554:THR:O	2:B:560:CYS:HB3	2.16	0.45
1:A:2:ASN:O	1:A:4:ASP:N	2.50	0.45
1:A:763:ALA:CB	1:A:959:LEU:HD21	2.46	0.45
2:B:31:LEU:HD12	2:B:32:PRO:HD2	1.99	0.45
2:B:33:LEU:HD23	2:B:33:LEU:HA	1.86	0.45
2:B:378:GLU:CD	2:B:633:ARG:HH21	2.16	0.45
1:A:471:LYS:HD3	1:A:481:PRO:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:437:CYS:SG	2:B:438:GLN:N	2.90	0.45
1:A:72:LEU:HA	1:A:88:LYS:HD3	1.99	0.45
2:B:85:PRO:HG2	2:B:88:ILE:HD11	1.99	0.44
1:A:612:LEU:HB3	1:A:733:SER:HB3	1.98	0.44
1:A:510:LEU:HD11	1:A:523:LEU:HG	1.98	0.44
1:A:763:ALA:CB	1:A:959:LEU:CD2	2.95	0.44
2:B:486:CYS:HB3	2:B:506:CYS:SG	2.57	0.44
1:A:751:ARG:HB2	2:B:603:THR:HG21	2.00	0.44
1:A:664:SER:N	1:A:670:GLU:O	2.50	0.44
2:B:496:SER:O	2:B:498:ARG:HG3	2.18	0.44
1:A:964:ILE:HA	2:B:693:ILE:CD1	2.22	0.44
2:B:215:ASN:ND2	2:B:220:GLU:OE1	2.49	0.44
1:A:48:GLU:OE1	1:A:48:GLU:N	2.51	0.44
1:A:394:GLY:HA2	1:A:399:LEU:HD23	2.00	0.44
2:B:195:THR:O	2:B:197:THR:HG23	2.17	0.44
1:A:910:TRP:HD1	1:A:913:SER:HG	1.65	0.43
2:B:243:SER:OG	2:B:352:ARG:NH2	2.47	0.43
1:A:144:SER:HB3	1:A:147:ARG:HE	1.83	0.43
1:A:793:THR:HG22	1:A:896:ALA:CB	2.48	0.43
1:A:900:ARG:CG	1:A:901:ALA:H	2.25	0.43
1:A:964:ILE:CG2	1:A:966:ILE:HG22	2.46	0.43
2:B:44:LEU:HD23	2:B:44:LEU:HA	1.90	0.43
5:E:1:NAG:H82	5:E:1:NAG:H2	1.84	0.43
1:A:939:VAL:HB	1:A:941:PRO:HG3	2.00	0.43
2:B:613:GLU:HA	2:B:616:GLU:HB2	2.00	0.43
2:B:435:CYS:H	2:B:438:GLN:NE2	2.17	0.43
1:A:781:GLU:HG2	1:A:905:VAL:O	2.19	0.43
1:A:820:PRO:HB2	1:A:821:GLN:H	1.57	0.43
1:A:785:GLU:CB	1:A:902:MET:HB3	2.48	0.43
1:A:791:PRO:O	1:A:897:ARG:CB	2.66	0.43
1:A:785:GLU:HG3	1:A:901:ALA:O	2.18	0.43
1:A:969:VAL:HG12	1:A:969:VAL:O	2.18	0.43
1:A:428:ASP:OD1	1:A:428:ASP:N	2.52	0.42
2:B:136:THR:O	2:B:140:THR:HG23	2.19	0.42
2:B:602:PRO:C	2:B:604:CYS:N	2.70	0.42
1:A:965:PRO:HD3	2:B:693:ILE:HG13	2.00	0.42
1:A:245:ASP:OD1	1:A:246:GLY:N	2.52	0.42
2:B:102:ILE:HD12	2:B:399:ILE:HD11	2.00	0.42
2:B:159:LYS:HA	2:B:160:PRO:HD3	1.89	0.42
2:B:261:ARG:HG3	2:B:266:VAL:HG12	2.01	0.42
2:B:308:PHE:HB2	2:B:330:VAL:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:LEU:HB2	1:A:400:ARG:HD2	2.02	0.42
1:A:782:HIS:HB3	1:A:951:VAL:HG21	2.00	0.42
1:A:894:GLU:O	1:A:895:MET:HB2	2.19	0.42
2:B:250:THR:HG22	2:B:310:VAL:HG12	2.02	0.42
2:B:637:ASP:HA	2:B:677:SER:HB2	2.01	0.42
1:A:6:VAL:HG13	1:A:7:GLN:HG2	2.02	0.42
1:A:25:PHE:CE2	1:A:427:ILE:HD12	2.54	0.42
1:A:812:LEU:HA	1:A:913:SER:HB2	2.01	0.42
1:A:914:LEU:O	1:A:916:GLN:N	2.52	0.42
2:B:90:LEU:HD23	2:B:92:LEU:HD21	2.00	0.42
2:B:380:ILE:HD12	2:B:383:LEU:HD23	2.02	0.42
1:A:611:GLN:HB2	1:A:641:GLY:N	2.35	0.42
1:A:667:GLU:O	1:A:669:PHE:N	2.52	0.42
2:B:24:ALA:HB2	2:B:56:PHE:CD2	2.54	0.42
2:B:161:VAL:HG22	2:B:162:SER:H	1.85	0.42
2:B:190:TYR:HB3	2:B:281:TYR:HB2	2.02	0.42
1:A:182:VAL:HG21	1:A:195:LEU:HD23	2.02	0.41
1:A:333:GLN:HE21	1:A:333:GLN:HB2	1.66	0.41
1:A:491:VAL:HG11	1:A:535:LEU:HG	2.02	0.41
1:A:608:CYS:HB3	1:A:643:GLY:O	2.20	0.41
1:A:794:VAL:HB	1:A:935:LEU:HD22	2.01	0.41
2:B:110:TYR:CD1	2:B:111:PRO:HD2	2.49	0.41
2:B:191:LYS:HE3	2:B:191:LYS:HB2	1.86	0.41
2:B:621:ASP:OD1	2:B:621:ASP:N	2.54	0.41
1:A:123:GLU:O	1:A:125:THR:HG23	2.20	0.41
1:A:522:LEU:HD11	1:A:527:GLN:C	2.41	0.41
1:A:664:SER:H	1:A:670:GLU:CA	2.33	0.41
1:A:356:PHE:CE1	1:A:390:LEU:HD13	2.55	0.41
1:A:555:GLU:OE1	1:A:561:LYS:NZ	2.39	0.41
2:B:65:GLU:HB2	2:B:86:GLN:HG2	2.02	0.41
2:B:138:LEU:HA	2:B:341:LEU:HD11	2.02	0.41
1:A:395:GLN:N	1:A:398:GLY:O	2.40	0.41
2:B:181:LYS:HA	2:B:181:LYS:HD3	1.61	0.41
1:A:484:CYS:HA	1:A:551:PHE:HA	2.03	0.41
2:B:531:TYR:HD1	2:B:532:LYS:HG3	1.86	0.41
1:A:120:GLU:HG3	1:A:121:GLU:N	2.36	0.41
1:A:662:ALA:O	1:A:663:LEU:HD23	2.21	0.41
2:B:467:LEU:HB2	2:B:474:SER:HA	2.03	0.41
2:B:488:PRO:HB2	2:B:489:ARG:HH11	1.85	0.41
2:B:702:GLY:O	2:B:706:LEU:HD23	2.21	0.41
1:A:320:ARG:HA	1:A:320:ARG:HD2	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:832:VAL:O	1:A:833:ASN:C	2.60	0.41
1:A:893:GLN:OE1	1:A:894:GLU:HB3	2.21	0.41
1:A:917:ARG:CB	1:A:920:ASP:HB2	2.50	0.41
1:A:925:GLN:HG2	1:A:926:SER:N	2.36	0.41
2:B:416:ILE:HD12	2:B:416:ILE:N	2.36	0.41
1:A:918:PRO:O	1:A:919:LEU:HD23	2.20	0.40
2:B:44:LEU:HD13	2:B:54:ILE:HG12	2.02	0.40
1:A:835:LEU:C	1:A:836:LYS:HG3	2.42	0.40
1:A:932:VAL:HB	1:A:945:PRO:HD2	2.03	0.40
2:B:134:LEU:HG	2:B:135:GLY:H	1.86	0.40
2:B:400:GLU:OE1	2:B:551:SER:OG	2.21	0.40
1:A:43:LEU:HB3	1:A:44:GLY:H	1.56	0.40
1:A:800:SER:HA	1:A:889:GLN:HG3	2.03	0.40
1:A:965:PRO:HG2	2:B:696:VAL:HG23	2.03	0.40
2:B:43:ASN:HA	2:B:46:LYS:HD3	2.03	0.40
2:B:179:ASP:O	2:B:181:LYS:NZ	2.55	0.40
1:A:36:VAL:HG22	1:A:55:LEU:HD12	2.04	0.40
1:A:141:ALA:HA	1:A:207:TYR:CD2	2.56	0.40
1:A:565:ILE:O	1:A:596:THR:N	2.48	0.40
2:B:185:LEU:HD13	2:B:211:SER:HB2	2.03	0.40
2:B:294:LEU:HD12	2:B:294:LEU:HA	1.91	0.40
2:B:654:ASN:HA	2:B:668:GLN:HA	2.03	0.40
1:A:107:CYS:HA	1:A:130:CYS:HA	2.04	0.40
1:A:134:GLN:O	1:A:138:GLY:HA3	2.22	0.40
1:A:837:VAL:HG12	1:A:838:ASP:N	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	934/1039 (90%)	850 (91%)	66 (7%)	18 (2%)	6	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	689/788 (87%)	627 (91%)	59 (9%)	3 (0%)	30	63
All	All	1623/1827 (89%)	1477 (91%)	125 (8%)	21 (1%)	13	37

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	667	GLU
1	A	668	GLY
1	A	836	LYS
1	A	837	VAL
1	A	895	MET
2	B	602	PRO
2	B	603	THR
1	A	820	PRO
2	B	670	TYR
1	A	3	LEU
1	A	825	GLN
1	A	961	GLU
1	A	965	PRO
1	A	67	SER
1	A	745	GLU
1	A	821	GLN
1	A	900	ARG
1	A	902	MET
1	A	960	GLU
1	A	962	ARG
1	A	123	GLU

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	779/864 (90%)	720 (92%)	59 (8%)	11	35
2	B	616/690 (89%)	587 (95%)	29 (5%)	22	53
All	All	1395/1554 (90%)	1307 (94%)	88 (6%)	17	43

