



## Full wwPDB EM Validation Report ⓘ

Jun 14, 2025 – 12:45 PM EDT

PDB ID : 9CU5 / pdb\_00009cu5  
EMDB ID : EMD-45928  
Title : LJF-085 Fab in complex with HIV Env JRFL NFL TD CC3+ trimer and 35O22 Fab  
Authors : Ozorowski, G.; Ward, A.B.  
Deposited on : 2024-07-25  
Resolution : 3.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
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) : 2.44

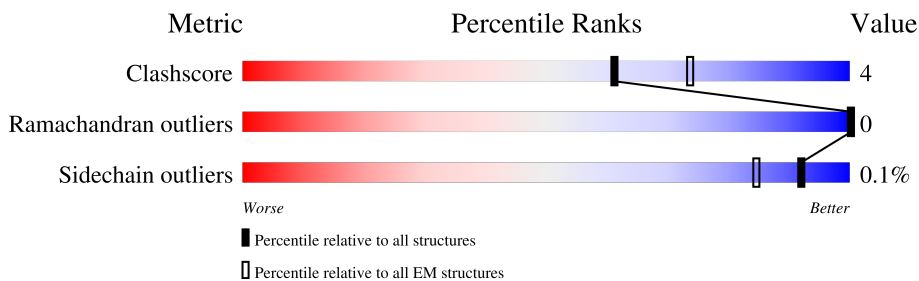
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	D	131	<div> <div>15%</div> <div>87%</div> <div>11%</div> <div>•</div> </div>
1	F	131	<div> <div>19%</div> <div>93%</div> <div>5%</div> <div>•</div> </div>
1	J	131	<div> <div>13%</div> <div>88%</div> <div>11%</div> <div>•</div> </div>
2	E	114	<div> <div>23%</div> <div>92%</div> <div>6%</div> <div>•</div> </div>
2	G	114	<div> <div>11%</div> <div>83%</div> <div>15%</div> <div>•</div> </div>
2	K	114	<div> <div>28%</div> <div>88%</div> <div>11%</div> <div>•</div> </div>
3	H	123	<div> <div>•</div> <div>90%</div> <div>8%</div> <div>•</div> </div>
3	I	123	<div> <div>•</div> <div>93%</div> <div>5%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
4	L	107	
4	M	107	
5	A	649	
5	B	649	
5	C	649	
6	N	5	
6	Q	5	
6	U	5	
7	O	2	
7	R	2	
7	S	2	
7	V	2	
8	P	5	
9	T	10	
10	W	4	

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 23538 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 35O22 heavy chain Fv.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	129	Total	C	N	O	S	0	0
			1009	646	170	188	5		
1	F	128	Total	C	N	O	S	0	0
			1003	643	169	186	5		
1	J	129	Total	C	N	O	S	0	0
			1009	646	170	188	5		

- Molecule 2 is a protein called 35O22 light chain Fv.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	112	Total	C	N	O	S	0	0
			851	533	141	171	6		
2	G	112	Total	C	N	O	S	0	0
			851	533	141	171	6		
2	K	112	Total	C	N	O	S	0	0
			851	533	141	171	6		

- Molecule 3 is a protein called LJF-085 heavy chain Fv.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	121	Total	C	N	O	S	0	0
			947	605	158	181	3		
3	I	121	Total	C	N	O	S	0	0
			947	605	158	181	3		

- Molecule 4 is a protein called LJF-085 light chain Fv.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	106	Total	C	N	O	S	0	0
			822	511	147	159	5		
4	M	106	Total	C	N	O	S	0	0
			822	511	147	159	5		

- Molecule 5 is a protein called HIV Env JRFL NFL TD CC3+ gp140.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	569	Total	C	N	O	S	0	0
			4529	2851	798	845	35		
5	B	561	Total	C	N	O	S	0	0
			4466	2813	784	835	34		
5	A	554	Total	C	N	O	S	0	0
			4405	2776	774	821	34		

There are 153 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	47	ASP	GLU	engineered mutation	UNP Q75760
C	49	GLU	THR	engineered mutation	UNP Q75760
C	65	LYS	VAL	engineered mutation	UNP Q75760
C	106	THR	GLU	engineered mutation	UNP Q75760
C	164	GLU	SER	engineered mutation	UNP Q75760
C	165	LEU	ILE	engineered mutation	UNP Q75760
C	168	LYS	GLU	engineered mutation	UNP Q75760
C	172	VAL	GLU	engineered mutation	UNP Q75760
C	302	TYR	ASN	engineered mutation	UNP Q75760
C	308	ARG	HIS	engineered mutation	UNP Q75760
C	320	MET	THR	engineered mutation	UNP Q75760
C	429	ARG	GLU	engineered mutation	UNP Q75760
C	432	GLN	LYS	engineered mutation	UNP Q75760
C	500	ARG	LYS	engineered mutation	UNP Q75760
C	501	CYS	ALA	engineered mutation	UNP Q75760
C	505C	GLY	-	insertion	UNP Q75760
C	505D	GLY	-	insertion	UNP Q75760
C	505E	GLY	-	insertion	UNP Q75760
C	505F	GLY	-	insertion	UNP Q75760
C	505G	SER	-	insertion	UNP Q75760
C	505H	GLY	-	insertion	UNP Q75760
C	505I	GLY	ARG	engineered mutation	UNP Q75760
C	505J	GLY	GLU	engineered mutation	UNP Q75760
C	505K	GLY	LYS	engineered mutation	UNP Q75760
C	505L	SER	ARG	engineered mutation	UNP Q75760
C	519	ARG	PHE	engineered mutation	UNP Q75760
C	520	ARG	LEU	engineered mutation	UNP Q75760
C	543	ASN	LEU	engineered mutation	UNP Q75760
C	551	PRO	GLN	engineered mutation	UNP Q75760
C	553	SER	ASN	engineered mutation	UNP Q75760
C	559	PRO	ILE	engineered mutation	UNP Q75760
C	569	GLY	THR	engineered mutation	UNP Q75760

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Chain	Residue	Modelled	Actual	Comment	Reference
C	588	ARG	GLY	engineered mutation	UNP Q75760
C	662	CYS	GLU	engineered mutation	UNP Q75760
C	665	GLY	-	expression tag	UNP Q75760
C	666	GLY	-	expression tag	UNP Q75760
C	667	GLY	-	expression tag	UNP Q75760
C	668	GLY	-	expression tag	UNP Q75760
C	669	SER	-	expression tag	UNP Q75760
C	670	HIS	-	expression tag	UNP Q75760
C	671	HIS	-	expression tag	UNP Q75760
C	672	HIS	-	expression tag	UNP Q75760
C	673	HIS	-	expression tag	UNP Q75760
C	674	HIS	-	expression tag	UNP Q75760
C	675	HIS	-	expression tag	UNP Q75760
C	676	HIS	-	expression tag	UNP Q75760
C	677	HIS	-	expression tag	UNP Q75760
C	678	GLY	-	expression tag	UNP Q75760
C	679	SER	-	expression tag	UNP Q75760
C	680	GLY	-	expression tag	UNP Q75760
C	681	CYS	-	expression tag	UNP Q75760
B	47	ASP	GLU	engineered mutation	UNP Q75760
B	49	GLU	THR	engineered mutation	UNP Q75760
B	65	LYS	VAL	engineered mutation	UNP Q75760
B	106	THR	GLU	engineered mutation	UNP Q75760
B	164	GLU	SER	engineered mutation	UNP Q75760
B	165	LEU	ILE	engineered mutation	UNP Q75760
B	168	LYS	GLU	engineered mutation	UNP Q75760
B	172	VAL	GLU	engineered mutation	UNP Q75760
B	302	TYR	ASN	engineered mutation	UNP Q75760
B	308	ARG	HIS	engineered mutation	UNP Q75760
B	320	MET	THR	engineered mutation	UNP Q75760
B	429	ARG	GLU	engineered mutation	UNP Q75760
B	432	GLN	LYS	engineered mutation	UNP Q75760
B	500	ARG	LYS	engineered mutation	UNP Q75760
B	501	CYS	ALA	engineered mutation	UNP Q75760
B	503E	GLY	-	insertion	UNP Q75760
B	503F	GLY	-	insertion	UNP Q75760
B	503G	GLY	-	insertion	UNP Q75760
B	503H	GLY	-	insertion	UNP Q75760
B	503I	SER	-	insertion	UNP Q75760
B	503J	GLY	-	insertion	UNP Q75760
B	503K	GLY	ARG	engineered mutation	UNP Q75760
B	503L	GLY	GLU	engineered mutation	UNP Q75760

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Chain	Residue	Modelled	Actual	Comment	Reference
B	503M	GLY	LYS	engineered mutation	UNP Q75760
B	503N	SER	ARG	engineered mutation	UNP Q75760
B	503V	ARG	PHE	engineered mutation	UNP Q75760
B	520	ARG	LEU	engineered mutation	UNP Q75760
B	543	ASN	LEU	engineered mutation	UNP Q75760
B	551	PRO	GLN	engineered mutation	UNP Q75760
B	553	SER	ASN	engineered mutation	UNP Q75760
B	559	PRO	ILE	engineered mutation	UNP Q75760
B	569	GLY	THR	engineered mutation	UNP Q75760
B	588	ARG	GLY	engineered mutation	UNP Q75760
B	662	CYS	GLU	engineered mutation	UNP Q75760
B	665	GLY	-	expression tag	UNP Q75760
B	666	GLY	-	expression tag	UNP Q75760
B	667	GLY	-	expression tag	UNP Q75760
B	668	GLY	-	expression tag	UNP Q75760
B	669	SER	-	expression tag	UNP Q75760
B	670	HIS	-	expression tag	UNP Q75760
B	671	HIS	-	expression tag	UNP Q75760
B	672	HIS	-	expression tag	UNP Q75760
B	673	HIS	-	expression tag	UNP Q75760
B	674	HIS	-	expression tag	UNP Q75760
B	675	HIS	-	expression tag	UNP Q75760
B	676	HIS	-	expression tag	UNP Q75760
B	677	HIS	-	expression tag	UNP Q75760
B	678	GLY	-	expression tag	UNP Q75760
B	679	SER	-	expression tag	UNP Q75760
B	680	GLY	-	expression tag	UNP Q75760
B	681	CYS	-	expression tag	UNP Q75760
A	47	ASP	GLU	engineered mutation	UNP Q75760
A	49	GLU	THR	engineered mutation	UNP Q75760
A	65	LYS	VAL	engineered mutation	UNP Q75760
A	106	THR	GLU	engineered mutation	UNP Q75760
A	164	GLU	SER	engineered mutation	UNP Q75760
A	165	LEU	ILE	engineered mutation	UNP Q75760
A	168	LYS	GLU	engineered mutation	UNP Q75760
A	172	VAL	GLU	engineered mutation	UNP Q75760
A	302	TYR	ASN	engineered mutation	UNP Q75760
A	308	ARG	HIS	engineered mutation	UNP Q75760
A	320	MET	THR	engineered mutation	UNP Q75760
A	429	ARG	GLU	engineered mutation	UNP Q75760
A	432	GLN	LYS	engineered mutation	UNP Q75760
A	500	ARG	LYS	engineered mutation	UNP Q75760

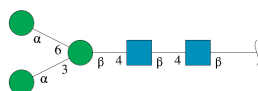
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Chain	Residue	Modelled	Actual	Comment	Reference
A	501	CYS	ALA	engineered mutation	UNP Q75760
A	503E	GLY	-	insertion	UNP Q75760
A	503F	GLY	-	insertion	UNP Q75760
A	503G	GLY	-	insertion	UNP Q75760
A	503H	GLY	-	insertion	UNP Q75760
A	503I	SER	-	insertion	UNP Q75760
A	503J	GLY	-	insertion	UNP Q75760
A	503K	GLY	ARG	engineered mutation	UNP Q75760
A	503L	GLY	GLU	engineered mutation	UNP Q75760
A	503M	GLY	LYS	engineered mutation	UNP Q75760
A	503N	SER	ARG	engineered mutation	UNP Q75760
A	519	ARG	PHE	engineered mutation	UNP Q75760
A	520	ARG	LEU	engineered mutation	UNP Q75760
A	543	ASN	LEU	engineered mutation	UNP Q75760
A	551	PRO	GLN	engineered mutation	UNP Q75760
A	553	SER	ASN	engineered mutation	UNP Q75760
A	559	PRO	ILE	engineered mutation	UNP Q75760
A	569	GLY	THR	engineered mutation	UNP Q75760
A	588	ARG	GLY	engineered mutation	UNP Q75760
A	662	CYS	GLU	engineered mutation	UNP Q75760
A	665	GLY	-	expression tag	UNP Q75760
A	666	GLY	-	expression tag	UNP Q75760
A	667	GLY	-	expression tag	UNP Q75760
A	668	GLY	-	expression tag	UNP Q75760
A	669	SER	-	expression tag	UNP Q75760
A	670	HIS	-	expression tag	UNP Q75760
A	671	HIS	-	expression tag	UNP Q75760
A	672	HIS	-	expression tag	UNP Q75760
A	673	HIS	-	expression tag	UNP Q75760
A	674	HIS	-	expression tag	UNP Q75760
A	675	HIS	-	expression tag	UNP Q75760
A	676	HIS	-	expression tag	UNP Q75760
A	677	HIS	-	expression tag	UNP Q75760
A	678	GLY	-	expression tag	UNP Q75760
A	679	SER	-	expression tag	UNP Q75760
A	680	GLY	-	expression tag	UNP Q75760
A	681	CYS	-	expression tag	UNP Q75760

- 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.





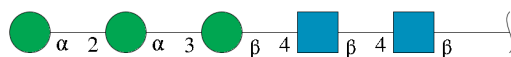
Mol	Chain	Residues	Atoms				AltConf	Trace
6	N	5	Total	C	N	O	0	0
			61	34	2	25		
6	Q	5	Total	C	N	O	0	0
			61	34	2	25		
6	U	5	Total	C	N	O	0	0
			61	34	2	25		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	2	Total	C	N	O	0	0
			28	16	2	10		
7	R	2	Total	C	N	O	0	0
			28	16	2	10		
7	S	2	Total	C	N	O	0	0
			28	16	2	10		
7	V	2	Total	C	N	O	0	0
			28	16	2	10		

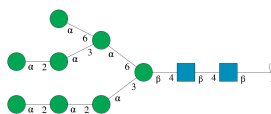
- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyra

nose-(1-3)-[alpha-D-mannopyranose-(1-6)]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.



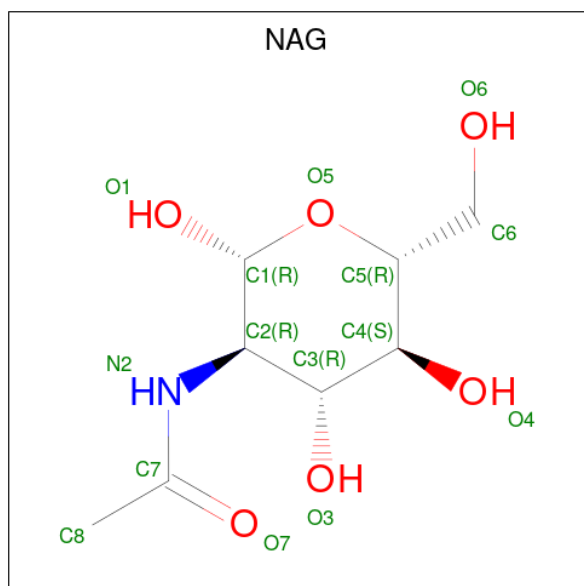
Mol	Chain	Residues	Atoms				AltConf	Trace
9	T	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 10 is an oligosaccharide called 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
10	W	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

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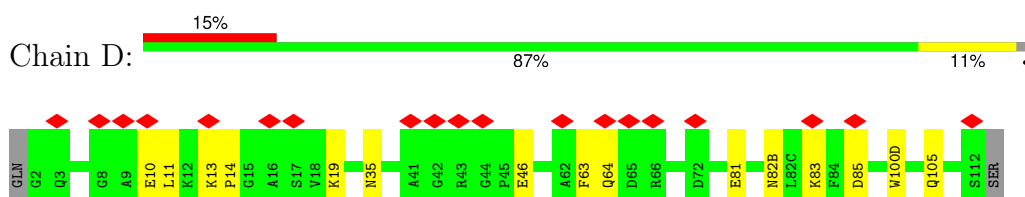
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Mol	Chain	Residues	Atoms				AltConf
11	B	1	Total	C	N	O	0
			14	8	1	5	
11	B	1	Total	C	N	O	0
			14	8	1	5	
11	A	1	Total	C	N	O	0
			14	8	1	5	
11	A	1	Total	C	N	O	0
			14	8	1	5	
11	A	1	Total	C	N	O	0
			14	8	1	5	
11	A	1	Total	C	N	O	0
			14	8	1	5	
11	A	1	Total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

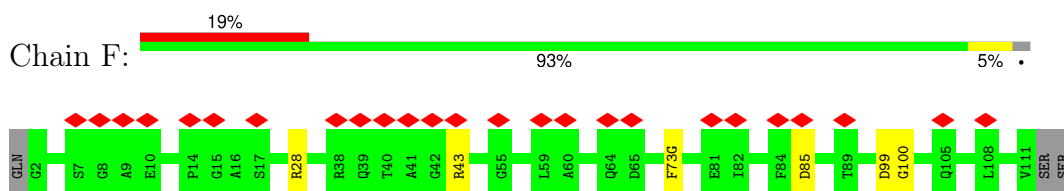
### 3 Residue-property plots [i](#)

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.

