



## Full wwPDB EM Validation Report ⓘ

Nov 10, 2024 – 02:26 AM EST

PDB ID : 6X5B  
EMDB ID : EMD-22048  
Title : Symmetric model of CD4- and 17-bound B41 HIV-1 Env SOSIP in complex with small molecule GO52  
Authors : Ozorowski, G.; Torres, J.L.; Ward, A.B.  
Deposited on : 2020-05-25  
Resolution : 3.60 Å(reported)  
Based on initial model : 5VN3

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

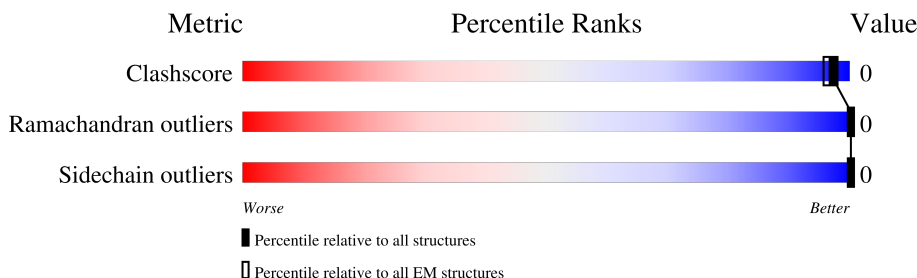
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	524	
1	D	524	
1	J	524	
2	B	153	
2	E	153	
2	K	153	
3	F	214	
3	L	214	

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Mol	Chain	Length	Quality of chain
3	M	214	
4	C	208	
4	G	208	
4	N	208	
5	H	229	
5	I	229	
5	O	229	
6	P	2	
6	R	2	
6	T	2	
7	Q	5	
7	S	5	
7	U	5	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 20232 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 Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	353	Total	C	N	O	S	0	0
			2769	1743	490	515	21		
1	D	353	Total	C	N	O	S	0	0
			2769	1743	490	515	21		
1	J	353	Total	C	N	O	S	0	0
			2769	1743	490	515	21		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	initiating methionine	UNP B3UES2
A	-3	ASP	-	expression tag	UNP B3UES2
A	-2	ALA	-	expression tag	UNP B3UES2
A	-1	MET	-	expression tag	UNP B3UES2
A	0	LYS	-	expression tag	UNP B3UES2
A	1	ARG	-	expression tag	UNP B3UES2
A	2	GLY	-	expression tag	UNP B3UES2
A	3	LEU	-	expression tag	UNP B3UES2
A	4	CYS	-	expression tag	UNP B3UES2
A	5	CYS	-	expression tag	UNP B3UES2
A	6	VAL	-	expression tag	UNP B3UES2
A	7	LEU	-	expression tag	UNP B3UES2
A	8	LEU	-	expression tag	UNP B3UES2
A	9	LEU	-	expression tag	UNP B3UES2
A	10	CYS	-	expression tag	UNP B3UES2
A	11	GLY	-	expression tag	UNP B3UES2
A	12	ALA	-	expression tag	UNP B3UES2
A	13	VAL	-	expression tag	UNP B3UES2
A	14	PHE	-	expression tag	UNP B3UES2
A	15	VAL	-	expression tag	UNP B3UES2
A	16	SER	-	expression tag	UNP B3UES2
A	17	PRO	-	expression tag	UNP B3UES2
A	18	SER	-	expression tag	UNP B3UES2
A	19	GLN	-	expression tag	UNP B3UES2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLU	-	expression tag	UNP B3UES2
A	21	ILE	-	expression tag	UNP B3UES2
A	22	HIS	-	expression tag	UNP B3UES2
A	23	ALA	-	expression tag	UNP B3UES2
A	24	ARG	-	expression tag	UNP B3UES2
A	25	PHE	-	expression tag	UNP B3UES2
A	26	ARG	-	expression tag	UNP B3UES2
A	27	ARG	-	expression tag	UNP B3UES2
A	28	GLY	-	expression tag	UNP B3UES2
A	29	ALA	-	expression tag	UNP B3UES2
A	30	ARG	-	expression tag	UNP B3UES2
A	501	CYS	ALA	engineered mutation	UNP B3UES2
A	509	ARG	GLU	engineered mutation	UNP B3UES2
A	510	ARG	LYS	engineered mutation	UNP B3UES2
A	512	ARG	ALA	engineered mutation	UNP B3UES2
A	513	ARG	VAL	engineered mutation	UNP B3UES2
D	-4	MET	-	initiating methionine	UNP B3UES2
D	-3	ASP	-	expression tag	UNP B3UES2
D	-2	ALA	-	expression tag	UNP B3UES2
D	-1	MET	-	expression tag	UNP B3UES2
D	0	LYS	-	expression tag	UNP B3UES2
D	1	ARG	-	expression tag	UNP B3UES2
D	2	GLY	-	expression tag	UNP B3UES2
D	3	LEU	-	expression tag	UNP B3UES2
D	4	CYS	-	expression tag	UNP B3UES2
D	5	CYS	-	expression tag	UNP B3UES2
D	6	VAL	-	expression tag	UNP B3UES2
D	7	LEU	-	expression tag	UNP B3UES2
D	8	LEU	-	expression tag	UNP B3UES2
D	9	LEU	-	expression tag	UNP B3UES2
D	10	CYS	-	expression tag	UNP B3UES2
D	11	GLY	-	expression tag	UNP B3UES2
D	12	ALA	-	expression tag	UNP B3UES2
D	13	VAL	-	expression tag	UNP B3UES2
D	14	PHE	-	expression tag	UNP B3UES2
D	15	VAL	-	expression tag	UNP B3UES2
D	16	SER	-	expression tag	UNP B3UES2
D	17	PRO	-	expression tag	UNP B3UES2
D	18	SER	-	expression tag	UNP B3UES2
D	19	GLN	-	expression tag	UNP B3UES2
D	20	GLU	-	expression tag	UNP B3UES2
D	21	ILE	-	expression tag	UNP B3UES2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	22	HIS	-	expression tag	UNP B3UES2
D	23	ALA	-	expression tag	UNP B3UES2
D	24	ARG	-	expression tag	UNP B3UES2
D	25	PHE	-	expression tag	UNP B3UES2
D	26	ARG	-	expression tag	UNP B3UES2
D	27	ARG	-	expression tag	UNP B3UES2
D	28	GLY	-	expression tag	UNP B3UES2
D	29	ALA	-	expression tag	UNP B3UES2
D	30	ARG	-	expression tag	UNP B3UES2
D	501	CYS	ALA	engineered mutation	UNP B3UES2
D	509	ARG	GLU	engineered mutation	UNP B3UES2
D	510	ARG	LYS	engineered mutation	UNP B3UES2
D	512	ARG	ALA	engineered mutation	UNP B3UES2
D	513	ARG	VAL	engineered mutation	UNP B3UES2
J	-4	MET	-	initiating methionine	UNP B3UES2
J	-3	ASP	-	expression tag	UNP B3UES2
J	-2	ALA	-	expression tag	UNP B3UES2
J	-1	MET	-	expression tag	UNP B3UES2
J	0	LYS	-	expression tag	UNP B3UES2
J	1	ARG	-	expression tag	UNP B3UES2
J	2	GLY	-	expression tag	UNP B3UES2
J	3	LEU	-	expression tag	UNP B3UES2
J	4	CYS	-	expression tag	UNP B3UES2
J	5	CYS	-	expression tag	UNP B3UES2
J	6	VAL	-	expression tag	UNP B3UES2
J	7	LEU	-	expression tag	UNP B3UES2
J	8	LEU	-	expression tag	UNP B3UES2
J	9	LEU	-	expression tag	UNP B3UES2
J	10	CYS	-	expression tag	UNP B3UES2
J	11	GLY	-	expression tag	UNP B3UES2
J	12	ALA	-	expression tag	UNP B3UES2
J	13	VAL	-	expression tag	UNP B3UES2
J	14	PHE	-	expression tag	UNP B3UES2
J	15	VAL	-	expression tag	UNP B3UES2
J	16	SER	-	expression tag	UNP B3UES2
J	17	PRO	-	expression tag	UNP B3UES2
J	18	SER	-	expression tag	UNP B3UES2
J	19	GLN	-	expression tag	UNP B3UES2
J	20	GLU	-	expression tag	UNP B3UES2
J	21	ILE	-	expression tag	UNP B3UES2
J	22	HIS	-	expression tag	UNP B3UES2
J	23	ALA	-	expression tag	UNP B3UES2

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Chain	Residue	Modelled	Actual	Comment	Reference
J	24	ARG	-	expression tag	UNP B3UES2
J	25	PHE	-	expression tag	UNP B3UES2
J	26	ARG	-	expression tag	UNP B3UES2
J	27	ARG	-	expression tag	UNP B3UES2
J	28	GLY	-	expression tag	UNP B3UES2
J	29	ALA	-	expression tag	UNP B3UES2
J	30	ARG	-	expression tag	UNP B3UES2
J	501	CYS	ALA	engineered mutation	UNP B3UES2
J	509	ARG	GLU	engineered mutation	UNP B3UES2
J	510	ARG	LYS	engineered mutation	UNP B3UES2
J	512	ARG	ALA	engineered mutation	UNP B3UES2
J	513	ARG	VAL	engineered mutation	UNP B3UES2

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	149	Total	C	N	O	S	0	0
			1184	751	206	219	8		
2	E	149	Total	C	N	O	S	0	0
			1184	751	206	219	8		
2	K	149	Total	C	N	O	S	0	0
			1184	751	206	219	8		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP B3UEZ6
B	605	CYS	THR	engineered mutation	UNP B3UEZ6
E	559	PRO	ILE	engineered mutation	UNP B3UEZ6
E	605	CYS	THR	engineered mutation	UNP B3UEZ6
K	559	PRO	ILE	engineered mutation	UNP B3UEZ6
K	605	CYS	THR	engineered mutation	UNP B3UEZ6

- Molecule 3 is a protein called 17b Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	106	Total	C	N	O	S	0	0
			812	508	140	162	2		
3	F	106	Total	C	N	O	S	0	0
			812	508	140	162	2		
3	M	106	Total	C	N	O	S	0	0
			812	508	140	162	2		

- Molecule 4 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	96	Total	C	N	O	S	0	0
			768	482	135	149	2		
4	G	96	Total	C	N	O	S	0	0
			768	482	135	149	2		
4	N	96	Total	C	N	O	S	0	0
			768	482	135	149	2		

There are 87 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	initiating methionine	UNP P01730
C	-18	GLU	-	expression tag	UNP P01730
C	-17	THR	-	expression tag	UNP P01730
C	-16	ASP	-	expression tag	UNP P01730
C	-15	THR	-	expression tag	UNP P01730
C	-14	LEU	-	expression tag	UNP P01730
C	-13	LEU	-	expression tag	UNP P01730
C	-12	LEU	-	expression tag	UNP P01730
C	-11	TRP	-	expression tag	UNP P01730
C	-10	VAL	-	expression tag	UNP P01730
C	-9	LEU	-	expression tag	UNP P01730
C	-8	LEU	-	expression tag	UNP P01730
C	-7	LEU	-	expression tag	UNP P01730
C	-6	TRP	-	expression tag	UNP P01730
C	-5	VAL	-	expression tag	UNP P01730
C	-4	PRO	-	expression tag	UNP P01730
C	-3	GLY	-	expression tag	UNP P01730
C	-2	SER	-	expression tag	UNP P01730
C	-1	THR	-	expression tag	UNP P01730
C	179	GLY	-	expression tag	UNP P01730
C	180	GLY	-	expression tag	UNP P01730
C	181	SER	-	expression tag	UNP P01730
C	182	GLY	-	expression tag	UNP P01730
C	183	HIS	-	expression tag	UNP P01730
C	184	HIS	-	expression tag	UNP P01730
C	185	HIS	-	expression tag	UNP P01730
C	186	HIS	-	expression tag	UNP P01730
C	187	HIS	-	expression tag	UNP P01730
C	188	HIS	-	expression tag	UNP P01730
G	-19	MET	-	initiating methionine	UNP P01730
G	-18	GLU	-	expression tag	UNP P01730
G	-17	THR	-	expression tag	UNP P01730

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-16	ASP	-	expression tag	UNP P01730
G	-15	THR	-	expression tag	UNP P01730
G	-14	LEU	-	expression tag	UNP P01730
G	-13	LEU	-	expression tag	UNP P01730
G	-12	LEU	-	expression tag	UNP P01730
G	-11	TRP	-	expression tag	UNP P01730
G	-10	VAL	-	expression tag	UNP P01730
G	-9	LEU	-	expression tag	UNP P01730
G	-8	LEU	-	expression tag	UNP P01730
G	-7	LEU	-	expression tag	UNP P01730
G	-6	TRP	-	expression tag	UNP P01730
G	-5	VAL	-	expression tag	UNP P01730
G	-4	PRO	-	expression tag	UNP P01730
G	-3	GLY	-	expression tag	UNP P01730
G	-2	SER	-	expression tag	UNP P01730
G	-1	THR	-	expression tag	UNP P01730
G	179	GLY	-	expression tag	UNP P01730
G	180	GLY	-	expression tag	UNP P01730
G	181	SER	-	expression tag	UNP P01730
G	182	GLY	-	expression tag	UNP P01730
G	183	HIS	-	expression tag	UNP P01730
G	184	HIS	-	expression tag	UNP P01730
G	185	HIS	-	expression tag	UNP P01730
G	186	HIS	-	expression tag	UNP P01730
G	187	HIS	-	expression tag	UNP P01730
G	188	HIS	-	expression tag	UNP P01730
N	-19	MET	-	initiating methionine	UNP P01730
N	-18	GLU	-	expression tag	UNP P01730
N	-17	THR	-	expression tag	UNP P01730
N	-16	ASP	-	expression tag	UNP P01730
N	-15	THR	-	expression tag	UNP P01730
N	-14	LEU	-	expression tag	UNP P01730
N	-13	LEU	-	expression tag	UNP P01730
N	-12	LEU	-	expression tag	UNP P01730
N	-11	TRP	-	expression tag	UNP P01730
N	-10	VAL	-	expression tag	UNP P01730
N	-9	LEU	-	expression tag	UNP P01730
N	-8	LEU	-	expression tag	UNP P01730
N	-7	LEU	-	expression tag	UNP P01730
N	-6	TRP	-	expression tag	UNP P01730
N	-5	VAL	-	expression tag	UNP P01730
N	-4	PRO	-	expression tag	UNP P01730

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-3	GLY	-	expression tag	UNP P01730
N	-2	SER	-	expression tag	UNP P01730
N	-1	THR	-	expression tag	UNP P01730
N	179	GLY	-	expression tag	UNP P01730
N	180	GLY	-	expression tag	UNP P01730
N	181	SER	-	expression tag	UNP P01730
N	182	GLY	-	expression tag	UNP P01730
N	183	HIS	-	expression tag	UNP P01730
N	184	HIS	-	expression tag	UNP P01730
N	185	HIS	-	expression tag	UNP P01730
N	186	HIS	-	expression tag	UNP P01730
N	187	HIS	-	expression tag	UNP P01730
N	188	HIS	-	expression tag	UNP P01730

- Molecule 5 is a protein called 17b Fab heavy chain.

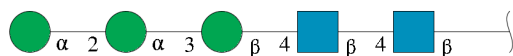
Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	125	Total	C	N	O	S	0	0
			971	614	166	188	3		
5	I	125	Total	C	N	O	S	0	0
			971	614	166	188	3		
5	O	125	Total	C	N	O	S	0	0
			971	614	166	188	3		

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



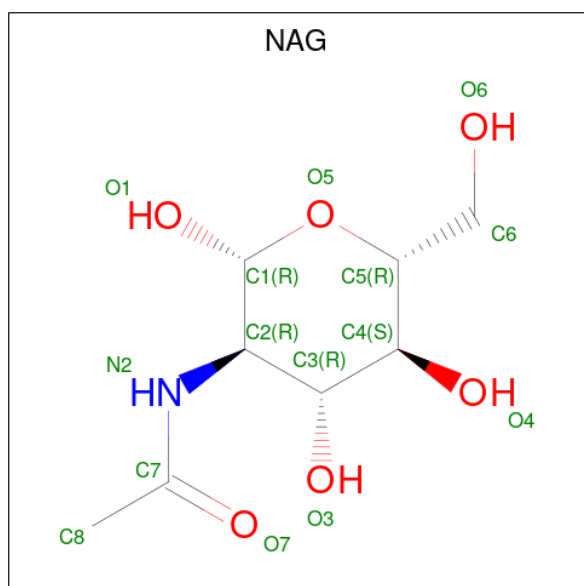
Mol	Chain	Residues	Atoms				AltConf	Trace
6	P	2	Total	C	N	O	0	0
			28	16	2	10		
6	R	2	Total	C	N	O	0	0
			28	16	2	10		
6	T	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 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
7	Q	5	Total	C	N	O	0	0
			61	34	2	25		
7	S	5	Total	C	N	O	0	0
			61	34	2	25		
7	U	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



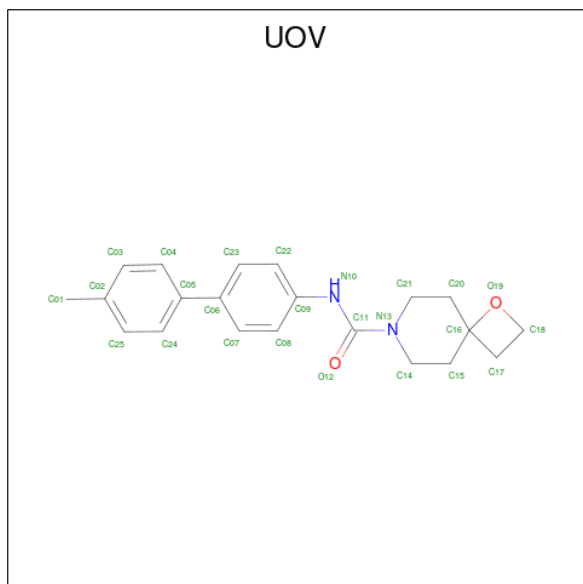
Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	

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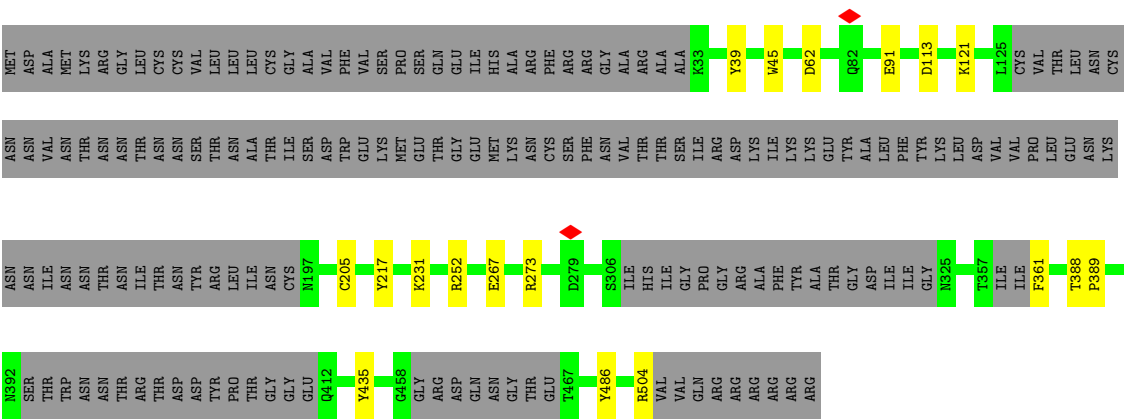
Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total 14	C 8	N 1	O 5	0
8	A	1	Total 14	C 8	N 1	O 5	0
8	B	1	Total 14	C 8	N 1	O 5	0
8	D	1	Total 14	C 8	N 1	O 5	0
8	D	1	Total 14	C 8	N 1	O 5	0
8	D	1	Total 14	C 8	N 1	O 5	0
8	D	1	Total 14	C 8	N 1	O 5	0
8	D	1	Total 14	C 8	N 1	O 5	0
8	D	1	Total 14	C 8	N 1	O 5	0
8	D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

