



wwPDB EM Validation Summary Report ⓘ

Oct 13, 2024 – 06:01 AM EDT

PDB ID : 7MLY
EMDB ID : EMD-23913
Title : Cryo-EM reveals partially and fully assembled native glycine receptors, heteromeric pentamer
Authors : Zhu, H.; Gouaux, E.
Deposited on : 2021-04-29
Resolution : 2.70 Å (reported)

This is a wwPDB EM Validation Summary 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	:	2022.3.0, CSD as543be (2022)
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

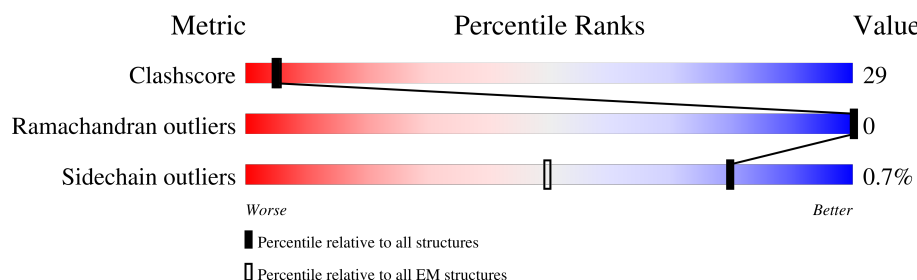
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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.



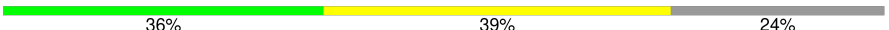


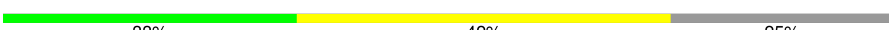
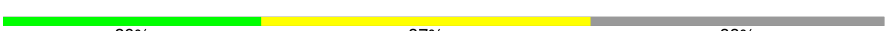
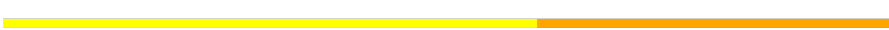




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	I	107	51% 45% .
1	J	107	52% 42% 6%
1	K	107	57% 38% 5%
1	M	107	51% 44% . .
2	F	118	60% 37% .
2	G	118	57% 41% .
2	H	118	59% 38% .
2	L	118	53% 45% .

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Mol	Chain	Length	Quality of chain
3	A	447	
3	B	447	
3	C	447	
3	D	447	
4	E	497	
5	T	5	
6	Z	5	
7	f	4	
7	l	4	
8	r	3	

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
15	GLY	B	501	-	X	-	-
15	GLY	C	501	-	-	X	-

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 21640 atoms, of which 658 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 3D1 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	101	Total	C	N	O	S	0	0
			766	478	133	151	4		
1	K	102	Total	C	N	O	S	0	0
			782	490	135	153	4		
1	M	103	Total	C	N	O	S	0	0
			783	490	136	153	4		
1	I	103	Total	C	N	O	S	0	0
			783	490	136	153	4		

- Molecule 2 is a protein called 3D1 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	115	Total	C	N	O	S	0	0
			891	565	150	171	5		
2	F	115	Total	C	N	O	S	0	0
			891	565	150	171	5		
2	L	115	Total	C	N	O	S	0	0
			891	565	150	171	5		
2	H	115	Total	C	N	O	S	0	0
			891	565	150	171	5		

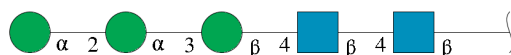
- Molecule 3 is a protein called Glycine receptor alpha 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	335	Total	C	N	O	S	0	0
			2724	1773	446	485	20		
3	A	340	Total	C	N	O	S	0	0
			2771	1801	458	491	21		
3	B	336	Total	C	N	O	S	0	0
			2732	1778	447	486	21		
3	C	347	Total	C	N	O	S	0	0
			2819	1830	464	504	21		

- Molecule 4 is a protein called Glycine receptor beta.

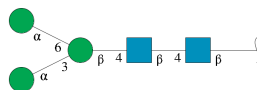
Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	331	Total	C	N	O	S	0	0
			2686	1765	428	477	16		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

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



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

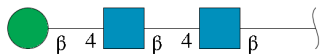
- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	f	4	Total	C	N	O	0	0
			50	28	2	20		
7	l	4	Total	C	N	O	0	0
			50	28	2	20		

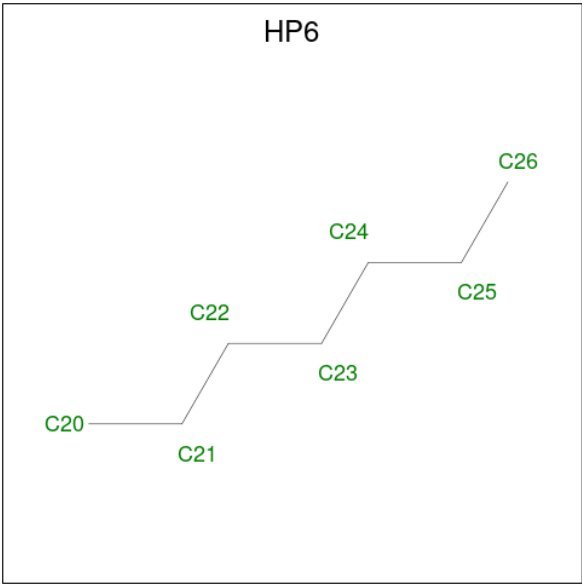
- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b

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



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

- Molecule 9 is HEPTANE (three-letter code: HP6) (formula: C₇H₁₆).



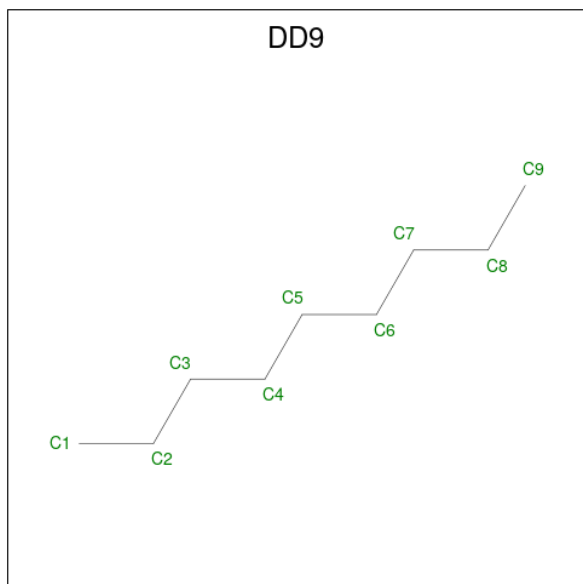
Mol	Chain	Residues	Atoms			AltConf
			Total	C	H	
9	D	1	23	7	16	0
9	D	1	23	7	16	0
9	A	1	23	7	16	0
9	A	1	23	7	16	0
9	B	1	23	7	16	0
9	B	1	23	7	16	0
9	E	1	23	7	16	0
9	E	1	23	7	16	0

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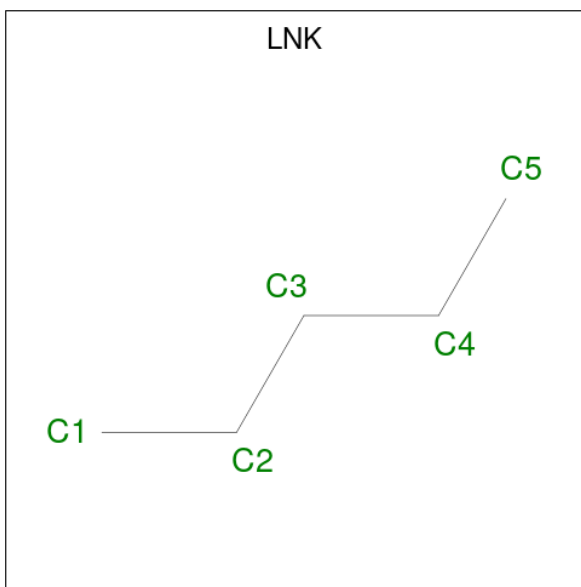
Mol	Chain	Residues	Atoms			AltConf
9	E	1	Total	C	H	0
			23	7	16	

- Molecule 10 is nonane (three-letter code: DD9) (formula: C_9H_{20}).



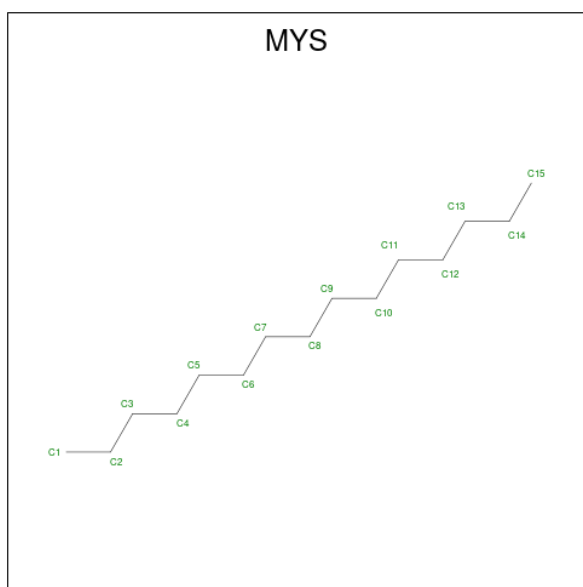
Mol	Chain	Residues	Atoms			AltConf
10	D	1	Total	C	H	0
			29	9	20	
10	A	1	Total	C	H	0
			29	9	20	
10	B	1	Total	C	H	0
			29	9	20	

- Molecule 11 is PENTANE (three-letter code: LNK) (formula: C_5H_{12}).



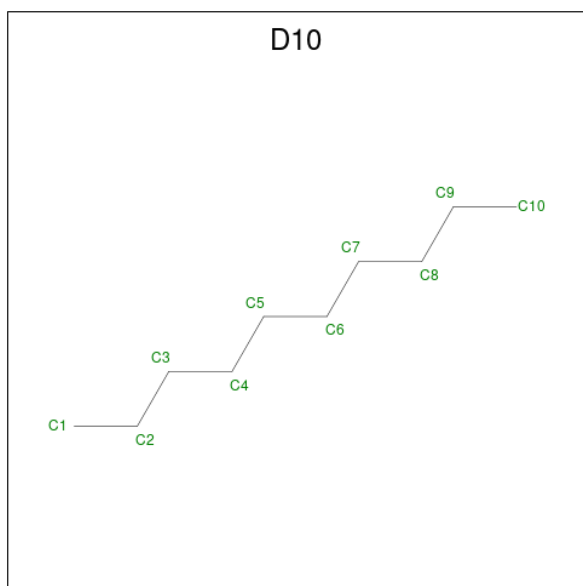
Mol	Chain	Residues	Atoms			AltConf
11	D	1	Total	C	H	0
			17	5	12	
11	D	1	Total	C	H	0
			17	5	12	
11	A	1	Total	C	H	0
			17	5	12	
11	A	1	Total	C	H	0
			17	5	12	
11	B	1	Total	C	H	0
			17	5	12	
11	B	1	Total	C	H	0
			17	5	12	
11	C	1	Total	C	H	0
			17	5	12	
11	C	1	Total	C	H	0
			17	5	12	
11	E	1	Total	C	H	0
			17	5	12	
11	E	1	Total	C	H	0
			17	5	12	

- Molecule 12 is PENTADECANE (three-letter code: MYS) (formula: C₁₅H₃₂).



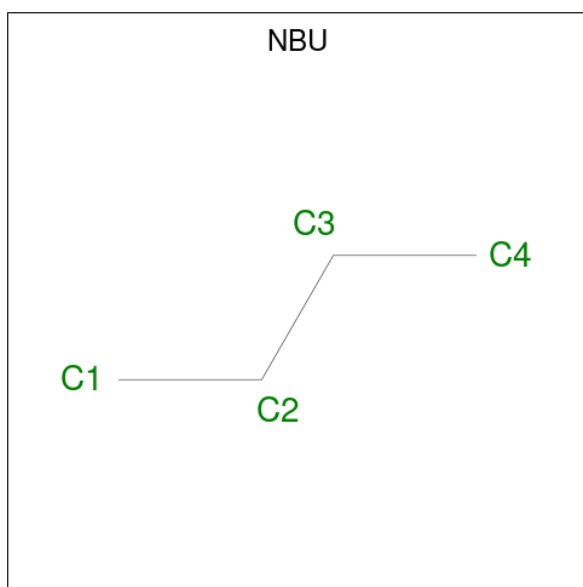
Mol	Chain	Residues	Atoms			AltConf
12	D	1	Total	C	H	0
			47	15	32	

- Molecule 13 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).



