



Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 09:13 pm BST

PDB ID : 5NER
EMDB ID : EMD-3633
Title : Localised reconstruction of alpha v beta 6 bound to Foot and Mouth Disease Virus O PanAsia - Pose A prime.
Authors : Kotecha, A.; Stuart, D.
Deposited on : 2017-03-11
Resolution : 11.50 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
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

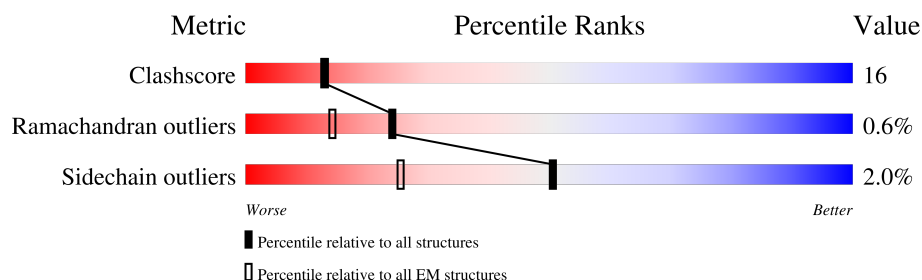
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY






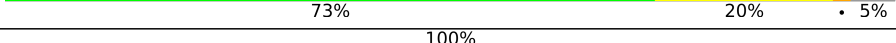
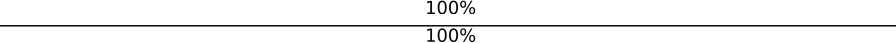

The reported resolution of this entry is 11.50 Å.

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



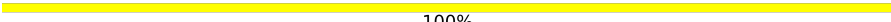


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	210	
2	2	214	
3	3	220	
4	4	70	
5	A	594	
6	B	470	
7	C	2	
8	D	3	

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Mol	Chain	Length	Quality of chain
9	E	2	 100%
10	F	4	 50%100%50%
11	G	4	 100%100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	NAG	F	1	-	-	X	-
10	MAN	F	4	X	-	-	-
11	NAG	G	1	-	-	X	-
11	NAG	G	2	-	-	X	-
11	MAN	G	3	-	-	X	-
13	NAG	B	501	X	-	-	-
9	MAN	E	2	X	-	-	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 13639 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called O PanAsia VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	210	Total	C	N	O	S	0	0
			1638	1033	295	306	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	155	VAL	ALA	conflict	UNP A0A1P8NWT0

- Molecule 2 is a protein called O PanAsia VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	214	Total	C	N	O	S	0	0
			1677	1065	286	319	7		

- Molecule 3 is a protein called O PanAsia VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	220	Total	C	N	O	S	0	0
			1686	1080	275	322	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	56	ARG	HIS	engineered mutation	UNP J3T9N5

- Molecule 4 is a protein called O PanAsia VP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	47	Total	C	N	O	S	0	1
			354	222	58	72	2		

- Molecule 5 is a protein called Integrin alpha-V.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	589	Total	C	N	O	S	0	0
			4564	2894	774	875	21		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	400	CYS	MET	conflict	UNP P06756

- Molecule 6 is a protein called Integrin beta-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	448	Total	C	N	O	S	0	0
			3438	2157	587	663	31		

There are 2 discrepancies between the modelled and reference sequences:

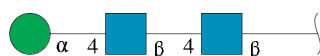
Chain	Residue	Modelled	Actual	Comment	Reference
B	267	CYS	ILE	conflict	UNP P18564
B	449	ASN	HIS	conflict	UNP P18564

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
7	C	2	Total	C	O	0	0
			22	12	10		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
8	D	3	Total	C	N	O	0	0
			40	22	2	16		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	2	Total	C	N	O	0	0
			25	14	1	10		

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



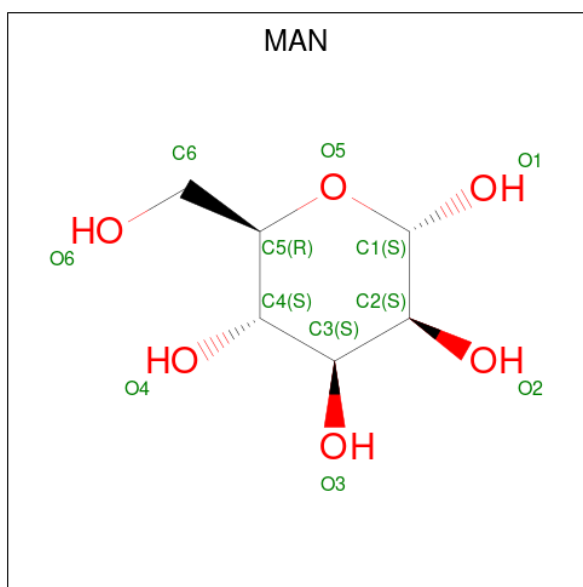
Mol	Chain	Residues	Atoms				AltConf	Trace
10	F	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
11	G	4	Total	C	N	O	0	0
			52	28	2	22		

- Molecule 12 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			AltConf
12	1	1	Total	C	O	0
			11	6	5	
12	1	1	Total	C	O	0
			11	6	5	
12	3	1	Total	C	O	0
			11	6	5	

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

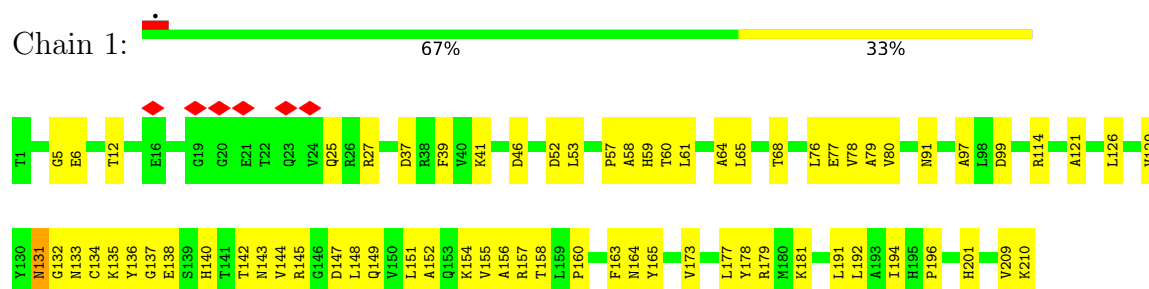
- Molecule 14 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
14	A	4	Total	Ca	0
			4	4	

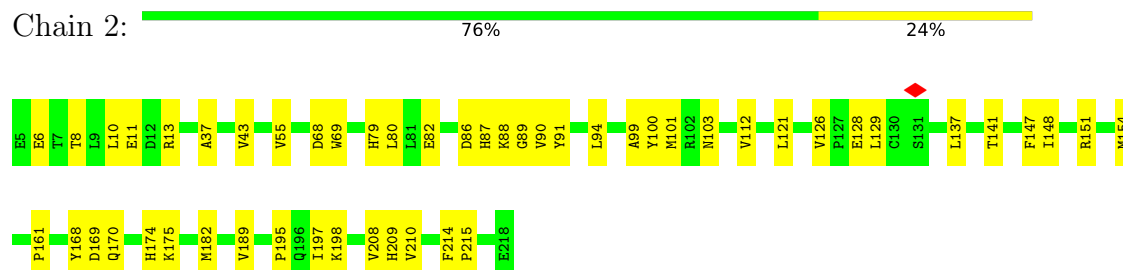
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

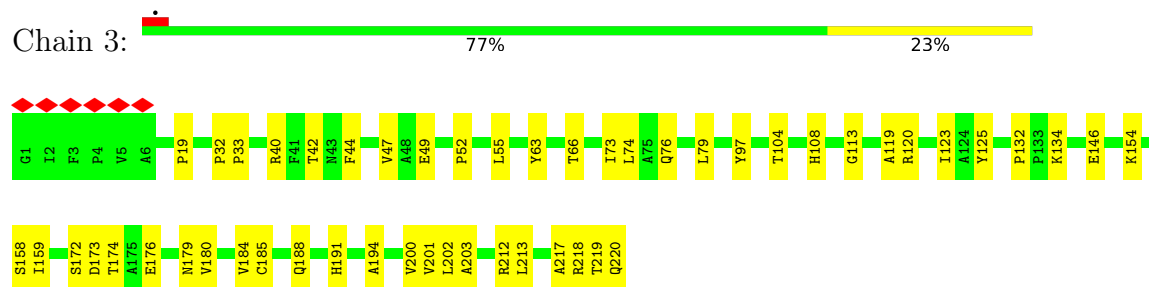
• Molecule 1: O PanAsia VP1



• Molecule 2: O PanAsia VP2



• Molecule 3: O PanAsia VP3



• Molecule 4: O PanAsia VP4







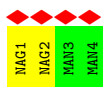
- Molecule 8: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13483	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	18	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	37037	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.038	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.005	Depositor
Map size (\AA)	172.8, 172.8, 172.8	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.35, 1.35, 1.35	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MAN, 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	1	0.48	0/1675	0.60	0/2289
2	2	0.53	0/1720	0.55	0/2348
3	3	0.53	0/1735	0.56	0/2370
4	4	0.42	0/360	0.58	0/483
5	A	0.23	0/4665	0.40	0/6312
6	B	0.22	0/3497	0.40	0/4729
All	All	0.37	0/13652	0.48	0/18531