- Molecule 9 is N-(4'-methyl[1,1'-biphenyl]-4-yl)-1-oxa-7-azaspiro[3.5]nonane-7-carboxamide (three-letter code: UOV) (formula: C<sub>21</sub>H<sub>24</sub>N<sub>2</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

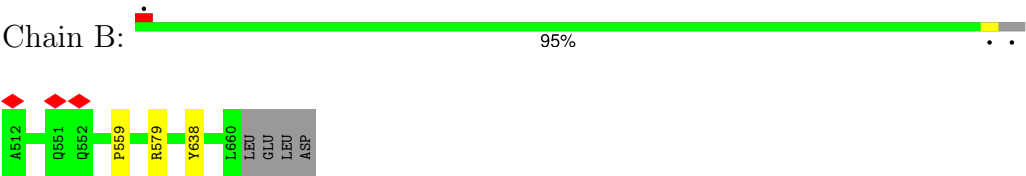


Mol	Chain	Residues	Atoms				AltConf
9	B	1	Total	C	N	O	0
			25	21	2	2	
9	E	1	Total	C	N	O	0
			25	21	2	2	
9	K	1	Total	C	N	O	0
			25	21	2	2	

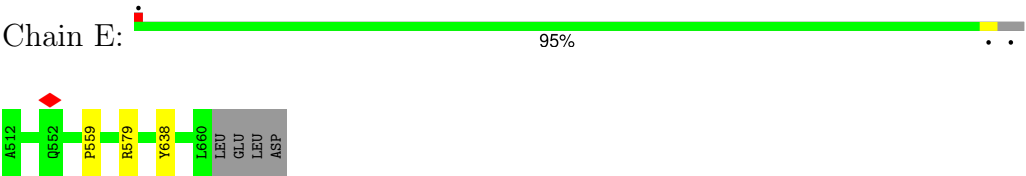




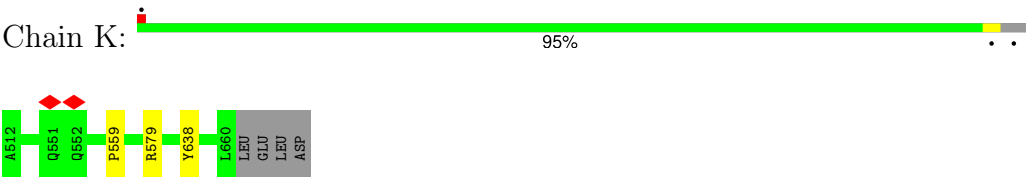
• Molecule 2: Envelope glycoprotein gp41



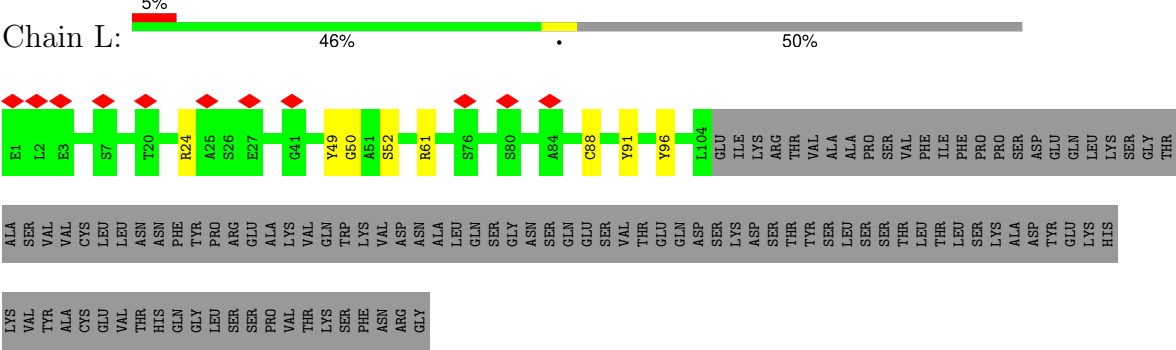
• Molecule 2: Envelope glycoprotein gp41



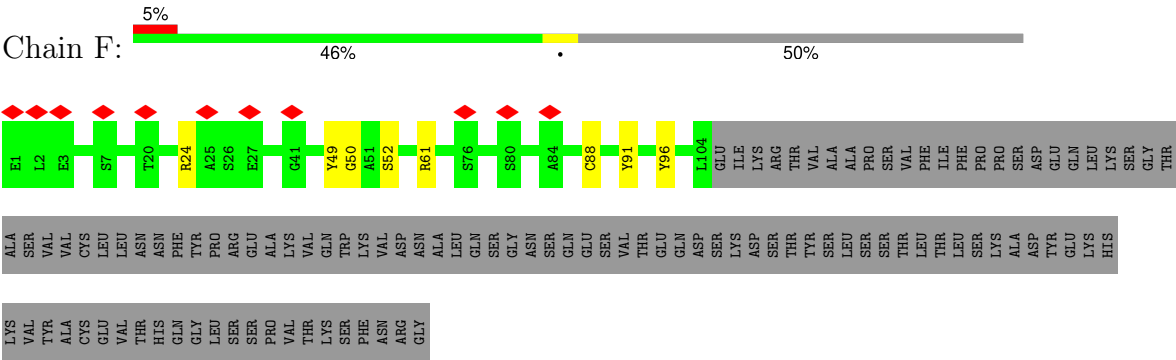
• Molecule 2: Envelope glycoprotein gp41



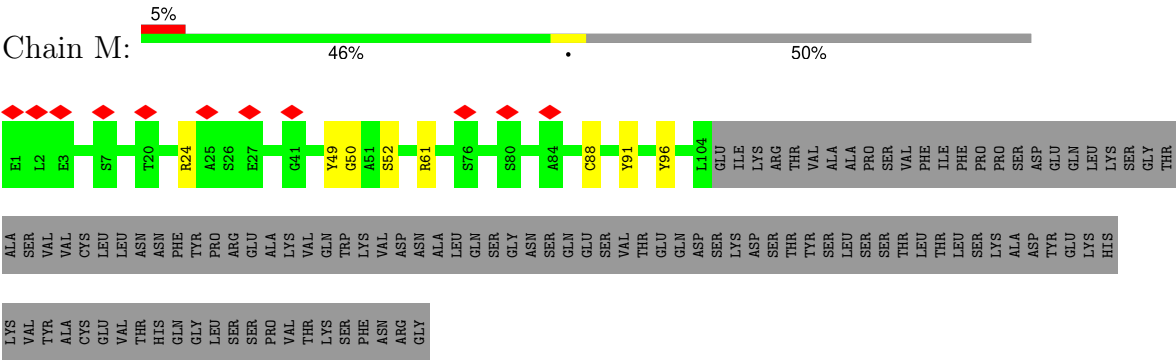
• Molecule 3: 17b Fab light chain



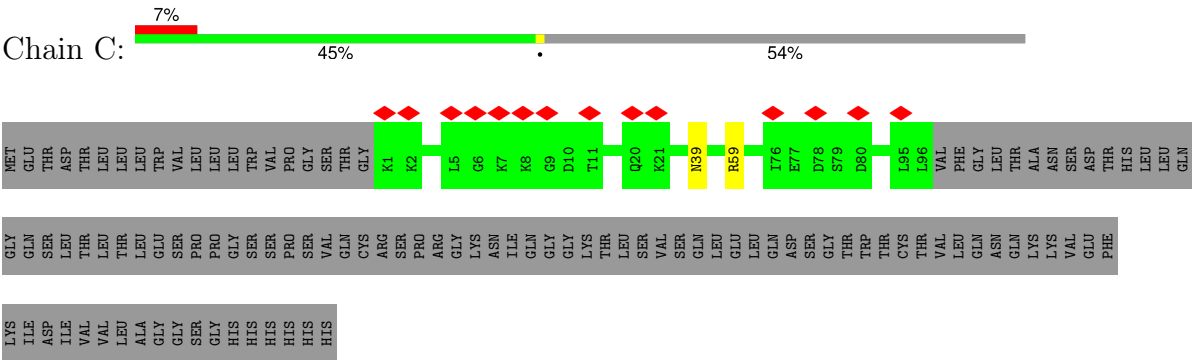
• Molecule 3: 17b Fab light chain



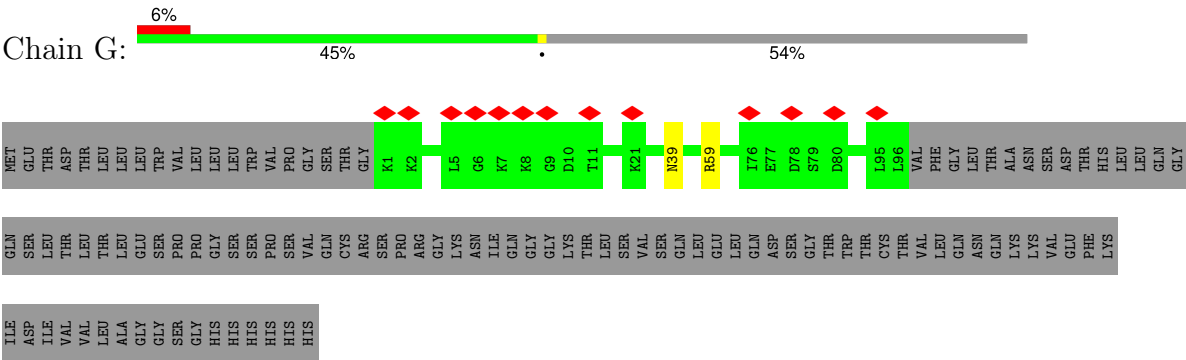
• Molecule 3: 17b Fab light chain



• Molecule 4: T-cell surface glycoprotein CD4

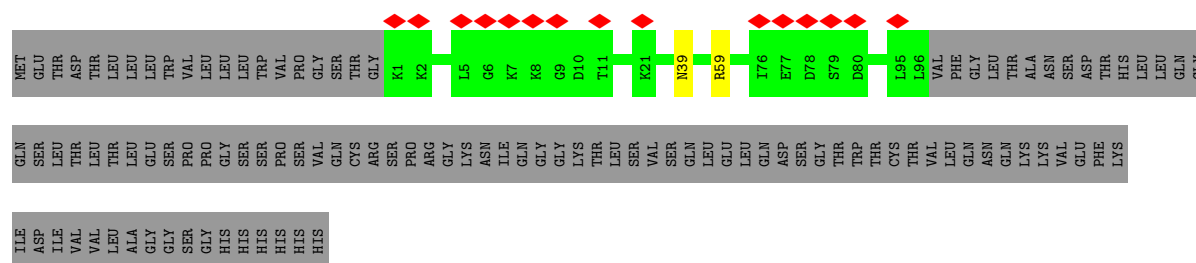
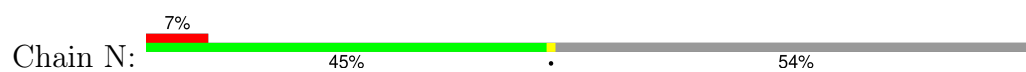


• Molecule 4: T-cell surface glycoprotein CD4

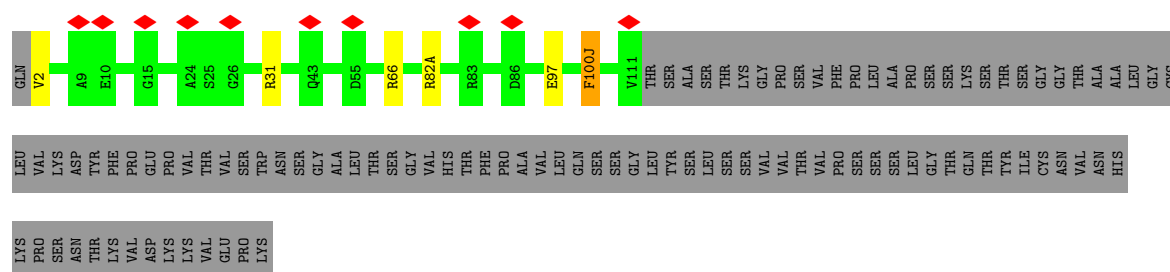


• Molecule 4: T-cell surface glycoprotein CD4

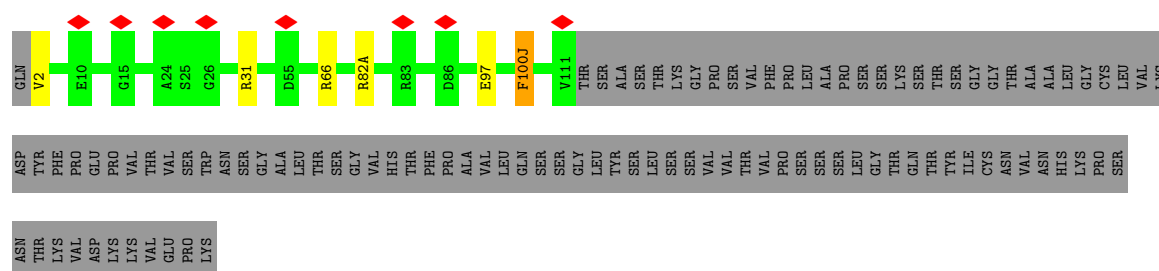




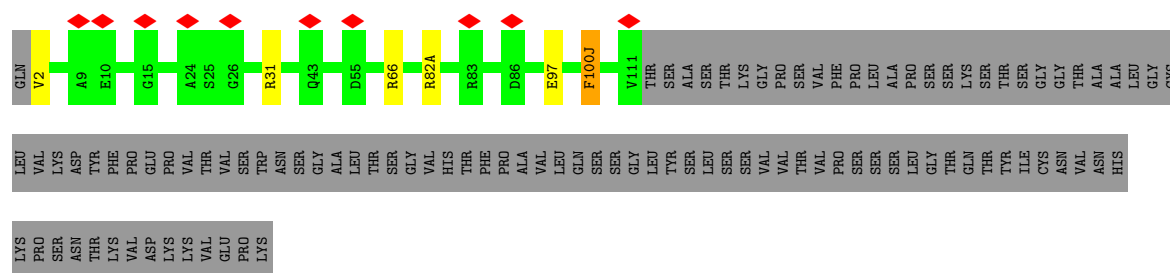
• Molecule 5: 17b Fab heavy chain



• Molecule 5: 17b Fab heavy chain



• Molecule 5: 17b Fab heavy chain



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

Chain P:  100%

MAG1  
MAG2

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

Chain R:  100%


MAG1  
MAG2

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

Chain T:  100%

MAG1  
MAG2

- Molecule 7: 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 Q:  100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

- Molecule 7: 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 S:  100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

- Molecule 7: 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 U:  100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	228502	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	49	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.183	Depositor
Minimum map value	-0.101	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	331.19998, 331.19998, 331.19998	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	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: UOV, BMA, NAG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.10	8/2828 (0.3%)	0.90	8/3841 (0.2%)
1	D	1.10	8/2828 (0.3%)	0.90	8/3841 (0.2%)
1	J	1.10	9/2828 (0.3%)	0.90	8/3841 (0.2%)
2	B	1.02	1/1206 (0.1%)	0.85	3/1637 (0.2%)
2	E	1.02	1/1206 (0.1%)	0.85	3/1637 (0.2%)
2	K	1.02	1/1206 (0.1%)	0.85	3/1637 (0.2%)
3	F	1.12	3/832 (0.4%)	1.02	3/1133 (0.3%)
3	L	1.12	3/832 (0.4%)	1.02	3/1133 (0.3%)
3	M	1.12	3/832 (0.4%)	1.02	3/1133 (0.3%)
4	C	1.01	0/778	0.89	1/1043 (0.1%)
4	G	1.01	0/778	0.89	1/1043 (0.1%)
4	N	1.01	0/778	0.89	1/1043 (0.1%)
5	H	1.09	4/992 (0.4%)	0.96	3/1346 (0.2%)
5	I	1.09	4/992 (0.4%)	0.96	3/1346 (0.2%)
5	O	1.09	4/992 (0.4%)	0.96	3/1346 (0.2%)
All	All	1.08	49/19908 (0.2%)	0.91	54/27000 (0.2%)

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	361	PHE	CG-CD1	7.20	1.49	1.38
1	A	361	PHE	CG-CD1	7.16	1.49	1.38
1	D	361	PHE	CG-CD1	7.13	1.49	1.38
1	D	205	CYS	CB-SG	-6.83	1.70	1.82
1	J	205	CYS	CB-SG	-6.82	1.70	1.82
1	A	45	TRP	CB-CG	-6.77	1.38	1.50
1	A	205	CYS	CB-SG	-6.77	1.70	1.82
1	J	45	TRP	CB-CG	-6.73	1.38	1.50
1	D	45	TRP	CB-CG	-6.72	1.38	1.50
1	A	361	PHE	CG-CD2	6.28	1.48	1.38
1	D	361	PHE	CG-CD2	6.23	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	361	PHE	CG-CD2	6.20	1.48	1.38
1	A	504	ARG	NE-CZ	5.88	1.40	1.33
1	D	504	ARG	NE-CZ	5.84	1.40	1.33
1	J	504	ARG	NE-CZ	5.82	1.40	1.33
3	F	91	TYR	CB-CG	-5.68	1.43	1.51
5	I	100(J)	PHE	CB-CG	-5.68	1.41	1.51
3	L	91	TYR	CB-CG	-5.67	1.43	1.51
3	M	91	TYR	CB-CG	-5.66	1.43	1.51
5	O	100(J)	PHE	CB-CG	-5.64	1.41	1.51
5	H	100(J)	PHE	CB-CG	-5.64	1.41	1.51
5	O	2	VAL	CB-CG1	5.59	1.64	1.52
5	I	2	VAL	CB-CG1	5.59	1.64	1.52
5	H	2	VAL	CB-CG1	5.57	1.64	1.52
2	B	638	TYR	CB-CG	-5.52	1.43	1.51
2	K	638	TYR	CB-CG	-5.49	1.43	1.51
2	E	638	TYR	CB-CG	-5.48	1.43	1.51
1	A	361	PHE	CE2-CZ	5.45	1.47	1.37
1	D	361	PHE	CE2-CZ	5.44	1.47	1.37
1	J	361	PHE	CE2-CZ	5.43	1.47	1.37
1	J	91	GLU	CD-OE1	-5.36	1.19	1.25
3	M	91	TYR	CD1-CE1	-5.34	1.31	1.39
1	D	91	GLU	CD-OE1	-5.31	1.19	1.25
1	A	91	GLU	CD-OE1	-5.29	1.19	1.25
3	F	91	TYR	CD1-CE1	-5.29	1.31	1.39
3	L	91	TYR	CD1-CE1	-5.27	1.31	1.39
1	D	39	TYR	CB-CG	-5.18	1.43	1.51
3	M	88	CYS	CB-SG	-5.18	1.73	1.81
3	L	88	CYS	CB-SG	-5.17	1.73	1.81
1	A	39	TYR	CB-CG	-5.17	1.44	1.51
1	J	39	TYR	CB-CG	-5.15	1.44	1.51
3	F	88	CYS	CB-SG	-5.13	1.73	1.81
5	I	97	GLU	CD-OE2	-5.08	1.20	1.25
5	H	97	GLU	CG-CD	-5.07	1.44	1.51
5	O	97	GLU	CG-CD	-5.07	1.44	1.51
5	O	97	GLU	CD-OE2	-5.06	1.20	1.25
5	I	97	GLU	CG-CD	-5.05	1.44	1.51
5	H	97	GLU	CD-OE2	-5.02	1.20	1.25
1	J	361	PHE	CE1-CZ	5.00	1.46	1.37