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	21	PHE
1	A	23	LEU
1	A	30	HIS
1	A	139	ARG
1	A	147	ARG
1	A	153	ARG
1	A	171	PHE
1	A	177	GLN
1	A	190	TYR
1	A	204	PHE
1	A	249	ASN
1	A	288	TYR
1	A	554	ASP
1	A	601	ASP
1	A	661	ARG
1	A	663	LEU
1	A	664	SER
1	A	667	GLU
1	A	669	PHE
1	A	670	GLU
1	A	673	ILE
1	A	743	ARG
1	A	750	LEU
1	A	761	VAL
1	A	798	HIS
1	A	799	LEU
1	A	810	SER
1	A	811	ASP
1	A	812	LEU
1	A	813	LEU
1	A	816	LEU
1	A	818	ILE
1	A	821	GLN
1	A	825	GLN
1	A	836	LYS
1	A	880	CYS
1	A	887	VAL
1	A	893	GLN
1	A	894	GLU
1	A	897	ARG
1	A	899	GLN

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Mol	Chain	Res	Type
1	A	900	ARG
1	A	902	MET
1	A	904	THR
1	A	914	LEU
1	A	915	TYR
1	A	916	GLN
1	A	917	ARG
1	A	921	GLN
1	A	927	HIS
1	A	930	PHE
1	A	932	VAL
1	A	939	VAL
1	A	942	LEU
1	A	957	ARG
1	A	959	LEU
1	A	967	TRP
1	A	968	TRP
2	B	16	CYS
2	B	26	CYS
2	B	109	ASP
2	B	110	TYR
2	B	117	LEU
2	B	127	ASP
2	B	133	ASN
2	B	198	ASP
2	B	241	ASP
2	B	281	TYR
2	B	322	SER
2	B	449	ASN
2	B	535	MET
2	B	543	SER
2	B	561	THR
2	B	568	MET
2	B	599	GLU
2	B	600	LYS
2	B	606	ASP
2	B	614	CYS
2	B	620	PHE
2	B	630	THR
2	B	636	ARG
2	B	637	ASP
2	B	647	ASP

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Mol	Chain	Res	Type
2	B	654	ASN
2	B	664	VAL
2	B	669	TYR
2	B	701	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	333	GLN
1	A	747	GLN
1	A	798	HIS
1	A	802	HIS
1	A	916	GLN
1	A	921	GLN
1	A	925	GLN
2	B	668	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

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	2,3	14,14,15	0.51	0	17,19,21	1.66	3 (17%)

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	0.43	0	17,19,21	1.59	2 (11%)
3	BMA	C	3	3	11,11,12	0.23	0	15,15,17	0.82	0
3	MAN	C	4	3	11,11,12	0.29	0	15,15,17	0.73	1 (6%)
3	BMA	C	5	3	11,11,12	0.22	0	15,15,17	0.49	0
4	NAG	D	1	4,2	14,14,15	0.56	0	17,19,21	0.88	1 (5%)
4	NAG	D	2	4	14,14,15	0.52	0	17,19,21	0.87	0
4	BMA	D	3	4	11,11,12	0.27	0	15,15,17	0.62	0
5	NAG	E	1	2,5	14,14,15	0.36	0	17,19,21	1.86	5 (29%)
5	NAG	E	2	5	14,14,15	0.32	0	17,19,21	0.99	0
5	NAG	F	1	2,5	14,14,15	0.43	0	17,19,21	1.04	2 (11%)
5	NAG	F	2	5	14,14,15	0.32	0	17,19,21	1.08	2 (11%)

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	2,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	1/1/5/7	4/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	BMA	C	5	3	-	1/2/19/22	0/1/1/1
4	NAG	D	1	4,2	-	3/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
5	NAG	E	1	2,5	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	4/6/23/26	0/1/1/1
5	NAG	F	1	2,5	-	3/6/23/26	0/1/1/1
5	NAG	F	2	5	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C1-O5-C5	4.54	118.26	112.19
3	C	2	NAG	C2-N2-C7	-4.19	117.28	122.90
5	E	1	NAG	O5-C1-C2	-4.18	104.83	111.29
3	C	2	NAG	C1-C2-N2	3.84	116.48	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C2-N2-C7	-3.82	117.78	122.90
5	E	1	NAG	C2-N2-C7	-3.49	118.22	122.90
5	F	2	NAG	C2-N2-C7	-3.28	118.50	122.90
5	E	1	NAG	C4-C3-C2	-3.17	106.37	111.02
5	F	1	NAG	C1-O5-C5	2.64	115.73	112.19
5	E	1	NAG	C3-C4-C5	-2.60	105.52	110.23
4	D	1	NAG	C1-O5-C5	2.26	115.21	112.19
5	E	1	NAG	O4-C4-C3	2.25	115.68	110.38
5	F	1	NAG	C6-C5-C4	-2.21	107.59	113.02
3	C	4	MAN	C1-O5-C5	2.18	115.11	112.19
5	F	2	NAG	C4-C3-C2	-2.15	107.87	111.02
3	C	1	NAG	O5-C5-C6	2.01	111.57	107.66

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	2	NAG	C1
5	E	1	NAG	C1

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1	NAG	C8-C7-N2-C2
5	E	1	NAG	O7-C7-N2-C2
5	E	2	NAG	C3-C2-N2-C7
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
5	F	1	NAG	C1-C2-N2-C7
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
5	F	2	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
5	F	1	NAG	C8-C7-N2-C2
4	D	1	NAG	C8-C7-N2-C2
4	D	2	NAG	C8-C7-N2-C2
5	F	1	NAG	O7-C7-N2-C2
4	D	1	NAG	O5-C5-C6-O6
5	F	2	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2

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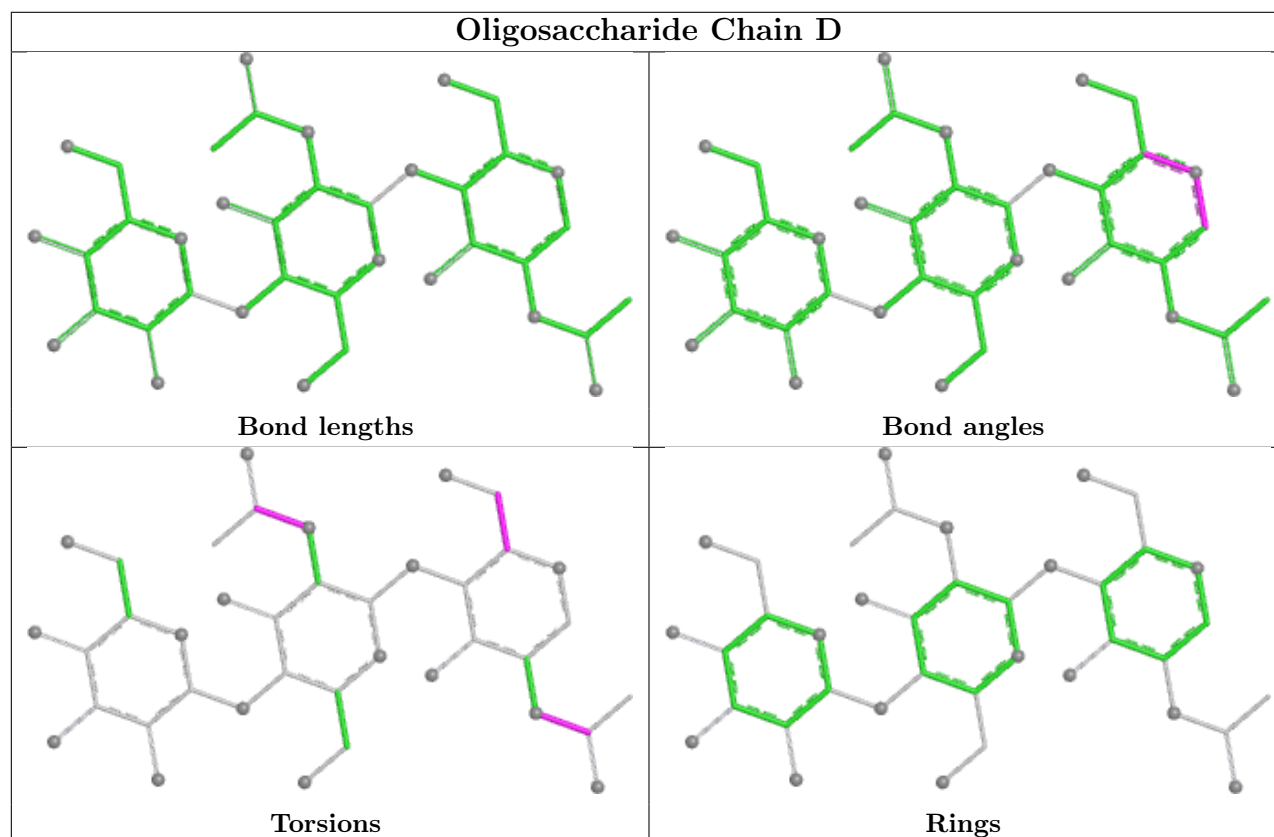
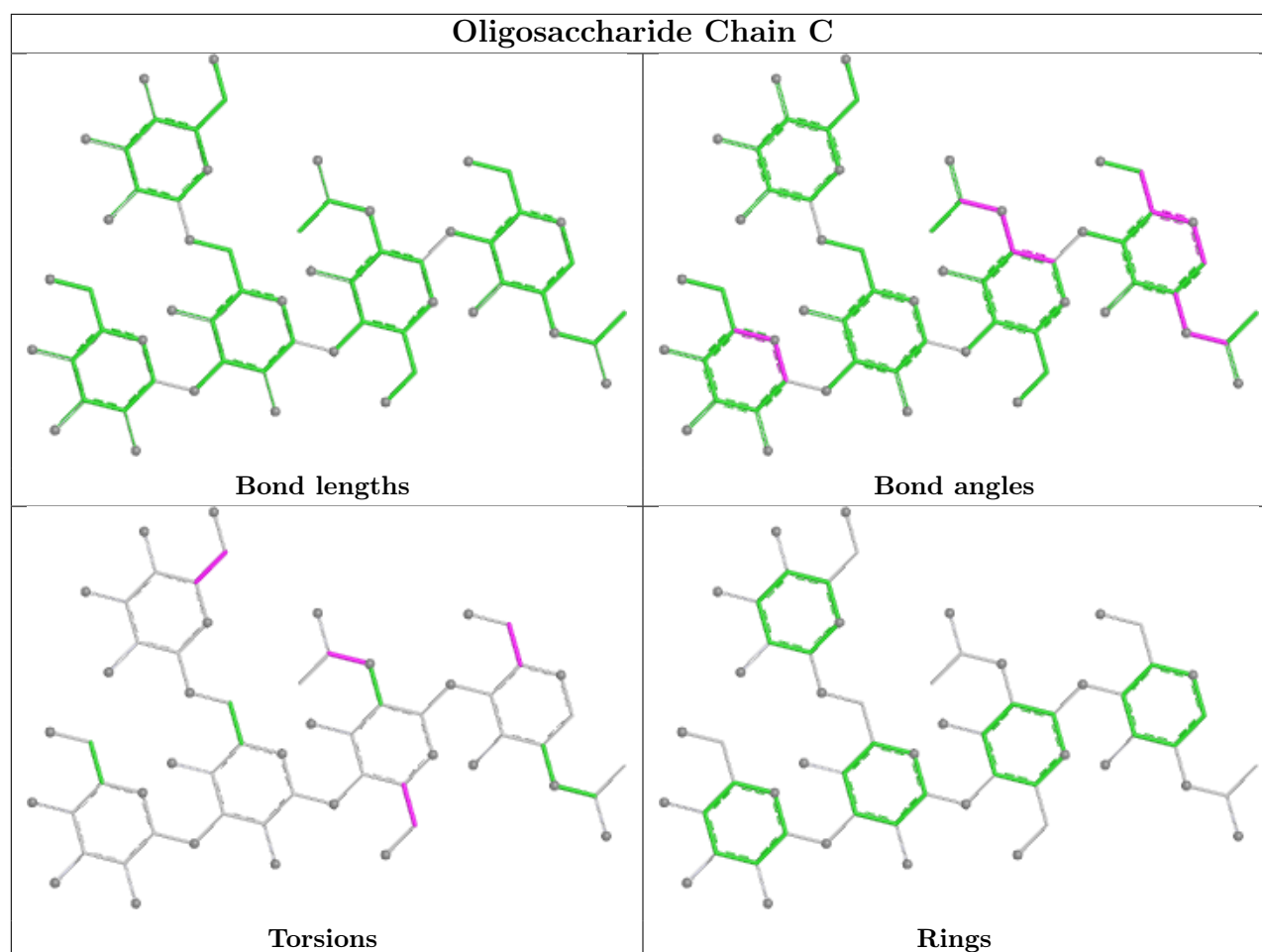
Mol	Chain	Res	Type	Atoms
5	F	2	NAG	O7-C7-N2-C2
5	E	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	5	BMA	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6

