



## Full wwPDB EM Validation Report ⓘ

Oct 7, 2025 – 12:13 PM EDT

PDB ID : 9E8A / pdb\_00009e8a  
EMDB ID : EMD-47713  
Title : Integrin  $\alpha$ IIb $\beta$ 3 bent conformation from human platelet membrane crude preparation  
Authors : Han, X.; Nieman, M.T.  
Deposited on : 2024-11-05  
Resolution : 2.75 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:

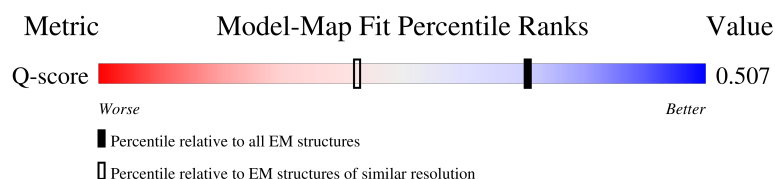
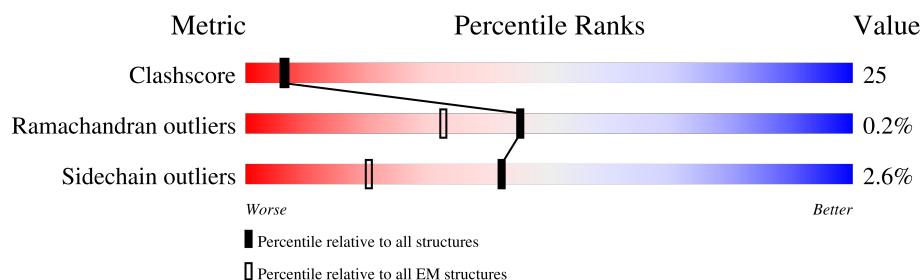
EMDB validation analysis : 0.0.1.dev129  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

# 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 2.75 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	10570 ( 2.25 - 3.25 )

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	4	
4	D	2	

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Mol	Chain	Length	Quality of chain
4	E	2	 100%
4	F	2	 100%
4	G	2	 50%50%
5	H	3	 67%33%
5	I	3	 67%33%
6	J	4	 25%25%50%

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 12589 atoms, of which 22 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	915	Total	C	N	O	S	1	0
			7002	4425	1220	1328	29		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	683	Total	C	N	O	S	0	0
			5234	3215	894	1055	70		

- Molecule 3 is a protein called GLY-ARG-GLY-ASP.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	4	Total	C	H	N	O	0	0
			49	14	22	7	6		

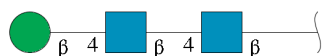
- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

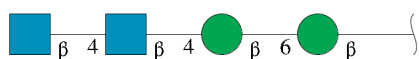
- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b

eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	H	3	Total	C	N	O	0	0
			39	22	2	15		
5	I	3	Total	C	N	O	0	0
			39	22	2	15		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
6	J	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

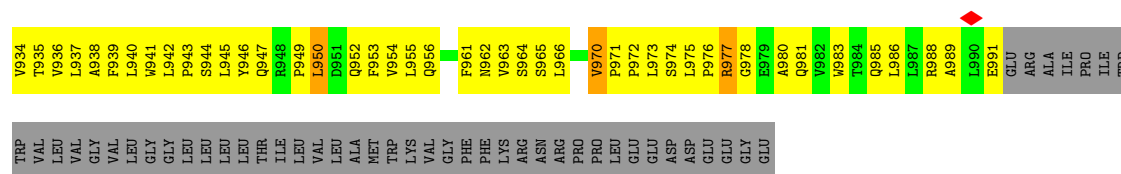


Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

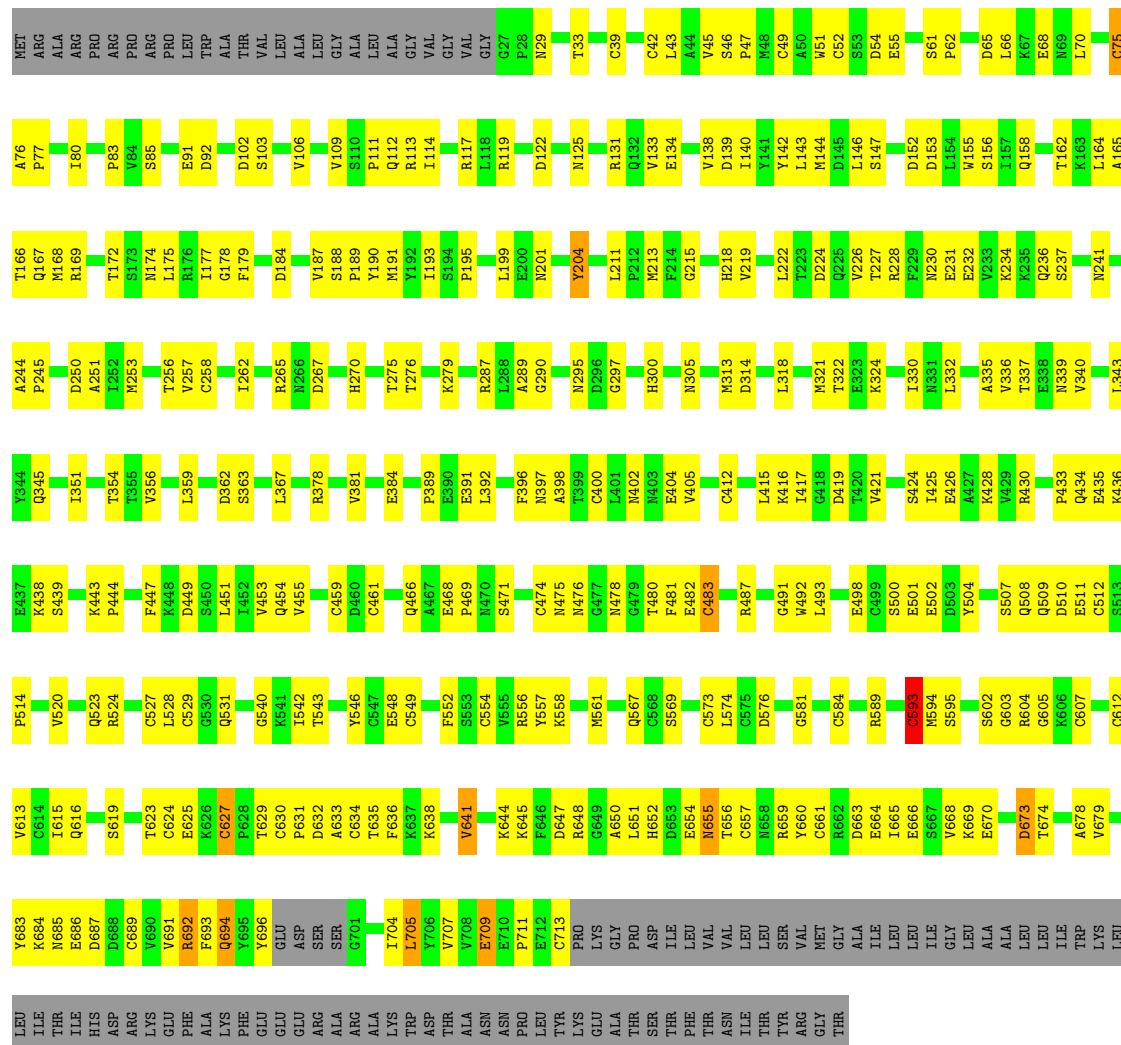
Mol	Chain	Residues	Atoms		AltConf
9	B	1	Total	Mg	0
			1	1	





### • Molecule 2: Integrin beta-3

Chain B: 48% 37% 13%



### • Molecule 3: GLY-ARG-GLY-ASP

Chain C: 50% 25% 25%



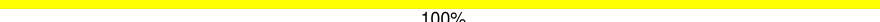
### • Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



Chain D:  50% 50%

NAG1  
NAG2

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

Chain E:  100%

NAG1  
NAG2

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

Chain F:  100%

NAG1  
NAG2

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

Chain G:  50% 50%

NAG1  
NAG2

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

Chain H:  67% 33%

NAG1  
NAG2  
BMA3

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

Chain I:  67% 33%

NAG1  
NAG2  
BMA3

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-mannopyranose-(1-6)-beta-D-mannopyranose

Chain J:  25% 25% 50%

BMA3  
BMA2  
NAG3  
NAG4

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	120965	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 ( $e^-/\text{\AA}^2$ )	36.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.115	Depositor
Minimum map value	-0.500	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	321.00003, 321.00003, 321.00003	wwPDB
Map dimensions	300, 300, 300	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: MG, NAG, CA, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.31	0/7171	0.38	0/9775
2	B	0.44	0/5328	0.57	2/7207 (0.0%)
3	C	0.88	0/26	1.29	0/32
All	All	0.38	0/12525	0.48	2/17014 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
3	C	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	593	CYS	CB-CA-C	-6.20	101.15	110.88
2	B	581	GLY	CA-C-O	-6.01	118.31	122.22

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	977	ARG	Sidechain
2	B	589	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	C	493	ARG	Sidechain

## 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	7002	0	6835	371	0
2	B	5234	0	4956	263	0
3	C	27	22	22	1	0
4	D	28	0	25	6	0
4	E	28	0	25	0	0
4	F	28	0	25	0	0
4	G	28	0	25	0	0
5	H	39	0	34	0	0
5	I	39	0	34	0	0
6	J	50	0	43	4	0
7	A	5	0	0	0	0
7	B	2	0	0	0	0
8	A	42	0	39	1	0
8	B	14	0	13	1	0
9	B	1	0	0	0	0
All	All	12567	22	12076	624	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 25.