All (54) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	61	ARG	NE-CZ-NH2	-8.44	116.08	120.30
3	F	61	ARG	NE-CZ-NH2	-8.37	116.12	120.30
3	L	61	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	J	273	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	D	273	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	A	273	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	D	252	ARG	NE-CZ-NH1	6.95	123.78	120.30
5	H	31	ARG	NE-CZ-NH2	-6.94	116.83	120.30
5	O	31	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	A	252	ARG	NE-CZ-NH1	6.89	123.74	120.30
5	I	31	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	J	252	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	J	486	TYR	CB-CG-CD1	-6.67	117.00	121.00
1	A	486	TYR	CB-CG-CD1	-6.65	117.01	121.00
1	D	486	TYR	CB-CG-CD1	-6.62	117.03	121.00
1	D	217	TYR	CB-CG-CD2	-6.55	117.07	121.00
1	A	217	TYR	CB-CG-CD2	-6.53	117.08	121.00
1	J	217	TYR	CB-CG-CD2	-6.53	117.08	121.00
3	M	24	ARG	NE-CZ-NH2	-6.46	117.07	120.30
2	E	579	ARG	NE-CZ-NH2	-6.44	117.08	120.30
2	B	579	ARG	NE-CZ-NH2	-6.44	117.08	120.30
2	K	579	ARG	NE-CZ-NH2	-6.42	117.09	120.30
3	F	24	ARG	NE-CZ-NH2	-6.41	117.10	120.30
3	L	24	ARG	NE-CZ-NH2	-6.37	117.12	120.30
2	E	579	ARG	NE-CZ-NH1	6.34	123.47	120.30
2	K	579	ARG	NE-CZ-NH1	6.25	123.42	120.30
2	B	579	ARG	NE-CZ-NH1	6.16	123.38	120.30
5	I	66	ARG	NE-CZ-NH2	-5.90	117.35	120.30
5	O	66	ARG	NE-CZ-NH2	-5.88	117.36	120.30
5	H	66	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	D	435	TYR	CB-CG-CD2	-5.75	117.55	121.00
4	C	59	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	A	435	TYR	CB-CG-CD2	-5.72	117.57	121.00
4	N	59	ARG	NE-CZ-NH2	-5.71	117.45	120.30
4	G	59	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	J	435	TYR	CB-CG-CD2	-5.69	117.59	121.00
3	L	96	TYR	CB-CG-CD2	-5.60	117.64	121.00
3	F	96	TYR	CB-CG-CD2	-5.56	117.67	121.00
3	M	96	TYR	CB-CG-CD2	-5.52	117.69	121.00
1	D	504	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	J	504	ARG	NE-CZ-NH1	5.39	122.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	504	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	D	252	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	J	273	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	J	252	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	252	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	D	273	ARG	NE-CZ-NH1	5.13	122.86	120.30
2	K	559	PRO	N-CA-C	5.07	125.28	112.10
2	B	559	PRO	N-CA-C	5.07	125.28	112.10
2	E	559	PRO	N-CA-C	5.07	125.28	112.10
1	A	273	ARG	NE-CZ-NH1	5.04	122.82	120.30
5	I	82(A)	ARG	NE-CZ-NH2	-5.04	117.78	120.30
5	H	82(A)	ARG	NE-CZ-NH2	-5.01	117.80	120.30
5	O	82(A)	ARG	NE-CZ-NH2	-5.00	117.80	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	A	2769	0	2720	3	0
1	D	2769	0	2720	4	0
1	J	2769	0	2720	4	0
2	B	1184	0	1174	0	0
2	E	1184	0	1174	0	0
2	K	1184	0	1174	0	0
3	F	812	0	776	2	0
3	L	812	0	776	2	0
3	M	812	0	776	2	0
4	C	768	0	786	1	0
4	G	768	0	786	1	0
4	N	768	0	786	1	0
5	H	971	0	940	1	0
5	I	971	0	940	1	0
5	O	971	0	940	1	0
6	P	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	28	0	25	0	0
6	T	28	0	25	0	0
7	Q	61	0	52	0	0
7	S	61	0	52	0	0
7	U	61	0	52	0	0
8	A	112	0	104	0	0
8	B	14	0	13	0	0
8	D	112	0	104	0	0
8	E	14	0	13	0	0
8	J	112	0	104	0	0
8	K	14	0	13	0	0
9	B	25	0	0	0	0
9	E	25	0	0	0	0
9	K	25	0	0	0	0
All	All	20232	0	19770	20	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 0.

All (20) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:388:THR:N	1:J:389:PRO:CD	2.74	0.51
1:D:388:THR:N	1:D:389:PRO:CD	2.74	0.50
1:A:388:THR:N	1:A:389:PRO:CD	2.74	0.50
1:A:113:ASP:OD1	1:A:121:LYS:NZ	2.45	0.49
1:J:113:ASP:OD1	1:J:121:LYS:NZ	2.45	0.49
1:D:113:ASP:OD1	1:D:121:LYS:NZ	2.45	0.49
4:G:39:ASN:N	4:G:39:ASN:OD1	2.45	0.48
3:L:49:TYR:HB2	5:H:100(J):PHE:CE2	2.49	0.48
3:F:49:TYR:HB2	5:I:100(J):PHE:CE2	2.49	0.48
3:M:49:TYR:HB2	5:O:100(J):PHE:CE2	2.49	0.47
1:J:62:ASP:OD1	1:J:62:ASP:N	2.46	0.47
1:A:231:LYS:NZ	1:A:267:GLU:OE1	2.49	0.43
4:C:39:ASN:OD1	4:C:39:ASN:N	2.45	0.43
1:J:231:LYS:NZ	1:J:267:GLU:OE1	2.49	0.42
1:D:231:LYS:NZ	1:D:267:GLU:OE1	2.49	0.42
3:F:50:GLY:O	3:F:52:SER:N	2.53	0.41
3:M:50:GLY:O	3:M:52:SER:N	2.53	0.41
3:L:50:GLY:O	3:L:52:SER:N	2.53	0.41
4:N:39:ASN:OD1	4:N:39:ASN:N	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:ASN:OD1	1:D:289:ASN:N	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	341/524 (65%)	332 (97%)	9 (3%)	0	100	100
1	D	341/524 (65%)	332 (97%)	9 (3%)	0	100	100
1	J	341/524 (65%)	332 (97%)	9 (3%)	0	100	100
2	B	147/153 (96%)	144 (98%)	3 (2%)	0	100	100
2	E	147/153 (96%)	144 (98%)	3 (2%)	0	100	100
2	K	147/153 (96%)	144 (98%)	3 (2%)	0	100	100
3	F	104/214 (49%)	101 (97%)	3 (3%)	0	100	100
3	L	104/214 (49%)	101 (97%)	3 (3%)	0	100	100
3	M	104/214 (49%)	101 (97%)	3 (3%)	0	100	100
4	C	94/208 (45%)	90 (96%)	4 (4%)	0	100	100
4	G	94/208 (45%)	90 (96%)	4 (4%)	0	100	100
4	N	94/208 (45%)	90 (96%)	4 (4%)	0	100	100
5	H	123/229 (54%)	122 (99%)	1 (1%)	0	100	100
5	I	123/229 (54%)	122 (99%)	1 (1%)	0	100	100
5	O	123/229 (54%)	122 (99%)	1 (1%)	0	100	100
All	All	2427/3984 (61%)	2367 (98%)	60 (2%)	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	A	312/461 (68%)	312 (100%)	0	100	100
1	D	312/461 (68%)	312 (100%)	0	100	100
1	J	312/461 (68%)	312 (100%)	0	100	100
2	B	126/130 (97%)	126 (100%)	0	100	100
2	E	126/130 (97%)	126 (100%)	0	100	100
2	K	126/130 (97%)	126 (100%)	0	100	100
3	F	87/184 (47%)	87 (100%)	0	100	100
3	L	87/184 (47%)	87 (100%)	0	100	100
3	M	87/184 (47%)	87 (100%)	0	100	100
4	C	88/186 (47%)	88 (100%)	0	100	100
4	G	88/186 (47%)	88 (100%)	0	100	100
4	N	88/186 (47%)	88 (100%)	0	100	100
5	H	103/193 (53%)	103 (100%)	0	100	100
5	I	103/193 (53%)	103 (100%)	0	100	100
5	O	103/193 (53%)	103 (100%)	0	100	100
All	All	2148/3462 (62%)	2148 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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
6	NAG	P	1	1,6	14,14,15	2.13	6 (42%)	17,19,21	1.16	1 (5%)
6	NAG	P	2	6	14,14,15	2.07	5 (35%)	17,19,21	0.88	1 (5%)
7	NAG	Q	1	1,7	14,14,15	2.10	4 (28%)	17,19,21	1.13	1 (5%)
7	NAG	Q	2	7	14,14,15	1.92	5 (35%)	17,19,21	1.11	2 (11%)
7	BMA	Q	3	7	11,11,12	0.58	0	15,15,17	0.76	1 (6%)
7	MAN	Q	4	7	11,11,12	0.65	0	15,15,17	0.95	1 (6%)
7	MAN	Q	5	7	11,11,12	1.81	3 (27%)	15,15,17	0.72	0
6	NAG	R	1	1,6	14,14,15	2.14	6 (42%)	17,19,21	1.16	1 (5%)
6	NAG	R	2	6	14,14,15	2.08	5 (35%)	17,19,21	0.88	1 (5%)
7	NAG	S	1	1,7	14,14,15	2.11	4 (28%)	17,19,21	1.13	1 (5%)
7	NAG	S	2	7	14,14,15	1.92	5 (35%)	17,19,21	1.11	2 (11%)
7	BMA	S	3	7	11,11,12	0.58	0	15,15,17	0.76	1 (6%)
7	MAN	S	4	7	11,11,12	0.64	0	15,15,17	0.95	1 (6%)
7	MAN	S	5	7	11,11,12	1.80	3 (27%)	15,15,17	0.72	0
6	NAG	T	1	1,6	14,14,15	2.13	6 (42%)	17,19,21	1.16	1 (5%)
6	NAG	T	2	6	14,14,15	2.07	6 (42%)	17,19,21	0.88	1 (5%)
7	NAG	U	1	1,7	14,14,15	2.11	4 (28%)	17,19,21	1.12	1 (5%)
7	NAG	U	2	7	14,14,15	1.93	5 (35%)	17,19,21	1.11	2 (11%)
7	BMA	U	3	7	11,11,12	0.57	0	15,15,17	0.76	1 (6%)
7	MAN	U	4	7	11,11,12	0.65	0	15,15,17	0.95	1 (6%)
7	MAN	U	5	7	11,11,12	1.82	3 (27%)	15,15,17	0.72	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
6	NAG	P	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	P	2	6	-	0/6/23/26	0/1/1/1
7	NAG	Q	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	0/6/23/26	0/1/1/1
7	BMA	Q	3	7	-	1/2/19/22	0/1/1/1
7	MAN	Q	4	7	-	2/2/19/22	0/1/1/1
7	MAN	Q	5	7	-	0/2/19/22	0/1/1/1
6	NAG	R	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	R	2	6	-	0/6/23/26	0/1/1/1
7	NAG	S	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	S	2	7	-	0/6/23/26	0/1/1/1
7	BMA	S	3	7	-	1/2/19/22	0/1/1/1
7	MAN	S	4	7	-	2/2/19/22	0/1/1/1
7	MAN	S	5	7	-	0/2/19/22	0/1/1/1
6	NAG	T	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	T	2	6	-	0/6/23/26	0/1/1/1
7	NAG	U	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	U	2	7	-	0/6/23/26	0/1/1/1
7	BMA	U	3	7	-	1/2/19/22	0/1/1/1
7	MAN	U	4	7	-	2/2/19/22	0/1/1/1
7	MAN	U	5	7	-	0/2/19/22	0/1/1/1

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	S	1	NAG	C1-C2	5.90	1.60	1.52
7	U	1	NAG	C1-C2	5.86	1.60	1.52
7	Q	1	NAG	C1-C2	5.84	1.60	1.52
6	R	1	NAG	C1-C2	5.71	1.60	1.52
6	P	1	NAG	C1-C2	5.67	1.60	1.52
6	T	1	NAG	C1-C2	5.66	1.60	1.52
6	R	2	NAG	C1-C2	4.89	1.59	1.52
6	P	2	NAG	C1-C2	4.87	1.59	1.52
6	T	2	NAG	C1-C2	4.85	1.58	1.52
7	U	2	NAG	C1-C2	4.65	1.58	1.52
7	S	2	NAG	C1-C2	4.64	1.58	1.52
7	Q	2	NAG	C1-C2	4.62	1.58	1.52
6	P	2	NAG	O5-C5	3.32	1.49	1.43
6	T	2	NAG	O5-C5	3.31	1.49	1.43
6	R	2	NAG	O5-C5	3.30	1.49	1.43
7	U	5	MAN	C2-C3	3.03	1.57	1.52
7	Q	5	MAN	C2-C3	3.01	1.57	1.52
7	S	5	MAN	C2-C3	2.99	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	U	5	MAN	O5-C5	2.94	1.49	1.43
7	Q	5	MAN	O5-C5	2.93	1.49	1.43
7	S	5	MAN	O5-C5	2.91	1.49	1.43
6	T	1	NAG	O5-C5	2.63	1.48	1.43
6	R	1	NAG	O5-C5	2.62	1.48	1.43
6	P	1	NAG	O5-C5	2.61	1.48	1.43
7	U	2	NAG	O5-C5	2.57	1.48	1.43
7	S	5	MAN	C1-C2	2.54	1.58	1.52
7	Q	5	MAN	C1-C2	2.54	1.58	1.52
7	U	5	MAN	C1-C2	2.54	1.58	1.52
7	Q	2	NAG	O5-C5	2.54	1.48	1.43
7	S	2	NAG	O5-C5	2.53	1.48	1.43
7	Q	1	NAG	O5-C5	2.46	1.48	1.43
6	P	2	NAG	C3-C2	2.46	1.57	1.52
7	S	1	NAG	O5-C5	2.46	1.48	1.43
6	R	2	NAG	C3-C2	2.46	1.57	1.52
6	T	2	NAG	C3-C2	2.46	1.57	1.52
7	U	1	NAG	O5-C5	2.45	1.48	1.43
6	P	1	NAG	C4-C5	2.39	1.58	1.53
6	T	1	NAG	C4-C5	2.37	1.58	1.53
6	R	1	NAG	C4-C5	2.36	1.58	1.53
7	U	2	NAG	C3-C2	2.34	1.57	1.52
7	S	2	NAG	C3-C2	2.34	1.57	1.52
6	R	2	NAG	C4-C5	2.34	1.58	1.53
6	T	2	NAG	C4-C5	2.33	1.58	1.53
7	Q	2	NAG	C3-C2	2.31	1.57	1.52
7	S	2	NAG	C4-C3	2.30	1.58	1.52
7	U	2	NAG	C4-C3	2.30	1.58	1.52
7	Q	2	NAG	C4-C3	2.29	1.58	1.52
6	P	2	NAG	C4-C5	2.28	1.57	1.53
6	T	2	NAG	C2-N2	2.25	1.50	1.46
7	U	1	NAG	O5-C1	2.24	1.47	1.43
6	R	2	NAG	C2-N2	2.24	1.50	1.46
6	P	2	NAG	C2-N2	2.23	1.50	1.46
7	S	1	NAG	O5-C1	2.23	1.47	1.43
7	Q	2	NAG	C4-C5	2.20	1.57	1.53
7	Q	1	NAG	O5-C1	2.20	1.47	1.43
7	Q	1	NAG	C3-C2	2.18	1.57	1.52
7	S	1	NAG	C3-C2	2.18	1.57	1.52
6	T	1	NAG	C3-C2	2.18	1.57	1.52
7	S	2	NAG	C4-C5	2.18	1.57	1.53
7	U	1	NAG	C3-C2	2.18	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	U	2	NAG	C4-C5	2.17	1.57	1.53
6	R	1	NAG	C3-C2	2.16	1.57	1.52
6	P	1	NAG	C3-C2	2.15	1.57	1.52
6	T	1	NAG	C4-C3	2.08	1.57	1.52
6	R	1	NAG	C4-C3	2.07	1.57	1.52
6	P	1	NAG	C4-C3	2.07	1.57	1.52
6	T	1	NAG	O5-C1	2.02	1.47	1.43
6	P	1	NAG	O5-C1	2.02	1.47	1.43
6	T	2	NAG	C4-C3	2.02	1.57	1.52
6	R	1	NAG	O5-C1	2.01	1.47	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	2	NAG	O7-C7-C8	-2.47	117.65	122.05
7	Q	2	NAG	O7-C7-C8	-2.45	117.70	122.05
7	S	2	NAG	O7-C7-C8	-2.44	117.72	122.05
7	S	4	MAN	C2-C3-C4	-2.34	106.74	110.86
7	U	4	MAN	C2-C3-C4	-2.34	106.75	110.86
7	S	1	NAG	C8-C7-N2	2.32	119.97	116.12
7	Q	4	MAN	C2-C3-C4	-2.32	106.78	110.86
7	Q	1	NAG	C8-C7-N2	2.32	119.97	116.12
7	U	3	BMA	C2-C3-C4	-2.31	106.80	110.86
7	U	1	NAG	C8-C7-N2	2.30	119.93	116.12
7	Q	3	BMA	C2-C3-C4	-2.30	106.82	110.86
7	S	3	BMA	C2-C3-C4	-2.28	106.85	110.86
7	S	2	NAG	O4-C4-C5	-2.21	103.88	109.32
7	U	2	NAG	O4-C4-C5	-2.21	103.88	109.32
7	Q	2	NAG	O4-C4-C5	-2.21	103.89	109.32
6	R	2	NAG	C8-C7-N2	2.19	119.75	116.12
6	P	1	NAG	C8-C7-N2	2.18	119.74	116.12
6	T	1	NAG	C8-C7-N2	2.18	119.74	116.12
6	R	1	NAG	C8-C7-N2	2.18	119.73	116.12
6	T	2	NAG	C8-C7-N2	2.18	119.73	116.12
6	P	2	NAG	C8-C7-N2	2.17	119.72	116.12

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	Q	4	MAN	O5-C5-C6-O6
7	U	4	MAN	O5-C5-C6-O6