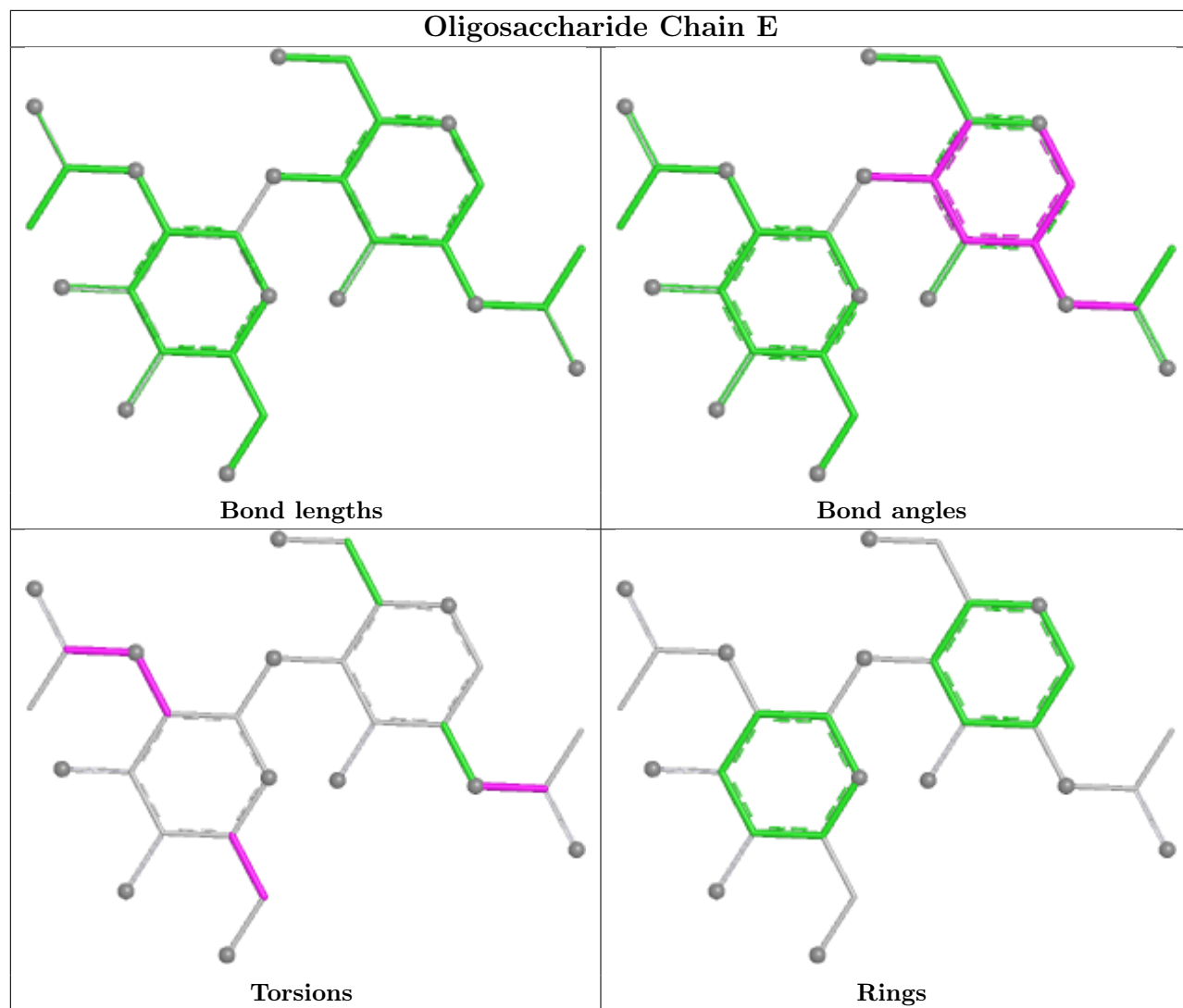
There are no ring outliers.

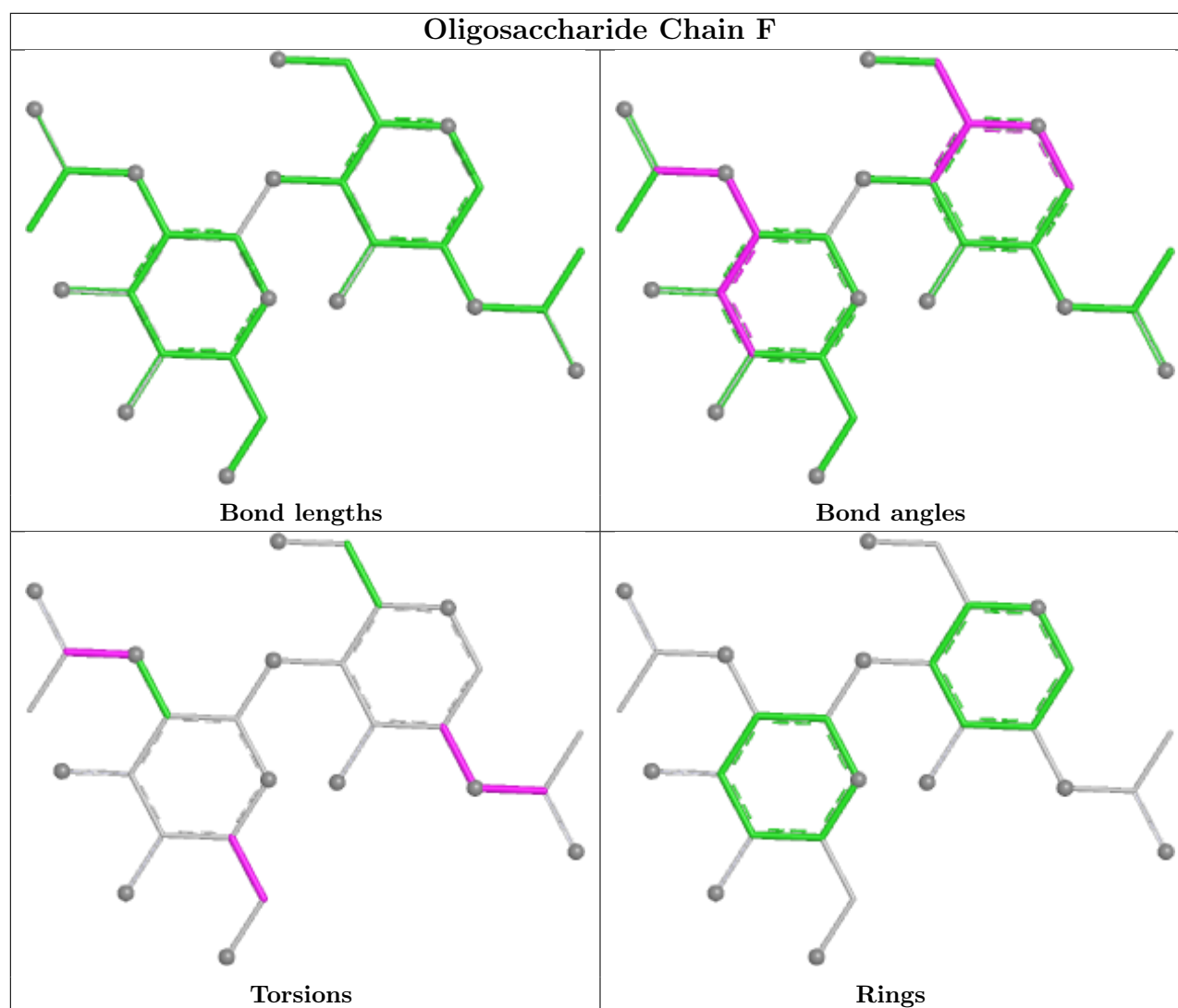
6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	1	0
5	F	1	NAG	1	0
5	E	2	NAG	3	0
5	F	2	NAG	1	0
5	E	1	NAG	5	0
3	C	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 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 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	$\# Z  > 2$
7	NAG	A	1107	1	14,14,15	0.28	0	17,19,21	1.22	2 (11%)
7	NAG	A	1108	1	14,14,15	0.31	0	17,19,21	0.75	0
7	NAG	A	1106	1	14,14,15	0.36	0	17,19,21	0.74	1 (5%)



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
7	NAG	A	1107	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1108	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1106	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1107	NAG	C4-C3-C2	-3.18	106.36	111.02
7	A	1107	NAG	C2-N2-C7	-2.68	119.30	122.90
7	A	1106	NAG	C4-C3-C2	-2.28	107.67	111.02

There are no chirality outliers.