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1638	0	1651	217	0
2	2	1677	0	1625	105	0
3	3	1686	0	1617	54	0
4	4	354	0	324	7	0
5	A	4564	0	4410	114	0
6	B	3438	0	3378	98	0
7	C	22	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	40	0	35	1	0
9	E	25	0	21	0	0
10	F	50	0	43	8	0
11	G	52	0	45	26	0
12	1	22	0	20	0	0
12	3	11	0	10	0	0
13	A	28	0	26	3	0
13	B	28	0	26	0	0
14	A	4	0	0	0	0
All	All	13639	0	13250	433	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 (433) 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)
2:2:99:ALA:HB2	2:2:214:PHE:CZ	1.27	1.61
1:1:134:CYS:SG	1:1:156:ALA:HB1	1.44	1.53
1:1:135:LYS:CD	2:2:80:LEU:HD23	1.08	1.52
1:1:135:LYS:HD3	2:2:80:LEU:CD2	1.01	1.46
5:A:585:ASN:ND2	11:G:1:NAG:C1	1.79	1.45
2:2:99:ALA:CB	2:2:214:PHE:CZ	1.97	1.42
5:A:585:ASN:CG	11:G:1:NAG:C1	1.87	1.40
1:1:142:THR:OG1	5:A:150:ASP:HB2	1.21	1.37
5:A:585:ASN:OD1	11:G:1:NAG:C1	1.69	1.36
1:1:145:ARG:N	5:A:178:TYR:CZ	1.81	1.34
1:1:135:LYS:NZ	2:2:80:LEU:HD21	1.37	1.34
1:1:138:GLU:OE1	2:2:79:HIS:ND1	1.59	1.34
1:1:151:LEU:HD22	6:B:123:ALA:CB	1.58	1.33
1:1:155:VAL:HG22	6:B:180:ILE:CD1	1.60	1.28
1:1:135:LYS:CD	2:2:80:LEU:CD2	1.76	1.28
1:1:142:THR:C	5:A:150:ASP:HB3	1.53	1.26
5:A:558:PHE:HE1	11:G:1:NAG:C8	1.47	1.26
2:2:99:ALA:HB2	2:2:214:PHE:CE1	1.71	1.25
1:1:135:LYS:N	2:2:82:GLU:OE2	1.70	1.23
6:B:110:ASP:CG	6:B:148:SER:HA	1.55	1.20
6:B:74:ARG:NH1	6:B:145:LYS:HA	1.57	1.19
1:1:135:LYS:HD2	2:2:80:LEU:HD23	1.26	1.18
5:A:585:ASN:HD21	11:G:1:NAG:C1	1.46	1.18
1:1:135:LYS:CE	2:2:80:LEU:CD2	2.24	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:145:ARG:HB3	5:A:178:TYR:CG	1.80	1.15
1:1:145:ARG:HB3	5:A:178:TYR:CD2	1.80	1.15
1:1:155:VAL:HG22	6:B:180:ILE:HD12	1.17	1.14
1:1:142:THR:O	5:A:178:TYR:HE2	1.29	1.13
1:1:142:THR:O	5:A:150:ASP:HB3	1.46	1.13
1:1:143:ASN:ND2	5:A:148:ASP:OD2	1.80	1.12
1:1:151:LEU:CD2	6:B:123:ALA:HB1	1.79	1.12
1:1:135:LYS:HD3	2:2:80:LEU:HD22	1.17	1.10
1:1:135:LYS:CE	2:2:80:LEU:HD21	1.81	1.10
11:G:1:NAG:H62	11:G:2:NAG:H82	1.33	1.10
1:1:134:CYS:SG	1:1:156:ALA:CB	2.38	1.10
6:B:74:ARG:CZ	6:B:145:LYS:HA	1.72	1.10
1:1:151:LEU:HB2	6:B:123:ALA:O	1.52	1.08
6:B:110:ASP:CG	6:B:148:SER:CA	2.14	1.07
1:1:142:THR:C	5:A:150:ASP:CB	2.21	1.07
1:1:135:LYS:NZ	2:2:129:LEU:CD2	2.18	1.07
2:2:99:ALA:CB	2:2:214:PHE:HZ	1.50	1.07
5:A:558:PHE:HE1	11:G:1:NAG:H81	1.09	1.06
5:A:558:PHE:CE1	11:G:1:NAG:C8	2.39	1.05
1:1:143:ASN:OD1	5:A:148:ASP:O	1.74	1.05
5:A:558:PHE:CE1	11:G:1:NAG:H81	1.91	1.05
1:1:135:LYS:NZ	2:2:129:LEU:HD21	1.72	1.05
1:1:142:THR:O	5:A:178:TYR:CE2	2.11	1.03
6:B:74:ARG:NH1	6:B:145:LYS:CA	2.21	1.02
6:B:74:ARG:CZ	6:B:145:LYS:CA	2.34	1.02
6:B:110:ASP:OD2	6:B:148:SER:HA	1.57	1.02
1:1:132:GLY:O	2:2:175:LYS:N	1.92	1.02
1:1:145:ARG:CD	5:A:218:ASP:OD2	2.08	1.01
1:1:137:GLY:H	2:2:80:LEU:CB	1.73	1.01
3:3:42:THR:HG1	4:4:65:ASN:N	1.58	1.00
1:1:135:LYS:NZ	2:2:80:LEU:CD2	2.21	0.99
1:1:142:THR:OG1	5:A:150:ASP:CB	2.10	0.99
1:1:145:ARG:HE	5:A:178:TYR:HB2	1.28	0.98
5:A:524:ASN:HD21	13:A:611:NAG:C1	1.75	0.98
1:1:135:LYS:HZ2	2:2:129:LEU:CD2	1.75	0.98
1:1:135:LYS:HE3	2:2:129:LEU:HG	1.47	0.97
1:1:145:ARG:CB	5:A:178:TYR:CE2	2.49	0.96
1:1:77:GLU:OE1	1:1:181:LYS:NZ	1.99	0.95
1:1:145:ARG:HE	5:A:178:TYR:CB	1.79	0.94
1:1:145:ARG:N	5:A:178:TYR:CE1	2.35	0.94
1:1:145:ARG:NE	5:A:218:ASP:OD2	2.00	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:145:ARG:NH2	5:A:177:PHE:C	2.22	0.93
1:1:135:LYS:HZ3	2:2:80:LEU:HD21	1.20	0.92
1:1:145:ARG:HB3	5:A:178:TYR:CD1	2.04	0.92
1:1:194:ILE:HD11	3:3:219:THR:OG1	1.69	0.92
1:1:145:ARG:NH2	5:A:177:PHE:O	2.02	0.92
1:1:136:TYR:O	2:2:80:LEU:O	1.88	0.91
1:1:145:ARG:HD2	5:A:218:ASP:OD2	1.70	0.91
1:1:145:ARG:CB	5:A:178:TYR:CD2	2.52	0.91
6:B:74:ARG:HH12	6:B:145:LYS:N	1.58	0.90
1:1:151:LEU:HD22	6:B:123:ALA:HB1	0.91	0.90
1:1:145:ARG:HB3	5:A:178:TYR:CE2	2.07	0.90
1:1:145:ARG:HH21	5:A:178:TYR:HB2	1.34	0.89
1:1:145:ARG:HH21	5:A:177:PHE:C	1.75	0.89
1:1:137:GLY:H	2:2:80:LEU:HB2	1.36	0.89
1:1:142:THR:HG1	5:A:150:ASP:HB2	1.06	0.89
1:1:129:VAL:HG11	2:2:128:GLU:O	1.72	0.88
1:1:77:GLU:OE2	1:1:114:ARG:NH2	2.06	0.87
1:1:145:ARG:NE	5:A:178:TYR:HB2	1.88	0.87
2:2:99:ALA:CA	2:2:214:PHE:CZ	2.58	0.86
1:1:155:VAL:CG2	6:B:180:ILE:HD12	2.04	0.86
2:2:99:ALA:HB1	2:2:214:PHE:HZ	1.37	0.86
1:1:132:GLY:O	2:2:174:HIS:HA	1.74	0.86
1:1:145:ARG:NH2	5:A:178:TYR:HB2	1.91	0.86
1:1:135:LYS:HZ1	2:2:129:LEU:HD21	1.40	0.86
5:A:585:ASN:ND2	11:G:1:NAG:O5	2.08	0.85
1:1:135:LYS:CE	2:2:129:LEU:HG	2.06	0.85
1:1:137:GLY:N	2:2:80:LEU:HB2	1.90	0.85
1:1:155:VAL:CG2	6:B:180:ILE:CD1	2.53	0.84
1:1:135:LYS:HZ2	2:2:80:LEU:HD21	1.41	0.84
1:1:145:ARG:CA	5:A:178:TYR:CZ	2.60	0.84
5:A:524:ASN:ND2	13:A:611:NAG:C1	2.41	0.83
6:B:74:ARG:NH1	6:B:145:LYS:N	2.18	0.83
1:1:137:GLY:CA	2:2:80:LEU:HB2	2.07	0.83
1:1:126:LEU:HD22	1:1:163:PHE:HB3	1.60	0.82
1:1:148:LEU:CD2	6:B:215:ASN:O	2.28	0.82
1:1:143:ASN:N	5:A:150:ASP:CB	2.40	0.82
1:1:91:ASN:CG	1:1:164:ASN:O	2.18	0.81
1:1:148:LEU:HG	6:B:215:ASN:O	1.81	0.80
1:1:135:LYS:HZ1	2:2:129:LEU:CD2	1.91	0.79
1:1:145:ARG:HB2	5:A:178:TYR:CE2	2.17	0.79
1:1:138:GLU:OE1	2:2:79:HIS:CG	2.36	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:74:ARG:NH2	6:B:146:LEU:N	2.30	0.79
1:1:148:LEU:CD1	6:B:216:ILE:HA	2.13	0.79
1:1:64:ALA:O	1:1:68:THR:HG23	1.82	0.79
6:B:111:TYR:HD1	6:B:352:ARG:HB2	1.48	0.78
1:1:145:ARG:CB	5:A:178:TYR:CZ	2.67	0.78
6:B:110:ASP:OD1	6:B:148:SER:N	2.18	0.77
1:1:145:ARG:O	5:A:178:TYR:CE1	2.37	0.77
1:1:132:GLY:HA2	2:2:174:HIS:HA	1.67	0.77
1:1:132:GLY:O	2:2:174:HIS:CA	2.33	0.77
1:1:134:CYS:CB	1:1:156:ALA:HB1	2.15	0.76
11:G:2:NAG:C3	11:G:3:MAN:H2	2.15	0.76
1:1:59:HIS:HA	3:3:220:GLN:HB2	1.65	0.76
1:1:145:ARG:CA	5:A:178:TYR:CE1	2.69	0.76
1:1:155:VAL:HG22	6:B:180:ILE:HD11	1.62	0.76
3:3:173:ASP:H	3:3:179:ASN:HD22	1.34	0.75
1:1:91:ASN:ND2	1:1:164:ASN:O	2.20	0.75
11:G:1:NAG:O3	11:G:2:NAG:O5	2.03	0.75
1:1:145:ARG:CZ	5:A:178:TYR:HB2	2.17	0.74
1:1:135:LYS:HZ1	2:2:129:LEU:CG	2.00	0.74
1:1:135:LYS:HZ2	2:2:129:LEU:HD23	1.51	0.74
2:2:99:ALA:HA	2:2:214:PHE:CE2	2.23	0.74
1:1:194:ILE:CD1	3:3:219:THR:OG1	2.36	0.73
10:F:1:NAG:H61	10:F:2:NAG:O7	1.89	0.73
1:1:58:ALA:O	3:3:220:GLN:HB2	1.89	0.73
6:B:110:ASP:OD1	6:B:148:SER:CA	2.36	0.73
6:B:147:THR:HG22	6:B:149:ASN:H	1.54	0.73
1:1:27:ARG:NH2	3:3:49:GLU:OE2	2.18	0.72
1:1:129:VAL:CG1	2:2:128:GLU:O	2.37	0.72
5:A:460:THR:HB	10:F:1:NAG:H62	1.71	0.72
5:A:558:PHE:HE1	11:G:1:NAG:H82	1.51	0.72
1:1:132:GLY:C	2:2:174:HIS:HA	2.09	0.72
2:2:11:GLU:OE2	2:2:13:ARG:NH2	2.22	0.72
1:1:58:ALA:HB1	3:3:220:GLN:OE1	1.89	0.72
1:1:137:GLY:N	2:2:80:LEU:CB	2.50	0.72
1:1:132:GLY:CA	2:2:174:HIS:HA	2.19	0.72
1:1:143:ASN:OD1	5:A:148:ASP:CB	2.38	0.71
1:1:148:LEU:CG	6:B:215:ASN:O	2.38	0.71
1:1:135:LYS:NZ	2:2:129:LEU:CG	2.53	0.71
6:B:74:ARG:NH2	6:B:145:LYS:C	2.43	0.71
11:G:1:NAG:H62	11:G:2:NAG:C8	2.17	0.71
3:3:174:THR:O	3:3:179:ASN:ND2	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:2:NAG:H3	11:G:3:MAN:H2	1.72	0.70
1:1:133:ASN:OD1	2:2:175:LYS:HG2	1.92	0.70
1:1:148:LEU:HG	6:B:216:ILE:HA	1.73	0.69
1:1:145:ARG:HB3	5:A:178:TYR:CE1	2.27	0.69
1:1:142:THR:CB	5:A:150:ASP:HB2	2.22	0.69
1:1:135:LYS:HZ2	2:2:80:LEU:CD2	1.99	0.69
2:2:86:ASP:OD2	2:2:88:LYS:NZ	2.25	0.69
1:1:151:LEU:CD2	6:B:123:ALA:CB	2.52	0.68
1:1:148:LEU:HD21	6:B:215:ASN:O	1.93	0.68
1:1:145:ARG:HB3	5:A:178:TYR:CZ	2.28	0.68
1:1:137:GLY:H	2:2:80:LEU:HB3	1.56	0.68
1:1:143:ASN:OD1	5:A:148:ASP:HB3	1.94	0.68
1:1:192:LEU:O	3:3:220:GLN:O	2.12	0.67
5:A:232:ASN:ND2	5:A:257:ASP:OD2	2.28	0.67
1:1:135:LYS:NZ	2:2:129:LEU:HG	2.09	0.67
1:1:137:GLY:HA3	2:2:80:LEU:HB2	1.77	0.66
1:1:57:PRO:HB2	1:1:60:THR:HG23	1.78	0.66
1:1:147:ASP:N	6:B:218:THR:HA	2.10	0.66
1:1:52:ASP:OD2	1:1:160:PRO:HB2	1.95	0.66
5:A:585:ASN:OD1	11:G:1:NAG:C2	2.44	0.65
2:2:55:VAL:HG11	2:2:94:LEU:HD21	1.78	0.65
2:2:101:MET:HG2	2:2:210:VAL:HG12	1.79	0.65
10:F:1:NAG:H61	10:F:2:NAG:C7	2.26	0.65
1:1:152:ALA:O	1:1:155:VAL:HG23	1.97	0.65
5:A:585:ASN:OD1	11:G:1:NAG:N2	2.29	0.65
1:1:132:GLY:O	2:2:174:HIS:C	2.35	0.65
1:1:145:ARG:C	5:A:178:TYR:CE1	2.71	0.65
6:B:417:PRO:HG2	6:B:420:LEU:HB2	1.77	0.65
2:2:99:ALA:CA	2:2:214:PHE:CE2	2.79	0.64
11:G:3:MAN:H3	11:G:4:MAN:O1	1.98	0.64
1:1:145:ARG:HH21	5:A:178:TYR:CB	2.09	0.64
6:B:158:VAL:HG21	6:B:213:SER:HB2	1.80	0.64
1:1:131:ASN:HD22	2:2:129:LEU:N	1.96	0.63
1:1:143:ASN:OD1	5:A:148:ASP:CG	2.37	0.63
1:1:64:ALA:CB	3:3:220:GLN:HG3	2.28	0.63
3:3:66:THR:OG1	3:3:194:ALA:O	2.12	0.63
6:B:363:THR:HB	6:B:366:LEU:HB2	1.79	0.63
3:3:108:HIS:HB2	3:3:202:LEU:HB2	1.81	0.63
1:1:148:LEU:CG	6:B:216:ILE:HA	2.28	0.63
1:1:136:TYR:N	1:1:137:GLY:HA2	2.13	0.63
1:1:77:GLU:HB3	1:1:179:ARG:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:147:ASP:HB2	6:B:218:THR:HA	1.82	0.62
1:1:64:ALA:HB1	3:3:220:GLN:HG3	1.82	0.61
3:3:52:PRO:HB2	3:3:202:LEU:HB3	1.82	0.61
1:1:135:LYS:O	2:2:82:GLU:CD	2.39	0.61
2:2:141:THR:OG1	3:3:52:PRO:O	2.14	0.61
5:A:558:PHE:CE1	11:G:1:NAG:H82	2.29	0.61
11:G:2:NAG:H5	11:G:3:MAN:O1	2.00	0.61
1:1:25:GLN:N	1:1:25:GLN:OE1	2.34	0.60
3:3:176:GLU:O	3:3:180:VAL:HG12	2.01	0.60
1:1:6:GLU:HB3	2:2:147:PHE:HB2	1.82	0.60
1:1:132:GLY:HA3	1:1:157:ARG:HG3	1.83	0.60
11:G:1:NAG:C6	11:G:2:NAG:H82	2.21	0.60
5:A:9:ALA:HB3	5:A:434:LEU:HB3	1.84	0.60
1:1:135:LYS:HZ2	2:2:129:LEU:HD21	1.45	0.60
2:2:214:PHE:HB3	2:2:215:PRO:HD2	1.82	0.60
1:1:78:VAL:O	1:1:114:ARG:HA	2.02	0.59
1:1:137:GLY:HA3	2:2:80:LEU:HD22	1.83	0.59
1:1:147:ASP:CB	6:B:218:THR:HA	2.32	0.59
2:2:69:TRP:HB3	2:2:197:ILE:HG23	1.83	0.59
3:3:76:GLN:HE21	3:3:132:PRO:HB2	1.68	0.59
1:1:135:LYS:CA	2:2:82:GLU:OE2	2.50	0.59
5:A:58:LYS:HB2	5:A:70:ILE:HD11	1.83	0.59
1:1:133:ASN:CG	2:2:175:LYS:HZ2	2.06	0.59
1:1:209:VAL:HG12	1:1:210:LYS:HG2	1.84	0.59
6:B:371:THR:HG22	6:B:381:GLN:HA	1.83	0.59
8:D:2:NAG:H3	8:D:3:MAN:O1	2.02	0.59
1:1:143:ASN:O	5:A:149:ALA:HB3	2.03	0.58