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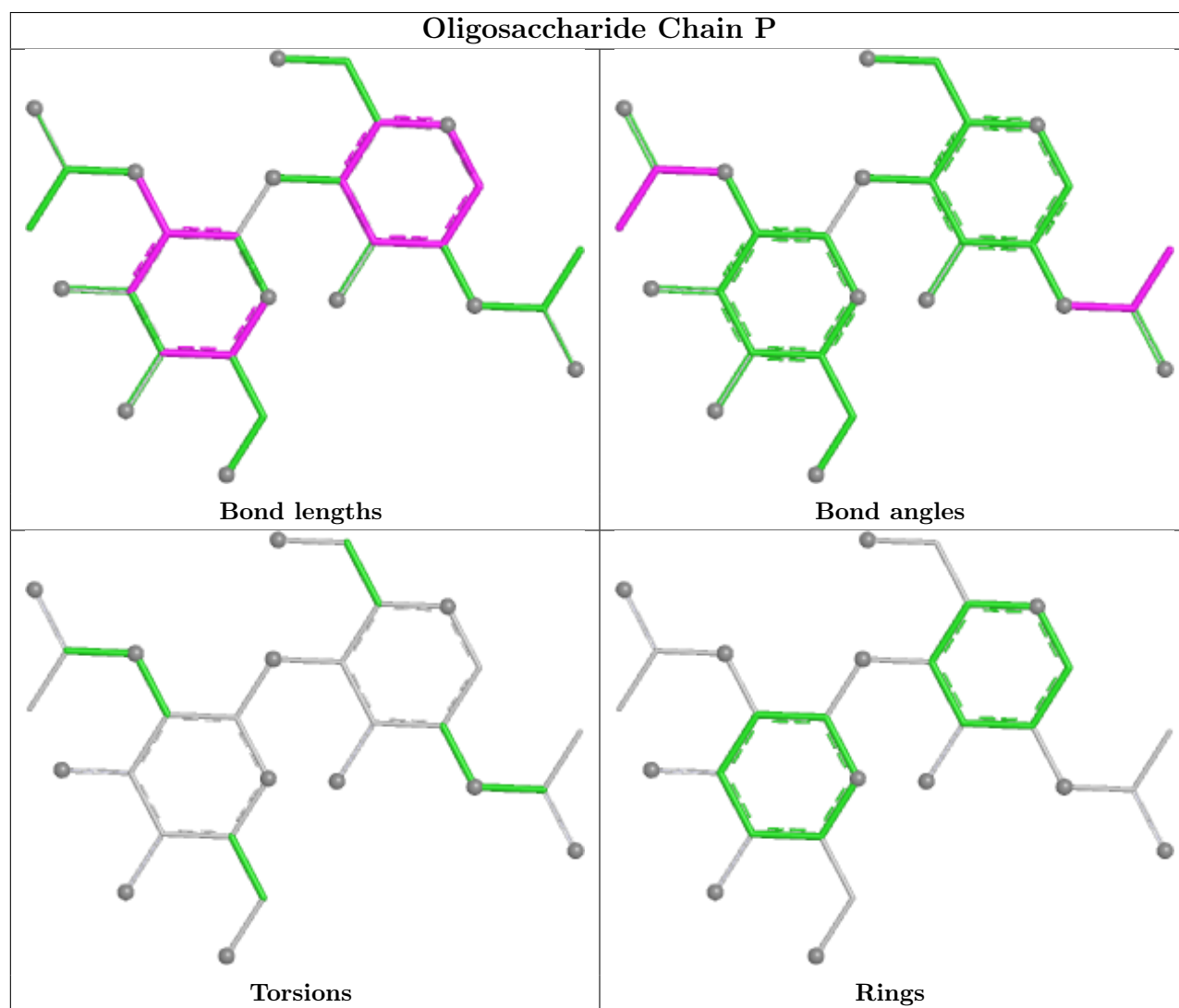
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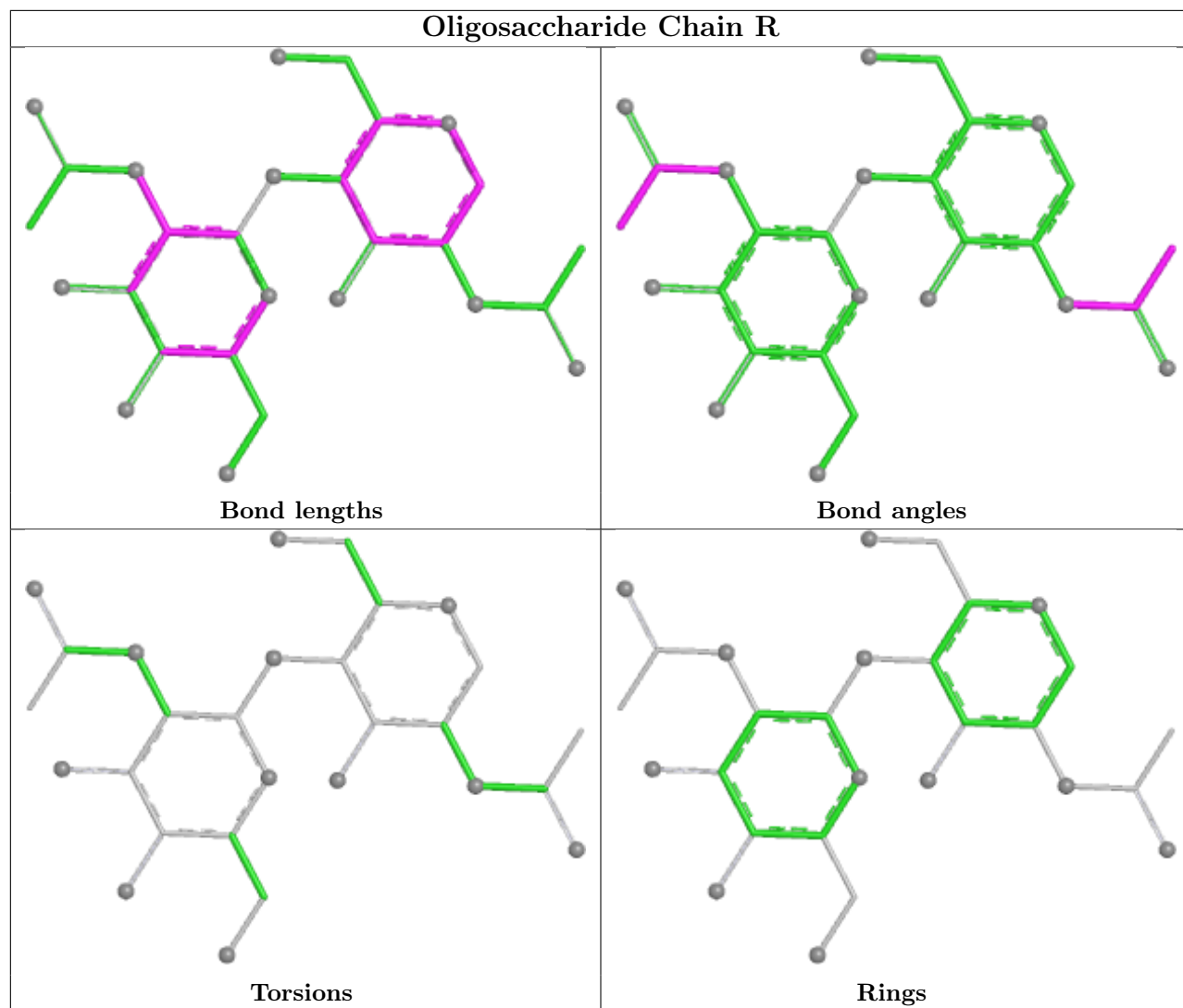
Mol	Chain	Res	Type	Atoms
7	S	4	MAN	O5-C5-C6-O6
7	Q	3	BMA	O5-C5-C6-O6
7	S	3	BMA	O5-C5-C6-O6
7	U	3	BMA	O5-C5-C6-O6
7	U	4	MAN	C4-C5-C6-O6
7	Q	4	MAN	C4-C5-C6-O6
7	S	4	MAN	C4-C5-C6-O6

There are no ring outliers.

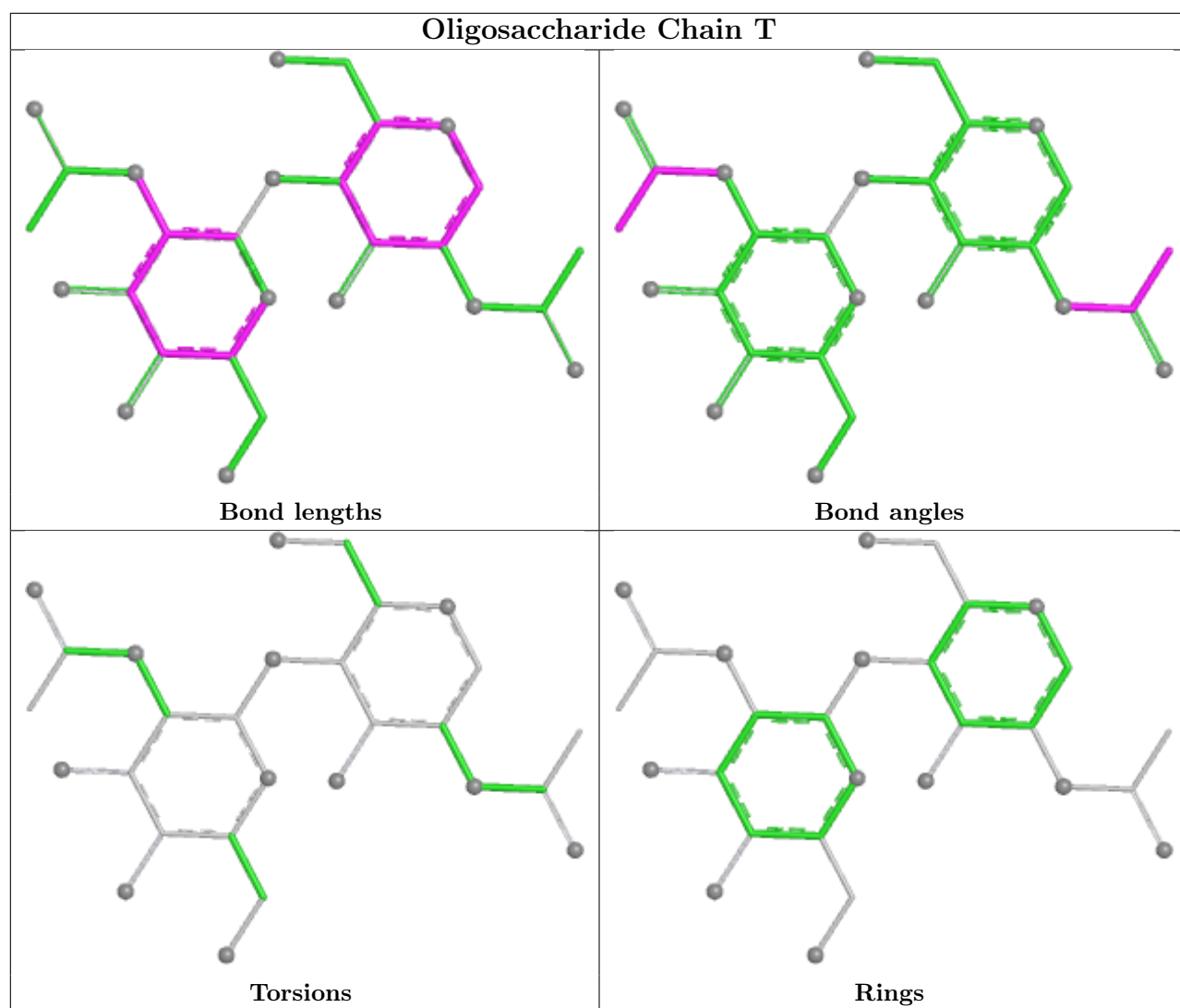
No monomer is involved in short contacts.

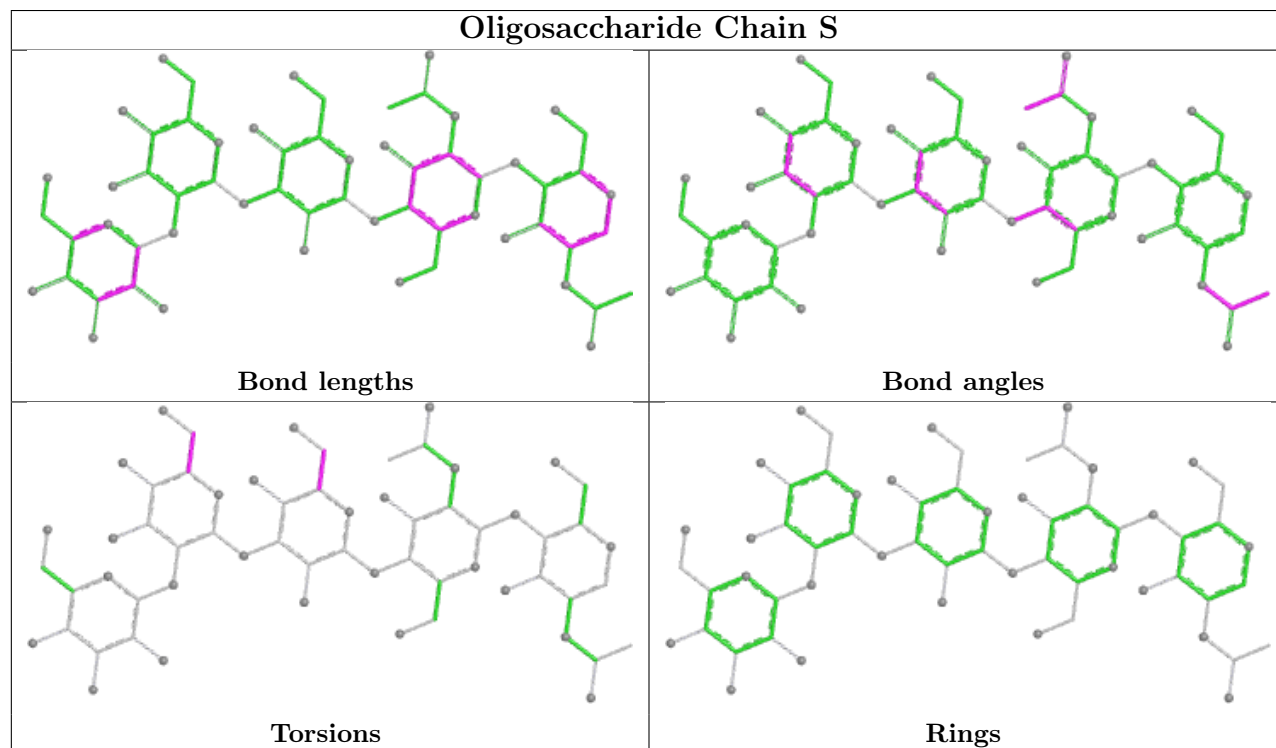
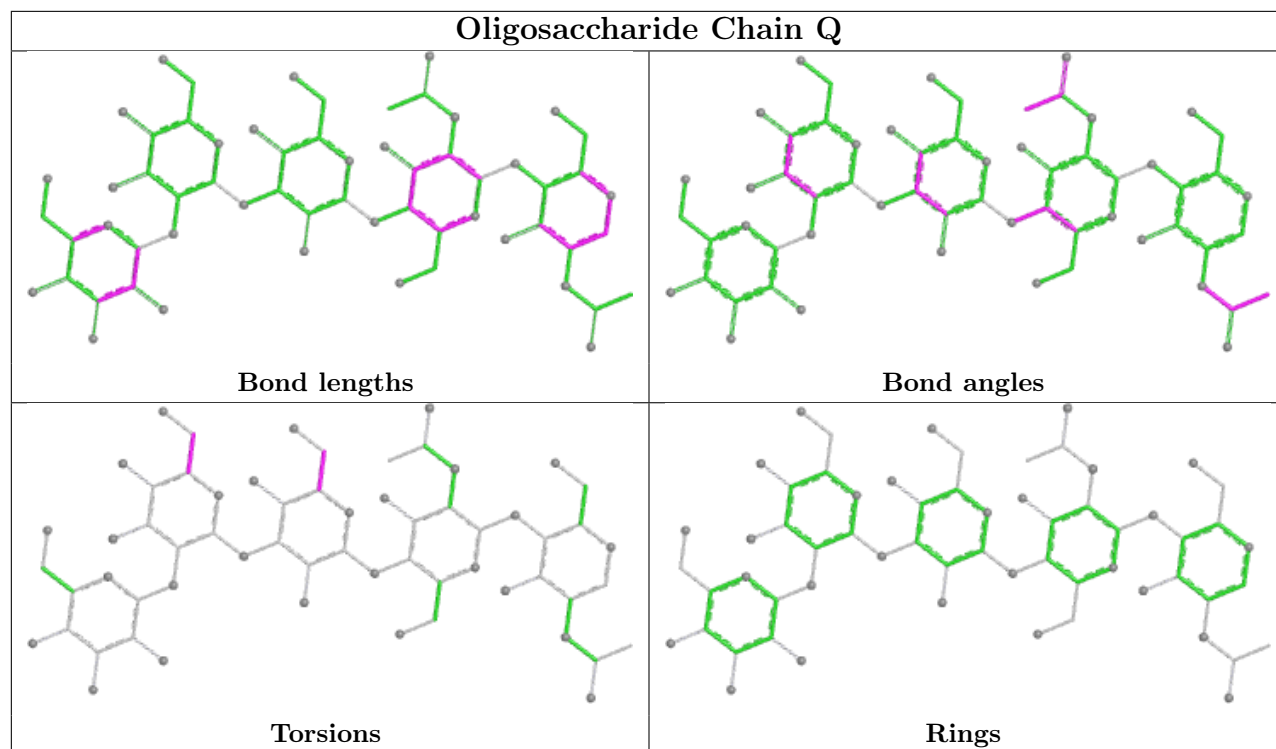
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