All (7) torsion outliers are listed below:

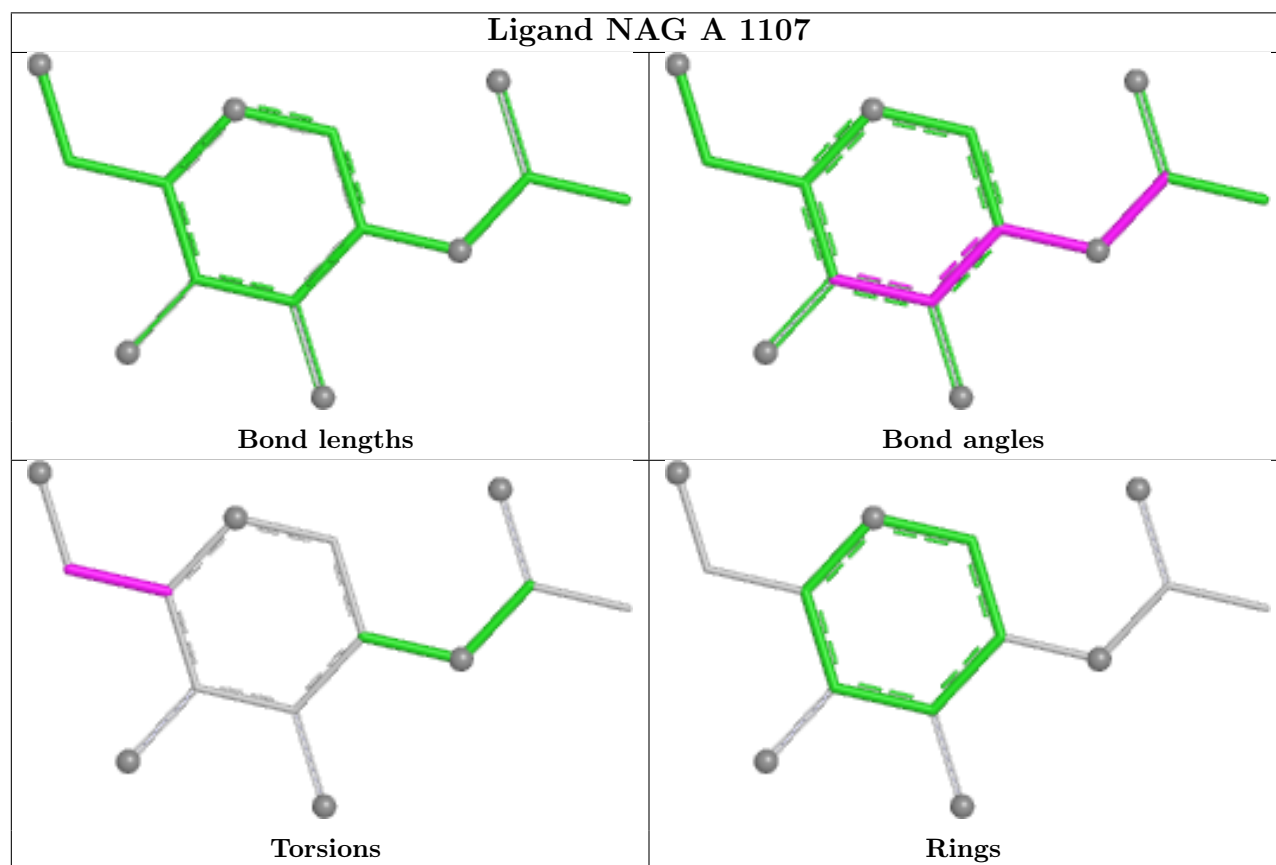
Mol	Chain	Res	Type	Atoms
7	A	1106	NAG	C1-C2-N2-C7
7	A	1106	NAG	C8-C7-N2-C2
7	A	1106	NAG	O7-C7-N2-C2
7	A	1108	NAG	C8-C7-N2-C2
7	A	1108	NAG	O7-C7-N2-C2
7	A	1107	NAG	C4-C5-C6-O6
7	A	1107	NAG	O5-C5-C6-O6

There are no ring outliers.

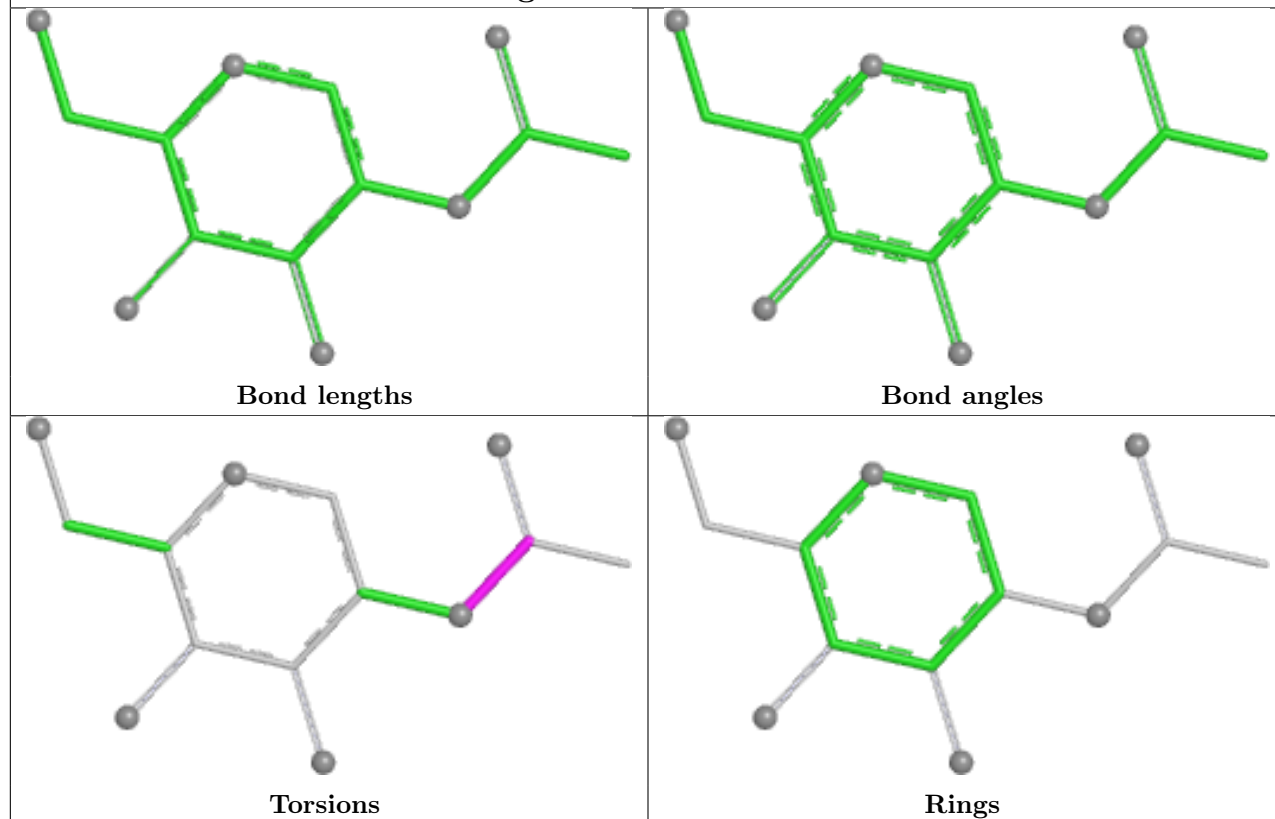
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

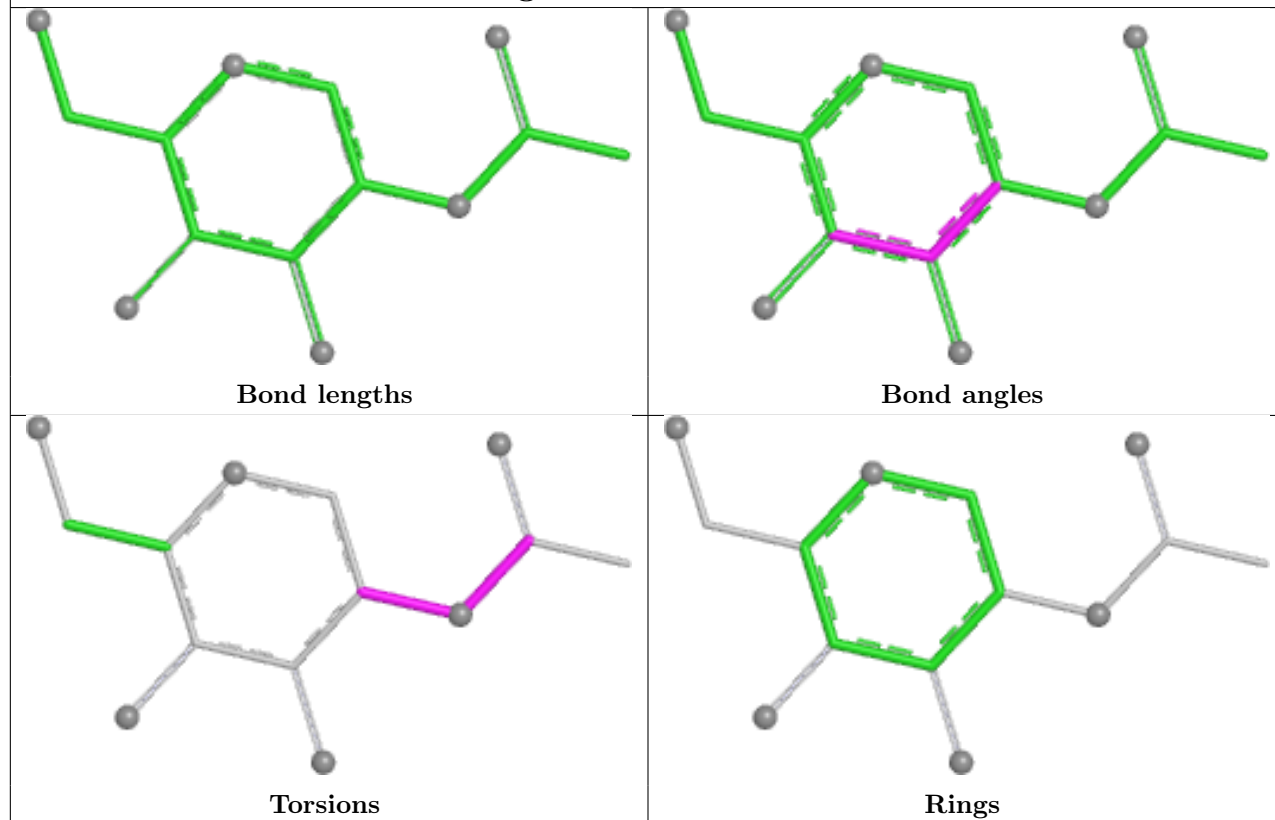
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## Ligand NAG A 1108



## Ligand NAG A 1106



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

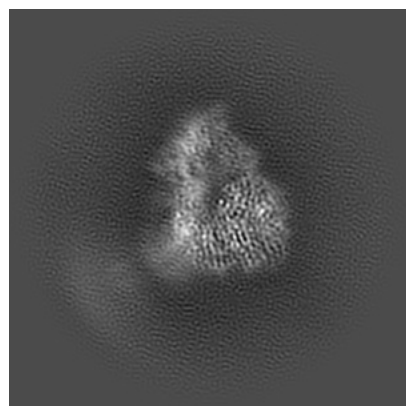
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29931. These allow visual inspection of the internal detail of the map and identification of artifacts.

