



## Full wwPDB EM Validation Report ⓘ

Nov 18, 2025 – 12:23 PM JST

PDB ID : 9LOC / pdb\_00009loc  
EMDB ID : EMD-63244  
Title : Cryo-EM structure of human FcRL5 bound to IgG-Fc  
Authors : Chen, S.H.; Xiao, J.Y.  
Deposited on : 2025-01-23  
Resolution : 3.56 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

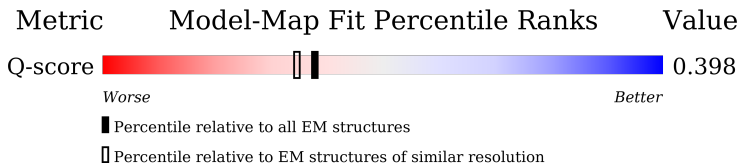
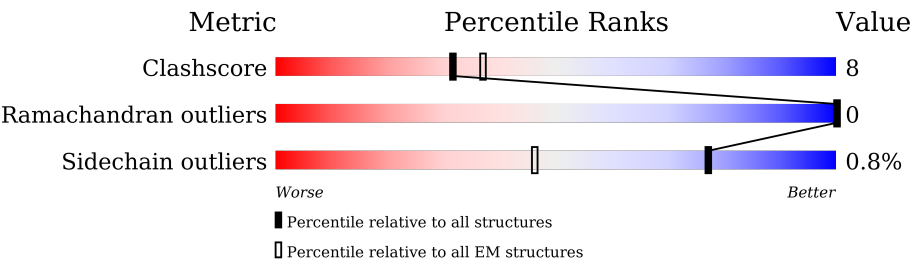
EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.56 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	12750 ( 3.06 - 4.06 )

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	860	<div><div></div><div>26%5%69%</div></div>
2	B	250	<div><div></div><div>71%17%12%</div></div>
2	C	250	<div><div>7%</div><div>68%20%12%</div></div>
2	D	250	<div><div>15%</div><div>69%18%12%</div></div>

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Mol	Chain	Length	Quality of chain
2	E	250	
2	F	250	
2	G	250	
2	H	250	
2	I	250	
2	J	250	
2	K	250	
2	L	250	
2	M	250	
3	N	6	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23545 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 Fc receptor-like protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	264	Total	C	N	O	S	0	0
			2121	1352	369	389	11		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	852	HIS	-	expression tag	UNP Q96RD9
A	853	HIS	-	expression tag	UNP Q96RD9
A	854	HIS	-	expression tag	UNP Q96RD9
A	855	HIS	-	expression tag	UNP Q96RD9
A	856	HIS	-	expression tag	UNP Q96RD9
A	857	HIS	-	expression tag	UNP Q96RD9
A	858	HIS	-	expression tag	UNP Q96RD9
A	859	HIS	-	expression tag	UNP Q96RD9
A	860	TRP	-	expression tag	UNP Q96RD9
A	861	ARG	-	expression tag	UNP Q96RD9
A	862	PRO	-	expression tag	UNP Q96RD9
A	863	LEU	-	expression tag	UNP Q96RD9
A	864	GLU	-	expression tag	UNP Q96RD9
A	865	SER	-	expression tag	UNP Q96RD9
A	866	ARG	-	expression tag	UNP Q96RD9
A	867	VAL	-	expression tag	UNP Q96RD9
A	868	ASP	-	expression tag	UNP Q96RD9
A	869	TYR	-	expression tag	UNP Q96RD9
A	870	LYS	-	expression tag	UNP Q96RD9
A	871	ASP	-	expression tag	UNP Q96RD9
A	872	ASP	-	expression tag	UNP Q96RD9
A	873	ASP	-	expression tag	UNP Q96RD9
A	874	ASP	-	expression tag	UNP Q96RD9
A	875	LYS	-	expression tag	UNP Q96RD9

- Molecule 2 is a protein called Immunoglobulin gamma-1 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	221	Total	C	N	O	S	0	0
			1764	1122	296	338	8		
2	C	221	Total	C	N	O	S	0	0
			1764	1122	296	338	8		
2	D	221	Total	C	N	O	S	0	0
			1764	1122	296	338	8		
2	E	221	Total	C	N	O	S	0	0
			1764	1122	296	338	8		
2	F	221	Total	C	N	O	S	0	0
			1764	1122	296	338	8		
2	G	221	Total	C	N	O	S	0	0
			1764	1122	296	338	8		
2	H	221	Total	C	N	O	S	0	0
			1764	1122	296	338	8		
2	I	221	Total	C	N	O	S	0	0
			1764	1122	296	338	8		
2	J	221	Total	C	N	O	S	0	0
			1764	1122	296	338	8		
2	K	221	Total	C	N	O	S	0	0
			1764	1122	296	338	8		
2	L	221	Total	C	N	O	S	0	0
			1764	1122	296	338	8		
2	M	221	Total	C	N	O	S	0	0
			1764	1122	296	338	8		

There are 300 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	309	CYS	LEU	conflict	UNP P0DOX5
B	442	ASP	-	expression tag	UNP P0DOX5
B	443	LYS	-	expression tag	UNP P0DOX5
B	444	SER	-	expression tag	UNP P0DOX5
B	445	THR	-	expression tag	UNP P0DOX5
B	446	GLY	-	expression tag	UNP P0DOX5
B	447	LYS	-	expression tag	UNP P0DOX5
B	448	PRO	-	expression tag	UNP P0DOX5
B	449	THR	-	expression tag	UNP P0DOX5
B	450	LEU	-	expression tag	UNP P0DOX5
B	451	TYR	-	expression tag	UNP P0DOX5
B	452	ASN	-	expression tag	UNP P0DOX5
B	453	VAL	-	expression tag	UNP P0DOX5
B	454	SER	-	expression tag	UNP P0DOX5
B	455	LEU	-	expression tag	UNP P0DOX5
B	456	ILE	-	expression tag	UNP P0DOX5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	457	MET	-	expression tag	UNP P0DOX5
B	458	SER	-	expression tag	UNP P0DOX5
B	459	ASP	-	expression tag	UNP P0DOX5
B	460	THR	-	expression tag	UNP P0DOX5
B	461	GLY	-	expression tag	UNP P0DOX5
B	462	GLY	-	expression tag	UNP P0DOX5
B	463	THR	-	expression tag	UNP P0DOX5
B	464	CYS	-	expression tag	UNP P0DOX5
B	465	TYR	-	expression tag	UNP P0DOX5
C	309	CYS	LEU	conflict	UNP P0DOX5
C	442	ASP	-	expression tag	UNP P0DOX5
C	443	LYS	-	expression tag	UNP P0DOX5
C	444	SER	-	expression tag	UNP P0DOX5
C	445	THR	-	expression tag	UNP P0DOX5
C	446	GLY	-	expression tag	UNP P0DOX5
C	447	LYS	-	expression tag	UNP P0DOX5
C	448	PRO	-	expression tag	UNP P0DOX5
C	449	THR	-	expression tag	UNP P0DOX5
C	450	LEU	-	expression tag	UNP P0DOX5
C	451	TYR	-	expression tag	UNP P0DOX5
C	452	ASN	-	expression tag	UNP P0DOX5
C	453	VAL	-	expression tag	UNP P0DOX5
C	454	SER	-	expression tag	UNP P0DOX5
C	455	LEU	-	expression tag	UNP P0DOX5
C	456	ILE	-	expression tag	UNP P0DOX5
C	457	MET	-	expression tag	UNP P0DOX5
C	458	SER	-	expression tag	UNP P0DOX5
C	459	ASP	-	expression tag	UNP P0DOX5
C	460	THR	-	expression tag	UNP P0DOX5
C	461	GLY	-	expression tag	UNP P0DOX5
C	462	GLY	-	expression tag	UNP P0DOX5
C	463	THR	-	expression tag	UNP P0DOX5
C	464	CYS	-	expression tag	UNP P0DOX5
C	465	TYR	-	expression tag	UNP P0DOX5
D	309	CYS	LEU	conflict	UNP P0DOX5
D	442	ASP	-	expression tag	UNP P0DOX5
D	443	LYS	-	expression tag	UNP P0DOX5
D	444	SER	-	expression tag	UNP P0DOX5
D	445	THR	-	expression tag	UNP P0DOX5
D	446	GLY	-	expression tag	UNP P0DOX5
D	447	LYS	-	expression tag	UNP P0DOX5
D	448	PRO	-	expression tag	UNP P0DOX5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	449	THR	-	expression tag	UNP P0DOX5
D	450	LEU	-	expression tag	UNP P0DOX5
D	451	TYR	-	expression tag	UNP P0DOX5
D	452	ASN	-	expression tag	UNP P0DOX5
D	453	VAL	-	expression tag	UNP P0DOX5
D	454	SER	-	expression tag	UNP P0DOX5
D	455	LEU	-	expression tag	UNP P0DOX5
D	456	ILE	-	expression tag	UNP P0DOX5
D	457	MET	-	expression tag	UNP P0DOX5
D	458	SER	-	expression tag	UNP P0DOX5
D	459	ASP	-	expression tag	UNP P0DOX5
D	460	THR	-	expression tag	UNP P0DOX5
D	461	GLY	-	expression tag	UNP P0DOX5
D	462	GLY	-	expression tag	UNP P0DOX5
D	463	THR	-	expression tag	UNP P0DOX5
D	464	CYS	-	expression tag	UNP P0DOX5
D	465	TYR	-	expression tag	UNP P0DOX5
E	309	CYS	LEU	conflict	UNP P0DOX5
E	442	ASP	-	expression tag	UNP P0DOX5
E	443	LYS	-	expression tag	UNP P0DOX5
E	444	SER	-	expression tag	UNP P0DOX5
E	445	THR	-	expression tag	UNP P0DOX5
E	446	GLY	-	expression tag	UNP P0DOX5
E	447	LYS	-	expression tag	UNP P0DOX5
E	448	PRO	-	expression tag	UNP P0DOX5
E	449	THR	-	expression tag	UNP P0DOX5
E	450	LEU	-	expression tag	UNP P0DOX5
E	451	TYR	-	expression tag	UNP P0DOX5
E	452	ASN	-	expression tag	UNP P0DOX5
E	453	VAL	-	expression tag	UNP P0DOX5
E	454	SER	-	expression tag	UNP P0DOX5
E	455	LEU	-	expression tag	UNP P0DOX5
E	456	ILE	-	expression tag	UNP P0DOX5
E	457	MET	-	expression tag	UNP P0DOX5
E	458	SER	-	expression tag	UNP P0DOX5
E	459	ASP	-	expression tag	UNP P0DOX5
E	460	THR	-	expression tag	UNP P0DOX5
E	461	GLY	-	expression tag	UNP P0DOX5
E	462	GLY	-	expression tag	UNP P0DOX5
E	463	THR	-	expression tag	UNP P0DOX5
E	464	CYS	-	expression tag	UNP P0DOX5
E	465	TYR	-	expression tag	UNP P0DOX5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	309	CYS	LEU	conflict	UNP P0DOX5
F	442	ASP	-	expression tag	UNP P0DOX5
F	443	LYS	-	expression tag	UNP P0DOX5
F	444	SER	-	expression tag	UNP P0DOX5
F	445	THR	-	expression tag	UNP P0DOX5
F	446	GLY	-	expression tag	UNP P0DOX5
F	447	LYS	-	expression tag	UNP P0DOX5
F	448	PRO	-	expression tag	UNP P0DOX5
F	449	THR	-	expression tag	UNP P0DOX5
F	450	LEU	-	expression tag	UNP P0DOX5
F	451	TYR	-	expression tag	UNP P0DOX5
F	452	ASN	-	expression tag	UNP P0DOX5
F	453	VAL	-	expression tag	UNP P0DOX5
F	454	SER	-	expression tag	UNP P0DOX5
F	455	LEU	-	expression tag	UNP P0DOX5
F	456	ILE	-	expression tag	UNP P0DOX5
F	457	MET	-	expression tag	UNP P0DOX5
F	458	SER	-	expression tag	UNP P0DOX5
F	459	ASP	-	expression tag	UNP P0DOX5
F	460	THR	-	expression tag	UNP P0DOX5
F	461	GLY	-	expression tag	UNP P0DOX5
F	462	GLY	-	expression tag	UNP P0DOX5
F	463	THR	-	expression tag	UNP P0DOX5
F	464	CYS	-	expression tag	UNP P0DOX5
F	465	TYR	-	expression tag	UNP P0DOX5
G	309	CYS	LEU	conflict	UNP P0DOX5
G	442	ASP	-	expression tag	UNP P0DOX5
G	443	LYS	-	expression tag	UNP P0DOX5
G	444	SER	-	expression tag	UNP P0DOX5
G	445	THR	-	expression tag	UNP P0DOX5
G	446	GLY	-	expression tag	UNP P0DOX5
G	447	LYS	-	expression tag	UNP P0DOX5
G	448	PRO	-	expression tag	UNP P0DOX5
G	449	THR	-	expression tag	UNP P0DOX5
G	450	LEU	-	expression tag	UNP P0DOX5
G	451	TYR	-	expression tag	UNP P0DOX5
G	452	ASN	-	expression tag	UNP P0DOX5
G	453	VAL	-	expression tag	UNP P0DOX5
G	454	SER	-	expression tag	UNP P0DOX5
G	455	LEU	-	expression tag	UNP P0DOX5
G	456	ILE	-	expression tag	UNP P0DOX5
G	457	MET	-	expression tag	UNP P0DOX5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	458	SER	-	expression tag	UNP P0DOX5
G	459	ASP	-	expression tag	UNP P0DOX5
G	460	THR	-	expression tag	UNP P0DOX5
G	461	GLY	-	expression tag	UNP P0DOX5
G	462	GLY	-	expression tag	UNP P0DOX5
G	463	THR	-	expression tag	UNP P0DOX5
G	464	CYS	-	expression tag	UNP P0DOX5
G	465	TYR	-	expression tag	UNP P0DOX5
H	309	CYS	LEU	conflict	UNP P0DOX5
H	442	ASP	-	expression tag	UNP P0DOX5
H	443	LYS	-	expression tag	UNP P0DOX5
H	444	SER	-	expression tag	UNP P0DOX5
H	445	THR	-	expression tag	UNP P0DOX5
H	446	GLY	-	expression tag	UNP P0DOX5
H	447	LYS	-	expression tag	UNP P0DOX5
H	448	PRO	-	expression tag	UNP P0DOX5
H	449	THR	-	expression tag	UNP P0DOX5
H	450	LEU	-	expression tag	UNP P0DOX5
H	451	TYR	-	expression tag	UNP P0DOX5
H	452	ASN	-	expression tag	UNP P0DOX5
H	453	VAL	-	expression tag	UNP P0DOX5
H	454	SER	-	expression tag	UNP P0DOX5
H	455	LEU	-	expression tag	UNP P0DOX5
H	456	ILE	-	expression tag	UNP P0DOX5
H	457	MET	-	expression tag	UNP P0DOX5
H	458	SER	-	expression tag	UNP P0DOX5
H	459	ASP	-	expression tag	UNP P0DOX5
H	460	THR	-	expression tag	UNP P0DOX5
H	461	GLY	-	expression tag	UNP P0DOX5
H	462	GLY	-	expression tag	UNP P0DOX5
H	463	THR	-	expression tag	UNP P0DOX5
H	464	CYS	-	expression tag	UNP P0DOX5
H	465	TYR	-	expression tag	UNP P0DOX5
I	309	CYS	LEU	conflict	UNP P0DOX5
I	442	ASP	-	expression tag	UNP P0DOX5
I	443	LYS	-	expression tag	UNP P0DOX5
I	444	SER	-	expression tag	UNP P0DOX5
I	445	THR	-	expression tag	UNP P0DOX5
I	446	GLY	-	expression tag	UNP P0DOX5
I	447	LYS	-	expression tag	UNP P0DOX5
I	448	PRO	-	expression tag	UNP P0DOX5
I	449	THR	-	expression tag	UNP P0DOX5

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Chain	Residue	Modelled	Actual	Comment	Reference
I	450	LEU	-	expression tag	UNP P0DOX5
I	451	TYR	-	expression tag	UNP P0DOX5
I	452	ASN	-	expression tag	UNP P0DOX5
I	453	VAL	-	expression tag	UNP P0DOX5
I	454	SER	-	expression tag	UNP P0DOX5
I	455	LEU	-	expression tag	UNP P0DOX5
I	456	ILE	-	expression tag	UNP P0DOX5
I	457	MET	-	expression tag	UNP P0DOX5
I	458	SER	-	expression tag	UNP P0DOX5
I	459	ASP	-	expression tag	UNP P0DOX5
I	460	THR	-	expression tag	UNP P0DOX5
I	461	GLY	-	expression tag	UNP P0DOX5
I	462	GLY	-	expression tag	UNP P0DOX5
I	463	THR	-	expression tag	UNP P0DOX5
I	464	CYS	-	expression tag	UNP P0DOX5
I	465	TYR	-	expression tag	UNP P0DOX5
J	309	CYS	LEU	conflict	UNP P0DOX5
J	442	ASP	-	expression tag	UNP P0DOX5
J	443	LYS	-	expression tag	UNP P0DOX5
J	444	SER	-	expression tag	UNP P0DOX5
J	445	THR	-	expression tag	UNP P0DOX5
J	446	GLY	-	expression tag	UNP P0DOX5
J	447	LYS	-	expression tag	UNP P0DOX5
J	448	PRO	-	expression tag	UNP P0DOX5
J	449	THR	-	expression tag	UNP P0DOX5
J	450	LEU	-	expression tag	UNP P0DOX5
J	451	TYR	-	expression tag	UNP P0DOX5
J	452	ASN	-	expression tag	UNP P0DOX5
J	453	VAL	-	expression tag	UNP P0DOX5
J	454	SER	-	expression tag	UNP P0DOX5
J	455	LEU	-	expression tag	UNP P0DOX5
J	456	ILE	-	expression tag	UNP P0DOX5
J	457	MET	-	expression tag	UNP P0DOX5
J	458	SER	-	expression tag	UNP P0DOX5
J	459	ASP	-	expression tag	UNP P0DOX5
J	460	THR	-	expression tag	UNP P0DOX5
J	461	GLY	-	expression tag	UNP P0DOX5
J	462	GLY	-	expression tag	UNP P0DOX5
J	463	THR	-	expression tag	UNP P0DOX5
J	464	CYS	-	expression tag	UNP P0DOX5
J	465	TYR	-	expression tag	UNP P0DOX5
K	309	CYS	LEU	conflict	UNP P0DOX5