All (624) 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:601:ASN:OD1	4:D:1:NAG:H83	1.45	1.14
1:A:844:LEU:HD13	1:A:955:LEU:HD13	1.34	1.06
1:A:806:SER:HB3	1:A:942:LEU:HB3	1.48	0.95
2:B:666:GLU:HA	2:B:707:VAL:HB	1.50	0.91
2:B:663:ASP:HB3	2:B:705:LEU:HB2	1.53	0.90
1:A:707:GLN:HE22	1:A:714:ARG:HB2	1.38	0.89
1:A:394:LEU:HD11	1:A:406:ALA:HB2	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:953:PHE:HB2	1:A:986:LEU:HD12	1.56	0.87
1:A:857:CYS:HB2	1:A:919:VAL:HB	1.55	0.85
1:A:956:GLN:HG2	1:A:983:TRP:HB3	1.58	0.85
2:B:685:ASN:HD21	2:B:689:CYS:HB2	1.42	0.85
2:B:689:CYS:HB3	2:B:711:PRO:HB2	1.59	0.84
1:A:852:GLN:HB3	1:A:933:MET:HG3	1.58	0.84
2:B:678:ALA:HA	2:B:694:GLN:HE22	1.40	0.84
1:A:861:PRO:HD2	1:A:917:THR:HG23	1.60	0.83
1:A:950:LEU:HA	1:A:991:GLU:HA	1.58	0.83
2:B:188:SER:OG	2:B:189:PRO:HD3	1.79	0.83
1:A:940:LEU:HB3	1:A:945:LEU:HD21	1.58	0.83
1:A:649:VAL:HG11	1:A:771:VAL:HG22	1.60	0.82
1:A:683:HIS:HB2	1:A:751:GLN:HB2	1.61	0.82
1:A:966:LEU:HB2	1:A:971:PRO:HB3	1.62	0.82
2:B:52:CYS:HB2	2:B:70:LEU:HD21	1.62	0.82
1:A:855:LEU:HD12	1:A:921:CYS:HB3	1.62	0.81
2:B:167:GLN:HG3	2:B:367:LEU:HD11	1.60	0.81
1:A:643:LEU:HB2	1:A:764:SER:HB3	1.63	0.80
2:B:552:PHE:HA	2:B:561:MET:HE1	1.64	0.80
2:B:187:VAL:HG21	2:B:289:ALA:HB1	1.64	0.78
1:A:692:ARG:HH11	1:A:694:LEU:HD23	1.49	0.77
2:B:76:ALA:HA	2:B:80:ILE:HD11	1.67	0.77
2:B:444:PRO:HG2	2:B:447:PHE:HB2	1.67	0.77
2:B:188:SER:OG	2:B:189:PRO:CD	2.33	0.77
1:A:774:ARG:HE	1:A:973:LEU:HD11	1.49	0.76
1:A:970:VAL:O	1:A:972:PRO:HD3	1.86	0.76
1:A:580:MET:HA	1:A:580:MET:HE2	1.67	0.75
1:A:496:SER:HB2	1:A:630:VAL:HG22	1.68	0.75
1:A:601:ASN:OD1	4:D:1:NAG:C1	2.34	0.75
2:B:644:LYS:HG2	2:B:657:CYS:HB3	1.69	0.74
2:B:693:PHE:HD2	2:B:705:LEU:HD11	1.52	0.74
2:B:569:SER:HB3	2:B:574:LEU:HD13	1.67	0.74
2:B:647:ASP:O	2:B:648:ARG:NH1	2.21	0.73
2:B:654:GLU:O	2:B:659:ARG:NH2	2.21	0.72
1:A:961:PHE:HB3	1:A:978:GLY:H	1.54	0.72
1:A:829:HIS:HB3	1:A:962:ASN:HB3	1.71	0.71
1:A:541:LEU:HB3	1:A:552:VAL:HG23	1.73	0.71
2:B:191:MET:HA	2:B:213:MET:HE1	1.71	0.70
2:B:689:CYS:HA	2:B:713:CYS:HA	1.73	0.70
2:B:322:THR:HG22	2:B:351:ILE:HG23	1.74	0.70
1:A:654:LEU:HD21	1:A:662:LEU:HD11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:941:TRP:HB3	1:A:944:SER:HB2	1.74	0.70
1:A:408:ALA:HB2	1:A:452:LEU:HD11	1.74	0.69
2:B:91:GLU:HG2	2:B:113:ARG:HB3	1.73	0.69
1:A:145:ASN:HB2	1:A:155:LYS:HB2	1.73	0.69
2:B:651:LEU:HD12	2:B:656:THR:HG21	1.75	0.69
2:B:119:ARG:HG3	2:B:122:ASP:HB2	1.75	0.69
2:B:165:ALA:HB2	2:B:226:VAL:HG11	1.76	0.68
1:A:542:ASP:O	1:A:550:ARG:NH1	2.27	0.68
2:B:644:LYS:NZ	2:B:663:ASP:O	2.27	0.68
1:A:138:CYS:HA	1:A:161:CYS:HA	1.74	0.68
1:A:684:LEU:HB2	1:A:714:ARG:HG3	1.74	0.68
2:B:228:ARG:NH2	2:B:232:GLU:OE2	2.26	0.68
1:A:654:LEU:HD21	1:A:662:LEU:HD21	1.76	0.67
1:A:866:LEU:HB2	1:A:870:TRP:CZ3	2.30	0.67
1:A:778:GLN:H	1:A:821:GLY:HA3	1.59	0.67
2:B:693:PHE:CD2	2:B:705:LEU:HD11	2.31	0.66
1:A:855:LEU:HB3	1:A:923:LEU:HB2	1.78	0.66
1:A:781:LEU:HD13	1:A:817:LEU:HD21	1.75	0.66
1:A:847:LEU:N	1:A:937:LEU:O	2.25	0.66
1:A:836:GLY:H	1:A:914:ALA:HB3	1.60	0.66
1:A:776:GLU:OE2	1:A:778:GLN:NE2	2.29	0.66
2:B:511:GLU:OE1	2:B:511:GLU:N	2.30	0.65
1:A:834:LEU:HD21	1:A:936:VAL:HG11	1.77	0.65
1:A:782:ARG:NH1	2:B:629:THR:OG1	2.30	0.65
1:A:394:LEU:HD21	1:A:466:LEU:HD13	1.77	0.65
2:B:623:THR:HG23	2:B:625:GLU:HB3	1.77	0.65
1:A:601:ASN:ND2	4:D:1:NAG:O5	2.21	0.64
2:B:633:ALA:HB3	2:B:679:VAL:HG11	1.79	0.64
2:B:265:ARG:O	2:B:270:HIS:NE2	2.22	0.64
2:B:52:CYS:HB2	2:B:70:LEU:HD11	1.78	0.64
1:A:224:GLY:HA3	1:A:266:TRP:HB3	1.80	0.64
1:A:849:ILE:HD12	1:A:919:VAL:HG11	1.78	0.64
2:B:113:ARG:NH1	2:B:454:GLN:OE1	2.31	0.63
2:B:133:VAL:O	2:B:378:ARG:NH2	2.27	0.63
1:A:785:SER:HB2	1:A:788:ALA:HA	1.79	0.63
1:A:845:TYR:HB2	1:A:941:TRP:HE3	1.64	0.63
1:A:860:GLN:HB3	1:A:861:PRO:HD3	1.79	0.63
1:A:835:PRO:HB3	1:A:910:SER:O	1.99	0.62
2:B:705:LEU:HD12	2:B:707:VAL:HG22	1.80	0.62
2:B:68:GLU:OE1	2:B:68:GLU:N	2.28	0.62
1:A:861:PRO:HD3	1:A:917:THR:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:ALA:HB1	2:B:169:ARG:NH1	2.15	0.62
1:A:680:LEU:HB2	1:A:720:LEU:HD11	1.81	0.62
2:B:668:VAL:HA	2:B:709:GLU:HG3	1.81	0.62
2:B:47:PRO:HA	2:B:119:ARG:HD2	1.82	0.62
2:B:444:PRO:HG2	2:B:447:PHE:CB	2.29	0.61
1:A:832:ILE:O	1:A:918:VAL:HA	1.98	0.61
2:B:142:TYR:CE1	2:B:144:MET:HB2	2.36	0.61
2:B:92:ASP:HB3	2:B:111:PRO:HB3	1.83	0.61
2:B:659:ARG:HD2	2:B:660:TYR:CE1	2.36	0.61
2:B:691:VAL:HA	2:B:711:PRO:HB3	1.82	0.61
2:B:502:GLU:OE1	2:B:502:GLU:N	2.31	0.61
1:A:509:THR:HG22	1:A:510:LYS:H	1.66	0.60
1:A:941:TRP:O	1:A:945:LEU:HG	2.01	0.60
2:B:142:TYR:HE1	2:B:144:MET:HB2	1.66	0.60
2:B:430:ARG:HD2	2:B:567:GLN:HB3	1.83	0.60
2:B:139:ASP:HB2	2:B:222:LEU:HD13	1.83	0.60
2:B:134:GLU:HG2	2:B:417:ILE:HG22	1.84	0.60
1:A:449:GLY:HA2	1:A:468:VAL:HG13	1.82	0.60
2:B:187:VAL:HG11	2:B:289:ALA:HB2	1.82	0.60
1:A:537:ALA:HB1	1:A:600:LEU:HD11	1.84	0.59
1:A:722:ASN:HB3	1:A:723:PRO:HD3	1.84	0.59
1:A:847:LEU:HG	1:A:848:ASP:H	1.66	0.59
6:J:2:BMA:H4	6:J:3:NAG:HN2	1.67	0.59
1:A:410:PRO:HA	1:A:448:PHE:O	2.01	0.59
1:A:534:SER:HA	1:A:567:ASP:HA	1.85	0.59
1:A:641:PRO:O	1:A:761:ASN:ND2	2.35	0.59
1:A:543:ARG:HD2	1:A:599:SER:HB2	1.84	0.59
1:A:830:LEU:HB3	1:A:921:CYS:HB2	1.84	0.59
1:A:961:PHE:HB3	1:A:978:GLY:N	2.17	0.59
1:A:90:ARG:NH2	1:A:95:GLN:O	2.34	0.59
1:A:690:TYR:HB2	1:A:716:VAL:HG11	1.85	0.58
2:B:389:PRO:HB3	2:B:438:LYS:HD3	1.85	0.58
1:A:67:VAL:HG22	1:A:86:LEU:HD13	1.86	0.58
1:A:643:LEU:CB	1:A:764:SER:HB3	2.33	0.58
2:B:625:GLU:OE1	2:B:625:GLU:N	2.35	0.58
1:A:941:TRP:HD1	1:A:944:SER:H	1.52	0.58
1:A:954:VAL:HG12	1:A:985:GLN:HG2	1.86	0.58
2:B:400:CYS:HA	2:B:421:VAL:HG12	1.84	0.58
2:B:619:SER:HA	2:B:627:CYS:HB2	1.86	0.58
2:B:256:THR:HG23	2:B:330:ILE:HD12	1.86	0.58
1:A:682:VAL:HG22	1:A:752:LEU:HD22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:GLU:O	1:A:773:VAL:N	2.27	0.58
1:A:647:ALA:HB2	1:A:752:LEU:HD12	1.86	0.57
1:A:747:SER:HA	1:A:773:VAL:HG23	1.85	0.57
1:A:966:LEU:HB2	1:A:971:PRO:CB	2.34	0.57
2:B:46:SER:OG	2:B:49:CYS:SG	2.60	0.57
2:B:55:GLU:OE1	2:B:55:GLU:N	2.37	0.57
2:B:602:SER:O	2:B:604:ARG:HG3	2.04	0.57
2:B:612:CYS:SG	2:B:623:THR:HA	2.44	0.57
1:A:710:GLU:O	1:A:711:ASN:C	2.47	0.57
2:B:187:VAL:HG22	2:B:188:SER:H	1.68	0.57
2:B:402:ASN:HB3	2:B:404:GLU:OE1	2.05	0.57
2:B:466:GLN:N	2:B:466:GLN:OE1	2.37	0.57
1:A:656:VAL:CG1	1:A:742:GLU:HG3	2.34	0.57
2:B:191:MET:HG3	2:B:213:MET:HE3	1.85	0.57
1:A:301:LEU:HD12	1:A:305:TYR:HA	1.85	0.57
1:A:585:ASP:HB3	1:A:588:ASP:OD1	2.04	0.57
2:B:645:LYS:HG3	2:B:666:GLU:HB3	1.85	0.57
2:B:51:TRP:NE1	2:B:483:CYS:SG	2.78	0.57
2:B:165:ALA:O	2:B:169:ARG:HD3	2.04	0.57
2:B:665:ILE:HG22	2:B:666:GLU:H	1.70	0.57
1:A:33:ASN:ND2	1:A:481:ALA:HB1	2.20	0.56
1:A:806:SER:HB3	1:A:943:PRO:HD3	1.86	0.56
1:A:856:GLN:OE1	1:A:856:GLN:N	2.38	0.56
1:A:944:SER:HA	1:A:947:GLN:HG3	1.88	0.56
1:A:146:VAL:HB	1:A:153:ALA:HB2	1.87	0.56
1:A:656:VAL:HG23	1:A:774:ARG:O	2.05	0.56
1:A:844:LEU:HD22	1:A:955:LEU:HD22	1.87	0.56
2:B:187:VAL:HG11	2:B:289:ALA:CB	2.35	0.56
2:B:297:GLY:O	2:B:324:LYS:NZ	2.38	0.56
2:B:318:LEU:O	2:B:322:THR:HG23	2.05	0.56
2:B:604:ARG:HB3	2:B:616:GLN:HB3	1.88	0.56
1:A:835:PRO:HB3	1:A:911:CYS:HA	1.87	0.56
2:B:416:LYS:HG2	2:B:419:ASP:OD2	2.06	0.56
2:B:652:HIS:HA	2:B:657:CYS:SG	2.45	0.56
1:A:806:SER:HA	1:A:870:TRP:CD1	2.40	0.56
1:A:71:PRO:HA	1:A:124:LEU:O	2.05	0.56
1:A:600:LEU:HB3	1:A:623:VAL:HG12	1.88	0.56
1:A:709:LYS:HA	1:A:714:ARG:HA	1.88	0.56
2:B:474:CYS:SG	2:B:481:PHE:HB2	2.46	0.56
1:A:750:PHE:O	1:A:768:LEU:HD12	2.04	0.56
2:B:434:GLN:HA	2:B:436:LYS:NZ	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:GLU:O	1:A:156:THR:HG23	2.06	0.56
1:A:656:VAL:HG12	1:A:742:GLU:HG3	1.86	0.56
2:B:168:MET:HB2	2:B:175:LEU:HD22	1.88	0.56
1:A:857:CYS:CB	1:A:919:VAL:HB	2.30	0.55
2:B:402:ASN:HD22	2:B:659:ARG:HG3	1.71	0.55
1:A:682:VAL:HB	1:A:716:VAL:CG2	2.36	0.55
2:B:651:LEU:HB3	2:B:656:THR:OG1	2.06	0.55
1:A:817:LEU:HD11	1:A:830:LEU:HD23	1.87	0.55
2:B:275:THR:HG22	2:B:335:ALA:HB3	1.87	0.55
1:A:661:VAL:HG13	1:A:691:MET:HE1	1.89	0.55
1:A:942:LEU:HB3	1:A:943:PRO:HD3	1.89	0.55
2:B:491:GLY:O	2:B:501:GLU:HB2	2.06	0.55
2:B:245:PRO:HA	2:B:279:LYS:O	2.07	0.55
2:B:391:GLU:HG2	2:B:433:PRO:HG3	1.87	0.55
2:B:655:ASN:O	2:B:655:ASN:ND2	2.36	0.55
2:B:674:THR:HA	2:B:678:ALA:HB2	1.88	0.55
1:A:845:TYR:HB2	1:A:941:TRP:CE3	2.41	0.55
1:A:649:VAL:HB	1:A:769:LEU:HD21	1.89	0.54
1:A:655:LEU:HD12	1:A:776:GLU:HB3	1.89	0.54
1:A:866:LEU:HD13	1:A:870:TRP:CH2	2.42	0.54
2:B:164:LEU:HA	2:B:367:LEU:HD21	1.90	0.54
2:B:508:GLN:HG2	2:B:509:GLN:OE1	2.07	0.54
2:B:548:GLU:OE1	2:B:548:GLU:N	2.30	0.54
2:B:678:ALA:HA	2:B:694:GLN:NE2	2.17	0.54
1:A:849:ILE:HG12	1:A:936:VAL:HG12	1.88	0.54
2:B:140:ILE:O	2:B:177:ILE:HA	2.07	0.54
1:A:863:VAL:HG13	1:A:864:ASN:ND2	2.22	0.54
2:B:138:VAL:HG12	2:B:172:THR:HG21	1.90	0.54
2:B:295:ASN:HB2	2:B:314:ASP:O	2.07	0.54
2:B:381:VAL:HG23	2:B:415:LEU:HD12	1.90	0.54
2:B:498:GLU:N	2:B:498:GLU:OE1	2.37	0.54
1:A:548:GLN:NE2	2:B:501:GLU:OE2	2.38	0.54
1:A:635:GLU:N	1:A:635:GLU:OE1	2.39	0.54
1:A:816:GLU:HB3	2:B:629:THR:HG21	1.90	0.54
2:B:689:CYS:SG	2:B:713:CYS:N	2.80	0.54
1:A:108[A]:ARG:HD3	1:A:243:LEU:H	1.73	0.54
1:A:580:MET:HA	1:A:580:MET:CE	2.36	0.54
2:B:404:GLU:OE1	2:B:404:GLU:N	2.37	0.54
1:A:849:ILE:CD1	1:A:919:VAL:HG11	2.37	0.54
1:A:837:GLN:H	1:A:842:ASP:HB2	1.73	0.53
1:A:847:LEU:HB3	1:A:937:LEU:HB2	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:LEU:HD23	1:A:855:LEU:H	1.73	0.53
2:B:482:GLU:OE2	2:B:487:ARG:NE	2.41	0.53
2:B:80:ILE:HD12	2:B:80:ILE:H	1.72	0.53
1:A:658:ALA:HB2	1:A:822:PRO:CB	2.39	0.53
1:A:835:PRO:CA	1:A:911:CYS:HA	2.39	0.53
2:B:253:MET:O	2:B:257:VAL:HG22	2.09	0.53
2:B:402:ASN:ND2	2:B:659:ARG:HG3	2.22	0.53
1:A:552:VAL:O	1:A:553:LEU:HD23	2.09	0.53
2:B:604:ARG:HD2	2:B:624:CYS:O	2.08	0.53
1:A:467:ILE:HG22	1:A:478:VAL:HG13	1.91	0.53
1:A:645:LEU:HD12	1:A:667:ASP:O	2.07	0.53
1:A:847:LEU:HD12	1:A:864:ASN:HB3	1.89	0.53
2:B:51:TRP:O	2:B:80:ILE:HA	2.09	0.53
2:B:500:SER:OG	2:B:501:GLU:N	2.41	0.53
2:B:434:GLN:HA	2:B:436:LYS:HZ2	1.73	0.53
2:B:633:ALA:HA	2:B:636:PHE:CZ	2.43	0.53
1:A:550:ARG:HG2	1:A:560:ALA:CB	2.38	0.53
1:A:683:HIS:CB	1:A:751:GLN:HB2	2.37	0.53
1:A:686:GLN:OE1	1:A:686:GLN:N	2.37	0.53
1:A:833:HIS:HB3	1:A:911:CYS:SG	2.48	0.53
1:A:965:SER:HA	1:A:975:LEU:CD1	2.38	0.52
2:B:552:PHE:HA	2:B:561:MET:CE	2.37	0.52
1:A:654:LEU:CD2	1:A:662:LEU:HD21	2.39	0.52
1:A:218:GLY:HA2	1:A:222:PHE:HA	1.91	0.52
1:A:719:GLU:N	1:A:719:GLU:OE1	2.43	0.52
2:B:109:VAL:O	2:B:112:GLN:NE2	2.35	0.52
2:B:131:ARG:HD2	2:B:133:VAL:HG12	1.91	0.52
2:B:493:LEU:HB3	2:B:531:GLN:NE2	2.24	0.52
1:A:202:PHE:CZ	2:B:287:ARG:HB3	2.45	0.52
1:A:675:ALA:HB3	1:A:724:MET:HB3	1.92	0.52
1:A:426:GLN:OE1	1:A:431:ARG:NH1	2.43	0.52
2:B:524:ARG:HH21	2:B:542:ILE:HG12	1.75	0.52
2:B:540:GLY:HA3	2:B:552:PHE:CD1	2.44	0.52
2:B:179:PHE:CE2	2:B:236:GLN:HG3	2.45	0.52
2:B:443:LYS:HG3	2:B:449:ASP:O	2.10	0.52
1:A:280:ASN:HB2	8:A:1105:NAG:HN2	1.75	0.51
1:A:553:LEU:HB2	1:A:582:PHE:CE1	2.45	0.51
2:B:29:ASN:O	2:B:33:THR:HG23	2.10	0.51
1:A:115:LEU:HB3	1:A:144:TRP:CH2	2.45	0.51
1:A:539:LEU:O	1:A:561:GLY:HA2	2.10	0.51
2:B:336:VAL:O	2:B:359:LEU:N	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:749:SER:HA	1:A:770:ASP:HA	1.92	0.51
2:B:162:THR:O	2:B:166:THR:HG23	2.11	0.51
1:A:835:PRO:HA	1:A:911:CYS:HA	1.92	0.51
1:A:954:VAL:HG12	1:A:985:GLN:HA	1.92	0.51
1:A:677:GLU:HG2	1:A:722:ASN:OD1	2.10	0.51
2:B:339:ASN:OD1	2:B:340:VAL:HG13	2.10	0.51
1:A:555:LEU:HD12	1:A:580:MET:HB3	1.91	0.51
2:B:147:SER:HB3	3:C:495:ASP:OD2	2.10	0.51
1:A:654:LEU:HB3	1:A:741:LEU:CD2	2.41	0.51
1:A:950:LEU:CA	1:A:991:GLU:HA	2.38	0.51
2:B:696:TYR:HB3	2:B:704:ILE:HG23	1.93	0.51
1:A:535:LEU:N	1:A:566:LEU:O	2.28	0.51
1:A:666:MET:SD	1:A:752:LEU:HD13	2.51	0.51
1:A:778:GLN:H	1:A:821:GLY:CA	2.23	0.51
1:A:941:TRP:CD1	1:A:944:SER:HG	2.28	0.51
2:B:190:TYR:O	2:B:241:ASN:HB2	2.11	0.51
2:B:218:HIS:O	2:B:305:ASN:HB3	2.11	0.51
1:A:774:ARG:NE	1:A:973:LEU:HD11	2.24	0.50
2:B:685:ASN:ND2	2:B:689:CYS:HB2	2.20	0.50
1:A:371:LEU:H	1:A:371:LEU:HD12	1.76	0.50
1:A:628:ARG:HD2	1:A:676:TYR:CD1	2.46	0.50
1:A:775:ALA:O	1:A:972:PRO:HD2	2.10	0.50
1:A:816:GLU:HA	1:A:933:MET:HA	1.93	0.50
2:B:39:CYS:HB3	2:B:483:CYS:SG	2.51	0.50
1:A:452:LEU:CD2	1:A:468:VAL:HG22	2.40	0.50
1:A:543:ARG:HA	1:A:550:ARG:HH12	1.77	0.50
1:A:596:ILE:N	1:A:627:THR:O	2.39	0.50
1:A:655:LEU:H	1:A:655:LEU:HD22	1.77	0.50
1:A:682:VAL:HB	1:A:716:VAL:HG22	1.93	0.50
2:B:253:MET:HE1	2:B:321:MET:HA	1.93	0.50
2:B:631:PRO:HB3	2:B:635:THR:HG21	1.94	0.50
1:A:285:VAL:HG11	1:A:337:LEU:HD11	1.94	0.50
2:B:556:ARG:HG2	2:B:561:MET:HA	1.94	0.50
1:A:152:GLU:HG3	1:A:154:GLU:H	1.76	0.50
1:A:677:GLU:O	1:A:679:GLU:HG3	2.12	0.50
1:A:944:SER:HA	1:A:947:GLN:CG	2.41	0.50
2:B:70:LEU:CD2	2:B:75:CYS:HB3	2.40	0.50
2:B:134:GLU:HG2	2:B:417:ILE:CG2	2.40	0.50
2:B:655:ASN:HD22	2:B:659:ARG:HB2	1.76	0.50
1:A:105:ASP:OD2	1:A:118:PHE:HA	2.11	0.50
1:A:645:LEU:HD13	1:A:754:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:ILE:HA	2:B:199:LEU:HD21	1.93	0.50
2:B:543:THR:O	2:B:549:CYS:HB2	2.12	0.49
2:B:573:CYS:HB3	2:B:584:CYS:SG	2.52	0.49
1:A:145:ASN:CB	1:A:155:LYS:HB2	2.41	0.49
1:A:198:CYS:HB3	1:A:216:ALA:HB1	1.95	0.49
1:A:817:LEU:O	1:A:931:ARG:HA	2.13	0.49
1:A:853:GLY:HA3	1:A:932:ALA:HB1	1.94	0.49
1:A:974:SER:O	1:A:975:LEU:HD13	2.11	0.49
1:A:408:ALA:HB2	1:A:452:LEU:CD1	2.42	0.49
2:B:664:GLU:OE1	2:B:704:ILE:HA	2.13	0.49
1:A:138:CYS:HB3	1:A:201:GLY:HA3	1.93	0.49
1:A:956:GLN:HA	1:A:983:TRP:HB3	1.93	0.49
2:B:201:ASN:O	2:B:204:TYR:HB3	2.13	0.49
2:B:569:SER:HB3	2:B:574:LEU:CD1	2.41	0.49
2:B:228:ARG:O	2:B:232:GLU:HG2	2.13	0.49
2:B:392:LEU:HD11	2:B:455:VAL:HG11	1.94	0.49
2:B:644:LYS:CG	2:B:657:CYS:HB3	2.42	0.49
1:A:376:LEU:HD21	1:A:378:LEU:HD21	1.95	0.49
1:A:743:GLU:OE1	1:A:743:GLU:N	2.46	0.49
1:A:807:TRP:O	1:A:942:LEU:HB2	2.12	0.49