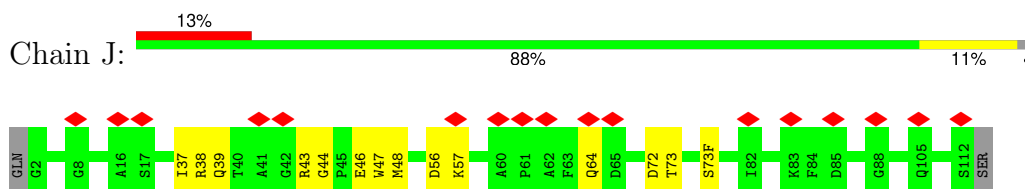
- Molecule 1: 35O22 heavy chain Fv



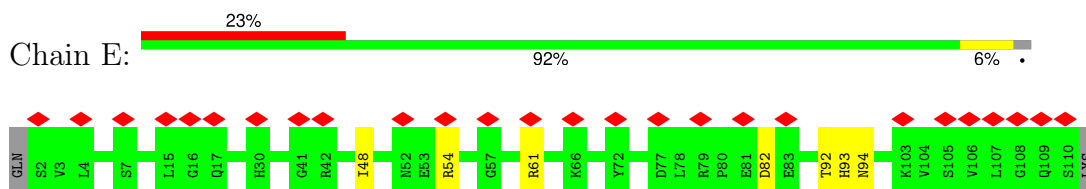
- Molecule 1: 35O22 heavy chain Fv



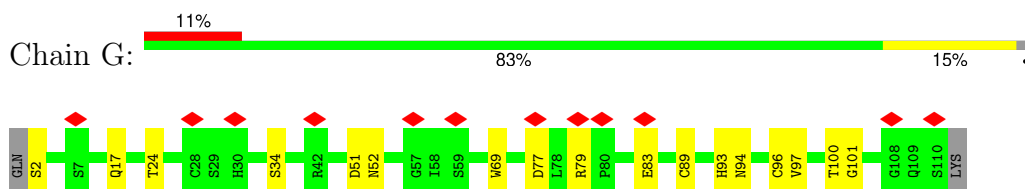
- Molecule 1: 35O22 heavy chain Fv



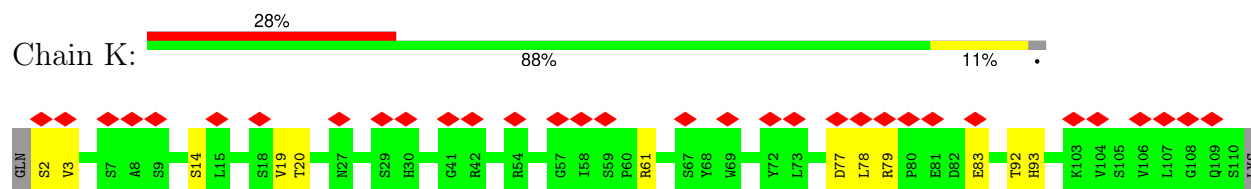
- Molecule 2: 35O22 light chain Fv



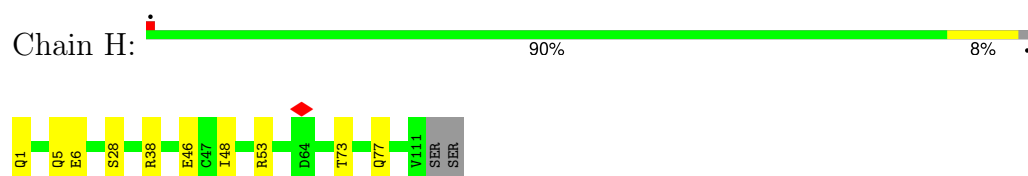
- Molecule 2: 35O22 light chain Fv



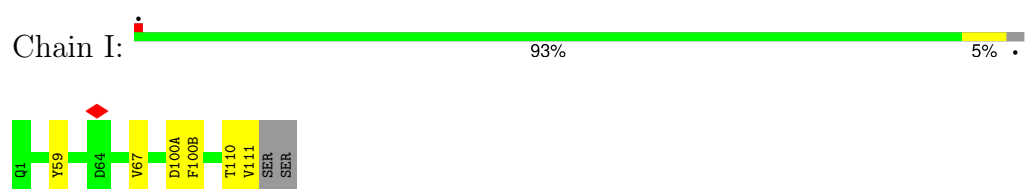
- Molecule 2: 35O22 light chain Fv



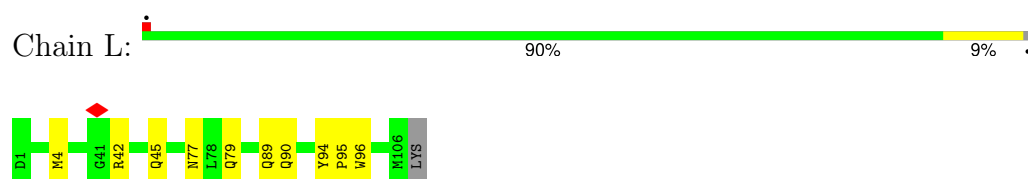
- Molecule 3: LJF-085 heavy chain Fv



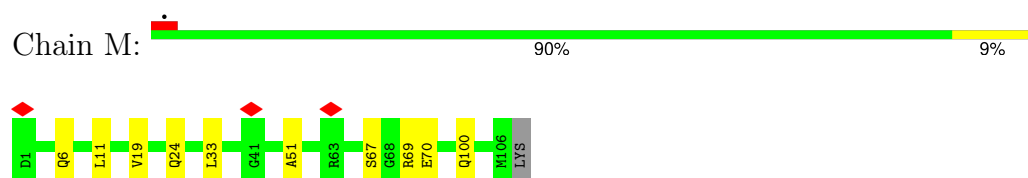
- Molecule 3: LJF-085 heavy chain Fv



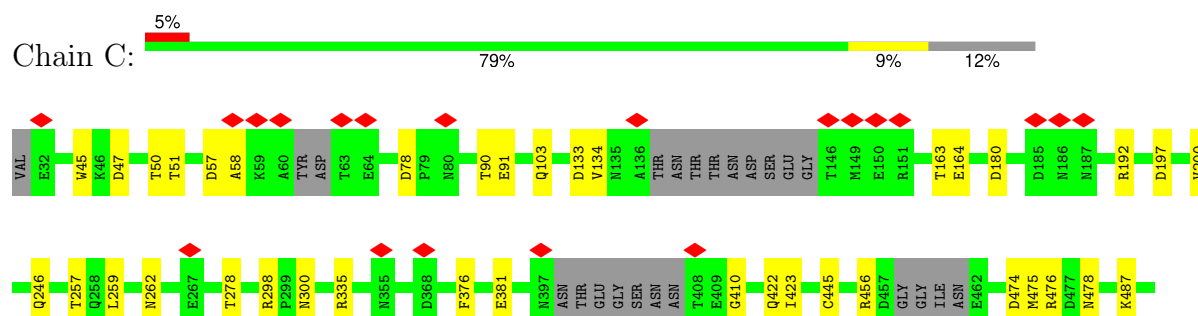
- Molecule 4: LJF-085 light chain Fv

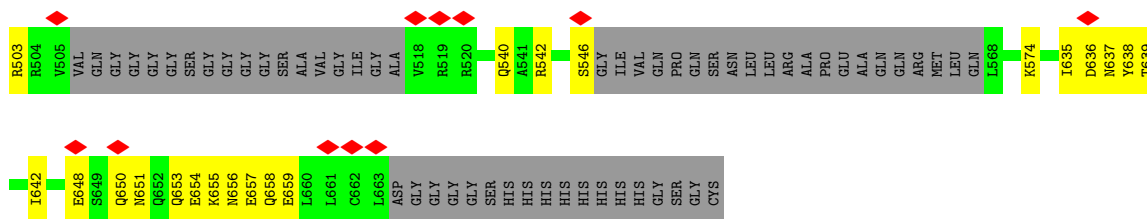


- Molecule 4: LJF-085 light chain Fv

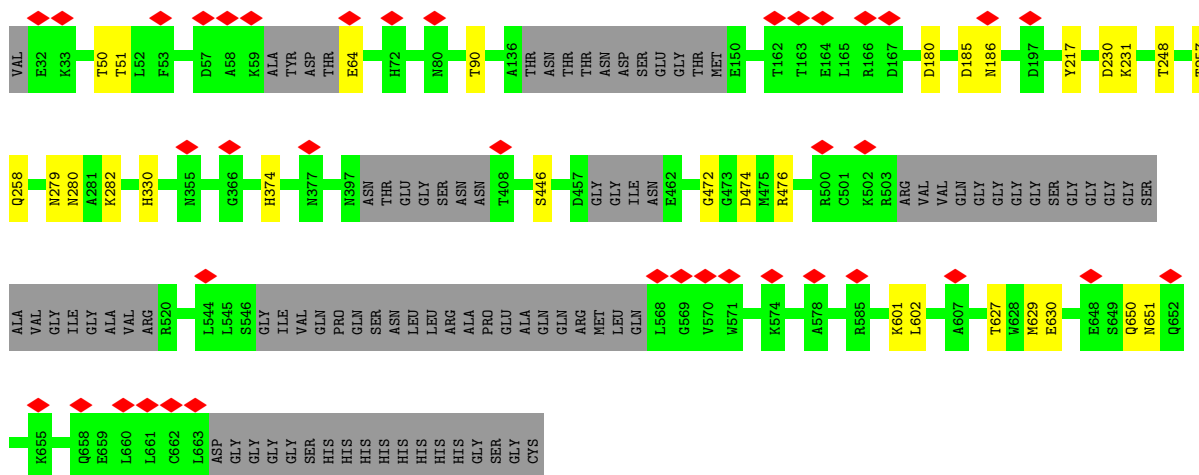
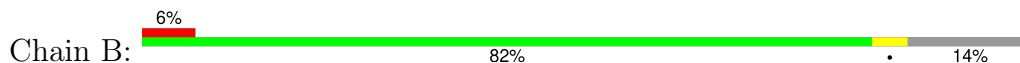


- Molecule 5: HIV Env JRFL NFL TD CC3+ gp140

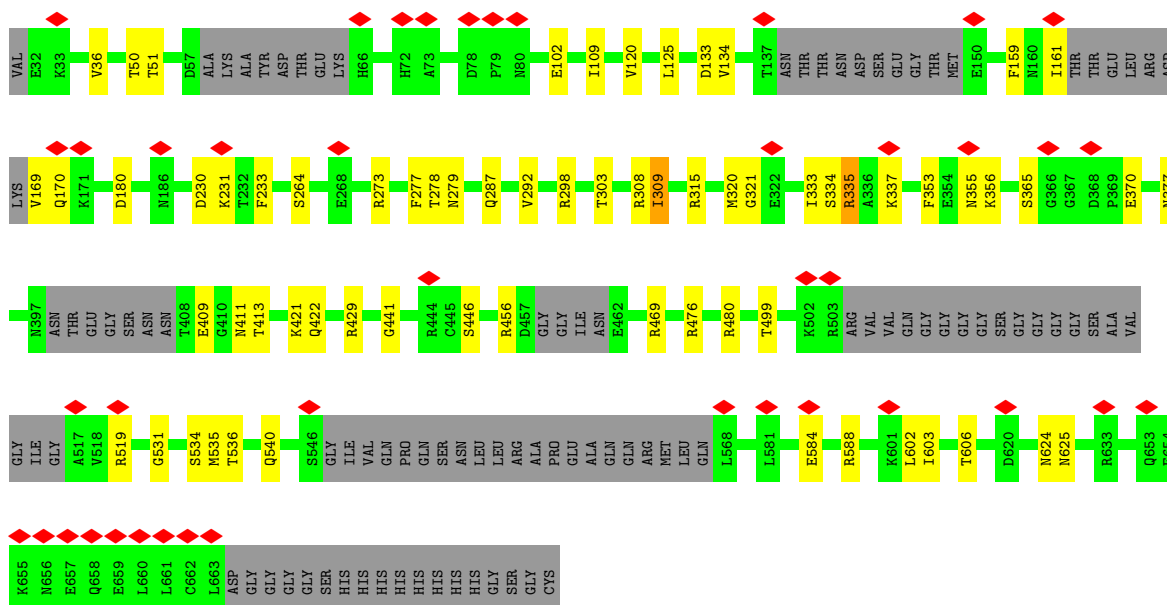
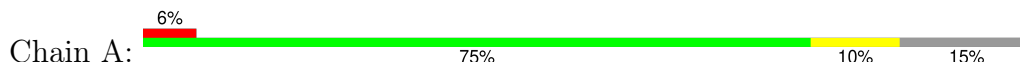




• Molecule 5: HIV Env JRFL NFL TD CC3+ gp140



• Molecule 5: HIV Env JRFL NFL TD CC3+ gp140



• 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-glucopyra

nose

Chain N: 



• 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 Q: 



• 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 U: 



• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 



• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R: 



• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S: 

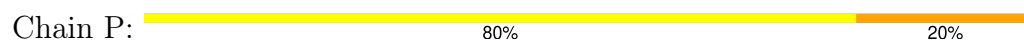


• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

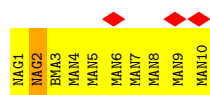
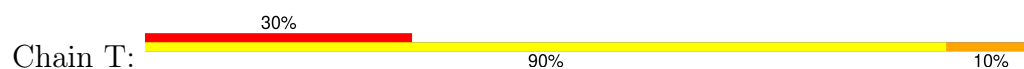




- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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 10: 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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	64443	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	190000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.786	Depositor
Minimum map value	-0.469	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	459.51358, 459.51358, 459.51358	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0257, 1.0257, 1.0257	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MAN, 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	D	0.33	0/1037	0.64	0/1408
1	F	0.38	0/1031	0.68	0/1400
1	J	0.31	0/1037	0.63	0/1408
2	E	0.25	0/875	0.55	0/1195
2	G	0.28	0/875	0.60	0/1195
2	K	0.31	0/875	0.62	0/1195
3	H	0.29	0/973	0.56	0/1329
3	I	0.24	0/973	0.56	0/1329
4	L	0.35	0/842	0.67	0/1141
4	M	0.33	0/842	0.51	0/1141
5	A	0.33	0/4492	0.64	1/6090 (0.0%)
5	B	0.25	0/4554	0.54	0/6172
5	C	0.23	0/4617	0.50	0/6257
All	All	0.29	0/23023	0.58	1/31260 (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( $^{\circ}$ )
5	A	309	ILE	N-CA-C	5.29	116.01	110.62

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	D	1009	0	980	13	0
1	F	1003	0	975	9	0
1	J	1009	0	980	11	0
2	E	851	0	800	4	0
2	G	851	0	800	12	0
2	K	851	0	800	9	0
3	H	947	0	911	6	0
3	I	947	0	911	4	0
4	L	822	0	788	10	0
4	M	822	0	788	9	0
5	A	4405	0	4329	56	0
5	B	4466	0	4393	20	0
5	C	4529	0	4465	45	0
6	N	61	0	52	0	0
6	Q	61	0	52	0	0
6	U	61	0	52	0	0
7	O	28	0	25	0	0
7	R	28	0	25	0	0
7	S	28	0	25	0	0
7	V	28	0	25	0	0
8	P	61	0	52	1	0
9	T	116	0	97	1	0
10	W	50	0	43	0	0
11	A	168	0	156	0	0
11	B	168	0	156	1	0
11	C	168	0	156	0	0
All	All	23538	0	22836	193	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 4.