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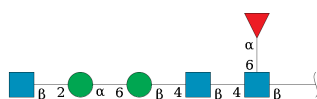
Chain	Residue	Modelled	Actual	Comment	Reference
K	442	ASP	-	expression tag	UNP P0DOX5
K	443	LYS	-	expression tag	UNP P0DOX5
K	444	SER	-	expression tag	UNP P0DOX5
K	445	THR	-	expression tag	UNP P0DOX5
K	446	GLY	-	expression tag	UNP P0DOX5
K	447	LYS	-	expression tag	UNP P0DOX5
K	448	PRO	-	expression tag	UNP P0DOX5
K	449	THR	-	expression tag	UNP P0DOX5
K	450	LEU	-	expression tag	UNP P0DOX5
K	451	TYR	-	expression tag	UNP P0DOX5
K	452	ASN	-	expression tag	UNP P0DOX5
K	453	VAL	-	expression tag	UNP P0DOX5
K	454	SER	-	expression tag	UNP P0DOX5
K	455	LEU	-	expression tag	UNP P0DOX5
K	456	ILE	-	expression tag	UNP P0DOX5
K	457	MET	-	expression tag	UNP P0DOX5
K	458	SER	-	expression tag	UNP P0DOX5
K	459	ASP	-	expression tag	UNP P0DOX5
K	460	THR	-	expression tag	UNP P0DOX5
K	461	GLY	-	expression tag	UNP P0DOX5
K	462	GLY	-	expression tag	UNP P0DOX5
K	463	THR	-	expression tag	UNP P0DOX5
K	464	CYS	-	expression tag	UNP P0DOX5
K	465	TYR	-	expression tag	UNP P0DOX5
L	309	CYS	LEU	conflict	UNP P0DOX5
L	442	ASP	-	expression tag	UNP P0DOX5
L	443	LYS	-	expression tag	UNP P0DOX5
L	444	SER	-	expression tag	UNP P0DOX5
L	445	THR	-	expression tag	UNP P0DOX5
L	446	GLY	-	expression tag	UNP P0DOX5
L	447	LYS	-	expression tag	UNP P0DOX5
L	448	PRO	-	expression tag	UNP P0DOX5
L	449	THR	-	expression tag	UNP P0DOX5
L	450	LEU	-	expression tag	UNP P0DOX5
L	451	TYR	-	expression tag	UNP P0DOX5
L	452	ASN	-	expression tag	UNP P0DOX5
L	453	VAL	-	expression tag	UNP P0DOX5
L	454	SER	-	expression tag	UNP P0DOX5
L	455	LEU	-	expression tag	UNP P0DOX5
L	456	ILE	-	expression tag	UNP P0DOX5
L	457	MET	-	expression tag	UNP P0DOX5
L	458	SER	-	expression tag	UNP P0DOX5

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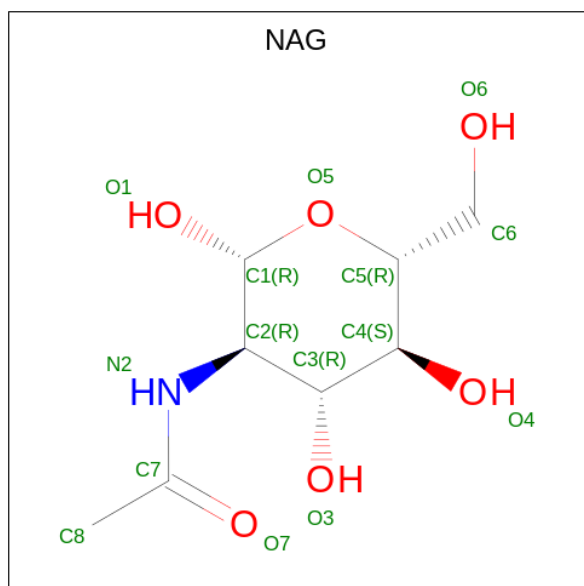
Chain	Residue	Modelled	Actual	Comment	Reference
L	459	ASP	-	expression tag	UNP P0DOX5
L	460	THR	-	expression tag	UNP P0DOX5
L	461	GLY	-	expression tag	UNP P0DOX5
L	462	GLY	-	expression tag	UNP P0DOX5
L	463	THR	-	expression tag	UNP P0DOX5
L	464	CYS	-	expression tag	UNP P0DOX5
L	465	TYR	-	expression tag	UNP P0DOX5
M	309	CYS	LEU	conflict	UNP P0DOX5
M	442	ASP	-	expression tag	UNP P0DOX5
M	443	LYS	-	expression tag	UNP P0DOX5
M	444	SER	-	expression tag	UNP P0DOX5
M	445	THR	-	expression tag	UNP P0DOX5
M	446	GLY	-	expression tag	UNP P0DOX5
M	447	LYS	-	expression tag	UNP P0DOX5
M	448	PRO	-	expression tag	UNP P0DOX5
M	449	THR	-	expression tag	UNP P0DOX5
M	450	LEU	-	expression tag	UNP P0DOX5
M	451	TYR	-	expression tag	UNP P0DOX5
M	452	ASN	-	expression tag	UNP P0DOX5
M	453	VAL	-	expression tag	UNP P0DOX5
M	454	SER	-	expression tag	UNP P0DOX5
M	455	LEU	-	expression tag	UNP P0DOX5
M	456	ILE	-	expression tag	UNP P0DOX5
M	457	MET	-	expression tag	UNP P0DOX5
M	458	SER	-	expression tag	UNP P0DOX5
M	459	ASP	-	expression tag	UNP P0DOX5
M	460	THR	-	expression tag	UNP P0DOX5
M	461	GLY	-	expression tag	UNP P0DOX5
M	462	GLY	-	expression tag	UNP P0DOX5
M	463	THR	-	expression tag	UNP P0DOX5
M	464	CYS	-	expression tag	UNP P0DOX5
M	465	TYR	-	expression tag	UNP P0DOX5

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



Mol	Chain	Residues	Atoms				AltConf	Trace
3	N	6	Total	C	N	O	0	0
			74	42	3	29		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	G	1	Total	C	N	O	0
			14	8	1	5	
4	H	1	Total	C	N	O	0
			14	8	1	5	
4	I	1	Total	C	N	O	0
			14	8	1	5	
4	J	1	Total	C	N	O	0
			14	8	1	5	

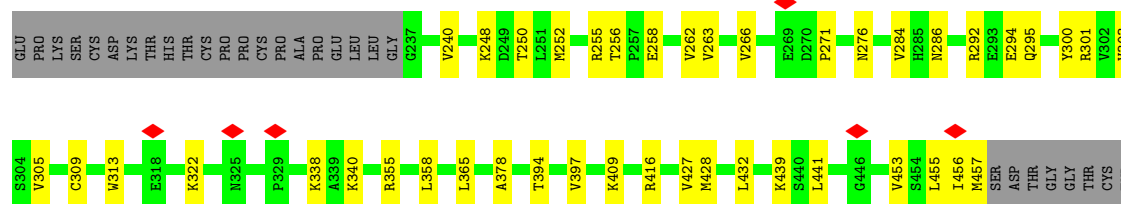
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Mol	Chain	Residues	Atoms				AltConf
4	K	1	Total	C	N	O	0
			14	8	1	5	
4	L	1	Total	C	N	O	0
			14	8	1	5	
4	M	1	Total	C	N	O	0
			14	8	1	5	

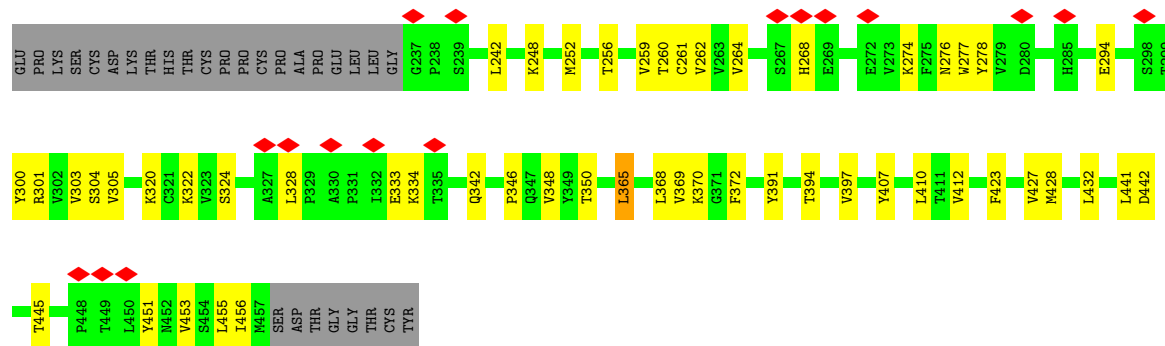


Chain B: 



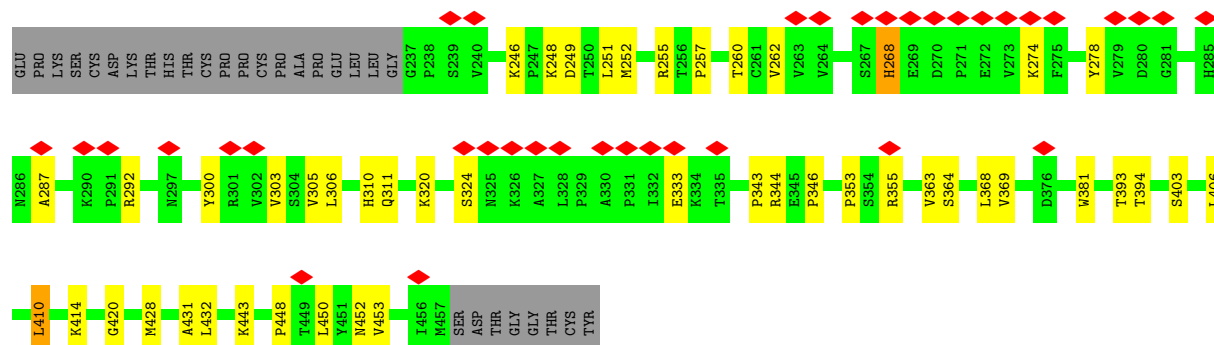
• Molecule 2: Immunoglobulin gamma-1 heavy chain

Chain C: 



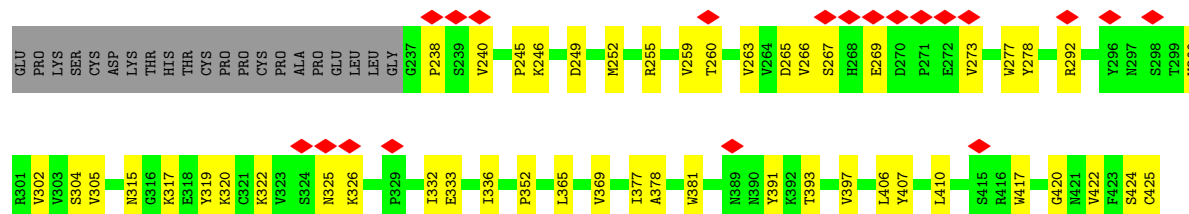
• Molecule 2: Immunoglobulin gamma-1 heavy chain

Chain D: 



• Molecule 2: Immunoglobulin gamma-1 heavy chain

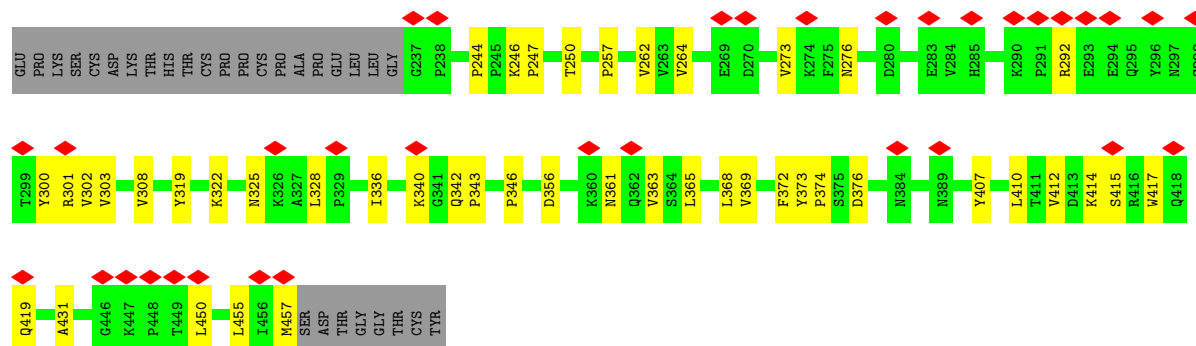
Chain E: 



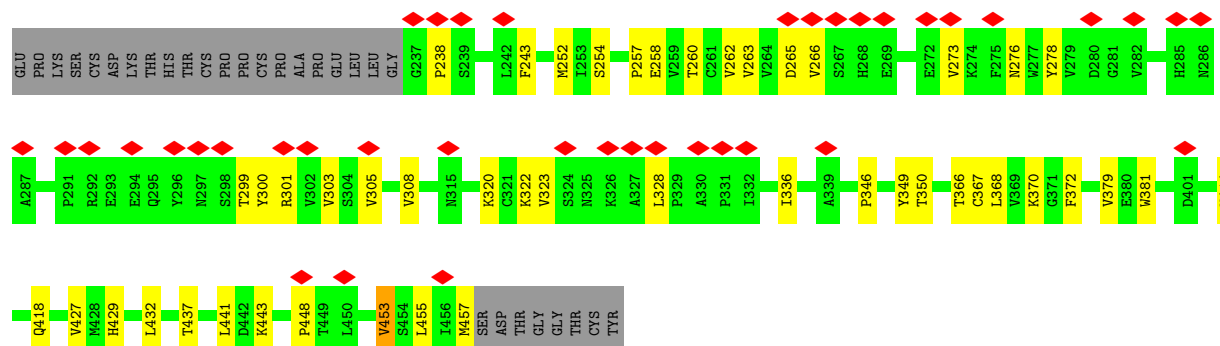




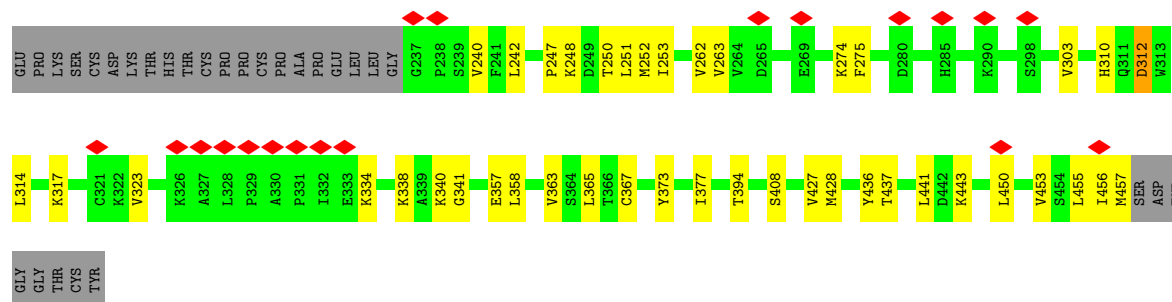
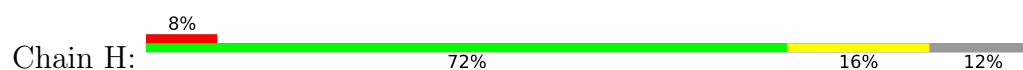
• Molecule 2: Immunoglobulin gamma-1 heavy chain



• Molecule 2: Immunoglobulin gamma-1 heavy chain

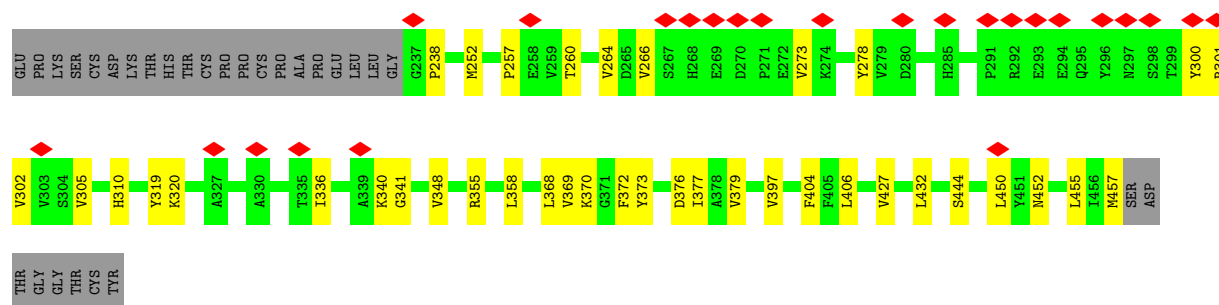


• Molecule 2: Immunoglobulin gamma-1 heavy chain

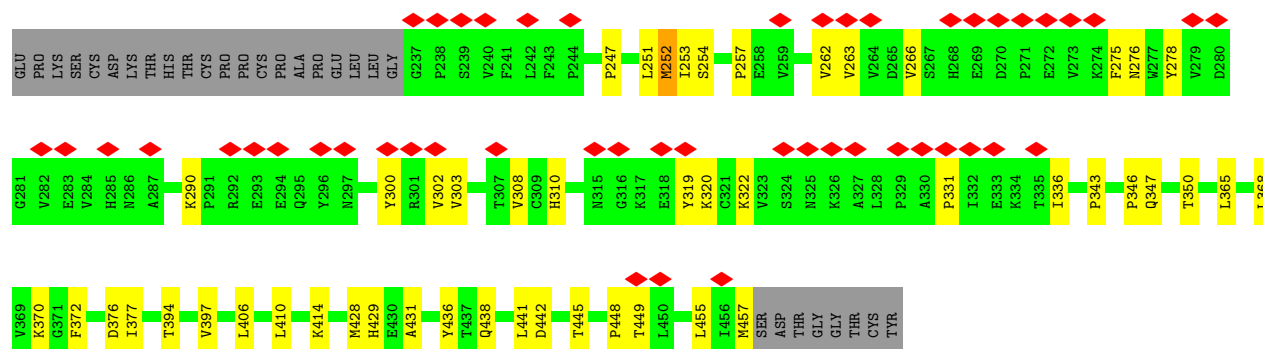


• Molecule 2: Immunoglobulin gamma-1 heavy chain

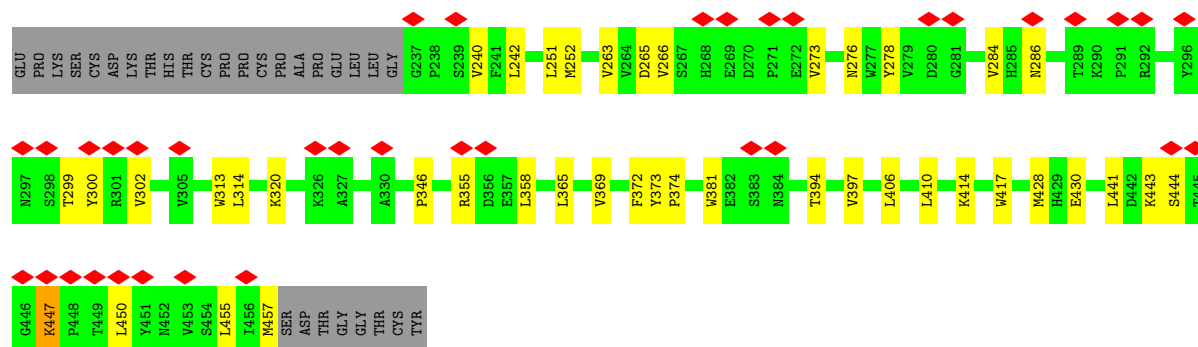
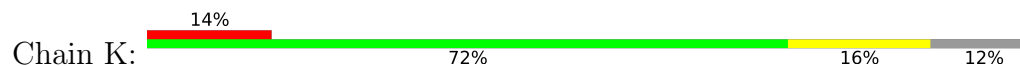