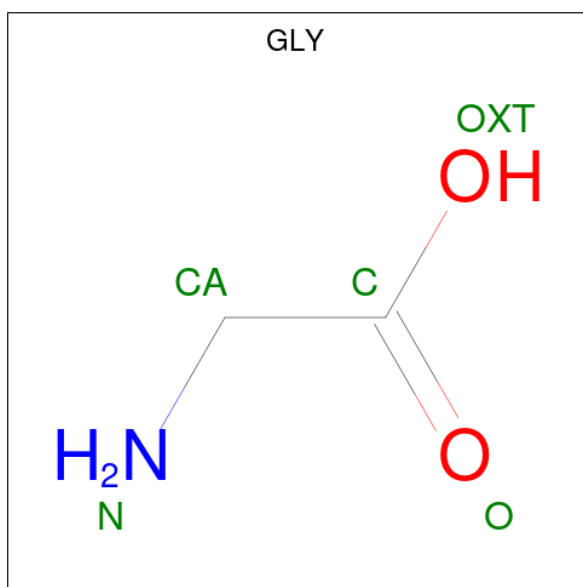
Mol	Chain	Residues	Atoms			AltConf
13	D	1	Total	C	H	0
			32	10	22	

- Molecule 14 is N-BUTANE (three-letter code: NBU) (formula: C_4H_{10}).



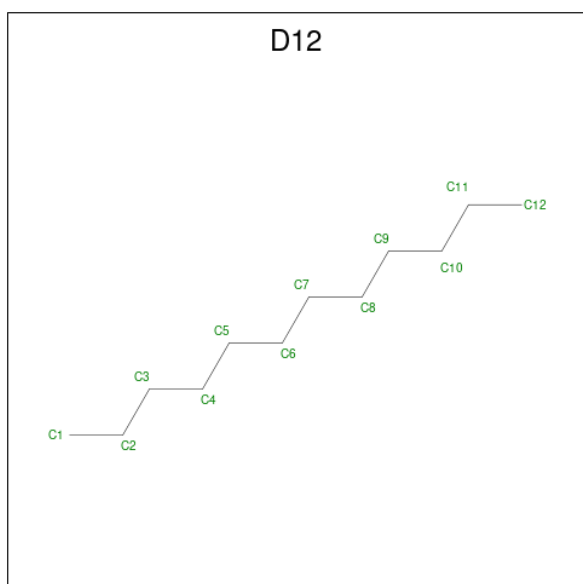
Mol	Chain	Residues	Atoms			AltConf
14	D	1	Total	C	H	0
			14	4	10	
14	D	1	Total	C	H	0
			14	4	10	
14	B	1	Total	C	H	0
			14	4	10	
14	B	1	Total	C	H	0
			14	4	10	
14	B	1	Total	C	H	0
			14	4	10	
14	C	1	Total	C	H	0
			14	4	10	
14	C	1	Total	C	H	0
			14	4	10	
14	C	1	Total	C	H	0
			14	4	10	

- Molecule 15 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).



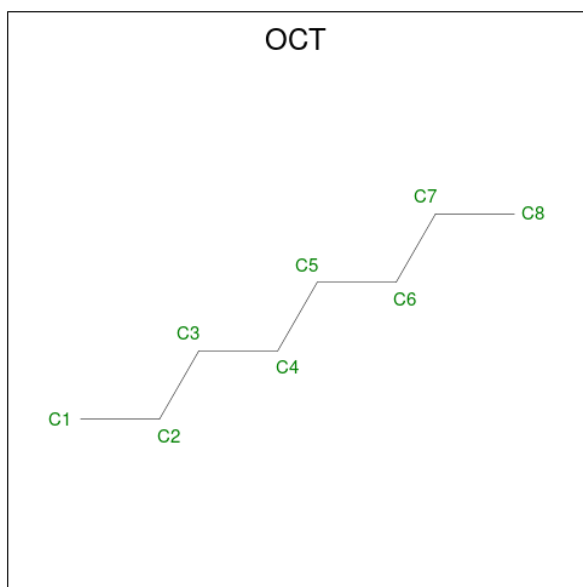
Mol	Chain	Residues	Atoms				AltConf
15	A	1	Total	C	N	O	0
			5	2	1	2	
15	A	1	Total	C	N	O	0
			5	2	1	2	
15	B	1	Total	C	N	O	0
			5	2	1	2	
15	C	1	Total	C	N	O	0
			5	2	1	2	
15	E	1	Total	C	N	O	0
			5	2	1	2	

- Molecule 16 is DODECANE (three-letter code: D12) (formula: C₁₂H₂₆).



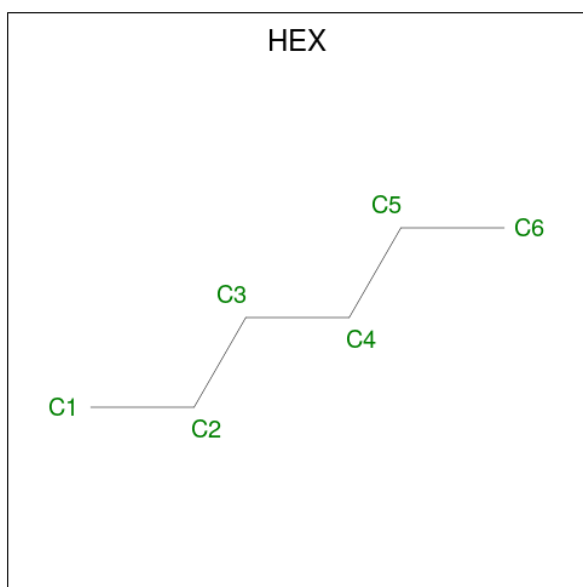
Mol	Chain	Residues	Atoms			AltConf
16	A	1	Total	C	H	0
			38	12	26	
16	C	1	Total	C	H	0
			38	12	26	

- Molecule 17 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}).



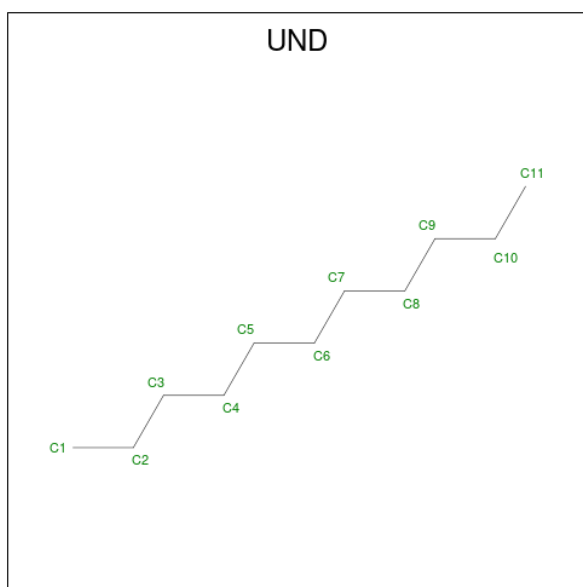
Mol	Chain	Residues	Atoms			AltConf
17	A	1	Total	C	H	0
			26	8	18	
17	A	1	Total	C	H	0
			26	8	18	
17	A	1	Total	C	H	0
			26	8	18	
17	C	1	Total	C	H	0
			26	8	18	

- Molecule 18 is HEXANE (three-letter code: HEX) (formula: C_6H_{14}).



Mol	Chain	Residues	Atoms			AltConf
18	A	1	Total	C	H	0
			20	6	14	
18	B	1	Total	C	H	0
			20	6	14	
18	C	1	Total	C	H	0
			20	6	14	

- Molecule 19 is UNDECANE (three-letter code: UND) (formula: $C_{11}H_{24}$).