2:B:153:ASP:OD2	2:B:363:SER:OG	2.26	0.49
1:A:452:LEU:HD22	1:A:468:VAL:HG22	1.95	0.49
2:B:638:LYS:HB2	2:B:683:TYR:CD1	2.48	0.49
1:A:780:GLU:O	1:A:817:LEU:HA	2.12	0.49
2:B:65:ASP:OD1	2:B:70:LEU:HB2	2.13	0.49
2:B:253:MET:HE2	2:B:321:MET:HG2	1.95	0.49
2:B:492:TRP:C	2:B:493:LEU:HD22	2.37	0.49
1:A:67:VAL:HG22	1:A:86:LEU:CD1	2.43	0.49
1:A:684:LEU:O	1:A:714:ARG:HG2	2.13	0.48
2:B:508:GLN:HG2	2:B:509:GLN:CD	2.38	0.48
1:A:55:ASP:OD1	1:A:56:PHE:N	2.46	0.48
1:A:536:ASN:HD21	1:A:565:ASN:HD22	1.61	0.48
1:A:658:ALA:HB2	1:A:822:PRO:HB2	1.95	0.48
1:A:705:CYS:HA	1:A:717:LEU:O	2.13	0.48
2:B:504:TYR:CD2	2:B:529:CYS:HA	2.48	0.48
2:B:648:ARG:HA	2:B:648:ARG:HH11	1.78	0.48
1:A:956:GLN:OE1	1:A:981:GLN:HB3	2.13	0.48
2:B:384:GLU:HG2	2:B:443:LYS:O	2.14	0.48
2:B:528:LEU:O	2:B:528:LEU:HD12	2.13	0.48
1:A:603:SER:CB	4:D:1:NAG:H62	2.44	0.48
2:B:655:ASN:ND2	2:B:659:ARG:HB2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:GLU:OE2	1:A:931:ARG:HD3	2.14	0.48
1:A:202:PHE:HZ	2:B:287:ARG:HB3	1.78	0.48
1:A:144:TRP:O	1:A:155:LYS:HA	2.13	0.48
1:A:330:ASN:HA	1:A:426:GLN:O	2.14	0.48
1:A:753:GLN:HE21	1:A:763:ASN:HB3	1.78	0.48
2:B:70:LEU:HD23	2:B:75:CYS:HB3	1.95	0.48
2:B:389:PRO:CB	2:B:438:LYS:HD3	2.44	0.48
1:A:552:VAL:HG13	1:A:596:ILE:HD13	1.95	0.48
1:A:554:LEU:HD12	1:A:562:THR:HG23	1.96	0.48
2:B:224:ASP:OD1	2:B:224:ASP:N	2.47	0.48
2:B:66:LEU:HB3	2:B:68:GLU:OE1	2.14	0.47
1:A:487:ALA:HB2	1:A:617:LEU:HD11	1.96	0.47
1:A:844:LEU:HD22	1:A:955:LEU:CD2	2.44	0.47
1:A:847:LEU:HD22	1:A:939:PHE:CE2	2.48	0.47
1:A:857:CYS:HB3	1:A:920:GLN:C	2.39	0.47
2:B:664:GLU:OE1	2:B:664:GLU:N	2.47	0.47
1:A:428:GLU:N	1:A:428:GLU:OE1	2.47	0.47
1:A:489:VAL:CG1	1:A:602:VAL:HG21	2.44	0.47
2:B:114:ILE:CG2	2:B:453:VAL:HG22	2.44	0.47
2:B:332:LEU:HB3	2:B:354:THR:HG22	1.97	0.47
2:B:345:GLN:HA	2:B:356:VAL:HG21	1.95	0.47
1:A:707:GLN:NE2	1:A:714:ARG:HB2	2.19	0.47
2:B:244:ALA:HB3	2:B:245:PRO:HD3	1.96	0.47
2:B:595:SER:HB3	2:B:623:THR:OG1	2.14	0.47
2:B:520:VAL:CG2	2:B:527:CYS:HB2	2.44	0.47
1:A:952:GLN:HA	1:A:988:ARG:HB2	1.97	0.47
2:B:54:ASP:CG	2:B:77:PRO:HG3	2.40	0.47
2:B:168:MET:CB	2:B:175:LEU:HD22	2.45	0.47
1:A:426:GLN:HG2	1:A:429:GLY:O	2.14	0.47
1:A:489:VAL:HG23	1:A:623:VAL:HB	1.97	0.47
1:A:822:PRO:O	1:A:928:ARG:HG3	2.15	0.47
1:A:949:PRO:HD2	1:A:950:LEU:HD23	1.97	0.47
2:B:178:GLY:N	2:B:222:LEU:HD23	2.29	0.47
2:B:554:CYS:HB2	2:B:561:MET:CG	2.44	0.47
2:B:593:CYS:O	2:B:594:MET:C	2.58	0.47
1:A:74:LEU:HD23	1:A:78:GLN:NE2	2.29	0.47
1:A:108[A]:ARG:HG2	1:A:243:LEU:HD12	1.97	0.47
1:A:677:GLU:N	1:A:722:ASN:O	2.47	0.47
2:B:47:PRO:HA	2:B:119:ARG:CD	2.44	0.47
1:A:327:THR:HG23	1:A:329:VAL:HG13	1.96	0.47
1:A:345:MET:HA	1:A:354:ALA:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:LEU:HD22	2:B:523:GLN:NE2	2.30	0.46
1:A:628:ARG:NH2	1:A:677:GLU:OE2	2.47	0.46
1:A:781:LEU:HA	1:A:817:LEU:HD23	1.97	0.46
1:A:781:LEU:HG	1:A:980:ALA:CB	2.45	0.46
2:B:512:CYS:CB	2:B:520:VAL:HG23	2.46	0.46
1:A:33:ASN:HD22	1:A:481:ALA:HB1	1.79	0.46
1:A:175:SER:OG	1:A:178:ARG:HG3	2.14	0.46
1:A:84:VAL:HG21	1:A:137:ALA:CB	2.45	0.46
1:A:629:ILE:HD12	1:A:629:ILE:H	1.81	0.46
1:A:685:PRO:HD2	1:A:688:ALA:HB3	1.97	0.46
1:A:836:GLY:N	1:A:914:ALA:HB3	2.30	0.46
1:A:851:PRO:HA	1:A:934:VAL:HG12	1.96	0.46
1:A:855:LEU:CD1	1:A:921:CYS:HB3	2.40	0.46
2:B:152:ASP:OD1	2:B:152:ASP:N	2.48	0.46
2:B:554:CYS:HB3	2:B:573:CYS:SG	2.56	0.46
2:B:648:ARG:NH1	2:B:648:ARG:HA	2.31	0.46
1:A:496:SER:HB2	1:A:630:VAL:CG2	2.44	0.46
1:A:810:LYS:HZ1	1:A:937:LEU:HA	1.80	0.46
1:A:848:ASP:OD2	1:A:850:GLN:NE2	2.47	0.46
1:A:966:LEU:HD22	1:A:966:LEU:H	1.81	0.46
2:B:650:ALA:C	2:B:652:HIS:H	2.23	0.46
1:A:36:PRO:O	1:A:39:LEU:HD11	2.16	0.46
1:A:845:TYR:N	1:A:939:PHE:O	2.49	0.46
2:B:103:SER:HB2	2:B:267:ASP:CG	2.41	0.46
1:A:552:VAL:CG1	1:A:596:ILE:HD13	2.45	0.46
1:A:835:PRO:CB	1:A:911:CYS:HA	2.46	0.46
1:A:837:GLN:H	1:A:842:ASP:CB	2.29	0.46
1:A:940:LEU:HD11	1:A:986:LEU:HD22	1.98	0.46
2:B:66:LEU:HD23	2:B:68:GLU:OE2	2.16	0.46
1:A:59:ASP:HB2	1:A:167:GLU:OE2	2.16	0.46
1:A:80:GLU:O	1:A:121:ARG:HA	2.16	0.46
1:A:693:ALA:C	1:A:694:LEU:HD22	2.40	0.46
2:B:179:PHE:HE2	2:B:236:GLN:HG3	1.80	0.46
2:B:469:PRO:HA	2:B:480:THR:HG23	1.97	0.46
1:A:703:LEU:HD11	1:A:732:ILE:HG12	1.98	0.46
1:A:828:LEU:HB3	1:A:923:LEU:HB3	1.98	0.46
2:B:276:THR:CG2	2:B:336:VAL:HG12	2.46	0.46
1:A:289:PRO:HA	1:A:320:PHE:O	2.16	0.46
1:A:293:TRP:HB3	2:B:343:LEU:HD13	1.97	0.46
1:A:493:VAL:HG21	1:A:598:LEU:CD1	2.46	0.46
1:A:793:ALA:HA	1:A:989:ALA:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:439:SER:HA	2:B:453:VAL:O	2.16	0.46
1:A:739:GLY:C	1:A:741:LEU:HD12	2.42	0.45
1:A:809:PRO:HG2	1:A:940:LEU:HD12	1.97	0.45
2:B:434:GLN:OE1	2:B:434:GLN:N	2.39	0.45
2:B:475:ASN:OD1	2:B:478:ASN:ND2	2.49	0.45
1:A:845:TYR:O	1:A:939:PHE:N	2.41	0.45
2:B:92:ASP:HB3	2:B:111:PRO:CB	2.45	0.45
2:B:514:PRO:HB3	2:B:546:TYR:CE2	2.51	0.45
1:A:376:LEU:O	1:A:377:LEU:HD23	2.17	0.45
1:A:791:VAL:HG11	2:B:684:LYS:NZ	2.32	0.45
2:B:144:MET:HE2	2:B:179:PHE:CE1	2.51	0.45
1:A:541:LEU:HB3	1:A:552:VAL:CG2	2.43	0.45
1:A:961:PHE:HE2	1:A:976:PRO:HB2	1.81	0.45
1:A:963:VAL:O	1:A:977:ARG:NH2	2.50	0.45
2:B:42:CYS:HA	2:B:45:VAL:HG23	1.97	0.45
2:B:230:ASN:O	2:B:234:LYS:HG3	2.16	0.45
1:A:586:GLU:HB3	1:A:592:LYS:NZ	2.32	0.45
1:A:677:GLU:OE1	1:A:757:LYS:HG3	2.16	0.45
2:B:52:CYS:HB2	2:B:70:LEU:CD2	2.42	0.45
6:J:2:BMA:H4	6:J:3:NAG:N2	2.31	0.45
2:B:43:LEU:HD12	2:B:459:CYS:O	2.17	0.45
1:A:342:PRO:HG3	1:A:389:SER:HA	1.98	0.45
1:A:658:ALA:O	1:A:660:ASN:ND2	2.50	0.45
1:A:835:PRO:HB3	1:A:910:SER:C	2.42	0.45
2:B:85:SER:OG	2:B:122:ASP:OD2	2.29	0.45
2:B:514:PRO:HB3	2:B:546:TYR:CD2	2.52	0.45
1:A:255:ASP:OD1	1:A:256:SER:N	2.49	0.45
1:A:453:ARG:O	1:A:466:LEU:HD12	2.16	0.45
1:A:684:LEU:HB2	1:A:714:ARG:CG	2.46	0.45
2:B:184:ASP:O	2:B:215:GLY:HA2	2.15	0.45
2:B:300:HIS:CE1	2:B:313:MET:HE1	2.51	0.45
2:B:504:TYR:HD2	2:B:529:CYS:HA	1.81	0.45
1:A:759:SER:HB2	1:A:760:GLN:OE1	2.17	0.45
1:A:972:PRO:C	1:A:973:LEU:HD12	2.42	0.45
2:B:119:ARG:HG3	2:B:122:ASP:CB	2.44	0.45
1:A:230:PRO:O	1:A:234:ILE:HG13	2.17	0.45
1:A:485:VAL:CG1	1:A:524:ALA:HB1	2.47	0.45
1:A:668:ALA:O	1:A:729:GLN:HA	2.16	0.44
1:A:941:TRP:CD1	1:A:943:PRO:HD2	2.52	0.44
1:A:753:GLN:NE2	1:A:763:ASN:HB3	2.32	0.44
2:B:111:PRO:O	2:B:451:LEU:HD13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LEU:HD23	1:A:305:TYR:HE1	1.82	0.44
1:A:855:LEU:HD21	1:A:934:VAL:HG13	1.99	0.44
1:A:113:GLN:HG2	1:A:148:GLU:HB2	1.99	0.44
1:A:195:LYS:HB3	1:A:198:CYS:SG	2.58	0.44
1:A:509:THR:O	1:A:510:LYS:HD3	2.17	0.44
1:A:628:ARG:HD2	1:A:676:TYR:CG	2.52	0.44
1:A:868:VAL:HG13	1:A:870:TRP:CE3	2.52	0.44
2:B:164:LEU:HA	2:B:367:LEU:CD2	2.47	0.44
2:B:227:THR:O	2:B:231:GLU:HG3	2.17	0.44
2:B:632:ASP:OD1	2:B:633:ALA:N	2.50	0.44
1:A:493:VAL:HG21	1:A:598:LEU:HD11	1.99	0.44
1:A:822:PRO:HA	1:A:928:ARG:HH11	1.82	0.44
2:B:61:SER:OG	2:B:62:PRO:HD2	2.18	0.44
2:B:468:GLU:HG2	2:B:471:SER:HB2	1.99	0.44
2:B:638:LYS:O	2:B:641:VAL:HG22	2.17	0.44
1:A:212:LEU:O	1:A:228:GLN:HA	2.18	0.44
1:A:639:CYS:HA	1:A:673:GLU:OE1	2.17	0.44
1:A:642:GLN:HB3	1:A:672:GLY:N	2.32	0.44
1:A:846:ILE:HA	1:A:938:ALA:HA	1.99	0.44
2:B:144:MET:HA	2:B:275:THR:OG1	2.18	0.44
2:B:398:ALA:HB1	2:B:412:CYS:SG	2.58	0.44
2:B:476:ASN:HD21	6:J:4:NAG:H4	1.82	0.44
1:A:658:ALA:HB2	1:A:822:PRO:HB3	1.99	0.44
1:A:683:HIS:CG	1:A:751:GLN:HB2	2.53	0.44
1:A:688:ALA:HA	1:A:737:SER:O	2.18	0.44
1:A:780:GLU:HB2	1:A:818:HIS:HB3	2.00	0.44
1:A:837:GLN:H	1:A:842:ASP:CG	2.26	0.44
2:B:140:ILE:HD11	2:B:168:MET:HE3	1.99	0.44
2:B:174:ASN:HB3	2:B:265:ARG:HH12	1.83	0.44
2:B:187:VAL:O	2:B:191:MET:HB3	2.17	0.44
1:A:654:LEU:HB3	1:A:741:LEU:HD21	1.99	0.43
2:B:685:ASN:OD1	2:B:689:CYS:N	2.50	0.43
1:A:547:ARG:HA	1:A:550:ARG:HD3	2.00	0.43
2:B:83:PRO:HD2	2:B:119:ARG:NH2	2.33	0.43
2:B:85:SER:HA	2:B:117:ARG:O	2.18	0.43
2:B:605:GLY:HA2	2:B:615:ILE:HG13	2.01	0.43
1:A:827:GLY:HA3	1:A:964:SER:HB3	1.99	0.43
1:A:955:LEU:O	1:A:983:TRP:HA	2.18	0.43
2:B:155:TRP:O	2:B:158:GLN:HB2	2.19	0.43
2:B:258:CYS:O	2:B:262:ILE:HG12	2.18	0.43
2:B:507:SER:OG	2:B:510:ASP:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:GLU:OE1	1:A:92:GLU:N	2.46	0.43
1:A:101:PHE:CE1	1:A:164:ALA:HB2	2.53	0.43
1:A:146:VAL:H	1:A:153:ALA:HB3	1.83	0.43
1:A:949:PRO:HA	1:A:988:ARG:HE	1.83	0.43
1:A:839:GLN:HB3	1:A:840:PRO:HD2	1.99	0.43
1:A:950:LEU:HA	1:A:991:GLU:CA	2.40	0.43
1:A:692:ARG:NH1	1:A:694:LEU:HD23	2.26	0.43
1:A:827:GLY:HA3	1:A:964:SER:CB	2.49	0.43
2:B:520:VAL:HG21	2:B:527:CYS:HB2	1.99	0.43
2:B:602:SER:C	2:B:604:ARG:H	2.26	0.43
1:A:223:LEU:HD12	1:A:262:PHE:HA	2.00	0.43
1:A:649:VAL:HG21	1:A:771:VAL:HG21	2.00	0.43
1:A:777:ALA:O	1:A:976:PRO:HG3	2.19	0.43
1:A:814:THR:HG21	1:A:933:MET:HE3	2.00	0.43
2:B:125:ASN:HA	2:B:426:GLU:HA	2.00	0.43
1:A:261:TYR:OH	1:A:310:ARG:NH2	2.47	0.43
1:A:328:ASP:O	1:A:403:ASN:HB2	2.18	0.43
1:A:776:GLU:O	1:A:822:PRO:HG2	2.18	0.43
1:A:809:PRO:HD2	1:A:945:LEU:HD11	2.01	0.43
2:B:435:GLU:HB3	2:B:438:LYS:HE2	2.01	0.43
1:A:118:PHE:HB2	1:A:143:HIS:HB2	2.01	0.43
1:A:520:MET:HE3	1:A:600:LEU:HD13	1.99	0.43
1:A:608:GLU:HG2	1:A:609:ALA:N	2.34	0.43
2:B:156:SER:OG	2:B:362:ASP:O	2.29	0.43
1:A:392:ALA:HB2	1:A:452:LEU:HB2	2.00	0.42
1:A:680:LEU:HD13	1:A:754:ILE:HG12	2.00	0.42
1:A:954:VAL:CG1	1:A:985:GLN:HG2	2.49	0.42
2:B:144:MET:HE3	2:B:146:LEU:HD21	2.00	0.42
1:A:34:LEU:O	1:A:36:PRO:HD3	2.18	0.42
1:A:458:ILE:HG22	1:A:465:ASP:OD2	2.18	0.42
1:A:552:VAL:HG12	1:A:583:LEU:HD12	2.01	0.42
2:B:501:GLU:OE1	2:B:502:GLU:HB3	2.19	0.42
2:B:692:ARG:HH22	2:B:694:GLN:HB3	1.84	0.42
1:A:145:ASN:CG	1:A:155:LYS:HB2	2.44	0.42
1:A:644:GLN:HG3	1:A:671:GLU:OE2	2.19	0.42
1:A:694:LEU:CD1	1:A:702:ARG:HG2	2.49	0.42
1:A:781:LEU:HG	1:A:980:ALA:HB2	2.01	0.42
2:B:102:ASP:O	2:B:106:VAL:HG23	2.19	0.42
1:A:809:PRO:HD2	1:A:940:LEU:HB2	2.01	0.42
2:B:645:LYS:CG	2:B:666:GLU:HB3	2.47	0.42
1:A:156:THR:OG1	1:A:196:ARG:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:LEU:HD21	1:A:516:PHE:CE1	2.55	0.42
1:A:268:TYR:OH	2:B:287:ARG:HG3	2.19	0.42
1:A:341:ALA:O	1:A:357:GLY:HA2	2.19	0.42
1:A:502:LYS:HD3	1:A:512:PRO:O	2.19	0.42
2:B:211:LEU:HG	2:B:237:SER:HB3	2.02	0.42
2:B:493:LEU:HB3	2:B:531:GLN:HE21	1.84	0.42
2:B:686:GLU:HG2	2:B:687:ASP:OD1	2.19	0.42
1:A:156:THR:HB	1:A:157:PRO:HD2	2.01	0.42
1:A:642:GLN:N	1:A:672:GLY:HA3	2.34	0.42
2:B:476:ASN:ND2	2:B:476:ASN:O	2.52	0.42
1:A:710:GLU:O	1:A:712:GLU:N	2.52	0.42
1:A:790:LEU:CD2	1:A:809:PRO:HB3	2.50	0.42
2:B:478:ASN:ND2	6:J:4:NAG:O3	2.45	0.42
2:B:641:VAL:O	2:B:645:LYS:N	2.52	0.42
1:A:506:LEU:CD2	1:A:558:GLN:HE21	2.32	0.42
1:A:507:PRO:HD2	1:A:558:GLN:NE2	2.34	0.42
1:A:839:GLN:CD	1:A:865:PRO:HG2	2.45	0.42
1:A:849:ILE:CG1	1:A:936:VAL:HG12	2.49	0.42
1:A:857:CYS:HB3	1:A:921:CYS:N	2.35	0.42
2:B:270:HIS:HB2	2:B:330:ILE:HA	2.02	0.42
2:B:438:LYS:HB2	2:B:455:VAL:CG1	2.50	0.42
2:B:557:TYR:CD2	2:B:558:LYS:HD3	2.54	0.42
2:B:655:ASN:HB3	2:B:659:ARG:NH2	2.35	0.42
2:B:692:ARG:HH12	2:B:694:GLN:HB2	1.85	0.42
1:A:847:LEU:O	1:A:863:VAL:HG21	2.19	0.42
1:A:927:ALA:HB3	1:A:930:GLN:HB2	2.01	0.42
2:B:114:ILE:HG22	2:B:453:VAL:HG22	2.02	0.42
1:A:528:ASN:O	1:A:528:ASN:ND2	2.52	0.41
1:A:531:GLN:O	1:A:569:GLY:HA3	2.20	0.41
1:A:837:GLN:HG2	1:A:837:GLN:O	2.20	0.41
1:A:837:GLN:OE1	1:A:841:SER:HB3	2.20	0.41
2:B:337:THR:OG1	2:B:339:ASN:ND2	2.53	0.41
2:B:468:GLU:CG	2:B:471:SER:HB2	2.50	0.41
2:B:673:ASP:C	8:B:804:NAG:H61	2.45	0.41
2:B:669:LYS:O	2:B:670:GLU:C	2.63	0.41
1:A:956:GLN:HA	1:A:983:TRP:CB	2.50	0.41
1:A:956:GLN:CG	1:A:983:TRP:HB3	2.40	0.41
2:B:193:ILE:HA	2:B:199:LEU:CD2	2.51	0.41
1:A:124:LEU:HD12	1:A:125:GLY:H	1.86	0.41
1:A:263:ASP:OD2	2:B:245:PRO:HD3	2.20	0.41
2:B:190:TYR:O	2:B:213:MET:HE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:PRO:HG2	2:B:204:TYR:OH	2.19	0.41
1:A:320:PHE:CZ	1:A:339:VAL:HG11	2.55	0.41
1:A:369:HIS:HB2	1:A:371:LEU:CD1	2.50	0.41
1:A:541:LEU:HA	1:A:598:LEU:HD23	2.03	0.41
1:A:593:LEU:HD22	2:B:523:GLN:HE22	1.85	0.41
1:A:703:LEU:HD11	1:A:732:ILE:CG1	2.50	0.41
2:B:396:PHE:CE2	2:B:425:ILE:HG12	2.56	0.41
2:B:512:CYS:HB3	2:B:520:VAL:HG23	2.01	0.41
1:A:965:SER:HA	1:A:975:LEU:HD11	2.00	0.41
2:B:143:LEU:HD11	2:B:251:ALA:HB1	2.01	0.41
1:A:538:GLU:HB3	1:A:601:ASN:HB3	2.02	0.41
1:A:620:ASP:OD1	1:A:620:ASP:N	2.54	0.41
1:A:942:LEU:HD11	1:A:946:TYR:OH	2.21	0.41
1:A:988:ARG:HB3	1:A:991:GLU:HB2	2.01	0.41
2:B:397:ASN:HB2	2:B:424:SER:OG	2.20	0.41
1:A:141:TRP:CZ2	2:B:290:GLY:HA2	2.55	0.41
1:A:145:ASN:ND2	1:A:147:LEU:HD21	2.35	0.41
1:A:806:SER:CB	1:A:943:PRO:HD3	2.48	0.41
1:A:849:ILE:CD1	1:A:936:VAL:HG12	2.50	0.41
1:A:861:PRO:CD	1:A:917:THR:HA	2.49	0.41
2:B:657:CYS:O	2:B:661:CYS:HB2	2.21	0.41
1:A:425:GLY:HA2	1:A:430:LEU:HD23	2.02	0.41
1:A:426:GLN:OE1	1:A:431:ARG:HG2	2.21	0.41
1:A:489:VAL:HG12	1:A:602:VAL:HG21	2.03	0.41
1:A:521:CYS:HA	1:A:576:CYS:HA	2.03	0.41
1:A:601:ASN:OD1	4:D:1:NAG:C2	2.68	0.41
1:A:741:LEU:HD23	1:A:773:VAL:HG13	2.03	0.41
1:A:839:GLN:NE2	1:A:865:PRO:HG2	2.35	0.41
2:B:634:CYS:O	2:B:635:THR:C	2.63	0.41
1:A:190:ASP:O	1:A:191:PHE:C	2.64	0.41
2:B:318:LEU:HD22	2:B:351:ILE:HD11	2.03	0.41
2:B:438:LYS:O	2:B:455:VAL:HG12	2.20	0.41
1:A:514:SER:O	1:A:582:PHE:HA	2.22	0.40
1:A:394:LEU:CD2	1:A:466:LEU:HD13	2.48	0.40
1:A:553:LEU:HB2	1:A:582:PHE:CZ	2.56	0.40
1:A:855:LEU:HD12	1:A:921:CYS:CB	2.41	0.40
2:B:428:LYS:HD3	2:B:576:ASP:HA	2.03	0.40
1:A:603:SER:HB3	4:D:1:NAG:H62	2.02	0.40
1:A:814:THR:HA	1:A:935:THR:HA	2.03	0.40
1:A:722:ASN:HB3	1:A:723:PRO:CD	2.50	0.40
1:A:770:ASP:OD1	1:A:770:ASP:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:404:GLU:HG2	2:B:404:GLU:O	2.21	0.40
1:A:311:LEU:CD1	1:A:337:LEU:HD23	2.52	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	910/1039 (88%)	868 (95%)	40 (4%)	2 (0%)	44	63
2	B	679/788 (86%)	636 (94%)	42 (6%)	1 (0%)	48	70
3	C	2/4 (50%)	2 (100%)	0	0	100	100
All	All	1591/1831 (87%)	1506 (95%)	82 (5%)	3 (0%)	45	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	602	VAL
1	A	711	ASN
2	B	603	GLY