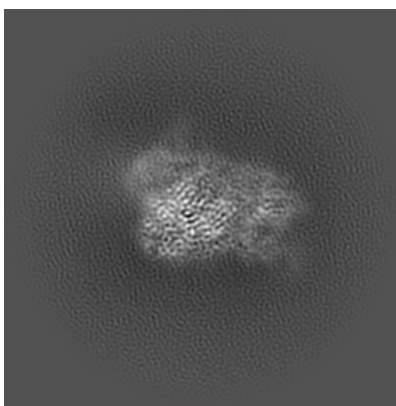
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

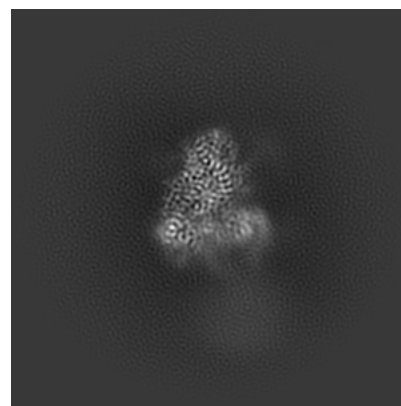
#### 6.1.1 Primary map



X

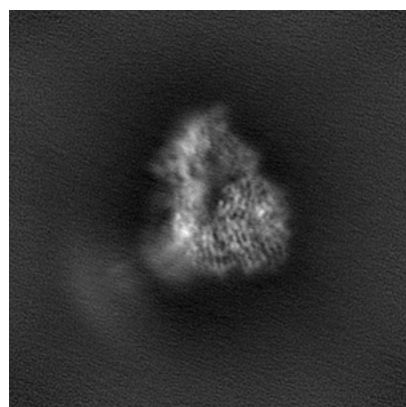


Y

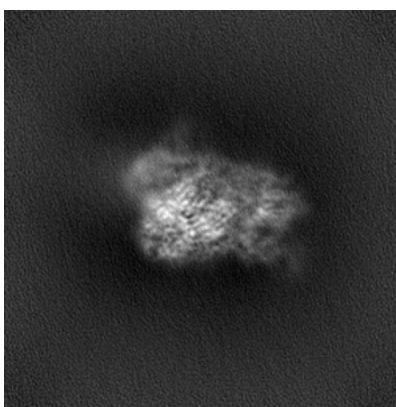


Z

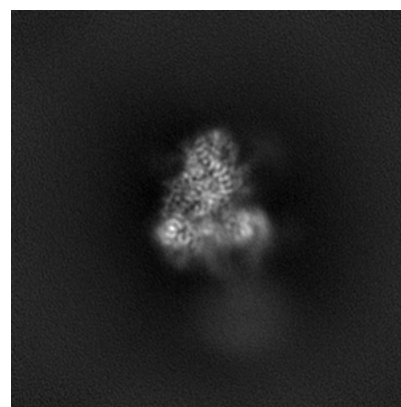
#### 6.1.2 Raw map



X



Y

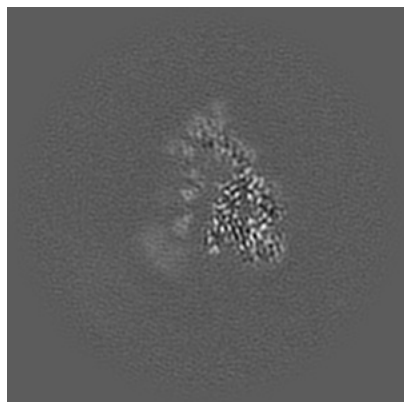


Z

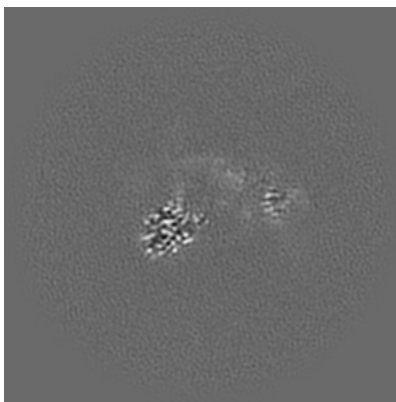
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

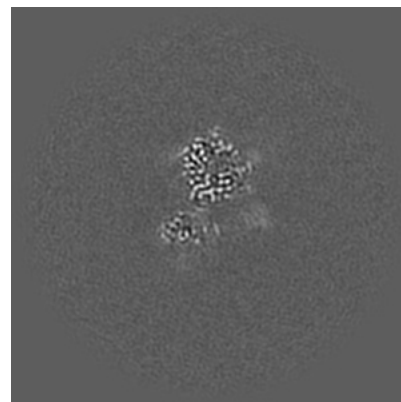
### 6.2.1 Primary map



X Index: 128

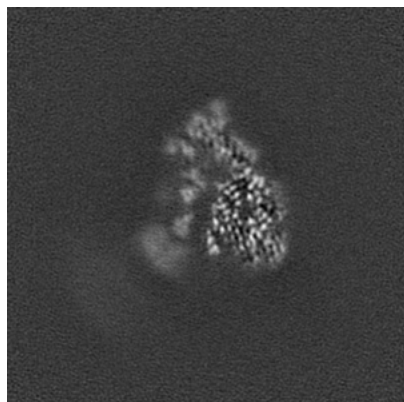


Y Index: 128

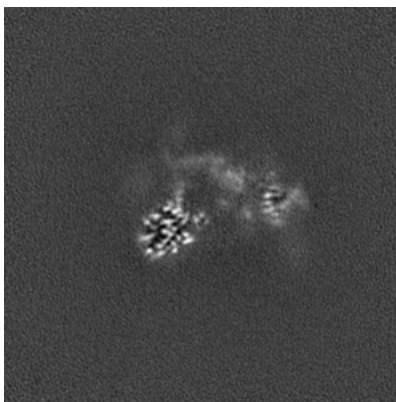


Z Index: 128

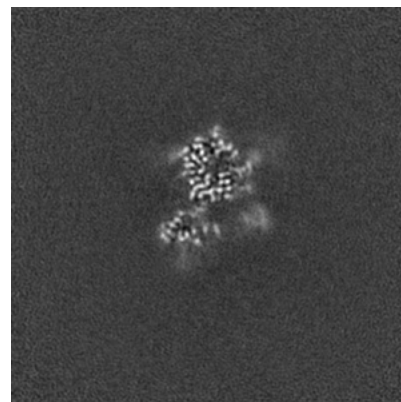
### 6.2.2 Raw map



X Index: 128



Y Index: 128

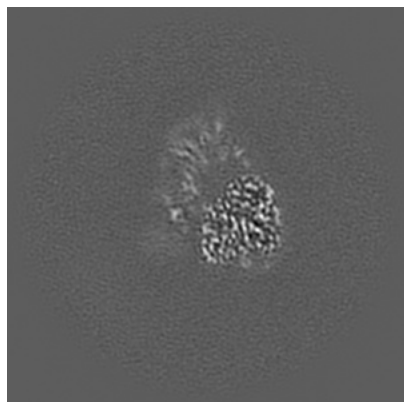


Z Index: 128

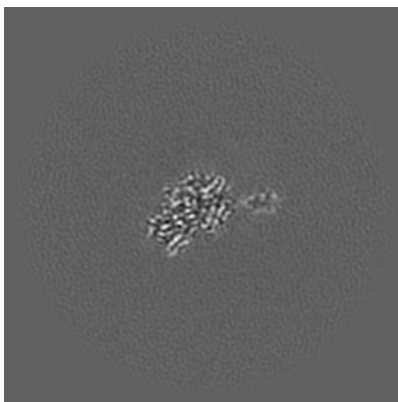
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