All (193) 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)
4:L:42:ARG:HH22	4:L:45:GLN:NE2	1.40	1.17
3:H:38:ARG:NH2	3:H:46:GLU:OE2	1.90	1.03
2:G:93:HIS:CD2	2:G:94:ASN:OD1	2.12	1.01
5:A:365:SER:HB3	5:A:469:ARG:NH1	1.75	1.01
4:L:42:ARG:HH22	4:L:45:GLN:HE21	1.10	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:ARG:NE	1:F:85:ASP:OD1	1.95	0.97
4:L:42:ARG:NH2	4:L:45:GLN:NE2	2.12	0.97
4:M:69:ARG:NH2	5:B:472:GLY:O	1.97	0.97
5:A:355:ASN:O	5:A:356:LYS:HG3	1.72	0.90
1:D:13:LYS:CG	1:D:14:PRO:HD2	2.02	0.89
5:C:103:GLN:NE2	5:C:574:LYS:HZ1	1.71	0.87
4:L:42:ARG:NH2	4:L:45:GLN:HE21	1.69	0.87
1:F:43:ARG:HE	1:F:85:ASP:CG	1.82	0.86
2:E:48:ILE:HG12	2:E:54:ARG:HG2	1.58	0.85
5:C:103:GLN:NE2	5:C:574:LYS:NZ	2.24	0.85
1:J:43:ARG:HD2	1:J:46:GLU:OE2	1.78	0.83
2:K:14:SER:O	2:K:78:LEU:HD12	1.80	0.80
2:G:93:HIS:HD2	2:G:94:ASN:OD1	1.61	0.80
5:C:200:VAL:HB	5:A:315:ARG:NH1	1.96	0.80
5:A:109:ILE:CG2	5:A:429:ARG:NH2	2.46	0.78
5:C:200:VAL:HB	5:A:315:ARG:HH11	1.51	0.76
5:C:503:ARG:NH1	5:C:654:GLU:OE2	2.18	0.76
1:D:13:LYS:HG2	1:D:14:PRO:HD2	1.66	0.75
5:A:365:SER:HB3	5:A:469:ARG:HH11	1.47	0.75
1:D:13:LYS:HG3	1:D:14:PRO:HD2	1.67	0.75
4:M:24:GLN:NE2	4:M:70:GLU:HG2	2.02	0.74
5:C:648:GLU:OE2	5:A:519:ARG:NH1	2.21	0.74
3:I:59:TYR:CD2	3:I:67:VAL:HG13	2.22	0.74
3:I:59:TYR:HD2	3:I:67:VAL:HG13	1.56	0.71
1:F:28:ARG:HD3	1:F:73(G):PHE:HA	1.73	0.71
5:C:475:MET:SD	5:C:478:ASN:ND2	2.64	0.70
5:A:169:VAL:N	5:A:170:GLN:OE1	2.25	0.70
2:K:61:ARG:HD2	2:K:77:ASP:HB3	1.72	0.69
5:A:109:ILE:HG23	5:A:429:ARG:NH2	2.06	0.69
5:A:109:ILE:CG2	5:A:429:ARG:HH22	2.05	0.69
5:C:650:GLN:O	5:C:654:GLU:HG2	1.91	0.69
1:J:38:ARG:HD3	1:J:48:MET:SD	2.32	0.69
1:J:38:ARG:NH2	1:J:46:GLU:OE1	2.26	0.69
1:J:72:ASP:OD1	1:J:73:THR:N	2.27	0.68
3:H:1:GLN:OE1	3:H:1:GLN:N	2.28	0.67
5:A:365:SER:CB	5:A:469:ARG:NH1	2.56	0.65
4:L:4:MET:SD	4:L:90:GLN:NE2	2.69	0.65
5:B:64:GLU:N	5:B:64:GLU:OE1	2.30	0.65
2:G:93:HIS:CD2	2:G:94:ASN:CG	2.75	0.64
5:C:659:GLU:OE2	5:A:499:THR:HG21	1.98	0.64
5:C:103:GLN:HE21	5:C:574:LYS:NZ	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:335:ARG:NE	5:C:410:GLY:O	2.30	0.63
1:D:46:GLU:N	1:D:46:GLU:OE1	2.32	0.62
5:C:103:GLN:HE21	5:C:574:LYS:HZ1	1.43	0.62
4:L:77:ASN:OD1	4:L:79:GLN:NE2	2.33	0.62
1:F:28:ARG:HD3	1:F:73(G):PHE:CA	2.29	0.62
5:C:659:GLU:OE2	5:A:499:THR:CG2	2.48	0.62
5:C:78:ASP:OD2	5:C:246:GLN:NE2	2.32	0.62
5:C:542:ARG:NH1	5:C:546:SER:OG	2.32	0.61
5:B:330:HIS:NE2	11:B:705:NAG:H3	2.16	0.60
5:C:655:LYS:HZ1	5:A:603:ILE:HG23	1.66	0.60
5:A:298:ARG:NH2	5:A:441:GLY:O	2.35	0.60
5:C:635:ILE:O	5:C:639:THR:N	2.33	0.60
2:G:96:CYS:SG	2:G:97:VAL:N	2.74	0.60
1:F:43:ARG:NE	1:F:85:ASP:CG	2.52	0.59
5:A:109:ILE:HG21	5:A:429:ARG:NH2	2.15	0.59
5:C:651:ASN:HA	5:C:654:GLU:OE2	2.02	0.59
1:D:10:GLU:OE1	1:D:10:GLU:N	2.35	0.59
5:C:180:ASP:OD2	5:C:422:GLN:HB2	2.03	0.59
1:D:35:ASN:ND2	1:D:100(D):TRP:O	2.35	0.58
5:C:262:ASN:OD1	8:P:1:NAG:N2	2.36	0.58
5:A:102:GLU:OE1	5:A:102:GLU:N	2.37	0.57
4:M:6:GLN:O	4:M:100:GLN:NE2	2.38	0.57
4:M:24:GLN:HE22	4:M:70:GLU:HG2	1.68	0.57
1:F:99:ASP:OD1	1:F:100:GLY:N	2.38	0.56
5:C:653:GLN:O	5:C:657:GLU:HG2	2.05	0.56
4:M:70:GLU:OE2	5:B:282:LYS:NZ	2.38	0.56
1:F:28:ARG:NH2	5:C:90:THR:OG1	2.38	0.56
1:J:38:ARG:CD	1:J:48:MET:SD	2.94	0.56
5:B:257:THR:O	5:B:374:HIS:ND1	2.39	0.56
2:G:24:THR:OG1	2:G:69:TRP:O	2.23	0.55
5:C:192:ARG:NH1	5:C:197:ASP:OD1	2.39	0.55
5:C:540:GLN:N	5:C:540:GLN:OE1	2.39	0.55
5:C:656:ASN:HD22	5:A:535:MET:HE1	1.70	0.55
2:G:17:GLN:OE1	2:G:17:GLN:N	2.41	0.54
1:J:43:ARG:CD	1:J:46:GLU:OE2	2.54	0.53
5:A:161:ILE:HG22	5:A:309:ILE:O	2.09	0.53
2:K:19:VAL:HG23	2:K:78:LEU:HD21	1.90	0.53
5:B:258:GLN:OE1	5:B:374:HIS:N	2.41	0.53
5:A:370:GLU:OE1	5:A:370:GLU:N	2.39	0.53
1:D:11:LEU:O	1:D:11:LEU:HG	2.09	0.53
5:B:474:ASP:OD1	5:B:474:ASP:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:42:ARG:HH22	4:L:45:GLN:CD	2.14	0.52
5:A:355:ASN:C	5:A:356:LYS:HG3	2.32	0.52
1:J:73(F):SER:O	5:B:90:THR:OG1	2.28	0.51
5:C:503:ARG:NH1	5:C:654:GLU:CD	2.68	0.51
5:C:180:ASP:CG	5:C:423:ILE:H	2.18	0.51
2:G:34:SER:OG	2:G:89:CYS:HB3	2.11	0.51
3:H:73:THR:OG1	3:H:77:GLN:N	2.43	0.51
5:A:125:LEU:CD1	5:A:309:ILE:HD12	2.41	0.51
5:A:320:MET:SD	5:A:422:GLN:NE2	2.85	0.50
2:K:19:VAL:CG2	2:K:78:LEU:HD21	2.41	0.50
2:K:83:GLU:OE1	2:K:83:GLU:N	2.43	0.50
1:D:13:LYS:HG2	1:D:14:PRO:CD	2.39	0.50
5:C:655:LYS:O	5:C:658:GLN:HG3	2.11	0.50
5:A:120:VAL:CG2	5:A:315:ARG:HE	2.25	0.50
5:C:45:TRP:NE1	5:C:91:GLU:OE2	2.44	0.50
2:K:77:ASP:O	2:K:79:ARG:HG3	2.12	0.49
5:A:377:ASN:O	5:A:377:ASN:OD1	2.29	0.49
1:J:64:GLN:N	1:J:64:GLN:OE1	2.45	0.49
3:H:38:ARG:HB2	3:H:48:ILE:HD11	1.94	0.49
5:C:50:THR:OG1	5:C:51:THR:N	2.45	0.49
5:A:355:ASN:O	5:A:356:LYS:CG	2.53	0.49
1:J:39:GLN:HE22	1:J:44:GLY:HA2	1.78	0.49
1:D:85:ASP:N	1:D:85:ASP:OD1	2.46	0.48
5:C:47:ASP:OD1	5:C:487:LYS:HE2	2.13	0.48
5:C:298:ARG:NE	5:C:381:GLU:OE1	2.46	0.48
5:B:446:SER:OG	9:T:2:NAG:O7	2.29	0.48
5:A:120:VAL:HG23	5:A:315:ARG:HE	1.79	0.48
3:I:110:THR:OG1	3:I:111:VAL:N	2.47	0.48
5:A:624:ASN:O	5:A:625:ASN:HB3	2.14	0.48
1:F:43:ARG:CD	1:F:85:ASP:OD1	2.61	0.47
5:C:638:TYR:O	5:C:642:ILE:HG13	2.13	0.47
5:A:109:ILE:HG21	5:A:429:ARG:HH22	1.73	0.47
2:E:61:ARG:NH2	2:E:82:ASP:OD2	2.48	0.47
3:H:28:SER:OG	3:H:53:ARG:NH2	2.47	0.47
1:J:56:ASP:OD1	1:J:57:LYS:N	2.48	0.47
5:C:474:ASP:OD2	5:C:476:ARG:NH1	2.46	0.47
5:B:50:THR:OG1	5:B:51:THR:N	2.47	0.47
5:A:303:THR:O	5:A:321:GLY:N	2.48	0.47
5:A:277:PHE:O	5:A:456:ARG:NH1	2.48	0.46
2:G:83:GLU:OE1	2:G:83:GLU:N	2.39	0.46
4:M:11:LEU:HD11	4:M:19:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2:SER:OG	2:G:100:THR:N	2.49	0.46
5:B:627:THR:OG1	5:B:630:GLU:OE1	2.33	0.46
5:A:278:THR:O	5:A:456:ARG:NH2	2.48	0.46
5:A:353:PHE:O	5:A:356:LYS:HD3	2.16	0.45
1:J:37:ILE:HD13	1:J:47:TRP:HA	1.99	0.45
5:A:36:VAL:O	5:A:606:THR:OG1	2.33	0.45
5:A:536:THR:O	5:A:540:GLN:NE2	2.47	0.45
5:C:300:ASN:OD1	5:C:300:ASN:N	2.49	0.45
3:I:100(A):ASP:OD1	3:I:100(B):PHE:N	2.48	0.45
5:A:159:PHE:CE1	5:A:309:ILE:HD11	2.52	0.45
2:E:93:HIS:ND1	2:E:94:ASN:OD1	2.48	0.45
5:A:584:GLU:OE2	5:A:588:ARG:NE	2.50	0.45
5:A:125:LEU:HD11	5:A:309:ILE:HD12	1.99	0.44
5:B:601:LYS:O	5:B:602:LEU:C	2.60	0.44
5:A:531:GLY:O	5:A:534:SER:OG	2.32	0.44
2:K:92:THR:OG1	2:K:93:HIS:N	2.50	0.44
5:C:133:ASP:OD1	5:C:134:VAL:N	2.50	0.44
5:C:278:THR:O	5:C:456:ARG:NH2	2.51	0.44
5:C:636:ASP:OD1	5:C:637:ASN:N	2.47	0.44
5:A:476:ARG:HH12	5:A:480:ARG:NH2	2.16	0.44
5:A:233:PHE:O	5:A:273:ARG:NE	2.42	0.44
2:G:100:THR:OG1	2:G:101:GLY:N	2.48	0.44
5:C:376:PHE:HE2	5:C:445:CYS:SG	2.41	0.44
5:B:279:ASN:O	5:B:280:ASN:HB3	2.18	0.43
5:A:50:THR:OG1	5:A:51:THR:N	2.51	0.43
5:A:335:ARG:HH12	5:A:409:GLU:HA	1.83	0.43
1:D:19:LYS:HE2	1:D:81:GLU:HB2	2.00	0.43
1:D:82(B):ASN:O	1:D:83:LYS:NZ	2.51	0.43
1:D:105:GLN:OE1	1:D:105:GLN:N	2.43	0.43
3:H:5:GLN:NE2	3:H:6:GLU:O	2.45	0.43
4:L:89:GLN:HE21	4:L:96:TRP:HB3	1.84	0.43
2:K:2:SER:OG	2:K:3:VAL:N	2.50	0.43
4:L:89:GLN:HE21	4:L:96:TRP:CB	2.32	0.43
5:B:230:ASP:OD1	5:B:231:LYS:N	2.48	0.43
4:L:94:TYR:CG	4:L:95:PRO:HA	2.54	0.42
5:A:133:ASP:OD1	5:A:134:VAL:N	2.53	0.42
5:A:180:ASP:OD1	5:A:421:LYS:HG3	2.19	0.42
5:C:655:LYS:NZ	5:A:602:LEU:HB2	2.34	0.42
5:A:333:ILE:HG12	5:A:334:SER:H	1.85	0.42
5:A:446:SER:O	5:A:446:SER:OG	2.38	0.42
5:C:655:LYS:HE2	5:A:603:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:217:TYR:H	5:B:248:THR:HG22	1.85	0.42
1:D:63:PHE:O	1:D:64:GLN:C	2.63	0.42
2:G:51:ASP:OD1	2:G:52:ASN:N	2.53	0.42
5:B:180:ASP:OD1	5:B:180:ASP:N	2.52	0.42
5:A:230:ASP:OD1	5:A:231:LYS:N	2.53	0.42
5:B:650:GLN:O	5:B:651:ASN:C	2.63	0.41
5:A:292:VAL:HG13	5:A:337:LYS:HB3	2.02	0.41
5:A:279:ASN:O	5:A:456:ARG:NH1	2.53	0.41
5:B:629:MET:HE3	5:B:629:MET:HA	2.02	0.41
5:C:257:THR:O	5:C:259:LEU:N	2.52	0.41
5:A:411:ASN:OD1	5:A:413:THR:N	2.52	0.41
4:M:67:SER:OG	5:B:476:ARG:NH2	2.54	0.41
5:B:185:ASP:OD1	5:B:186:ASN:N	2.51	0.41
2:K:20:THR:HG22	2:K:20:THR:O	2.21	0.41
5:C:57:ASP:OD1	5:C:58:ALA:N	2.53	0.41
4:M:33:LEU:O	4:M:51:ALA:N	2.54	0.41
2:E:92:THR:OG1	2:E:93:HIS:N	2.54	0.41
1:F:28:ARG:CD	1:F:73(G):PHE:HA	2.48	0.41
5:C:163:THR:OG1	5:C:164:GLU:OE1	2.38	0.40
5:A:264:SER:O	5:A:287:GLN:NE2	2.49	0.40
5:A:429:ARG:O	5:A:429:ARG:HG3	2.21	0.40
5:C:655:LYS:NZ	5:A:603:ILE:HG23	2.32	0.40
2:G:77:ASP:OD1	2:G:79:ARG:NH1	2.54	0.40
4:M:11:LEU:HD11	4:M:19:VAL:CG1	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	127/131 (97%)	118 (93%)	9 (7%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	126/131 (96%)	119 (94%)	7 (6%)	0	100	100
1	J	127/131 (97%)	125 (98%)	2 (2%)	0	100	100
2	E	110/114 (96%)	104 (94%)	6 (6%)	0	100	100
2	G	110/114 (96%)	95 (86%)	15 (14%)	0	100	100
2	K	110/114 (96%)	96 (87%)	14 (13%)	0	100	100
3	H	119/123 (97%)	114 (96%)	5 (4%)	0	100	100
3	I	119/123 (97%)	115 (97%)	4 (3%)	0	100	100
4	L	104/107 (97%)	98 (94%)	6 (6%)	0	100	100
4	M	104/107 (97%)	98 (94%)	6 (6%)	0	100	100
5	A	538/649 (83%)	482 (90%)	56 (10%)	0	100	100
5	B	547/649 (84%)	515 (94%)	32 (6%)	0	100	100
5	C	555/649 (86%)	536 (97%)	19 (3%)	0	100	100
All	All	2796/3142 (89%)	2615 (94%)	181 (6%)	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	D	107/109 (98%)	107 (100%)	0	100	100
1	F	106/109 (97%)	106 (100%)	0	100	100
1	J	107/109 (98%)	107 (100%)	0	100	100
2	E	98/100 (98%)	98 (100%)	0	100	100
2	G	98/100 (98%)	98 (100%)	0	100	100
2	K	98/100 (98%)	98 (100%)	0	100	100
3	H	104/106 (98%)	104 (100%)	0	100	100
3	I	104/106 (98%)	104 (100%)	0	100	100
4	L	90/91 (99%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	M	90/91 (99%)	90 (100%)	0	100	100
5	A	493/562 (88%)	491 (100%)	2 (0%)	89	93
5	B	500/562 (89%)	500 (100%)	0	100	100
5	C	507/562 (90%)	507 (100%)	0	100	100
All	All	2502/2707 (92%)	2500 (100%)	2 (0%)	92	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	308	ARG
5	A	335	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	39	GLN
1	F	30	ASN
2	G	93	HIS
1	J	39	GLN
4	L	45	GLN
5	C	103	GLN
5	C	432	GLN
5	C	656	ASN
5	B	114	GLN
5	B	651	ASN
5	A	66	HIS
5	A	92	HIS
5	A	229	ASN
5	A	377	ASN
5	A	425	ASN
5	A	428	GLN
5	A	656	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 ⓘ

42 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	$\# Z  > 2$
6	NAG	N	1	6,5	14,14,15	0.80	0	17,19,21	1.01	0
6	NAG	N	2	6	14,14,15	0.75	0	17,19,21	1.11	1 (5%)
6	BMA	N	3	6	11,11,12	0.75	0	15,15,17	2.29	3 (20%)
6	MAN	N	4	6	11,11,12	0.75	0	15,15,17	0.99	1 (6%)
6	MAN	N	5	6	11,11,12	0.69	0	15,15,17	1.24	1 (6%)
7	NAG	O	1	5,7	14,14,15	0.70	0	17,19,21	1.08	1 (5%)
7	NAG	O	2	7	14,14,15	0.70	0	17,19,21	1.56	1 (5%)
8	NAG	P	1	8,5	14,14,15	0.84	0	17,19,21	1.30	2 (11%)
8	NAG	P	2	8	14,14,15	0.71	0	17,19,21	1.14	1 (5%)
8	BMA	P	3	8	11,11,12	0.75	0	15,15,17	2.53	3 (20%)
8	MAN	P	4	8	11,11,12	0.73	0	15,15,17	1.15	1 (6%)
8	MAN	P	5	8	11,11,12	0.74	0	15,15,17	1.00	1 (6%)
6	NAG	Q	1	6,5	14,14,15	0.76	0	17,19,21	1.39	3 (17%)
6	NAG	Q	2	6	14,14,15	0.74	0	17,19,21	0.90	1 (5%)
6	BMA	Q	3	6	11,11,12	0.79	0	15,15,17	2.82	5 (33%)
6	MAN	Q	4	6	11,11,12	0.74	0	15,15,17	1.00	1 (6%)
6	MAN	Q	5	6	11,11,12	0.72	0	15,15,17	1.10	1 (6%)
7	NAG	R	1	5,7	14,14,15	0.70	0	17,19,21	1.31	2 (11%)
7	NAG	R	2	7	14,14,15	0.71	0	17,19,21	1.05	0
7	NAG	S	1	5,7	14,14,15	0.74	0	17,19,21	1.56	1 (5%)
7	NAG	S	2	7	14,14,15	0.71	0	17,19,21	1.02	0
9	NAG	T	1	9,5	14,14,15	0.73	0	17,19,21	1.06	1 (5%)
9	MAN	T	10	9	11,11,12	0.71	0	15,15,17	1.03	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	T	2	9	14,14,15	0.75	0	17,19,21	1.07	1 (5%)
9	BMA	T	3	9	11,11,12	0.81	0	15,15,17	1.35	1 (6%)
9	MAN	T	4	9	11,11,12	0.78	0	15,15,17	0.97	1 (6%)
9	MAN	T	5	9	11,11,12	0.75	0	15,15,17	0.95	1 (6%)
9	MAN	T	6	9	11,11,12	0.61	0	15,15,17	2.76	3 (20%)
9	MAN	T	7	9	11,11,12	0.68	0	15,15,17	1.17	1 (6%)
9	MAN	T	8	9	11,11,12	0.67	0	15,15,17	1.54	3 (20%)
9	MAN	T	9	9	11,11,12	0.71	0	15,15,17	1.29	1 (6%)
6	NAG	U	1	6,5	14,14,15	0.84	0	17,19,21	0.89	1 (5%)
6	NAG	U	2	6	14,14,15	0.74	0	17,19,21	0.96	0
6	BMA	U	3	6	11,11,12	0.71	0	15,15,17	1.27	1 (6%)
6	MAN	U	4	6	11,11,12	0.73	0	15,15,17	1.10	1 (6%)
6	MAN	U	5	6	11,11,12	0.69	0	15,15,17	1.20	1 (6%)
7	NAG	V	1	5,7	14,14,15	0.69	0	17,19,21	1.18	2 (11%)
7	NAG	V	2	7	14,14,15	0.72	0	17,19,21	1.08	1 (5%)
10	NAG	W	1	10,5	14,14,15	0.71	0	17,19,21	1.03	1 (5%)
10	NAG	W	2	10	14,14,15	0.74	0	17,19,21	0.83	0
10	BMA	W	3	10	11,11,12	0.86	0	15,15,17	1.28	1 (6%)
10	MAN	W	4	10	11,11,12	0.72	0	15,15,17	1.04	1 (6%)