### 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	758/864 (88%)	743 (98%)	15 (2%)	50	70
2	B	603/690 (87%)	584 (97%)	19 (3%)	34	55
3	C	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	1363/1556 (88%)	1328 (97%)	35 (3%)	42	63

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	197	TYR
1	A	301	LEU
1	A	319	TYR
1	A	547	ARG
1	A	580	MET
1	A	640	VAL
1	A	770	ASP
1	A	828	LEU
1	A	830	LEU
1	A	844	LEU
1	A	857	CYS
1	A	924	GLN
1	A	950	LEU
1	A	970	VAL
2	B	75	CYS
2	B	204	TYR
2	B	219	VAL
2	B	250	ASP
2	B	405	VAL
2	B	461	CYS
2	B	483	CYS
2	B	593	CYS
2	B	607	CYS
2	B	613	VAL
2	B	627	CYS
2	B	630	CYS
2	B	641	VAL
2	B	655	ASN
2	B	673	ASP
2	B	692	ARG
2	B	694	GLN
2	B	705	LEU
2	B	709	GLU

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Mol	Chain	Res	Type
3	C	495	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	46	ASN
1	A	78	GLN
1	A	95	GLN
1	A	116	GLN
1	A	335	HIS
1	A	482	GLN
1	A	490	GLN
1	A	517	ASN
1	A	528	ASN
1	A	558	GLN
1	A	565	ASN
1	A	622	HIS
1	A	626	GLN
1	A	642	GLN
1	A	644	GLN
1	A	753	GLN
1	A	761	ASN
1	A	930	GLN
1	A	947	GLN
1	A	981	GLN
2	B	105	GLN
2	B	158	GLN
2	B	167	GLN
2	B	300	HIS
2	B	331	ASN
2	B	339	ASN
2	B	470	ASN
2	B	496	GLN
2	B	518	GLN
2	B	531	GLN
2	B	597	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

18 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$
4	NAG	D	1	4	14,14,15	0.38	0	17,19,21	0.59	0
4	NAG	D	2	4	14,14,15	0.38	0	17,19,21	0.55	0
4	NAG	E	1	4,2	14,14,15	0.38	0	17,19,21	0.99	1 (5%)
4	NAG	E	2	4	14,14,15	0.35	0	17,19,21	0.84	1 (5%)
4	NAG	F	1	4,2	14,14,15	0.38	0	17,19,21	0.60	0
4	NAG	F	2	4	14,14,15	0.38	0	17,19,21	0.54	0
4	NAG	G	1	1,4	14,14,15	0.37	0	17,19,21	0.95	2 (11%)
4	NAG	G	2	4	14,14,15	0.39	0	17,19,21	0.45	0
5	NAG	H	1	5,2	14,14,15	0.38	0	17,19,21	0.49	0
5	NAG	H	2	5	14,14,15	0.36	0	17,19,21	0.79	1 (5%)
5	BMA	H	3	5	11,11,12	0.28	0	15,15,17	0.53	0
5	NAG	I	1	5,2	14,14,15	0.40	0	17,19,21	0.88	1 (5%)
5	NAG	I	2	5	14,14,15	0.40	0	17,19,21	0.57	0
5	BMA	I	3	5	11,11,12	0.28	0	15,15,17	0.58	0
6	BMA	J	1	6	11,11,12	0.30	0	15,15,17	0.56	0
6	BMA	J	2	6	11,11,12	0.26	0	15,15,17	0.65	0
6	NAG	J	3	6	14,14,15	0.41	0	17,19,21	1.07	1 (5%)
6	NAG	J	4	6	14,14,15	0.40	0	17,19,21	1.03	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
4	NAG	D	1	4	-	4/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	4,2	-	3/6/23/26	0/1/1/1
4	NAG	E	2	4	-	3/6/23/26	0/1/1/1
4	NAG	F	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
5	NAG	H	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	1/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	NAG	I	1	5,2	-	3/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
6	BMA	J	1	6	-	2/2/19/22	0/1/1/1
6	BMA	J	2	6	-	0/2/19/22	0/1/1/1
6	NAG	J	3	6	-	3/6/23/26	0/1/1/1
6	NAG	J	4	6	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	3	NAG	C2-N2-C7	4.00	128.26	122.90
4	E	1	NAG	C2-N2-C7	3.58	127.70	122.90
6	J	4	NAG	C1-C2-N2	3.56	116.05	110.43
4	E	2	NAG	C2-N2-C7	2.85	126.72	122.90
5	I	1	NAG	C1-O5-C5	2.82	115.97	112.19
4	G	1	NAG	C1-O5-C5	2.62	115.69	112.19
5	H	2	NAG	C2-N2-C7	2.38	126.09	122.90
4	G	1	NAG	C2-N2-C7	2.37	126.08	122.90

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C1-C2-N2-C7
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	E	1	NAG	C3-C2-N2-C7