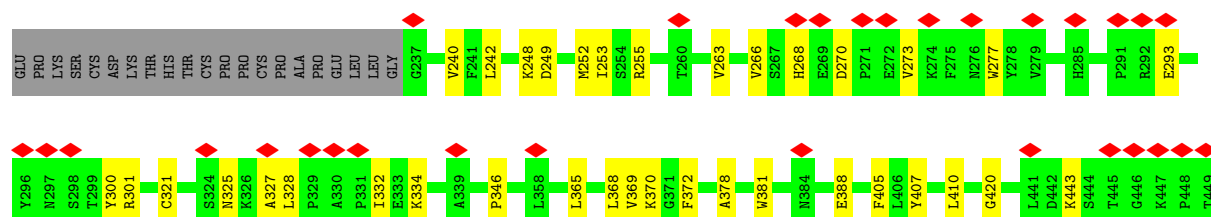
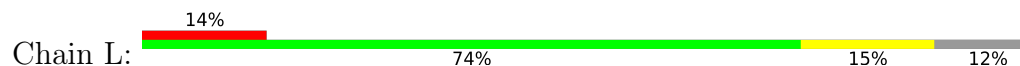
• Molecule 2: Immunoglobulin gamma-1 heavy chain

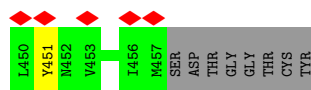


• Molecule 2: Immunoglobulin gamma-1 heavy chain



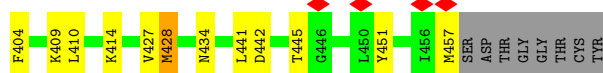
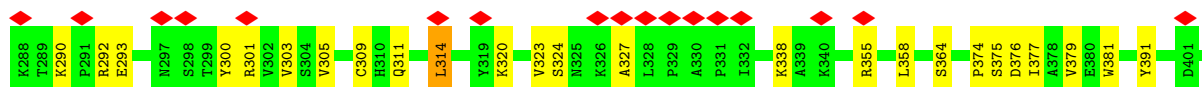
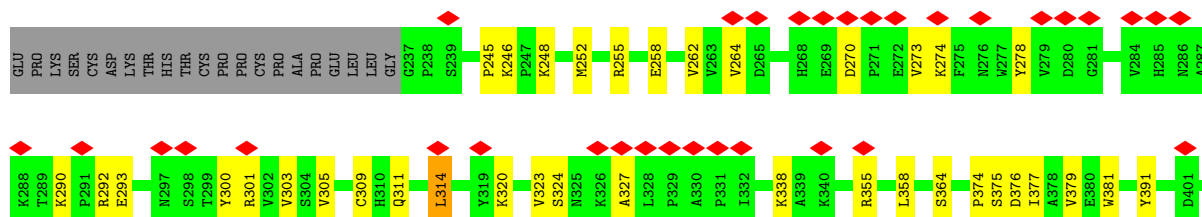
• Molecule 2: Immunoglobulin gamma-1 heavy chain





• Molecule 2: Immunoglobulin gamma-1 heavy chain

Chain M: 15% 69% 19% 12%



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

Chain N: 33% 67%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	257893	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)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.003	Depositor
Minimum map value	-0.547	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.167	Depositor
Map size (Å)	406.6, 406.6, 406.6	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, 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	A	0.20	0/2179	0.35	0/2964
2	B	0.26	0/1812	0.41	0/2468
2	C	0.26	0/1812	0.39	0/2468
2	D	0.23	0/1812	0.39	0/2468
2	E	0.23	0/1812	0.40	0/2468
2	F	0.21	0/1812	0.41	2/2468 (0.1%)
2	G	0.18	0/1812	0.36	0/2468
2	H	0.21	0/1812	0.37	0/2468
2	I	0.22	0/1812	0.33	0/2468
2	J	0.19	0/1812	0.37	0/2468
2	K	0.17	0/1812	0.32	0/2468
2	L	0.19	0/1812	0.38	0/2468
2	M	0.21	0/1812	0.42	0/2468
All	All	0.21	0/23923	0.38	2/32580 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	F	342	GLN	CA-C-N	-5.38	114.05	120.13
2	F	342	GLN	C-N-CA	-5.38	114.05	120.13

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2121	0	2086	28	0
2	B	1764	0	1731	35	0
2	C	1764	0	1732	41	0
2	D	1764	0	1732	34	0
2	E	1764	0	1732	38	0
2	F	1764	0	1732	34	0
2	G	1764	0	1732	31	0
2	H	1764	0	1732	35	0
2	I	1764	0	1733	28	0
2	J	1764	0	1733	39	0
2	K	1764	0	1732	28	0
2	L	1764	0	1732	25	0
2	M	1764	0	1732	35	0
3	N	74	0	64	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
4	E	14	0	13	1	0
4	F	14	0	13	0	0
4	G	14	0	13	0	0
4	H	14	0	13	0	0
4	I	14	0	13	1	0
4	J	14	0	13	0	0
4	K	14	0	13	0	0
4	L	14	0	13	0	0
4	M	14	0	13	0	0
All	All	23545	0	23104	394	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 8.