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
6	NAG	N	1	6,5	-	1/6/23/26	0/1/1/1
6	NAG	N	2	6	-	0/6/23/26	0/1/1/1
6	BMA	N	3	6	-	2/2/19/22	0/1/1/1
6	MAN	N	4	6	-	2/2/19/22	0/1/1/1
6	MAN	N	5	6	-	1/2/19/22	0/1/1/1
7	NAG	O	1	5,7	-	0/6/23/26	0/1/1/1
7	NAG	O	2	7	-	3/6/23/26	0/1/1/1
8	NAG	P	1	8,5	-	0/6/23/26	0/1/1/1
8	NAG	P	2	8	-	0/6/23/26	0/1/1/1
8	BMA	P	3	8	-	1/2/19/22	0/1/1/1
8	MAN	P	4	8	-	1/2/19/22	0/1/1/1
8	MAN	P	5	8	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	Q	1	6,5	-	0/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	0/6/23/26	0/1/1/1
6	BMA	Q	3	6	-	2/2/19/22	0/1/1/1
6	MAN	Q	4	6	-	1/2/19/22	0/1/1/1
6	MAN	Q	5	6	-	2/2/19/22	0/1/1/1
7	NAG	R	1	5,7	-	2/6/23/26	0/1/1/1
7	NAG	R	2	7	-	1/6/23/26	0/1/1/1
7	NAG	S	1	5,7	-	2/6/23/26	0/1/1/1
7	NAG	S	2	7	-	1/6/23/26	0/1/1/1
9	NAG	T	1	9,5	-	0/6/23/26	0/1/1/1
9	MAN	T	10	9	-	1/2/19/22	0/1/1/1
9	NAG	T	2	9	-	0/6/23/26	0/1/1/1
9	BMA	T	3	9	-	0/2/19/22	0/1/1/1
9	MAN	T	4	9	-	2/2/19/22	0/1/1/1
9	MAN	T	5	9	-	1/2/19/22	0/1/1/1
9	MAN	T	6	9	-	0/2/19/22	0/1/1/1
9	MAN	T	7	9	-	2/2/19/22	0/1/1/1
9	MAN	T	8	9	-	2/2/19/22	0/1/1/1
9	MAN	T	9	9	-	2/2/19/22	0/1/1/1
6	NAG	U	1	6,5	-	0/6/23/26	0/1/1/1
6	NAG	U	2	6	-	0/6/23/26	0/1/1/1
6	BMA	U	3	6	-	2/2/19/22	0/1/1/1
6	MAN	U	4	6	-	0/2/19/22	0/1/1/1
6	MAN	U	5	6	-	0/2/19/22	0/1/1/1
7	NAG	V	1	5,7	-	0/6/23/26	0/1/1/1
7	NAG	V	2	7	-	2/6/23/26	0/1/1/1
10	NAG	W	1	10,5	-	0/6/23/26	0/1/1/1
10	NAG	W	2	10	-	0/6/23/26	0/1/1/1
10	BMA	W	3	10	-	1/2/19/22	0/1/1/1
10	MAN	W	4	10	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Q	3	BMA	C1-O5-C5	9.30	124.64	112.19
9	T	6	MAN	C1-O5-C5	9.03	124.29	112.19
8	P	3	BMA	C1-O5-C5	8.50	123.58	112.19
6	N	3	BMA	C1-O5-C5	7.32	122.00	112.19
7	S	1	NAG	C2-N2-C7	5.08	129.71	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	2	NAG	C2-N2-C7	4.93	129.51	122.90
10	W	3	BMA	C1-O5-C5	4.05	117.61	112.19
9	T	3	BMA	C1-O5-C5	4.04	117.60	112.19
9	T	9	MAN	C1-O5-C5	4.02	117.58	112.19
6	N	5	MAN	C1-O5-C5	3.80	117.28	112.19
6	U	5	MAN	C1-O5-C5	3.58	116.98	112.19
6	U	3	BMA	C1-O5-C5	3.46	116.82	112.19
9	T	6	MAN	C1-C2-C3	3.44	114.66	109.64
9	T	8	MAN	C1-O5-C5	3.43	116.78	112.19
7	R	1	NAG	O5-C1-C2	-3.37	106.08	111.29
9	T	7	MAN	C1-O5-C5	3.36	116.69	112.19
8	P	4	MAN	C1-O5-C5	3.34	116.66	112.19
6	Q	1	NAG	C1-O5-C5	3.27	116.57	112.19
6	U	4	MAN	C1-O5-C5	3.08	116.32	112.19
6	Q	5	MAN	C1-O5-C5	3.01	116.22	112.19
8	P	1	NAG	C1-O5-C5	2.97	116.17	112.19
9	T	1	NAG	C2-N2-C7	2.96	126.87	122.90
8	P	1	NAG	O5-C1-C2	-2.93	106.76	111.29
6	Q	1	NAG	O5-C1-C2	-2.90	106.80	111.29
8	P	2	NAG	O5-C1-C2	-2.87	106.86	111.29
9	T	8	MAN	O2-C2-C1	-2.86	102.67	109.22
7	O	1	NAG	O5-C1-C2	-2.84	106.90	111.29
9	T	2	NAG	O5-C1-C2	-2.84	106.90	111.29
9	T	10	MAN	C1-O5-C5	2.81	115.95	112.19
6	Q	3	BMA	C3-C4-C5	2.79	115.28	110.23
10	W	4	MAN	C1-O5-C5	2.74	115.86	112.19
7	V	2	NAG	C1-O5-C5	2.74	115.86	112.19
6	Q	4	MAN	C1-O5-C5	2.70	115.81	112.19
7	R	1	NAG	C1-O5-C5	2.66	115.75	112.19
7	V	1	NAG	C1-O5-C5	2.60	115.68	112.19
9	T	4	MAN	C1-O5-C5	2.57	115.63	112.19
8	P	5	MAN	C1-O5-C5	2.57	115.63	112.19
6	N	4	MAN	C1-O5-C5	2.53	115.58	112.19
9	T	6	MAN	O5-C1-C2	2.40	116.53	110.79
6	Q	3	BMA	C2-C3-C4	2.34	114.98	110.86
7	V	1	NAG	C4-C3-C2	-2.28	107.68	111.02
6	N	3	BMA	O4-C4-C3	-2.26	105.04	110.38
9	T	8	MAN	O2-C2-C3	2.26	114.84	110.15
6	N	2	NAG	C2-N2-C7	2.23	125.89	122.90
6	Q	2	NAG	C4-C3-C2	-2.18	107.82	111.02
10	W	1	NAG	C1-O5-C5	2.18	115.11	112.19
8	P	3	BMA	O4-C4-C3	-2.18	105.25	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Q	3	BMA	O4-C4-C3	-2.15	105.31	110.38
8	P	3	BMA	C3-C4-C5	2.12	114.08	110.23
6	U	1	NAG	O5-C1-C2	-2.09	108.06	111.29
6	Q	3	BMA	O5-C5-C4	2.08	115.88	110.83
6	Q	1	NAG	O4-C4-C3	-2.03	105.59	110.38
9	T	5	MAN	C1-O5-C5	2.03	114.90	112.19
6	N	3	BMA	C3-C4-C5	2.02	113.89	110.23

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	R	1	NAG	O5-C5-C6-O6
9	T	9	MAN	O5-C5-C6-O6
9	T	7	MAN	C4-C5-C6-O6
9	T	4	MAN	O5-C5-C6-O6
6	Q	3	BMA	O5-C5-C6-O6
6	N	4	MAN	O5-C5-C6-O6
6	N	3	BMA	C4-C5-C6-O6
6	N	4	MAN	C4-C5-C6-O6
6	U	3	BMA	C4-C5-C6-O6
8	P	5	MAN	O5-C5-C6-O6
9	T	9	MAN	C4-C5-C6-O6
7	R	1	NAG	C4-C5-C6-O6
7	O	2	NAG	C8-C7-N2-C2
7	O	2	NAG	O7-C7-N2-C2
7	S	1	NAG	C8-C7-N2-C2
7	S	1	NAG	O7-C7-N2-C2
6	N	3	BMA	O5-C5-C6-O6
6	U	3	BMA	O5-C5-C6-O6
9	T	7	MAN	O5-C5-C6-O6
9	T	8	MAN	O5-C5-C6-O6
9	T	5	MAN	O5-C5-C6-O6
9	T	4	MAN	C4-C5-C6-O6
8	P	4	MAN	O5-C5-C6-O6
8	P	5	MAN	C4-C5-C6-O6
7	R	2	NAG	O5-C5-C6-O6
10	W	3	BMA	O5-C5-C6-O6
6	N	5	MAN	O5-C5-C6-O6
7	O	2	NAG	O5-C5-C6-O6
7	S	2	NAG	O5-C5-C6-O6
8	P	3	BMA	O5-C5-C6-O6

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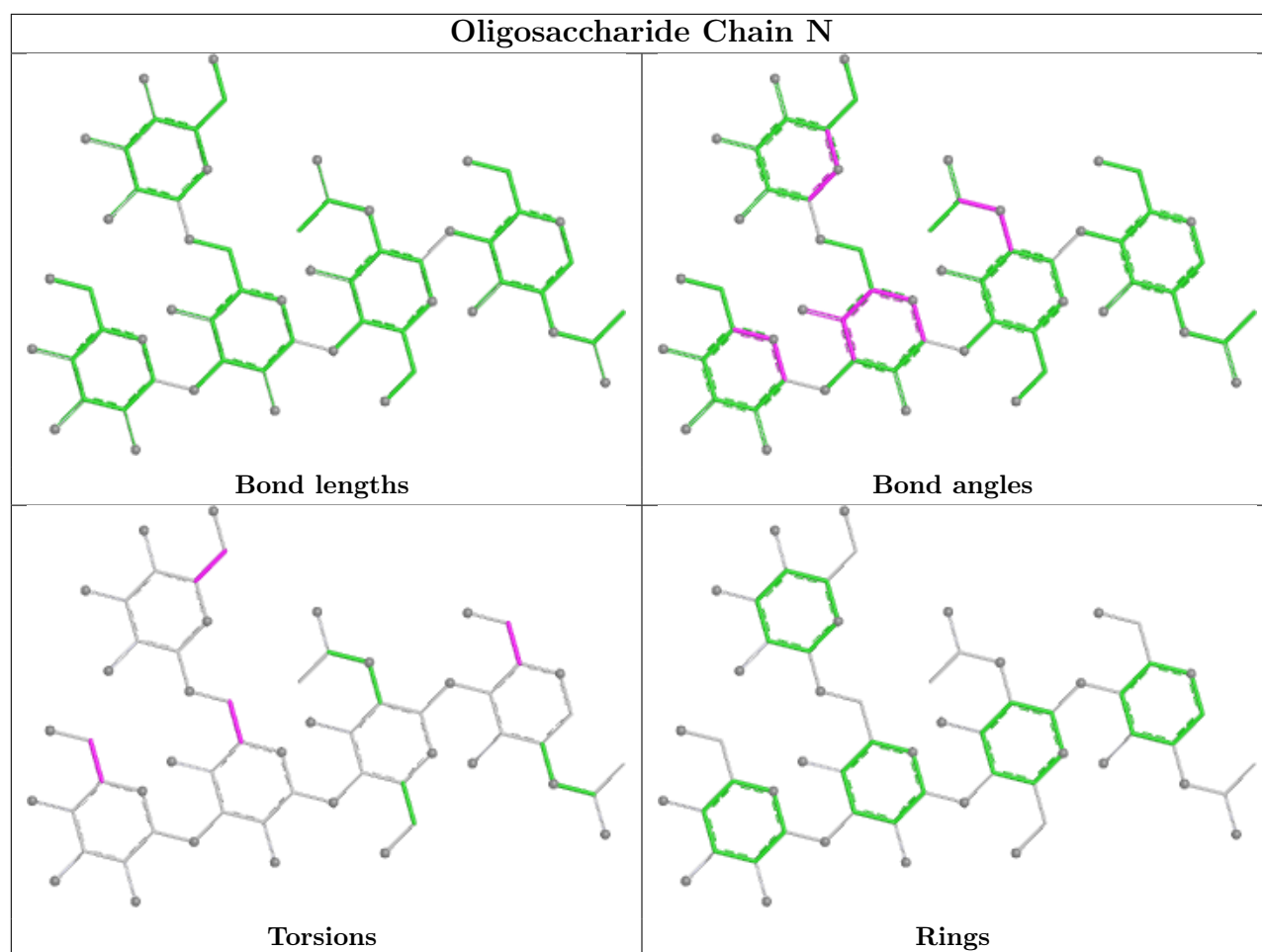
Mol	Chain	Res	Type	Atoms
6	Q	4	MAN	O5-C5-C6-O6
10	W	4	MAN	O5-C5-C6-O6
9	T	10	MAN	O5-C5-C6-O6
6	Q	3	BMA	C4-C5-C6-O6
6	Q	5	MAN	C4-C5-C6-O6
9	T	8	MAN	C4-C5-C6-O6
6	Q	5	MAN	O5-C5-C6-O6
6	N	1	NAG	C4-C5-C6-O6
7	V	2	NAG	C4-C5-C6-O6
7	V	2	NAG	O5-C5-C6-O6

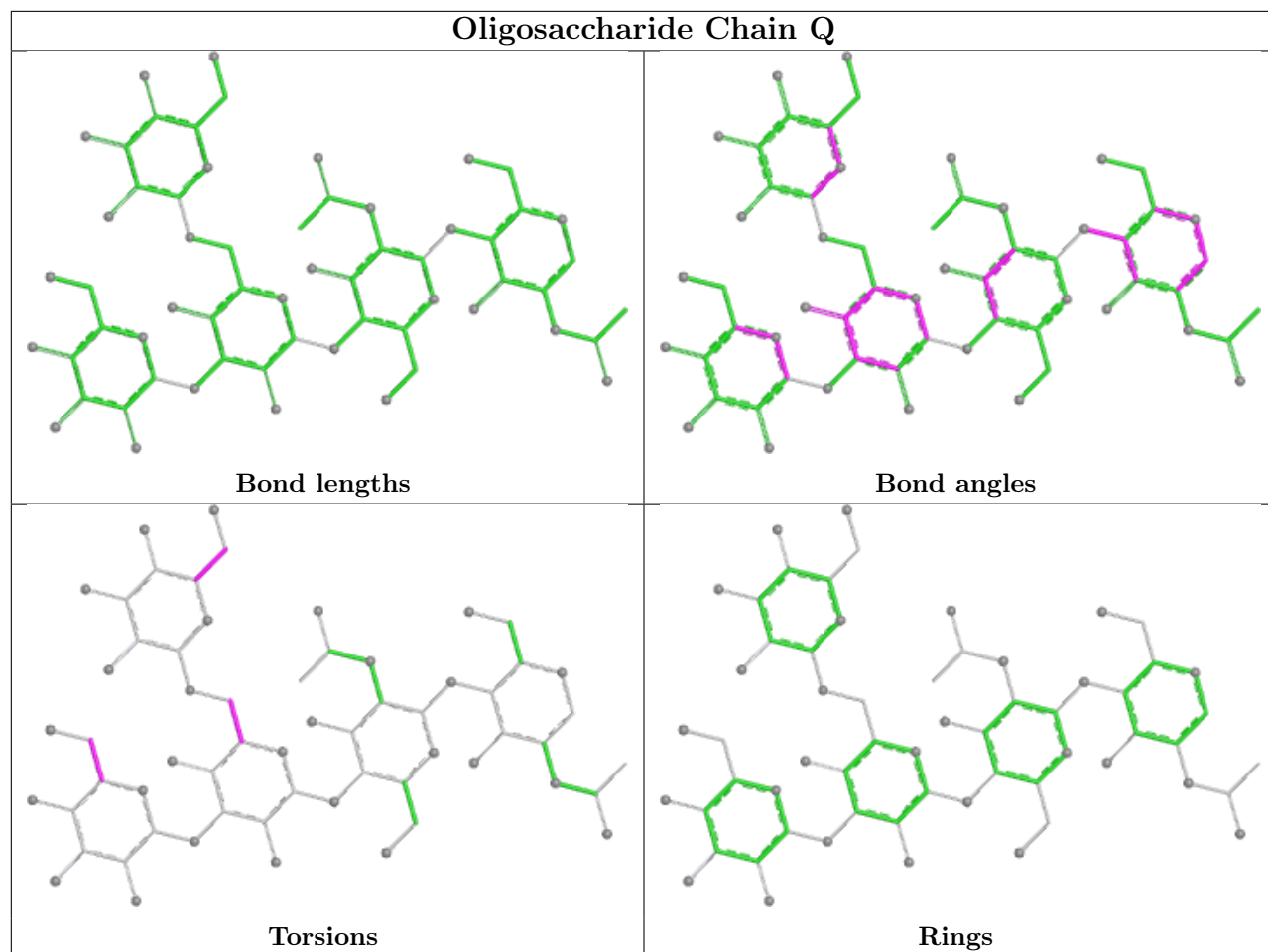
There are no ring outliers.

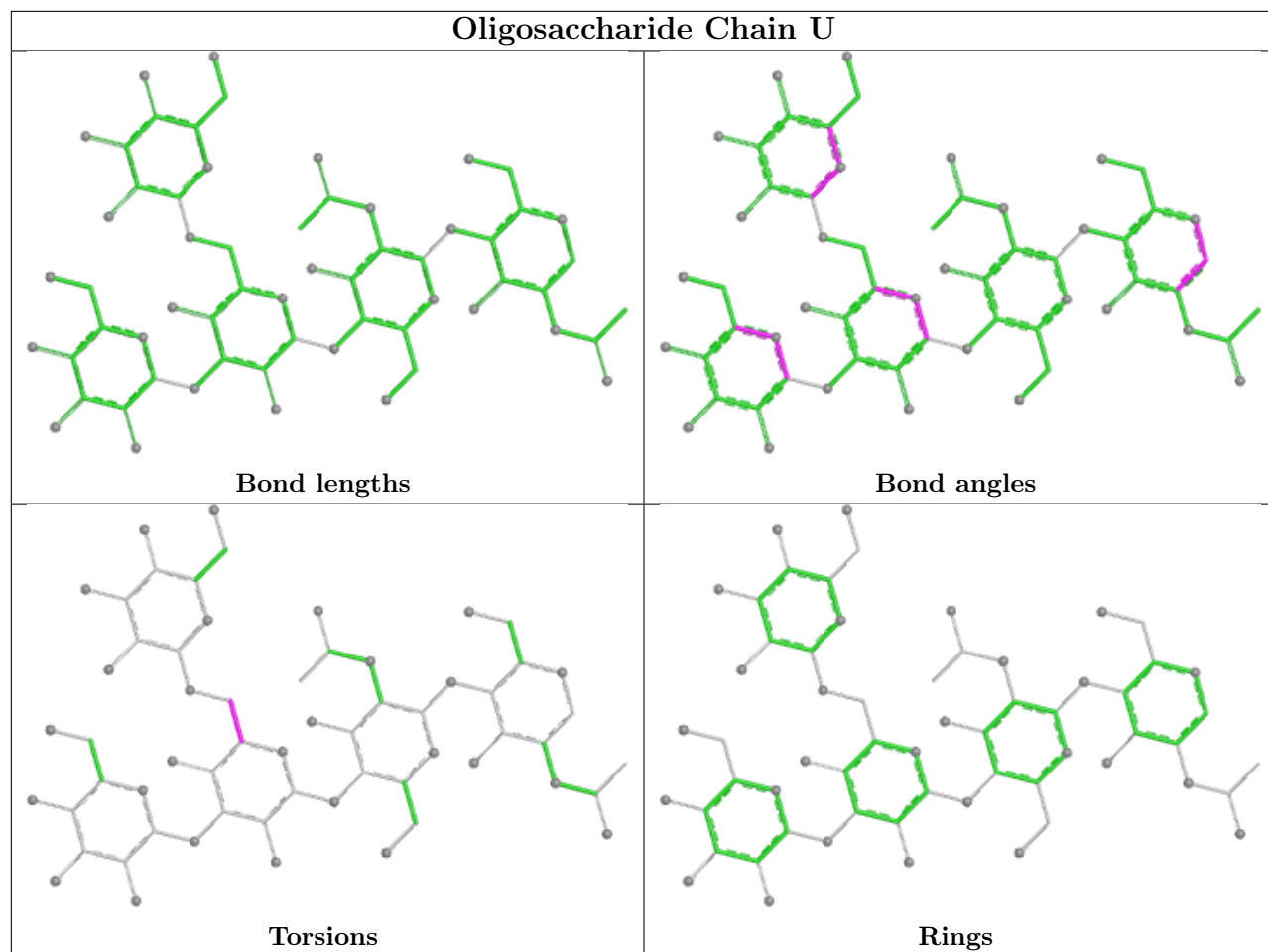
2 monomers are involved in 2 short contacts:

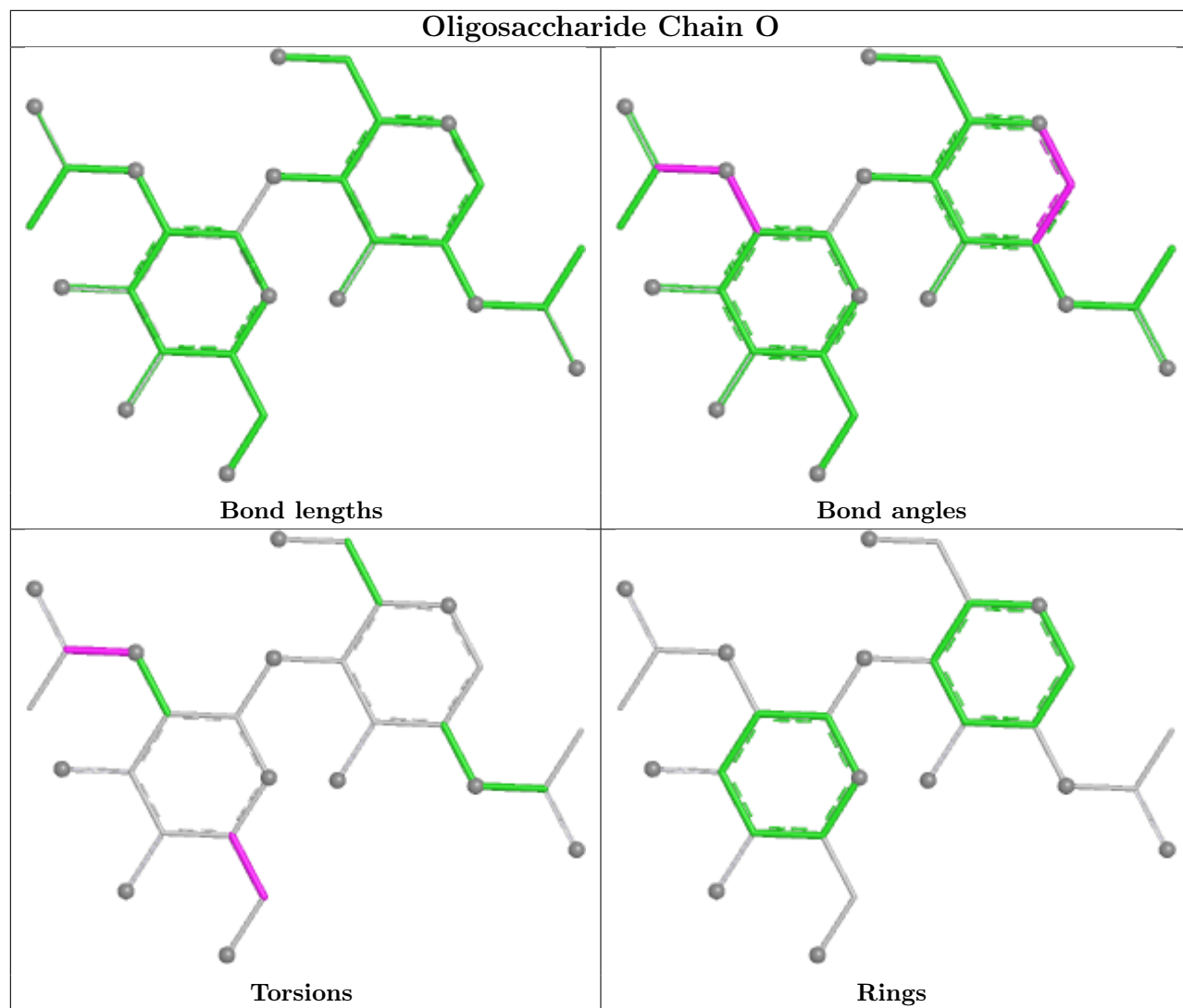
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	P	1	NAG	1	0
9	T	2	NAG	1	0

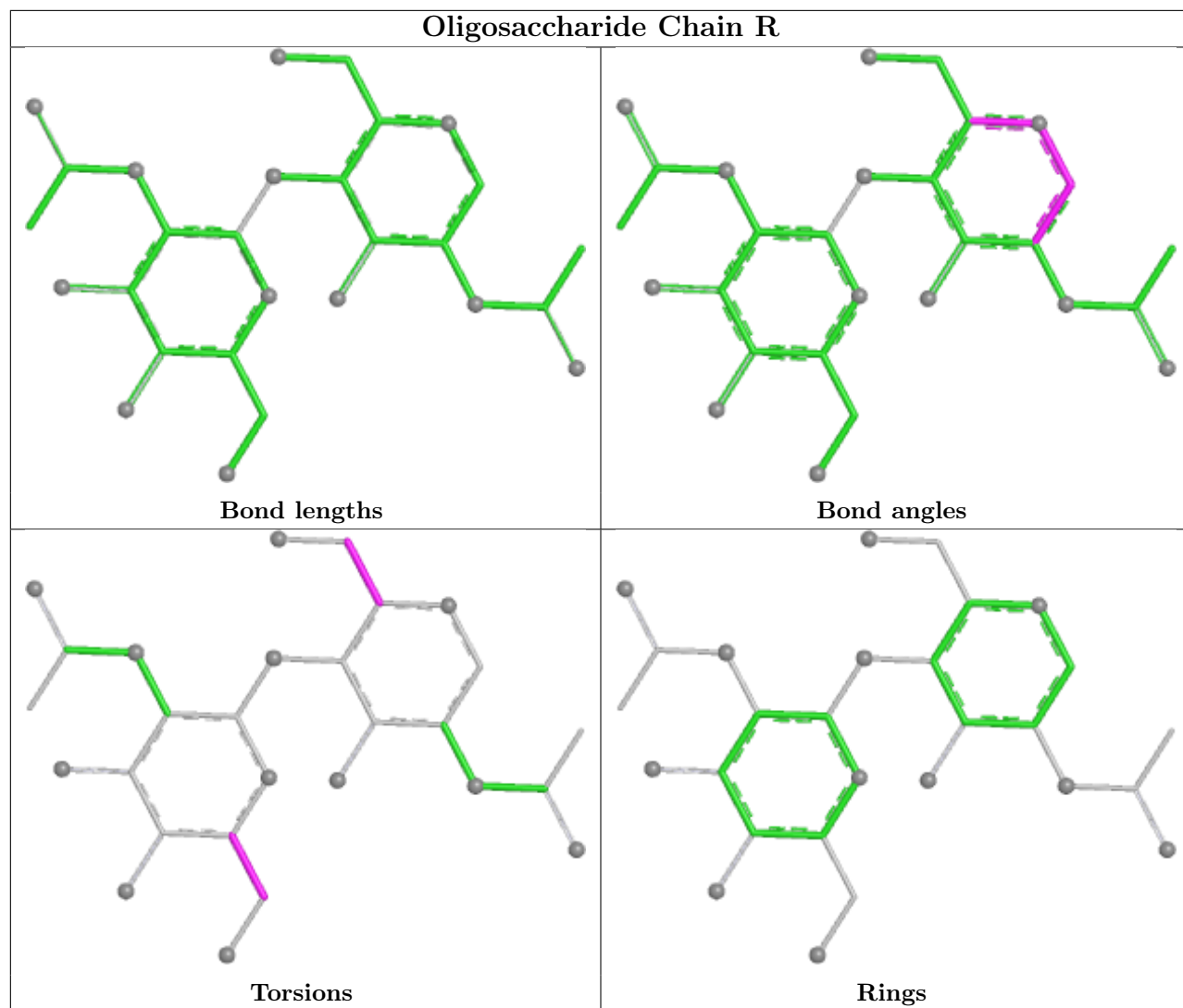
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