6:B:362:ASP:O	6:B:411:ARG:NH1	2.36	0.58
1:1:58:ALA:O	3:3:220:GLN:OE1	2.21	0.58
1:1:138:GLU:OE1	2:2:79:HIS:HA	2.03	0.58
5:A:544:ASP:HB3	5:A:547:GLU:HG3	1.86	0.58
6:B:111:TYR:HA	6:B:352:ARG:HG3	1.86	0.58
5:A:492:ASN:HA	5:A:526:THR:HA	1.85	0.58
1:1:145:ARG:HH21	5:A:178:TYR:N	2.02	0.58
1:1:194:ILE:CG1	3:3:219:THR:OG1	2.52	0.58
1:1:134:CYS:SG	1:1:157:ARG:N	2.77	0.57
1:1:37:ASP:HB3	4:4:17:ASN:HB2	1.85	0.57
1:1:143:ASN:CG	5:A:148:ASP:OD2	2.41	0.57
5:A:460:THR:CB	10:F:1:NAG:H62	2.34	0.57
1:1:78:VAL:HG12	1:1:80:VAL:HG23	1.85	0.57
2:2:99:ALA:HA	2:2:214:PHE:CZ	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:145:ARG:NE	5:A:178:TYR:CD2	2.72	0.56
11:G:2:NAG:O3	11:G:3:MAN:H2	2.03	0.56
1:1:148:LEU:HD11	6:B:216:ILE:HA	1.87	0.56
2:2:91:TYR:OH	2:2:103:ASN:ND2	2.38	0.56
6:B:91:LEU:HD22	6:B:93:LEU:HG	1.87	0.56
1:1:65:LEU:HD12	3:3:44:PHE:CZ	2.42	0.55
5:A:24:ASP:OD1	5:A:25:PHE:N	2.37	0.55
6:B:260:SER:HB2	6:B:265:ILE:HB	1.89	0.55
5:A:510:ARG:NH1	5:A:553:THR:O	2.36	0.55
6:B:84:ILE:HD12	6:B:417:PRO:HD3	1.87	0.55
1:1:148:LEU:HD12	6:B:216:ILE:HG23	1.88	0.55
1:1:145:ARG:CB	5:A:178:TYR:CE1	2.89	0.55
2:2:126:VAL:HG11	2:2:129:LEU:HD13	1.88	0.54
5:A:50:ILE:HD13	5:A:89:LYS:HB2	1.88	0.54
6:B:74:ARG:HH12	6:B:145:LYS:CA	2.01	0.54
2:2:68:ASP:OD1	2:2:198:LYS:HG2	2.07	0.54
5:A:558:PHE:CE1	11:G:1:NAG:C7	2.89	0.54
6:B:274:HIS:CD2	6:B:283:MET:HG3	2.43	0.54
1:1:145:ARG:HA	1:1:149:GLN:HB2	1.89	0.54
5:A:319:LEU:HB2	5:A:327:GLN:HB3	1.90	0.54
2:2:37:ALA:HB3	2:2:161:PRO:HG3	1.88	0.54
6:B:187:THR:OG1	6:B:214:ALA:O	2.23	0.54
1:1:151:LEU:CG	6:B:123:ALA:HB1	2.38	0.54
1:1:135:LYS:HZ1	2:2:129:LEU:HG	1.70	0.54
1:1:147:ASP:N	6:B:218:THR:CA	2.70	0.54
1:1:155:VAL:CG2	6:B:180:ILE:HD11	2.32	0.54
5:A:115:ARG:NH1	5:A:116:THR:O	2.40	0.54
1:1:143:ASN:OD1	5:A:148:ASP:C	2.45	0.53
1:1:145:ARG:O	5:A:178:TYR:HE1	1.88	0.53
3:3:79:LEU:HD22	3:3:125:TYR:HE1	1.74	0.53
6:B:18:LEU:HA	6:B:94:ARG:HH21	1.74	0.53
2:2:103:ASN:HB3	2:2:208:VAL:HG12	1.90	0.53
1:1:91:ASN:HD22	1:1:121:ALA:HA	1.75	0.52
1:1:133:ASN:CG	2:2:175:LYS:NZ	2.62	0.52
1:1:68:THR:HG21	1:1:191:LEU:HD22	1.91	0.52
1:1:79:ALA:HB3	1:1:177:LEU:HB2	1.92	0.52
1:1:196:PRO:HB3	1:1:201:HIS:HB2	1.92	0.52
1:1:53:LEU:HD11	1:1:76:LEU:HD13	1.92	0.52
6:B:61:GLN:HB3	6:B:92:LYS:HE2	1.92	0.51
6:B:151:ARG:NH2	6:B:237:GLY:O	2.43	0.51
5:A:144:SER:OG	5:A:145:GLN:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:65:LEU:HD12	3:3:44:PHE:CE1	2.46	0.51
6:B:219:PRO:HB3	6:B:253:ASP:HB2	1.93	0.51
1:1:145:ARG:HH22	5:A:177:PHE:C	2.13	0.51
2:2:128:GLU:OE1	2:2:174:HIS:HE1	1.94	0.50
3:3:218:ARG:HG2	3:3:219:THR:N	2.27	0.50
5:A:29:SER:O	5:A:32:SER:N	2.45	0.50
5:A:585:ASN:OD1	11:G:1:NAG:C7	2.58	0.50
2:2:10:LEU:H	2:2:10:LEU:HD23	1.77	0.50
2:2:151:ARG:HD2	3:3:113:GLY:O	2.11	0.49
1:1:147:ASP:H	6:B:218:THR:CA	2.25	0.49
1:1:61:LEU:HD12	1:1:65:LEU:HD23	1.93	0.49
1:1:12:THR:O	4:4:77:SER:HA	2.12	0.49
1:1:151:LEU:CB	6:B:123:ALA:O	2.43	0.49
1:1:147:ASP:H	6:B:218:THR:HA	1.76	0.49
5:A:148:ASP:O	5:A:150:ASP:N	2.46	0.49
6:B:191:LYS:HG2	6:B:280:GLU:HG2	1.93	0.49
6:B:273:CYS:O	6:B:274:HIS:ND1	2.46	0.49
1:1:6:GLU:CB	2:2:147:PHE:HB2	2.42	0.49
2:2:99:ALA:CB	2:2:214:PHE:CE1	2.63	0.48
1:1:135:LYS:HD3	2:2:80:LEU:HD23	0.64	0.48
5:A:1:PHE:HA	5:A:389:GLN:HB2	1.95	0.48
6:B:217:ASP:OD2	6:B:255:HIS:NE2	2.46	0.48
3:3:123:ILE:HD11	3:3:184:VAL:CG2	2.44	0.48
1:1:53:LEU:HD11	1:1:76:LEU:CD1	2.44	0.48
3:3:120:ARG:HD3	3:3:146:GLU:OE2	2.14	0.47
6:B:71:SER:HG	6:B:82:VAL:H	1.59	0.47
2:2:87:HIS:CE1	2:2:91:TYR:HB3	2.49	0.47
6:B:74:ARG:NH2	6:B:146:LEU:H	2.11	0.47
5:A:50:ILE:HD11	5:A:76:GLY:HA2	1.96	0.47
5:A:458:ASN:ND2	10:F:1:NAG:H82	2.28	0.47
6:B:362:ASP:HA	6:B:413:ILE:HG12	1.97	0.47
1:1:142:THR:CB	5:A:150:ASP:CB	2.88	0.47
3:3:76:GLN:HG3	3:3:185:CYS:SG	2.55	0.47
3:3:217:ALA:O	3:3:218:ARG:HB2	2.15	0.47
6:B:319:GLU:HG3	6:B:330:VAL:HG21	1.97	0.47
1:1:136:TYR:C	2:2:80:LEU:O	2.50	0.47
3:3:19:PRO:HB3	4:4:18:THR:HA	1.98	0.46
2:2:87:HIS:CE1	2:2:89:GLY:HA3	2.50	0.46
3:3:212:ARG:CZ	3:3:213:LEU:HD13	2.45	0.46
6:B:180:ILE:O	6:B:182:TYR:N	2.49	0.46
6:B:436:CYS:HB2	6:B:456:CYS:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:41:LYS:HA	1:1:177:LEU:HD23	1.96	0.46
1:1:145:ARG:N	5:A:178:TYR:CE2	2.69	0.46
6:B:353:SER:HB2	6:B:389:MET:H	1.80	0.46
1:1:59:HIS:HA	3:3:220:GLN:CB	2.41	0.46
3:3:63:TYR:HB3	3:3:200:VAL:HG12	1.98	0.46
1:1:138:GLU:H	2:2:80:LEU:H	1.63	0.46
3:3:79:LEU:CD1	3:3:159:ILE:HG21	2.46	0.46
4:4:22:ILE:HD12	4:4:22:ILE:O	2.16	0.46
1:1:77:GLU:OE1	1:1:181:LYS:CE	2.63	0.46
1:1:134:CYS:SG	1:1:156:ALA:CA	3.04	0.46
6:B:138:ARG:HB3	6:B:341:LEU:HD11	1.98	0.46
6:B:308:PHE:HB2	6:B:330:VAL:HG12	1.98	0.46
3:3:55:LEU:HD11	3:3:203:ALA:HB2	1.98	0.46
5:A:494:GLN:NE2	13:A:611:NAG:H3	2.31	0.46
6:B:84:ILE:HG13	6:B:105:VAL:HG22	1.98	0.46
3:3:40:ARG:HB3	4:4:66:ASP:HB2	1.98	0.45
5:A:116:THR:HG23	5:A:147:ILE:HG21	1.97	0.45
1:1:53:LEU:HD13	1:1:165:TYR:CE1	2.51	0.45
2:2:100:TYR:HE1	2:2:170:GLN:HE21	1.65	0.45
2:2:99:ALA:HA	2:2:214:PHE:HE2	1.80	0.45
11:G:3:MAN:H62	11:G:4:MAN:O5	2.17	0.45
1:1:5:GLY:HA2	3:3:154:LYS:HB2	1.97	0.45
2:2:189:VAL:HG11	2:2:195:PRO:HA	1.99	0.45
5:A:455:ASN:HA	5:A:593:LEU:HD11	1.97	0.45
6:B:448:HIS:O	6:B:451:ASN:ND2	2.35	0.45
3:3:79:LEU:HD22	3:3:125:TYR:CE1	2.51	0.45
10:F:1:NAG:HO3	10:F:2:NAG:C1	2.30	0.45
1:1:194:ILE:HG12	3:3:219:THR:OG1	2.16	0.45
2:2:90:VAL:O	2:2:94:LEU:HD13	2.17	0.45
6:B:363:THR:HG22	6:B:365:GLY:H	1.82	0.45
10:F:1:NAG:O3	10:F:2:NAG:C1	2.65	0.45
1:1:144:VAL:HG13	1:1:148:LEU:HB3	1.99	0.44
3:3:44:PHE:O	3:3:47:VAL:HG22	2.16	0.44
6:B:18:LEU:HD13	6:B:58:PRO:HG3	1.99	0.44
1:1:59:HIS:HA	3:3:220:GLN:H	1.82	0.44
1:1:65:LEU:O	1:1:68:THR:OG1	2.31	0.44
6:B:261:LYS:HG2	6:B:266:VAL:HG12	1.98	0.44
1:1:143:ASN:HD21	5:A:148:ASP:CG	2.10	0.44
5:A:253:VAL:HB	5:A:267:PHE:HB2	1.99	0.44
5:A:569:ALA:HB1	5:A:573:GLY:HA2	1.99	0.44
1:1:148:LEU:CD1	6:B:216:ILE:HG23	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:111:TYR:CD1	6:B:352:ARG:HB2	2.39	0.44
6:B:123:ALA:HB2	6:B:214:ALA:HB2	1.98	0.44
2:2:43:VAL:HG11	2:2:209:HIS:CD2	2.53	0.44
5:A:47:GLN:HA	5:A:48:PRO:HD3	1.90	0.44
5:A:242:GLY:HA2	5:A:253:VAL:HG22	1.99	0.44
3:3:104:THR:HG21	3:3:158:SER:HB3	2.00	0.44
5:A:554:PRO:HB3	5:A:591:HIS:CE1	2.52	0.44
1:1:138:GLU:OE1	2:2:79:HIS:CB	2.66	0.44
2:2:189:VAL:HG23	2:2:189:VAL:O	2.17	0.44
1:1:135:LYS:HA	1:1:140:HIS:HE1	1.83	0.43
1:1:144:VAL:HG11	1:1:152:ALA:HB2	2.00	0.43
5:A:569:ALA:HB2	5:A:575:GLN:HG2	2.00	0.43
6:B:94:ARG:HD2	6:B:95:PRO:HD2	2.00	0.43
1:1:136:TYR:H	1:1:137:GLY:HA2	1.82	0.43
5:A:373:VAL:HB	5:A:391:LEU:HB2	2.00	0.43
6:B:197:THR:OG1	6:B:198:ASN:N	2.51	0.43
3:3:172:SER:HA	3:3:179:ASN:HB2	2.01	0.43
1:1:142:THR:CA	5:A:150:ASP:CB	2.96	0.43
1:1:154:LYS:O	1:1:155:VAL:C	2.57	0.43
1:1:134:CYS:C	2:2:82:GLU:OE2	2.48	0.42
1:1:137:GLY:N	2:2:80:LEU:O	2.52	0.42
6:B:312:GLN:HA	6:B:315:VAL:HG23	2.01	0.42
3:3:218:ARG:HG2	3:3:219:THR:H	1.84	0.42
1:1:64:ALA:HB2	3:3:220:GLN:HG3	2.01	0.42
3:3:73:ILE:HD11	3:3:134:LYS:O	2.19	0.42
1:1:137:GLY:HA3	2:2:80:LEU:CB	2.48	0.42
3:3:123:ILE:HG23	3:3:123:ILE:O	2.19	0.42
6:B:71:SER:OG	6:B:82:VAL:N	2.41	0.42
2:2:103:ASN:CB	2:2:208:VAL:HG12	2.49	0.42
2:2:6:GLU:HG3	2:2:8:THR:H	1.84	0.42
5:A:364:TYR:HB3	5:A:369:LYS:HE2	2.02	0.42
3:3:74:LEU:HD11	3:3:188:GLN:HB2	2.00	0.42
5:A:449:VAL:HG21	5:A:557:ILE:HD13	2.01	0.42
2:2:6:GLU:HG2	2:2:10:LEU:HG	2.02	0.42
6:B:258:MET:SD	6:B:258:MET:N	2.93	0.42
3:3:219:THR:O	3:3:220:GLN:C	2.58	0.42
6:B:118:LEU:HD11	6:B:225:ALA:HB1	2.01	0.42
6:B:429:SER:HA	6:B:430:PRO:HD3	1.85	0.42
1:1:134:CYS:HG	1:1:156:ALA:HB1	1.64	0.41
6:B:244:HIS:HB2	6:B:304:VAL:HA	2.02	0.41
1:1:61:LEU:HD13	3:3:97:TYR:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:518:SER:HA	5:A:519:PRO:HD3	1.87	0.41
3:3:119:ALA:HA	3:3:191:HIS:HA	2.02	0.41
5:A:350:LEU:HA	5:A:420:PRO:HG2	2.02	0.41
1:1:157:ARG:HD2	1:1:157:ARG:HA	1.85	0.41
6:B:151:ARG:NH2	6:B:239:ARG:HG2	2.35	0.41
2:2:169:ASP:OD1	2:2:170:GLN:N	2.52	0.41
5:A:149:ALA:H	5:A:154:PHE:HD1	1.67	0.41
6:B:223:PHE:HB3	6:B:290:PRO:HG2	2.01	0.41
1:1:39:PHE:HA	1:1:178:TYR:O	2.21	0.41
1:1:131:ASN:ND2	2:2:129:LEU:N	2.66	0.41
1:1:97:ALA:C	1:1:99:ASP:H	2.24	0.41
1:1:132:GLY:CA	1:1:157:ARG:HG3	2.48	0.41
4:4:66:ASP:O	4:4:70:LYS:HE2	2.21	0.41
6:B:435:ASP:HA	6:B:438:LYS:NZ	2.36	0.41
5:A:436:ARG:HH12	5:A:572:THR:HG1	1.62	0.41
5:A:463:LEU:HD21	5:A:517:ARG:HE	1.86	0.41
6:B:171:GLU:CD	6:B:171:GLU:H	2.25	0.41
11:G:1:NAG:HO3	11:G:2:NAG:C1	2.25	0.41
3:3:55:LEU:HB2	3:3:201:VAL:HG13	2.03	0.41
5:A:164:THR:HB	5:A:237:ASP:HB2	2.03	0.41
5:A:458:ASN:ND2	10:F:1:NAG:C7	2.84	0.41
1:1:135:LYS:CE	2:2:129:LEU:CG	2.88	0.40
5:A:196:ASP:HB3	5:A:199:VAL:HB	2.03	0.40
5:A:575:GLN:HA	5:A:576:PRO:HD3	1.91	0.40
1:1:46:ASP:O	1:1:173:VAL:HG12	2.20	0.40
1:1:147:ASP:N	6:B:218:THR:CB	2.82	0.40
2:2:121:LEU:HB2	2:2:148:ILE:HB	2.04	0.40
3:3:32:PRO:HA	3:3:33:PRO:HD3	1.96	0.40
5:A:371:GLY:HA3	5:A:404:PHE:HB3	2.02	0.40
6:B:51:GLN:O	6:B:55:ILE:HG13	2.21	0.40
6:B:71:SER:HB2	6:B:75:GLN:NE2	2.36	0.40
1:1:147:ASP:CA	6:B:218:THR:HA	2.51	0.40
2:2:100:TYR:HB3	2:2:168:TYR:HB3	2.04	0.40
2:2:137:LEU:HB3	2:2:182:MET:SD	2.61	0.40
6:B:15:GLU:HG3	6:B:432:CYS:O	2.21	0.40
6:B:152:LEU:O	6:B:196:LEU:HA	2.21	0.40
2:2:112:VAL:HG12	2:2:154:MET:SD	2.62	0.40
3:3:74:LEU:CD1	3:3:188:GLN:HB2	2.52	0.40
1:1:134:CYS:CB	1:1:156:ALA:CB	2.93	0.40
5:A:156:GLN:OE1	6:B:164:PRO:HG3	2.22	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	1	208/210 (99%)	192 (92%)	15 (7%)	1 (0%)	25	64
2	2	212/214 (99%)	199 (94%)	13 (6%)	0	100	100
3	3	218/220 (99%)	203 (93%)	15 (7%)	0	100	100
4	4	43/70 (61%)	39 (91%)	4 (9%)	0	100	100
5	A	581/594 (98%)	550 (95%)	27 (5%)	4 (1%)	19	57
6	B	434/470 (92%)	397 (92%)	32 (7%)	5 (1%)	11	44
All	All	1696/1778 (95%)	1580 (93%)	106 (6%)	10 (1%)	24	60