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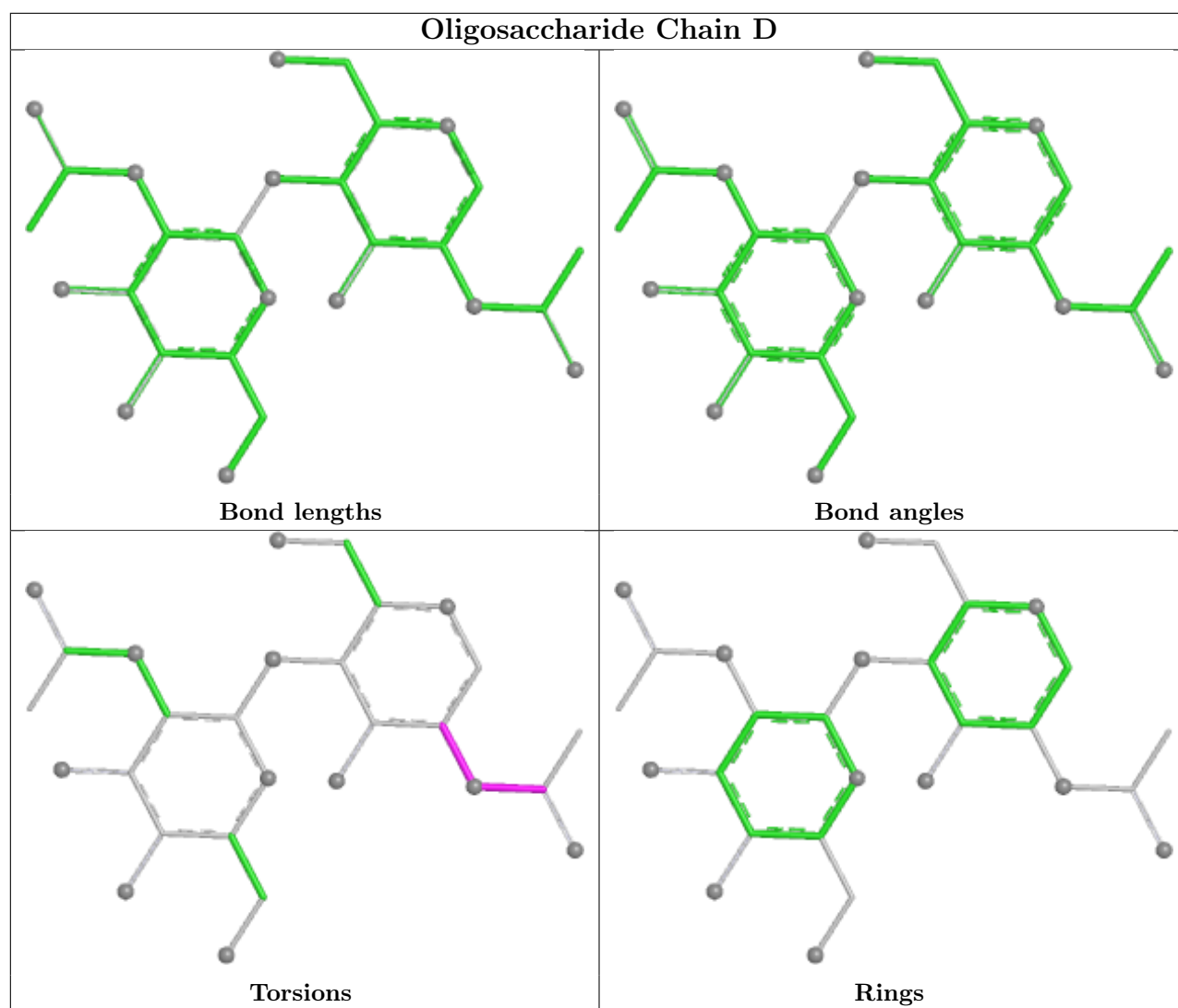
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	E	2	NAG	C3-C2-N2-C7
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
4	G	1	NAG	C3-C2-N2-C7
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
6	J	3	NAG	C8-C7-N2-C2
6	J	3	NAG	O7-C7-N2-C2
6	J	1	BMA	C4-C5-C6-O6
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
5	I	1	NAG	C8-C7-N2-C2
5	I	1	NAG	O7-C7-N2-C2
6	J	1	BMA	O5-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C3-C2-N2-C7
6	J	4	NAG	C1-C2-N2-C7
5	H	2	NAG	C3-C2-N2-C7
6	J	3	NAG	C3-C2-N2-C7
6	J	4	NAG	C3-C2-N2-C7

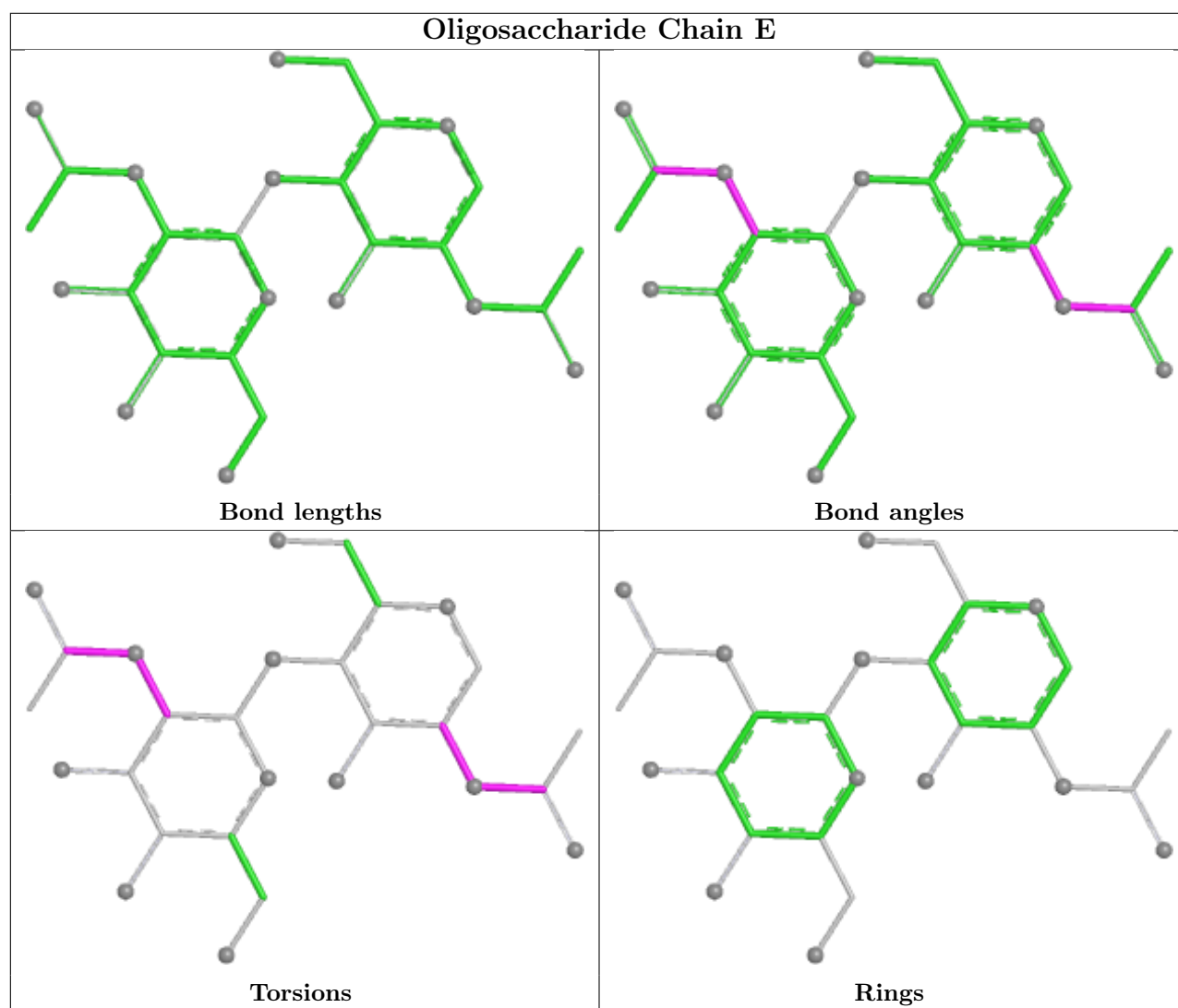
There are no ring outliers.

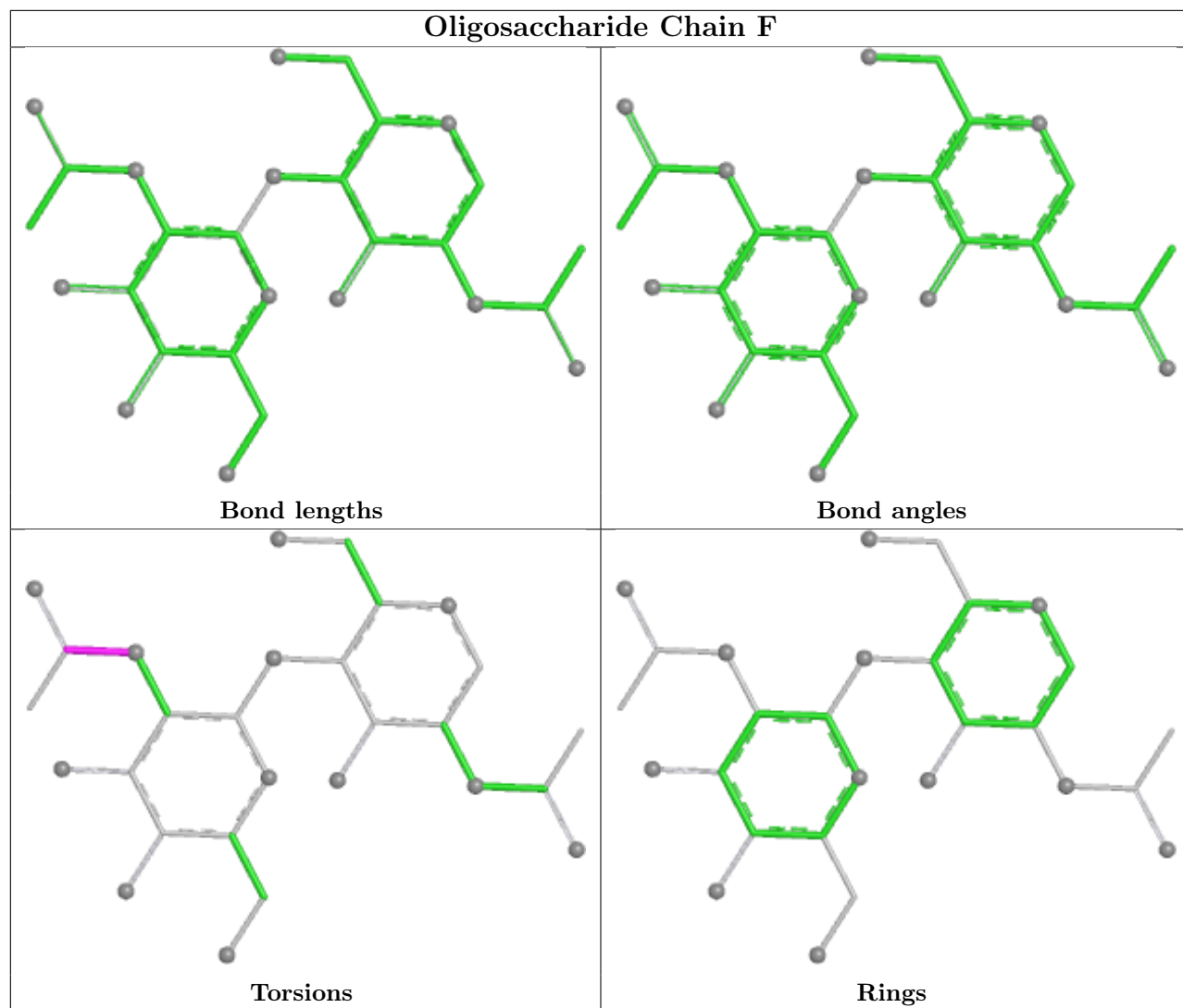
4 monomers are involved in 10 short contacts:

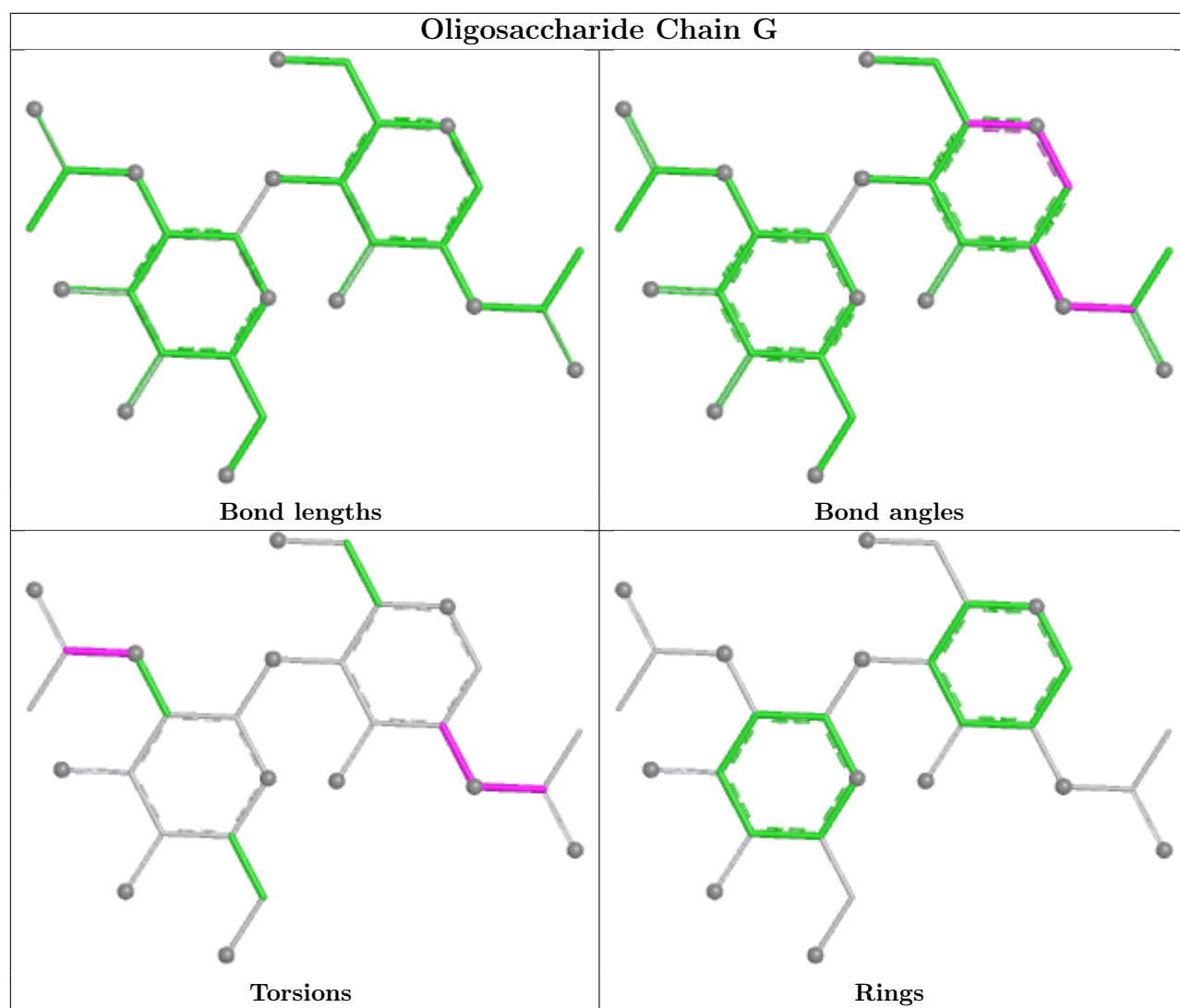
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	4	NAG	2	0
4	D	1	NAG	6	0
6	J	2	BMA	2	0
6	J	3	NAG	2	0