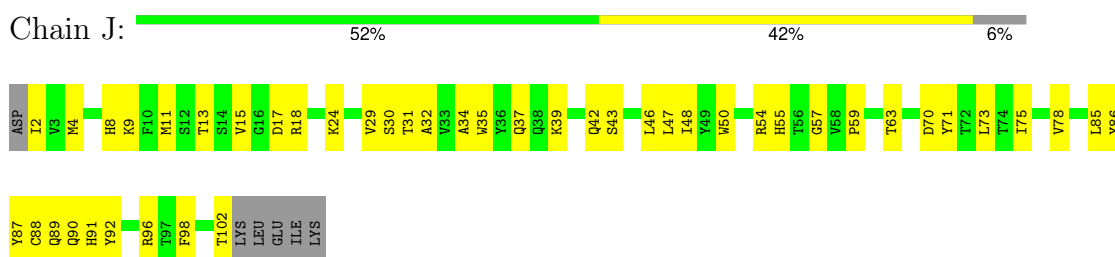


Mol	Chain	Residues	Atoms			AltConf
19	E	1	Total	C	H	0
			35	11	24	

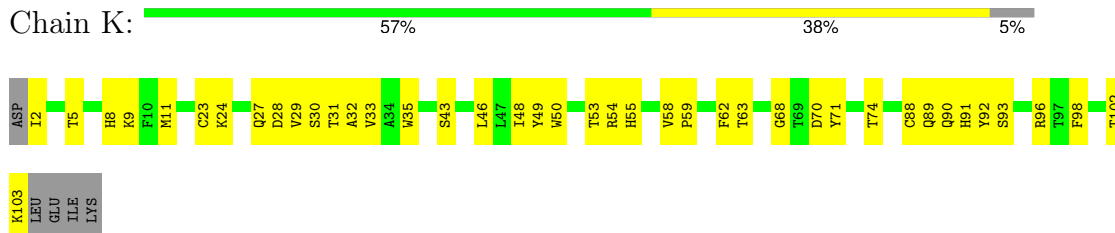
3 Residue-property plots

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: 3D1 Fab Light Chain



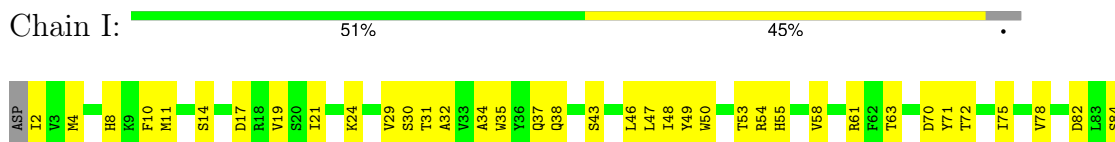
• Molecule 1: 3D1 Fab Light Chain



• Molecule 1: 3D1 Fab Light Chain



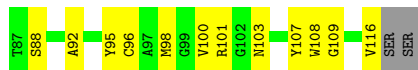
• Molecule 1: 3D1 Fab Light Chain





• Molecule 2: 3D1 Fab Heavy Chain

Chain G: 57% 41%



• Molecule 2: 3D1 Fab Heavy Chain

Chain F: 60% 37%



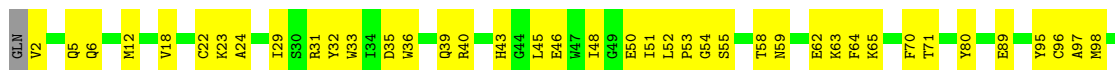
• Molecule 2: 3D1 Fab Heavy Chain

Chain L: 53% 45%



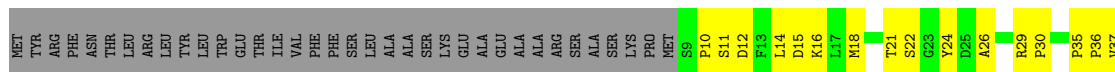
• Molecule 2: 3D1 Fab Heavy Chain

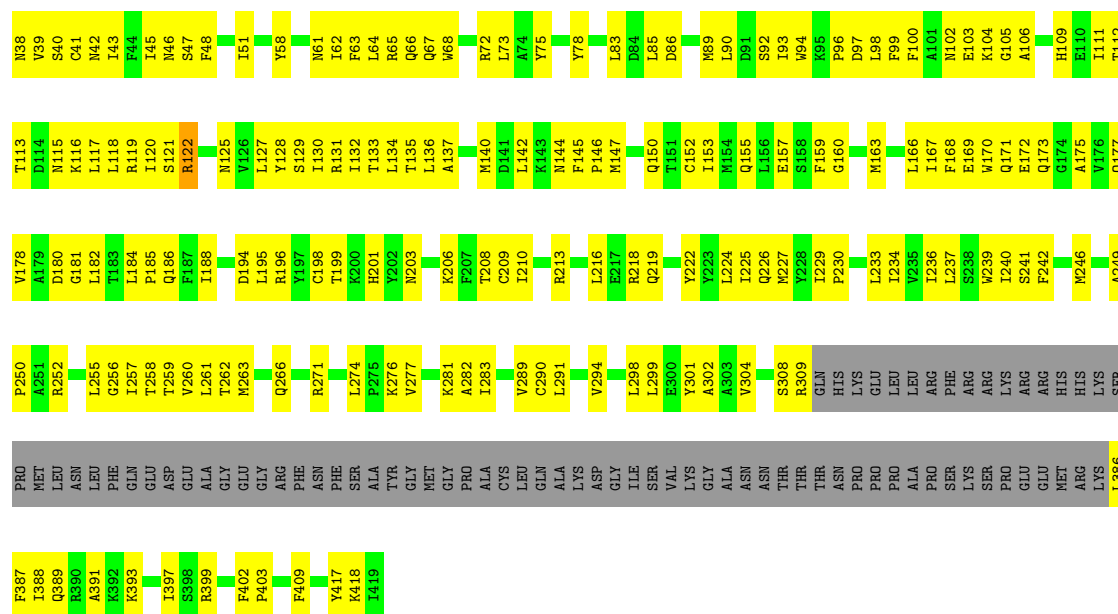
Chain H: 59% 38%



• Molecule 3: Glycine receptor alpha 1

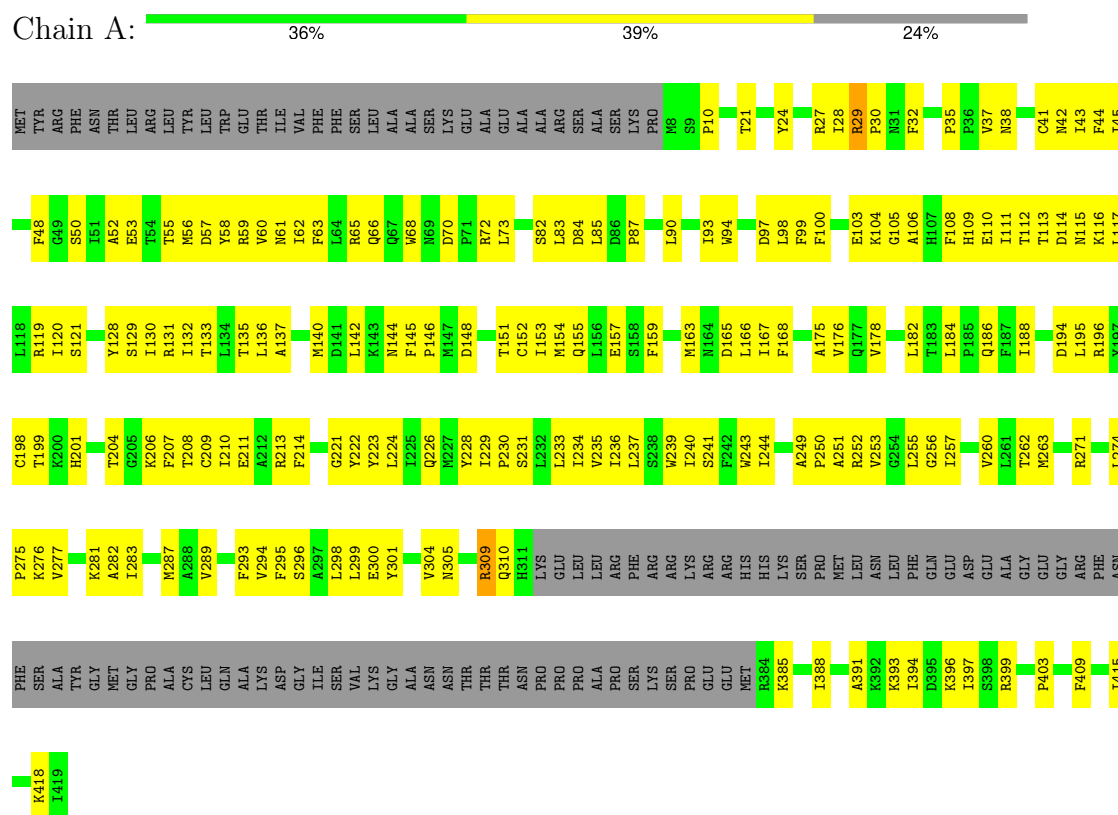
Chain D: 33% 42% 25%





• Molecule 3: Glycine receptor alpha 1

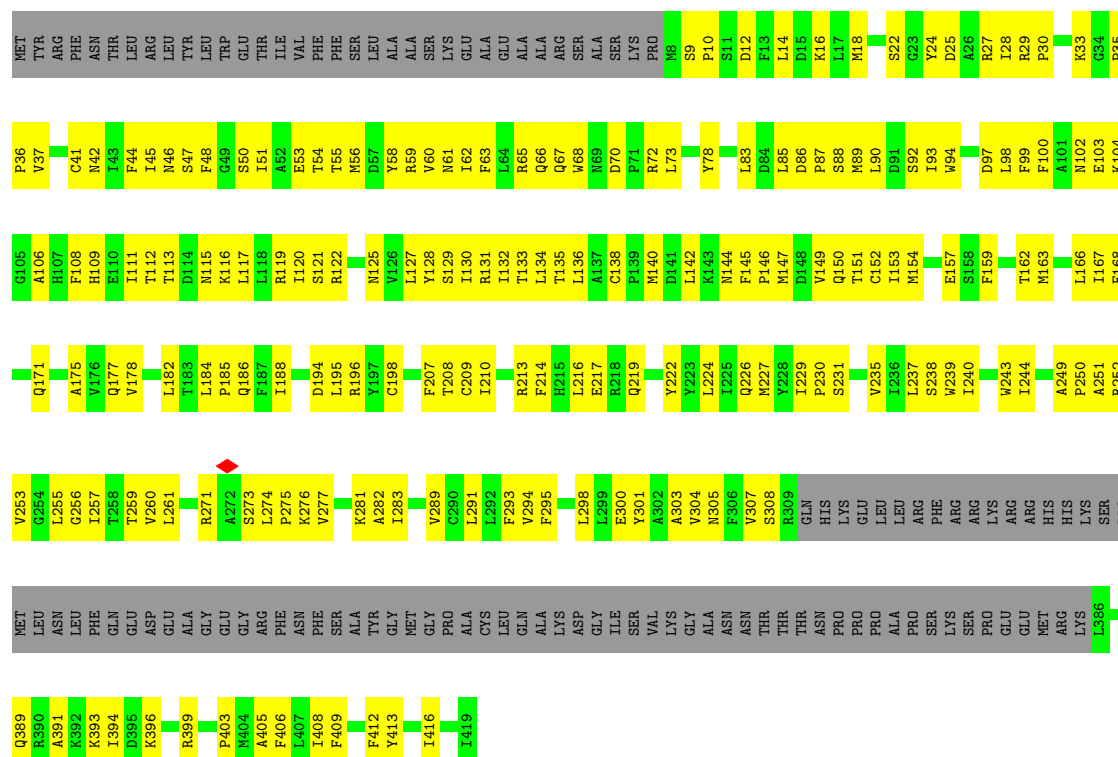
Chain A:



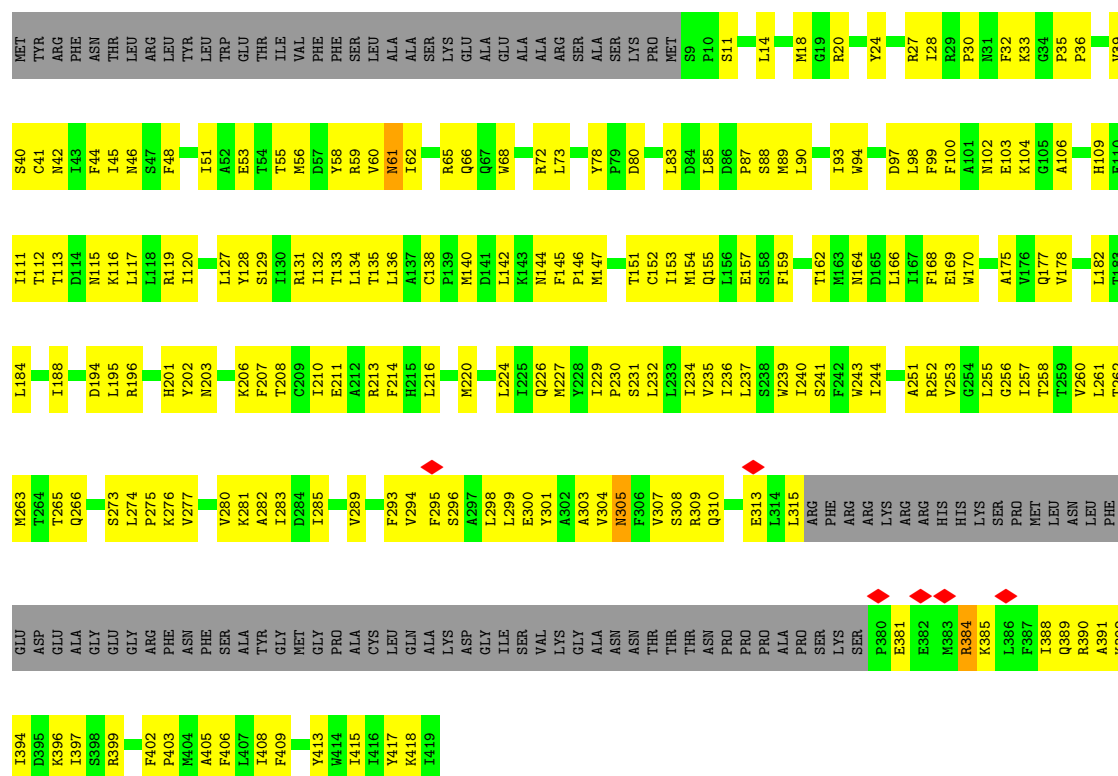
• Molecule 3: Glycine receptor alpha 1

Chain B:



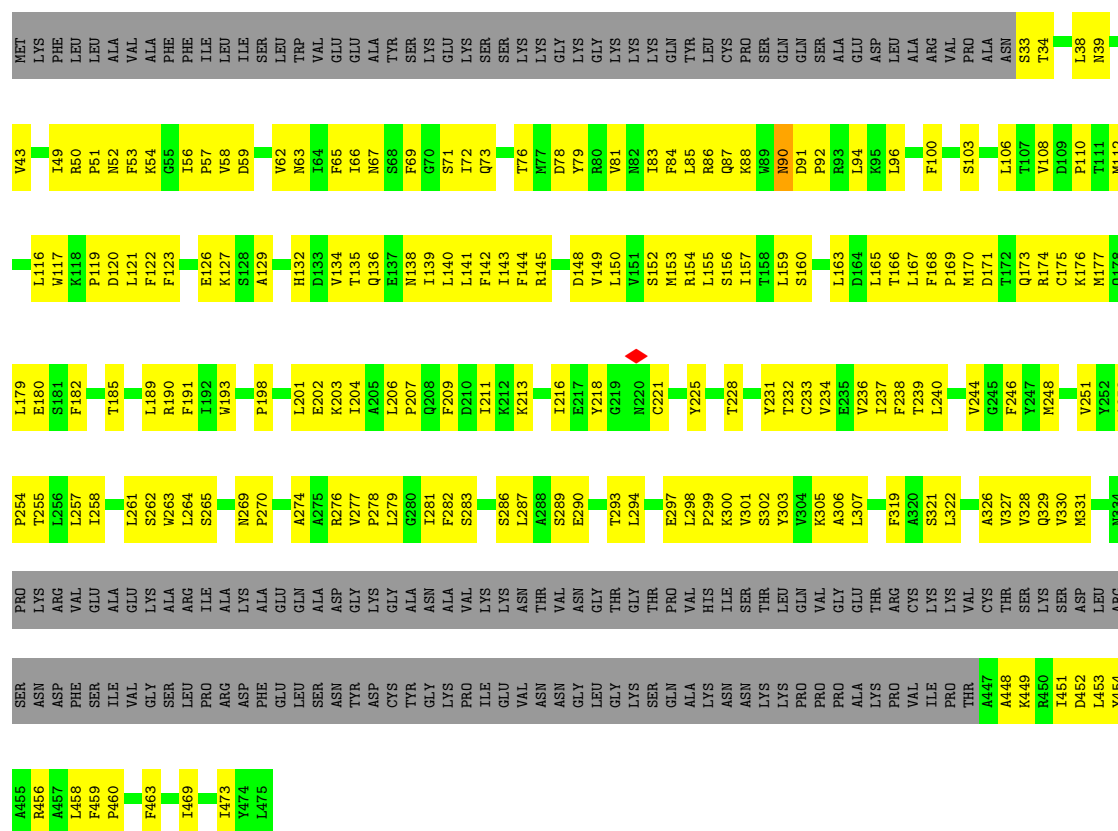


• Molecule 3: Glycine receptor alpha 1



• Molecule 4: Glycine receptor beta

Chain E: 




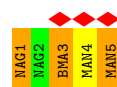
- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T: 



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

Chain Z: 



- Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f: 



- Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-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, C1	Depositor
Number of particles used	527075	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.970	Depositor
Minimum map value	-0.307	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.133	Depositor
Map size (Å)	396.47998, 396.47998, 396.47998	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.826, 0.826, 0.826	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: HEX, MYS, DD9, D10, MAN, LNK, HP6, OCT, D12, NBU, UND, NAG, 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	I	0.27	0/801	0.49	0/1087
1	J	0.27	0/784	0.49	0/1065
1	K	0.27	0/801	0.47	0/1087
1	M	0.27	0/801	0.47	0/1087
2	F	0.27	0/913	0.45	0/1235
2	G	0.28	0/913	0.46	0/1235
2	H	0.29	0/913	0.45	0/1235
2	L	0.27	0/913	0.46	0/1235
3	A	0.29	0/2841	0.44	0/3846
3	B	0.28	0/2801	0.45	0/3794
3	C	0.27	0/2888	0.44	0/3909
3	D	0.30	0/2793	0.46	1/3784 (0.0%)
4	E	0.28	0/2756	0.44	0/3748
All	All	0.28	0/20918	0.45	1/28347 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	D	399	ARG	NE-CZ-NH1	-5.32	117.64	120.30

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	I	783	0	760	42	0
1	J	766	0	736	36	0
1	K	782	0	756	41	0
1	M	783	0	760	48	0
2	F	891	0	859	33	0
2	G	891	0	859	38	0
2	H	891	0	859	39	0
2	L	891	0	859	43	0
3	A	2771	0	2768	201	0
3	B	2732	0	2727	216	0
3	C	2819	0	2817	207	0
3	D	2724	0	2718	211	0
4	E	2686	0	2692	191	0
5	T	61	0	52	2	0
6	Z	61	0	52	3	0
7	f	50	0	43	0	0
7	l	50	0	43	0	0
8	r	39	0	34	0	0
9	A	14	32	32	1	0
9	B	14	32	32	0	0
9	D	14	32	32	0	0
9	E	21	48	48	0	0
10	A	9	20	20	0	0
10	B	9	20	20	1	0
10	D	9	20	20	0	0
11	A	10	24	24	0	0
11	B	10	24	24	0	0
11	C	10	24	24	0	0
11	D	10	24	24	0	0
11	E	10	24	24	0	0
12	D	15	32	32	0	0
13	D	10	22	22	0	0
14	B	12	30	30	0	0
14	C	16	40	40	0	0
14	D	8	20	20	1	0
15	A	10	0	4	1	0
15	B	5	0	2	1	0
15	C	5	0	2	4	0
15	E	5	0	2	2	0
16	A	12	26	26	0	0
16	C	12	26	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	A	24	54	54	1	0
17	C	8	18	18	0	0
18	A	6	14	14	0	0
18	B	6	14	14	0	0
18	C	6	14	14	0	0
19	E	11	24	24	0	0
All	All	20982	658	21062	1207	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 29.