All (394) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:407:TYR:OH	2:G:366:THR:HG22	1.69	0.91
2:F:410:LEU:HG	2:F:412:VAL:HG23	1.53	0.91
2:D:260:THR:HG22	2:D:305:VAL:HG12	1.52	0.90
2:B:276:ASN:HB3	2:B:322:LYS:HB3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:275:PHE:HZ	2:J:302:VAL:HG12	1.46	0.78
2:H:456:ILE:O	2:H:456:ILE:HG22	1.86	0.76
2:J:350:THR:HB	2:J:441:LEU:HD13	1.69	0.74
2:F:343:PRO:HB2	2:F:431:ALA:HB2	1.74	0.70
2:L:365:LEU:HB2	2:L:410:LEU:HB3	1.74	0.70
2:J:278:TYR:HB2	2:J:320:LYS:HB3	1.73	0.69
2:C:262:VAL:HG23	2:C:303:VAL:HG22	1.72	0.69
2:C:350:THR:HB	2:C:441:LEU:CD1	2.24	0.68
2:J:308:VAL:HG11	2:J:319:TYR:HE2	1.58	0.68
1:A:176:VAL:HG22	2:B:294:GLU:HB3	1.76	0.68
2:G:346:PRO:HB3	2:G:372:PHE:HB3	1.77	0.66
2:K:266:VAL:HB	2:K:300:TYR:HB2	1.77	0.66
2:I:260:THR:HG22	2:I:305:VAL:HG22	1.76	0.66
2:K:365:LEU:HB2	2:K:410:LEU:HB3	1.78	0.66
2:B:248:LYS:HA	2:B:378:ALA:HB2	1.79	0.65
2:D:260:THR:HG22	2:D:305:VAL:CG1	2.25	0.65
2:B:262:VAL:HG23	2:B:303:VAL:HG12	1.79	0.65
2:E:393:THR:HG23	2:E:407:TYR:O	1.98	0.64
2:E:442:ASP:H	2:E:445:THR:HB	1.63	0.64
2:E:377:ILE:HD11	2:E:427:VAL:HG13	1.80	0.63
1:A:189:PHE:HB3	1:A:215:LEU:HD23	1.80	0.63
2:C:242:LEU:HD13	2:C:261:CYS:HB3	1.81	0.63
2:D:249:ASP:HB3	2:D:257:PRO:HA	1.81	0.62
2:H:365:LEU:HD12	2:H:441:LEU:HD21	1.82	0.62
2:B:252:MET:HE1	2:M:434:ASN:HA	1.80	0.62
2:E:240:VAL:HG22	2:E:263:VAL:HG22	1.82	0.62
2:G:266:VAL:HB	2:G:300:TYR:HB2	1.81	0.62
2:F:369:VAL:HG12	2:F:372:PHE:CD2	2.34	0.62
2:H:247:PRO:O	2:H:251:LEU:HB2	1.99	0.62
2:L:240:VAL:HG22	2:L:263:VAL:HG22	1.82	0.62
2:C:350:THR:HB	2:C:441:LEU:HD13	1.83	0.61
2:J:308:VAL:CG1	2:J:319:TYR:HE2	2.13	0.61
2:B:250:THR:HG1	2:B:313:TRP:CD1	2.19	0.61
2:I:310:HIS:HB3	2:J:253:ILE:HD11	1.83	0.61
2:G:368:LEU:HD11	2:G:370:LYS:HB3	1.83	0.61
2:J:266:VAL:HB	2:J:300:TYR:HB2	1.83	0.61
2:L:268:HIS:HA	2:L:300:TYR:HE2	1.67	0.60
2:F:346:PRO:HB3	2:F:372:PHE:HB3	1.83	0.60
2:G:457:MET:HE3	2:G:457:MET:HA	1.82	0.60
2:J:455:LEU:HB3	2:J:457:MET:SD	2.42	0.59
1:A:222:VAL:HG22	1:A:265:MET:HE1	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:THR:CG2	2:M:311:GLN:HE21	2.14	0.59
2:B:256:THR:HG22	2:M:311:GLN:HE21	1.66	0.59
2:J:308:VAL:HG11	2:J:319:TYR:CE2	2.37	0.59
2:M:274:LYS:HB3	2:M:324:SER:HB2	1.84	0.59
2:M:246:LYS:HD3	2:M:248:LYS:HE2	1.84	0.59
2:K:355:ARG:HA	2:K:358:LEU:HG	1.85	0.59
2:G:265:ASP:HA	2:G:299:THR:HB	1.84	0.58
2:K:273:VAL:HG11	2:K:302:VAL:HG21	1.84	0.58
2:K:252:MET:HE3	2:K:428:MET:HG2	1.84	0.57
2:G:276:ASN:HB2	2:G:322:LYS:HB3	1.87	0.57
2:B:271:PRO:HB2	2:B:292:ARG:HH11	1.70	0.57
2:M:377:ILE:HG13	2:M:428:MET:O	2.04	0.57
2:E:424:SER:HB3	2:E:438:GLN:HE21	1.69	0.57
2:F:250:THR:HG22	2:F:257:PRO:HB3	1.87	0.56
2:G:263:VAL:HG21	2:G:273:VAL:HG21	1.87	0.56
2:F:410:LEU:CG	2:F:412:VAL:HG23	2.32	0.56
2:K:443:LYS:HD2	2:K:444:SER:HB2	1.86	0.56
2:I:444:SER:HB2	2:J:449:THR:HG21	1.88	0.56
2:F:407:TYR:OH	2:G:366:THR:CG2	2.49	0.56
2:J:257:PRO:HD3	2:J:310:HIS:CE1	2.42	0.55
2:L:368:LEU:HD11	2:L:370:LYS:HB3	1.88	0.55
2:C:274:LYS:HB3	2:C:324:SER:HB2	1.88	0.55
2:D:343:PRO:HB2	2:D:431:ALA:HB2	1.88	0.55
2:H:242:LEU:HD22	2:H:334:LYS:HB3	1.88	0.55
2:J:448:PRO:HB3	2:K:450:LEU:HD23	1.87	0.55
2:H:252:MET:HG2	2:H:428:MET:HG3	1.88	0.55
2:M:270:ASP:HB2	2:M:327:ALA:HB2	1.89	0.55
1:A:80:SER:HB2	1:A:100:PHE:HB2	1.89	0.55
2:K:240:VAL:HG22	2:K:263:VAL:HG12	1.89	0.54
2:C:391:TYR:HB3	2:C:410:LEU:HD13	1.88	0.54
2:I:273:VAL:HG21	2:I:302:VAL:HG11	1.88	0.54
2:J:290:LYS:HB3	2:J:303:VAL:HB	1.88	0.54
2:M:355:ARG:HG3	2:M:358:LEU:HD12	1.88	0.54
2:C:350:THR:HB	2:C:441:LEU:HD12	1.88	0.54
2:C:350:THR:CB	2:C:441:LEU:HD12	2.37	0.54
2:C:278:TYR:HB2	2:C:320:LYS:HB2	1.90	0.54
2:C:365:LEU:HD23	2:C:410:LEU:HB3	1.89	0.54
2:D:251:LEU:HD12	2:D:428:MET:HB2	1.88	0.54
2:H:456:ILE:O	2:H:456:ILE:CG2	2.55	0.54
2:K:251:LEU:HD21	2:K:430:GLU:HG2	1.88	0.54
2:E:365:LEU:HD11	2:E:441:LEU:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:278:TYR:HD2	2:M:320:LYS:HB3	1.72	0.54
2:H:240:VAL:HG22	2:H:263:VAL:HG12	1.88	0.54
2:J:365:LEU:HB2	2:J:410:LEU:HB3	1.89	0.54
2:C:346:PRO:HD2	2:C:432:LEU:HG	1.90	0.53
2:D:448:PRO:HD2	2:E:450:LEU:HB3	1.89	0.53
2:H:457:MET:HG3	2:I:457:MET:HB2	1.88	0.53
2:B:266:VAL:HB	2:B:300:TYR:HB2	1.90	0.53
2:H:428:MET:HE1	2:H:436:TYR:HD2	1.72	0.53
2:L:293:GLU:HG2	2:L:301:ARG:HB3	1.91	0.53
2:F:361:ASN:HA	2:F:414:LYS:HE3	1.91	0.53
2:H:428:MET:HE1	2:H:436:TYR:CD2	2.44	0.53
2:M:442:ASP:HB3	2:M:445:THR:HG23	1.88	0.53
2:G:278:TYR:HB2	2:G:320:LYS:HB3	1.91	0.53
2:F:292:ARG:HB3	2:F:302:VAL:HG13	1.91	0.53
2:C:256:THR:HG22	2:D:311:GLN:HG3	1.91	0.53
2:L:266:VAL:HB	2:L:300:TYR:HB2	1.91	0.53
2:B:284:VAL:HG22	2:B:286:ASN:H	1.72	0.52
2:H:450:LEU:HB2	2:I:450:LEU:HD11	1.92	0.52
1:A:59:HIS:HE1	1:A:81:GLY:HA3	1.75	0.52
2:H:358:LEU:HD12	2:H:358:LEU:H	1.73	0.52
1:A:215:LEU:HD21	1:A:224:LEU:HD21	1.92	0.52
1:A:57:TRP:CG	1:A:75:LEU:HD22	2.45	0.52
2:F:373:TYR:HD1	2:F:374:PRO:HA	1.75	0.52
2:J:262:VAL:HG13	2:J:303:VAL:HG22	1.92	0.52
2:D:268:HIS:HA	2:D:300:TYR:HE2	1.74	0.52
2:D:346:PRO:HD2	2:D:432:LEU:HG	1.92	0.52
2:H:427:VAL:HB	2:H:437:THR:HG22	1.92	0.52
2:H:253:ILE:HA	2:H:310:HIS:CE1	2.45	0.52
2:B:455:LEU:HD13	2:C:455:LEU:HD13	1.92	0.51
2:B:256:THR:HG22	2:M:311:GLN:NE2	2.25	0.51
2:C:346:PRO:HB3	2:C:372:PHE:HB3	1.91	0.51
2:F:276:ASN:HB3	2:F:322:LYS:HB2	1.91	0.51
2:G:257:PRO:HG2	2:G:308:VAL:HB	1.92	0.51
2:H:377:ILE:HD11	2:H:427:VAL:HG13	1.93	0.51
2:C:294:GLU:HG3	2:C:300:TYR:HE1	1.76	0.51
2:H:275:PHE:CD1	2:H:323:VAL:HG22	2.45	0.51
2:I:264:VAL:HG12	2:I:301:ARG:HG3	1.93	0.51
2:I:452:ASN:HD22	4:I:700:NAG:H83	1.75	0.51
2:L:368:LEU:HB2	2:L:407:TYR:HE1	1.76	0.51
2:D:363:VAL:HG12	2:D:364:SER:N	2.26	0.50
2:H:341:GLY:HA3	2:H:373:TYR:HE2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:245:PRO:HB3	2:M:258:GLU:H	1.75	0.50
2:B:248:LYS:HD2	2:B:255:ARG:HH22	1.76	0.50
2:G:418:GLN:HA	2:G:443:LYS:HD2	1.94	0.50
2:K:373:TYR:HD1	2:K:374:PRO:HA	1.76	0.50
2:E:420:GLY:HA2	2:E:443:LYS:HB2	1.94	0.50
2:F:368:LEU:HD12	2:F:407:TYR:CZ	2.47	0.50
2:L:328:LEU:HD13	2:L:332:ILE:HG13	1.94	0.50
2:M:252:MET:HG3	2:M:255:ARG:HE	1.75	0.50
2:E:273:VAL:HG12	2:E:325:ASN:HD22	1.75	0.50
2:L:369:VAL:HG12	2:L:372:PHE:CD2	2.46	0.50
2:B:258:GLU:HB3	2:B:305:VAL:CG2	2.41	0.50
2:H:251:LEU:HB3	2:H:428:MET:HB3	1.94	0.50
2:G:429:HIS:H	2:G:432:LEU:HD12	1.76	0.50
2:I:376:ASP:C	2:I:377:ILE:HD12	2.37	0.49
1:A:57:TRP:CZ3	1:A:85:CYS:HB3	2.47	0.49
2:B:258:GLU:HB3	2:B:305:VAL:HG23	1.93	0.49
2:E:245:PRO:HD3	2:E:259:VAL:HG12	1.94	0.49
2:I:266:VAL:HB	2:I:300:TYR:HB2	1.94	0.49
2:I:368:LEU:HD21	2:I:370:LYS:HB3	1.93	0.49
2:C:262:VAL:HG23	2:C:303:VAL:CG2	2.39	0.49
2:I:379:VAL:HG22	2:I:427:VAL:HG22	1.94	0.49
2:J:322:LYS:HE3	2:J:331:PRO:HB3	1.93	0.49
1:A:27:LEU:HD23	1:A:29:PRO:O	2.12	0.49
1:A:225:ARG:HG3	1:A:267:TYR:HE1	1.77	0.49
2:E:352:PRO:HB3	2:E:446:GLY:HA3	1.93	0.49
2:J:397:VAL:HG21	2:K:394:THR:HA	1.94	0.49
1:A:265:MET:SD	1:A:266:PRO:HD3	2.52	0.49
2:D:268:HIS:HA	2:D:300:TYR:CE2	2.47	0.49
2:J:257:PRO:HG2	2:J:308:VAL:HG23	1.95	0.49
2:E:369:VAL:HB	2:E:406:LEU:HD23	1.95	0.49
2:E:266:VAL:HB	2:E:300:TYR:HB2	1.93	0.49
2:F:373:TYR:CD1	2:F:374:PRO:HA	2.48	0.49
2:I:341:GLY:HA3	2:I:373:TYR:HE1	1.77	0.49
2:C:277:TRP:HZ2	2:C:304:SER:HB3	1.78	0.48
2:G:457:MET:HE1	2:H:457:MET:HE2	1.95	0.48
2:D:394:THR:HA	2:E:397:VAL:HG21	1.95	0.48
2:E:238:PRO:HA	2:E:265:ASP:HB3	1.95	0.48
2:I:319:TYR:HB2	2:I:336:ILE:HG23	1.94	0.48
2:J:247:PRO:HB3	2:J:376:ASP:HB3	1.94	0.48
2:K:313:TRP:HD1	2:K:314:LEU:HD23	1.79	0.48
2:K:365:LEU:HD23	2:K:441:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ARG:HD2	1:A:239:TRP:CE2	2.48	0.48
2:C:252:MET:HG2	2:C:428:MET:SD	2.53	0.48
2:D:257:PRO:HD3	2:D:310:HIS:NE2	2.29	0.48
2:D:353:PRO:HG2	2:D:363:VAL:CG1	2.43	0.48
2:D:381:TRP:CD2	2:D:410:LEU:HD12	2.49	0.48
2:G:379:VAL:HG22	2:G:427:VAL:HG22	1.96	0.48
2:C:262:VAL:HG21	2:C:301:ARG:HE	1.78	0.48
2:D:248:LYS:HE2	2:D:255:ARG:HH12	1.78	0.48
2:J:275:PHE:HZ	2:J:302:VAL:CG1	2.19	0.48
2:E:278:TYR:HB2	2:E:320:LYS:HB3	1.96	0.48
2:J:275:PHE:CZ	2:J:302:VAL:HG12	2.36	0.48
2:L:242:LEU:HD12	2:L:242:LEU:HA	1.76	0.48
1:A:251:TRP:HB2	1:A:253:LYS:HG2	1.96	0.48
2:F:410:LEU:CD2	2:F:412:VAL:CG2	2.92	0.48
2:F:450:LEU:H	2:G:448:PRO:HD3	1.79	0.48
2:M:262:VAL:HG22	2:M:303:VAL:HG22	1.96	0.48
2:B:457:MET:HG3	2:M:457:MET:HB2	1.96	0.47
2:D:414:LYS:HB3	2:D:414:LYS:HE2	1.62	0.47
2:F:257:PRO:HG2	2:F:308:VAL:HG23	1.96	0.47
2:M:377:ILE:HD11	2:M:427:VAL:HG13	1.96	0.47
2:B:416:ARG:HE	2:B:416:ARG:HB3	1.54	0.47
2:K:284:VAL:HG12	2:K:286:ASN:H	1.79	0.47
2:K:381:TRP:NE1	2:K:410:LEU:HB2	2.30	0.47
1:A:57:TRP:CD1	1:A:75:LEU:HD13	2.49	0.47
1:A:103:ALA:HB3	1:A:106:ILE:HD11	1.97	0.47
1:A:187:GLU:HB3	2:C:342:GLN:HB3	1.97	0.47
2:M:273:VAL:HG23	2:M:323:VAL:HG13	1.97	0.47
2:D:453:VAL:HG21	2:G:455:LEU:HD21	1.97	0.47
2:M:314:LEU:HD13	2:M:338:LYS:HZ1	1.80	0.47
2:H:274:LYS:O	2:H:323:VAL:HA	2.15	0.47
2:I:348:VAL:HG22	2:I:369:VAL:HG13	1.97	0.47
2:F:363:VAL:HG21	2:F:417:TRP:CD1	2.50	0.46
2:H:248:LYS:O	2:H:252:MET:HG3	2.14	0.46
1:A:131:LEU:HD12	1:A:147:LYS:HD2	1.97	0.46
2:H:253:ILE:HA	2:H:310:HIS:HE1	1.80	0.46
2:J:263:VAL:HB	2:J:302:VAL:HB	1.97	0.46
2:J:276:ASN:HB2	2:J:322:LYS:HD3	1.98	0.46
2:B:256:THR:CG2	2:M:311:GLN:NE2	2.78	0.46
2:C:276:ASN:HB3	2:C:322:LYS:HB3	1.96	0.46
2:D:320:LYS:HD3	2:D:333:GLU:HB3	1.98	0.46
2:H:312:ASP:HA	2:H:317:LYS:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:HD23	1:A:67:LEU:HA	1.75	0.46
2:D:246:LYS:HG3	2:D:249:ASP:HB2	1.97	0.46
2:E:260:THR:HG22	2:E:305:VAL:HG22	1.97	0.46
2:M:364:SER:HB3	2:M:409:LYS:HG3	1.98	0.46
2:B:394:THR:HA	2:C:397:VAL:HG21	1.98	0.46
2:I:455:LEU:HB3	2:I:457:MET:SD	2.56	0.46
2:K:455:LEU:HG	2:K:457:MET:HG2	1.97	0.46
2:J:252:MET:HG2	2:J:254:SER:H	1.81	0.46
2:K:346:PRO:HB3	2:K:372:PHE:HB3	1.97	0.46
2:G:453:VAL:HA	2:H:453:VAL:HB	1.98	0.46
2:K:369:VAL:HB	2:K:406:LEU:HD23	1.96	0.45
2:E:443:LYS:HB3	2:E:443:LYS:HE2	1.73	0.45
2:F:264:VAL:HG12	2:F:301:ARG:HG2	1.97	0.45
2:F:273:VAL:HB	2:F:325:ASN:HD22	1.81	0.45
2:G:252:MET:HE1	2:G:254:SER:OG	2.16	0.45
2:D:420:GLY:HA2	2:D:443:LYS:HB3	1.97	0.45
2:I:340:LYS:HA	2:I:340:LYS:HD3	1.73	0.45
2:J:414:LYS:HE2	2:J:414:LYS:HB3	1.79	0.45
2:E:377:ILE:HD12	2:E:378:ALA:H	1.80	0.45
1:A:135:ILE:HD12	1:A:166:CYS:HB3	1.98	0.45
2:C:334:LYS:HD3	2:C:334:LYS:HA	1.78	0.45
2:D:393:THR:HG23	2:D:406:LEU:HD13	1.98	0.45
2:M:379:VAL:HG22	2:M:427:VAL:HG22	1.98	0.45
2:C:348:VAL:HG21	2:C:427:VAL:HG11	1.97	0.45
2:C:455:LEU:HD12	2:C:456:ILE:H	1.82	0.45
2:G:243:PHE:HB2	2:G:260:THR:HB	1.99	0.45
2:H:455:LEU:HB3	2:H:457:MET:SD	2.56	0.45
2:K:365:LEU:HD22	2:K:410:LEU:HD23	1.99	0.45
2:M:414:LYS:HB3	2:M:414:LYS:HE2	1.83	0.45
2:C:348:VAL:HG22	2:C:369:VAL:HG22	1.98	0.45
2:J:368:LEU:HD21	2:J:370:LYS:HB3	1.99	0.45
1:A:135:ILE:HG23	1:A:142:LEU:HB3	1.99	0.45
2:D:355:ARG:H	2:D:355:ARG:HG3	1.65	0.45
2:E:292:ARG:HA	2:E:302:VAL:HG22	1.97	0.45
2:H:338:LYS:HB2	2:H:338:LYS:HE2	1.78	0.45
2:K:414:LYS:HE2	2:K:414:LYS:HB2	1.79	0.45
2:F:325:ASN:HB3	2:F:328:LEU:HD23	1.97	0.44
2:J:436:TYR:HE1	2:J:438:GLN:HE21	1.64	0.44
2:M:248:LYS:HD2	2:M:255:ARG:HH12	1.82	0.44
2:F:308:VAL:HG11	2:F:319:TYR:CE2	2.52	0.44
2:J:343:PRO:HB2	2:J:431:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:369:VAL:HB	2:I:406:LEU:HD23	1.99	0.44
2:K:276:ASN:HB3	2:K:278:TYR:CE1	2.52	0.44
2:M:264:VAL:HG12	2:M:301:ARG:HG2	1.98	0.44
2:F:300:TYR:HD1	2:F:301:ARG:H	1.63	0.44
2:L:420:GLY:HA2	2:L:443:LYS:HG3	2.00	0.44
2:C:451:TYR:CD2	2:I:457:MET:HE3	2.53	0.44
2:B:340:LYS:HA	2:B:340:LYS:HD2	1.75	0.44
2:M:381:TRP:CE3	2:M:410:LEU:HD13	2.53	0.44
2:B:240:VAL:HG12	2:B:263:VAL:HG12	2.00	0.44
2:E:381:TRP:CH2	2:E:425:CYS:HB3	2.53	0.44
2:E:447:LYS:HA	2:E:447:LYS:HD2	1.85	0.44
2:L:369:VAL:HG12	2:L:372:PHE:CE2	2.53	0.44
2:B:305:VAL:O	2:B:305:VAL:HG13	2.18	0.44
2:B:378:ALA:HB3	2:B:428:MET:HE3	2.00	0.44
2:B:397:VAL:HG21	2:C:394:THR:HA	2.00	0.44
2:H:443:LYS:HB3	2:H:443:LYS:HE3	1.72	0.44
2:D:450:LEU:HB2	2:E:450:LEU:HD13	1.98	0.43
2:H:367:CYS:HB3	2:H:408:SER:OG	2.18	0.43
2:J:251:LEU:HD23	2:J:251:LEU:HA	1.72	0.43
2:L:240:VAL:HG23	2:L:332:ILE:HD12	2.00	0.43
2:L:381:TRP:HB2	2:L:388:GLU:HB2	1.99	0.43
2:M:290:LYS:HD2	2:M:290:LYS:HA	1.74	0.43
2:D:368:LEU:HD12	2:D:369:VAL:N	2.33	0.43
2:F:410:LEU:HD21	2:F:412:VAL:CG2	2.48	0.43
2:G:258:GLU:HB2	2:G:305:VAL:HG23	1.99	0.43
2:F:369:VAL:HG12	2:F:372:PHE:HD2	1.82	0.43
1:A:20:THR:HG22	1:A:22:ARG:HB2	2.00	0.43
1:A:29:PRO:HD2	1:A:40:VAL:HG23	1.99	0.43
2:E:315:ASN:HD21	2:E:317:LYS:NZ	2.16	0.43
2:E:381:TRP:CD1	2:E:410:LEU:HB2	2.54	0.43
2:H:340:LYS:HE3	2:H:340:LYS:HB2	1.88	0.43
2:K:265:ASP:HA	2:K:299:THR:HB	2.01	0.43
2:M:441:LEU:HA	2:M:441:LEU:HD23	1.71	0.43
2:D:278:TYR:HB2	2:D:320:LYS:HB3	2.00	0.43
2:D:287:ALA:HB2	2:D:306:LEU:HD13	1.99	0.43
2:G:336:ILE:HD12	2:G:336:ILE:HA	1.91	0.43
2:J:275:PHE:CZ	2:J:302:VAL:CG1	2.99	0.43
2:B:439:LYS:HA	2:B:439:LYS:HD2	1.79	0.43
2:F:246:LYS:O	2:F:250:THR:HG23	2.18	0.43
2:G:262:VAL:HG13	2:G:303:VAL:HG22	2.00	0.43
2:I:238:PRO:HB3	2:I:266:VAL:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:242:LEU:HD22	2:L:334:LYS:HB2	1.99	0.43
2:L:249:ASP:OD1	2:L:255:ARG:HB3	2.18	0.43
2:L:277:TRP:CH2	2:L:321:CYS:HB2	2.54	0.43
2:B:295:GLN:NE2	2:B:301:ARG:HB3	2.33	0.43
2:C:412:VAL:HG21	2:C:423:PHE:CZ	2.53	0.43
2:G:367:CYS:HB2	2:G:381:TRP:CZ2	2.54	0.43
2:I:278:TYR:HB2	2:I:320:LYS:HB3	2.00	0.43
2:I:355:ARG:HA	2:I:358:LEU:HD23	2.00	0.43
2:J:346:PRO:HB3	2:J:372:PHE:HB3	2.00	0.43
2:B:355:ARG:HA	2:B:358:LEU:HD12	2.01	0.43
2:F:247:PRO:HG3	2:F:376:ASP:HB2	2.01	0.43
2:G:262:VAL:HG11	2:G:301:ARG:CZ	2.49	0.43
2:C:260:THR:HG22	2:C:305:VAL:HG22	2.01	0.42
2:G:350:THR:HG22	2:G:367:CYS:SG	2.59	0.42
2:H:250:THR:HG23	2:H:251:LEU:HD23	2.01	0.42
2:H:263:VAL:HG11	2:H:323:VAL:HG11	2.00	0.42
2:J:394:THR:HA	2:K:397:VAL:HG21	1.99	0.42
2:J:442:ASP:H	2:J:445:THR:HG21	1.84	0.42
2:K:447:LYS:H	2:K:447:LYS:HG3	1.74	0.42
2:B:309:CYS:HB2	2:M:309:CYS:HB3	1.82	0.42
2:C:268:HIS:HA	2:C:300:TYR:HE2	1.83	0.42
2:E:451:TYR:HE2	2:F:455:LEU:HD13	1.84	0.42
2:C:328:LEU:HA	2:C:328:LEU:HD23	1.82	0.42
2:D:262:VAL:HA	2:D:303:VAL:HG22	2.02	0.42
2:E:422:VAL:HA	2:E:442:ASP:HB3	2.02	0.42
2:G:273:VAL:HG13	2:G:323:VAL:HG13	2.01	0.42
2:B:456:ILE:HA	2:C:456:ILE:HB	2.01	0.42
2:E:381:TRP:HD1	2:E:391:TYR:CG	2.38	0.42
2:J:347:GLN:OE1	2:J:347:GLN:HA	2.20	0.42
1:A:107:LEU:HD22	1:A:165:ARG:HA	2.01	0.42
1:A:215:LEU:HG	1:A:224:LEU:HD11	2.01	0.42
2:F:244:PRO:HB3	2:F:336:ILE:HD11	2.02	0.42
2:L:451:TYR:O	2:M:451:TYR:HA	2.19	0.42
2:M:374:PRO:HG2	2:M:376:ASP:OD1	2.20	0.42
2:E:246:LYS:HB2	2:E:249:ASP:CG	2.44	0.42
2:L:252:MET:HG2	2:L:255:ARG:HG3	2.02	0.42
2:M:391:TYR:HB3	2:M:410:LEU:HD12	2.02	0.42
2:C:368:LEU:HD21	2:C:370:LYS:HB3	2.02	0.42
2:D:452:ASN:HB3	4:E:700:NAG:H5	2.01	0.42
2:H:334:LYS:HD3	2:H:334:LYS:HA	1.70	0.42
2:H:394:THR:HA	2:I:397:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:290:LYS:HE2	2:J:290:LYS:HB2	1.95	0.42
1:A:85:CYS:H	1:A:93:SER:HB3	1.85	0.42
2:B:427:VAL:O	2:B:427:VAL:HG13	2.19	0.42
2:E:240:VAL:HG23	2:E:332:ILE:HD11	2.01	0.42
2:E:267:SER:HB2	2:E:269:GLU:OE1	2.19	0.42
2:K:278:TYR:HB2	2:K:320:LYS:HE3	2.01	0.42
2:C:248:LYS:H	2:C:248:LYS:HG3	1.62	0.41
2:G:238:PRO:HG2	2:G:328:LEU:HG	2.02	0.41
2:H:357:GLU:HB3	2:H:363:VAL:HG12	2.02	0.41
2:I:257:PRO:HD3	2:I:310:HIS:NE2	2.35	0.41
2:L:270:ASP:OD2	2:L:327:ALA:HB2	2.20	0.41
2:M:375:SER:HB3	2:M:404:PHE:CD2	2.55	0.41
1:A:23:PRO:HG2	1:A:93:SER:HB2	2.02	0.41
2:C:264:VAL:HG12	2:C:301:ARG:HG2	2.02	0.41
2:E:322:LYS:HA	2:E:333:GLU:HG2	2.02	0.41
2:F:262:VAL:HG13	2:F:301:ARG:HD3	2.01	0.41
2:J:346:PRO:HG3	2:J:429:HIS:HB3	2.02	0.41
2:L:381:TRP:CE2	2:L:410:LEU:HB2	2.55	0.41
2:C:442:ASP:H	2:C:445:THR:HG23	1.85	0.41
2:M:293:GLU:HG2	2:M:301:ARG:O	2.20	0.41
2:H:262:VAL:HG22	2:H:303:VAL:HG12	2.02	0.41
2:I:358:LEU:HD13	2:I:358:LEU:HA	1.95	0.41
2:K:242:LEU:HD12	2:K:242:LEU:HA	1.81	0.41
2:C:320:LYS:HE3	2:C:333:GLU:HB3	2.02	0.41
2:D:252:MET:HE2	2:D:255:ARG:HG3	2.01	0.41
2:F:415:SER:O	2:F:419:GLN:HG3	2.21	0.41
2:D:274:LYS:HB3	2:D:324:SER:HB2	2.02	0.41
2:D:292:ARG:HD2	2:D:300:TYR:HB3	2.02	0.41
2:L:273:VAL:HG23	2:L:325:ASN:HB2	2.02	0.41
2:F:262:VAL:HG22	2:F:303:VAL:HG23	2.01	0.41
2:F:356:ASP:HB2	2:G:349:TYR:HD1	1.85	0.41
2:F:365:LEU:HD13	2:F:365:LEU:HA	1.93	0.41
2:I:372:PHE:CE1	2:I:404:PHE:HB2	2.56	0.41
2:L:346:PRO:HB3	2:L:372:PHE:HB3	2.02	0.41
2:D:344:ARG:NH1	2:D:403:SER:HB3	2.36	0.41
2:E:252:MET:HE2	2:E:255:ARG:HG2	2.02	0.41
2:E:277:TRP:HZ2	2:E:304:SER:HB3	1.85	0.41
2:E:326:LYS:HB3	2:E:326:LYS:HE3	1.93	0.41
2:G:432:LEU:HD22	2:G:437:THR:HB	2.03	0.41
2:D:246:LYS:H	2:D:246:LYS:HG2	1.64	0.41
2:G:414:LYS:HB3	2:G:414:LYS:HE2	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:432:LEU:HD12	2:I:432:LEU:HA	1.82	0.41
2:J:257:PRO:HD3	2:J:310:HIS:HE1	1.84	0.41
2:K:381:TRP:CE2	2:K:410:LEU:HB2	2.56	0.41
2:K:417:TRP:CH2	2:K:443:LYS:HA	2.56	0.41
2:L:248:LYS:HB2	2:L:378:ALA:HB3	2.01	0.41
2:M:258:GLU:HB2	2:M:305:VAL:HG13	2.03	0.41
2:B:432:LEU:HD23	2:B:432:LEU:HA	1.88	0.41
2:C:259:VAL:HG13	2:C:277:TRP:HZ3	1.85	0.41
2:I:257:PRO:HD3	2:I:310:HIS:CE1	2.56	0.41
1:A:227:ARG:HB2	1:A:239:TRP:CE3	2.55	0.40
1:A:255:SER:HB3	1:A:280:VAL:HG23	2.02	0.40
2:B:409:LYS:HB2	2:C:407:TYR:OH	2.21	0.40
2:E:319:TYR:HB2	2:E:336:ILE:O	2.21	0.40
2:J:336:ILE:HD12	2:J:336:ILE:HA	1.88	0.40
2:J:377:ILE:HG12	2:J:429:HIS:HB2	2.03	0.40
2:M:292:ARG:HD2	2:M:300:TYR:CG	2.55	0.40
2:B:453:VAL:O	2:C:453:VAL:HA	2.22	0.40
2:E:252:MET:HE2	2:E:252:MET:HB3	1.93	0.40
2:E:417:TRP:CH2	2:E:443:LYS:HA	2.56	0.40
2:L:370:LYS:HA	2:L:405:PHE:HB2	2.01	0.40
2:B:338:LYS:HE3	2:B:338:LYS:HB3	1.76	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	262/860 (30%)	246 (94%)	16 (6%)	0	100	100
2	B	219/250 (88%)	207 (94%)	12 (6%)	0	100	100
2	C	219/250 (88%)	214 (98%)	5 (2%)	0	100	100
2	D	219/250 (88%)	211 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	219/250 (88%)	208 (95%)	11 (5%)	0	100	100
2	F	219/250 (88%)	211 (96%)	8 (4%)	0	100	100
2	G	219/250 (88%)	208 (95%)	11 (5%)	0	100	100
2	H	219/250 (88%)	209 (95%)	10 (5%)	0	100	100
2	I	219/250 (88%)	211 (96%)	8 (4%)	0	100	100
2	J	219/250 (88%)	213 (97%)	6 (3%)	0	100	100
2	K	219/250 (88%)	209 (95%)	10 (5%)	0	100	100
2	L	219/250 (88%)	207 (94%)	12 (6%)	0	100	100
2	M	219/250 (88%)	214 (98%)	5 (2%)	0	100	100
All	All	2890/3860 (75%)	2768 (96%)	122 (4%)	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	240/740 (32%)	238 (99%)	2 (1%)	79	89
2	B	206/231 (89%)	204 (99%)	2 (1%)	73	85
2	C	206/231 (89%)	205 (100%)	1 (0%)	86	93
2	D	206/231 (89%)	204 (99%)	2 (1%)	73	85
2	E	206/231 (89%)	204 (99%)	2 (1%)	73	85
2	F	206/231 (89%)	204 (99%)	2 (1%)	73	85
2	G	206/231 (89%)	204 (99%)	2 (1%)	73	85
2	H	206/231 (89%)	204 (99%)	2 (1%)	73	85
2	I	206/231 (89%)	205 (100%)	1 (0%)	86	93
2	J	206/231 (89%)	203 (98%)	3 (2%)	60	78
2	K	206/231 (89%)	205 (100%)	1 (0%)	86	93
2	L	206/231 (89%)	205 (100%)	1 (0%)	86	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	206/231 (89%)	204 (99%)	2 (1%)	73	85
All	All	2712/3512 (77%)	2689 (99%)	23 (1%)	77	89