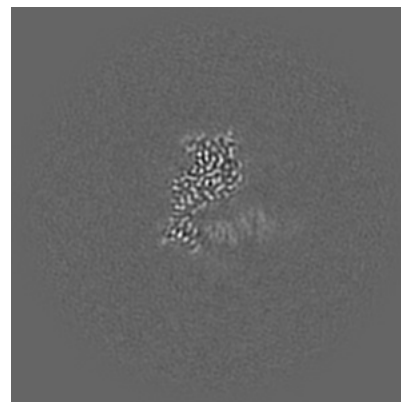
### 6.3.1 Primary map



X Index: 122

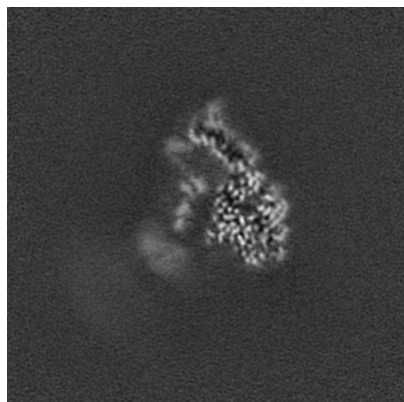


Y Index: 144

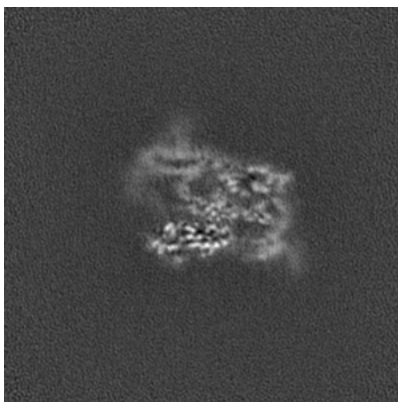


Z Index: 117

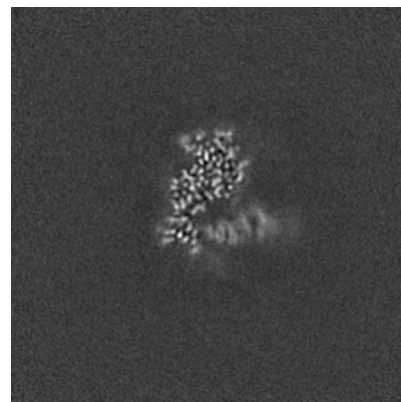
### 6.3.2 Raw map



X Index: 131



Y Index: 116



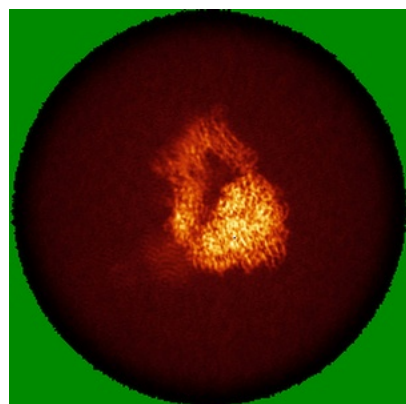
Z Index: 116

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

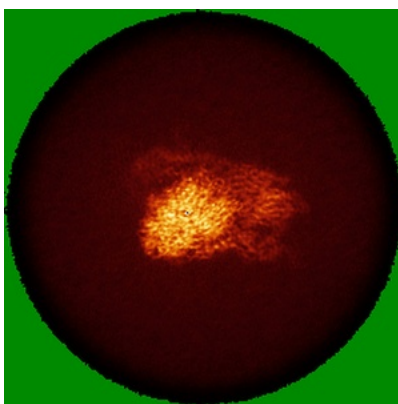


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

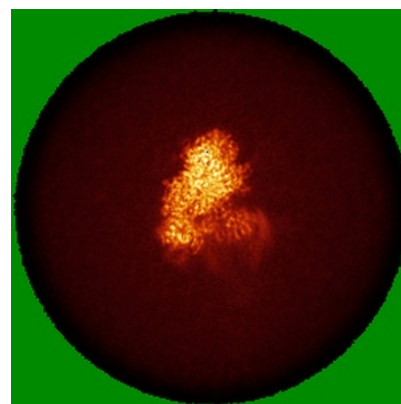
### 6.4.1 Primary map



X

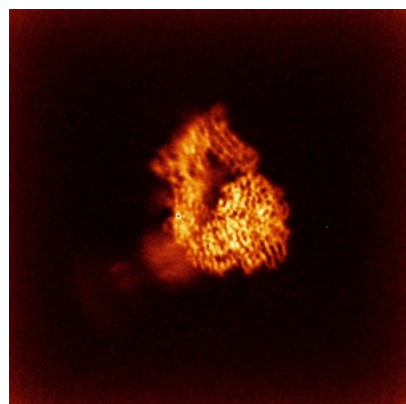


Y

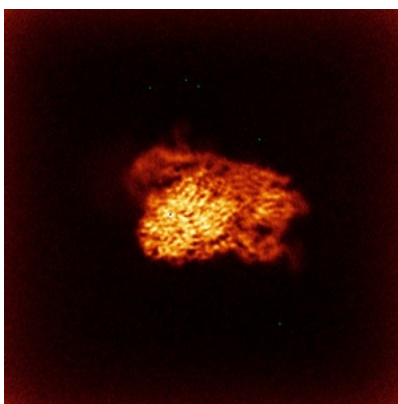


Z

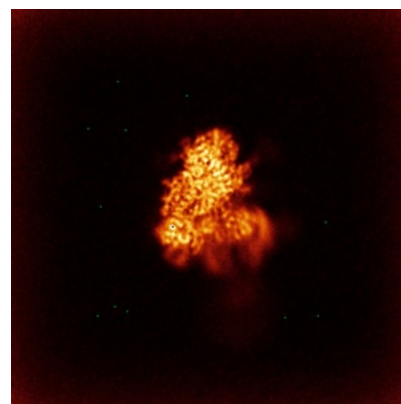
### 6.4.2 Raw map



X



Y



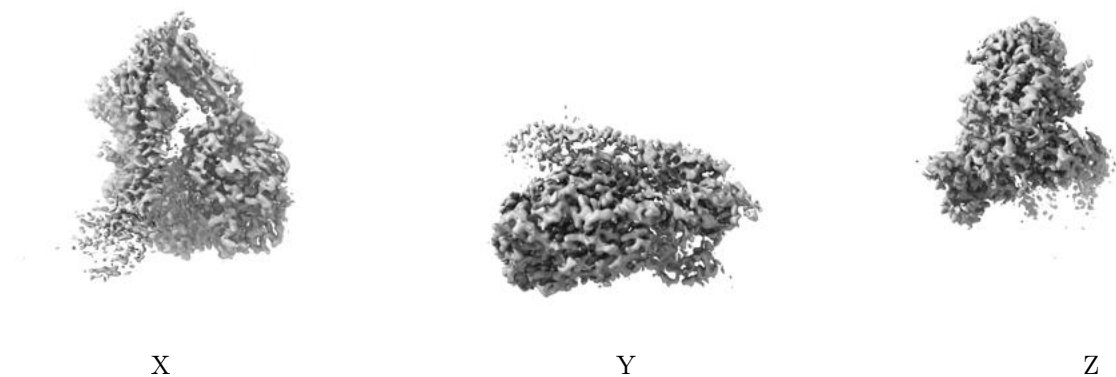
Z

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.



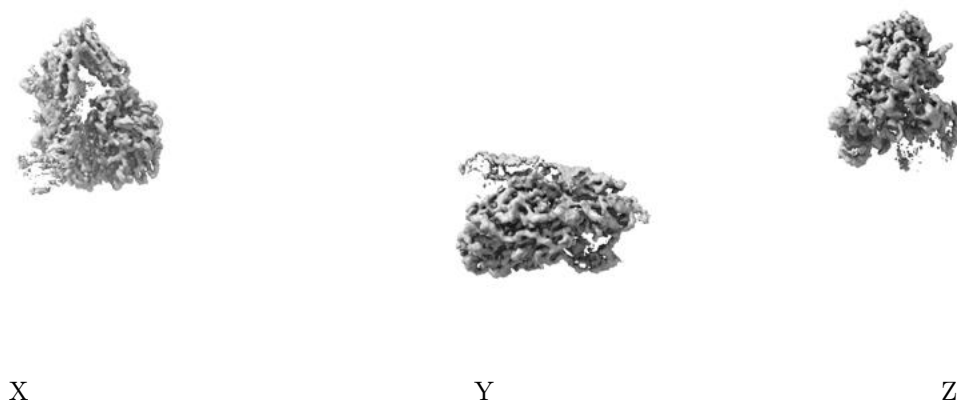
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.468. 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.

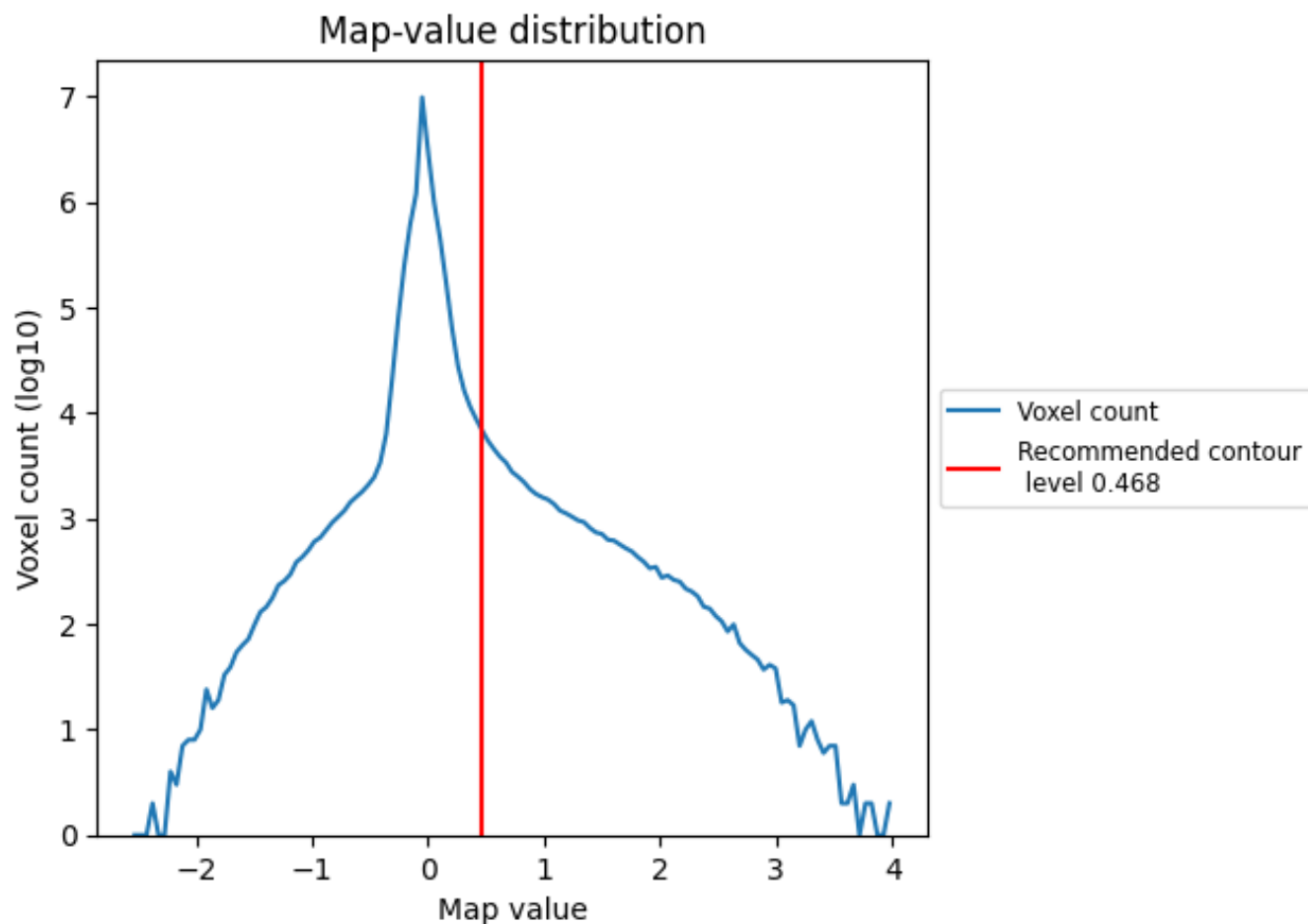
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