The worst 5 of 1207 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)
3:D:168:PHE:H	3:D:208:THR:HG21	1.20	1.03
3:A:100:PHE:HB2	3:A:103:GLU:HB3	1.39	1.03
3:A:233:LEU:HD12	3:A:236:ILE:HD11	1.37	1.03
3:A:103:GLU:HA	3:A:136:LEU:HD23	1.44	0.98
4:E:191:PHE:H	4:E:232:THR:HG21	1.26	0.98

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	I	101/107 (94%)	86 (85%)	15 (15%)	0	100	100
1	J	99/107 (92%)	84 (85%)	15 (15%)	0	100	100
1	K	100/107 (94%)	87 (87%)	13 (13%)	0	100	100
1	M	101/107 (94%)	93 (92%)	8 (8%)	0	100	100
2	F	113/118 (96%)	108 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
2	H	113/118 (96%)	107 (95%)	6 (5%)	0	100	100
2	L	113/118 (96%)	107 (95%)	6 (5%)	0	100	100
3	A	336/447 (75%)	317 (94%)	19 (6%)	0	100	100
3	B	332/447 (74%)	314 (95%)	18 (5%)	0	100	100
3	C	343/447 (77%)	323 (94%)	20 (6%)	0	100	100
3	D	331/447 (74%)	313 (95%)	18 (5%)	0	100	100
4	E	327/497 (66%)	307 (94%)	20 (6%)	0	100	100
All	All	2522/3185 (79%)	2354 (93%)	168 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	I	87/92 (95%)	87 (100%)	0	100	100
1	J	85/92 (92%)	85 (100%)	0	100	100
1	K	87/92 (95%)	87 (100%)	0	100	100
1	M	87/92 (95%)	86 (99%)	1 (1%)	70	87
2	F	93/96 (97%)	93 (100%)	0	100	100
2	G	93/96 (97%)	93 (100%)	0	100	100
2	H	93/96 (97%)	93 (100%)	0	100	100
2	L	93/96 (97%)	93 (100%)	0	100	100
3	A	305/394 (77%)	301 (99%)	4 (1%)	65	85
3	B	301/394 (76%)	301 (100%)	0	100	100
3	C	310/394 (79%)	306 (99%)	4 (1%)	65	85
3	D	300/394 (76%)	297 (99%)	3 (1%)	73	89
4	E	299/439 (68%)	296 (99%)	3 (1%)	73	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2233/2767 (81%)	2218 (99%)	15 (1%)	80 93

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	310	GLN
4	E	154	ARG
3	C	18	MET
4	E	213	LYS
3	C	384	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
4	E	36	ASN
4	E	90	ASN
3	A	150	GLN
3	A	125	ASN
4	E	136	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

21 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
5	NAG	T	1	3,5	14,14,15	0.51	0	17,19,21	0.92	1 (5%)
5	NAG	T	2	5	14,14,15	0.38	0	17,19,21	0.63	0
5	BMA	T	3	5	11,11,12	0.78	0	15,15,17	1.20	2 (13%)
5	MAN	T	4	5	11,11,12	0.57	0	15,15,17	0.98	2 (13%)
5	MAN	T	5	5	11,11,12	0.90	0	15,15,17	0.93	1 (6%)
6	NAG	Z	1	3,6	14,14,15	0.45	0	17,19,21	1.03	1 (5%)
6	NAG	Z	2	6	14,14,15	0.19	0	17,19,21	0.50	0
6	BMA	Z	3	6	11,11,12	0.82	0	15,15,17	0.96	1 (6%)
6	MAN	Z	4	6	11,11,12	0.57	0	15,15,17	0.97	2 (13%)
6	MAN	Z	5	6	11,11,12	0.70	0	15,15,17	1.30	2 (13%)
7	NAG	f	1	3,7	14,14,15	0.51	0	17,19,21	1.22	1 (5%)
7	NAG	f	2	7	14,14,15	0.42	0	17,19,21	0.66	0
7	BMA	f	3	7	11,11,12	0.52	0	15,15,17	0.72	0
7	MAN	f	4	7	11,11,12	0.61	0	15,15,17	1.09	2 (13%)
7	NAG	l	1	3,7	14,14,15	0.25	0	17,19,21	0.35	0
7	NAG	l	2	7	14,14,15	0.27	0	17,19,21	0.45	0
7	BMA	l	3	7	11,11,12	1.13	2 (18%)	15,15,17	1.32	2 (13%)
7	MAN	l	4	7	11,11,12	0.67	0	15,15,17	1.07	2 (13%)
8	NAG	r	1	8,4	14,14,15	1.15	1 (7%)	17,19,21	1.53	3 (17%)
8	NAG	r	2	8	14,14,15	0.62	1 (7%)	17,19,21	1.07	1 (5%)
8	BMA	r	3	8	11,11,12	0.54	0	15,15,17	0.79	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
5	NAG	T	1	3,5	-	4/6/23/26	0/1/1/1
5	NAG	T	2	5	-	1/6/23/26	0/1/1/1
5	BMA	T	3	5	-	0/2/19/22	0/1/1/1
5	MAN	T	4	5	-	0/2/19/22	0/1/1/1
5	MAN	T	5	5	-	2/2/19/22	0/1/1/1
6	NAG	Z	1	3,6	-	6/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	4/6/23/26	0/1/1/1
6	BMA	Z	3	6	-	2/2/19/22	0/1/1/1
6	MAN	Z	4	6	-	0/2/19/22	0/1/1/1
6	MAN	Z	5	6	-	0/2/19/22	1/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	f	1	3,7	-	1/6/23/26	0/1/1/1
7	NAG	f	2	7	-	0/6/23/26	0/1/1/1
7	BMA	f	3	7	-	2/2/19/22	0/1/1/1
7	MAN	f	4	7	-	0/2/19/22	1/1/1/1
7	NAG	l	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	l	2	7	-	2/6/23/26	0/1/1/1
7	BMA	l	3	7	-	1/2/19/22	0/1/1/1
7	MAN	l	4	7	-	1/2/19/22	1/1/1/1
8	NAG	r	1	8,4	-	6/6/23/26	0/1/1/1
8	NAG	r	2	8	-	2/6/23/26	0/1/1/1
8	BMA	r	3	8	-	1/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	r	1	NAG	O5-C1	-4.09	1.36	1.43
7	l	3	BMA	C1-C2	2.71	1.58	1.52
7	l	3	BMA	C2-C3	2.32	1.56	1.52
8	r	2	NAG	O5-C1	2.22	1.47	1.43

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	f	1	NAG	C1-O5-C5	4.75	118.56	112.19
8	r	2	NAG	C1-O5-C5	4.06	117.62	112.19
6	Z	5	MAN	C1-O5-C5	4.04	117.60	112.19
8	r	1	NAG	C3-C4-C5	3.73	116.99	110.23
8	r	1	NAG	C2-N2-C7	3.39	127.44	122.90

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	T	1	NAG	O5-C5-C6-O6
6	Z	2	NAG	O5-C5-C6-O6
7	l	2	NAG	O5-C5-C6-O6
7	f	3	BMA	C4-C5-C6-O6
6	Z	1	NAG	O5-C5-C6-O6

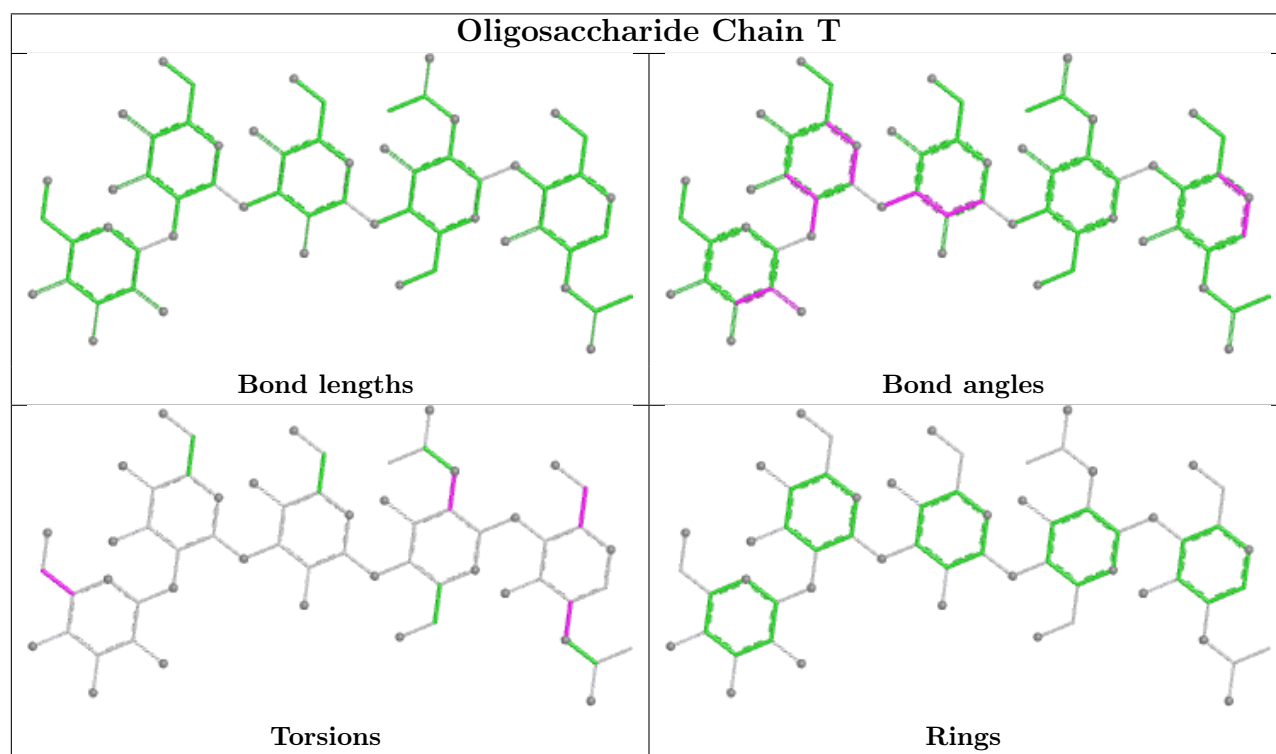
All (3) ring outliers are listed below:

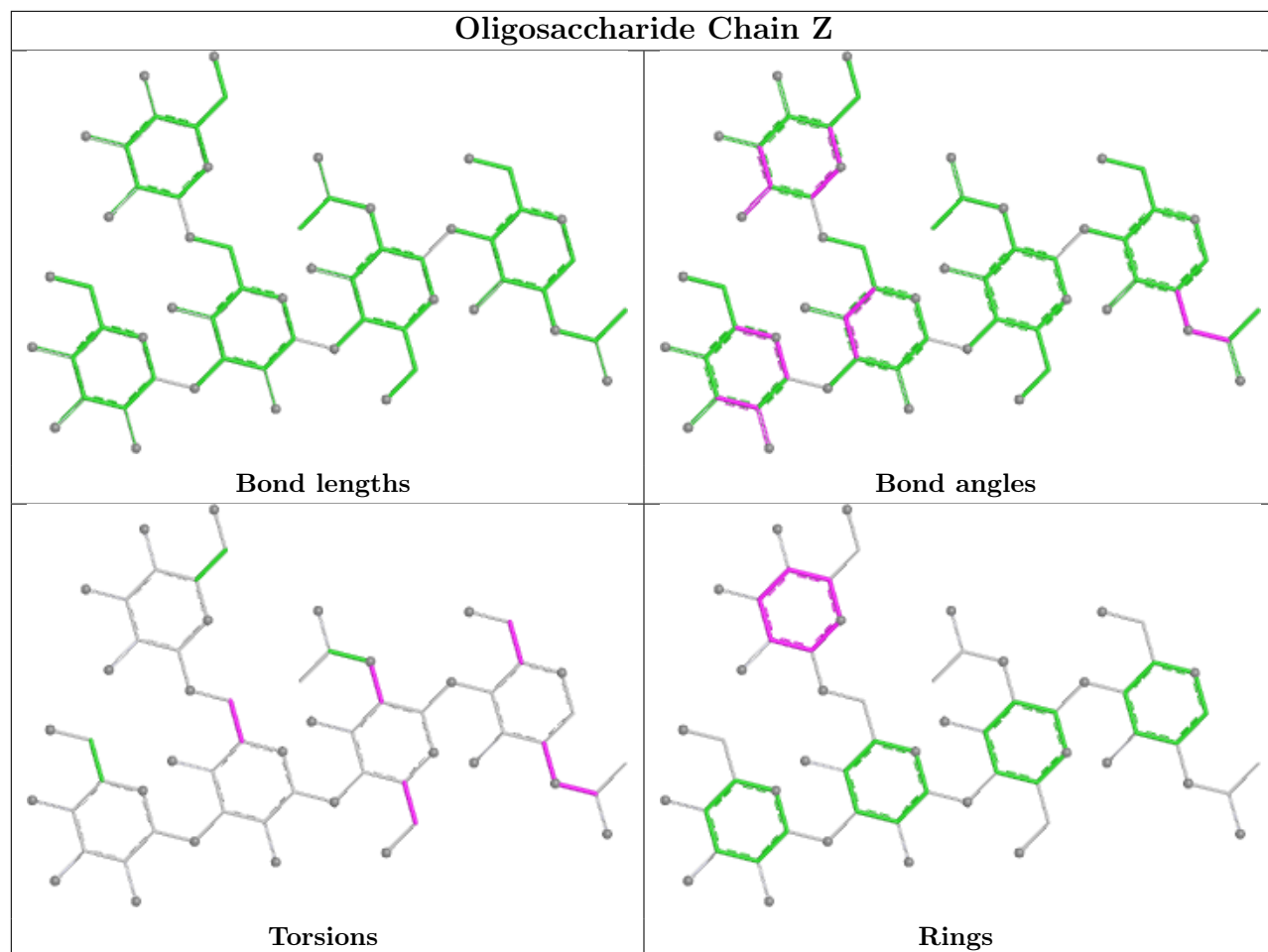
Mol	Chain	Res	Type	Atoms
7	f	4	MAN	C1-C2-C3-C4-C5-O5
7	l	4	MAN	C1-C2-C3-C4-C5-O5
6	Z	5	MAN	C1-C2-C3-C4-C5-O5

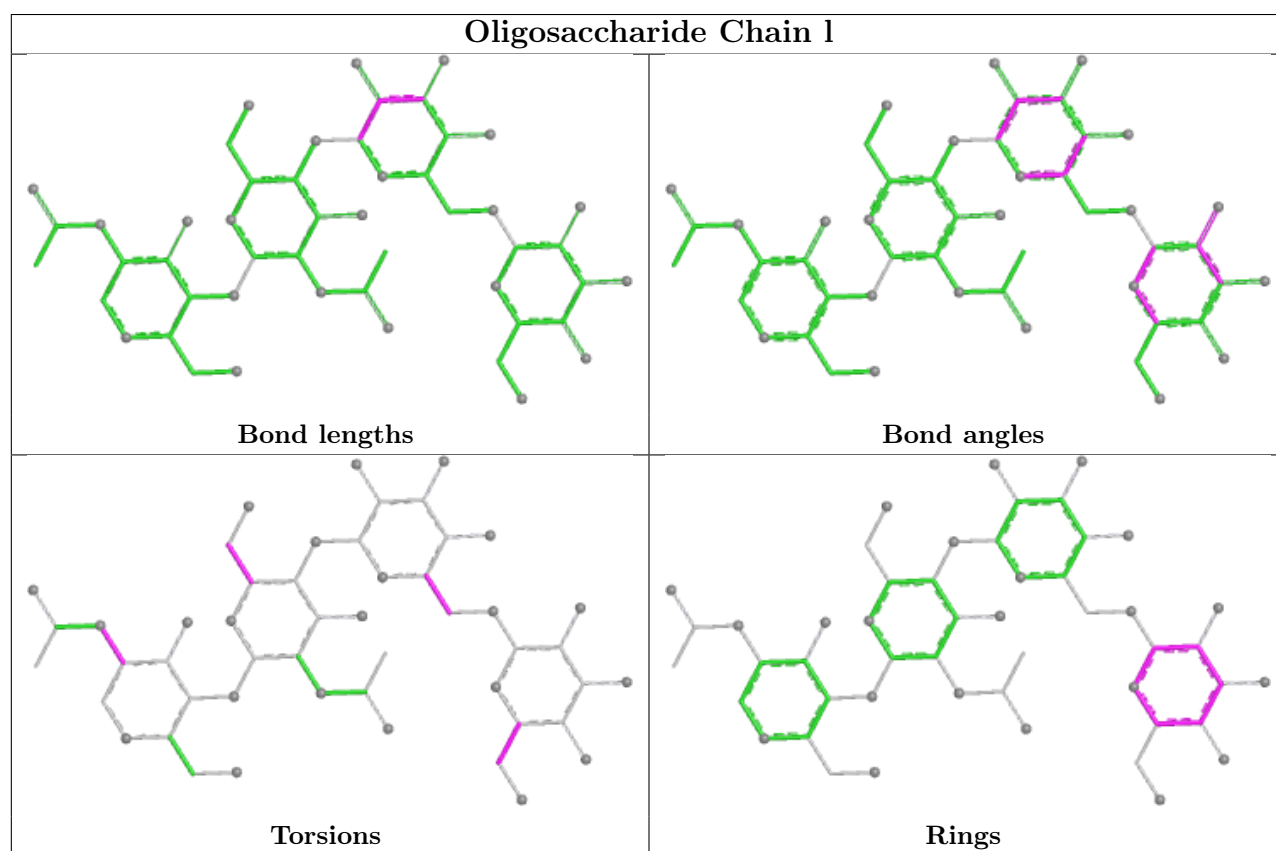
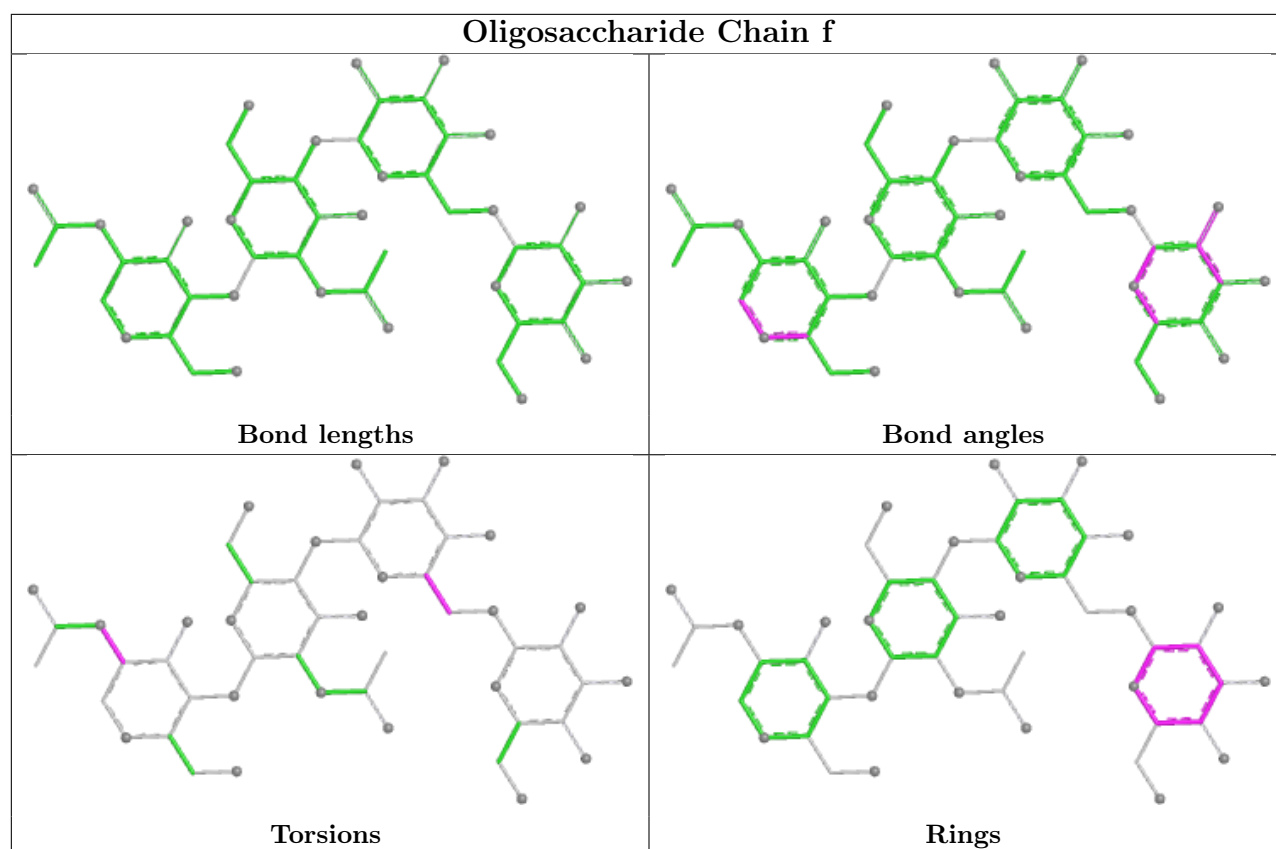
6 monomers are involved in 5 short contacts:

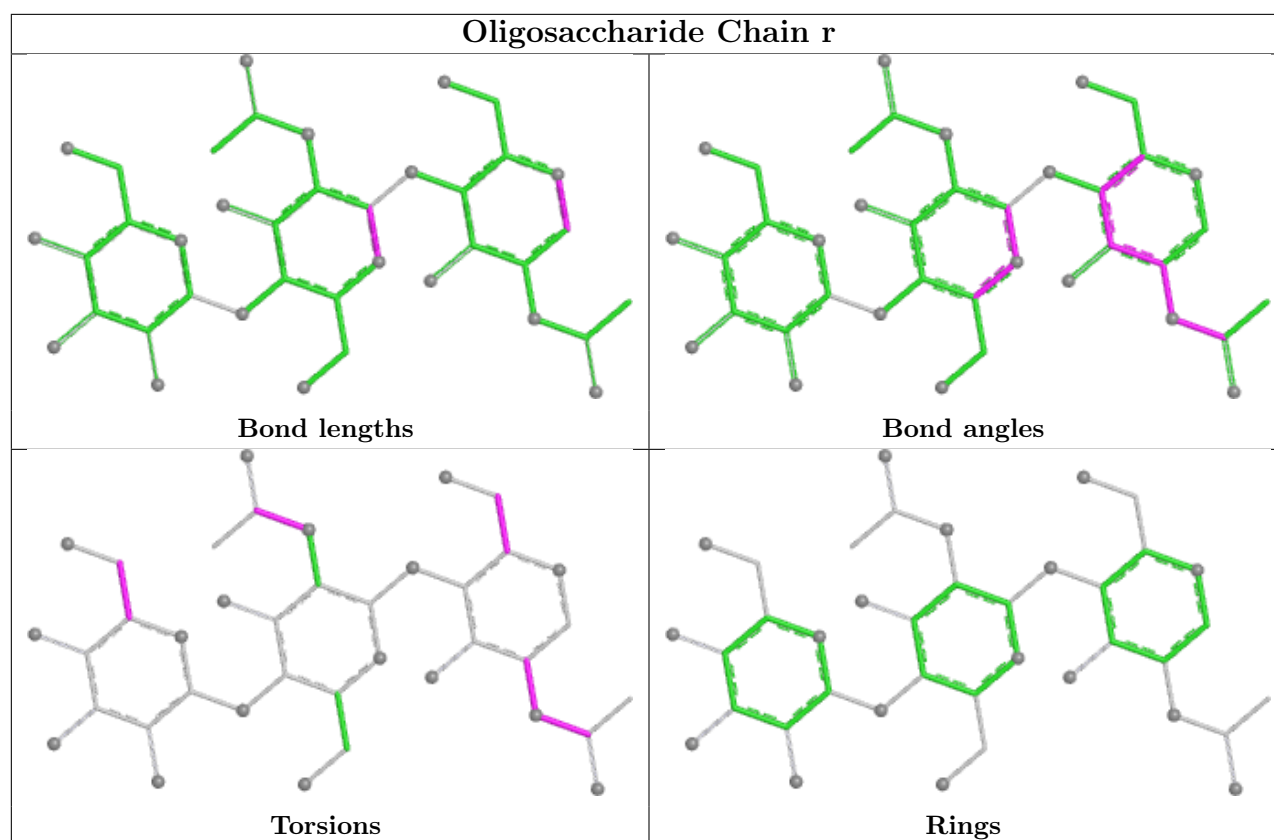
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Z	3	BMA	1	0
5	T	3	BMA	1	0
6	Z	5	MAN	1	0
6	Z	1	NAG	2	0
5	T	2	NAG	1	0
5	T	1	NAG	1	0