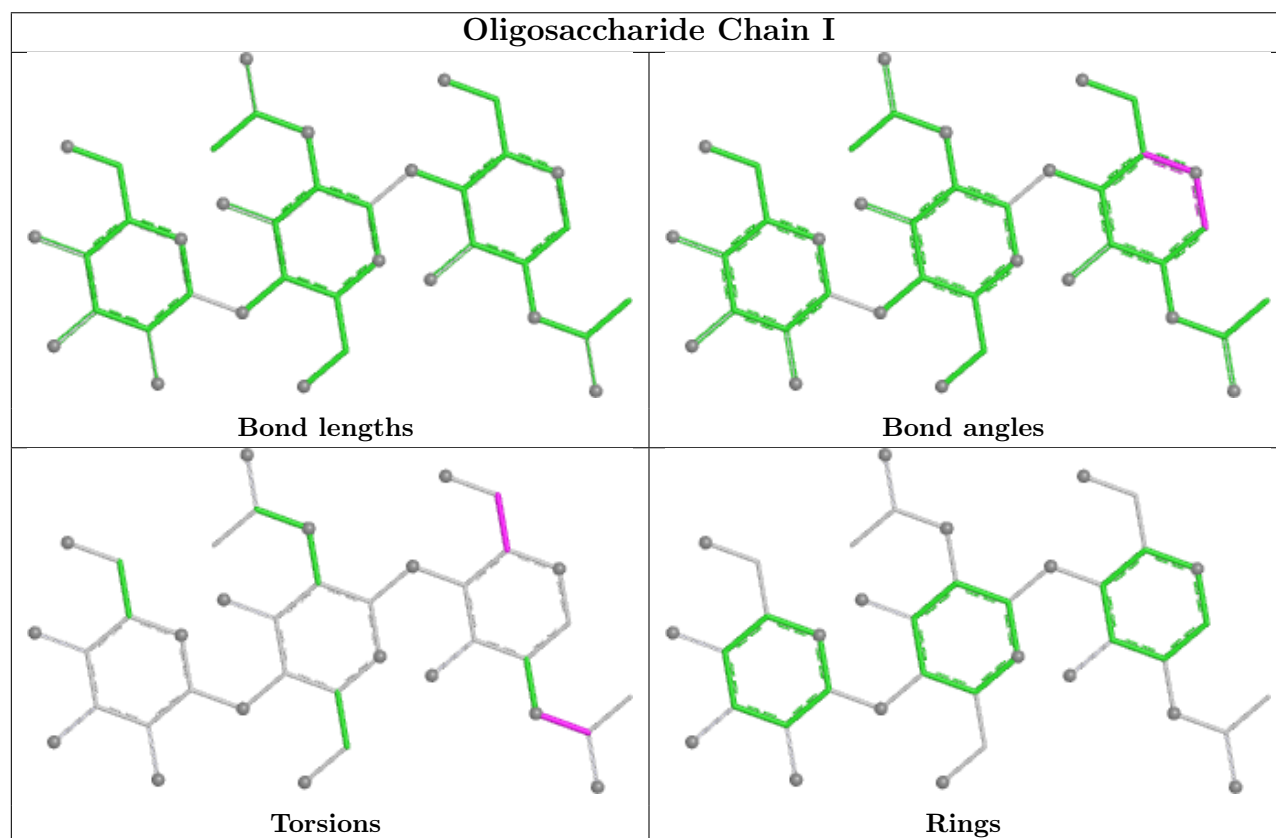
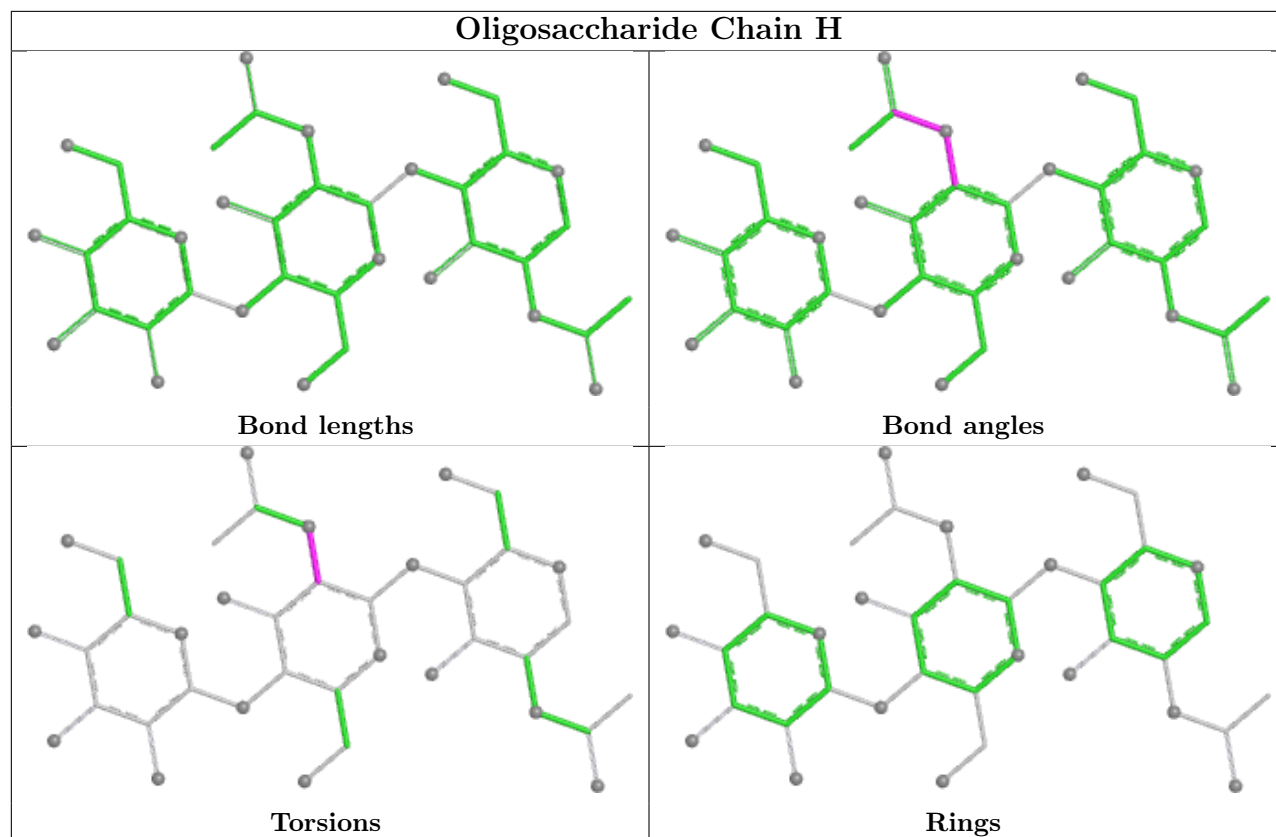
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

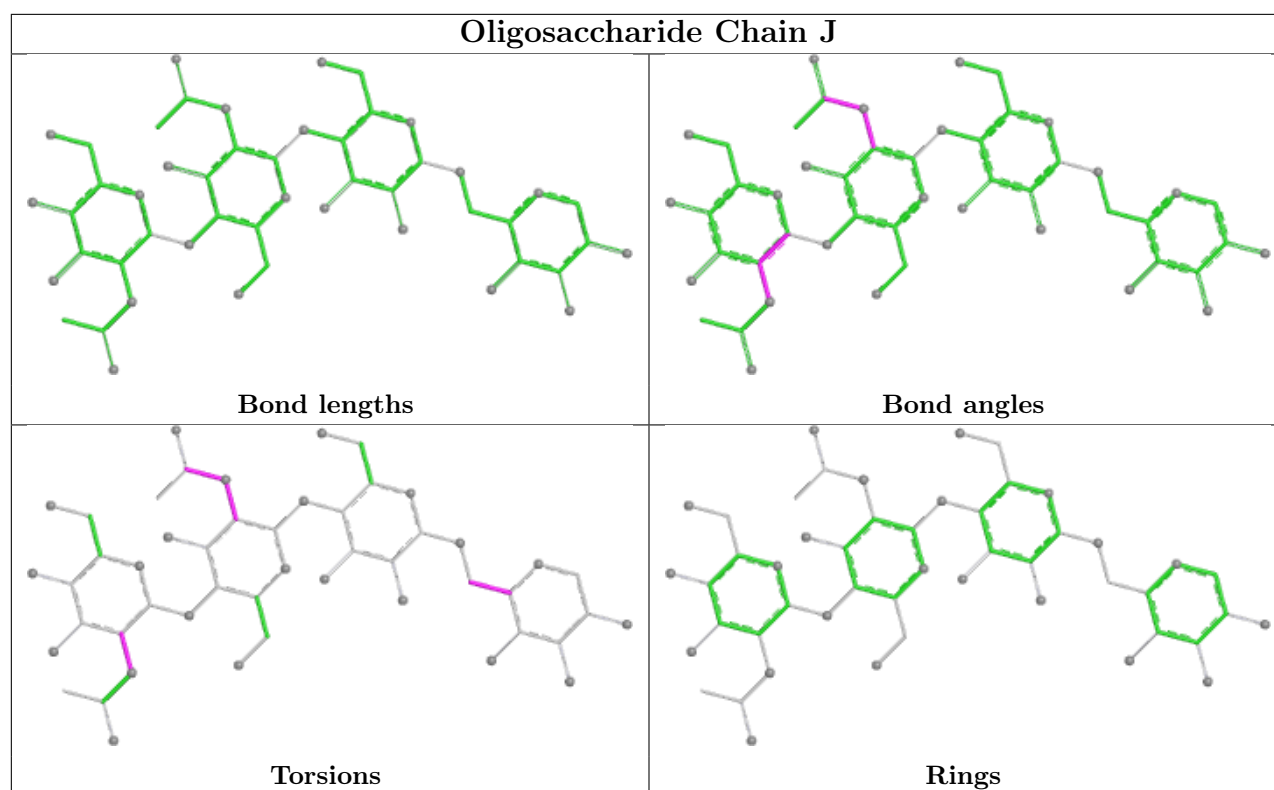












## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
8	NAG	A	1105	1	14,14,15	0.26	0	17,19,21	0.53	0
8	NAG	B	804	2	14,14,15	0.38	0	17,19,21	0.57	0
8	NAG	A	1106	-	14,14,15	0.38	0	17,19,21	0.55	0
8	NAG	A	1108	1	14,14,15	0.39	0	17,19,21	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	1105	1	-	2/6/23/26	0/1/1/1
8	NAG	B	804	2	-	2/6/23/26	0/1/1/1
8	NAG	A	1106	-	-	0/6/23/26	0/1/1/1
8	NAG	A	1108	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1105	NAG	C4-C5-C6-O6
8	A	1105	NAG	O5-C5-C6-O6
8	A	1108	NAG	C8-C7-N2-C2
8	A	1108	NAG	O7-C7-N2-C2
8	B	804	NAG	C8-C7-N2-C2
8	B	804	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1105	NAG	1	0
8	B	804	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



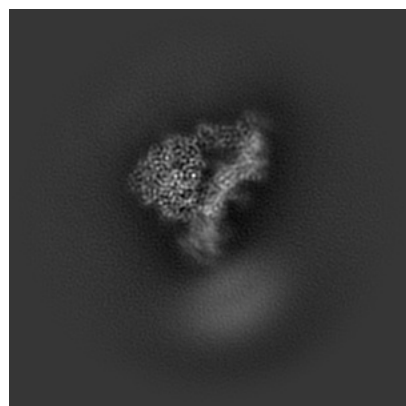
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47713. These allow visual inspection of the internal detail of the map and identification of artifacts.

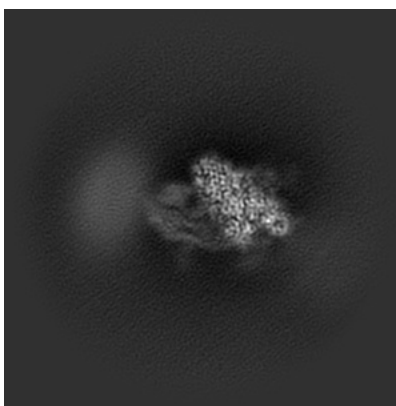
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

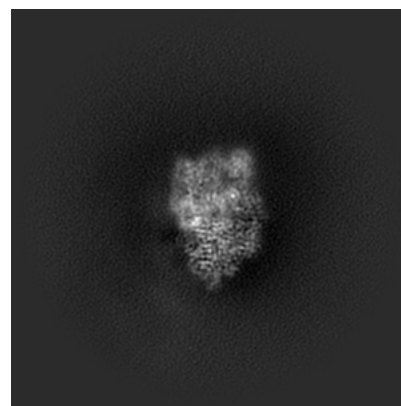
#### 6.1.1 Primary map



X

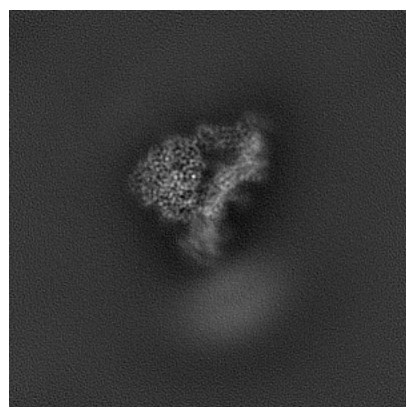


Y

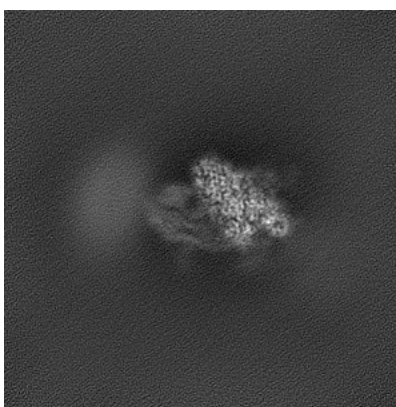


Z

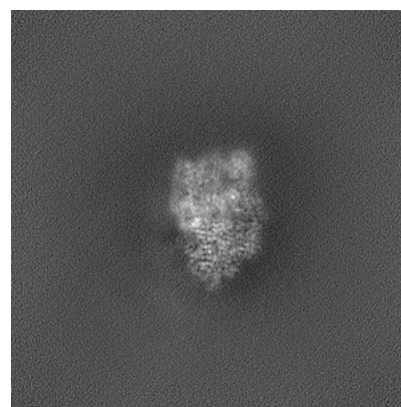
#### 6.1.2 Raw map



X



Y

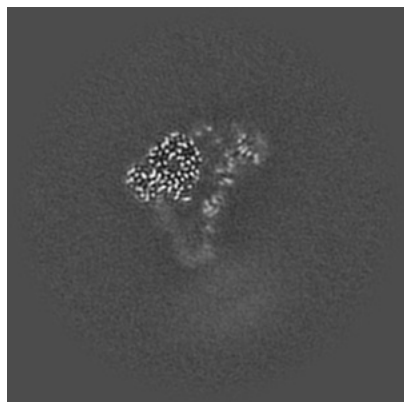


Z

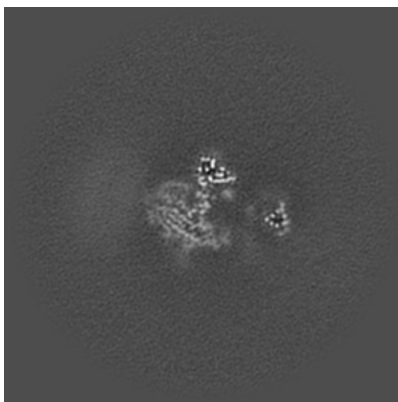
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

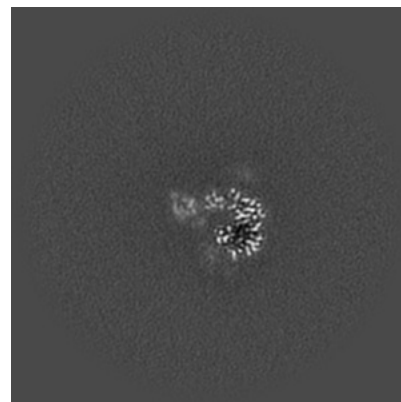
### 6.2.1 Primary map



X Index: 150

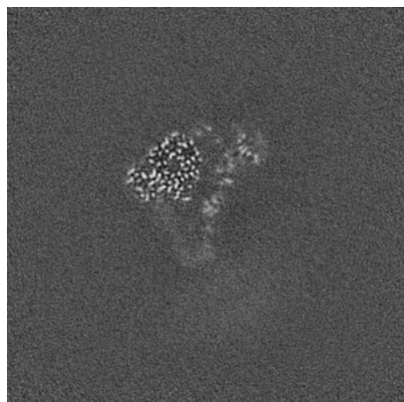


Y Index: 150

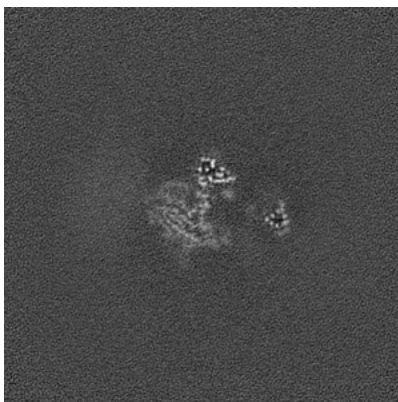


Z Index: 150

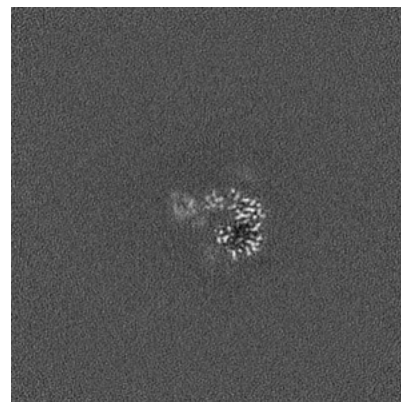
### 6.2.2 Raw map



X Index: 150



Y Index: 150

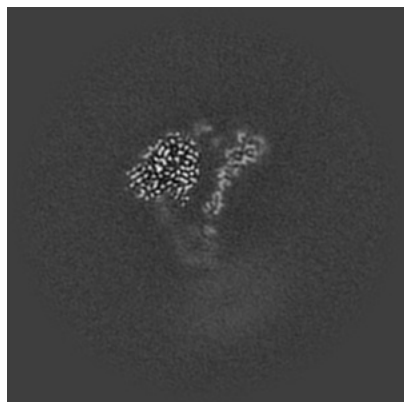


Z Index: 150

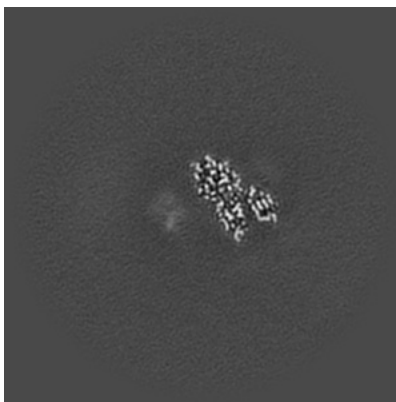
The images above show central slices of the map in three orthogonal directions.