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	117	ASP
2	B	365	LEU
2	B	441	LEU
2	C	365	LEU
2	D	268	HIS
2	D	410	LEU
2	E	442	ASP
2	E	443	LYS
2	F	340	LYS
2	F	457	MET
2	G	441	LEU
2	G	453	VAL
2	H	312	ASP
2	H	314	LEU
2	I	252	MET
2	J	252	MET
2	J	406	LEU
2	J	428	MET
2	K	447	LYS
2	L	253	ILE
2	M	314	LEU
2	M	428	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
2	C	362	GLN
2	D	276	ASN
2	D	325	ASN
2	D	386	GLN
2	D	418	GLN
2	E	268	HIS
2	E	286	ASN

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Mol	Chain	Res	Type
2	E	315	ASN
2	E	325	ASN
2	F	311	GLN
2	F	347	GLN
2	G	435	HIS
2	H	325	ASN
2	I	362	GLN
2	J	435	HIS
2	K	347	GLN
2	K	362	GLN
2	K	386	GLN
2	K	434	ASN
2	L	315	ASN
2	L	362	GLN
2	L	419	GLN
2	M	295	GLN
2	M	311	GLN
2	M	435	HIS

### 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 ⓘ

6 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	$\# Z  > 2$
3	NAG	N	1	2,3	14,14,15	0.77	0	17,19,21	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	N	2	3	14,14,15	0.80	0	17,19,21	0.97	0
3	BMA	N	3	3	11,11,12	0.84	0	15,15,17	2.62	5 (33%)
3	MAN	N	4	3	11,11,12	0.80	0	15,15,17	1.02	1 (6%)
3	NAG	N	5	3	14,14,15	0.74	0	17,19,21	0.87	1 (5%)
3	FUC	N	6	3	10,10,11	0.87	1 (10%)	14,14,16	1.07	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
3	NAG	N	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	BMA	N	3	3	-	0/2/19/22	0/1/1/1
3	MAN	N	4	3	-	2/2/19/22	0/1/1/1
3	NAG	N	5	3	-	0/6/23/26	0/1/1/1
3	FUC	N	6	3	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	6	FUC	O5-C1	-2.01	1.40	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	3	BMA	C1-O5-C5	7.90	122.90	112.19
3	N	3	BMA	C3-C4-C5	2.91	115.42	110.24
3	N	3	BMA	O4-C4-C3	-2.80	103.88	110.35
3	N	4	MAN	C1-O5-C5	2.47	115.54	112.19
3	N	3	BMA	C2-C3-C4	2.46	115.15	110.89
3	N	3	BMA	O3-C3-C2	-2.30	105.59	109.99
3	N	5	NAG	O5-C1-C2	-2.08	108.01	111.29

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	N	4	MAN	O5-C5-C6-O6

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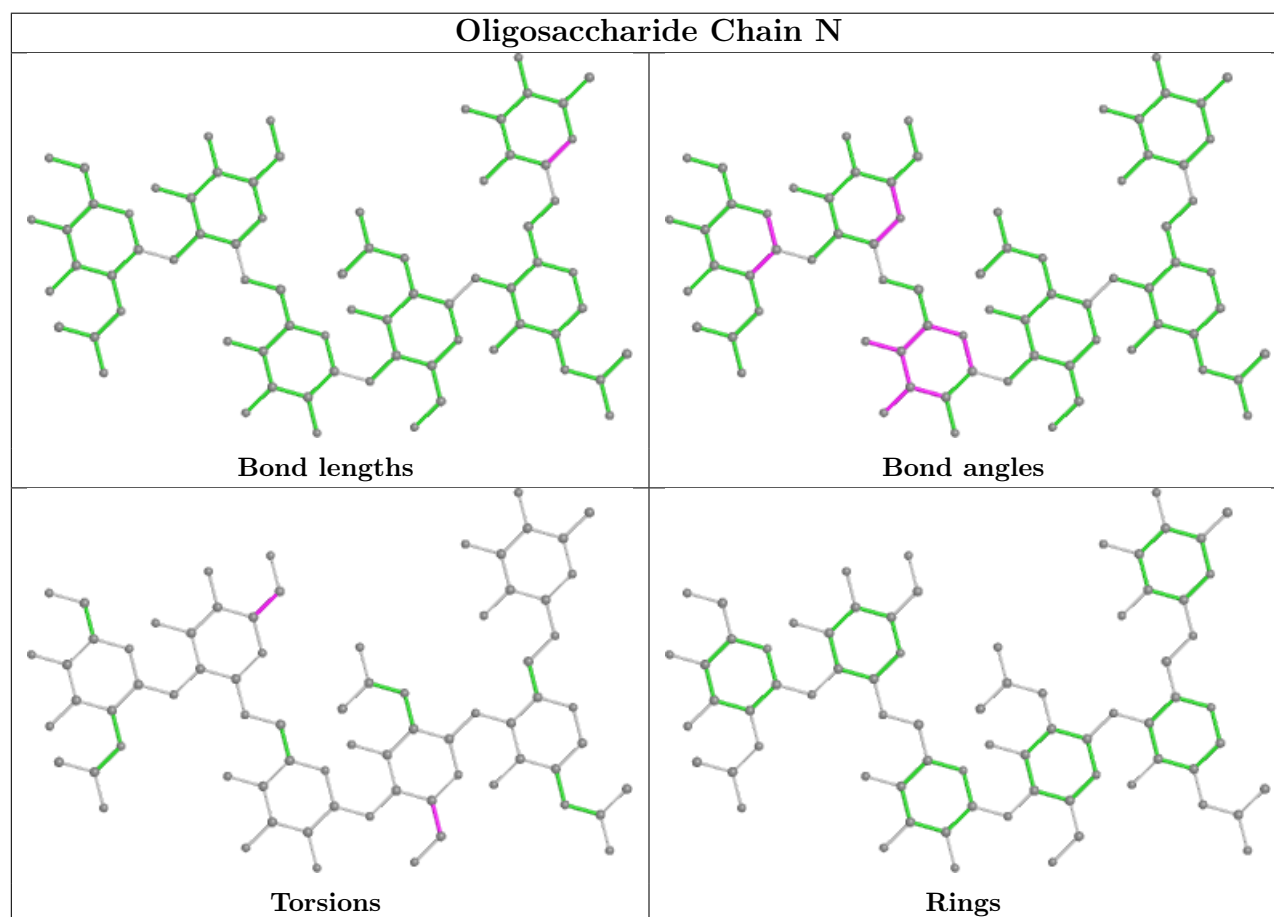
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Mol	Chain	Res	Type	Atoms
3	N	4	MAN	C4-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6

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](#)

13 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	$\# Z  > 2$
4	NAG	D	700	2	14,14,15	0.74	0	17,19,21	1.12	1 (5%)
4	NAG	E	700	2	14,14,15	0.73	0	17,19,21	0.88	0
4	NAG	G	700	2	14,14,15	0.72	0	17,19,21	0.76	0
4	NAG	K	700	2	14,14,15	0.73	0	17,19,21	0.95	1 (5%)
4	NAG	B	700	2	14,14,15	0.71	0	17,19,21	0.82	0
4	NAG	J	700	2	14,14,15	0.75	0	17,19,21	0.93	1 (5%)
4	NAG	H	700	2	14,14,15	0.74	0	17,19,21	0.92	1 (5%)
4	NAG	L	700	2	14,14,15	0.72	0	17,19,21	0.86	0
4	NAG	M	700	2	14,14,15	0.73	0	17,19,21	0.89	0
4	NAG	A	901	1	14,14,15	0.75	0	17,19,21	0.86	0
4	NAG	F	700	2	14,14,15	0.72	0	17,19,21	0.87	0
4	NAG	I	700	2	14,14,15	0.72	0	17,19,21	0.97	1 (5%)
4	NAG	C	700	2	14,14,15	0.74	0	17,19,21	0.80	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
4	NAG	D	700	2	-	0/6/23/26	0/1/1/1
4	NAG	E	700	2	-	0/6/23/26	0/1/1/1
4	NAG	G	700	2	-	0/6/23/26	0/1/1/1
4	NAG	K	700	2	-	3/6/23/26	0/1/1/1
4	NAG	B	700	2	-	2/6/23/26	0/1/1/1
4	NAG	J	700	2	-	0/6/23/26	0/1/1/1
4	NAG	H	700	2	-	3/6/23/26	0/1/1/1
4	NAG	L	700	2	-	2/6/23/26	0/1/1/1
4	NAG	M	700	2	-	2/6/23/26	0/1/1/1
4	NAG	A	901	1	-	0/6/23/26	0/1/1/1
4	NAG	F	700	2	-	0/6/23/26	0/1/1/1
4	NAG	I	700	2	-	2/6/23/26	0/1/1/1
4	NAG	C	700	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	700	NAG	C1-O5-C5	2.81	116.01	112.19
4	K	700	NAG	C2-N2-C7	2.48	126.44	122.90
4	I	700	NAG	C2-N2-C7	2.46	126.41	122.90
4	J	700	NAG	C1-O5-C5	2.23	115.22	112.19
4	H	700	NAG	C2-N2-C7	2.05	125.82	122.90

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	700	NAG	C8-C7-N2-C2
4	H	700	NAG	O7-C7-N2-C2
4	I	700	NAG	C8-C7-N2-C2
4	I	700	NAG	O7-C7-N2-C2
4	K	700	NAG	C8-C7-N2-C2
4	K	700	NAG	O7-C7-N2-C2
4	M	700	NAG	C8-C7-N2-C2
4	M	700	NAG	O7-C7-N2-C2
4	L	700	NAG	O5-C5-C6-O6
4	K	700	NAG	O5-C5-C6-O6
4	B	700	NAG	C4-C5-C6-O6
4	H	700	NAG	O5-C5-C6-O6
4	L	700	NAG	C4-C5-C6-O6
4	B	700	NAG	O5-C5-C6-O6

There are no ring outliers.

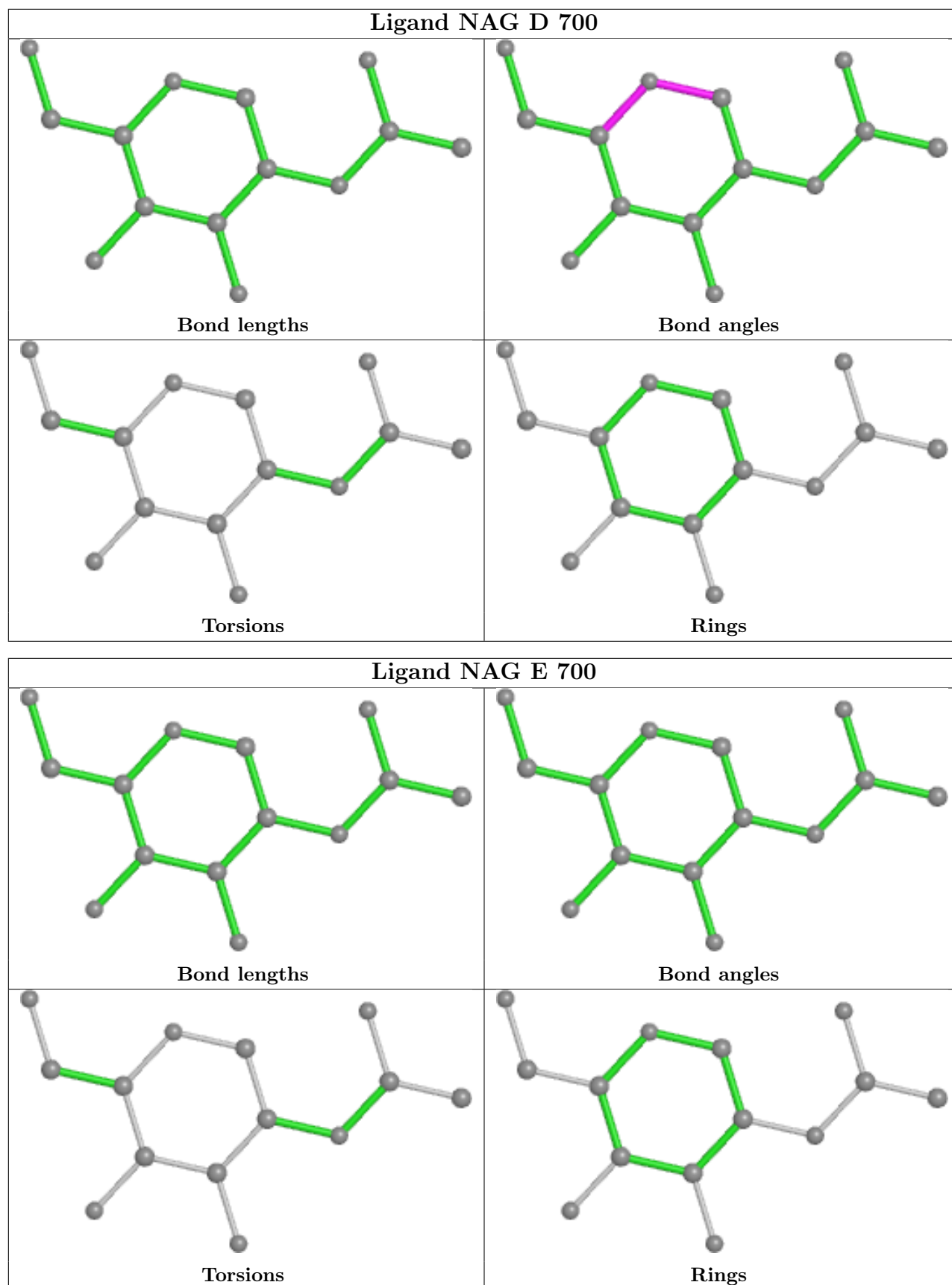
2 monomers are involved in 2 short contacts:

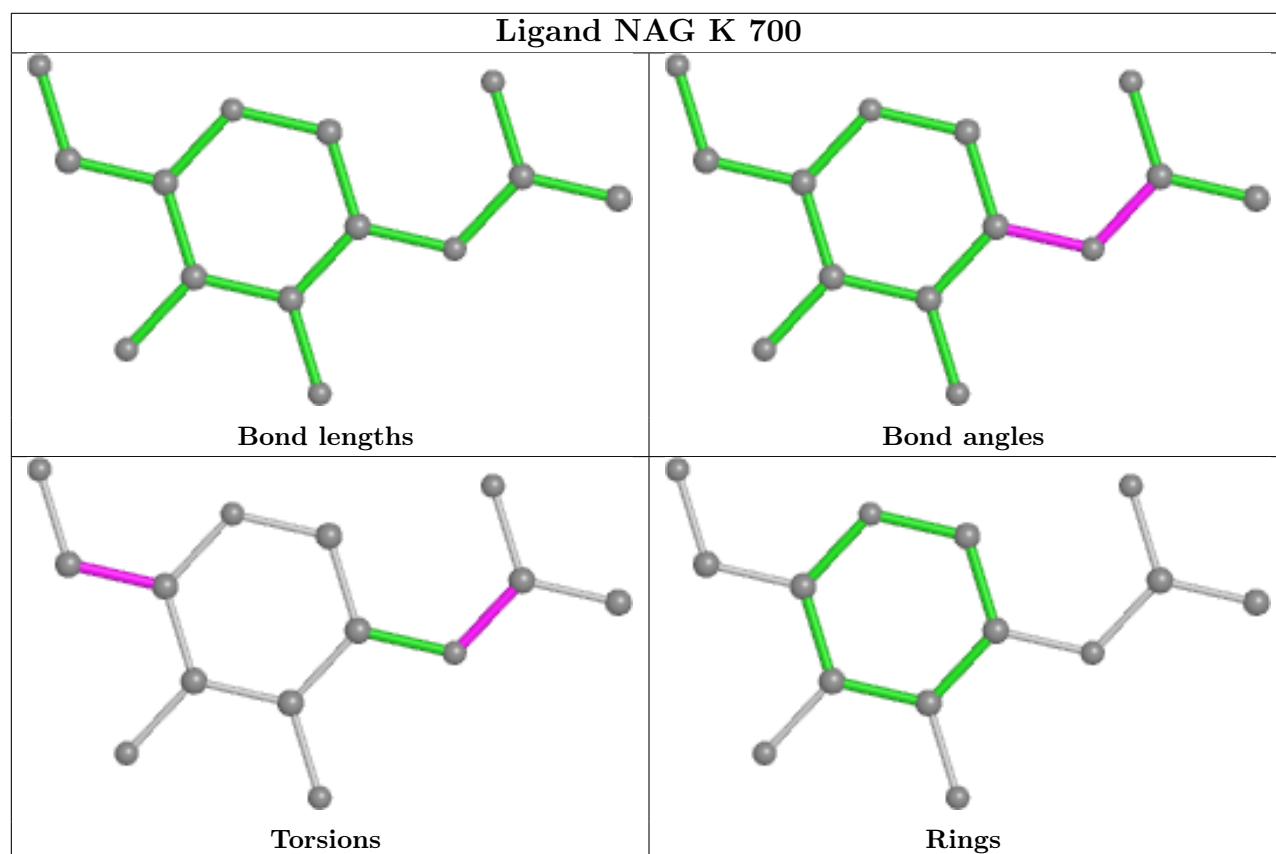
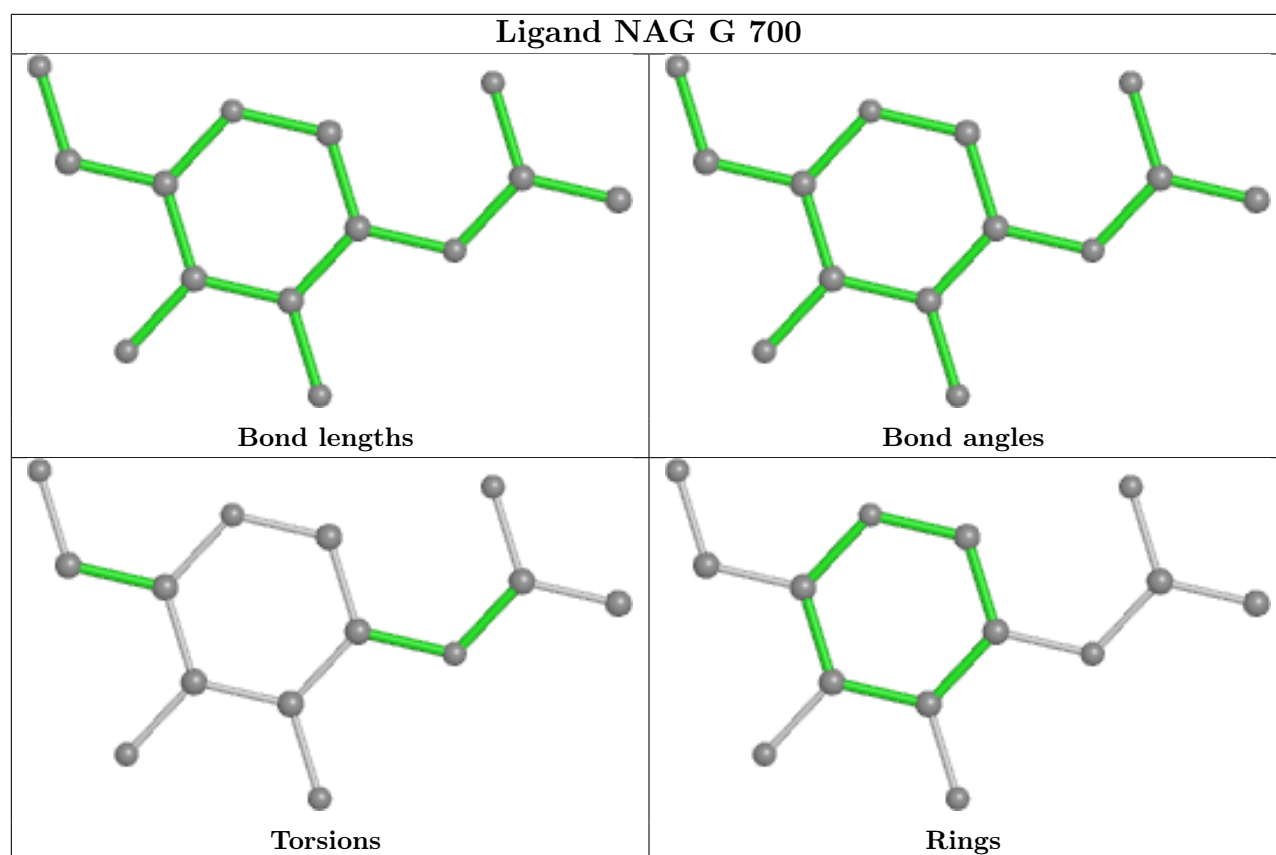
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	700	NAG	1	0
4	I	700	NAG	1	0

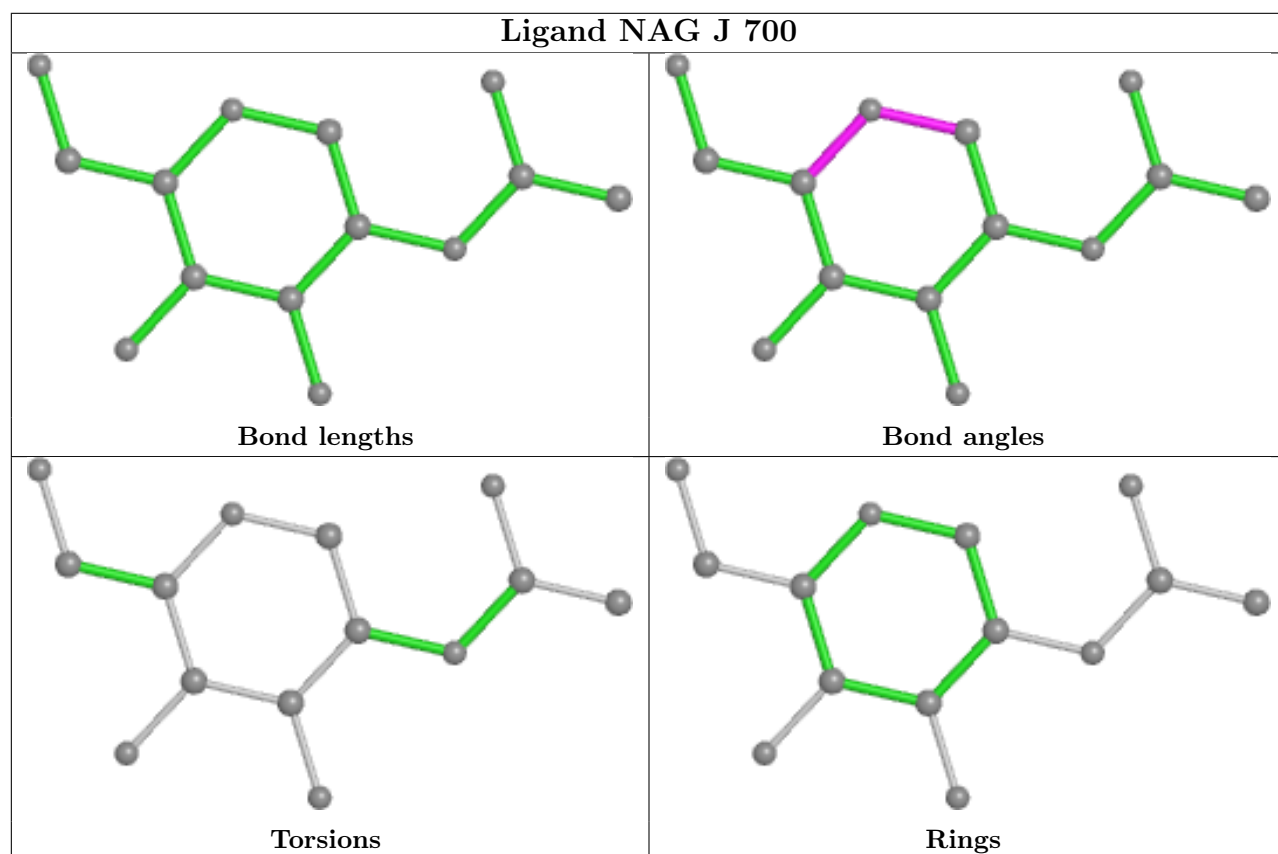
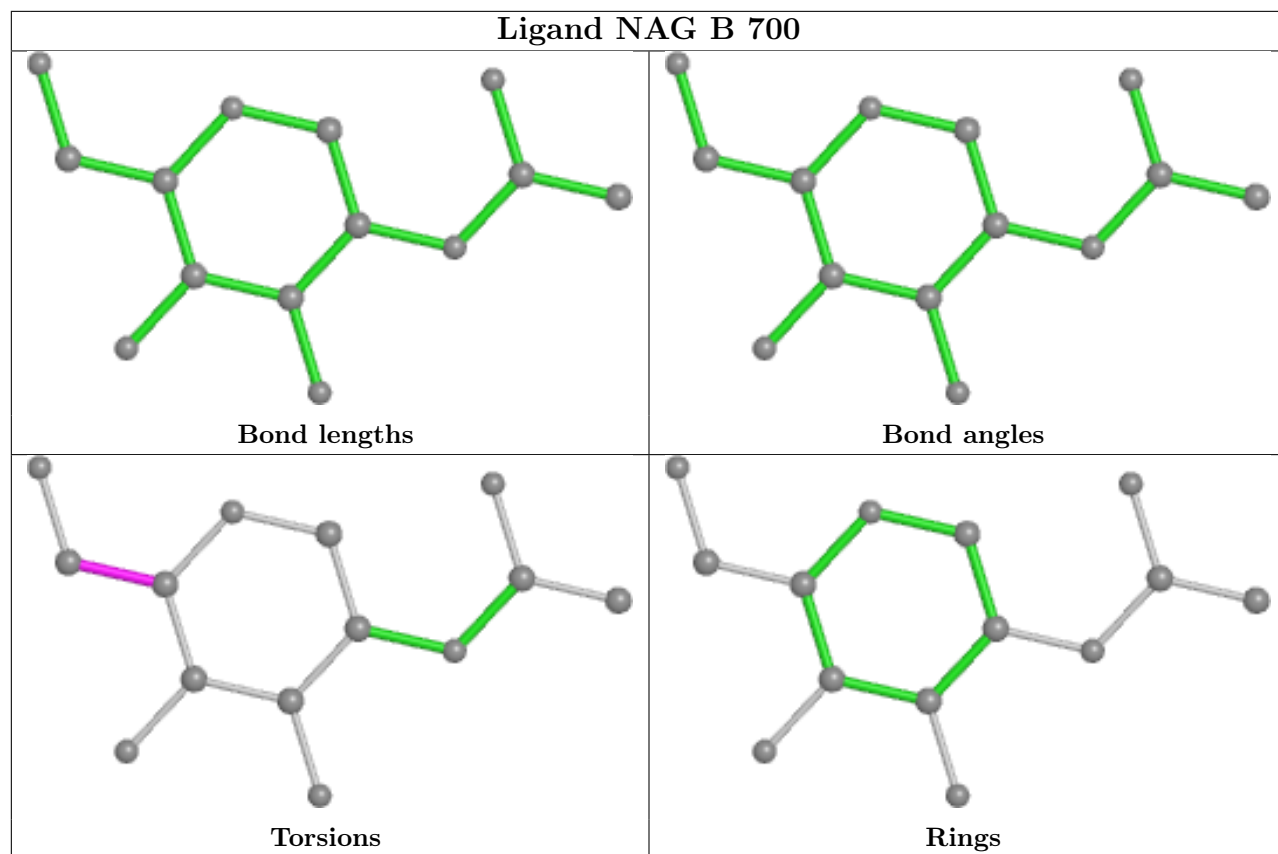
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

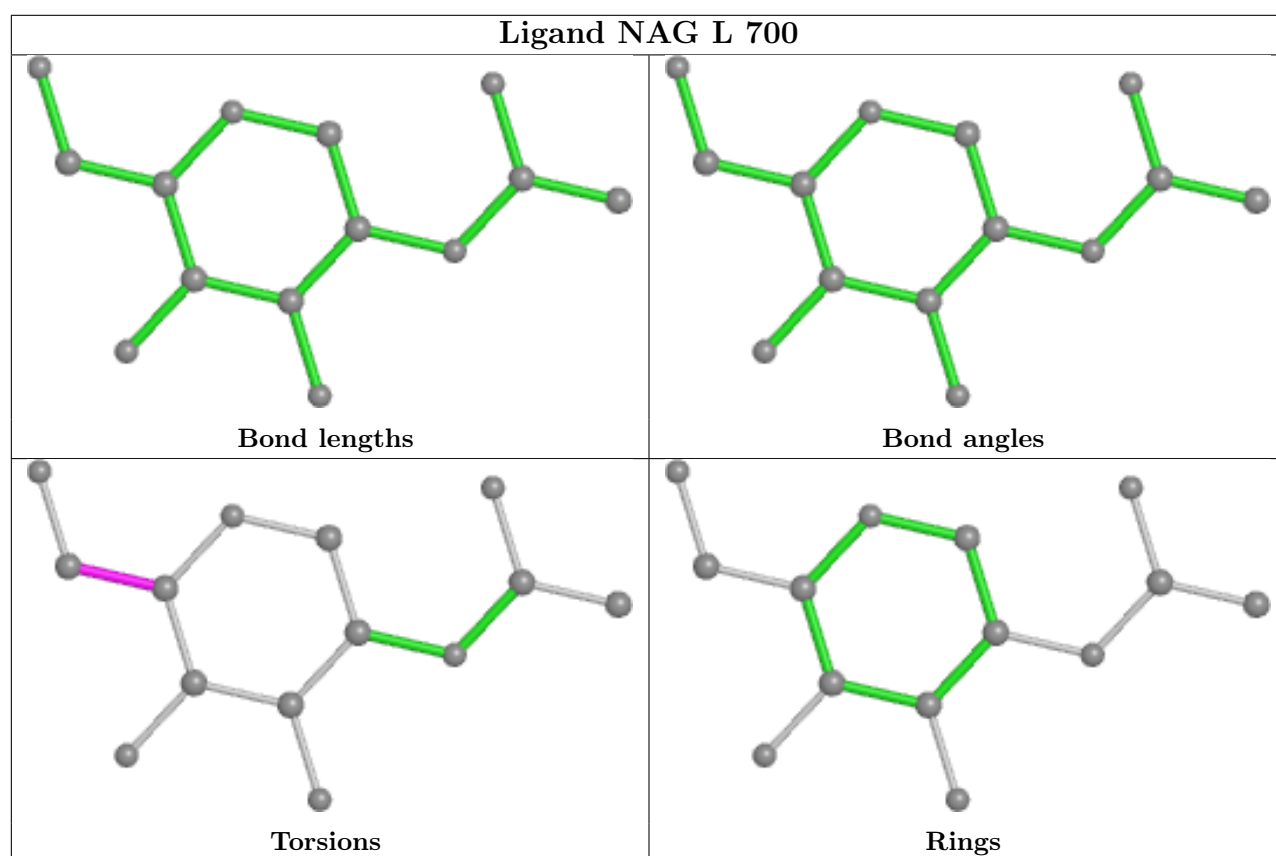
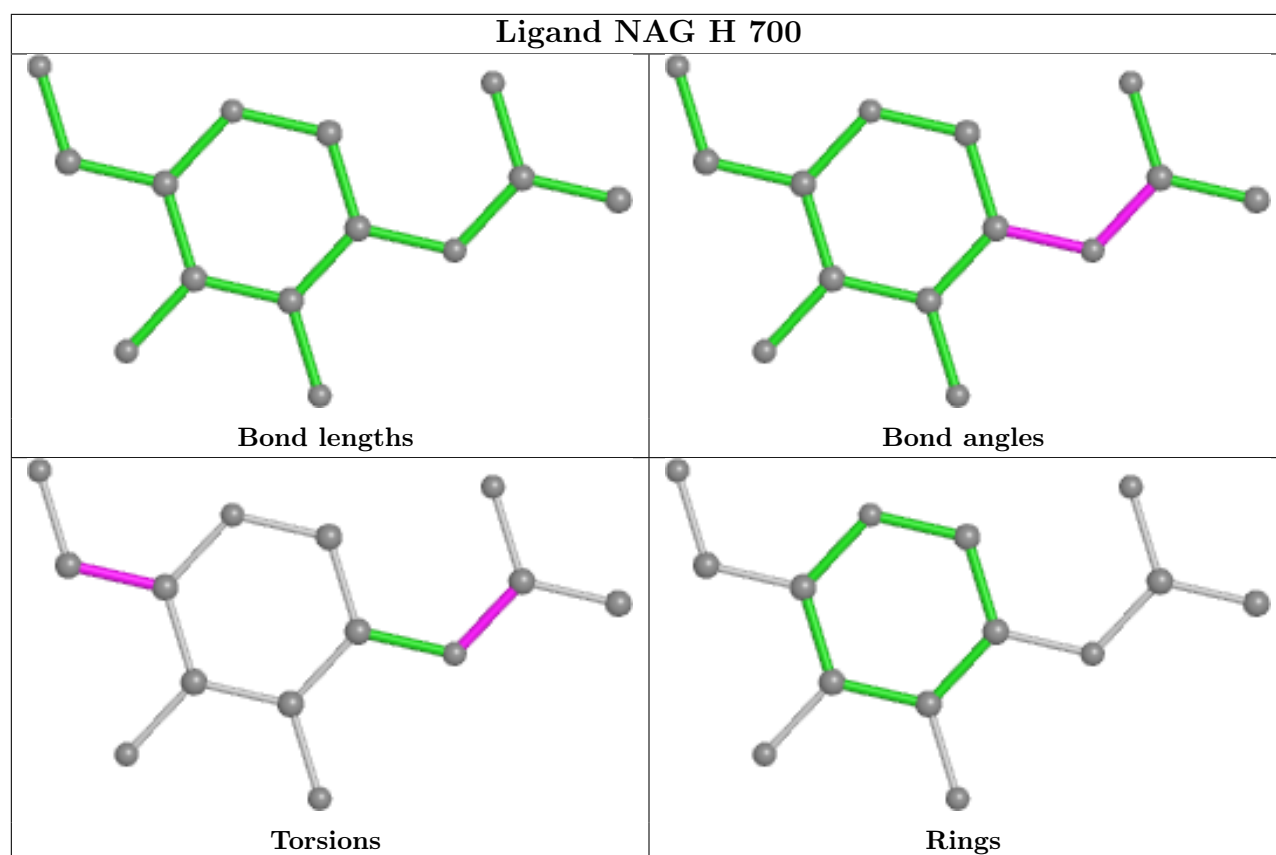