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](#)

48 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	LNK	D	504	-	4,4,4	0.31	0	3,3,3	0.55	0
17	OCT	A	507	-	7,7,7	0.27	0	6,6,6	0.74	0
15	GLY	C	501	-	4,4,4	1.18	1 (25%)	3,4,4	1.71	1 (33%)
11	LNK	B	504	-	4,4,4	0.31	0	3,3,3	0.54	0
19	UND	E	506	-	10,10,10	0.27	0	9,9,9	0.81	0
9	HP6	E	503	-	6,6,6	0.28	0	5,5,5	0.72	0
9	HP6	D	501	-	6,6,6	0.28	0	5,5,5	0.74	0
11	LNK	A	509	-	4,4,4	0.30	0	3,3,3	0.60	0
16	D12	C	502	-	11,11,11	0.26	0	10,10,10	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	OCT	A	511	-	7,7,7	0.29	0	6,6,6	0.67	0
14	NBU	B	509	-	3,3,3	0.39	0	2,2,2	0.74	0
14	NBU	C	506	-	3,3,3	0.36	0	2,2,2	0.77	0
11	LNK	C	505	-	4,4,4	0.31	0	3,3,3	0.63	0
9	HP6	E	504	-	6,6,6	0.30	0	5,5,5	0.69	0
14	NBU	D	508	-	3,3,3	0.40	0	2,2,2	0.75	0
14	NBU	C	508	-	3,3,3	0.40	0	2,2,2	0.72	0
14	NBU	B	507	-	3,3,3	0.39	0	2,2,2	0.75	0
9	HP6	B	510	-	6,6,6	0.30	0	5,5,5	0.71	0
10	DD9	D	503	-	8,8,8	0.23	0	7,7,7	0.84	0
14	NBU	B	508	-	3,3,3	0.38	0	2,2,2	0.74	0
11	LNK	A	506	-	4,4,4	0.28	0	3,3,3	0.63	0
14	NBU	C	509	-	3,3,3	0.39	0	2,2,2	0.74	0
11	LNK	C	503	-	4,4,4	0.32	0	3,3,3	0.54	0
18	HEX	A	510	-	5,5,5	0.31	0	4,4,4	0.61	0
9	HP6	B	502	-	6,6,6	0.29	0	5,5,5	0.68	0
14	NBU	D	509	-	3,3,3	0.39	0	2,2,2	0.74	0
17	OCT	A	508	-	7,7,7	0.31	0	6,6,6	0.62	0
11	LNK	E	507	-	4,4,4	0.32	0	3,3,3	0.56	0
18	HEX	B	505	-	5,5,5	0.30	0	4,4,4	0.64	0
15	GLY	E	501	-	4,4,4	1.18	1 (25%)	3,4,4	1.64	1 (33%)
16	D12	A	503	-	11,11,11	0.26	0	10,10,10	0.84	0
17	OCT	C	504	-	7,7,7	0.29	0	6,6,6	0.64	0
11	LNK	E	505	-	4,4,4	0.32	0	3,3,3	0.58	0
9	HP6	E	502	-	6,6,6	0.30	0	5,5,5	0.64	0
13	D10	D	506	-	9,9,9	0.27	0	8,8,8	0.84	0
15	GLY	A	501	-	4,4,4	1.20	1 (25%)	3,4,4	1.70	1 (33%)
18	HEX	C	510	-	5,5,5	0.30	0	4,4,4	0.59	0
12	MYS	D	505	-	14,14,14	0.27	0	13,13,13	0.86	0
9	HP6	A	505	-	6,6,6	0.30	0	5,5,5	0.68	0
10	DD9	A	512	-	8,8,8	0.29	0	7,7,7	0.80	0
10	DD9	B	503	-	8,8,8	0.29	0	7,7,7	0.81	0
9	HP6	D	502	-	6,6,6	0.29	0	5,5,5	0.69	0
11	LNK	B	506	-	4,4,4	0.32	0	3,3,3	0.58	0
14	NBU	C	507	-	3,3,3	0.38	0	2,2,2	0.75	0
11	LNK	D	507	-	4,4,4	0.31	0	3,3,3	0.59	0
9	HP6	A	504	-	6,6,6	0.26	0	5,5,5	0.71	0
15	GLY	B	501	-	4,4,4	1.18	1 (25%)	3,4,4	1.61	1 (33%)
15	GLY	A	502	-	4,4,4	1.19	1 (25%)	3,4,4	1.66	1 (33%)

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
11	LNK	D	504	-	-	0/2/2/2	-
17	OCT	A	507	-	-	0/5/5/5	-
15	GLY	C	501	-	-	1/2/2/2	-
11	LNK	B	504	-	-	0/2/2/2	-
19	UND	E	506	-	-	3/8/8/8	-
9	HP6	E	503	-	-	0/4/4/4	-
9	HP6	D	501	-	-	1/4/4/4	-
11	LNK	A	509	-	-	0/2/2/2	-
16	D12	C	502	-	-	0/9/9/9	-
17	OCT	A	511	-	-	0/5/5/5	-
14	NBU	B	509	-	-	0/1/1/1	-
14	NBU	C	506	-	-	0/1/1/1	-
11	LNK	C	505	-	-	0/2/2/2	-
9	HP6	E	504	-	-	1/4/4/4	-
14	NBU	D	508	-	-	0/1/1/1	-
14	NBU	C	508	-	-	0/1/1/1	-
14	NBU	B	507	-	-	0/1/1/1	-
9	HP6	B	510	-	-	0/4/4/4	-
10	DD9	D	503	-	-	1/6/6/6	-
14	NBU	B	508	-	-	0/1/1/1	-
11	LNK	A	506	-	-	0/2/2/2	-
14	NBU	C	509	-	-	0/1/1/1	-
11	LNK	C	503	-	-	1/2/2/2	-
18	HEX	A	510	-	-	0/3/3/3	-
9	HP6	B	502	-	-	0/4/4/4	-
14	NBU	D	509	-	-	0/1/1/1	-
17	OCT	A	508	-	-	1/5/5/5	-
11	LNK	E	507	-	-	0/2/2/2	-
18	HEX	B	505	-	-	0/3/3/3	-
15	GLY	E	501	-	-	0/2/2/2	-
16	D12	A	503	-	-	3/9/9/9	-
17	OCT	C	504	-	-	1/5/5/5	-
11	LNK	E	505	-	-	1/2/2/2	-
9	HP6	E	502	-	-	0/4/4/4	-
13	D10	D	506	-	-	1/7/7/7	-
15	GLY	A	501	-	-	0/2/2/2	-
18	HEX	C	510	-	-	1/3/3/3	-
12	MYS	D	505	-	-	3/12/12/12	-
9	HP6	A	505	-	-	0/4/4/4	-
10	DD9	A	512	-	-	0/6/6/6	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	DD9	B	503	-	-	1/6/6/6	-
9	HP6	D	502	-	-	1/4/4/4	-
11	LNK	B	506	-	-	1/2/2/2	-
14	NBU	C	507	-	-	0/1/1/1	-
11	LNK	D	507	-	-	1/2/2/2	-
9	HP6	A	504	-	-	0/4/4/4	-
15	GLY	B	501	-	-	2/2/2/2	-
15	GLY	A	502	-	-	0/2/2/2	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	501	GLY	OXT-C	-2.30	1.23	1.30
15	A	502	GLY	OXT-C	-2.30	1.23	1.30
15	C	501	GLY	OXT-C	-2.26	1.23	1.30
15	E	501	GLY	OXT-C	-2.23	1.23	1.30
15	B	501	GLY	OXT-C	-2.22	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	501	GLY	OXT-C-O	-2.20	117.67	123.33
15	A	502	GLY	OXT-C-O	-2.19	117.69	123.33
15	A	501	GLY	OXT-C-O	-2.19	117.69	123.33
15	E	501	GLY	OXT-C-O	-2.05	118.05	123.33
15	B	501	GLY	OXT-C-O	-2.03	118.11	123.33

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	B	501	GLY	O-C-CA-N
15	B	501	GLY	OXT-C-CA-N
19	E	506	UND	C5-C6-C7-C8
12	D	505	MYS	C10-C11-C12-C13
17	C	504	OCT	C2-C3-C4-C5

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	507	OCT	1	0
15	C	501	GLY	4	0
14	D	508	NBU	1	0
15	E	501	GLY	2	0
15	A	501	GLY	1	0
10	B	503	DD9	1	0
9	A	504	HP6	1	0
15	B	501	GLY	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.

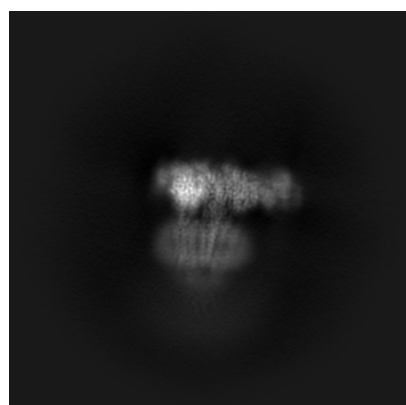
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23913. These allow visual inspection of the internal detail of the map and identification of artifacts.

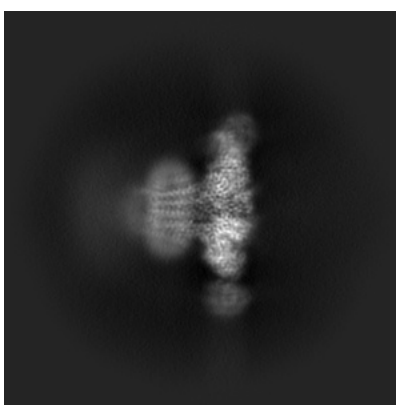
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

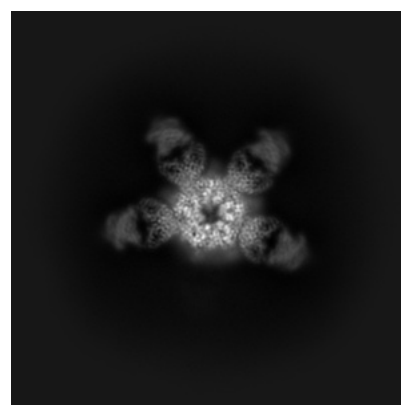
6.1.1 Primary map



X



Y

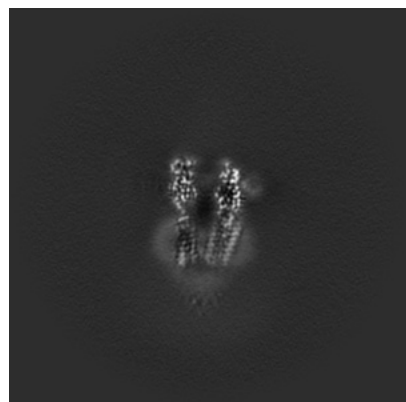


Z

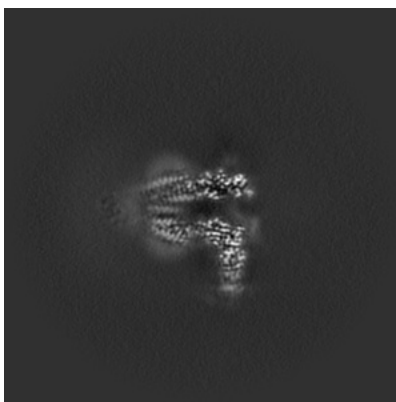
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

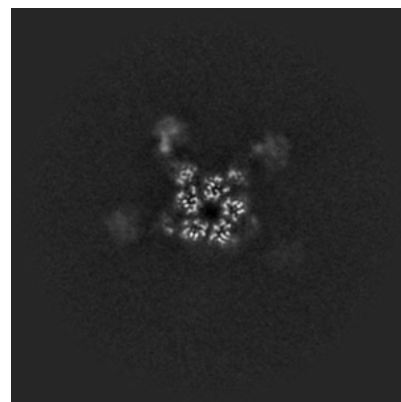
6.2.1 Primary map



X Index: 240



Y Index: 240

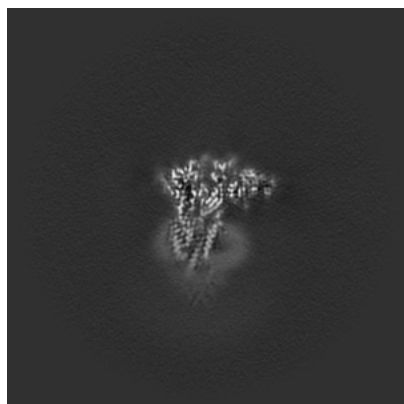


Z Index: 240

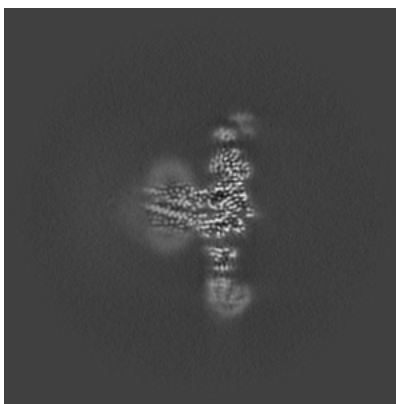
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