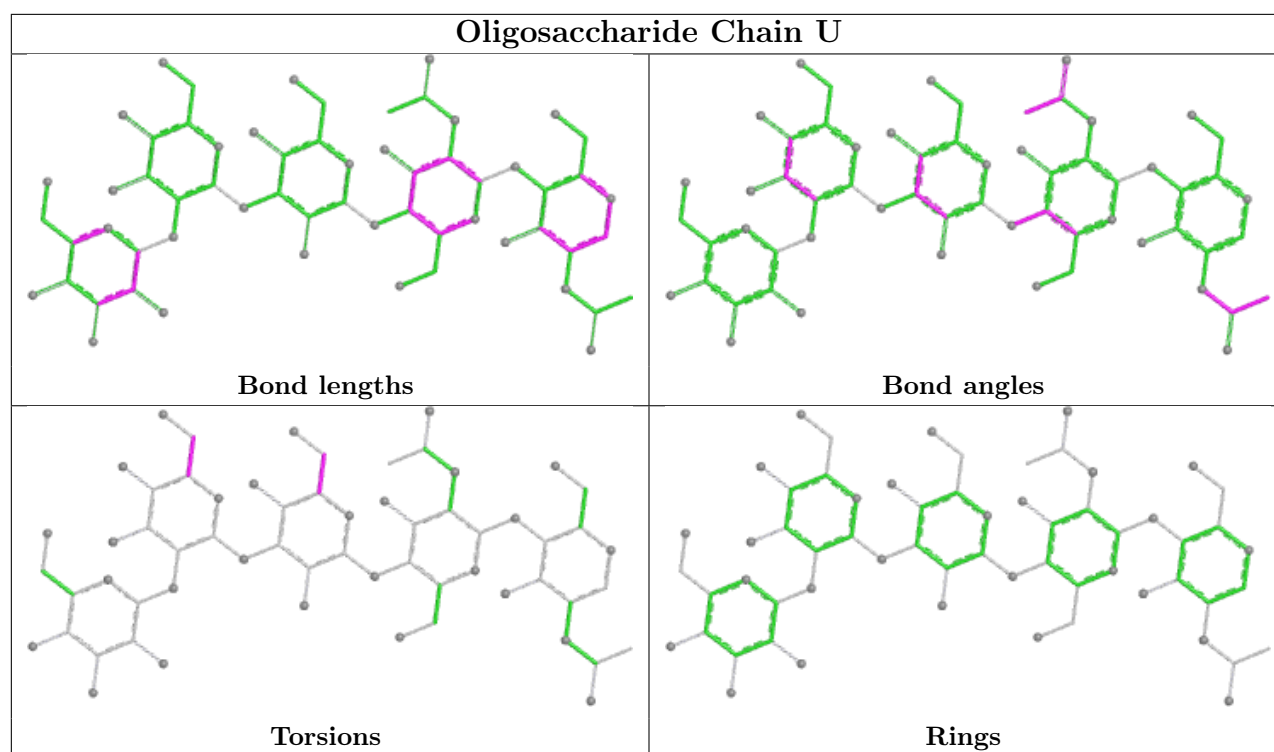












## 5.6 Ligand geometry [i](#)

30 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	$\# Z  > 2$
8	NAG	D	610	1	14,14,15	2.25	5 (35%)	17,19,21	1.05	2 (11%)
8	NAG	J	607	1	14,14,15	2.17	5 (35%)	17,19,21	1.04	1 (5%)
8	NAG	A	611	1	14,14,15	2.25	5 (35%)	17,19,21	0.90	0
9	UOV	E	702	-	24,28,28	3.41	20 (83%)	32,40,40	2.15	7 (21%)
8	NAG	J	613	1	14,14,15	2.18	7 (50%)	17,19,21	1.09	2 (11%)
8	NAG	D	614	1	14,14,15	2.22	6 (42%)	17,19,21	1.03	1 (5%)
8	NAG	J	608	1	14,14,15	2.18	5 (35%)	17,19,21	1.07	1 (5%)
8	NAG	J	611	1	14,14,15	2.26	5 (35%)	17,19,21	0.90	0
8	NAG	D	607	1	14,14,15	2.16	5 (35%)	17,19,21	1.05	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	A	613	1	14,14,15	2.18	6 (42%)	17,19,21	1.08	2 (11%)
8	NAG	A	610	1	14,14,15	2.24	5 (35%)	17,19,21	1.05	2 (11%)
8	NAG	D	611	1	14,14,15	2.25	5 (35%)	17,19,21	0.90	0
8	NAG	D	608	1	14,14,15	2.18	5 (35%)	17,19,21	1.06	1 (5%)
8	NAG	J	610	1	14,14,15	2.24	6 (42%)	17,19,21	1.05	2 (11%)
8	NAG	A	609	1	14,14,15	2.19	6 (42%)	17,19,21	1.15	2 (11%)
8	NAG	A	607	1	14,14,15	2.17	5 (35%)	17,19,21	1.04	1 (5%)
8	NAG	J	609	1	14,14,15	2.20	6 (42%)	17,19,21	1.15	2 (11%)
8	NAG	J	614	1	14,14,15	2.22	6 (42%)	17,19,21	1.03	1 (5%)
8	NAG	B	701	2	14,14,15	2.24	7 (50%)	17,19,21	1.14	2 (11%)
8	NAG	K	701	2	14,14,15	2.24	7 (50%)	17,19,21	1.14	2 (11%)
8	NAG	A	614	1	14,14,15	2.24	6 (42%)	17,19,21	1.03	1 (5%)
8	NAG	D	613	1	14,14,15	2.19	7 (50%)	17,19,21	1.09	2 (11%)
8	NAG	E	701	2	14,14,15	2.23	7 (50%)	17,19,21	1.14	2 (11%)
8	NAG	A	608	1	14,14,15	2.19	5 (35%)	17,19,21	1.06	1 (5%)
9	UOV	K	702	-	24,28,28	3.41	20 (83%)	32,40,40	2.15	7 (21%)
8	NAG	D	609	1	14,14,15	2.19	6 (42%)	17,19,21	1.16	2 (11%)
8	NAG	A	612	1	14,14,15	2.15	5 (35%)	17,19,21	1.03	1 (5%)
9	UOV	B	702	-	24,28,28	3.41	20 (83%)	32,40,40	2.15	7 (21%)
8	NAG	J	612	1	14,14,15	2.16	5 (35%)	17,19,21	1.03	1 (5%)
8	NAG	D	612	1	14,14,15	2.16	5 (35%)	17,19,21	1.03	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	D	610	1	-	1/6/23/26	0/1/1/1
8	NAG	J	607	1	-	0/6/23/26	0/1/1/1
8	NAG	A	611	1	-	0/6/23/26	0/1/1/1
9	UOV	E	702	-	-	0/12/32/32	0/4/4/4
8	NAG	J	613	1	-	0/6/23/26	0/1/1/1
8	NAG	D	614	1	-	0/6/23/26	0/1/1/1
8	NAG	J	608	1	-	0/6/23/26	0/1/1/1
8	NAG	J	611	1	-	0/6/23/26	0/1/1/1
8	NAG	D	607	1	-	0/6/23/26	0/1/1/1
8	NAG	A	613	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	610	1	-	1/6/23/26	0/1/1/1
8	NAG	D	611	1	-	0/6/23/26	0/1/1/1
8	NAG	D	608	1	-	0/6/23/26	0/1/1/1
8	NAG	J	610	1	-	1/6/23/26	0/1/1/1
8	NAG	A	609	1	-	1/6/23/26	0/1/1/1
8	NAG	A	607	1	-	0/6/23/26	0/1/1/1
8	NAG	J	609	1	-	1/6/23/26	0/1/1/1
8	NAG	J	614	1	-	0/6/23/26	0/1/1/1
8	NAG	B	701	2	-	0/6/23/26	0/1/1/1
8	NAG	K	701	2	-	0/6/23/26	0/1/1/1
8	NAG	A	614	1	-	0/6/23/26	0/1/1/1
8	NAG	D	613	1	-	0/6/23/26	0/1/1/1
8	NAG	E	701	2	-	0/6/23/26	0/1/1/1
8	NAG	A	608	1	-	0/6/23/26	0/1/1/1
9	UOV	K	702	-	-	0/12/32/32	0/4/4/4
8	NAG	D	609	1	-	1/6/23/26	0/1/1/1
8	NAG	A	612	1	-	1/6/23/26	0/1/1/1
9	UOV	B	702	-	-	0/12/32/32	0/4/4/4
8	NAG	J	612	1	-	1/6/23/26	0/1/1/1
8	NAG	D	612	1	-	1/6/23/26	0/1/1/1

All (213) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	702	UOV	C11-N13	6.66	1.48	1.36
9	E	702	UOV	C11-N13	6.65	1.48	1.36
9	B	702	UOV	C11-N13	6.63	1.48	1.36
8	J	611	NAG	C1-C2	6.08	1.60	1.52
8	D	611	NAG	C1-C2	6.04	1.60	1.52
8	A	611	NAG	C1-C2	6.04	1.60	1.52
8	J	609	NAG	C1-C2	5.94	1.60	1.52
8	A	609	NAG	C1-C2	5.91	1.60	1.52
8	D	609	NAG	C1-C2	5.89	1.60	1.52
8	D	610	NAG	C1-C2	5.82	1.60	1.52
8	A	610	NAG	C1-C2	5.80	1.60	1.52
8	J	610	NAG	C1-C2	5.79	1.60	1.52
8	J	607	NAG	C1-C2	5.61	1.60	1.52
8	A	607	NAG	C1-C2	5.60	1.60	1.52
8	D	607	NAG	C1-C2	5.57	1.59	1.52
8	A	614	NAG	C1-C2	5.57	1.59	1.52
8	D	614	NAG	C1-C2	5.54	1.59	1.52
8	A	608	NAG	C1-C2	5.52	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	614	NAG	C1-C2	5.51	1.59	1.52
8	D	608	NAG	C1-C2	5.49	1.59	1.52
8	J	608	NAG	C1-C2	5.48	1.59	1.52
8	A	612	NAG	C1-C2	5.29	1.59	1.52
8	J	612	NAG	C1-C2	5.27	1.59	1.52
8	D	612	NAG	C1-C2	5.26	1.59	1.52
8	K	701	NAG	C1-C2	5.21	1.59	1.52
8	B	701	NAG	C1-C2	5.21	1.59	1.52
8	D	613	NAG	C1-C2	5.17	1.59	1.52
8	E	701	NAG	C1-C2	5.17	1.59	1.52
8	A	613	NAG	C1-C2	5.17	1.59	1.52
8	J	613	NAG	C1-C2	5.13	1.59	1.52
9	B	702	UOV	C15-C16	4.63	1.59	1.52
9	K	702	UOV	C15-C16	4.63	1.59	1.52
9	E	702	UOV	C15-C16	4.61	1.59	1.52
9	E	702	UOV	C22-C09	4.47	1.46	1.39
9	K	702	UOV	C22-C09	4.45	1.46	1.39
9	B	702	UOV	C22-C09	4.42	1.46	1.39
9	K	702	UOV	C08-C09	4.41	1.46	1.39
9	E	702	UOV	C08-C09	4.40	1.46	1.39
9	B	702	UOV	C08-C09	4.39	1.46	1.39
9	B	702	UOV	C14-N13	4.29	1.54	1.47
9	E	702	UOV	C14-N13	4.28	1.54	1.47
9	K	702	UOV	C14-N13	4.25	1.54	1.47
9	B	702	UOV	C11-N10	4.22	1.44	1.37
9	K	702	UOV	C11-N10	4.20	1.44	1.37
9	E	702	UOV	C11-N10	4.18	1.44	1.37
9	E	702	UOV	C08-C07	3.76	1.44	1.38
9	B	702	UOV	C08-C07	3.76	1.44	1.38
9	B	702	UOV	C23-C06	3.76	1.46	1.39
9	K	702	UOV	C08-C07	3.76	1.44	1.38
9	E	702	UOV	C23-C06	3.75	1.46	1.39
9	K	702	UOV	C23-C06	3.74	1.46	1.39
9	B	702	UOV	C04-C03	3.70	1.44	1.38
9	K	702	UOV	C04-C03	3.69	1.44	1.38
9	E	702	UOV	C04-C03	3.68	1.44	1.38
8	A	614	NAG	O5-C5	3.53	1.50	1.43
8	D	608	NAG	O5-C5	3.52	1.50	1.43
8	A	608	NAG	O5-C5	3.51	1.50	1.43
8	J	614	NAG	O5-C5	3.50	1.50	1.43
8	J	608	NAG	O5-C5	3.50	1.50	1.43
8	J	613	NAG	O5-C5	3.46	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	614	NAG	O5-C5	3.45	1.50	1.43
8	D	613	NAG	O5-C5	3.44	1.50	1.43
8	D	612	NAG	O5-C5	3.43	1.50	1.43
8	A	613	NAG	O5-C5	3.42	1.50	1.43
8	J	612	NAG	O5-C5	3.40	1.50	1.43
9	E	702	UOV	C20-C16	3.39	1.57	1.52
8	E	701	NAG	O5-C5	3.39	1.50	1.43
9	K	702	UOV	C20-C16	3.38	1.57	1.52
8	K	701	NAG	O5-C5	3.38	1.50	1.43
8	A	612	NAG	O5-C5	3.38	1.50	1.43
8	B	701	NAG	O5-C5	3.37	1.50	1.43
9	B	702	UOV	C20-C16	3.34	1.57	1.52
9	B	702	UOV	C04-C05	3.28	1.45	1.39
9	E	702	UOV	C04-C05	3.28	1.45	1.39
9	K	702	UOV	C04-C05	3.28	1.45	1.39
9	E	702	UOV	C06-C05	3.27	1.56	1.49
9	K	702	UOV	C06-C05	3.27	1.56	1.49
9	B	702	UOV	C06-C05	3.25	1.56	1.49
8	D	610	NAG	O5-C5	3.18	1.49	1.43
8	J	611	NAG	O5-C5	3.18	1.49	1.43
8	J	610	NAG	O5-C5	3.17	1.49	1.43
8	A	611	NAG	O5-C5	3.16	1.49	1.43
8	A	610	NAG	O5-C5	3.16	1.49	1.43
8	D	607	NAG	O5-C5	3.15	1.49	1.43
8	D	611	NAG	O5-C5	3.15	1.49	1.43
8	A	607	NAG	O5-C5	3.14	1.49	1.43
8	J	607	NAG	O5-C5	3.12	1.49	1.43
9	E	702	UOV	C03-C02	3.00	1.46	1.38
9	B	702	UOV	C03-C02	2.99	1.45	1.38
9	K	702	UOV	C03-C02	2.99	1.45	1.38
9	K	702	UOV	C24-C05	2.99	1.45	1.39
9	B	702	UOV	C24-C05	2.98	1.45	1.39
9	E	702	UOV	C24-C05	2.97	1.45	1.39
9	B	702	UOV	C09-N10	2.92	1.47	1.41
9	K	702	UOV	C09-N10	2.92	1.47	1.41
9	E	702	UOV	C09-N10	2.91	1.47	1.41
8	B	701	NAG	C2-N2	2.81	1.50	1.46
8	D	612	NAG	O5-C1	2.81	1.48	1.43
8	J	613	NAG	O5-C1	2.81	1.48	1.43
8	D	613	NAG	O5-C1	2.80	1.48	1.43
8	A	613	NAG	O5-C1	2.80	1.48	1.43
8	A	612	NAG	O5-C1	2.79	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	612	NAG	O5-C1	2.78	1.48	1.43
8	K	701	NAG	C2-N2	2.78	1.50	1.46
8	J	609	NAG	O5-C5	2.76	1.48	1.43
8	D	609	NAG	O5-C5	2.76	1.48	1.43
8	A	614	NAG	O5-C1	2.75	1.48	1.43
8	D	614	NAG	O5-C1	2.75	1.48	1.43
8	A	609	NAG	O5-C5	2.75	1.48	1.43
8	J	614	NAG	O5-C1	2.75	1.48	1.43
8	E	701	NAG	C2-N2	2.74	1.50	1.46
8	K	701	NAG	O5-C1	2.71	1.48	1.43
8	B	701	NAG	O5-C1	2.70	1.48	1.43
8	E	701	NAG	O5-C1	2.67	1.48	1.43
9	B	702	UOV	C25-C24	2.62	1.43	1.38
8	J	608	NAG	O5-C1	2.61	1.48	1.43
8	A	608	NAG	O5-C1	2.60	1.48	1.43
9	E	702	UOV	C25-C24	2.60	1.43	1.38
8	D	608	NAG	O5-C1	2.60	1.48	1.43
8	J	610	NAG	O5-C1	2.58	1.48	1.43
8	D	610	NAG	O5-C1	2.58	1.48	1.43
8	A	610	NAG	O5-C1	2.58	1.48	1.43
9	K	702	UOV	C25-C24	2.57	1.43	1.38
8	D	610	NAG	C3-C2	2.53	1.57	1.52
8	A	610	NAG	C3-C2	2.52	1.57	1.52
8	J	610	NAG	C3-C2	2.51	1.57	1.52
9	K	702	UOV	C07-C06	2.50	1.44	1.39
9	B	702	UOV	C07-C06	2.49	1.44	1.39
9	E	702	UOV	C07-C06	2.47	1.44	1.39
9	B	702	UOV	C23-C22	2.47	1.42	1.38
8	D	611	NAG	O5-C1	2.45	1.47	1.43
8	J	611	NAG	O5-C1	2.45	1.47	1.43
9	E	702	UOV	C23-C22	2.45	1.42	1.38
8	A	611	NAG	O5-C1	2.44	1.47	1.43
9	K	702	UOV	C23-C22	2.42	1.42	1.38
8	J	607	NAG	O5-C1	2.41	1.47	1.43
8	J	607	NAG	C3-C2	2.41	1.57	1.52
8	D	611	NAG	C3-C2	2.40	1.57	1.52
8	A	611	NAG	C3-C2	2.39	1.57	1.52
8	A	607	NAG	C3-C2	2.38	1.57	1.52
8	D	607	NAG	O5-C1	2.38	1.47	1.43
8	J	611	NAG	C3-C2	2.38	1.57	1.52
8	A	607	NAG	O5-C1	2.38	1.47	1.43
9	E	702	UOV	C20-C21	2.37	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	702	UOV	C20-C21	2.37	1.59	1.52
8	B	701	NAG	C4-C5	2.36	1.58	1.53
8	D	607	NAG	C3-C2	2.35	1.57	1.52
9	B	702	UOV	C20-C21	2.35	1.59	1.52
8	E	701	NAG	C4-C5	2.35	1.58	1.53
8	K	701	NAG	C4-C5	2.34	1.58	1.53
8	D	609	NAG	C2-N2	2.34	1.50	1.46
8	J	609	NAG	C2-N2	2.32	1.50	1.46
8	J	613	NAG	C3-C2	2.32	1.57	1.52
8	D	613	NAG	C3-C2	2.31	1.57	1.52
9	B	702	UOV	C25-C02	2.31	1.44	1.38
9	E	702	UOV	C25-C02	2.30	1.44	1.38
8	A	609	NAG	C2-N2	2.30	1.50	1.46
9	K	702	UOV	C25-C02	2.30	1.44	1.38
8	A	613	NAG	C3-C2	2.29	1.57	1.52
8	A	609	NAG	O5-C1	2.27	1.47	1.43
8	K	701	NAG	C3-C2	2.27	1.57	1.52
8	J	609	NAG	O5-C1	2.26	1.47	1.43
8	D	610	NAG	C2-N2	2.26	1.50	1.46
8	D	613	NAG	C4-C5	2.26	1.57	1.53
8	B	701	NAG	C3-C2	2.25	1.57	1.52
8	E	701	NAG	C3-C2	2.25	1.57	1.52
8	A	613	NAG	C4-C5	2.24	1.57	1.53
8	J	610	NAG	C2-N2	2.24	1.50	1.46
8	J	612	NAG	C3-C2	2.24	1.57	1.52
8	A	610	NAG	C2-N2	2.23	1.50	1.46
8	D	609	NAG	O5-C1	2.23	1.47	1.43
8	A	614	NAG	C4-C5	2.23	1.57	1.53
8	D	614	NAG	C4-C5	2.23	1.57	1.53
8	A	608	NAG	C4-C5	2.23	1.57	1.53
8	J	608	NAG	C4-C5	2.22	1.57	1.53
8	J	609	NAG	C3-C2	2.22	1.57	1.52
8	D	612	NAG	C3-C2	2.22	1.57	1.52
8	A	609	NAG	C3-C2	2.22	1.57	1.52
8	D	609	NAG	C3-C2	2.22	1.57	1.52
8	J	613	NAG	C4-C5	2.22	1.57	1.53
8	J	614	NAG	C4-C5	2.21	1.57	1.53
8	J	613	NAG	C2-N2	2.20	1.49	1.46
8	D	608	NAG	C4-C5	2.20	1.57	1.53
8	A	608	NAG	C3-C2	2.20	1.57	1.52
8	J	608	NAG	C3-C2	2.20	1.57	1.52
8	A	612	NAG	C3-C2	2.19	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	614	NAG	C3-C2	2.19	1.57	1.52
8	D	608	NAG	C3-C2	2.19	1.57	1.52
8	A	611	NAG	C4-C5	2.18	1.57	1.53
8	D	614	NAG	C3-C2	2.18	1.57	1.52
8	A	613	NAG	C2-N2	2.18	1.49	1.46
8	J	614	NAG	C3-C2	2.17	1.57	1.52
8	D	613	NAG	C2-N2	2.17	1.49	1.46
8	A	609	NAG	C4-C5	2.17	1.57	1.53
8	J	609	NAG	C4-C5	2.16	1.57	1.53
8	D	611	NAG	C4-C5	2.16	1.57	1.53
8	E	701	NAG	C4-C3	2.15	1.57	1.52
8	J	611	NAG	C4-C5	2.15	1.57	1.53
8	J	607	NAG	C4-C5	2.15	1.57	1.53
8	K	701	NAG	C4-C3	2.14	1.57	1.52
8	A	607	NAG	C4-C5	2.14	1.57	1.53
8	D	607	NAG	C4-C5	2.13	1.57	1.53
8	D	609	NAG	C4-C5	2.13	1.57	1.53
8	A	612	NAG	C4-C5	2.12	1.57	1.53
8	D	612	NAG	C4-C5	2.10	1.57	1.53
8	J	612	NAG	C4-C5	2.10	1.57	1.53
8	B	701	NAG	C4-C3	2.10	1.57	1.52
8	A	614	NAG	C2-N2	2.02	1.49	1.46
8	D	613	NAG	C4-C3	2.01	1.57	1.52
8	J	614	NAG	C2-N2	2.01	1.49	1.46
8	J	610	NAG	C4-C5	2.01	1.57	1.53
8	D	614	NAG	C2-N2	2.00	1.49	1.46
8	J	613	NAG	C4-C3	2.00	1.57	1.52