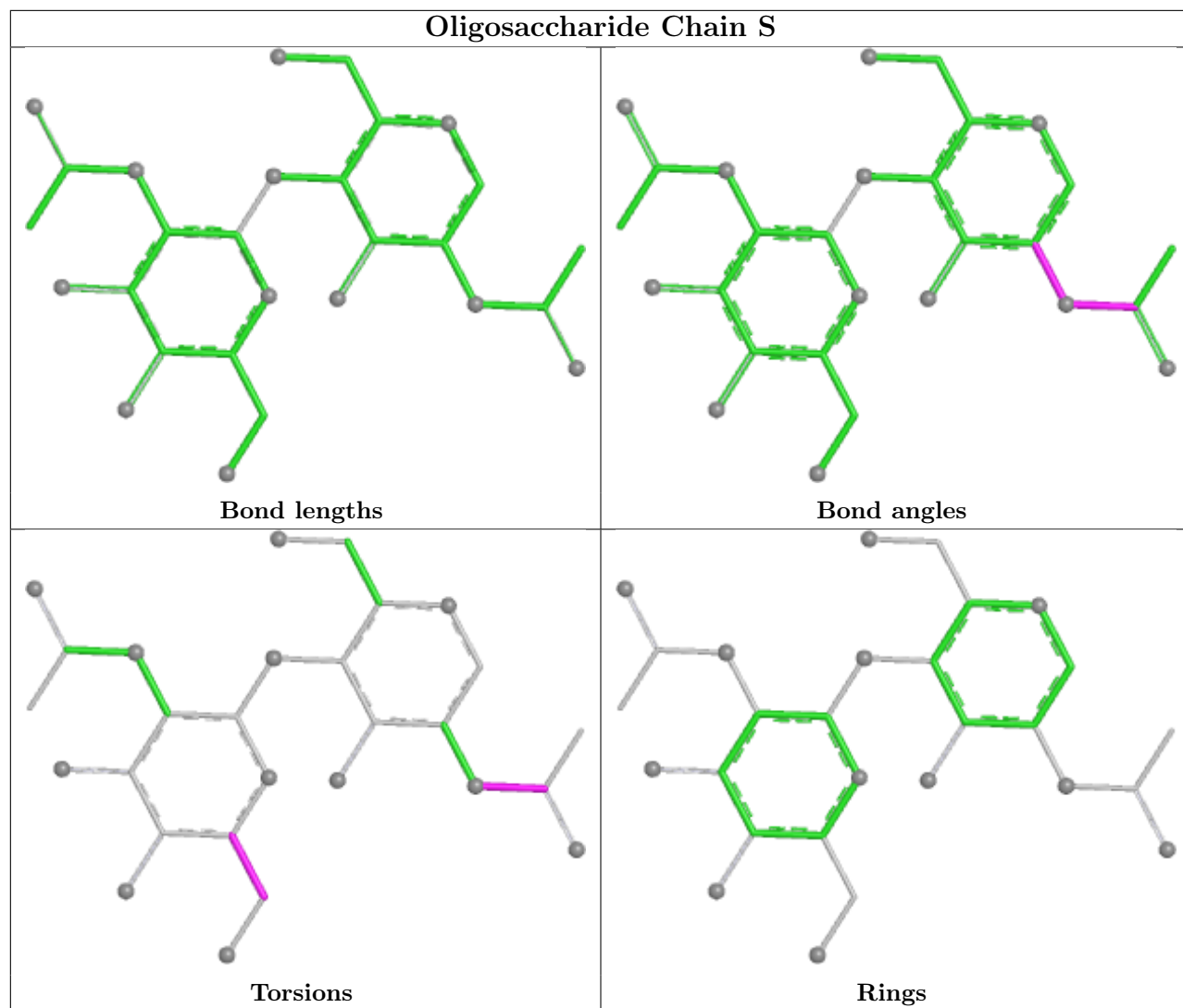


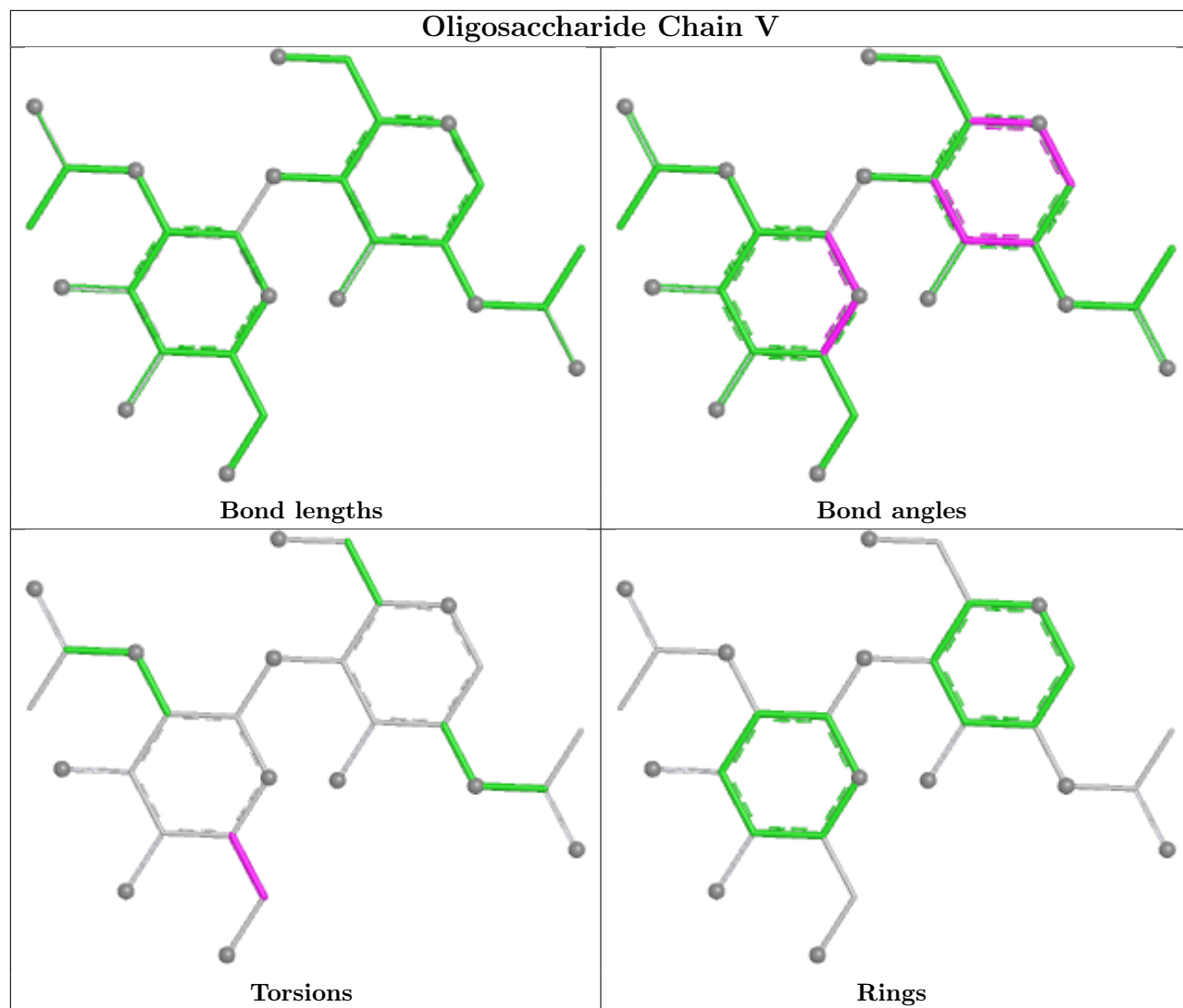




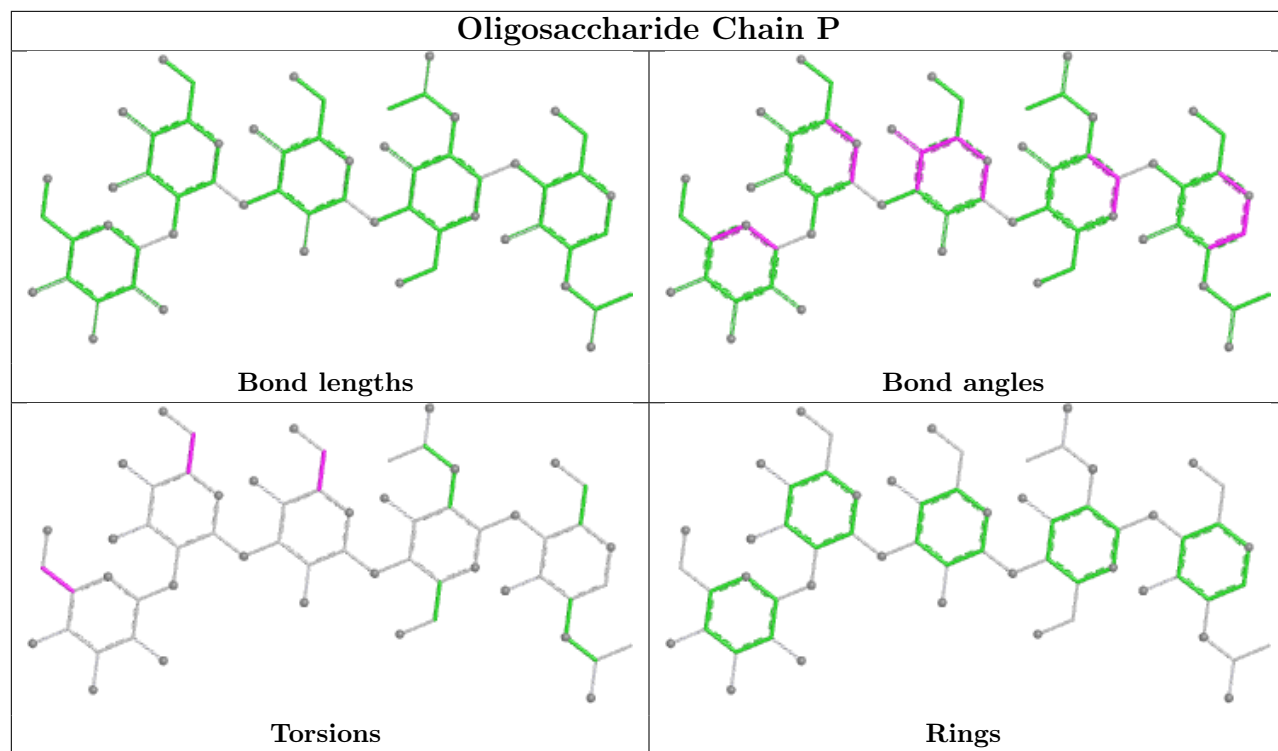


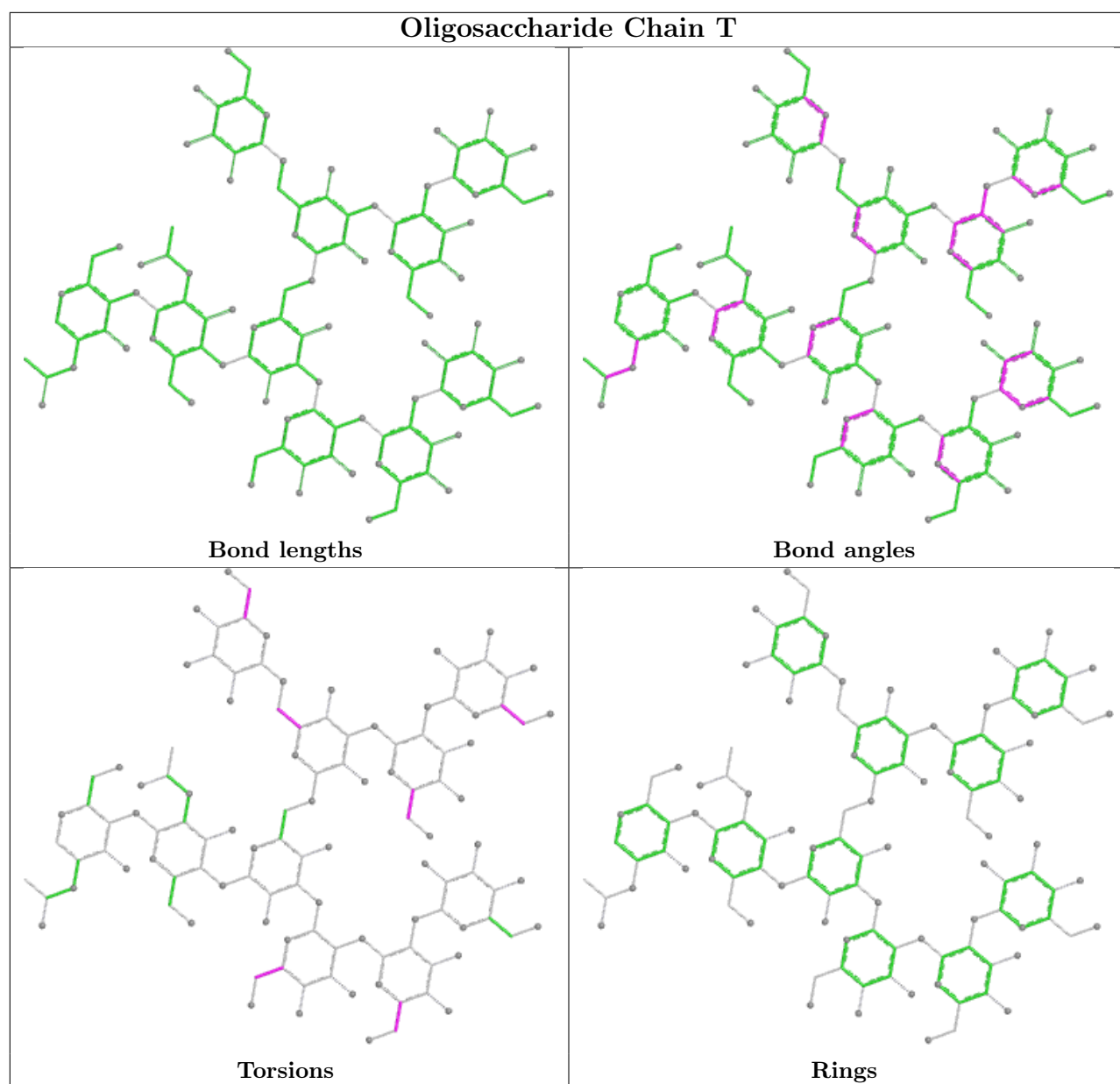


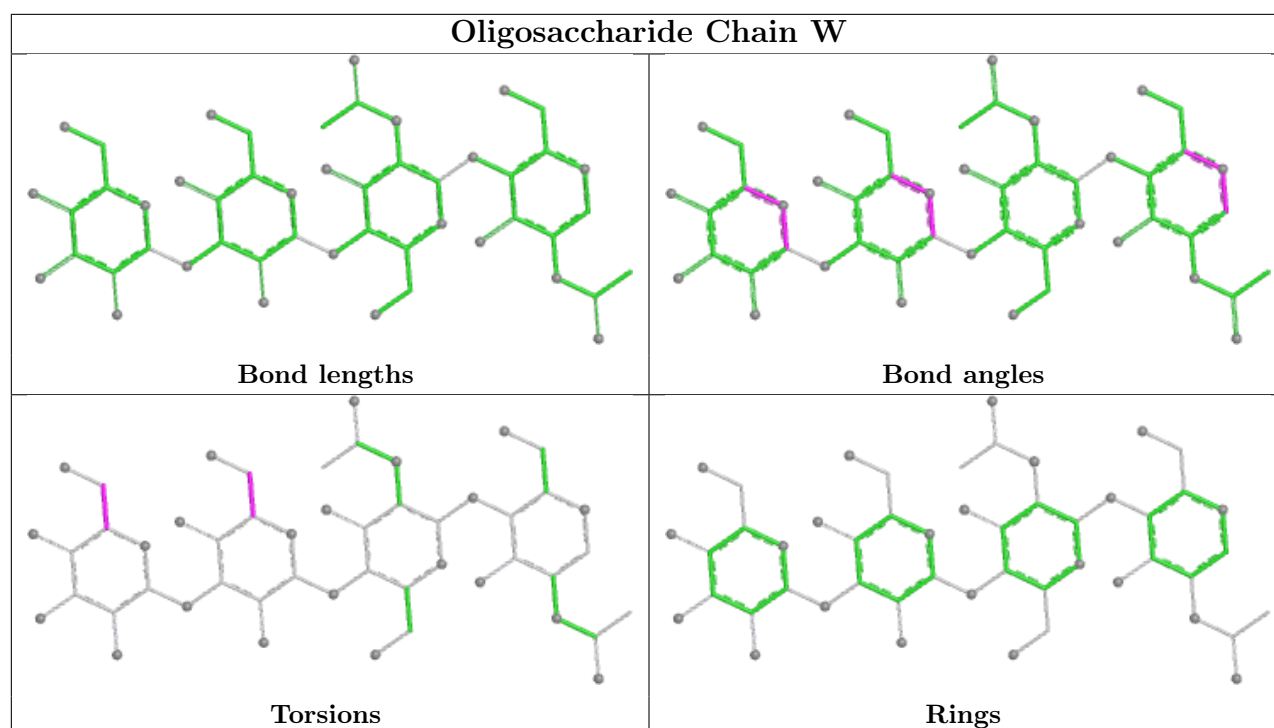












## 5.6 Ligand geometry [i](#)

36 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	NAG	C	703	5	14,14,15	0.71	0	17,19,21	0.97	0
11	NAG	C	707	5	14,14,15	0.68	0	17,19,21	1.27	1 (5%)
11	NAG	A	704	5	14,14,15	0.79	0	17,19,21	0.92	0
11	NAG	B	709	5	14,14,15	0.67	0	17,19,21	1.16	1 (5%)
11	NAG	C	701	5	14,14,15	0.75	0	17,19,21	1.30	2 (11%)
11	NAG	B	712	5	14,14,15	0.69	0	17,19,21	1.58	1 (5%)
11	NAG	A	703	5	14,14,15	0.70	0	17,19,21	1.22	1 (5%)
11	NAG	A	702	5	14,14,15	0.70	0	17,19,21	0.96	0
11	NAG	C	711	5	14,14,15	0.69	0	17,19,21	1.04	1 (5%)
11	NAG	C	709	5	14,14,15	0.72	0	17,19,21	1.03	0
11	NAG	B	705	5	14,14,15	0.71	0	17,19,21	1.06	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	NAG	B	711	5	14,14,15	0.73	0	17,19,21	1.52	4 (23%)
11	NAG	B	706	5	14,14,15	0.72	0	17,19,21	1.77	2 (11%)
11	NAG	C	712	5	14,14,15	0.66	0	17,19,21	1.21	1 (5%)
11	NAG	A	707	5	14,14,15	0.70	0	17,19,21	1.17	2 (11%)
11	NAG	C	706	5	14,14,15	0.71	0	17,19,21	0.87	0
11	NAG	C	705	5	14,14,15	0.68	0	17,19,21	1.15	1 (5%)
11	NAG	B	704	5	14,14,15	0.73	0	17,19,21	1.21	2 (11%)
11	NAG	C	702	5	14,14,15	0.71	0	17,19,21	0.93	0
11	NAG	B	710	5	14,14,15	0.75	0	17,19,21	1.30	1 (5%)
11	NAG	A	709	5	14,14,15	0.69	0	17,19,21	0.97	0
11	NAG	C	710	5	14,14,15	0.71	0	17,19,21	1.06	0
11	NAG	A	706	5	14,14,15	0.69	0	17,19,21	1.00	0
11	NAG	A	711	5	14,14,15	0.66	0	17,19,21	1.29	2 (11%)
11	NAG	C	704	5	14,14,15	0.69	0	17,19,21	1.03	0
11	NAG	A	708	5	14,14,15	0.75	0	17,19,21	1.29	3 (17%)
11	NAG	A	712	5	14,14,15	0.70	0	17,19,21	0.90	0
11	NAG	B	708	5	14,14,15	0.70	0	17,19,21	1.03	1 (5%)
11	NAG	A	701	5	14,14,15	0.72	0	17,19,21	1.10	1 (5%)
11	NAG	A	710	5	14,14,15	0.70	0	17,19,21	0.98	0
11	NAG	B	703	5	14,14,15	0.71	0	17,19,21	1.03	0
11	NAG	C	708	5	14,14,15	0.75	0	17,19,21	1.07	2 (11%)
11	NAG	B	701	5	14,14,15	0.75	0	17,19,21	1.02	0
11	NAG	B	702	5	14,14,15	0.73	0	17,19,21	1.05	0
11	NAG	A	705	5	14,14,15	0.70	0	17,19,21	0.91	0
11	NAG	B	707	5	14,14,15	0.72	0	17,19,21	1.04	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
11	NAG	C	703	5	-	1/6/23/26	0/1/1/1
11	NAG	C	707	5	-	3/6/23/26	0/1/1/1
11	NAG	A	704	5	-	0/6/23/26	0/1/1/1
11	NAG	B	709	5	-	1/6/23/26	0/1/1/1
11	NAG	C	701	5	-	2/6/23/26	0/1/1/1
11	NAG	B	712	5	-	3/6/23/26	0/1/1/1
11	NAG	A	703	5	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	A	702	5	-	1/6/23/26	0/1/1/1
11	NAG	C	711	5	-	1/6/23/26	0/1/1/1
11	NAG	C	709	5	-	1/6/23/26	0/1/1/1
11	NAG	B	705	5	-	1/6/23/26	0/1/1/1
11	NAG	B	711	5	-	0/6/23/26	0/1/1/1
11	NAG	B	706	5	-	2/6/23/26	0/1/1/1
11	NAG	C	712	5	-	2/6/23/26	0/1/1/1
11	NAG	A	707	5	-	0/6/23/26	0/1/1/1
11	NAG	C	706	5	-	1/6/23/26	0/1/1/1
11	NAG	C	705	5	-	1/6/23/26	0/1/1/1
11	NAG	B	704	5	-	1/6/23/26	0/1/1/1
11	NAG	C	702	5	-	1/6/23/26	0/1/1/1
11	NAG	B	710	5	-	0/6/23/26	0/1/1/1
11	NAG	A	709	5	-	1/6/23/26	0/1/1/1
11	NAG	C	710	5	-	1/6/23/26	0/1/1/1
11	NAG	A	706	5	-	1/6/23/26	0/1/1/1
11	NAG	A	711	5	-	0/6/23/26	0/1/1/1
11	NAG	C	704	5	-	1/6/23/26	0/1/1/1
11	NAG	A	708	5	-	1/6/23/26	0/1/1/1
11	NAG	A	712	5	-	0/6/23/26	0/1/1/1
11	NAG	B	708	5	-	0/6/23/26	0/1/1/1
11	NAG	A	701	5	-	0/6/23/26	0/1/1/1
11	NAG	A	710	5	-	1/6/23/26	0/1/1/1
11	NAG	B	703	5	-	1/6/23/26	0/1/1/1
11	NAG	C	708	5	-	1/6/23/26	0/1/1/1
11	NAG	B	701	5	-	1/6/23/26	0/1/1/1
11	NAG	B	702	5	-	1/6/23/26	0/1/1/1
11	NAG	A	705	5	-	1/6/23/26	0/1/1/1
11	NAG	B	707	5	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	706	NAG	C2-N2-C7	5.70	130.54	122.90
11	B	712	NAG	C2-N2-C7	5.13	129.78	122.90
11	C	701	NAG	O5-C1-C2	-3.86	105.32	111.29
11	C	707	NAG	C1-O5-C5	3.79	117.27	112.19
11	B	710	NAG	C2-N2-C7	3.75	127.92	122.90
11	A	711	NAG	C2-N2-C7	3.66	127.80	122.90
11	A	703	NAG	C1-O5-C5	3.27	116.57	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	708	NAG	O5-C1-C2	-2.96	106.71	111.29
11	B	709	NAG	C1-O5-C5	2.90	116.07	112.19
11	C	705	NAG	O5-C1-C2	-2.87	106.86	111.29
11	B	711	NAG	O5-C1-C2	-2.85	106.87	111.29
11	B	704	NAG	O5-C1-C2	-2.72	107.08	111.29
11	B	711	NAG	O4-C4-C3	-2.61	104.22	110.38
11	A	701	NAG	O5-C1-C2	-2.59	107.28	111.29
11	B	711	NAG	O4-C4-C5	2.50	115.47	109.32
11	B	706	NAG	C8-C7-N2	2.41	120.11	116.12
11	B	711	NAG	C1-O5-C5	2.35	115.33	112.19
11	B	708	NAG	C1-O5-C5	2.33	115.31	112.19
11	C	712	NAG	O5-C1-C2	-2.32	107.70	111.29
11	C	711	NAG	C1-O5-C5	2.32	115.29	112.19
11	A	708	NAG	C1-C2-N2	2.26	114.00	110.43
11	A	707	NAG	O5-C1-C2	-2.20	107.89	111.29
11	C	701	NAG	C2-N2-C7	2.12	125.74	122.90
11	B	705	NAG	O5-C1-C2	-2.12	108.01	111.29
11	B	704	NAG	C1-O5-C5	2.11	115.02	112.19
11	C	708	NAG	C1-O5-C5	2.05	114.93	112.19
11	A	707	NAG	C4-C3-C2	-2.04	108.02	111.02
11	A	708	NAG	C1-O5-C5	2.03	114.90	112.19
11	A	711	NAG	O4-C4-C3	-2.01	105.63	110.38
11	C	708	NAG	C1-C2-N2	2.01	113.60	110.43

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	707	NAG	C1-C2-N2-C7
11	B	706	NAG	C8-C7-N2-C2
11	B	706	NAG	O7-C7-N2-C2
11	B	712	NAG	C8-C7-N2-C2
11	B	712	NAG	O7-C7-N2-C2
11	C	701	NAG	O5-C5-C6-O6
11	A	705	NAG	O5-C5-C6-O6
11	A	706	NAG	O5-C5-C6-O6
11	A	709	NAG	O5-C5-C6-O6
11	B	702	NAG	O5-C5-C6-O6
11	B	712	NAG	O5-C5-C6-O6
11	B	703	NAG	O5-C5-C6-O6
11	C	702	NAG	O5-C5-C6-O6
11	C	706	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
11	C	707	NAG	O5-C5-C6-O6
11	B	709	NAG	O5-C5-C6-O6
11	A	702	NAG	O5-C5-C6-O6
11	A	710	NAG	O5-C5-C6-O6
11	B	704	NAG	O5-C5-C6-O6
11	B	707	NAG	O5-C5-C6-O6
11	C	703	NAG	O5-C5-C6-O6
11	C	708	NAG	O5-C5-C6-O6
11	C	704	NAG	O5-C5-C6-O6
11	A	708	NAG	O5-C5-C6-O6
11	C	710	NAG	O5-C5-C6-O6
11	C	705	NAG	O5-C5-C6-O6
11	C	709	NAG	O5-C5-C6-O6
11	A	703	NAG	O5-C5-C6-O6
11	B	705	NAG	O5-C5-C6-O6
11	C	711	NAG	O5-C5-C6-O6
11	B	701	NAG	O5-C5-C6-O6
11	C	707	NAG	C3-C2-N2-C7
11	C	701	NAG	C4-C5-C6-O6
11	C	712	NAG	O5-C5-C6-O6
11	C	712	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	705	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



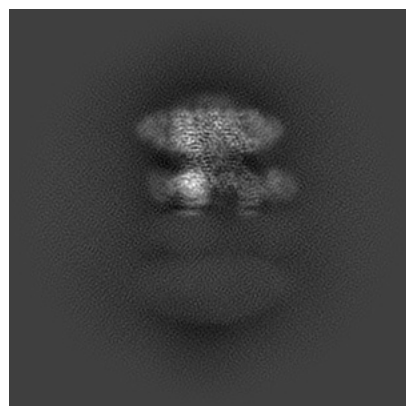
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45928. These allow visual inspection of the internal detail of the map and identification of artifacts.

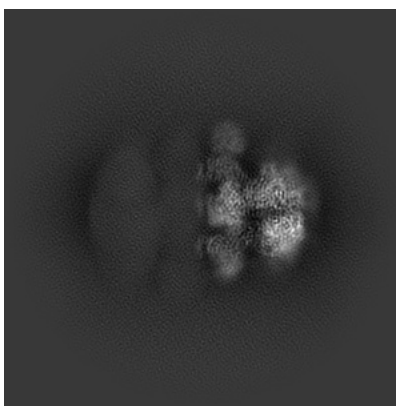
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

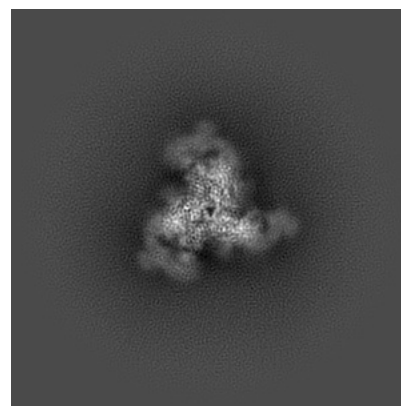
#### 6.1.1 Primary map



X

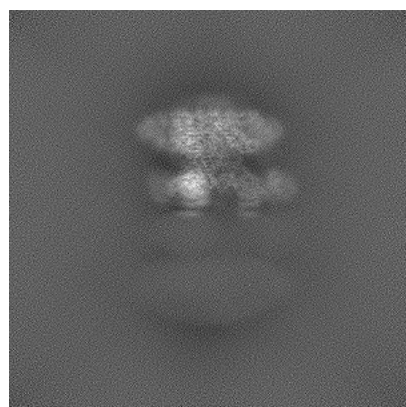


Y

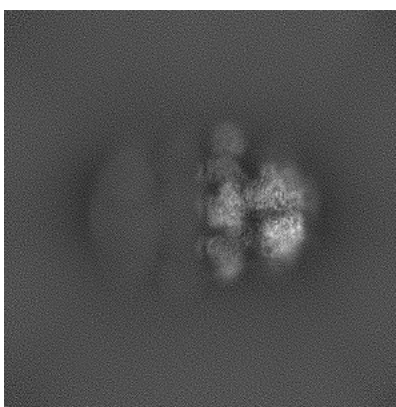


Z

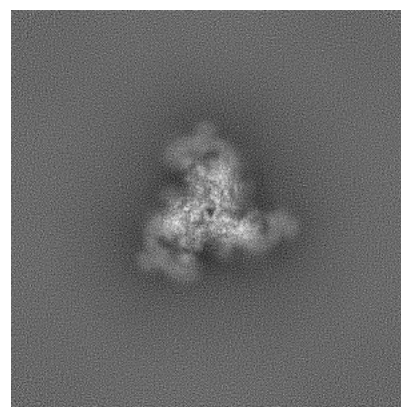
#### 6.1.2 Raw map



X



Y



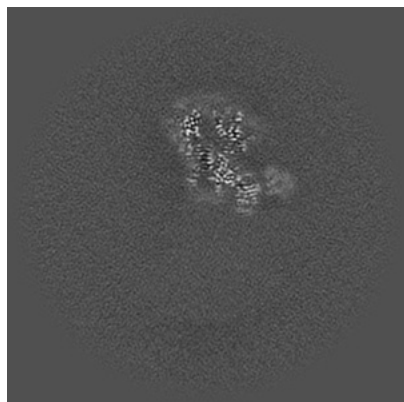
Z

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

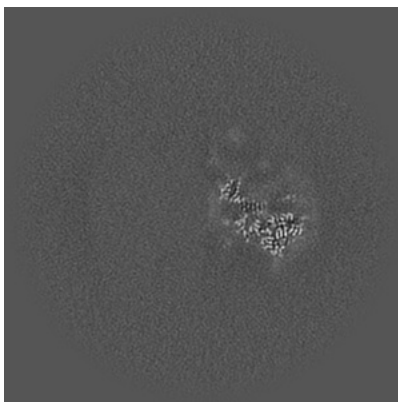


## 6.2 Central slices [i](#)

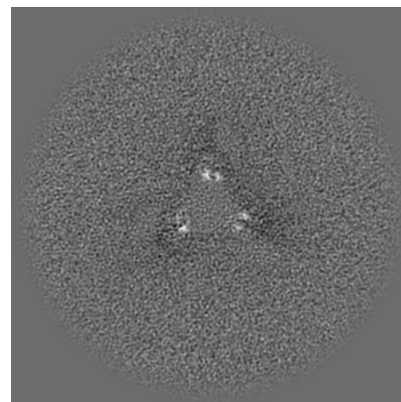
### 6.2.1 Primary map



X Index: 224

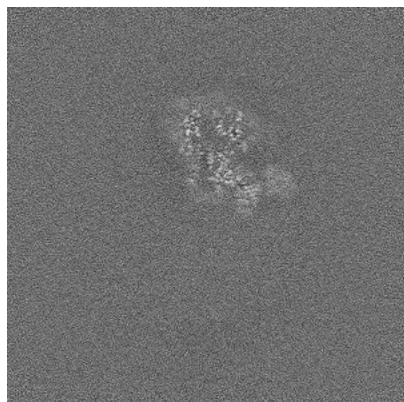


Y Index: 224



Z Index: 224

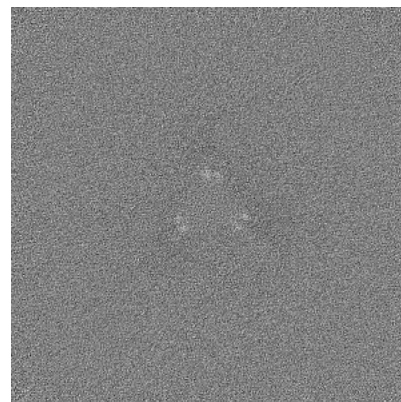
### 6.2.2 Raw map



X Index: 224



Y Index: 224

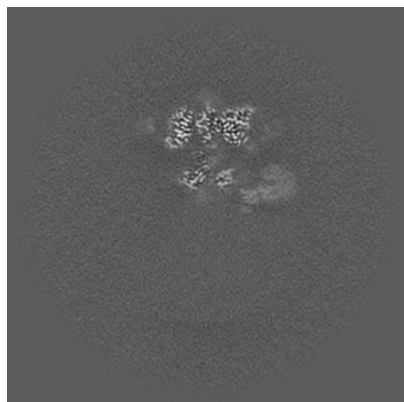


Z Index: 224

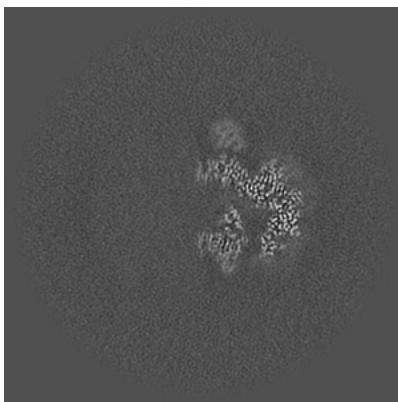
The images above show central slices of the map in three orthogonal directions.