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

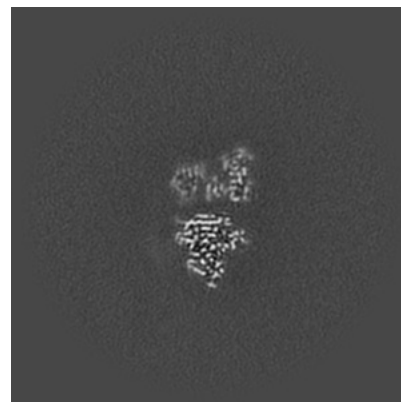
### 6.3.1 Primary map



X Index: 152

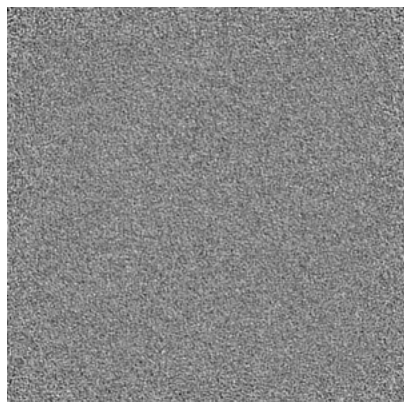


Y Index: 129

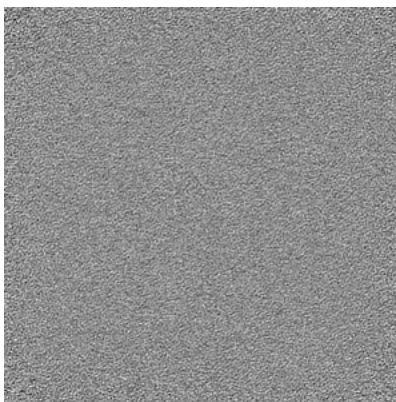


Z Index: 175

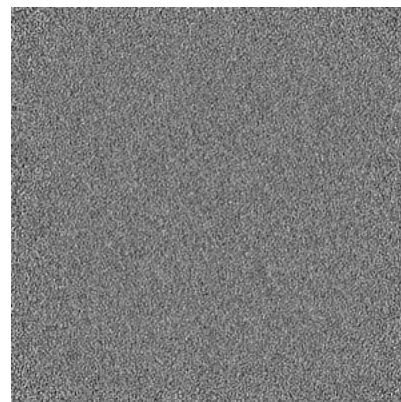
### 6.3.2 Raw map



X Index: 0



Y Index: 0



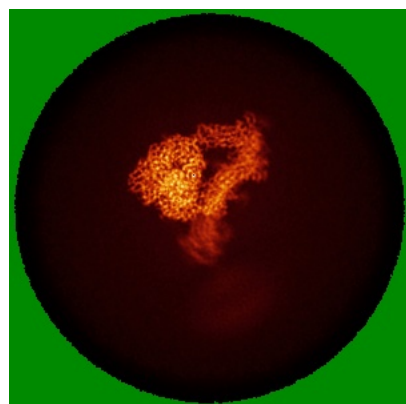
Z Index: 0

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

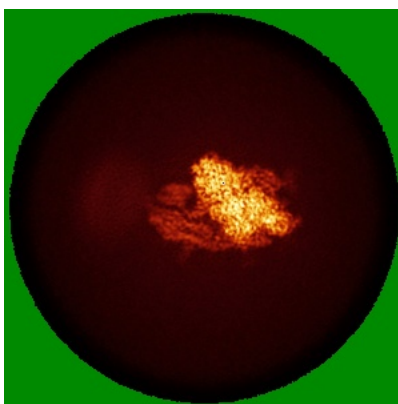


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

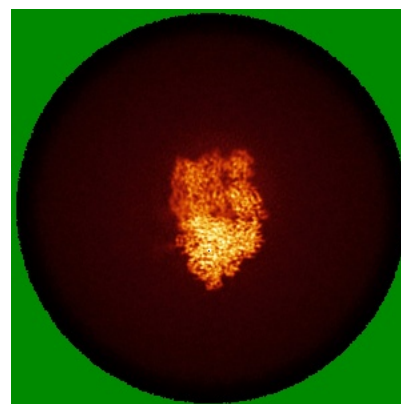
### 6.4.1 Primary map



X

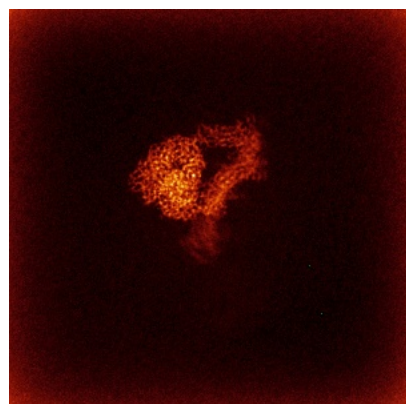


Y

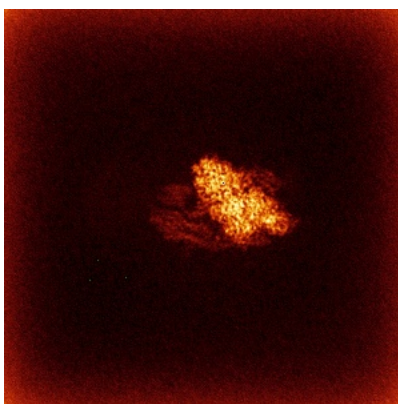


Z

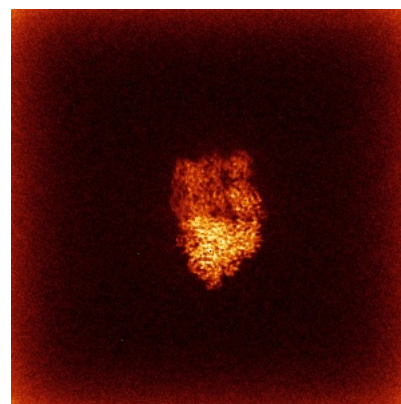
### 6.4.2 Raw map



X



Y

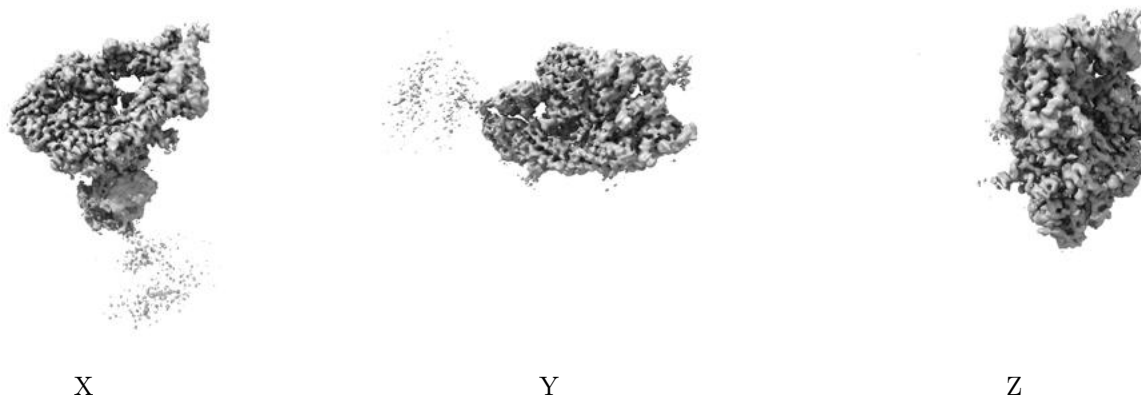


Z

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.

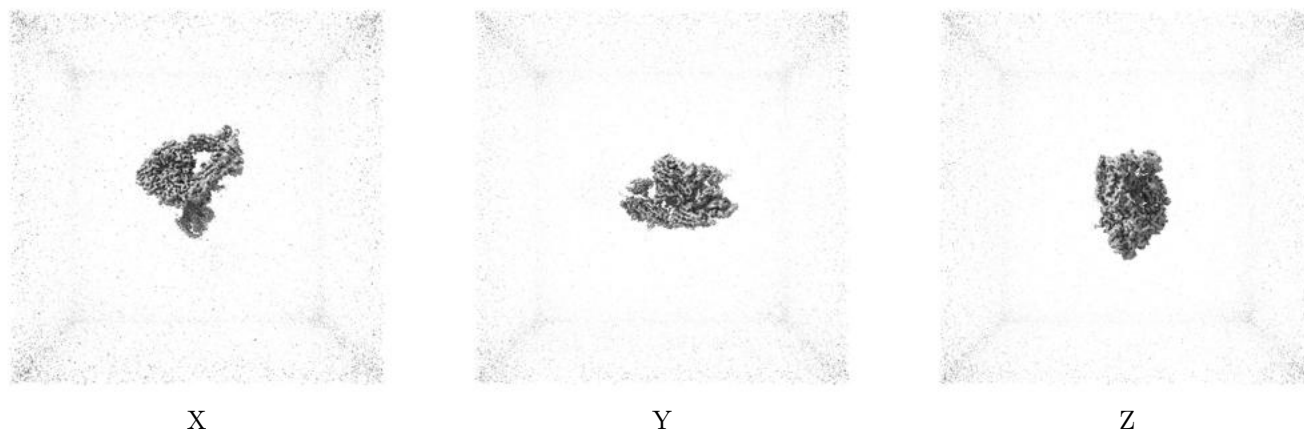
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

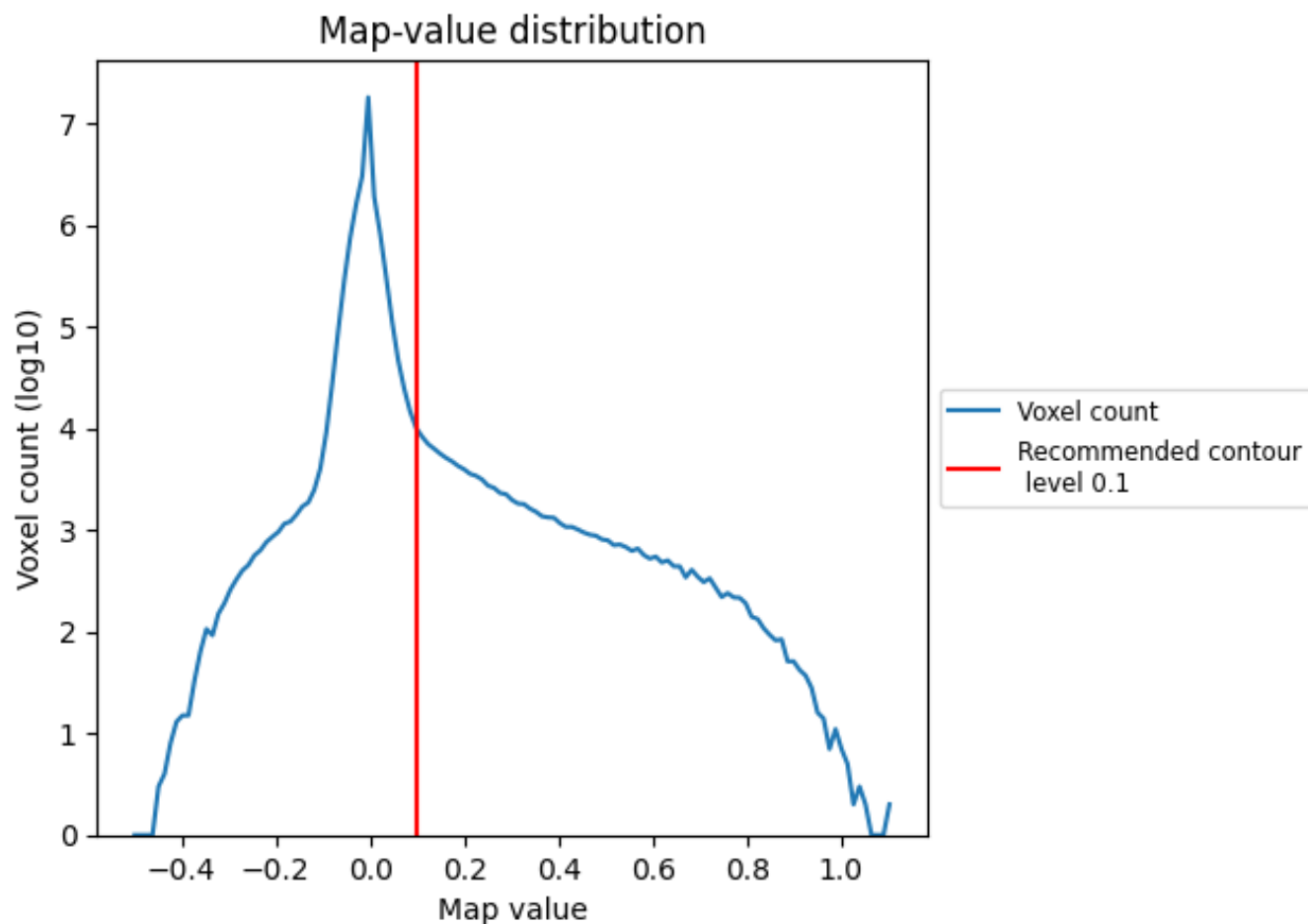
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

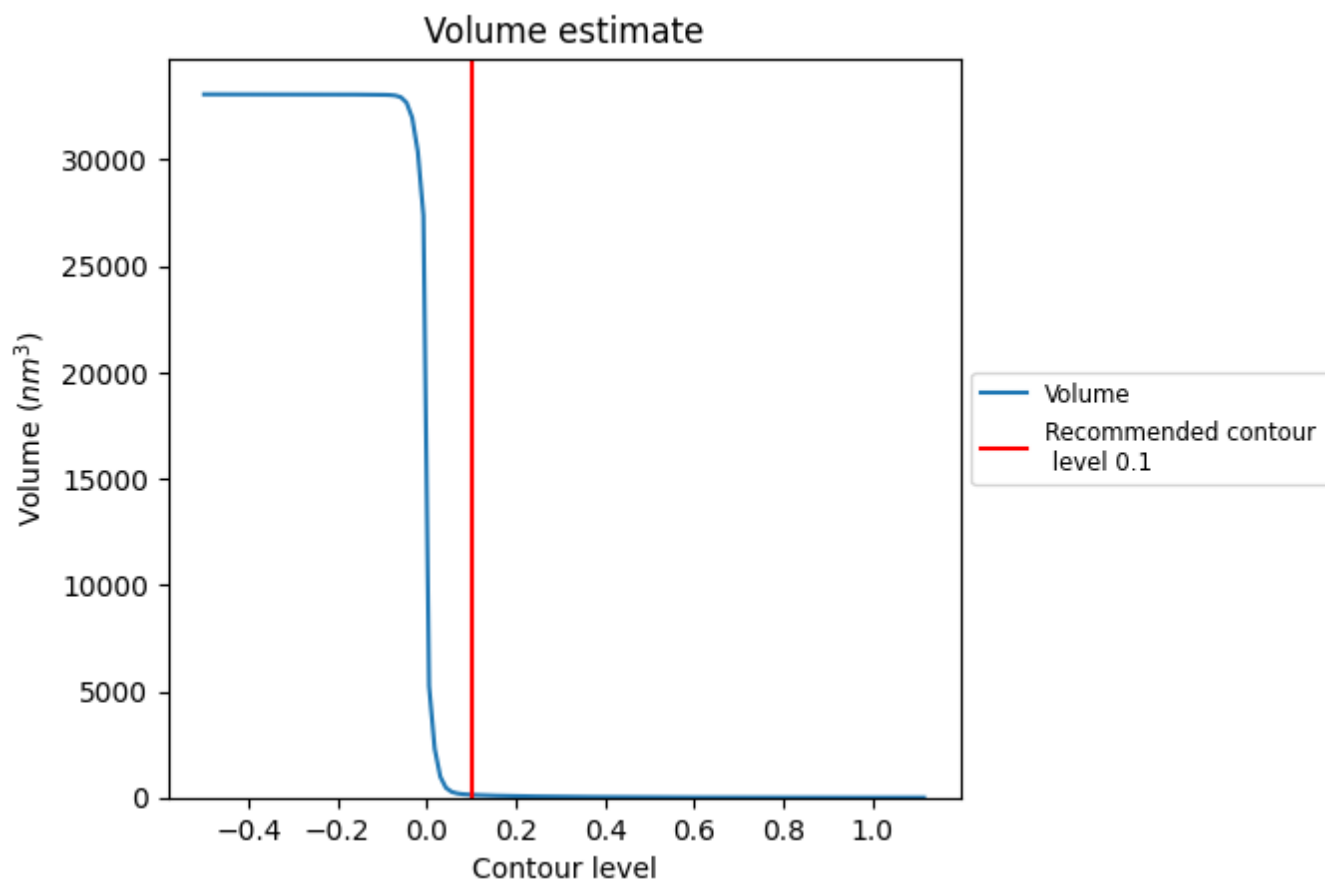
This section contains the results of statistical analysis of the map.