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	B	375	ASN
5	A	149	ALA
5	A	571	THR
5	A	28	PRO
6	B	9	GLY
1	1	158	THR
5	A	516	SER
6	B	124	SER
6	B	181	PRO
6	B	391	VAL

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	1	177/177 (100%)	176 (99%)	1 (1%)	84	88
2	2	186/188 (99%)	186 (100%)	0	100	100
3	3	176/176 (100%)	176 (100%)	0	100	100
4	4	37/57 (65%)	37 (100%)	0	100	100
5	A	483/487 (99%)	472 (98%)	11 (2%)	45	64
6	B	394/410 (96%)	377 (96%)	17 (4%)	25	46
All	All	1453/1495 (97%)	1424 (98%)	29 (2%)	50	68

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	131	ASN
5	A	116	THR
5	A	119	LYS
5	A	145	GLN
5	A	147	ILE
5	A	183	LEU
5	A	275	TYR
5	A	368	ASP
5	A	494	GLN
5	A	512	LEU
5	A	538	LEU
5	A	593	LEU
6	B	61	GLN
6	B	72	VAL
6	B	77	ASN
6	B	91	LEU
6	B	131	THR
6	B	145	LYS
6	B	163	SER
6	B	196	LEU
6	B	209	ASN
6	B	215	ASN
6	B	246	LEU
6	B	261	LYS
6	B	319	GLU
6	B	341	LEU
6	B	408	ARG
6	B	416	LYS
6	B	430	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	131	ASN
3	3	76	GLN
5	A	524	ASN
6	B	215	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 ⓘ

15 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	$\# Z > 2$
7	MAN	C	1	7	11,11,12	0.55	0	15,15,17	2.03	6 (40%)
7	MAN	C	2	7	11,11,12	0.63	0	15,15,17	2.02	6 (40%)
8	NAG	D	1	8	14,14,15	0.49	0	17,19,21	0.63	0
8	NAG	D	2	8	14,14,15	0.49	0	17,19,21	0.73	0
8	MAN	D	3	8	12,12,12	0.43	0	17,17,17	0.53	0
9	NAG	E	1	9	14,14,15	0.52	0	17,19,21	1.39	3 (17%)
9	MAN	E	2	9	11,11,12	0.66	0	15,15,17	1.46	3 (20%)
10	NAG	F	1	5,10	14,14,15	0.26	0	17,19,21	0.60	0
10	NAG	F	2	10	14,14,15	0.26	0	17,19,21	0.60	0
10	MAN	F	3	10	11,11,12	0.25	0	15,15,17	0.58	0
10	MAN	F	4	10	11,11,12	0.24	0	15,15,17	0.55	0
11	NAG	G	1	11	14,14,15	0.28	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	NAG	G	2	11	14,14,15	0.34	0	17,19,21	0.66	0
11	MAN	G	3	11	12,12,12	0.48	0	17,17,17	0.62	0
11	MAN	G	4	11	12,12,12	0.44	0	17,17,17	0.55	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
7	MAN	C	1	7	-	0/2/19/22	0/1/1/1
7	MAN	C	2	7	-	0/2/19/22	0/1/1/1
8	NAG	D	1	8	-	2/6/23/26	0/1/1/1
8	NAG	D	2	8	-	0/6/23/26	0/1/1/1
8	MAN	D	3	8	-	0/2/22/22	0/1/1/1
9	NAG	E	1	9	-	0/6/23/26	0/1/1/1
9	MAN	E	2	9	1/1/4/5	2/2/19/22	0/1/1/1
10	NAG	F	1	5,10	-	2/6/23/26	0/1/1/1
10	NAG	F	2	10	-	0/6/23/26	0/1/1/1
10	MAN	F	3	10	-	0/2/19/22	0/1/1/1
10	MAN	F	4	10	1/1/4/5	1/2/19/22	0/1/1/1
11	NAG	G	1	11	-	0/6/23/26	0/1/1/1
11	NAG	G	2	11	-	3/6/23/26	0/1/1/1
11	MAN	G	3	11	-	0/2/22/22	0/1/1/1
11	MAN	G	4	11	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1	MAN	O4-C4-C3	-3.98	101.16	110.35
9	E	1	NAG	O5-C5-C6	-3.56	101.62	107.20
7	C	2	MAN	O4-C4-C3	-3.45	102.38	110.35
7	C	2	MAN	C2-C3-C4	3.23	116.49	110.89
7	C	1	MAN	O4-C4-C5	3.17	117.16	109.30
9	E	2	MAN	O2-C2-C3	2.95	116.04	110.14
7	C	2	MAN	O5-C5-C6	-2.94	102.60	107.20
7	C	1	MAN	O5-C5-C6	-2.87	102.70	107.20
9	E	2	MAN	O4-C4-C5	-2.64	102.74	109.30
7	C	2	MAN	O5-C1-C2	2.57	114.73	110.77
7	C	2	MAN	O3-C3-C2	2.47	114.72	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	2	MAN	C6-C5-C4	-2.38	107.42	113.00
9	E	1	NAG	O5-C1-C2	-2.36	107.56	111.29
7	C	2	MAN	C1-O5-C5	2.29	115.29	112.19
7	C	1	MAN	O3-C3-C2	-2.26	105.66	109.99
7	C	1	MAN	C1-O5-C5	2.17	115.14	112.19
9	E	1	NAG	C4-C3-C2	-2.17	107.84	111.02
7	C	1	MAN	O5-C1-C2	2.03	113.90	110.77

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	E	2	MAN	C1
10	F	4	MAN	C1

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	F	1	NAG	C8-C7-N2-C2
10	F	1	NAG	O7-C7-N2-C2
11	G	2	NAG	C8-C7-N2-C2
11	G	2	NAG	O7-C7-N2-C2
8	D	1	NAG	C8-C7-N2-C2
8	D	1	NAG	O7-C7-N2-C2
10	F	4	MAN	O5-C5-C6-O6
11	G	2	NAG	O5-C5-C6-O6
9	E	2	MAN	C4-C5-C6-O6
9	E	2	MAN	O5-C5-C6-O6