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

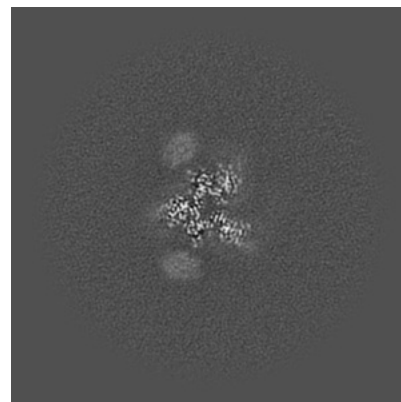
### 6.3.1 Primary map



X Index: 211

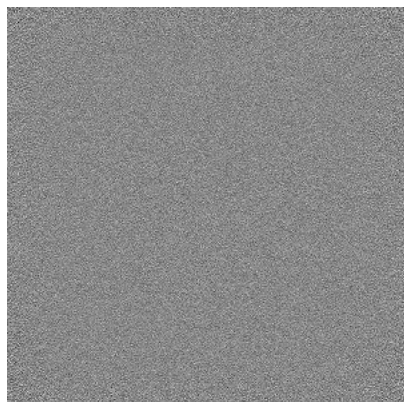


Y Index: 202

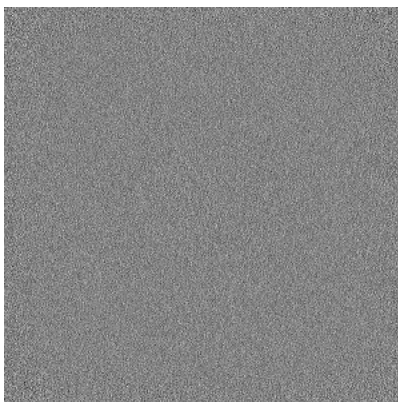


Z Index: 310

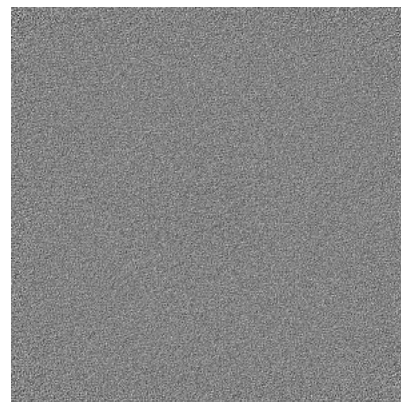
### 6.3.2 Raw map



X Index: 0



Y Index: 0

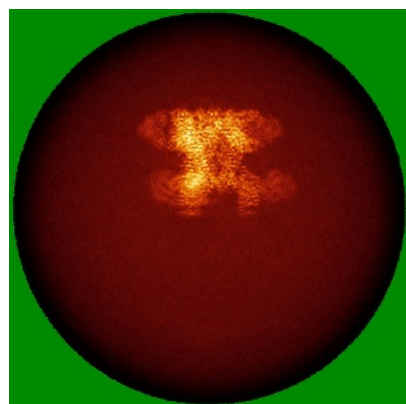


Z Index: 0

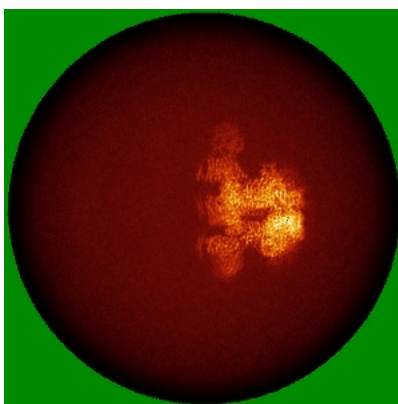
The images above show the largest variance slices of the map in three orthogonal directions.

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

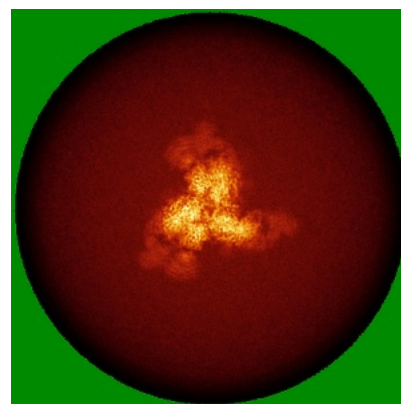
### 6.4.1 Primary map



X

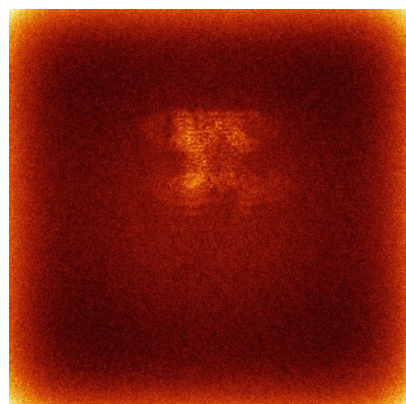


Y

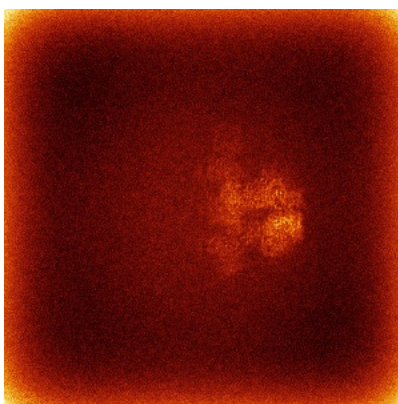


Z

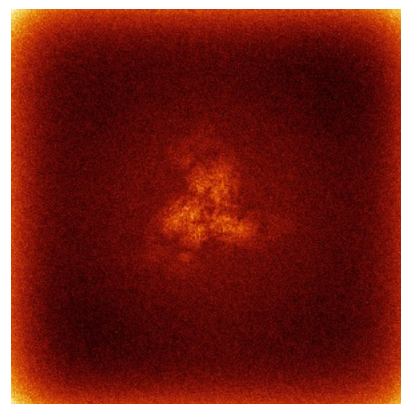
### 6.4.2 Raw map



X



Y



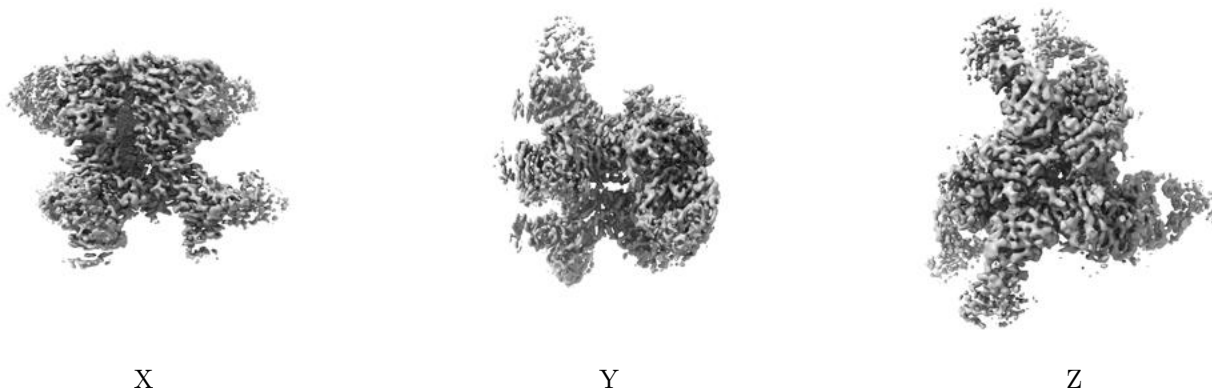
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



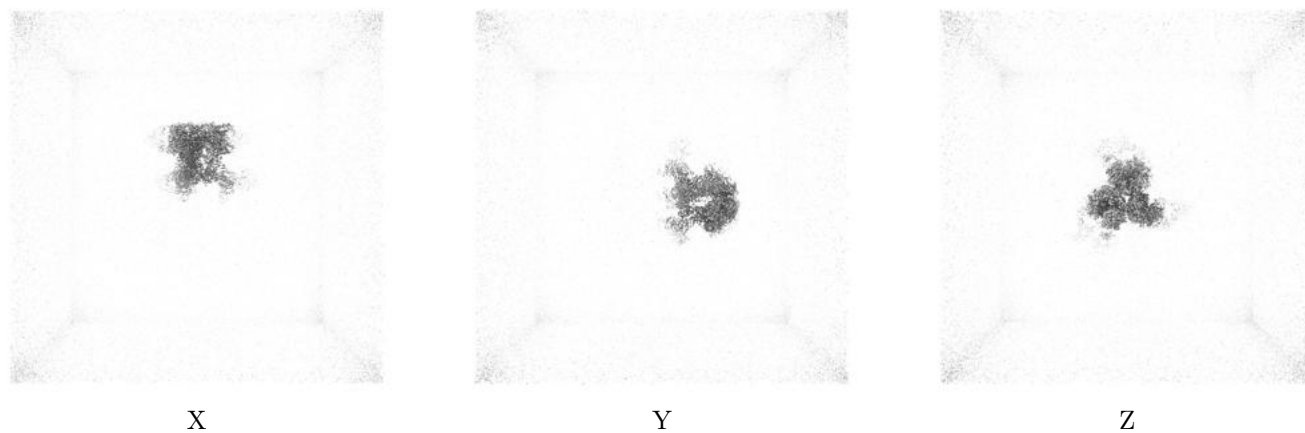
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

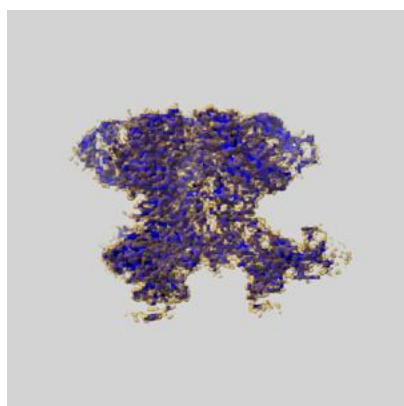
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

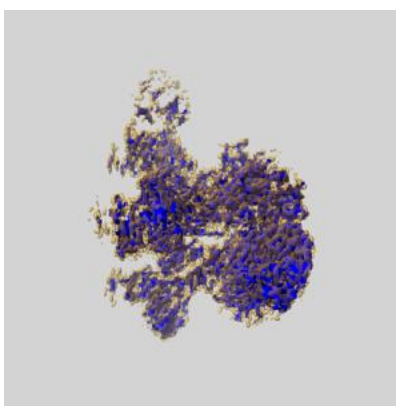
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

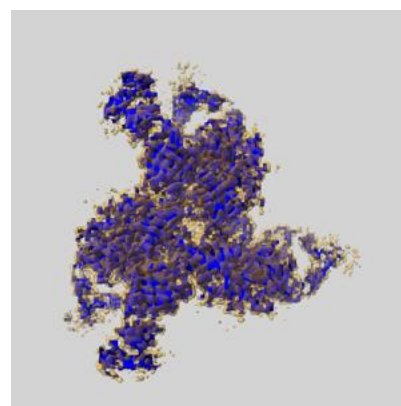
### 6.6.1 emd\_45928\_msk\_1.map [i](#)



X



Y

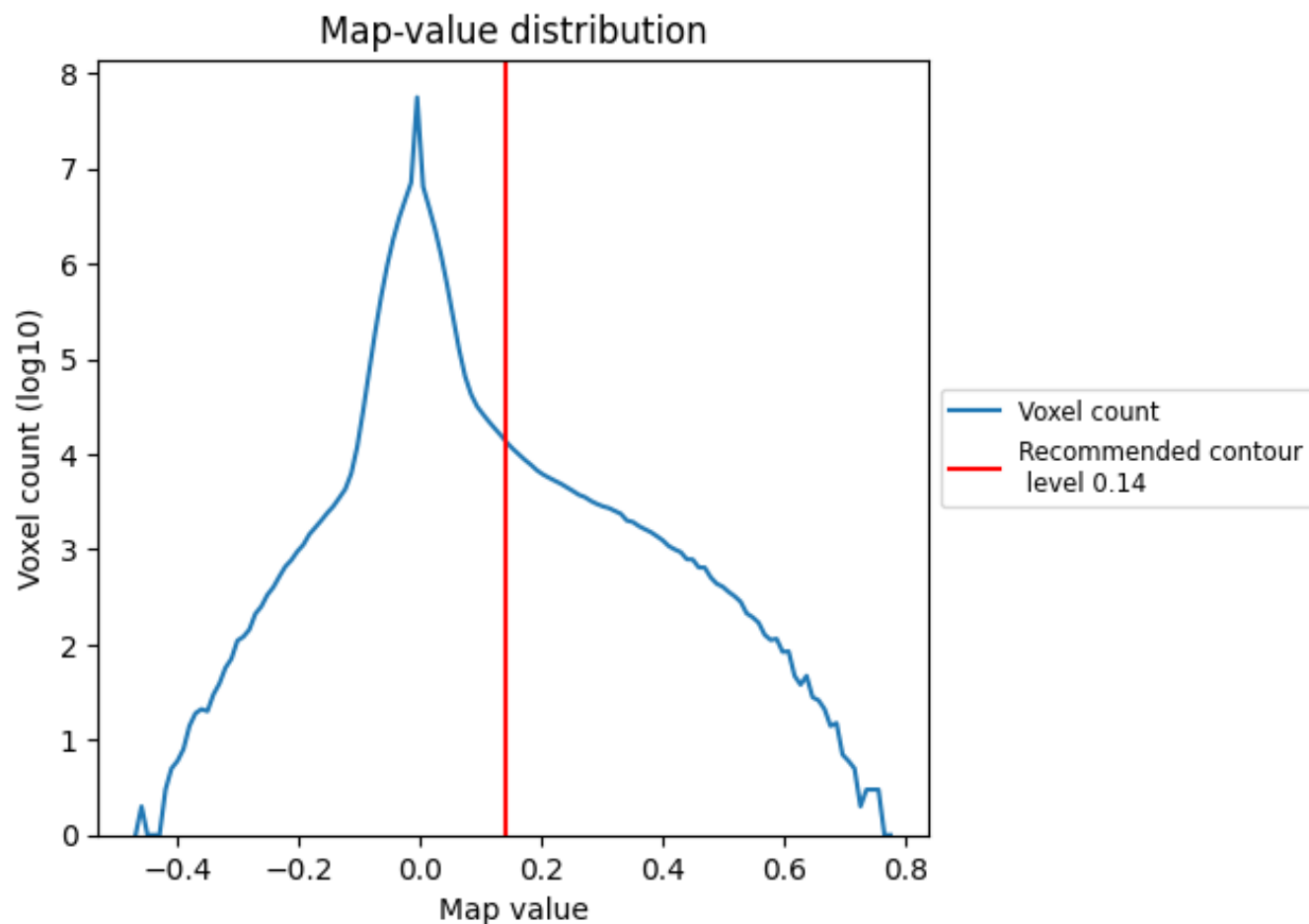


Z

## 7 Map analysis [i](#)

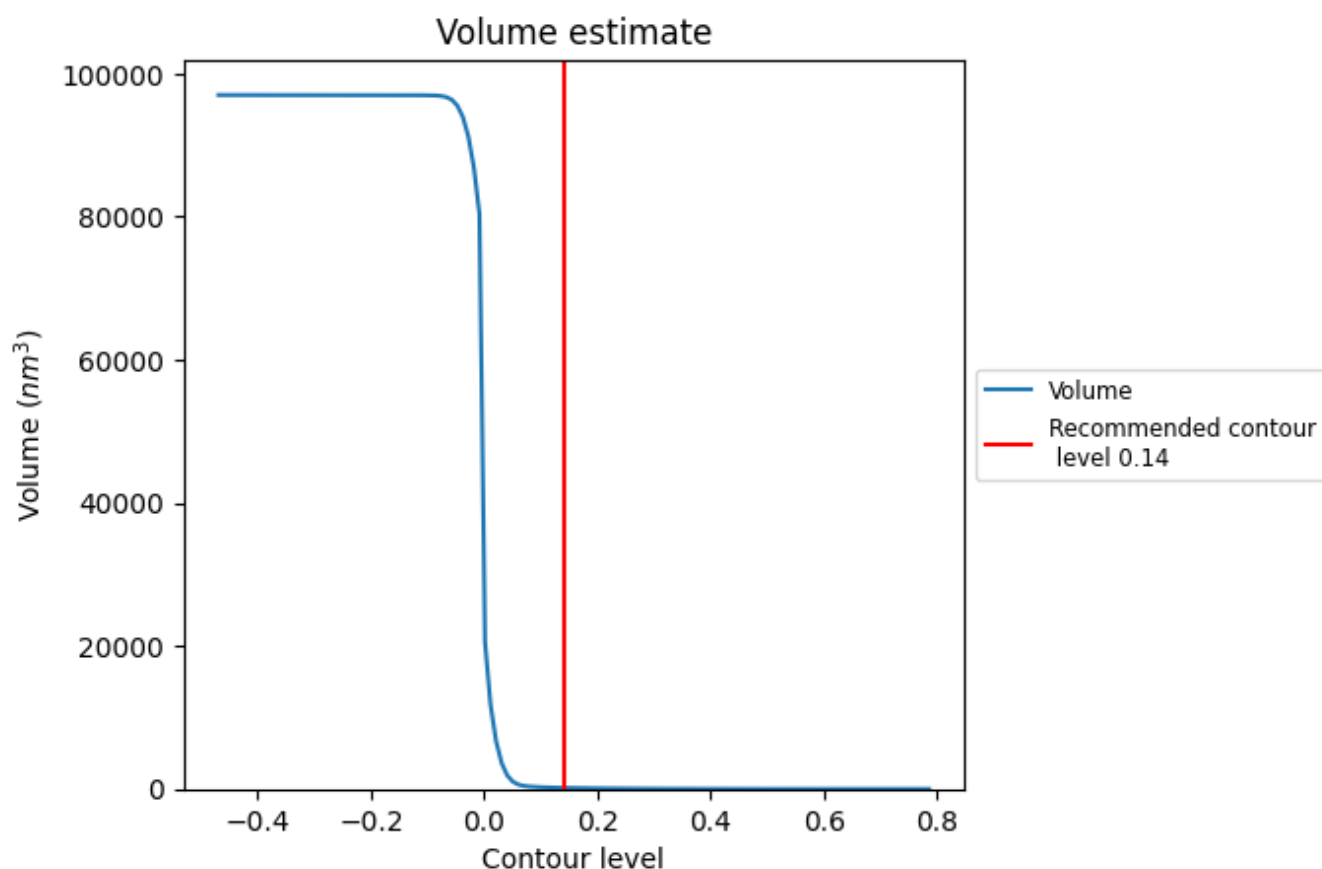
This section contains the results of statistical analysis of the map.