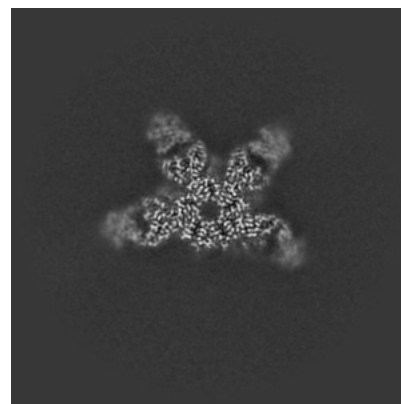
6.3.1 Primary map



X Index: 222



Y Index: 209

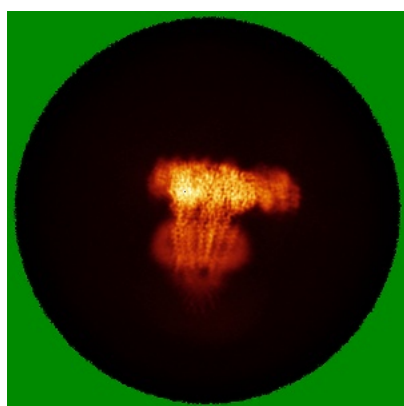


Z Index: 262

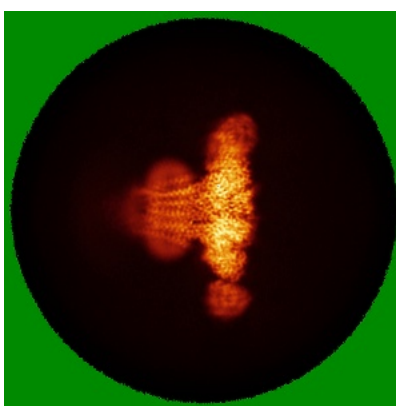
The images above show the largest variance slices of the map in three orthogonal directions.

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

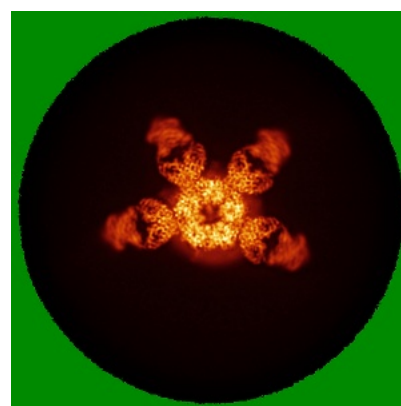
6.4.1 Primary map



X



Y

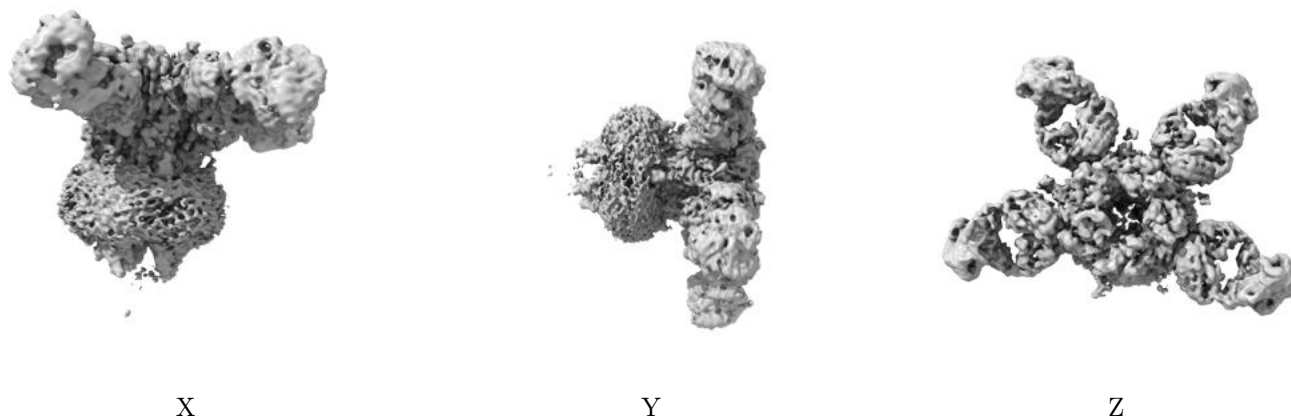


Z

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

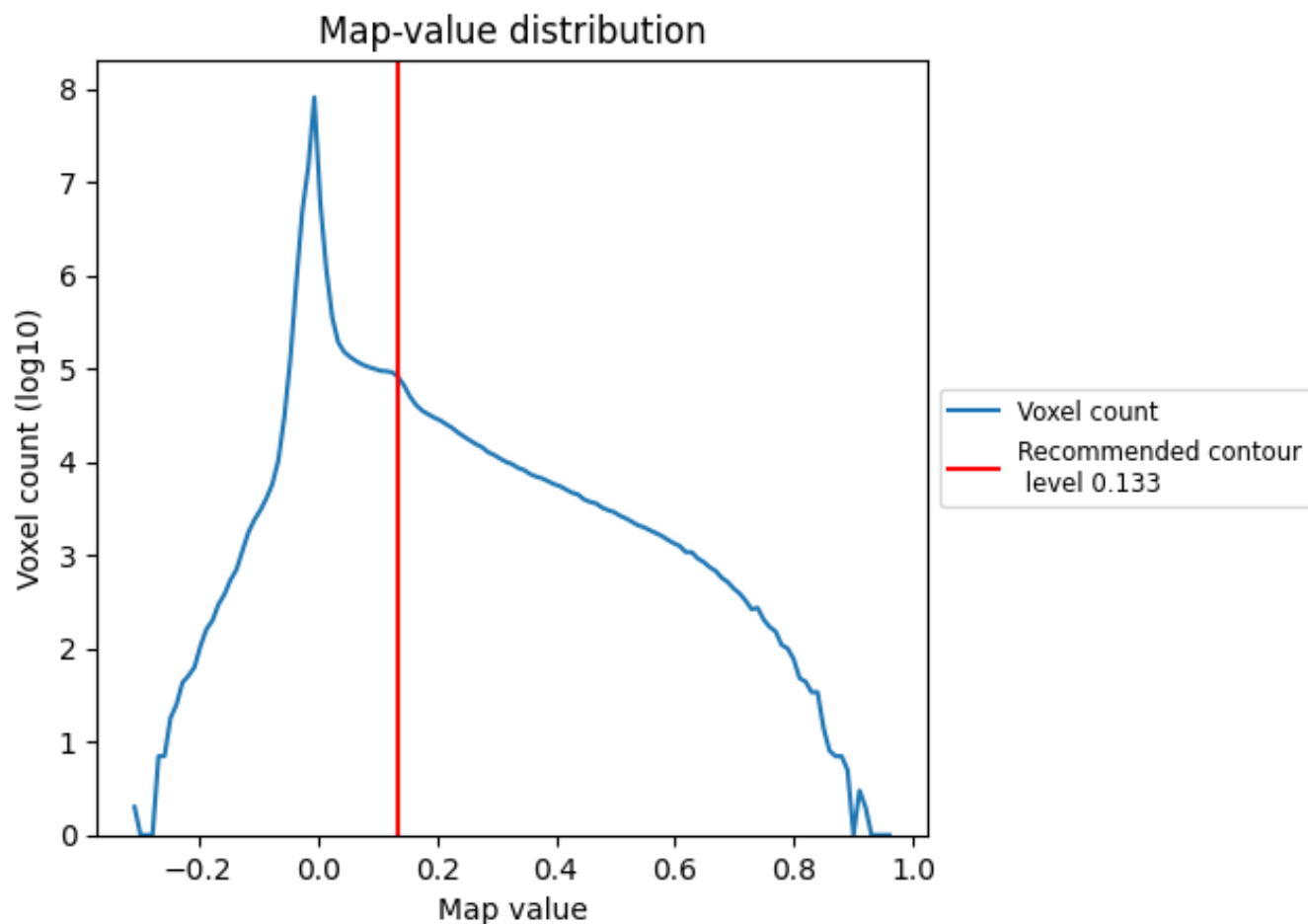
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

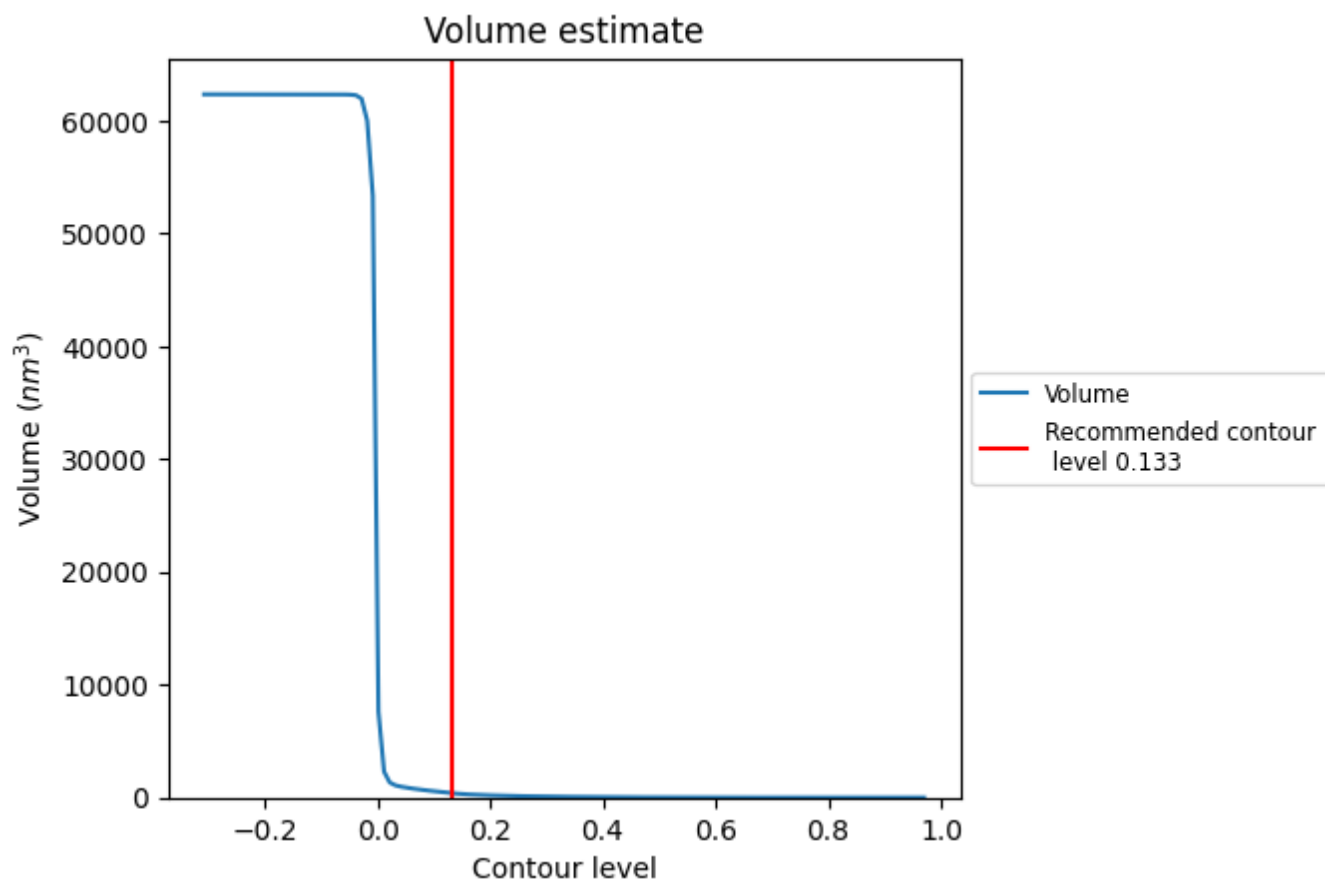
This section contains the results of statistical analysis of the map.

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.