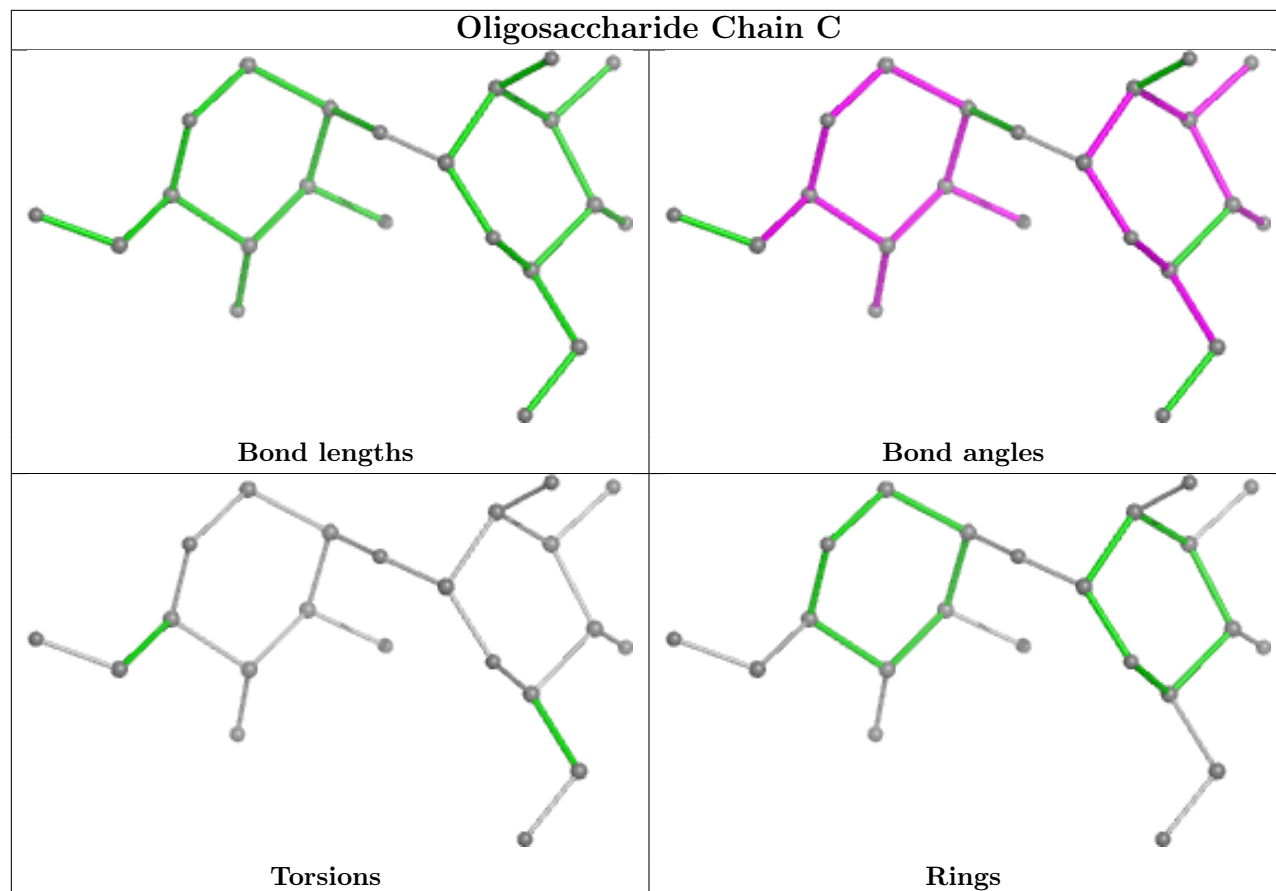
There are no ring outliers.

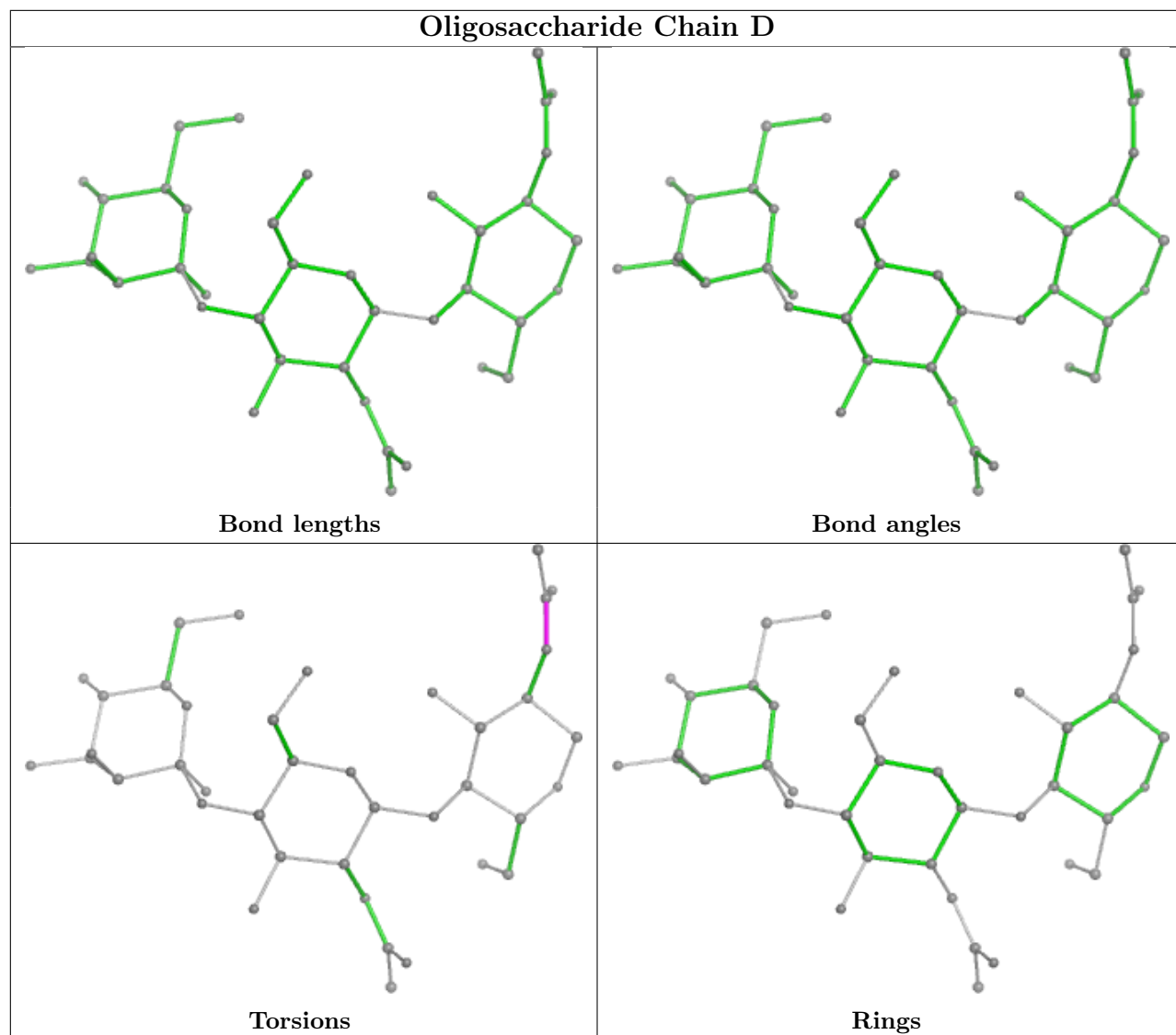
8 monomers are involved in 35 short contacts:

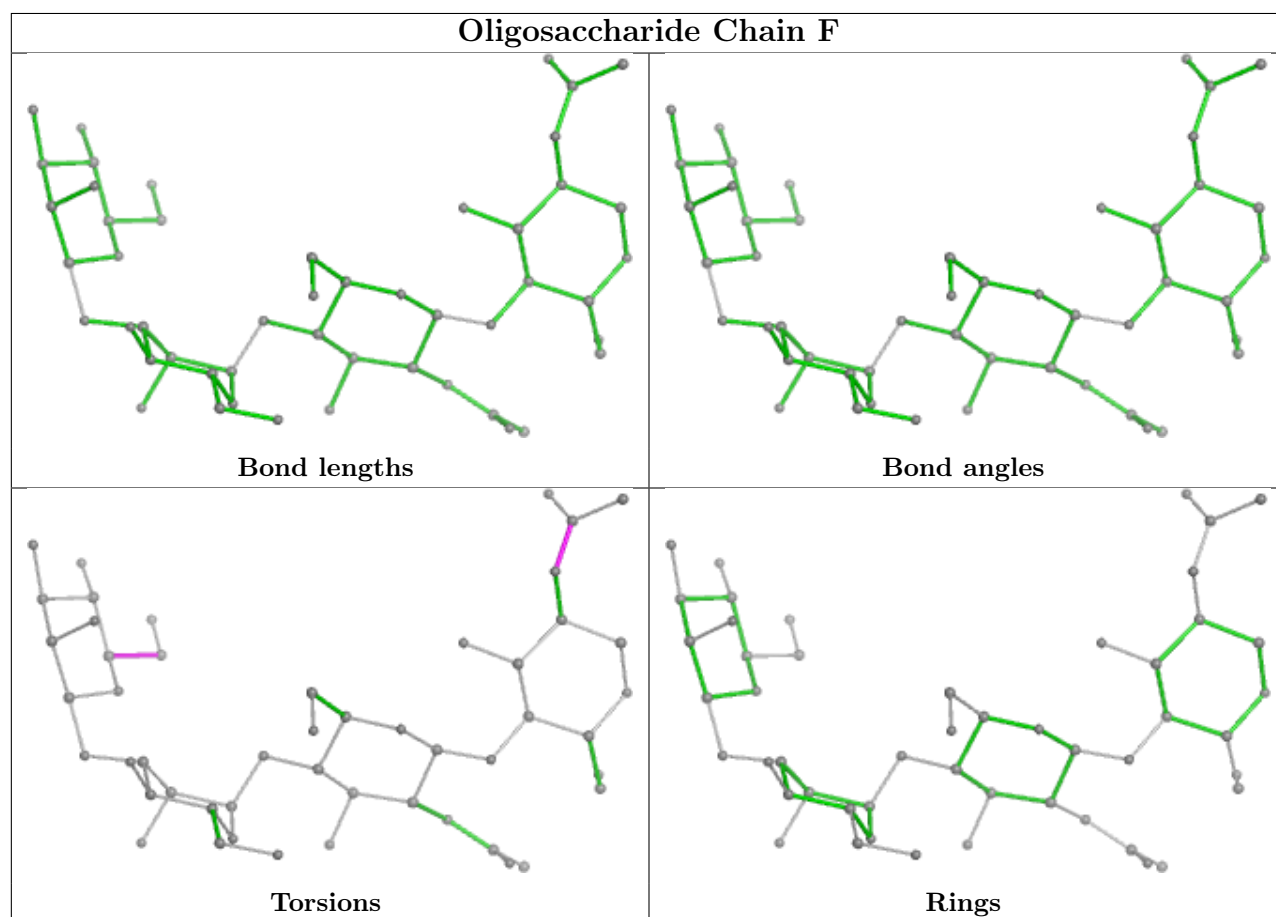
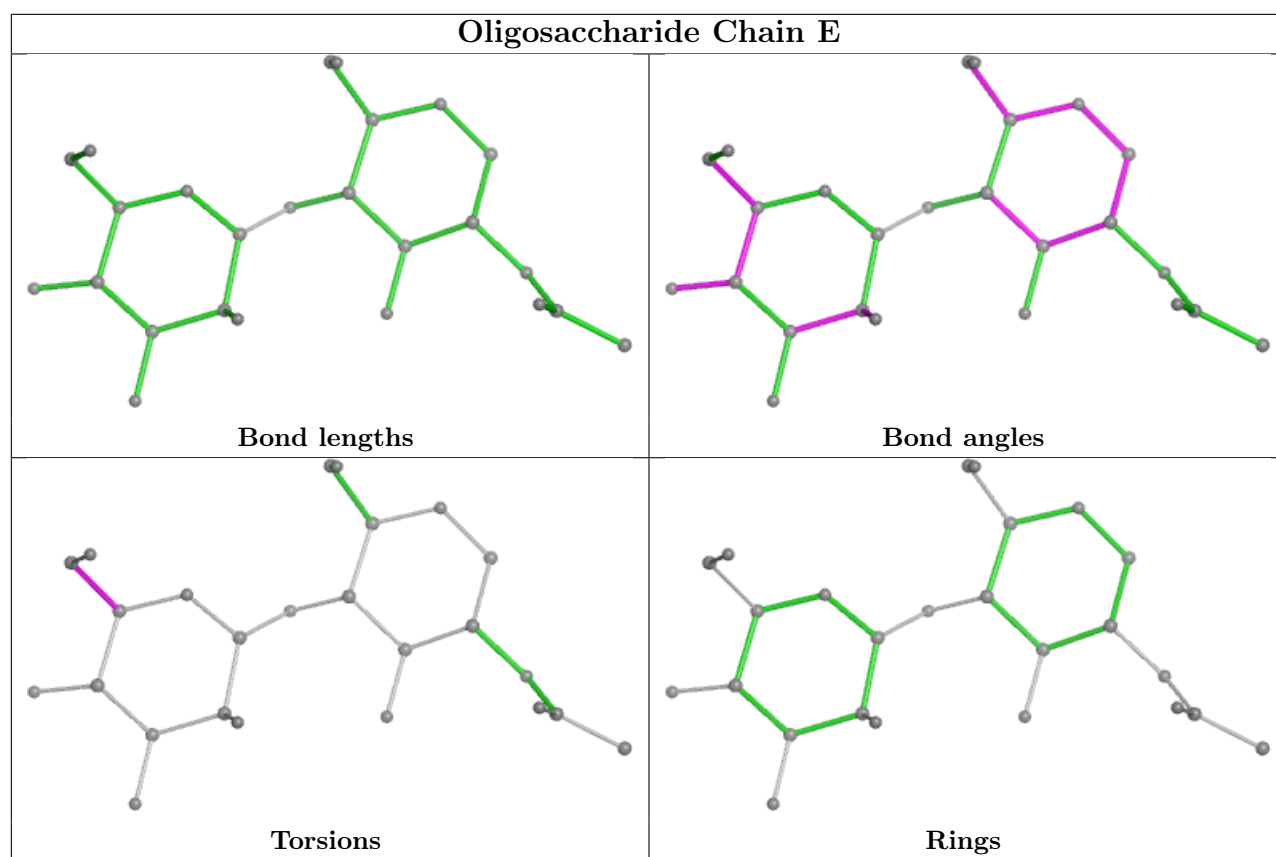
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	F	2	NAG	4	0
11	G	2	NAG	9	0
8	D	3	MAN	1	0
11	G	4	MAN	2	0
11	G	3	MAN	6	0
10	F	1	NAG	8	0
8	D	2	NAG	1	0
11	G	1	NAG	20	0