### 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.

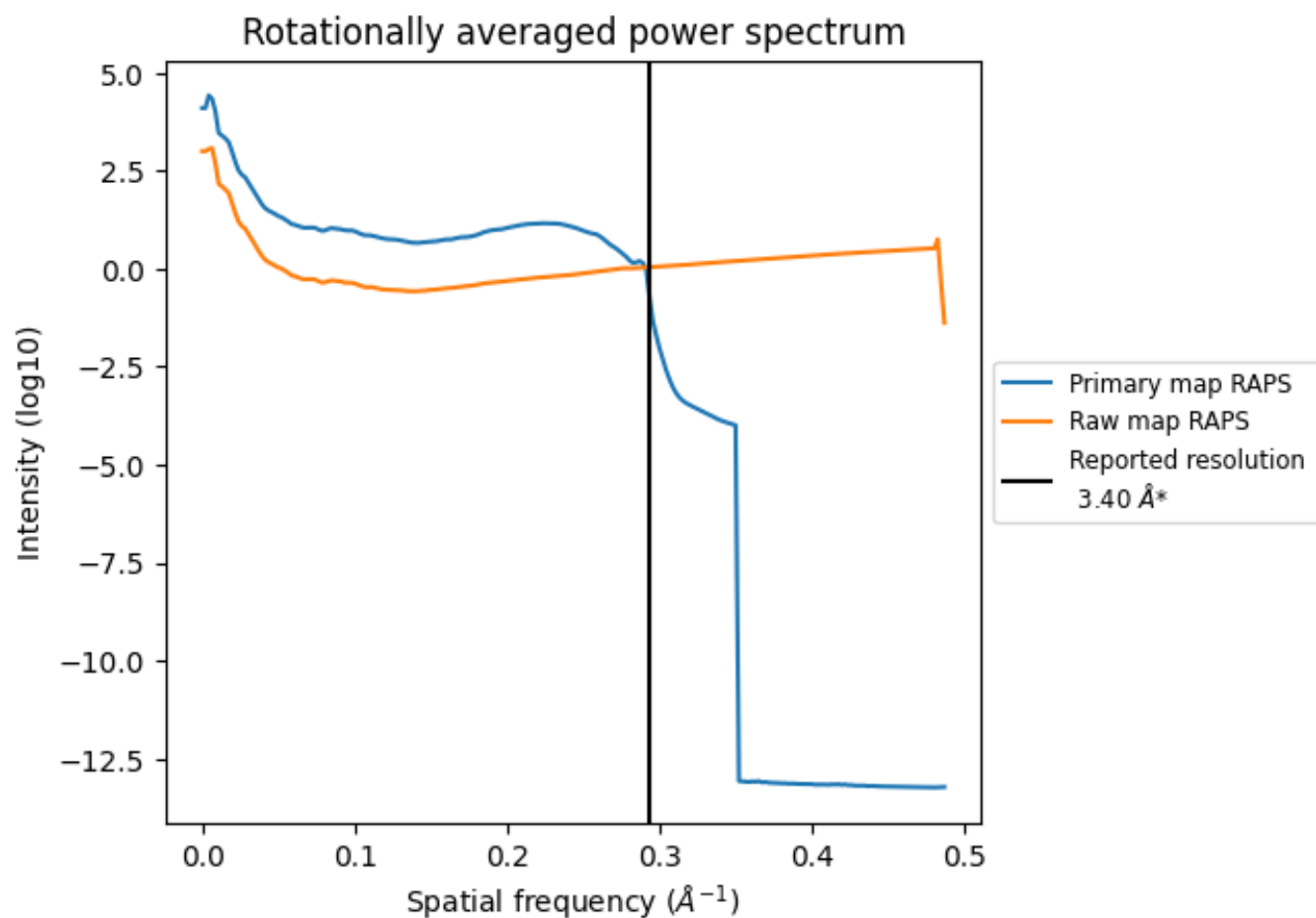
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 150 nm<sup>3</sup>; this corresponds to an approximate mass of 136 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 ⓘ



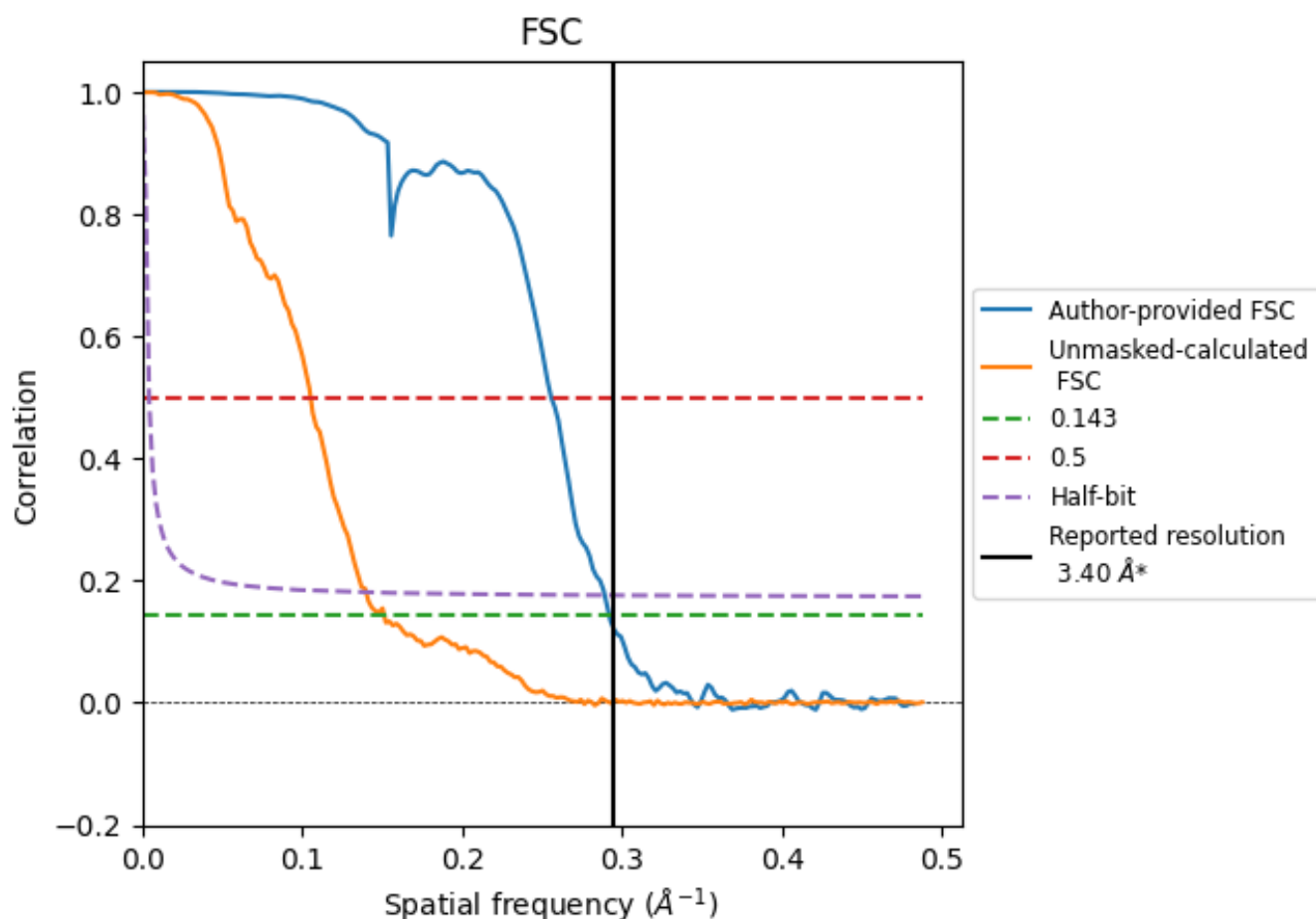
\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.294  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

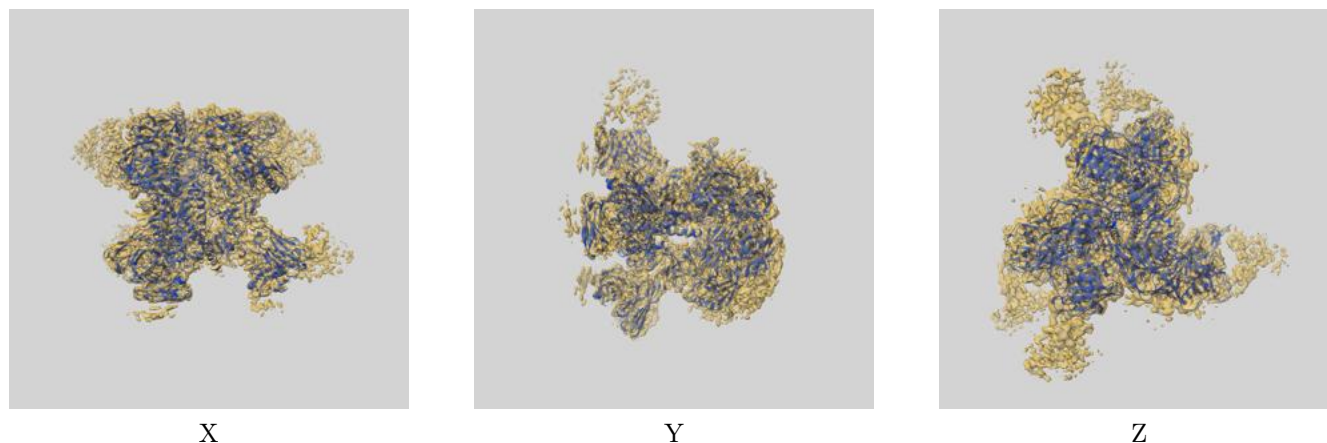
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.43	3.91	3.46
Unmasked-calculated*	6.61	9.51	7.15

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.61 differs from the reported value 3.4 by more than 10 %

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

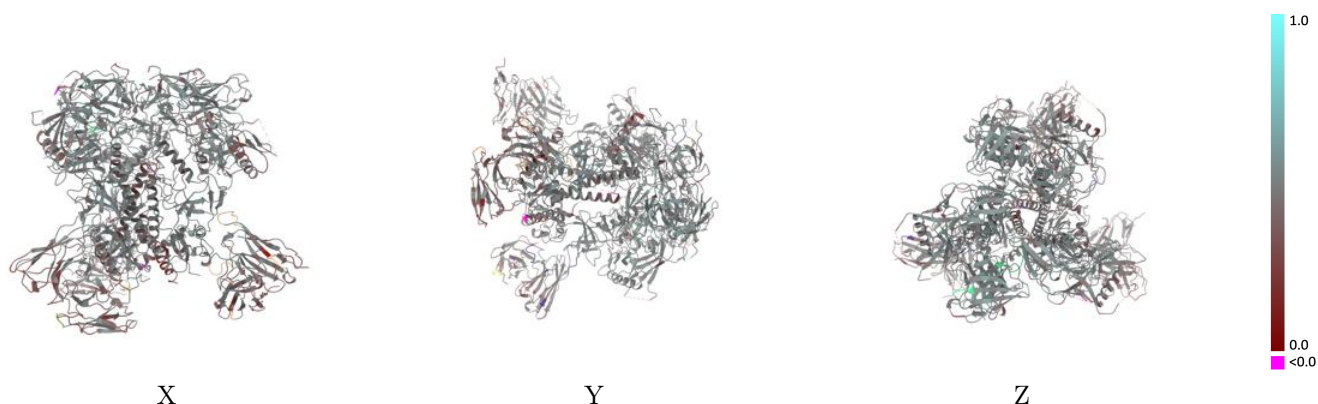
This section contains information regarding the fit between EMDB map EMD-45928 and PDB model 9CU5. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

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



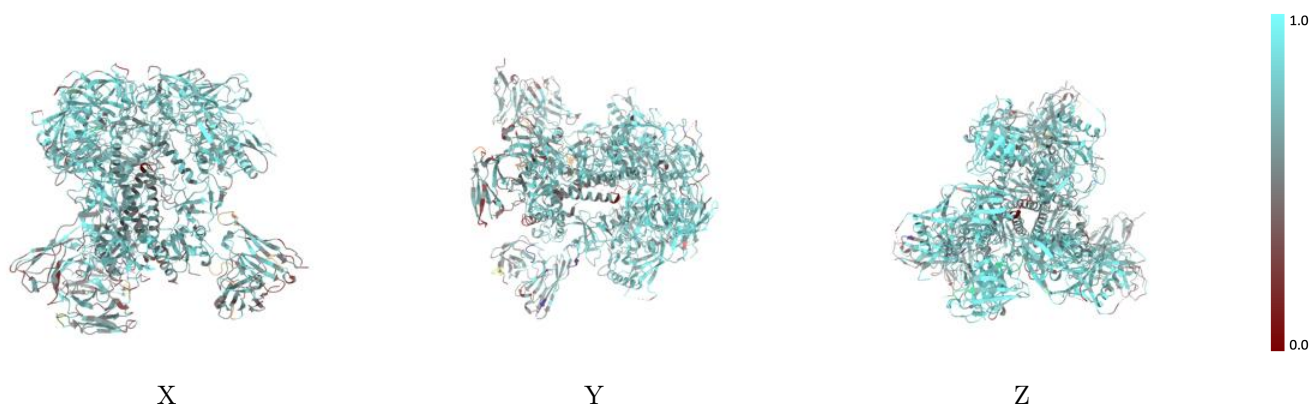
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



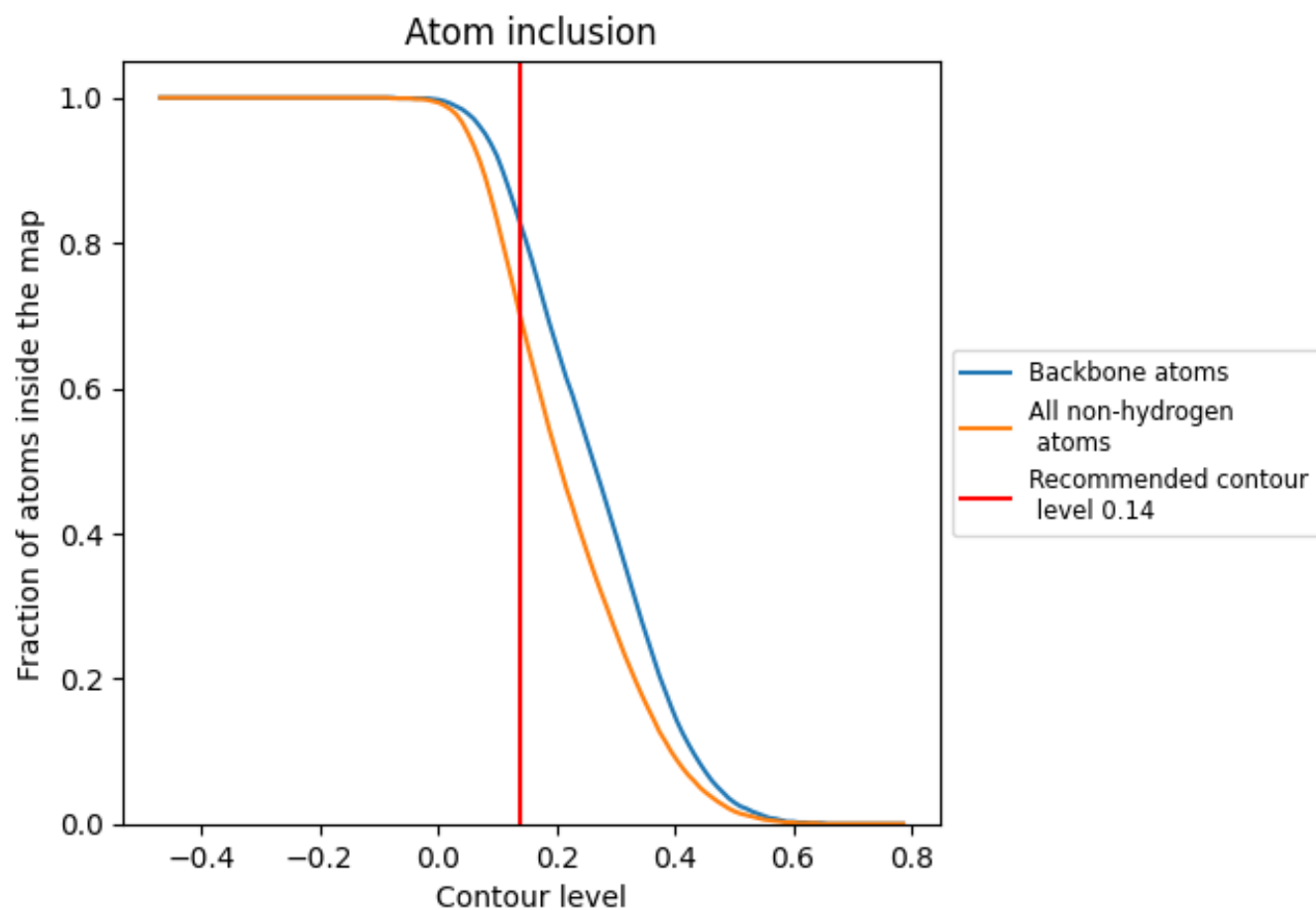
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.14).

















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 70% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6960	 0.4610
A	 0.6880	 0.4650
B	 0.7220	 0.4730
C	 0.7270	 0.4730
D	 0.6290	 0.4350
E	 0.5640	 0.4010
F	 0.6170	 0.4110
G	 0.5900	 0.4160
H	 0.8150	 0.5080
I	 0.8120	 0.5030
J	 0.6360	 0.4250
K	 0.5360	 0.3910
L	 0.7770	 0.4980
M	 0.7800	 0.5050
N	 0.7870	 0.4190
O	 0.5360	 0.4420
P	 0.6890	 0.4640
Q	 0.6720	 0.4020
R	 0.6070	 0.4470
S	 0.5710	 0.4500
T	 0.5860	 0.4710
U	 0.7870	 0.4700
V	 0.4290	 0.3650
W	 0.5000	 0.4110