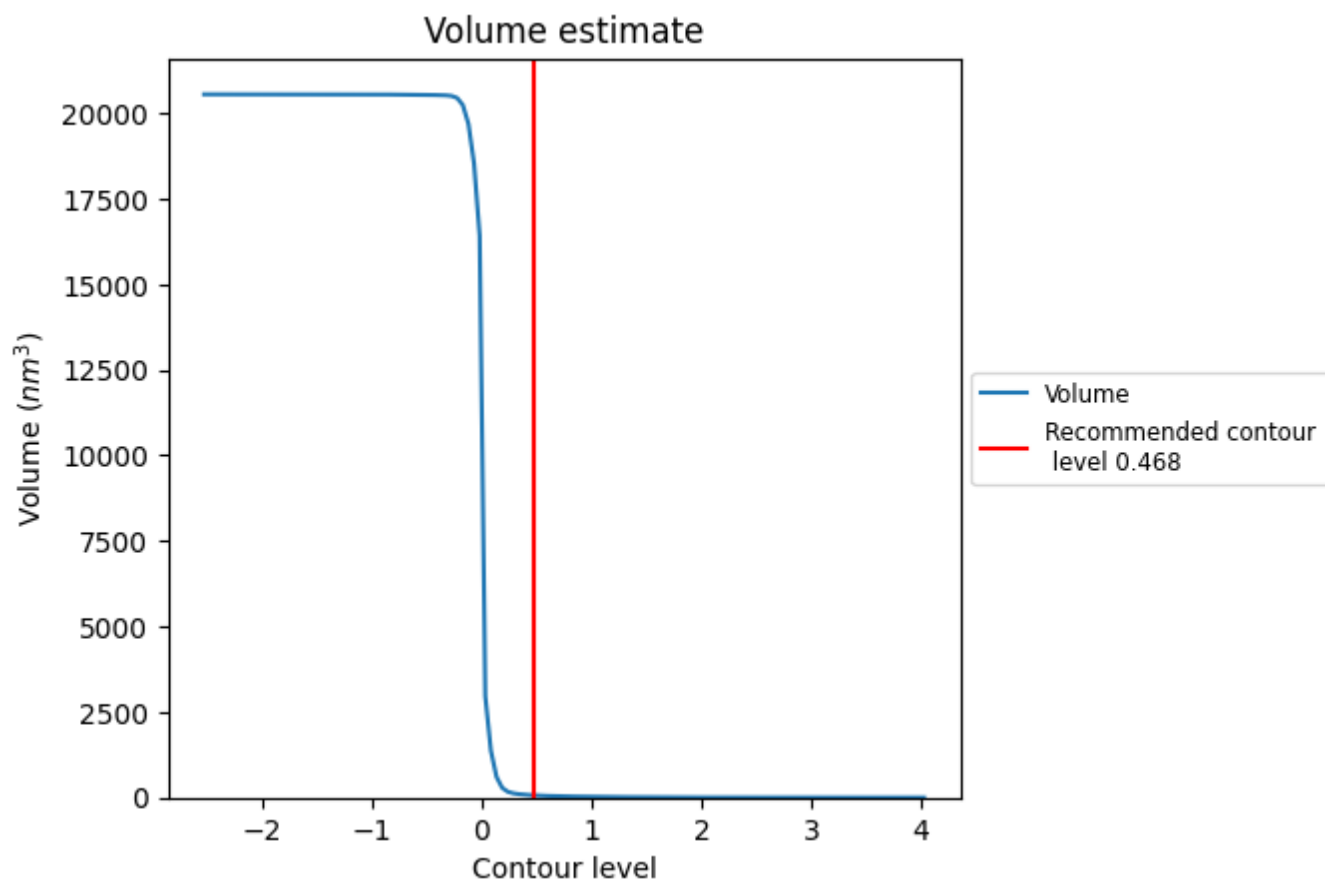
This section contains the results of statistical analysis of the map.

### 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.

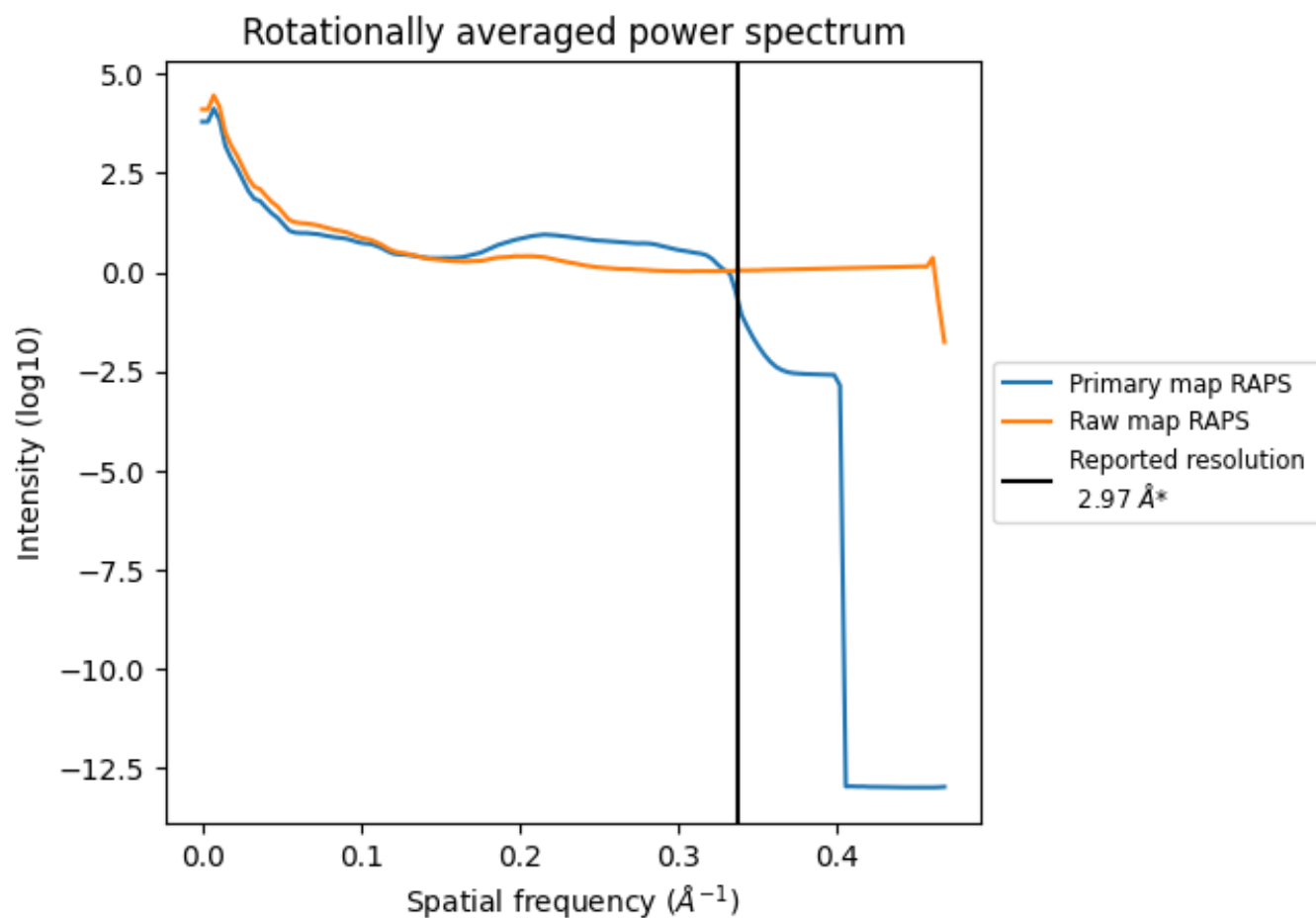
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 66 nm<sup>3</sup>; this corresponds to an approximate mass of 60 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 ⓘ

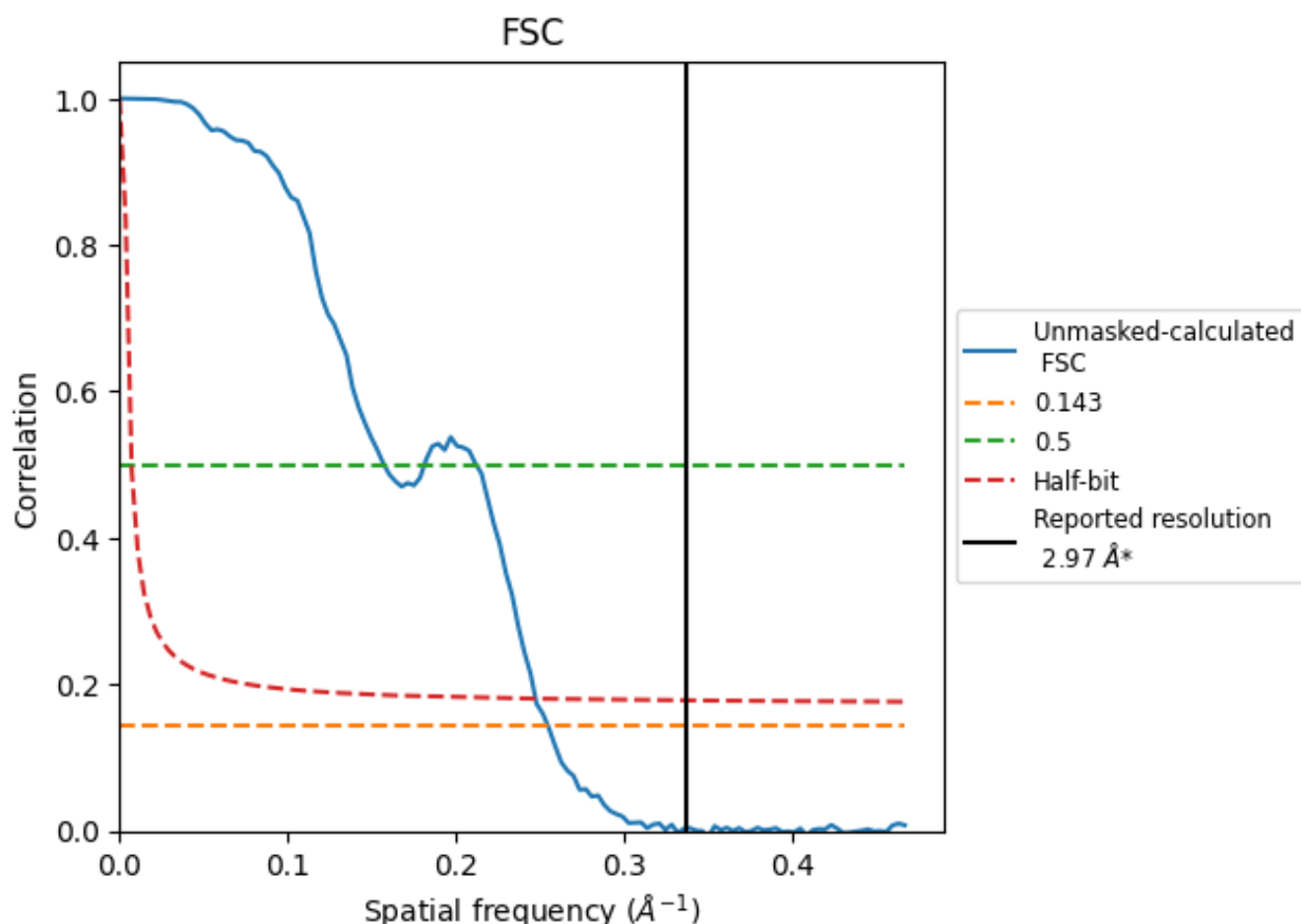


\*Reported resolution corresponds to spatial frequency of 0.337 Å<sup>-1</sup>

## 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 0.337 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

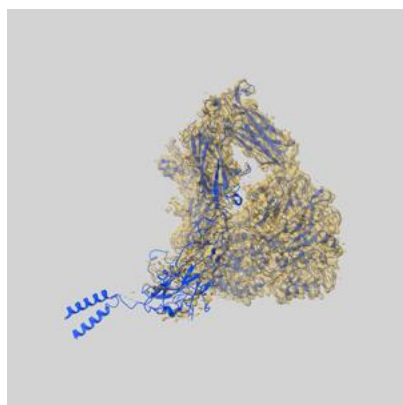
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.92	6.35	4.04