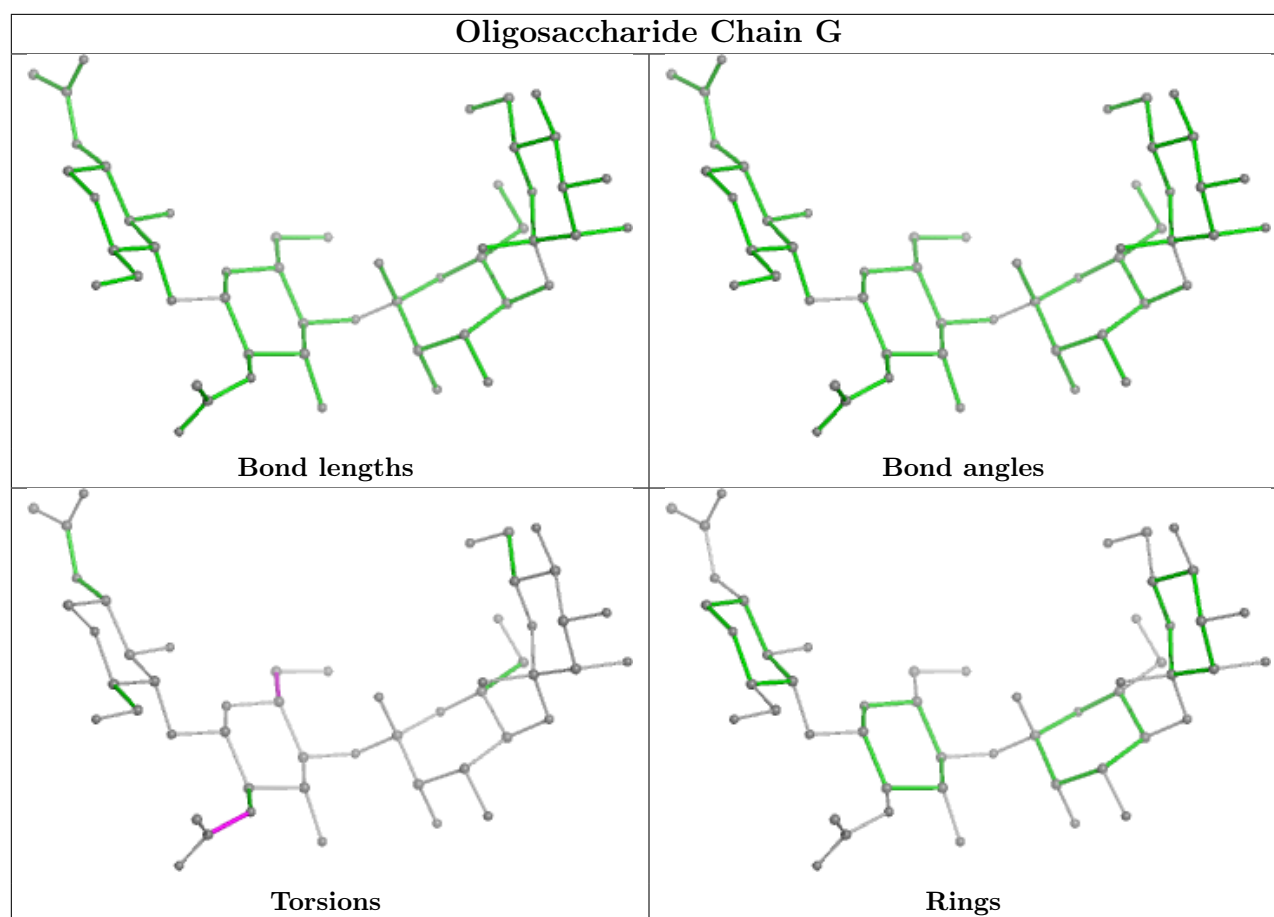
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	$\# Z > 2$
13	NAG	B	501	6	14,14,15	0.55	0	17,19,21	0.61	0
13	NAG	A	604	-	14,14,15	0.48	0	17,19,21	2.23	3 (17%)
13	NAG	A	611	-	14,14,15	0.28	0	17,19,21	0.59	0
12	MAN	1	302	-	11,11,12	0.64	0	15,15,17	2.42	7 (46%)
13	NAG	B	502	-	14,14,15	0.48	0	17,19,21	0.68	0
12	MAN	1	301	-	11,11,12	0.59	0	15,15,17	2.41	7 (46%)
12	MAN	3	301	-	11,11,12	0.62	0	15,15,17	2.52	4 (26%)

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
13	NAG	B	501	6	1/1/5/7	2/6/23/26	0/1/1/1
13	NAG	A	604	-	-	1/6/23/26	0/1/1/1
13	NAG	A	611	-	-	1/6/23/26	0/1/1/1
12	MAN	1	302	-	-	0/2/19/22	0/1/1/1
13	NAG	B	502	-	-	2/6/23/26	0/1/1/1
12	MAN	1	301	-	-	0/2/19/22	0/1/1/1
12	MAN	3	301	-	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	604	NAG	O5-C1-C2	-7.37	99.65	111.29
12	3	301	MAN	C1-C2-C3	6.93	118.19	109.67
12	1	302	MAN	C1-O5-C5	5.83	120.09	112.19
12	1	301	MAN	C6-C5-C4	-5.09	101.09	113.00
12	3	301	MAN	C2-C3-C4	-4.04	103.90	110.89
12	1	301	MAN	O4-C4-C3	-3.51	102.25	110.35
12	3	301	MAN	O5-C1-C2	-3.46	105.42	110.77
12	1	301	MAN	O5-C5-C6	3.43	112.58	107.20
12	1	302	MAN	C3-C4-C5	3.38	116.27	110.24
12	1	301	MAN	C3-C4-C5	-3.12	104.68	110.24
12	1	302	MAN	O2-C2-C1	2.96	115.21	109.15
12	1	301	MAN	O2-C2-C3	-2.87	104.39	110.14
12	1	302	MAN	O4-C4-C5	2.82	116.30	109.30
13	A	604	NAG	O7-C7-C8	-2.69	117.07	122.06
13	A	604	NAG	C4-C3-C2	-2.68	107.09	111.02
12	1	302	MAN	O5-C5-C6	-2.55	103.21	107.20
12	1	301	MAN	O2-C2-C1	2.39	114.05	109.15
12	1	302	MAN	C1-C2-C3	-2.19	106.97	109.67
12	1	301	MAN	C2-C3-C4	2.13	114.58	110.89
12	3	301	MAN	O5-C5-C6	-2.08	103.94	107.20
12	1	302	MAN	O4-C4-C3	-2.04	105.64	110.35

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	B	501	NAG	C1

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	B	502	NAG	C8-C7-N2-C2
13	B	502	NAG	O7-C7-N2-C2
13	B	501	NAG	O5-C5-C6-O6
13	B	501	NAG	C4-C5-C6-O6
13	A	611	NAG	C8-C7-N2-C2
13	A	604	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	611	NAG	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	351:LEU	C	352:ARG	N	15.18
1	B	110:ASP	C	111:TYR	N	8.73

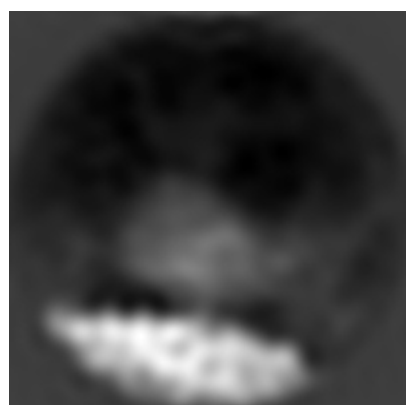
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3633. These allow visual inspection of the internal detail of the map and identification of artifacts.

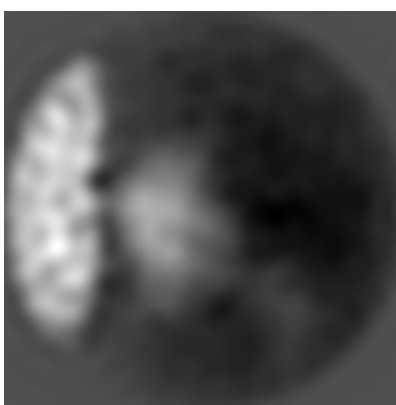
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

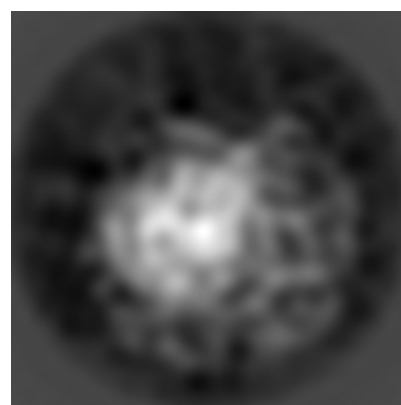
6.1.1 Primary map



X



Y

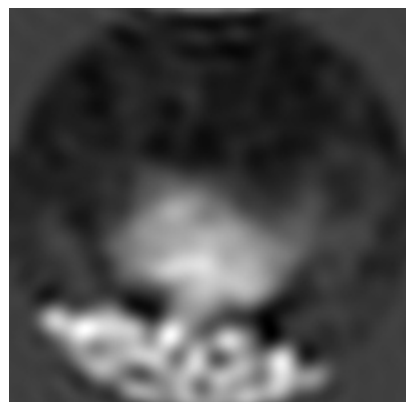


Z

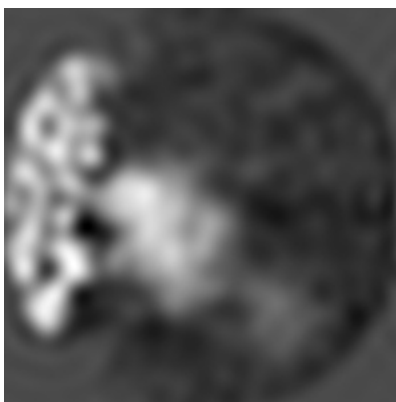
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

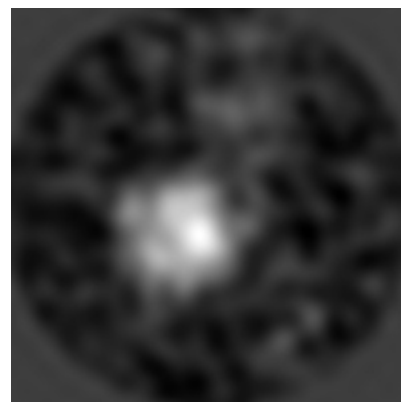
6.2.1 Primary map



X Index: 64



Y Index: 64

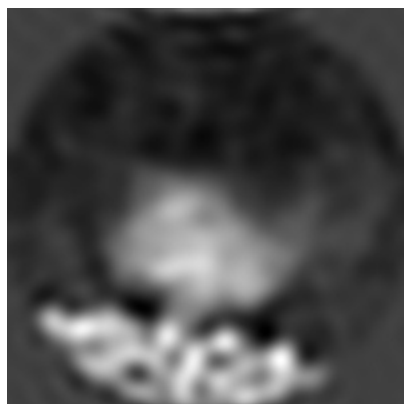


Z Index: 64

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

6.3 Largest variance slices [i](#)

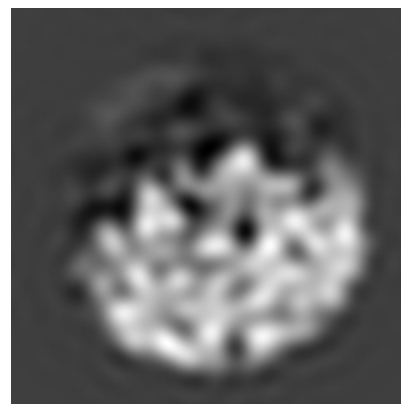
6.3.1 Primary map



X Index: 62



Y Index: 59

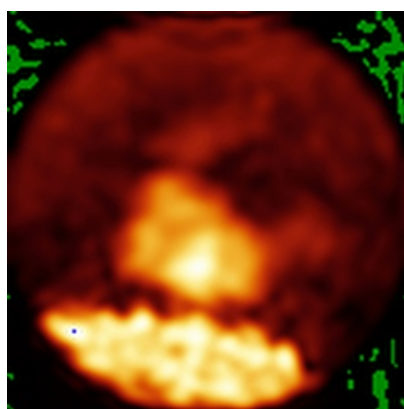


Z Index: 24

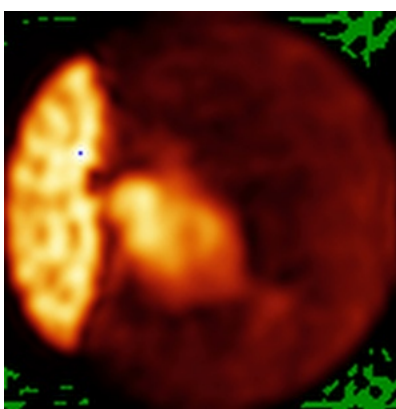
The images above show the largest variance slices of the map in three orthogonal directions.