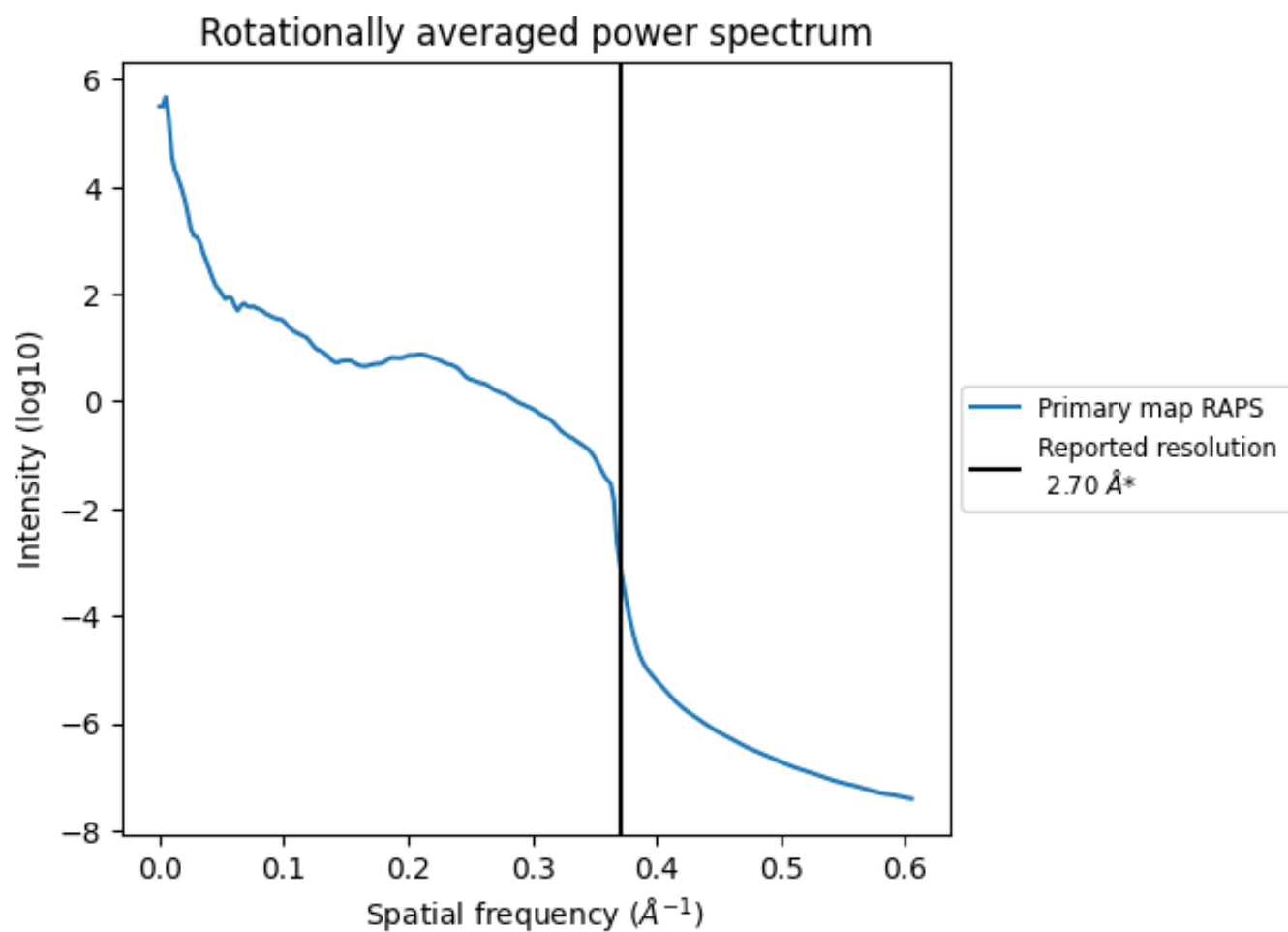
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 390 nm³; this corresponds to an approximate mass of 352 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 0.370 \AA^{-1}

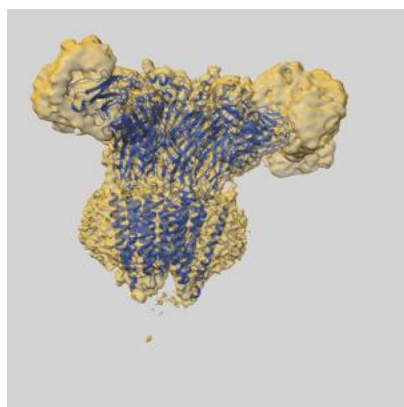
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

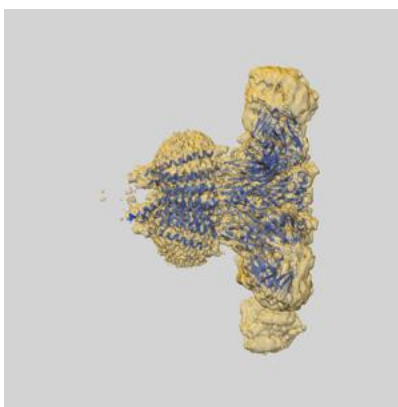
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23913 and PDB model 7MLY. Per-residue inclusion information can be found in section [3](#) on page [14](#).

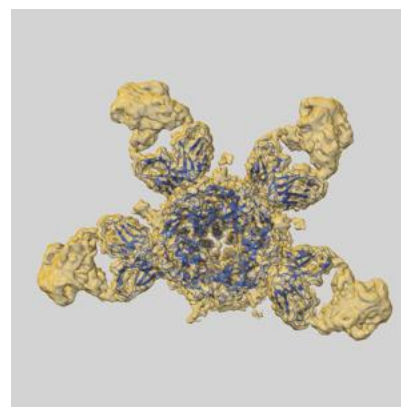
9.1 Map-model overlay [i](#)



X



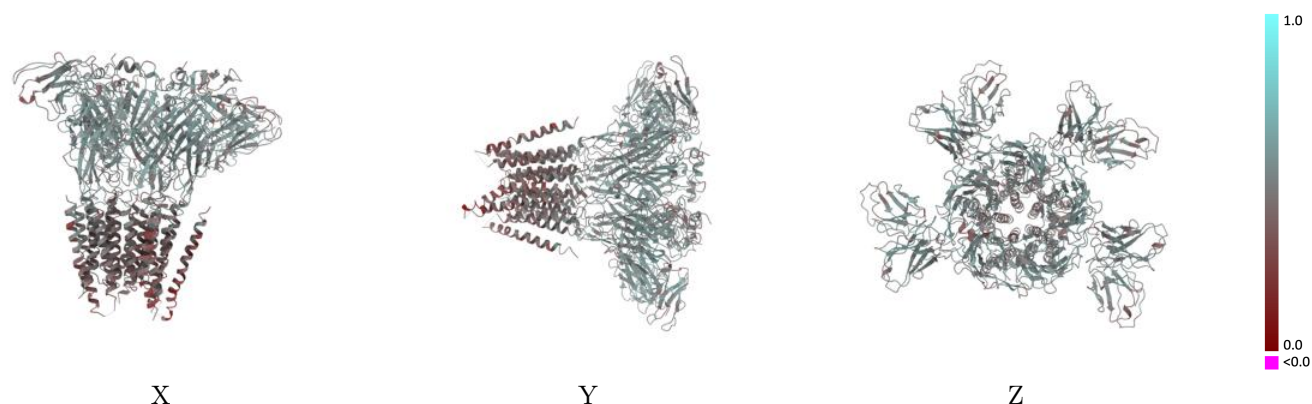
Y



Z

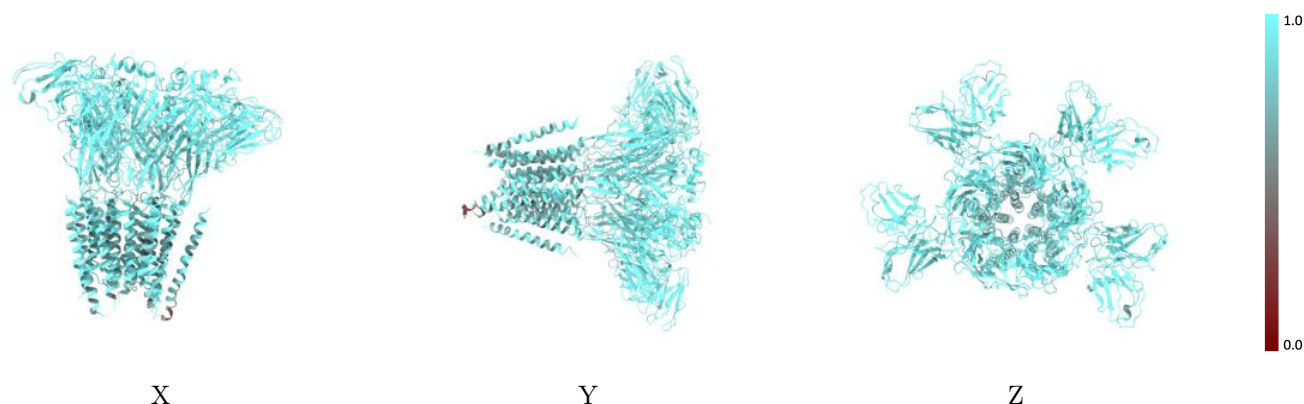
The images above show the 3D surface view of the map at the recommended contour level 0.133 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



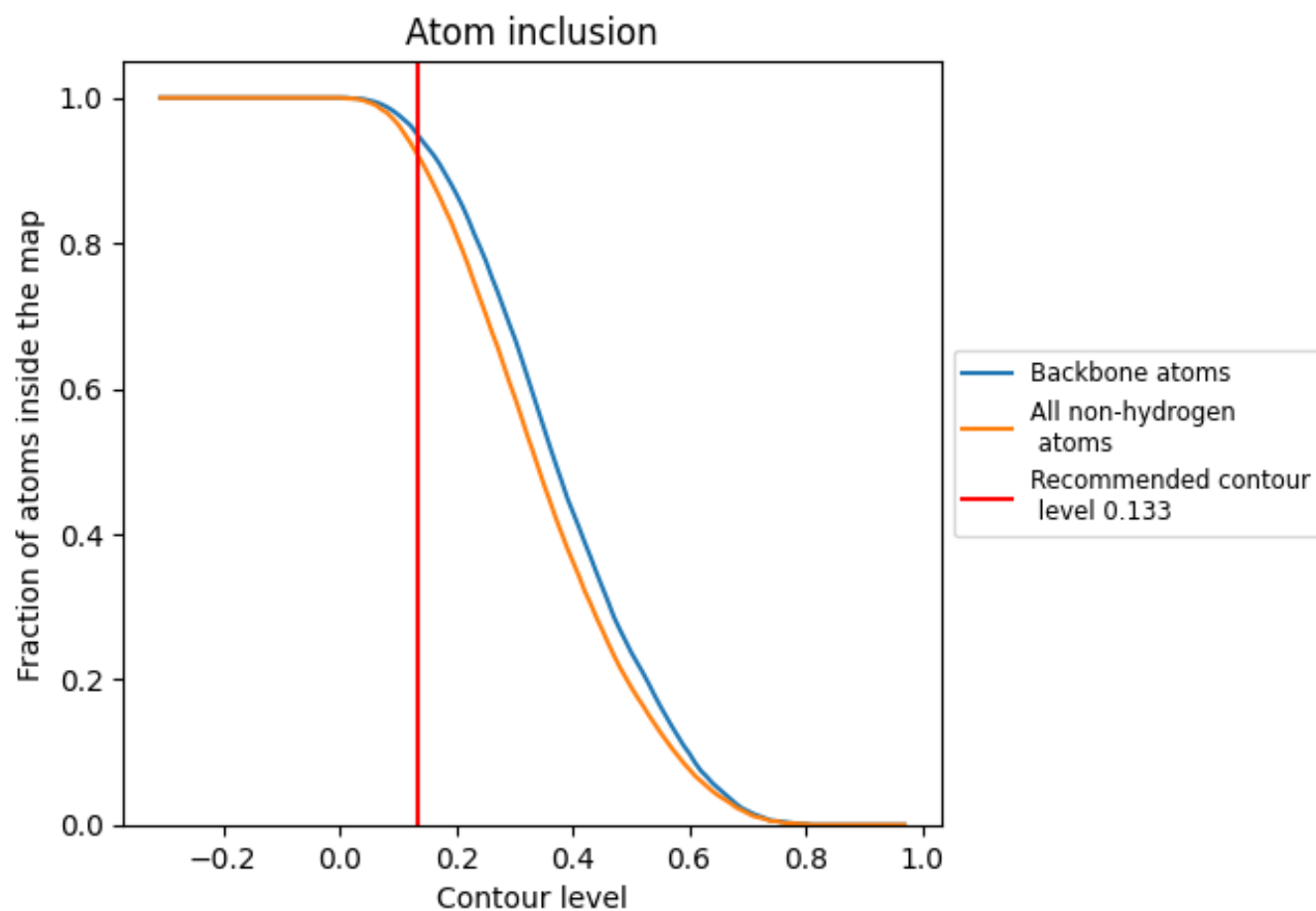
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.133).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 92% 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 (0.133) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9230	 0.4900
A	 0.9270	 0.4950
B	 0.9180	 0.4810
C	 0.9020	 0.4740
D	 0.9180	 0.4900
E	 0.9230	 0.4860
F	 0.9520	 0.5230
G	 0.9550	 0.5150
H	 0.9550	 0.5180
I	 0.9410	 0.4820
J	 0.9520	 0.4830
K	 0.9600	 0.5070
L	 0.9540	 0.5150
M	 0.9280	 0.4860
T	 0.9510	 0.4550
Z	 0.4750	 0.3890
f	 0.7000	 0.3830
l	 0.8800	 0.4110
r	 0.8210	 0.3670