\*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 3.92 differs from the reported value 2.97 by more than 10 %

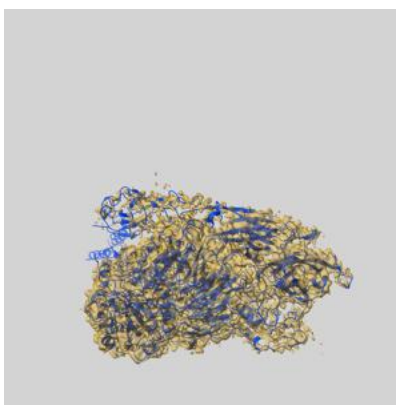
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29931 and PDB model 8GCD. Per-residue inclusion information can be found in section [3](#) on page [7](#).

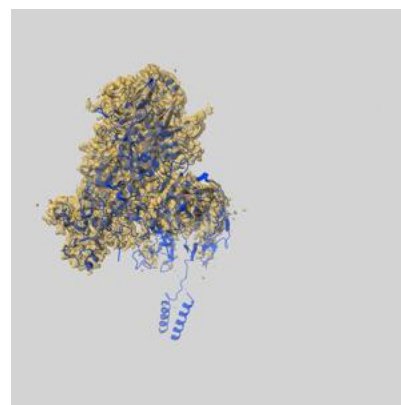
### 9.1 Map-model overlay [i](#)



X



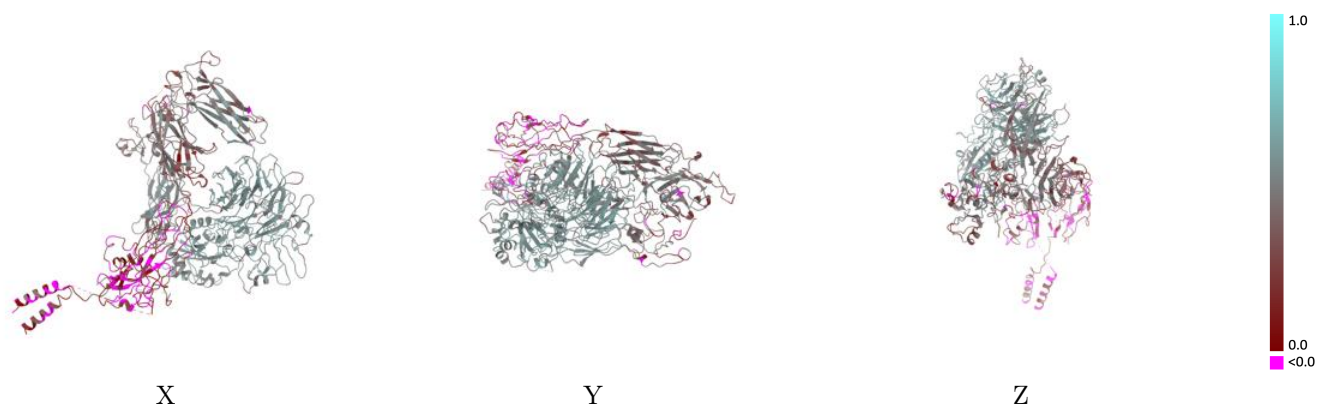
Y



Z

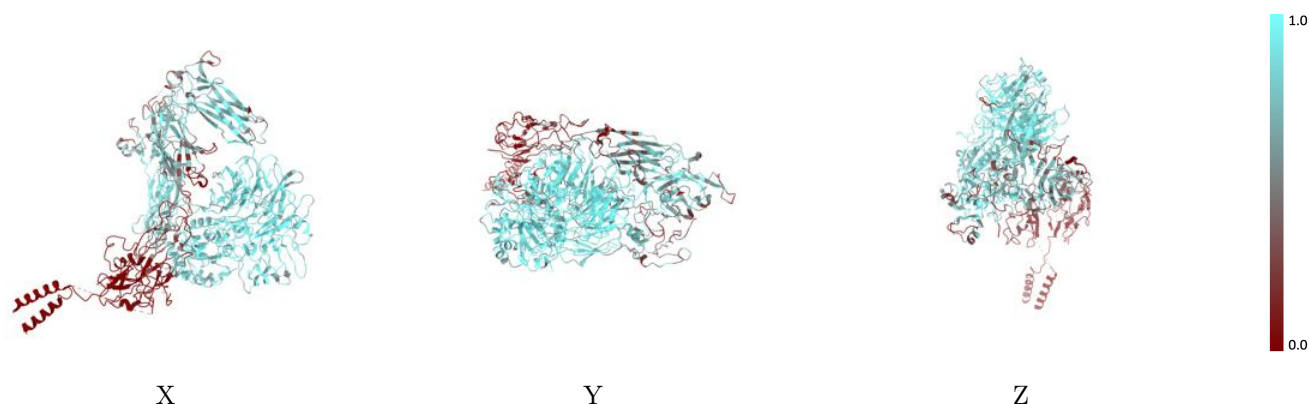
The images above show the 3D surface view of the map at the recommended contour level 0.468 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

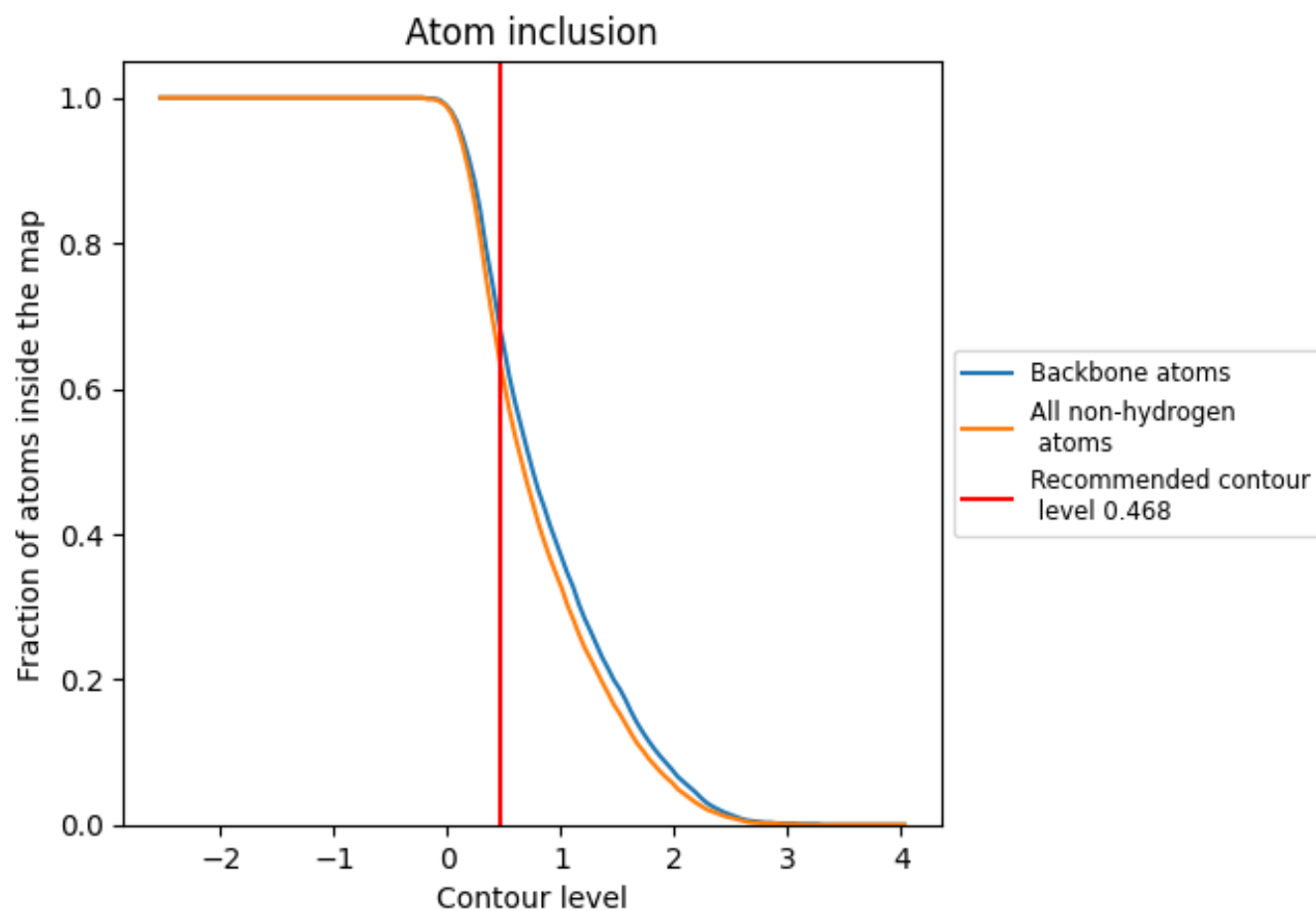
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.468).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 63% 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 (0.468) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.6310</div>	<div><div></div>0.4090</div>
A	<div><div></div>0.6210</div>	<div><div></div>0.4080</div>
B	<div><div></div>0.6450</div>	<div><div></div>0.4090</div>
C	<div><div></div>0.3440</div>	<div><div></div>0.3990</div>
D	<div><div></div>0.5640</div>	<div><div></div>0.4390</div>
E	<div><div></div>0.3930</div>	<div><div></div>0.3710</div>
F	<div><div></div>0.3570</div>	<div><div></div>0.4120</div>

1.0

0.0

<0.0