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	702	UOV	N10-C11-N13	9.08	126.57	115.91
9	K	702	UOV	N10-C11-N13	9.07	126.57	115.91
9	E	702	UOV	N10-C11-N13	9.06	126.56	115.91
9	B	702	UOV	O12-C11-N10	-3.53	115.71	123.46
9	E	702	UOV	O12-C11-N10	-3.53	115.71	123.46
9	K	702	UOV	O12-C11-N10	-3.52	115.74	123.46
8	K	701	NAG	C8-C7-N2	3.17	121.37	116.12
8	E	701	NAG	C8-C7-N2	3.15	121.34	116.12
8	B	701	NAG	C8-C7-N2	3.12	121.30	116.12
9	E	702	UOV	C09-N10-C11	2.91	131.93	126.04
9	K	702	UOV	C09-N10-C11	2.89	131.88	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	702	UOV	C09-N10-C11	2.89	131.88	126.04
9	E	702	UOV	C22-C09-C08	-2.88	115.22	119.04
9	B	702	UOV	C22-C09-C08	-2.88	115.22	119.04
9	K	702	UOV	C22-C09-C08	-2.88	115.22	119.04
9	K	702	UOV	O12-C11-N13	-2.85	117.69	121.67
9	B	702	UOV	O12-C11-N13	-2.84	117.71	121.67
9	E	702	UOV	O12-C11-N13	-2.82	117.73	121.67
8	D	613	NAG	C8-C7-N2	2.66	120.53	116.12
8	A	613	NAG	C8-C7-N2	2.65	120.52	116.12
8	J	613	NAG	C8-C7-N2	2.65	120.51	116.12
8	J	610	NAG	C8-C7-N2	2.56	120.37	116.12
8	D	610	NAG	C8-C7-N2	2.56	120.37	116.12
8	A	610	NAG	C8-C7-N2	2.55	120.35	116.12
8	D	614	NAG	C8-C7-N2	2.52	120.29	116.12
8	J	614	NAG	C8-C7-N2	2.51	120.28	116.12
9	B	702	UOV	C15-C16-C17	-2.51	112.52	117.31
9	K	702	UOV	C15-C16-C17	-2.50	112.53	117.31
8	A	614	NAG	C8-C7-N2	2.50	120.27	116.12
8	D	609	NAG	C8-C7-N2	2.49	120.25	116.12
9	E	702	UOV	C15-C16-C17	-2.49	112.55	117.31
8	J	609	NAG	C8-C7-N2	2.49	120.24	116.12
8	A	609	NAG	C8-C7-N2	2.48	120.23	116.12
8	J	608	NAG	C8-C7-N2	2.44	120.16	116.12
8	A	608	NAG	C8-C7-N2	2.42	120.13	116.12
8	D	608	NAG	C8-C7-N2	2.41	120.11	116.12
8	E	701	NAG	O7-C7-C8	-2.29	117.97	122.05
8	K	701	NAG	O7-C7-C8	-2.29	117.98	122.05
9	B	702	UOV	C23-C22-C09	2.28	122.92	120.30
8	B	701	NAG	O7-C7-C8	-2.27	118.01	122.05
9	E	702	UOV	C23-C22-C09	2.27	122.91	120.30
9	K	702	UOV	C23-C22-C09	2.26	122.90	120.30
8	D	610	NAG	O7-C7-C8	-2.24	118.07	122.05
8	J	610	NAG	O7-C7-C8	-2.23	118.08	122.05
8	D	607	NAG	C8-C7-N2	2.22	119.80	116.12
8	D	612	NAG	C8-C7-N2	2.22	119.80	116.12
8	J	612	NAG	C8-C7-N2	2.22	119.80	116.12
8	A	610	NAG	O7-C7-C8	-2.22	118.11	122.05
8	A	612	NAG	C8-C7-N2	2.20	119.77	116.12
8	A	607	NAG	C8-C7-N2	2.20	119.77	116.12
8	D	609	NAG	C1-O5-C5	2.20	115.13	112.19
8	J	607	NAG	C8-C7-N2	2.19	119.75	116.12
8	J	613	NAG	O7-C7-C8	-2.19	118.16	122.05

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	613	NAG	O7-C7-C8	-2.19	118.16	122.05
8	J	609	NAG	C1-O5-C5	2.17	115.10	112.19
8	A	609	NAG	C1-O5-C5	2.17	115.09	112.19
8	A	613	NAG	O7-C7-C8	-2.16	118.20	122.05

There are no chirality outliers.

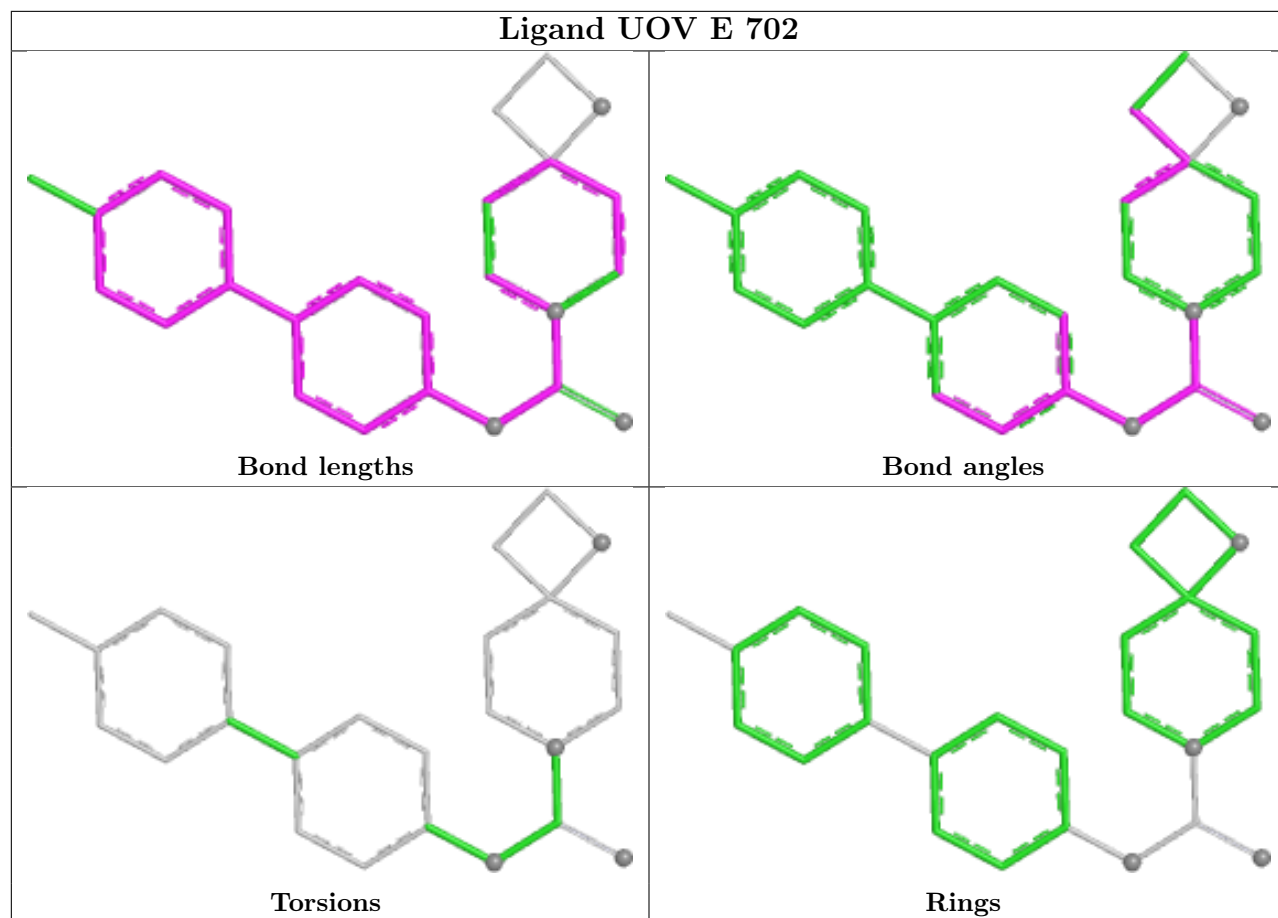
All (9) torsion outliers are listed below:

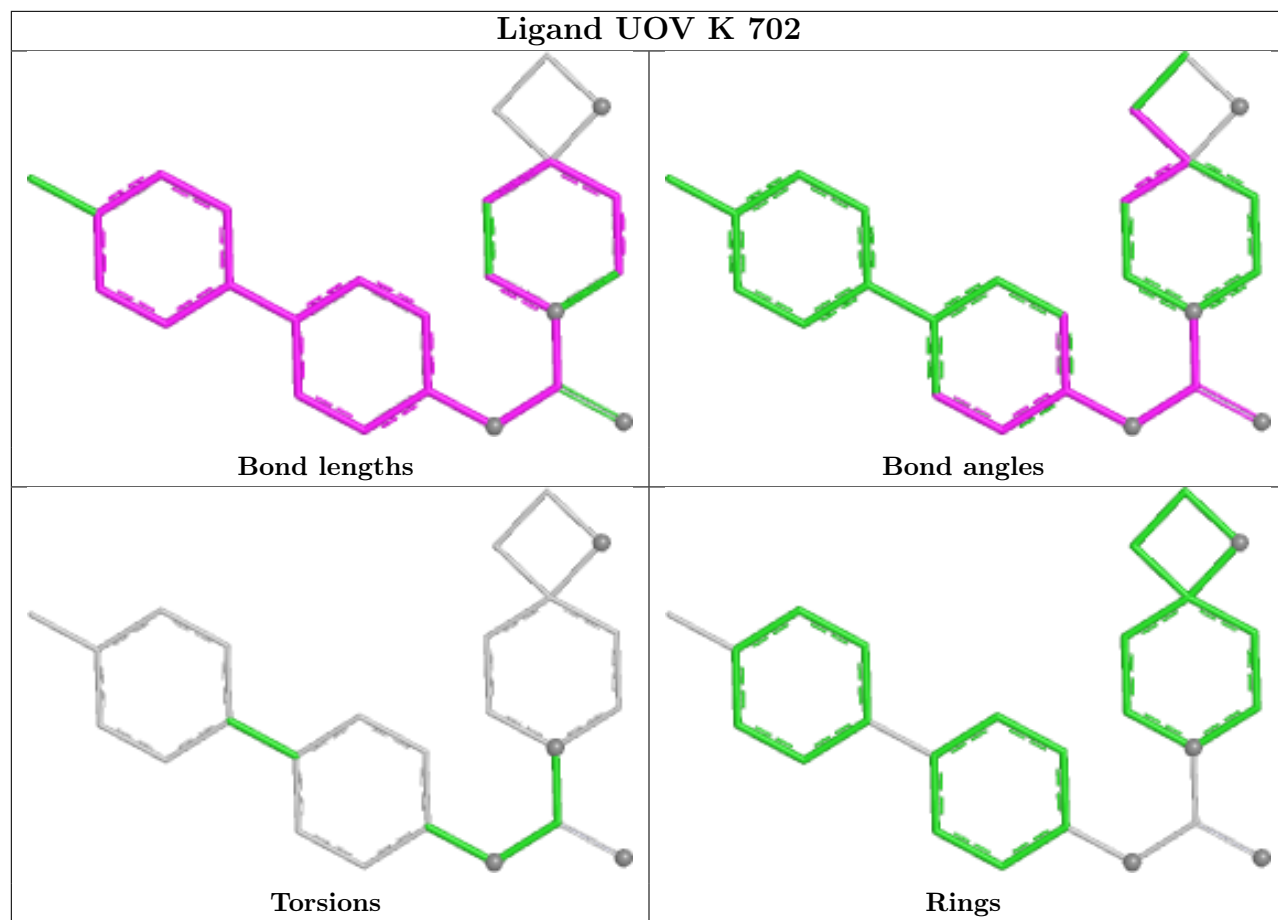
Mol	Chain	Res	Type	Atoms
8	A	612	NAG	O5-C5-C6-O6
8	J	612	NAG	O5-C5-C6-O6
8	D	612	NAG	O5-C5-C6-O6
8	A	609	NAG	O5-C5-C6-O6
8	D	609	NAG	O5-C5-C6-O6
8	J	609	NAG	O5-C5-C6-O6
8	A	610	NAG	C1-C2-N2-C7
8	D	610	NAG	C1-C2-N2-C7
8	J	610	NAG	C1-C2-N2-C7

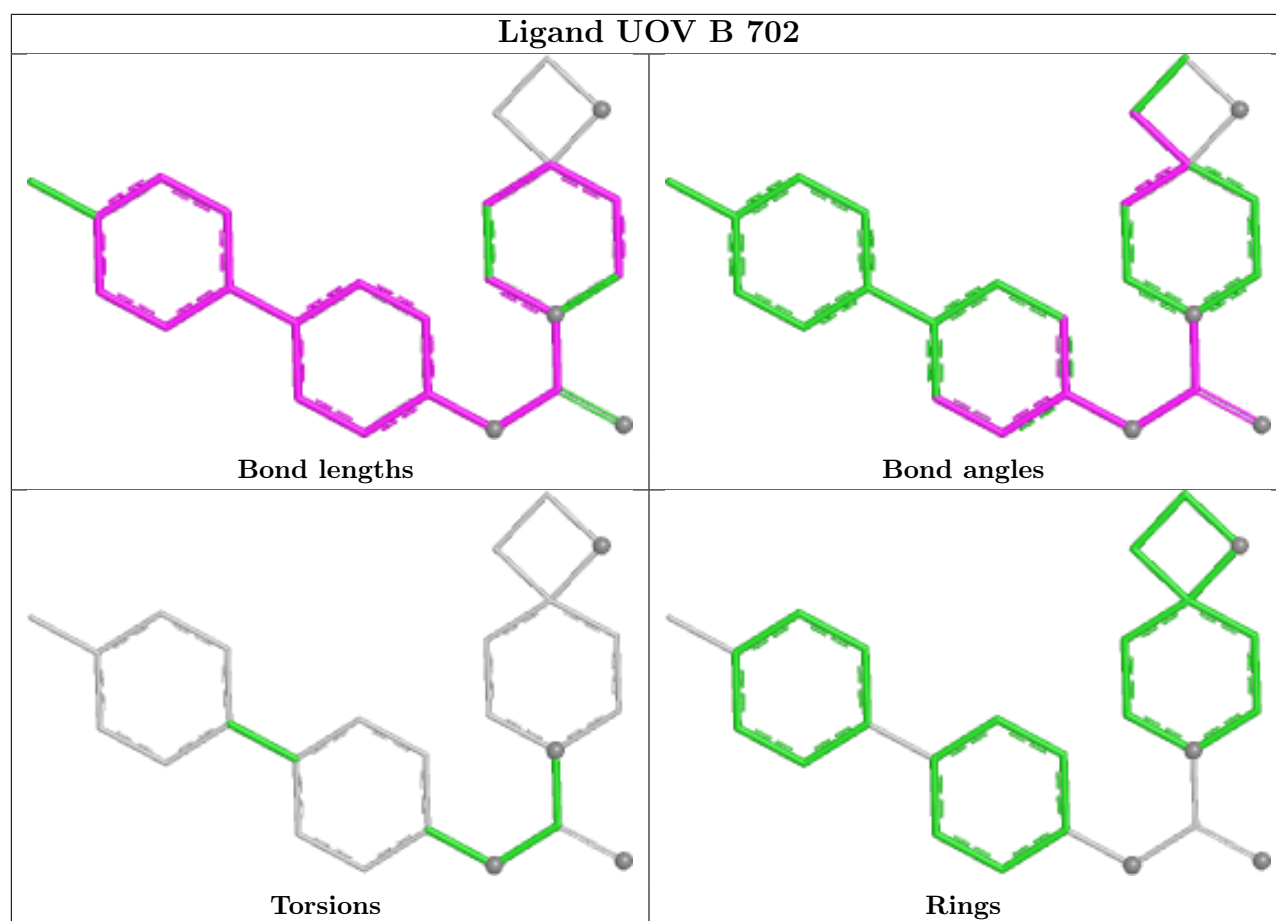
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 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.

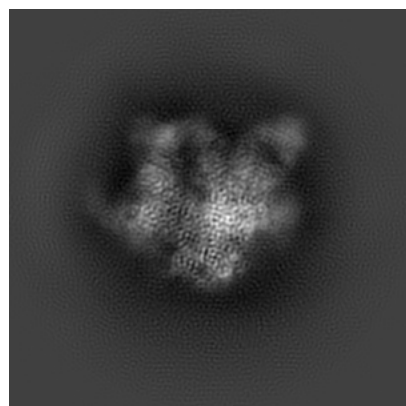
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22048. These allow visual inspection of the internal detail of the map and identification of artifacts.