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

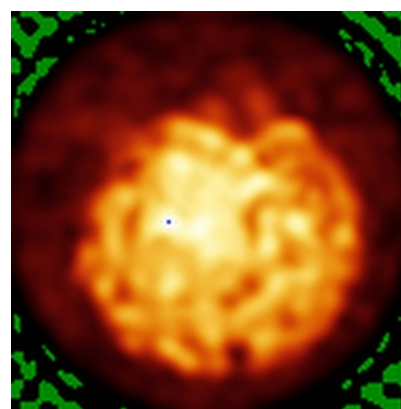
6.4.1 Primary map



X



Y

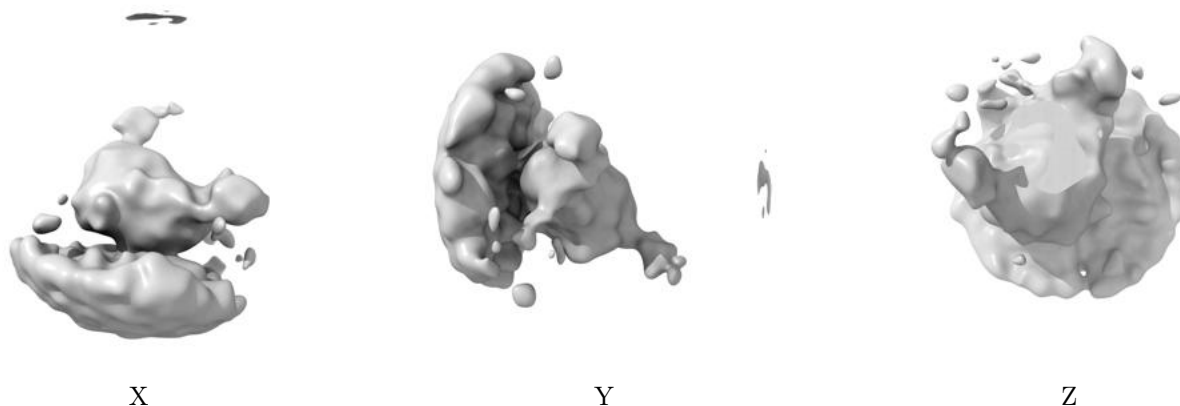


Z

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 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

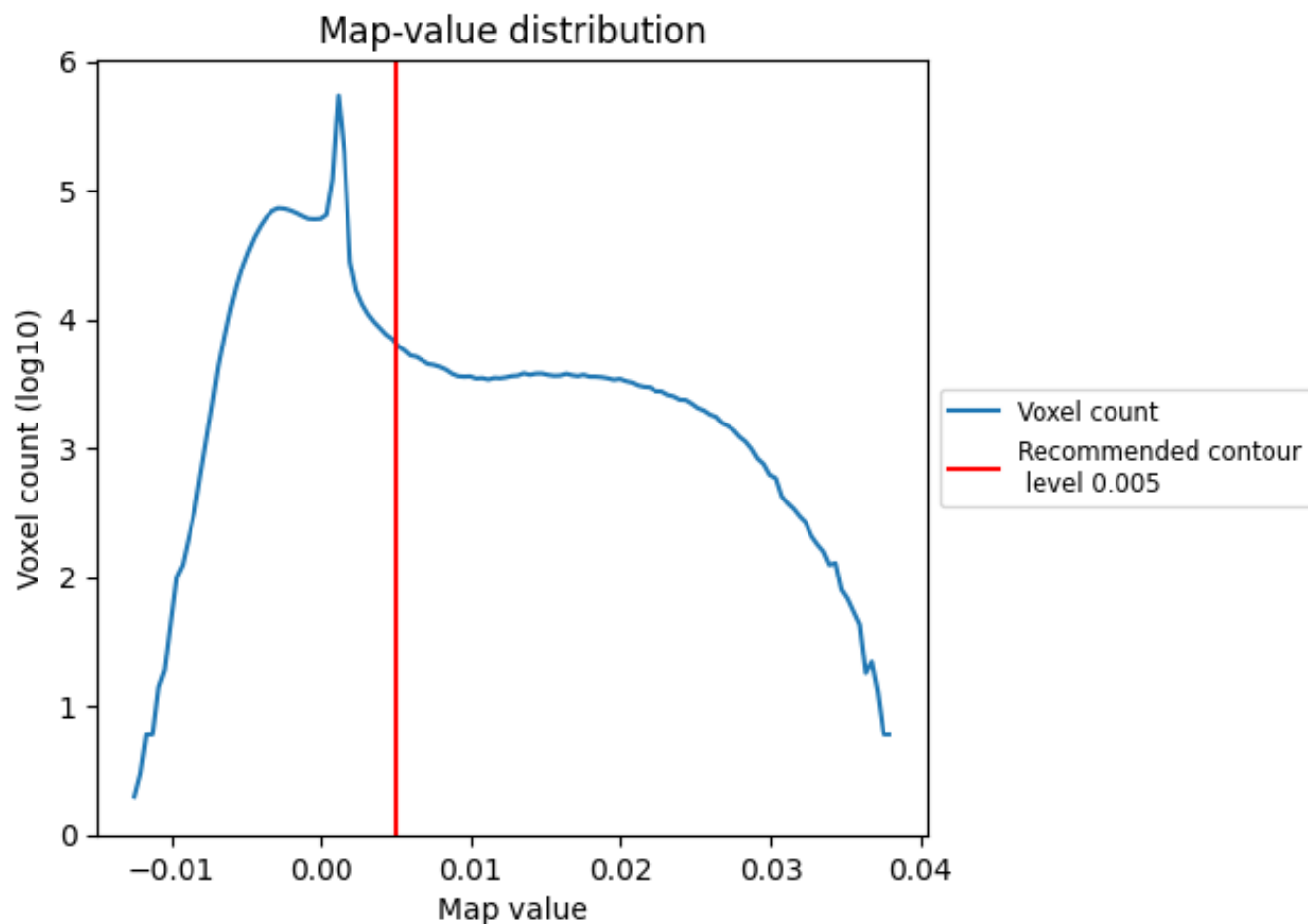
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

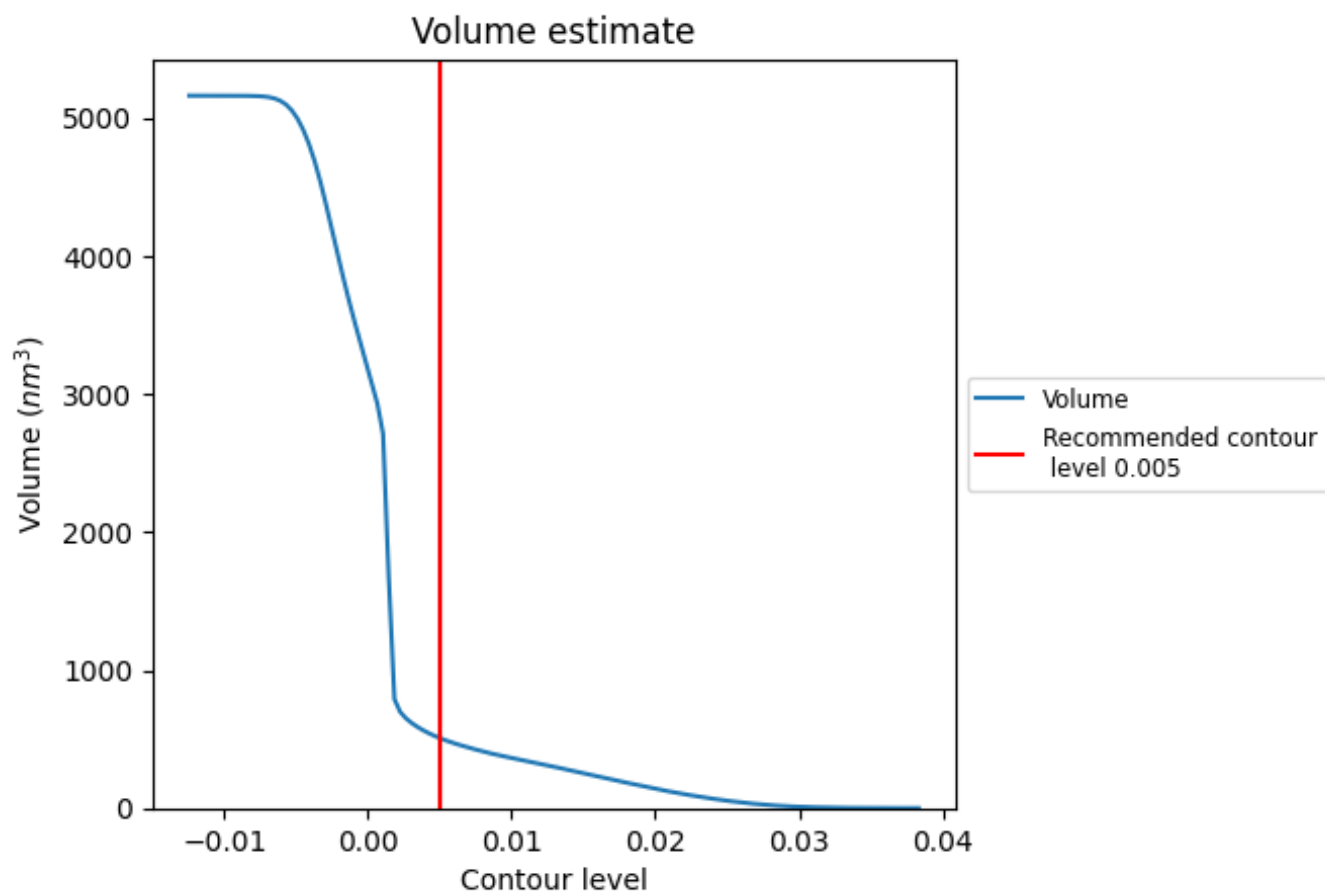
This section contains the results of statistical analysis of the map.

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.

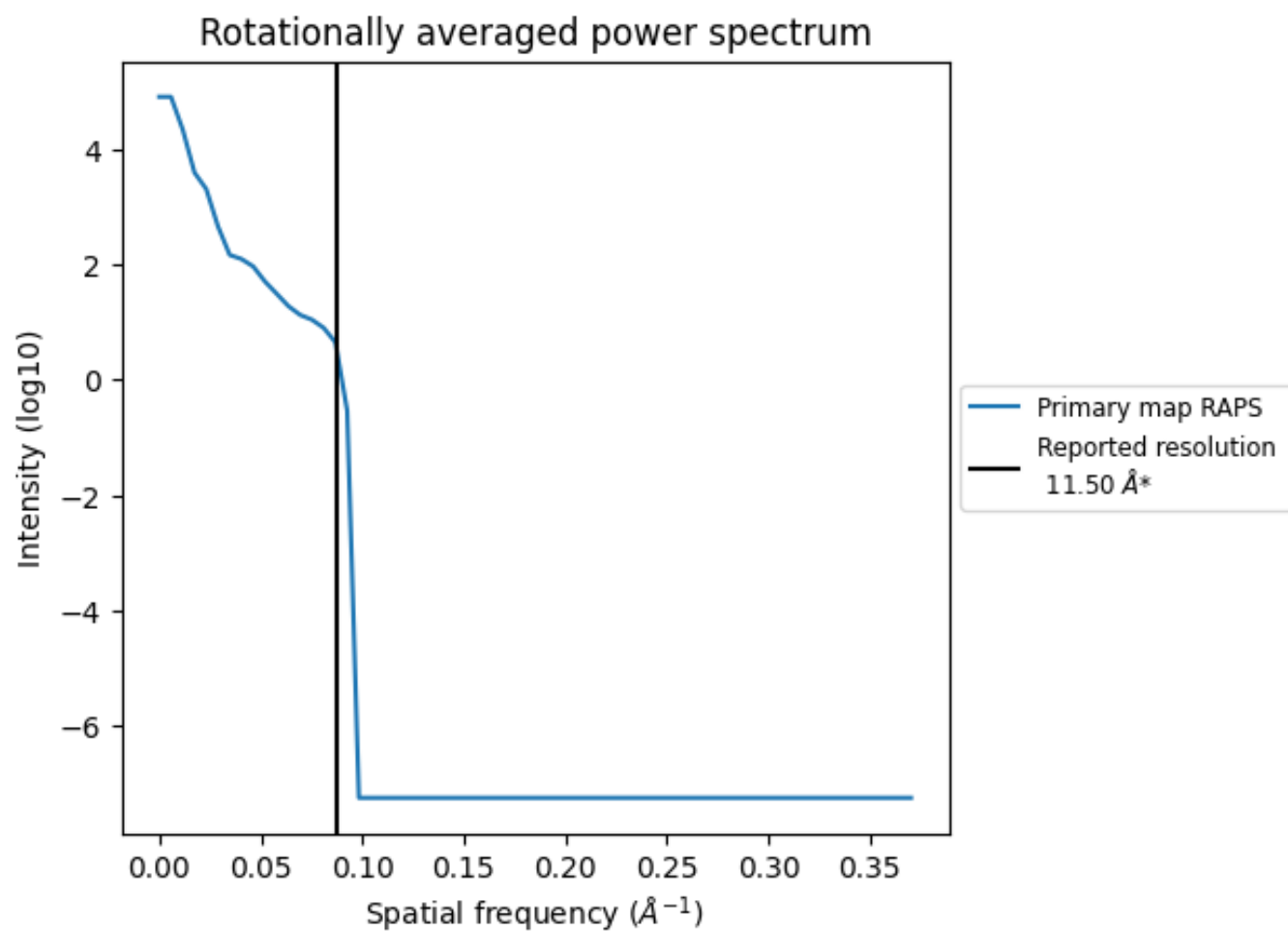
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 508 nm^3 ; this corresponds to an approximate mass of 459 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 ⓘ