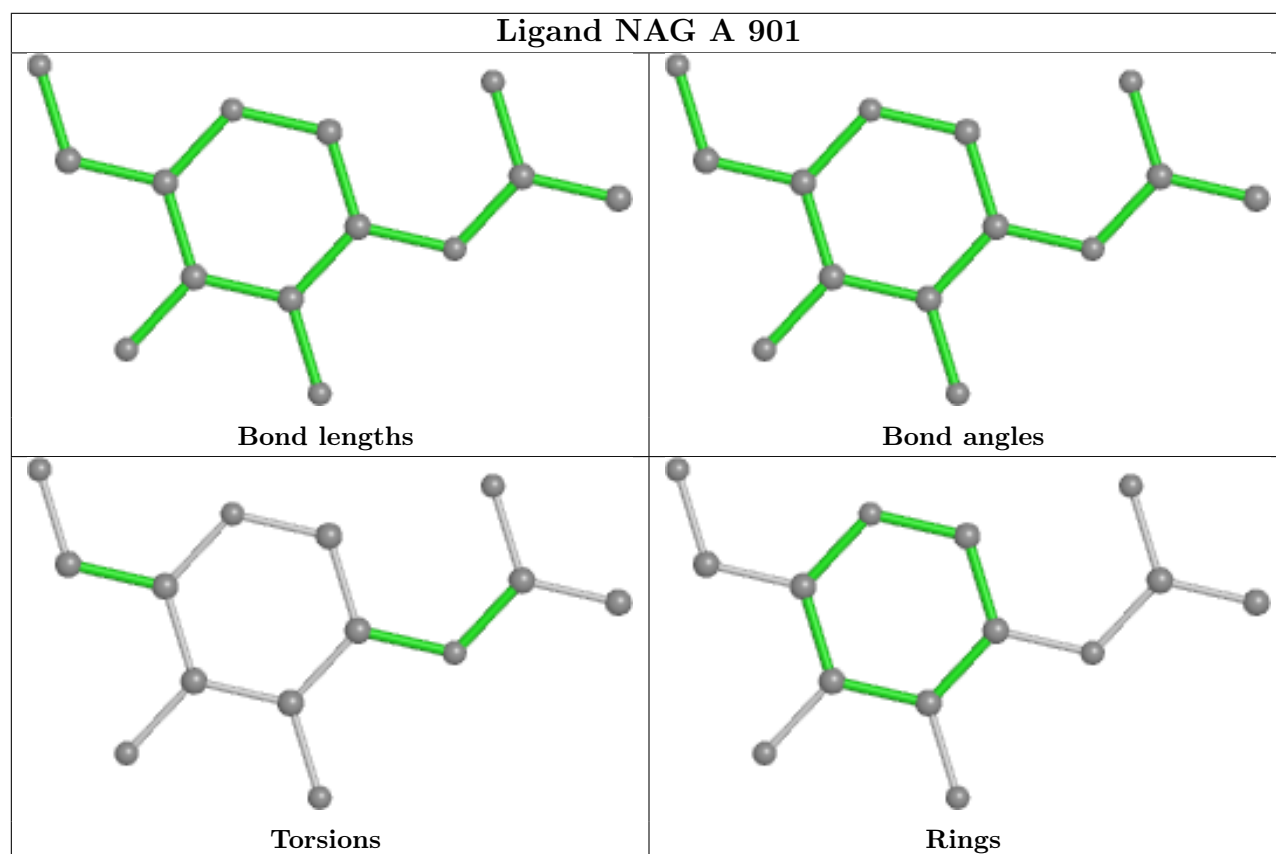
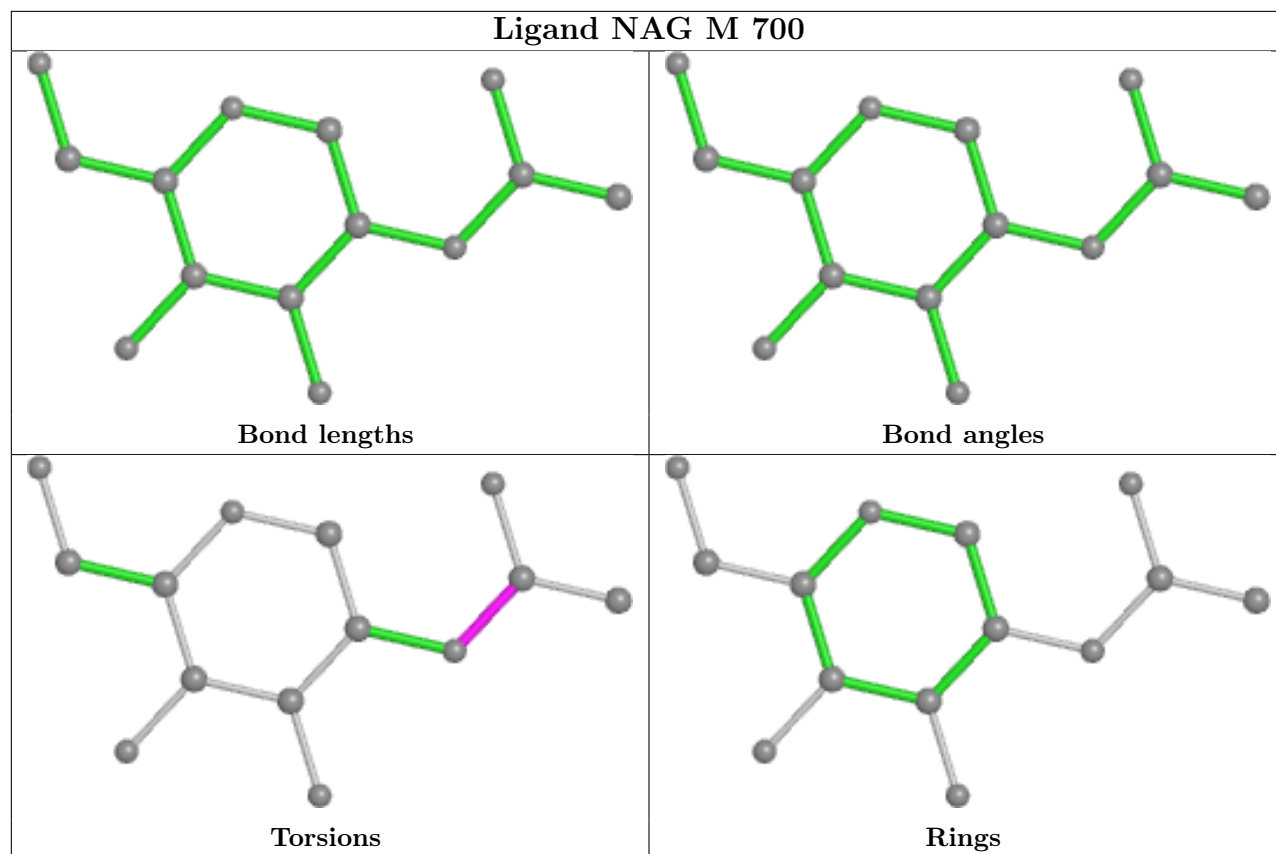
equivalents in the CSD to analyse the geometry.

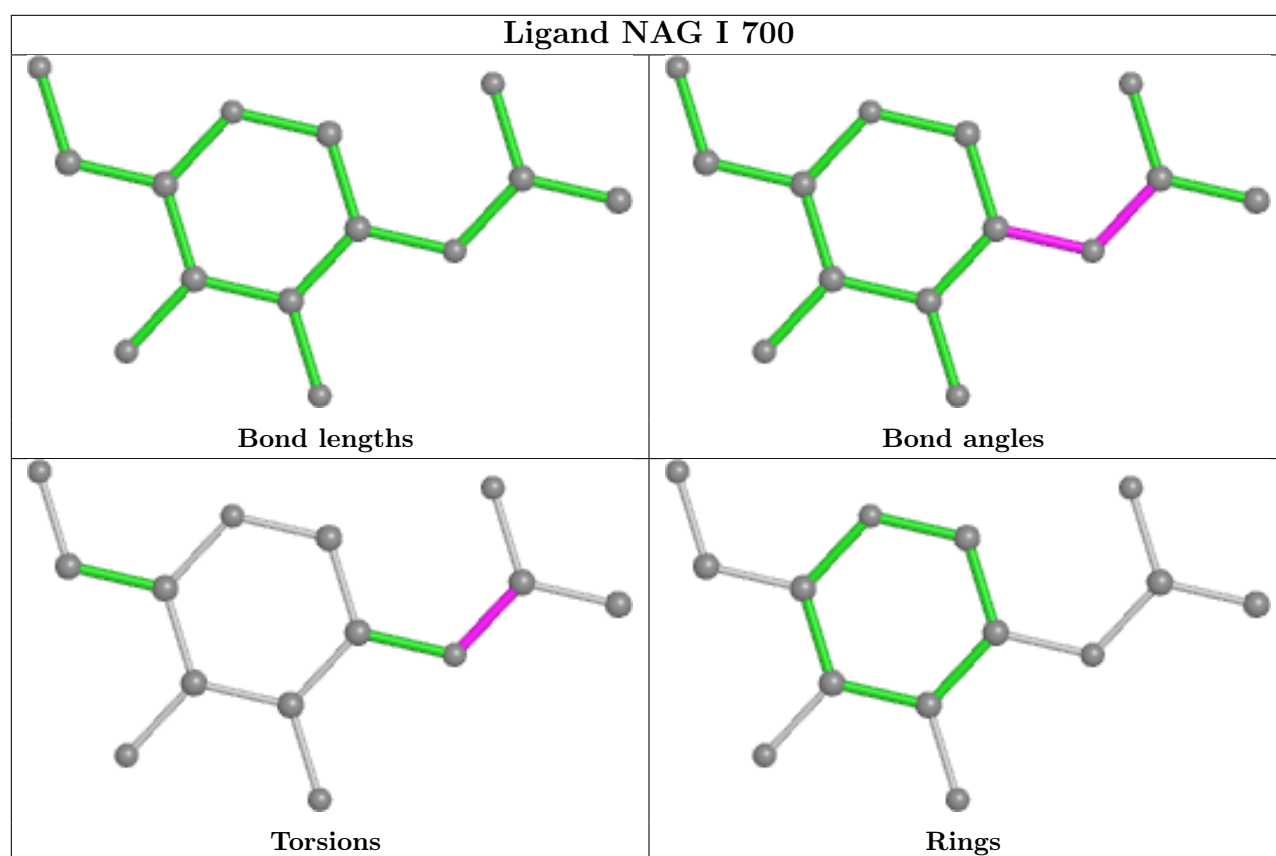
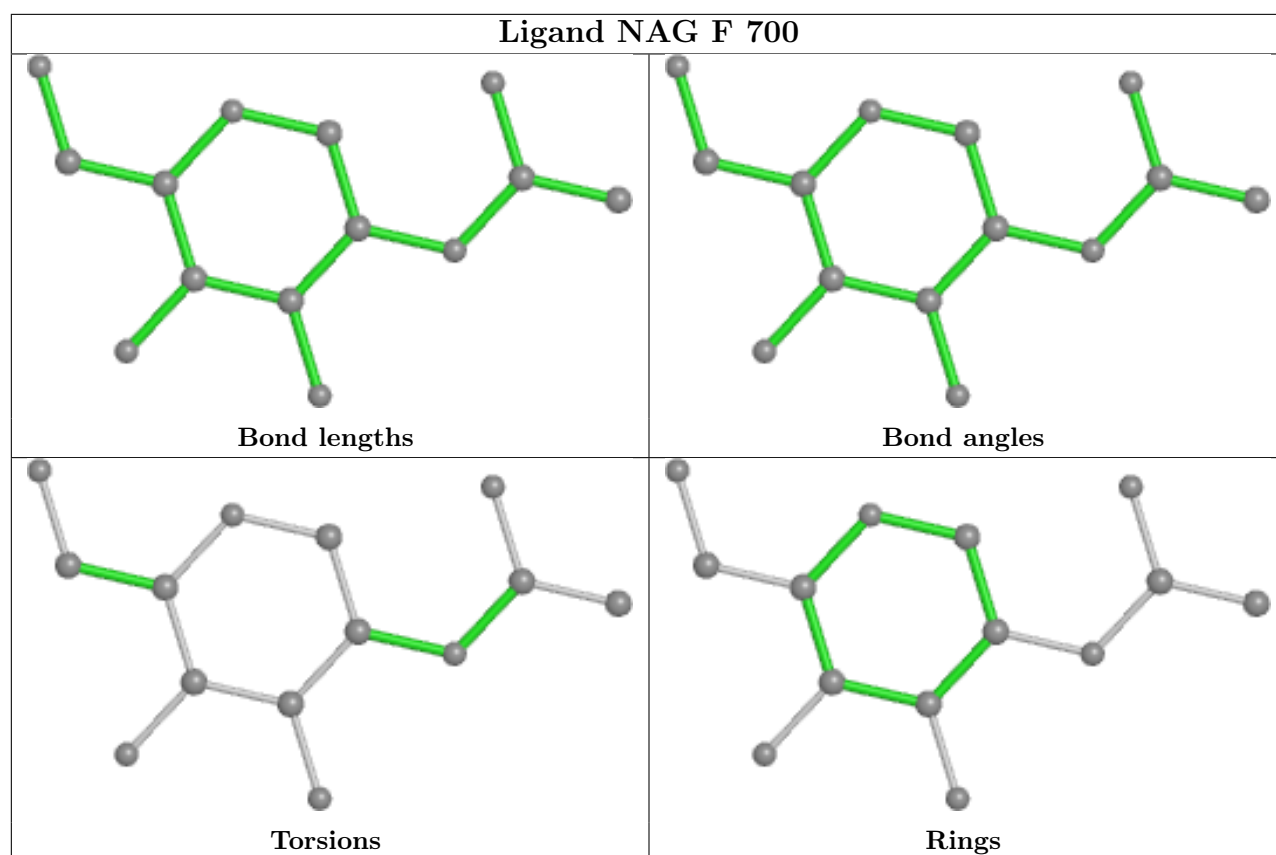


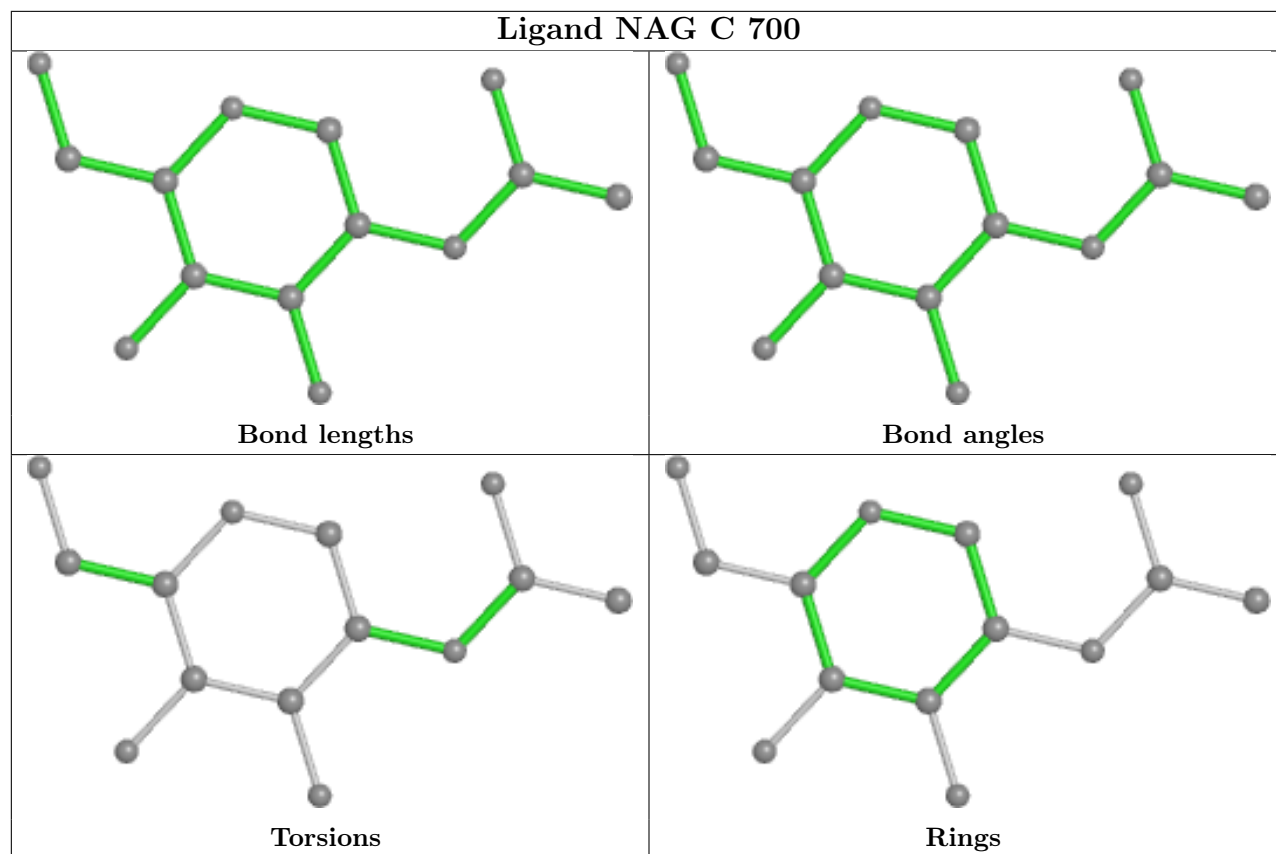












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

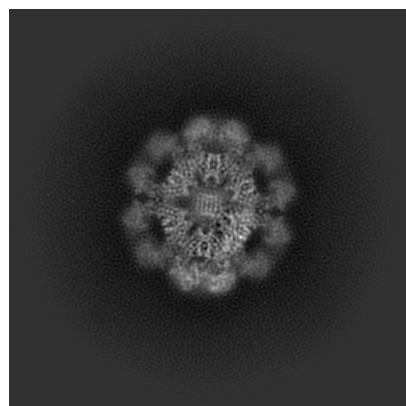
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63244. These allow visual inspection of the internal detail of the map and identification of artifacts.