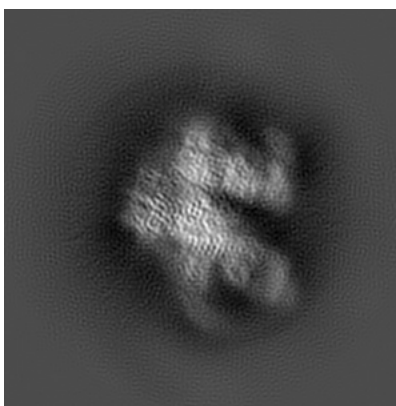
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

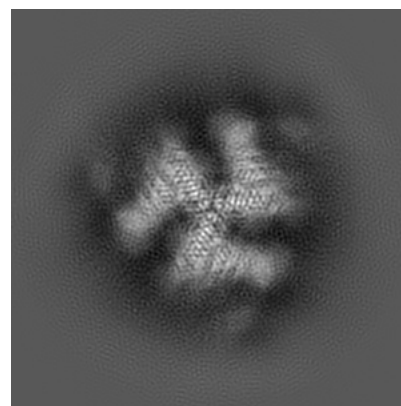
#### 6.1.1 Primary map



X

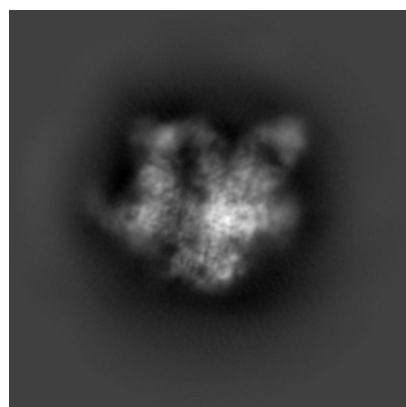


Y

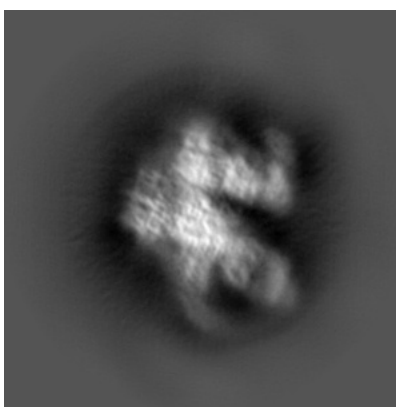


Z

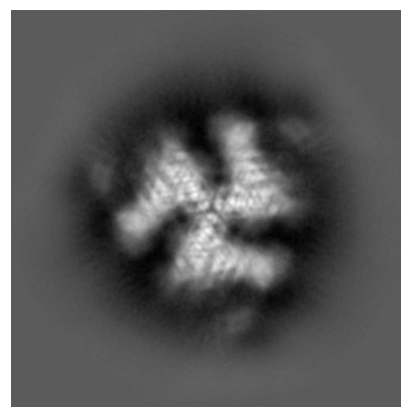
#### 6.1.2 Raw map



X



Y



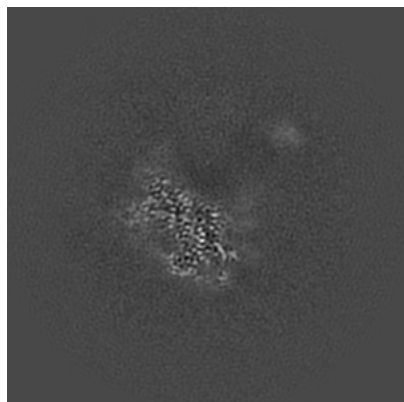
Z

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

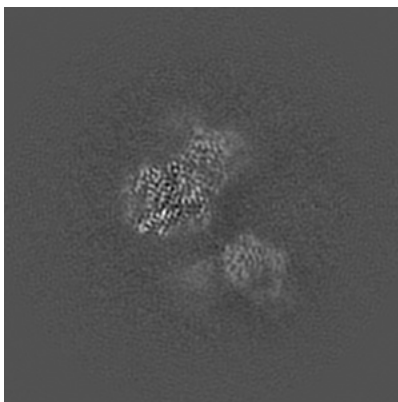


## 6.2 Central slices [i](#)

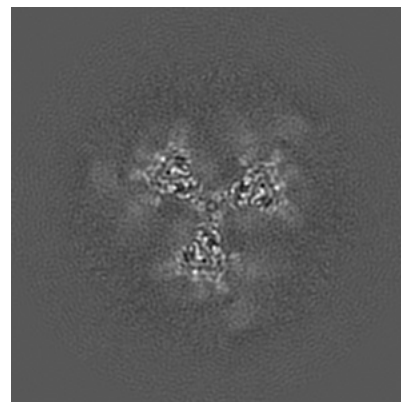
### 6.2.1 Primary map



X Index: 144

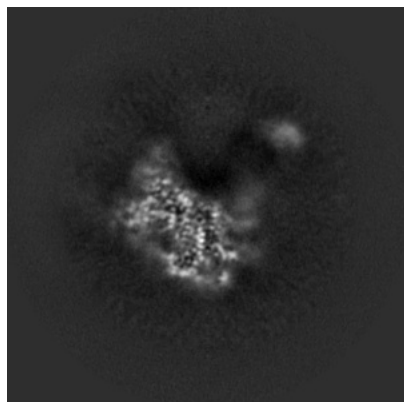


Y Index: 144

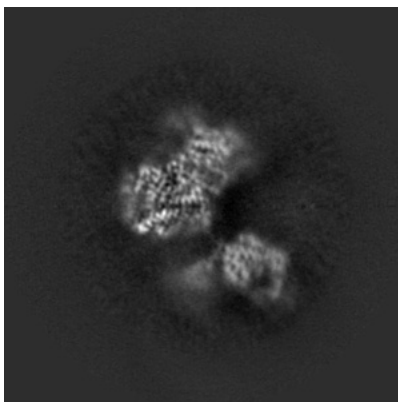


Z Index: 144

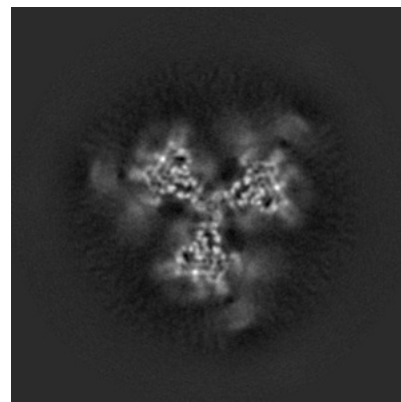
### 6.2.2 Raw map



X Index: 144



Y Index: 144

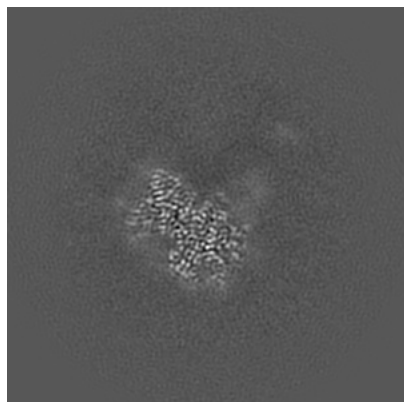


Z Index: 144

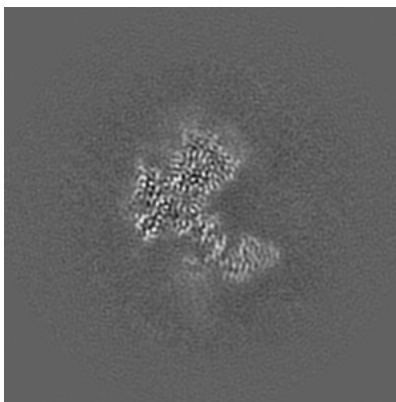
The images above show central slices of the map in three orthogonal directions.

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

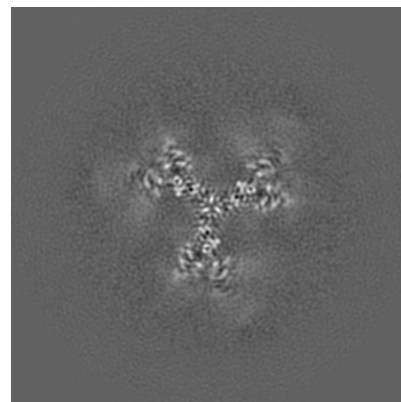
### 6.3.1 Primary map



X Index: 139

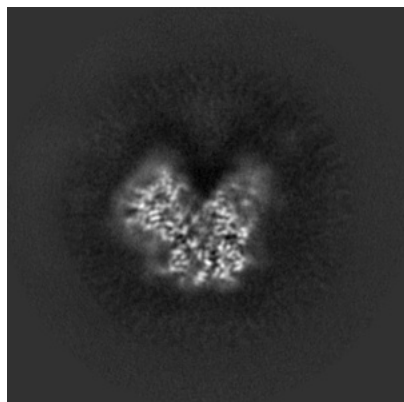


Y Index: 151

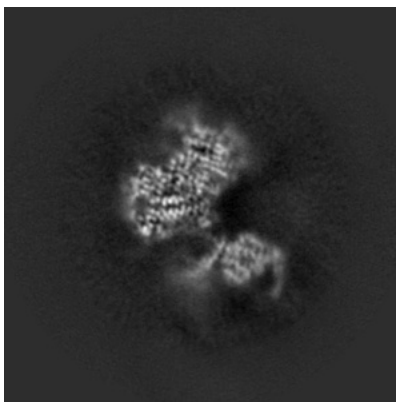


Z Index: 138

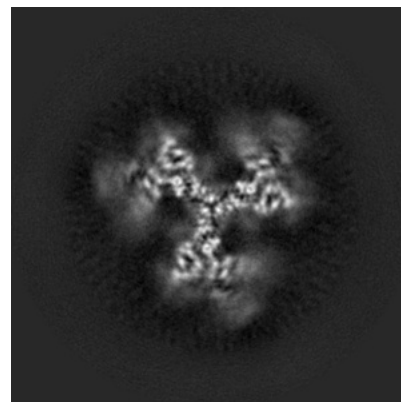
### 6.3.2 Raw map



X Index: 133



Y Index: 147

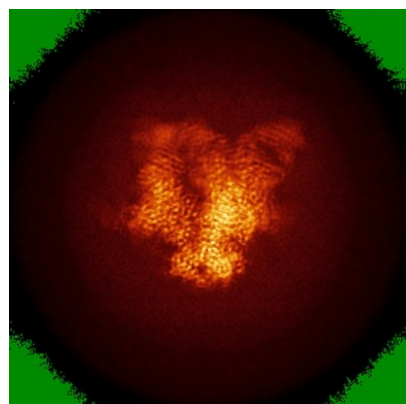


Z Index: 138

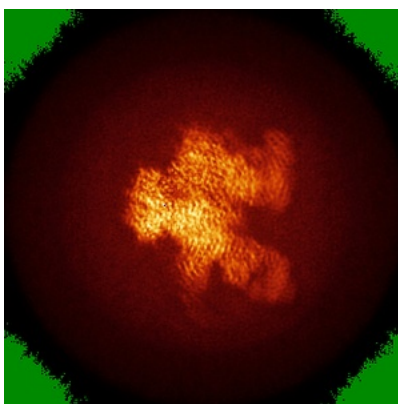
The images above show the largest variance slices of the map in three orthogonal directions.

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

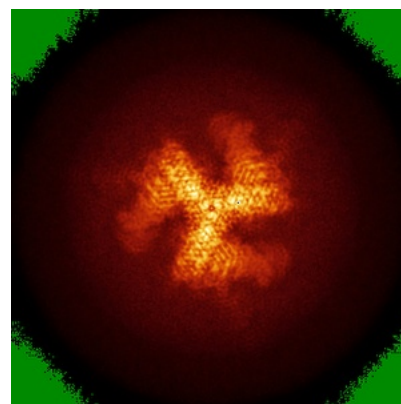
### 6.4.1 Primary map



X

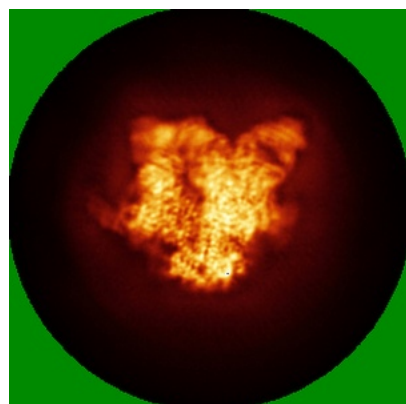


Y

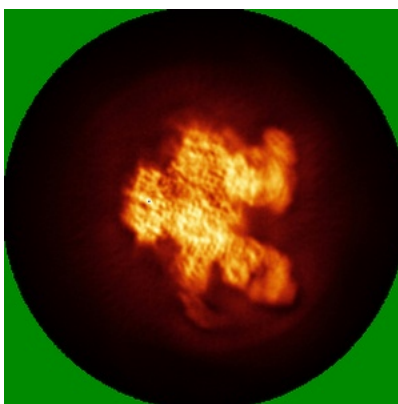


Z

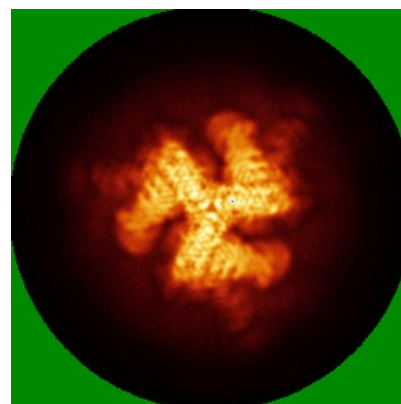
### 6.4.2 Raw map



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.

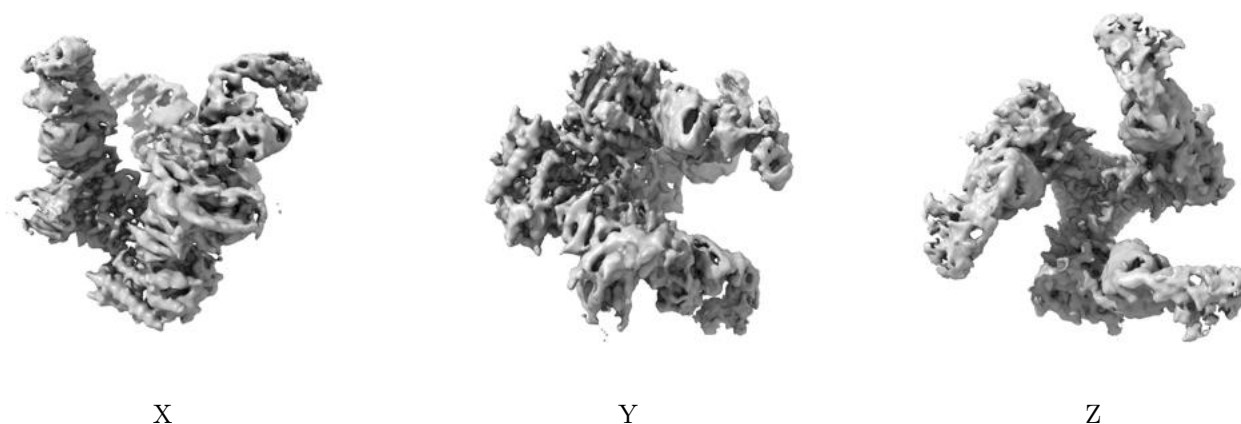
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

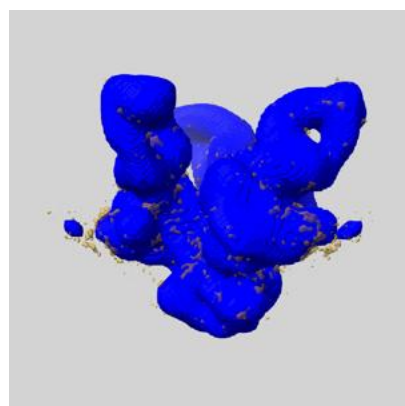
## 6.6 Mask visualisation [i](#)

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

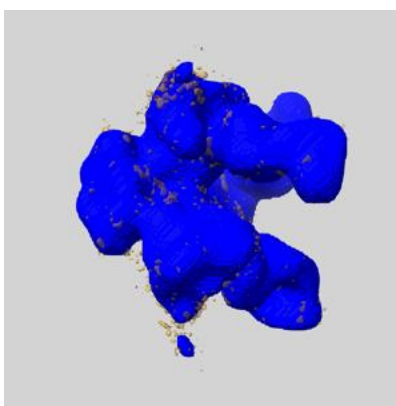
A mask typically either:

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

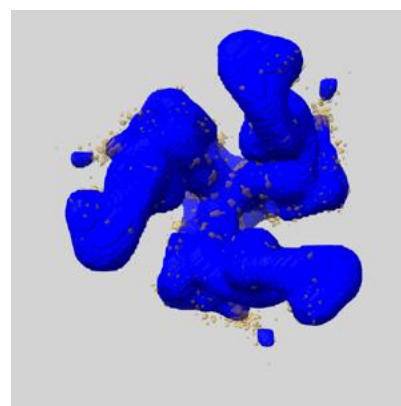
### 6.6.1 emd\_22048\_msk\_1.map [i](#)



X



Y

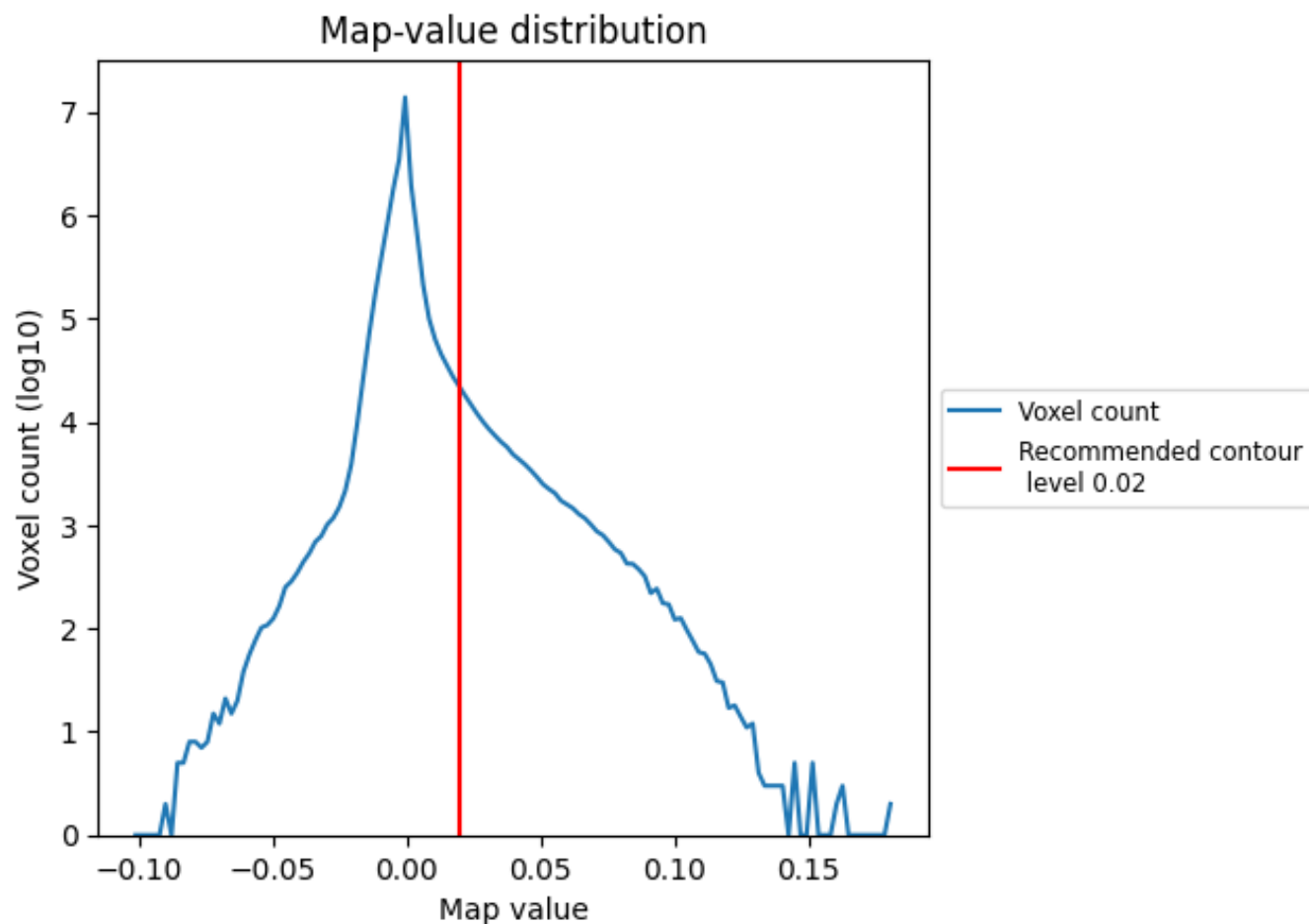


Z

## 7 Map analysis [i](#)

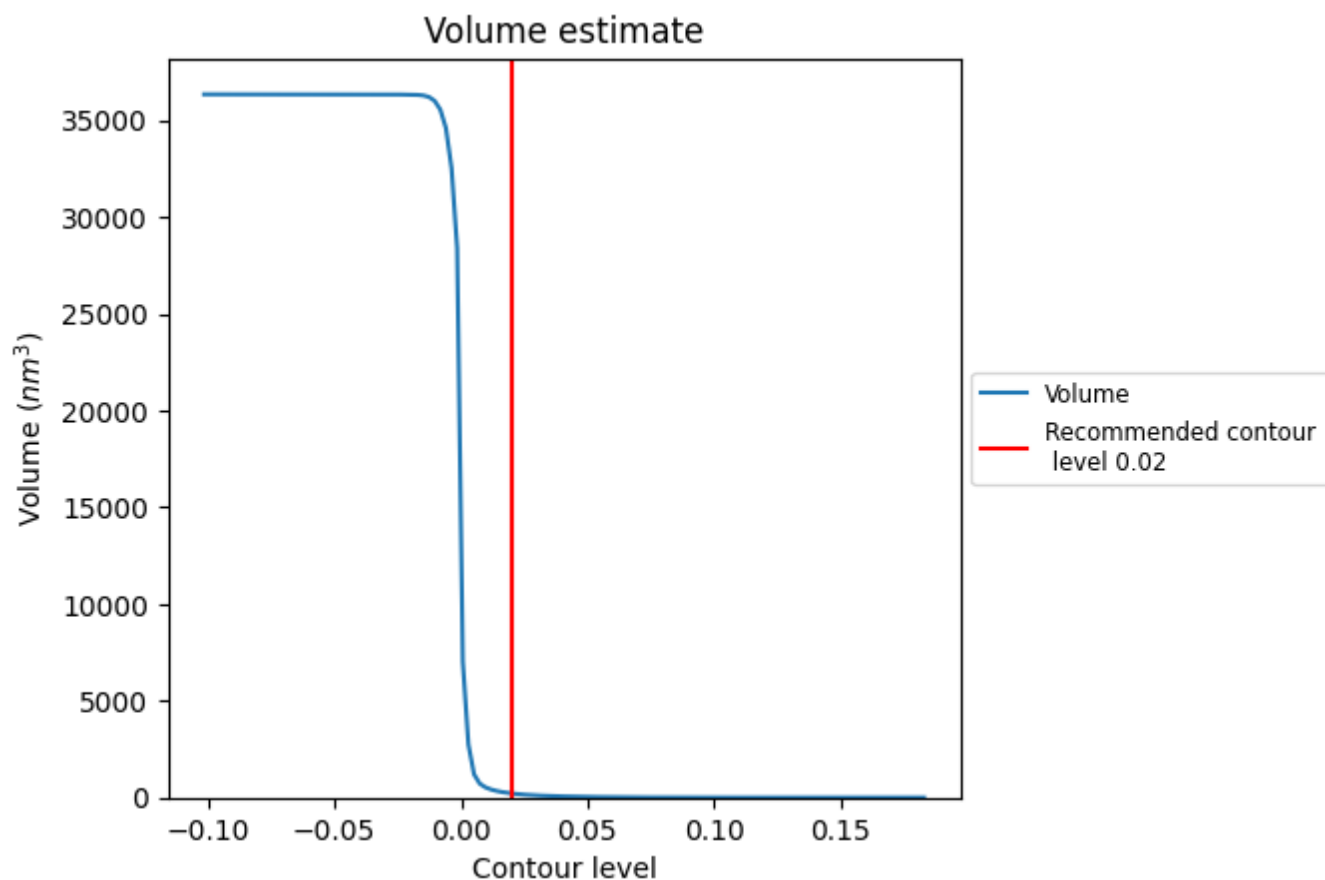
This section contains the results of statistical analysis of the map.