### 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.

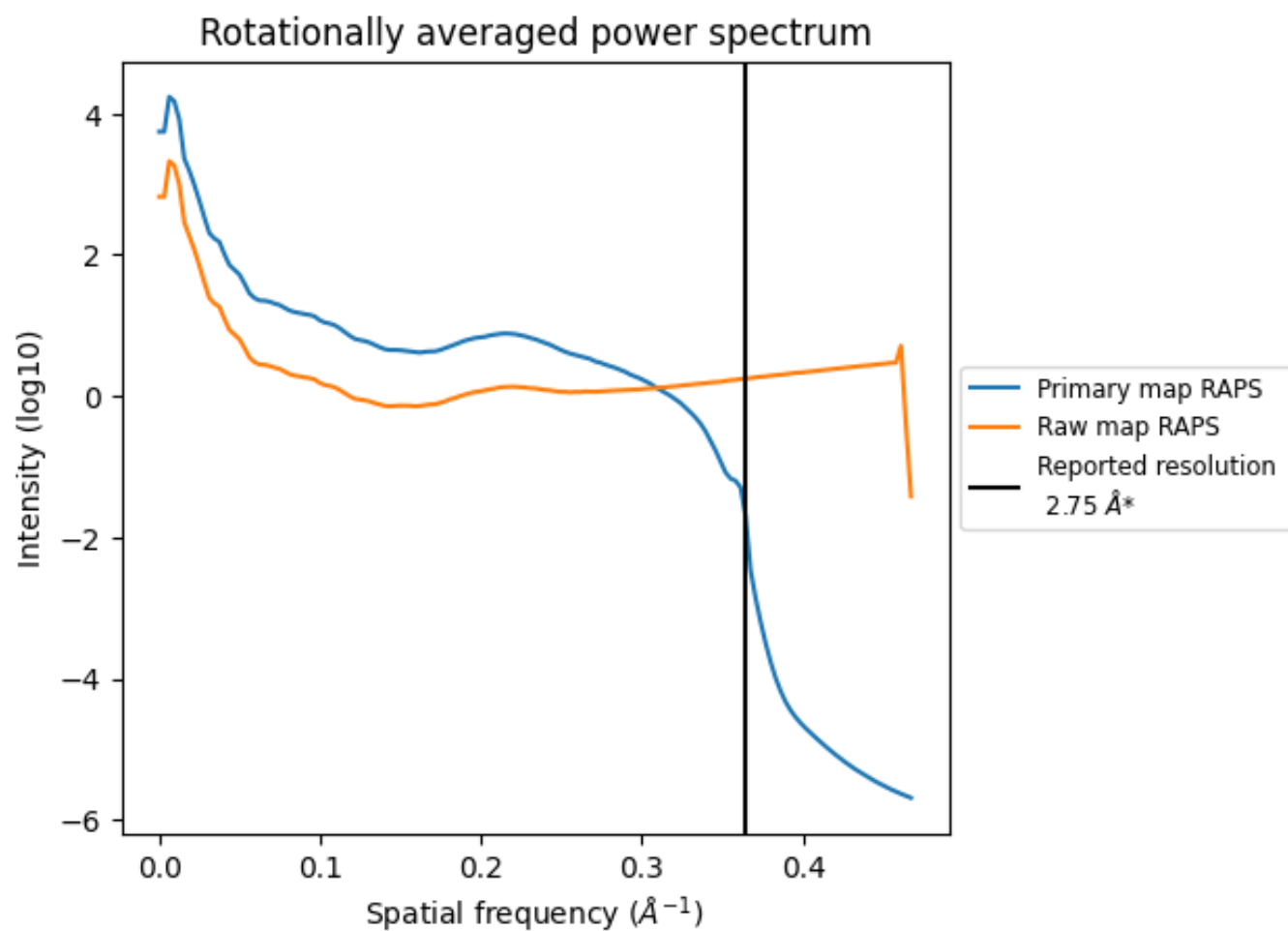
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 130 nm<sup>3</sup>; this corresponds to an approximate mass of 117 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 ⓘ



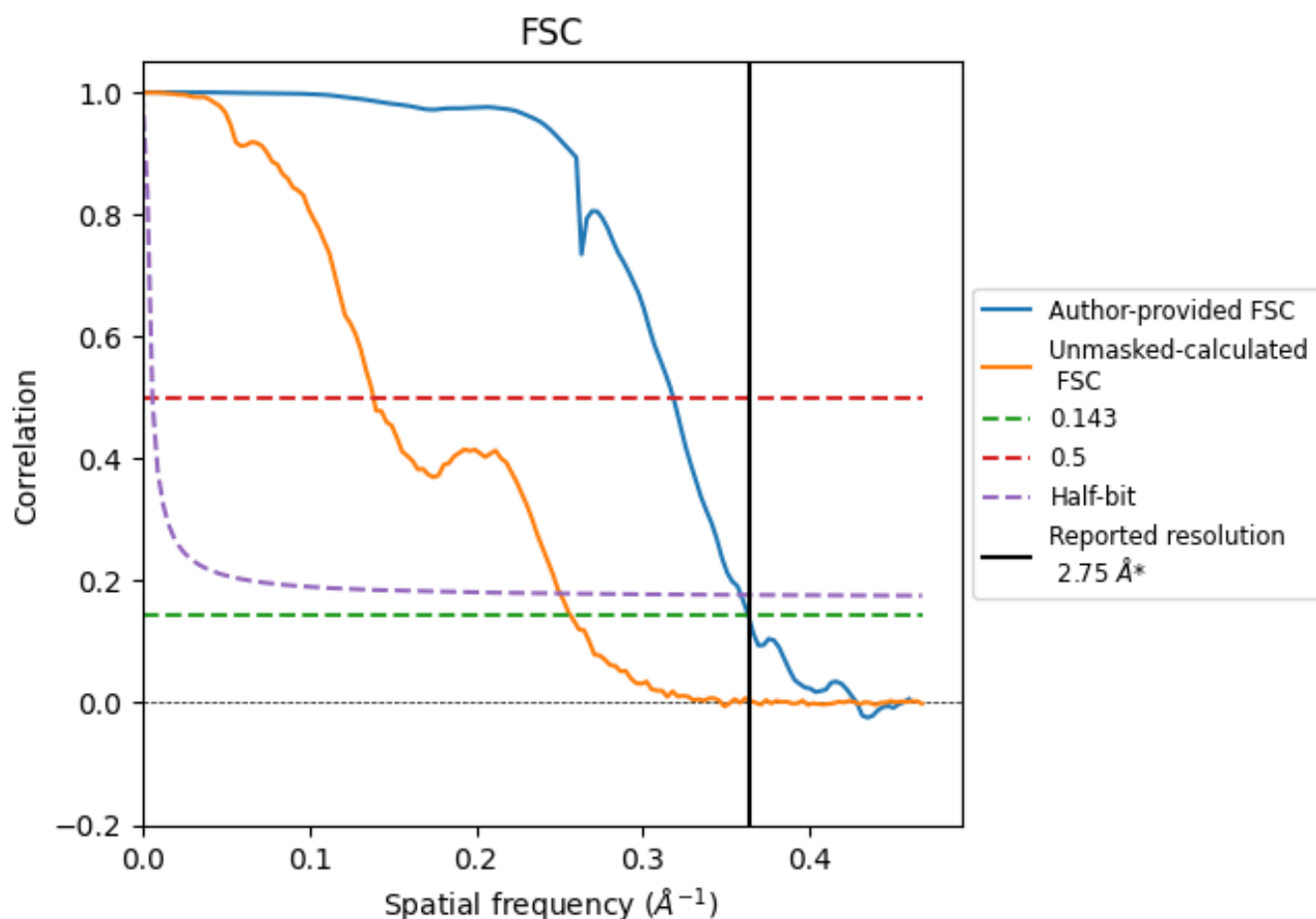
\*Reported resolution corresponds to spatial frequency of 0.364  $\text{\AA}^{-1}$



## 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 0.364 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

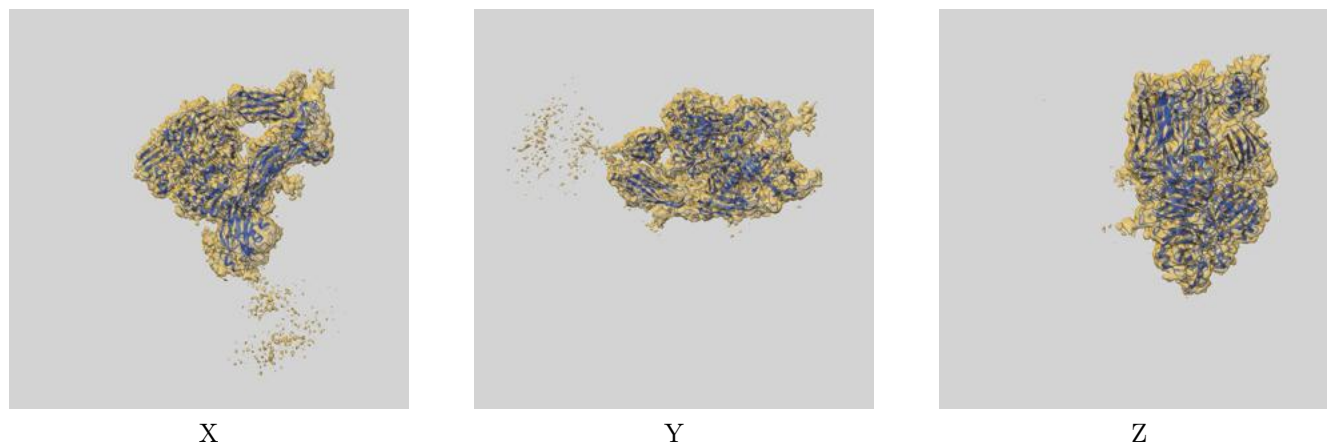
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.75	-	-
Author-provided FSC curve	2.75	3.14	2.79
Unmasked-calculated*	3.90	7.22	3.99

\*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 3.90 differs from the reported value 2.75 by more than 10 %

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

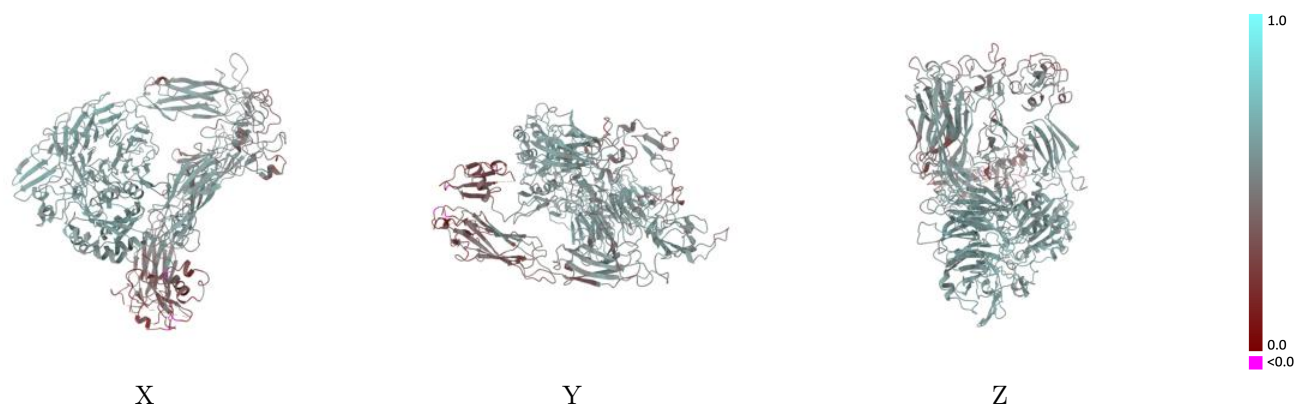
This section contains information regarding the fit between EMDB map EMD-47713 and PDB model 9E8A. Per-residue inclusion information can be found in section [3](#) on page [7](#).

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



The images above show the 3D surface view of the map at the recommended contour level 0.1 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](#)



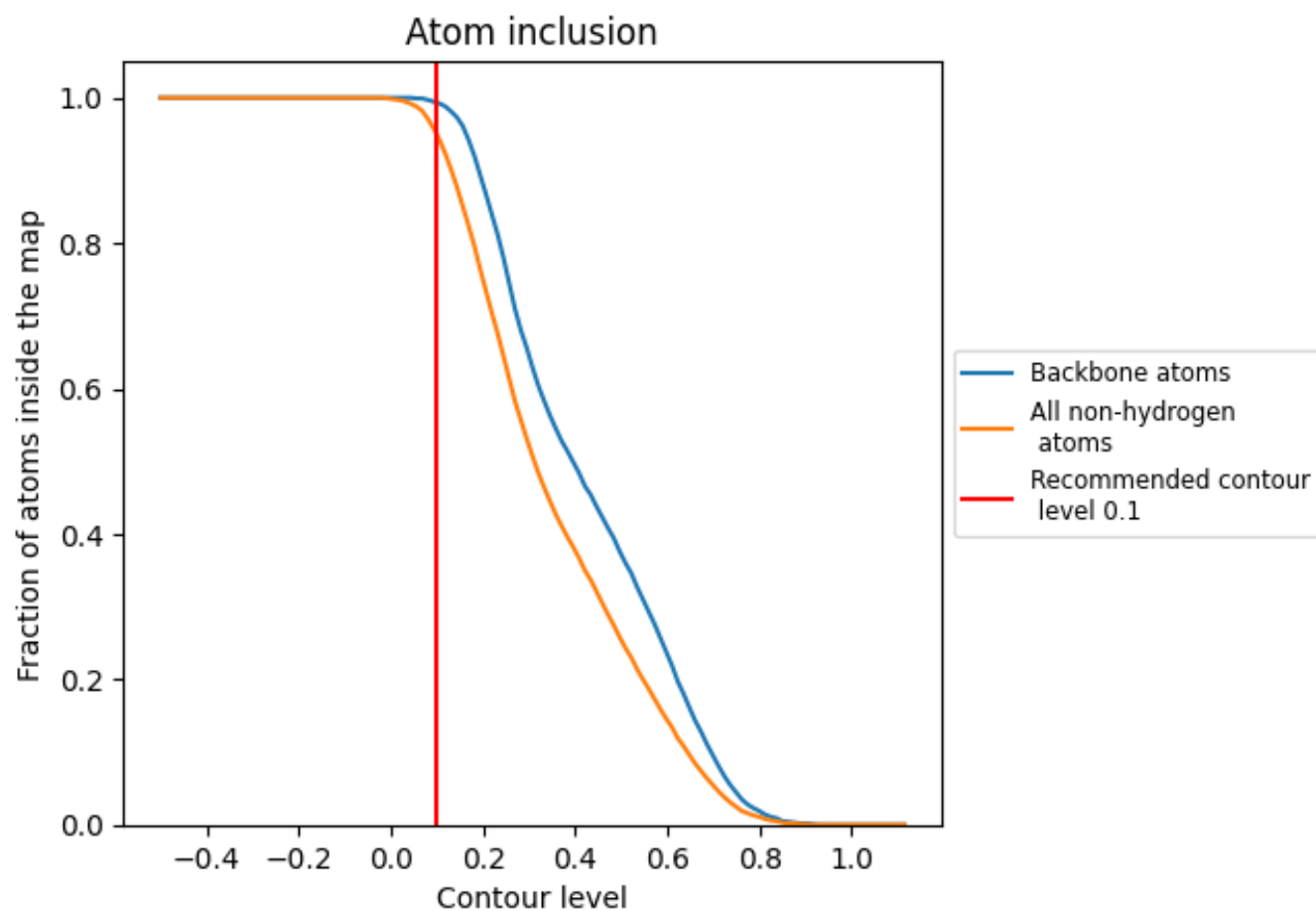
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 95% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9500	<div></div> 0.5070
A	<div></div> 0.9540	<div></div> 0.5140
B	<div></div> 0.9510	<div></div> 0.5050
C	<div></div> 0.9600	<div></div> 0.5120
D	<div></div> 0.7500	<div></div> 0.4480
E	<div></div> 0.8570	<div></div> 0.3860
F	<div></div> 0.7500	<div></div> 0.3480
G	<div></div> 0.6790	<div></div> 0.1300
H	<div></div> 0.9740	<div></div> 0.4980
I	<div></div> 0.8460	<div></div> 0.4060
J	<div></div> 0.7600	<div></div> 0.2570