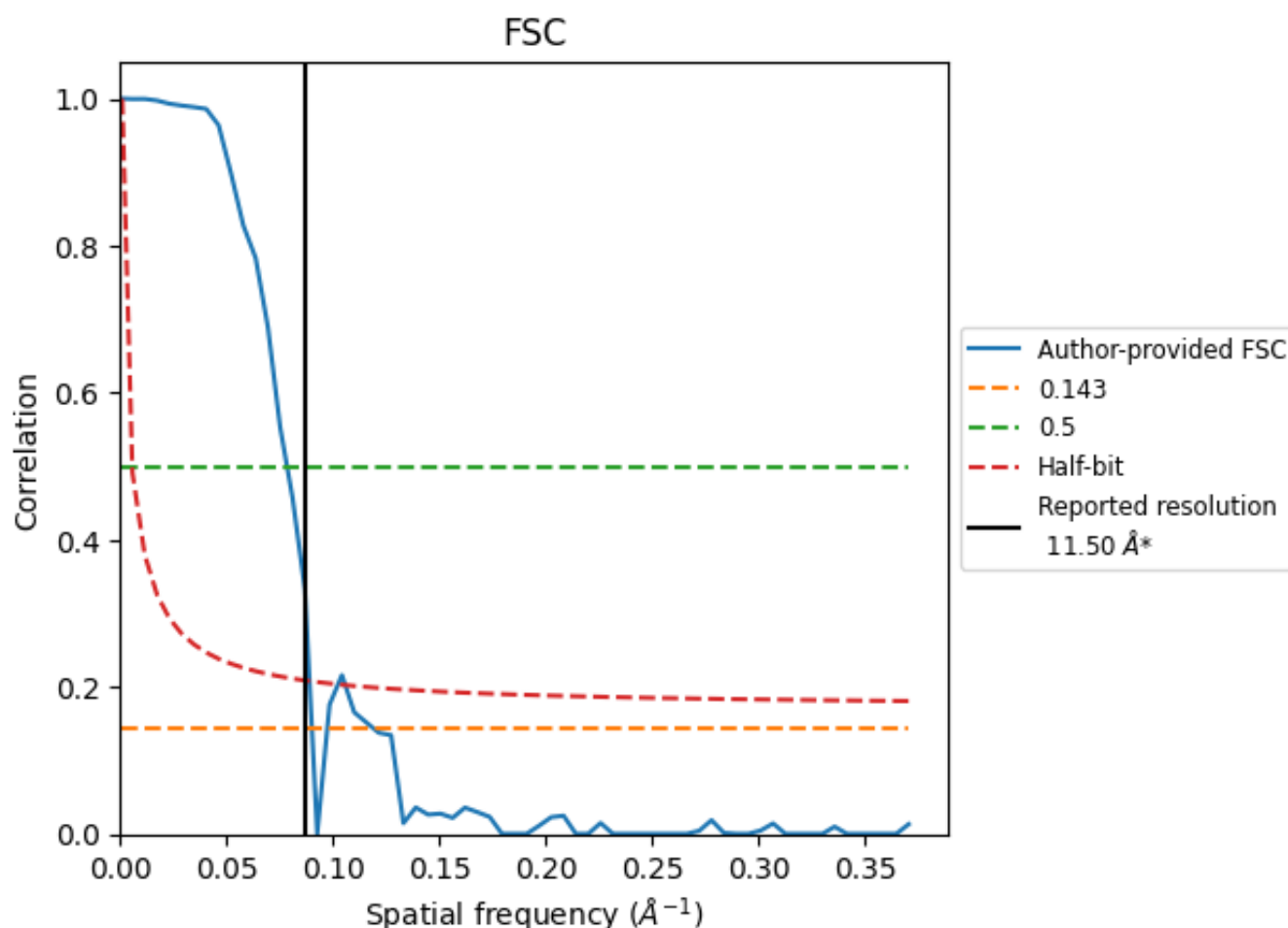


*Reported resolution corresponds to spatial frequency of 0.087 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.087 \AA^{-1}

8.2 Resolution estimates [i](#)

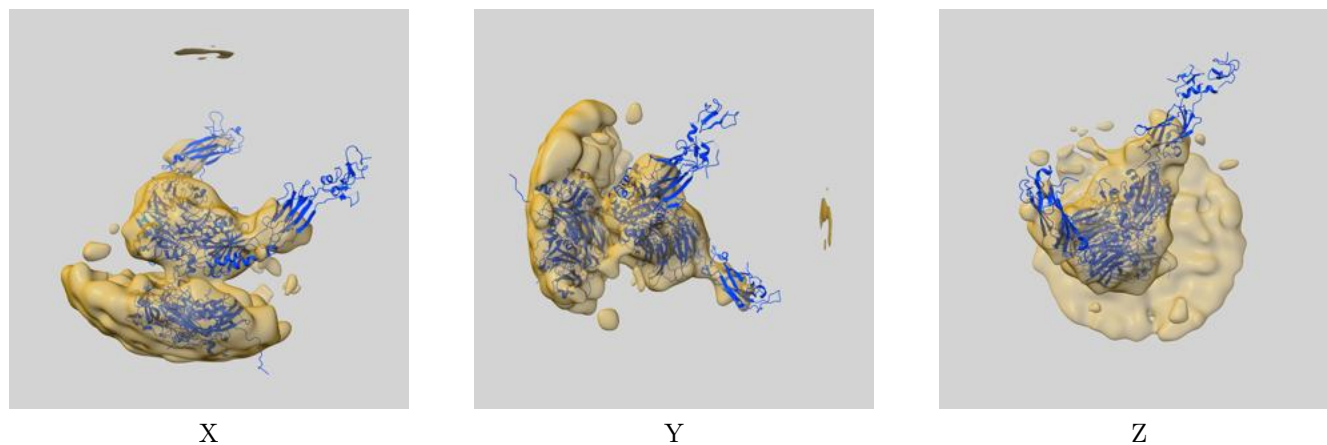
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	11.50	-	-
Author-provided FSC curve	11.10	12.76	11.24
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

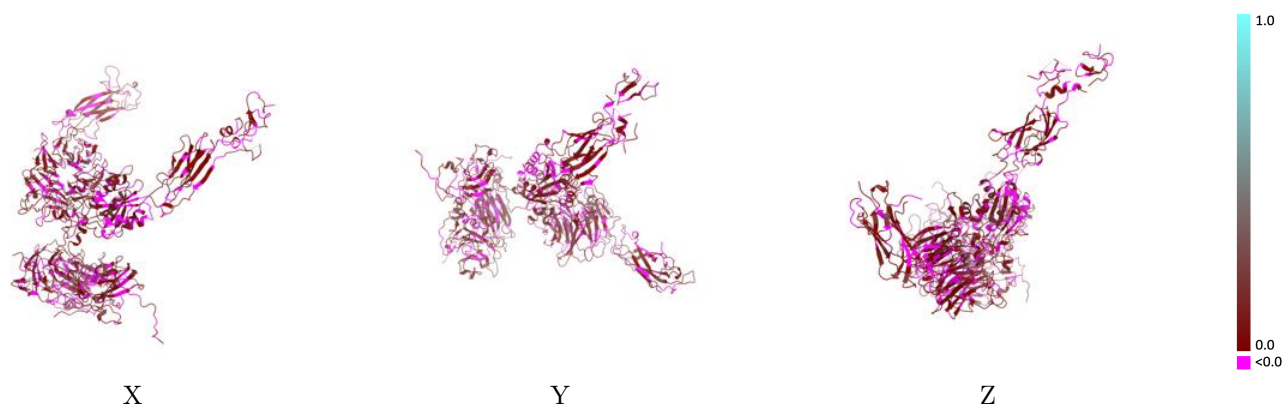
This section contains information regarding the fit between EMDB map EMD-3633 and PDB model 5NER. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



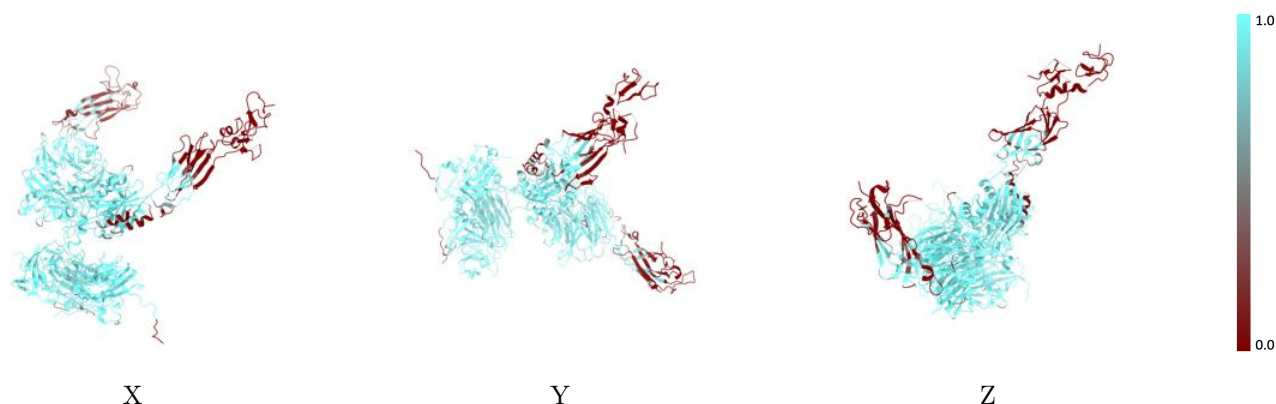
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



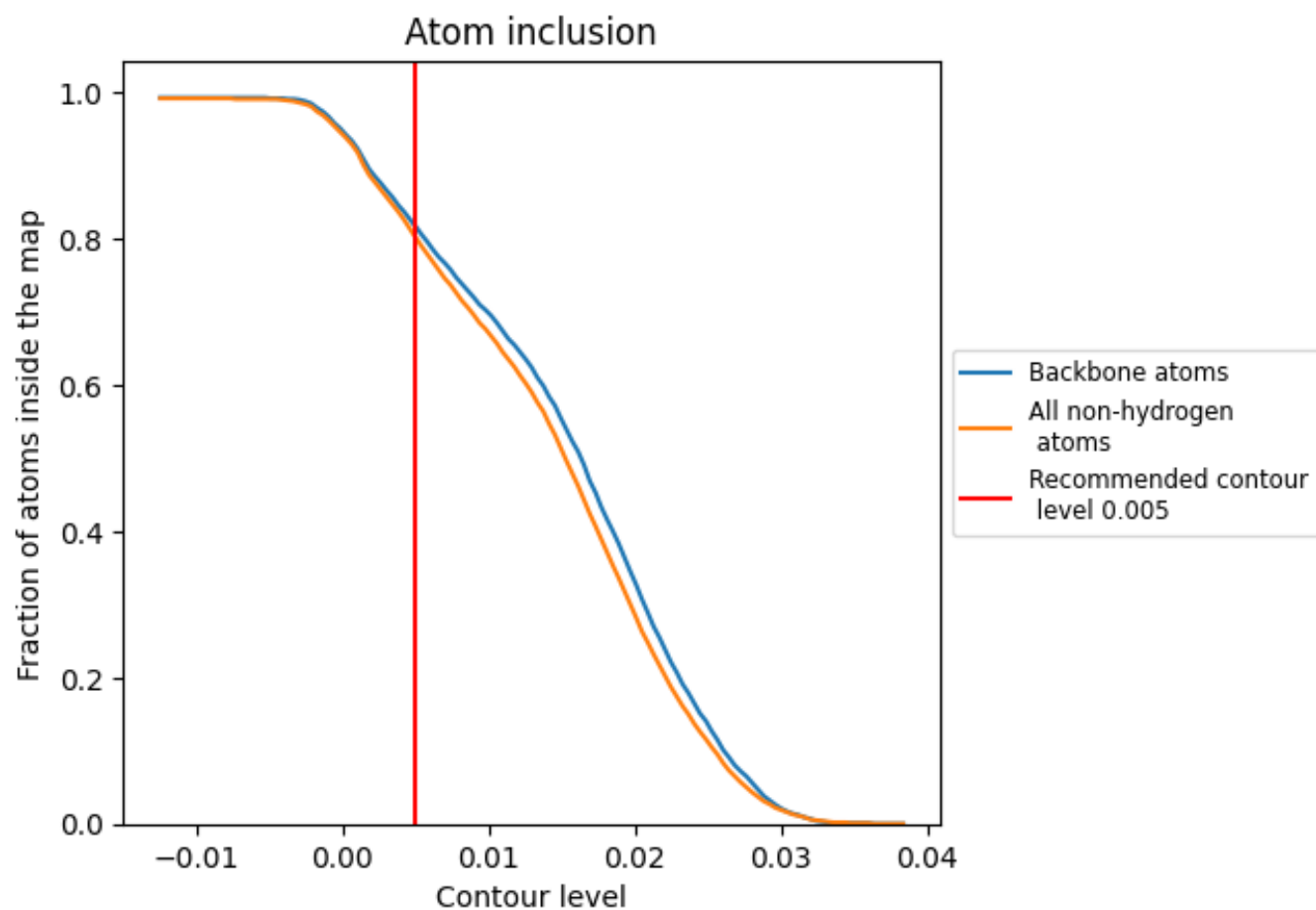
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 80% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8020	<div></div> 0.0600
1	<div></div> 0.9710	<div></div> 0.0750
2	<div></div> 0.9980	<div></div> 0.0670
3	<div></div> 0.9640	<div></div> 0.0630
4	<div></div> 0.8600	<div></div> 0.1230
A	<div></div> 0.7790	<div></div> 0.0590
B	<div></div> 0.6080	<div></div> 0.0430
C	<div></div> 0.0910	<div></div> -0.0920
D	<div></div> 0.2000	<div></div> 0.1310
E	<div></div> 1.0000	<div></div> 0.1080
F	<div></div> 0.0600	<div></div> 0.0790
G	<div></div> 0.0000	<div></div> 0.0430

1.0
0.0
-0.0