### 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.

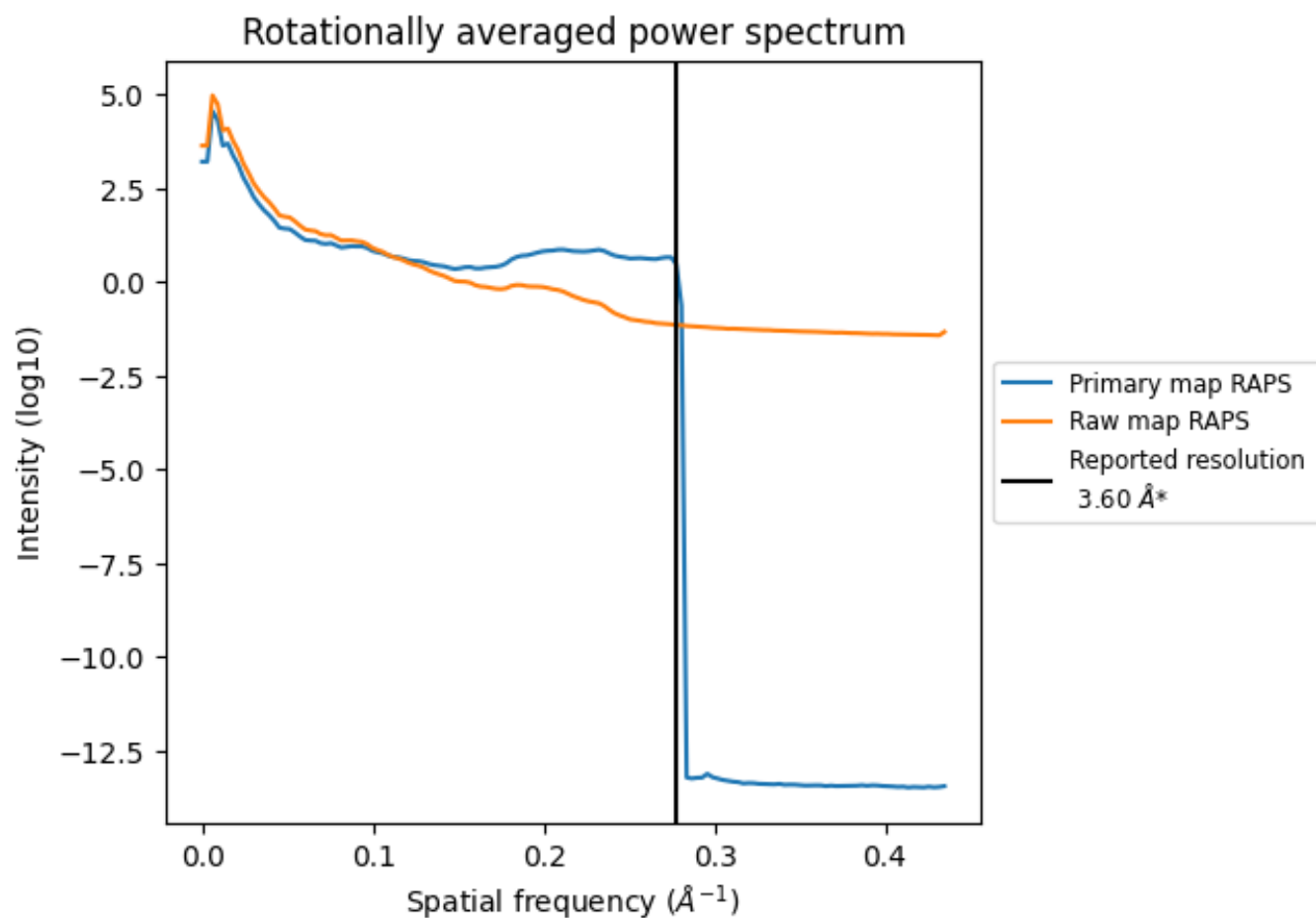
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 213 nm<sup>3</sup>; this corresponds to an approximate mass of 193 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 ⓘ



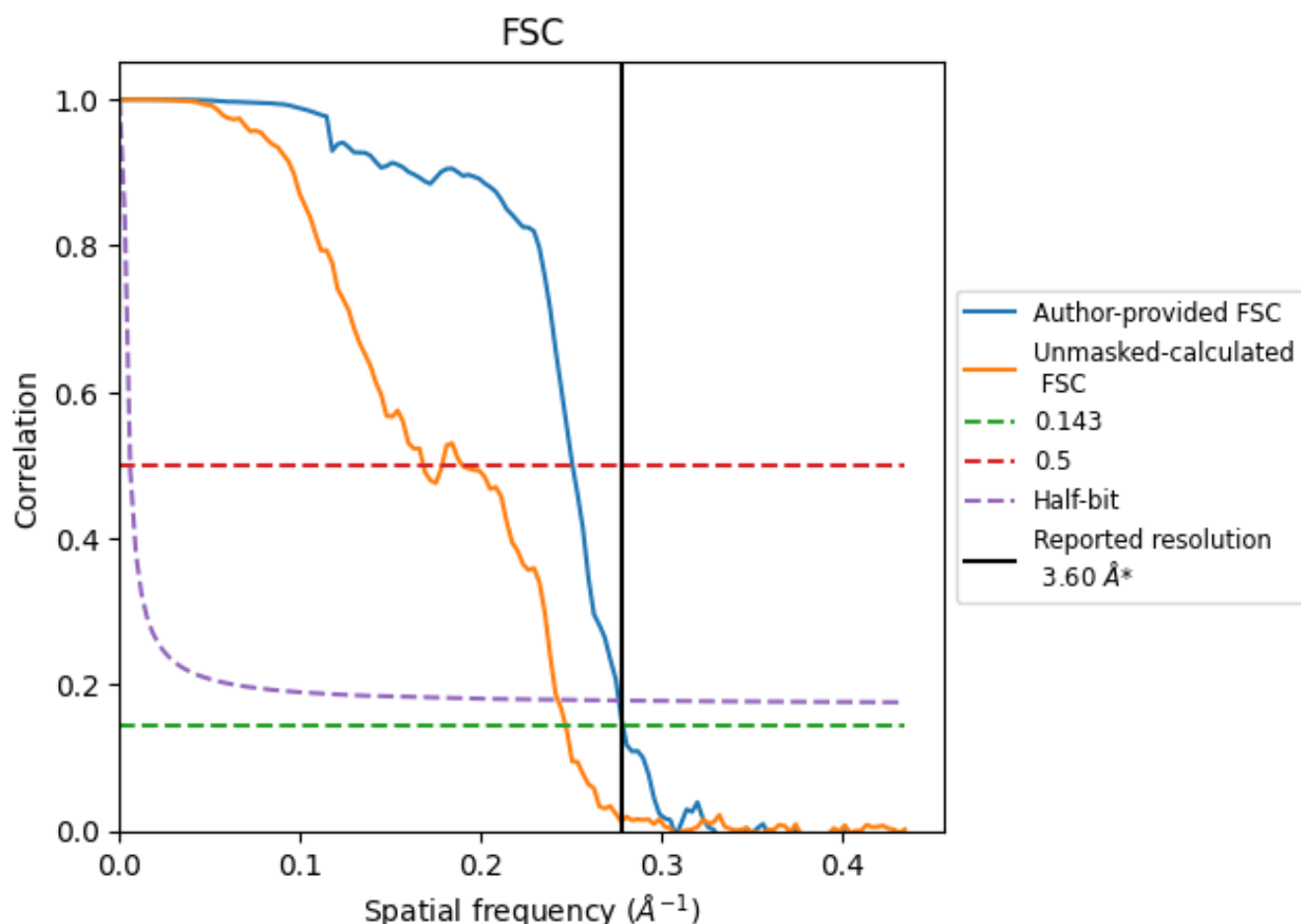
\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>



## 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 0.278  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

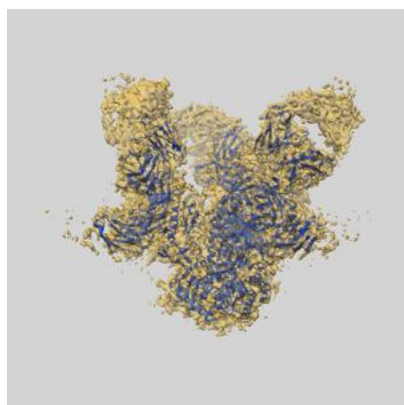
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.59	3.99	3.62
Unmasked-calculated*	4.05	5.95	4.12

\*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 4.05 differs from the reported value 3.6 by more than 10 %

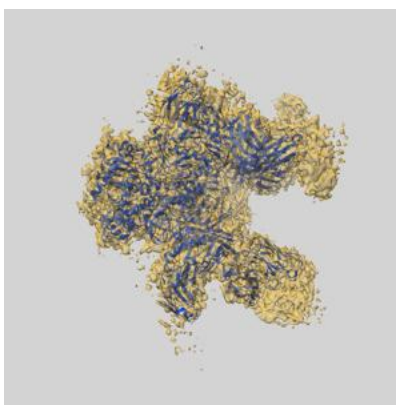
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22048 and PDB model 6X5B. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

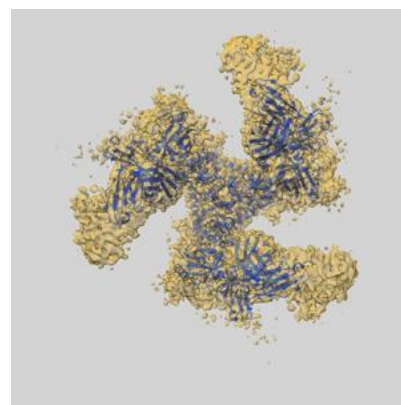
### 9.1 Map-model overlay [i](#)



X



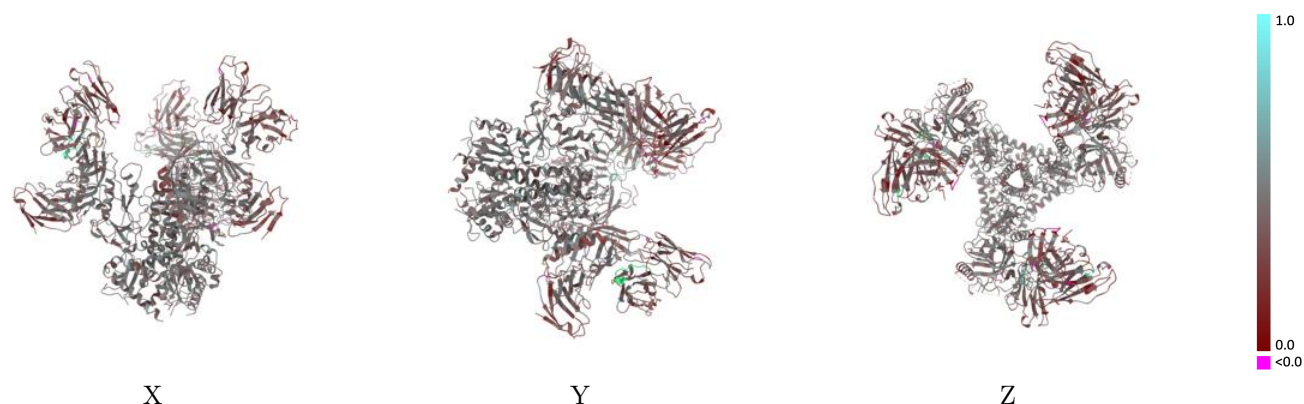
Y



Z

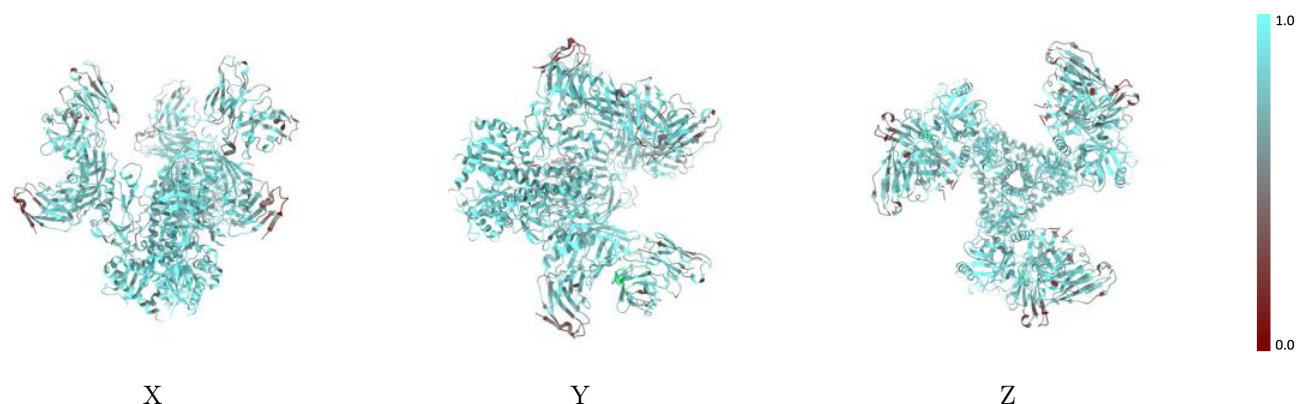
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



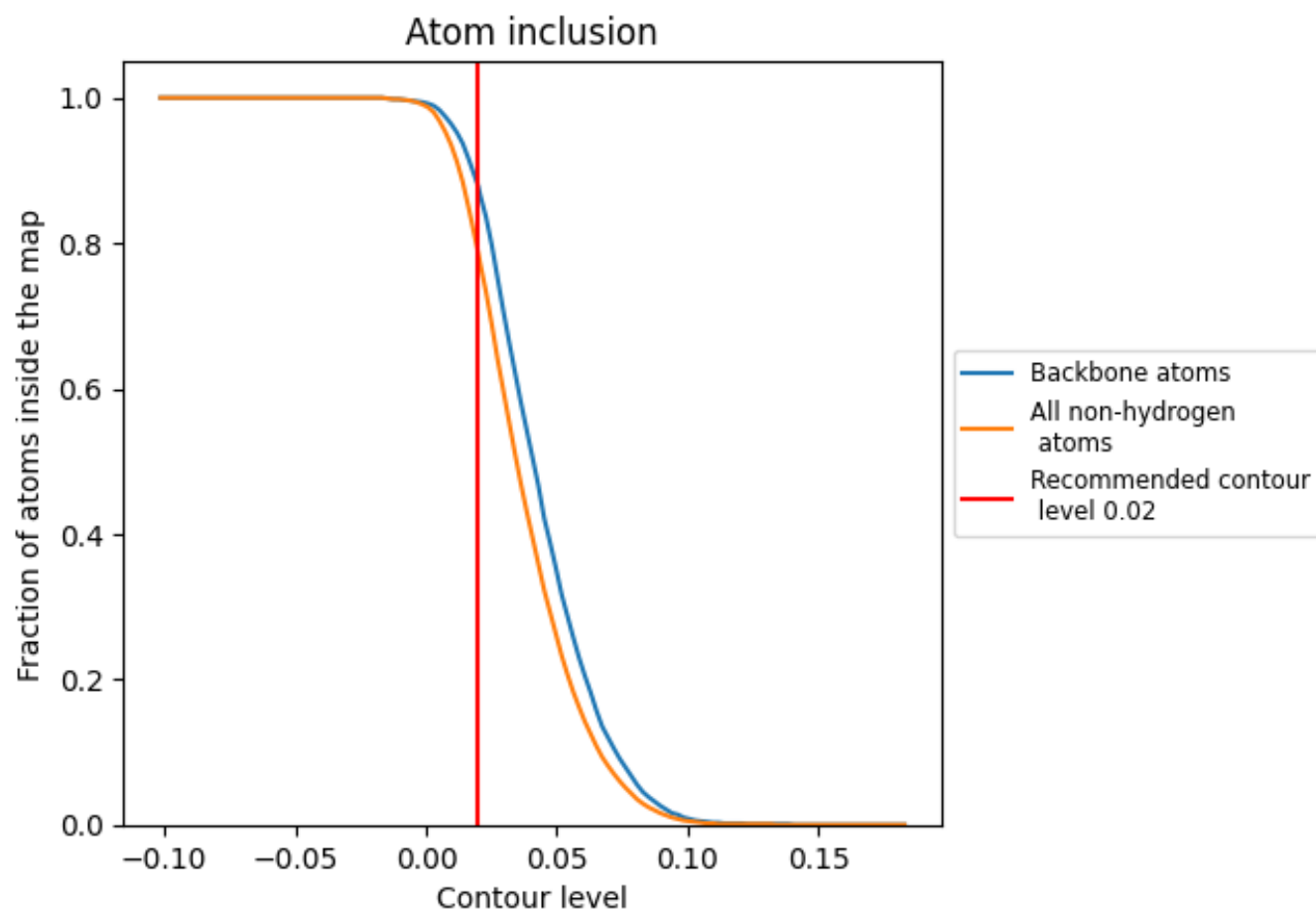
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).













































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 79% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7860	 0.3960
A	 0.8310	 0.4240
B	 0.8430	 0.4390
C	 0.6510	 0.3610
D	 0.8320	 0.4230
E	 0.8430	 0.4390
F	 0.7250	 0.3250
G	 0.6520	 0.3600
H	 0.7340	 0.3410
I	 0.7380	 0.3420
J	 0.8310	 0.4240
K	 0.8380	 0.4400
L	 0.7250	 0.3250
M	 0.7290	 0.3260
N	 0.6490	 0.3590
O	 0.7380	 0.3430
P	 0.6430	 0.3330
Q	 0.8850	 0.4630
R	 0.6430	 0.3280
S	 0.8850	 0.4480
T	 0.6790	 0.3430
U	 0.8850	 0.4660