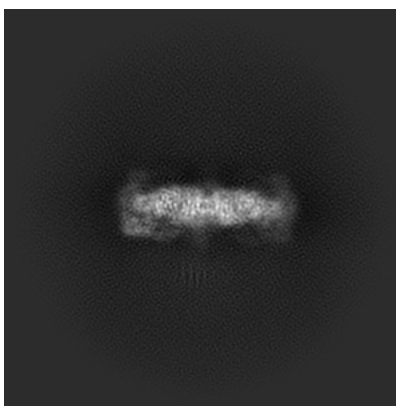
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

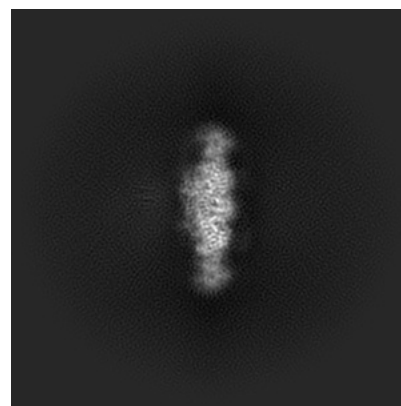
#### 6.1.1 Primary map



X

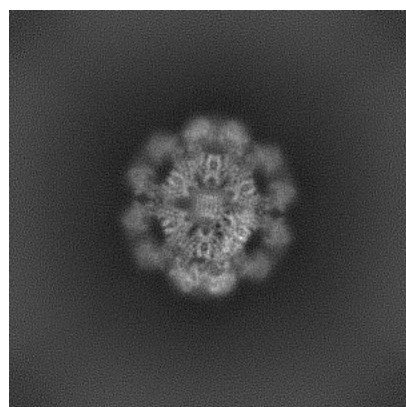


Y

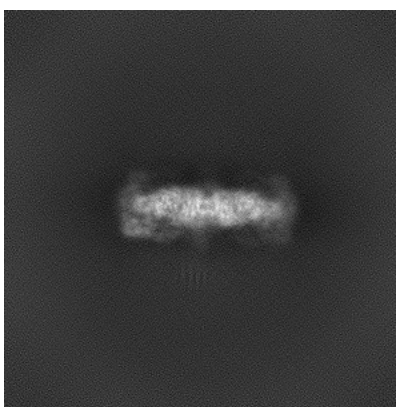


Z

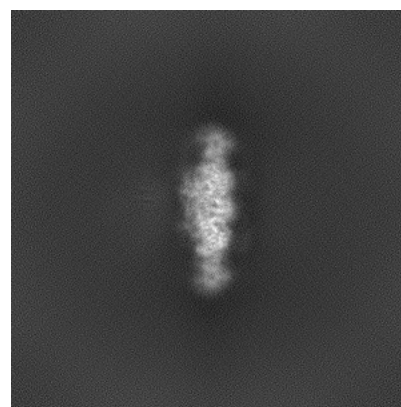
#### 6.1.2 Raw map



X



Y



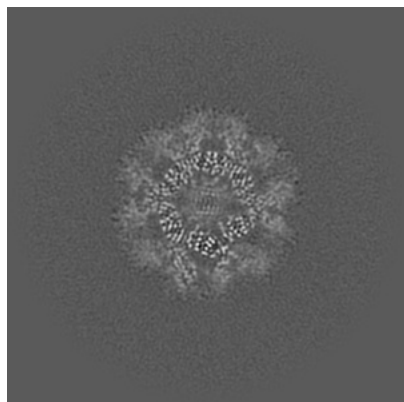
Z

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

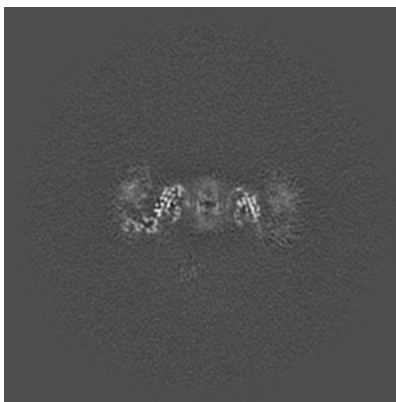


## 6.2 Central slices [i](#)

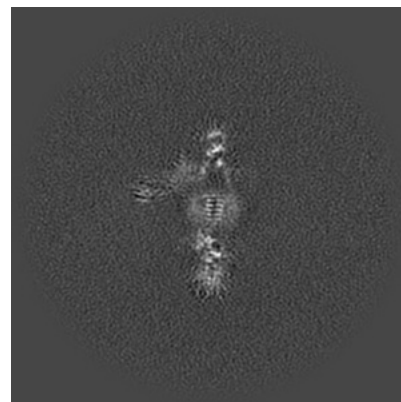
### 6.2.1 Primary map



X Index: 190

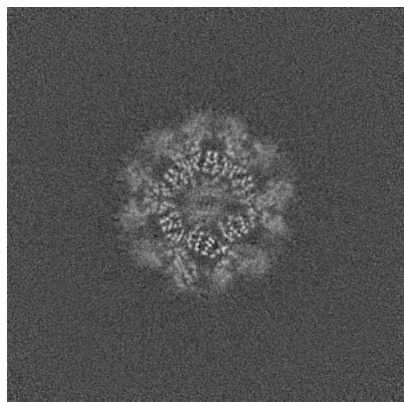


Y Index: 190

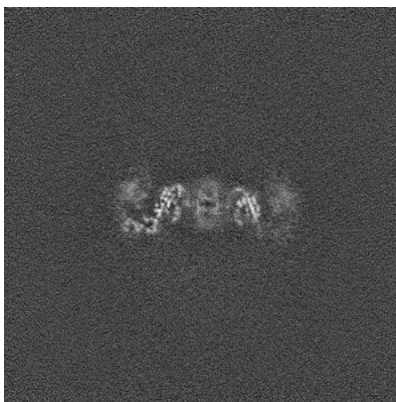


Z Index: 190

### 6.2.2 Raw map



X Index: 190



Y Index: 190

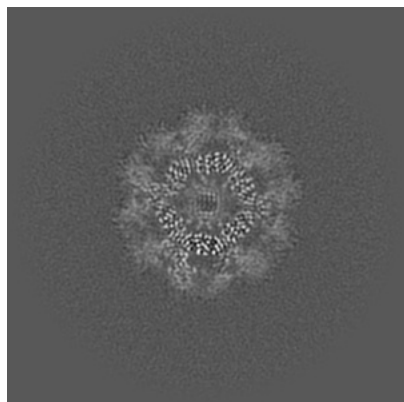


Z Index: 190

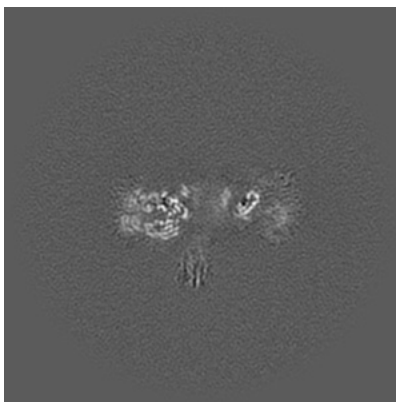
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 193

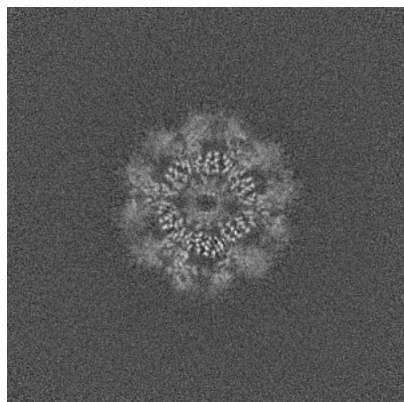


Y Index: 206

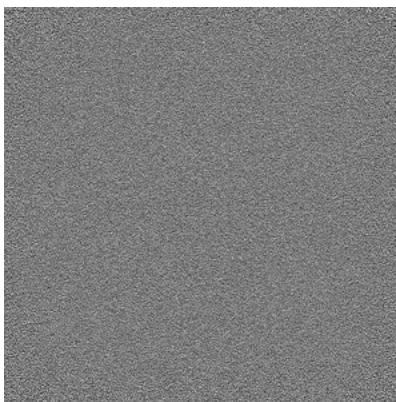


Z Index: 163

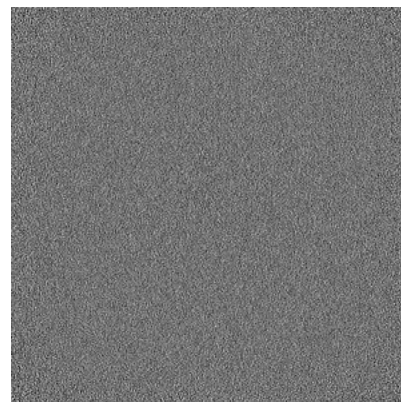
### 6.3.2 Raw map



X Index: 192



Y Index: 0

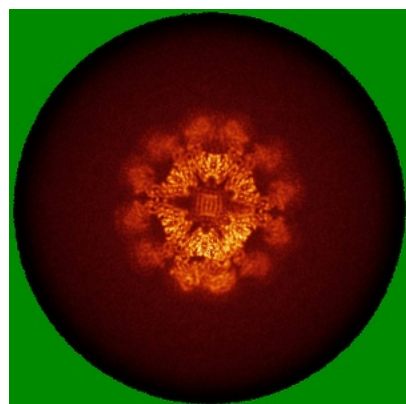


Z Index: 0

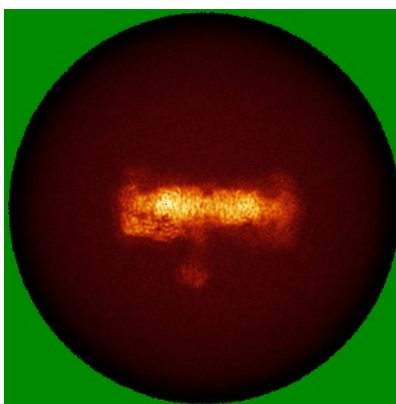
The images above show the largest variance slices of the map in three orthogonal directions.

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

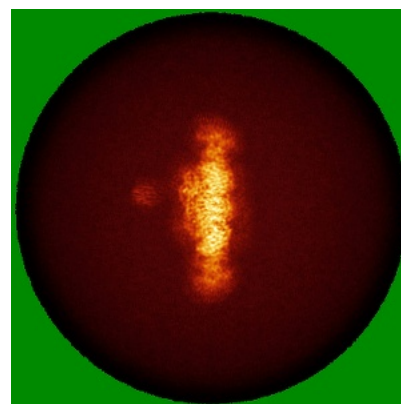
### 6.4.1 Primary map



X

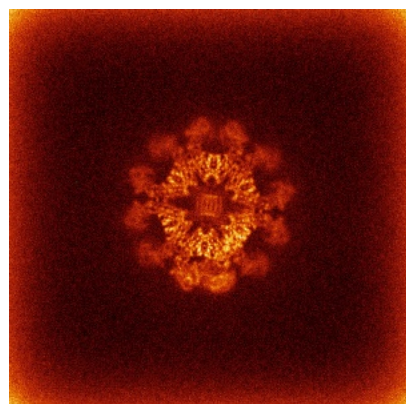


Y

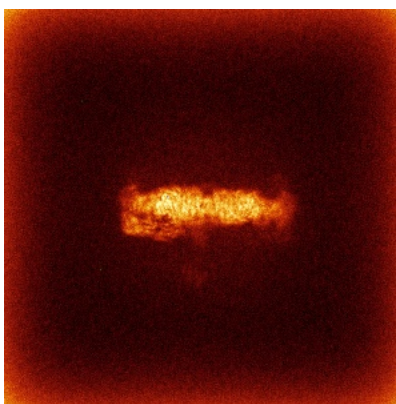


Z

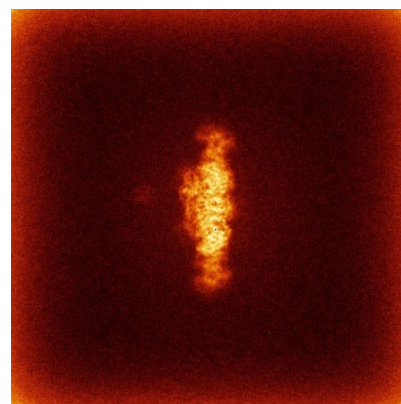
### 6.4.2 Raw map



X



Y

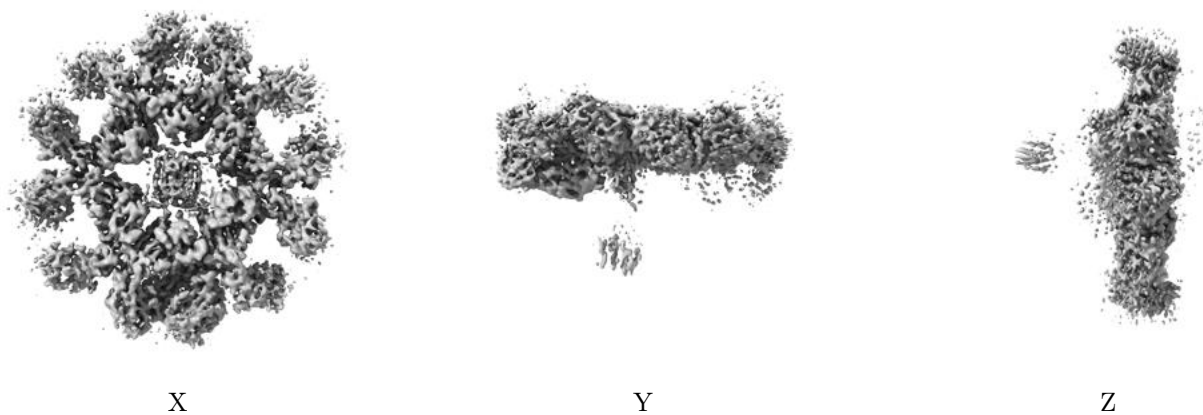


Z

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.

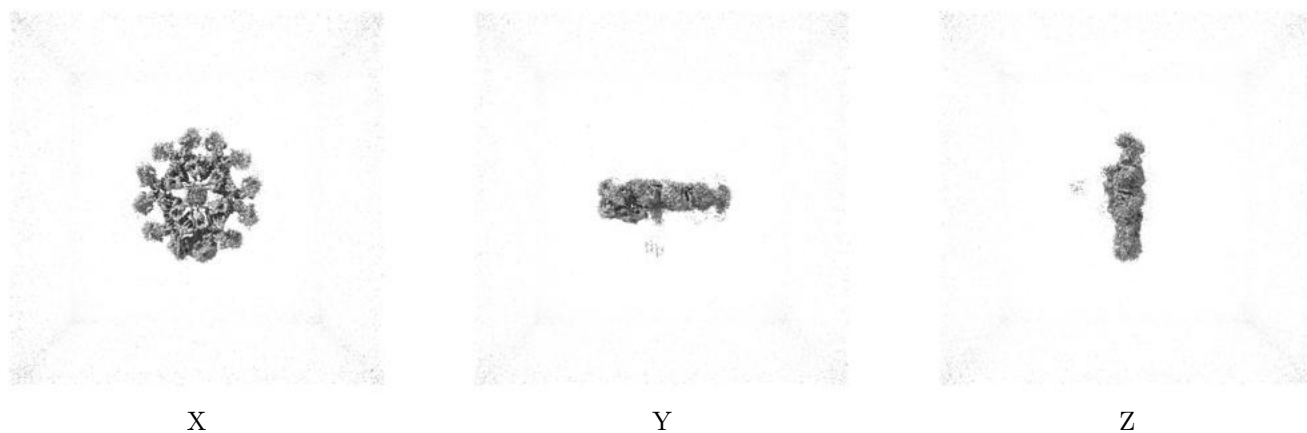
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.167. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

## 6.6 Mask visualisation [i](#)

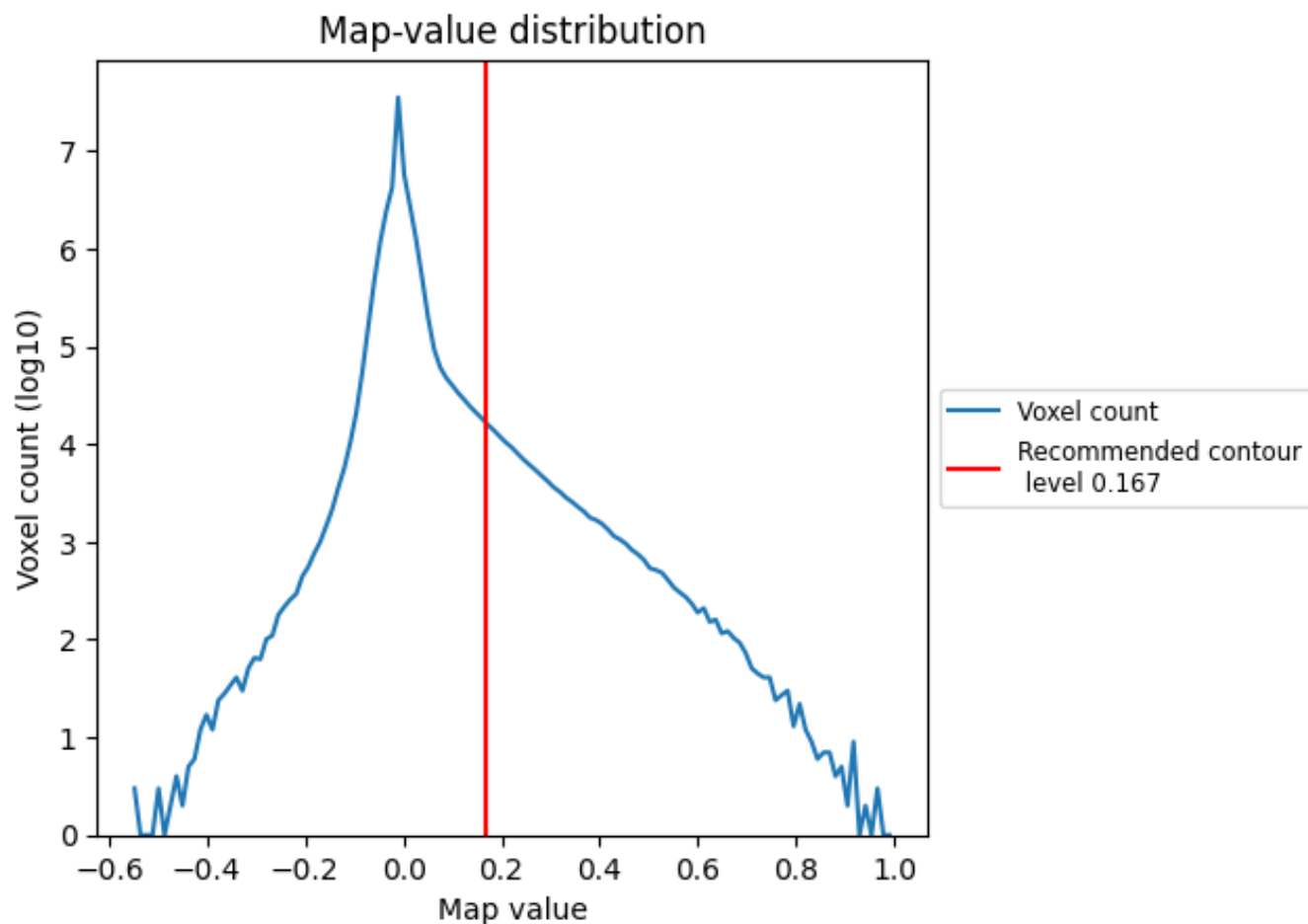
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

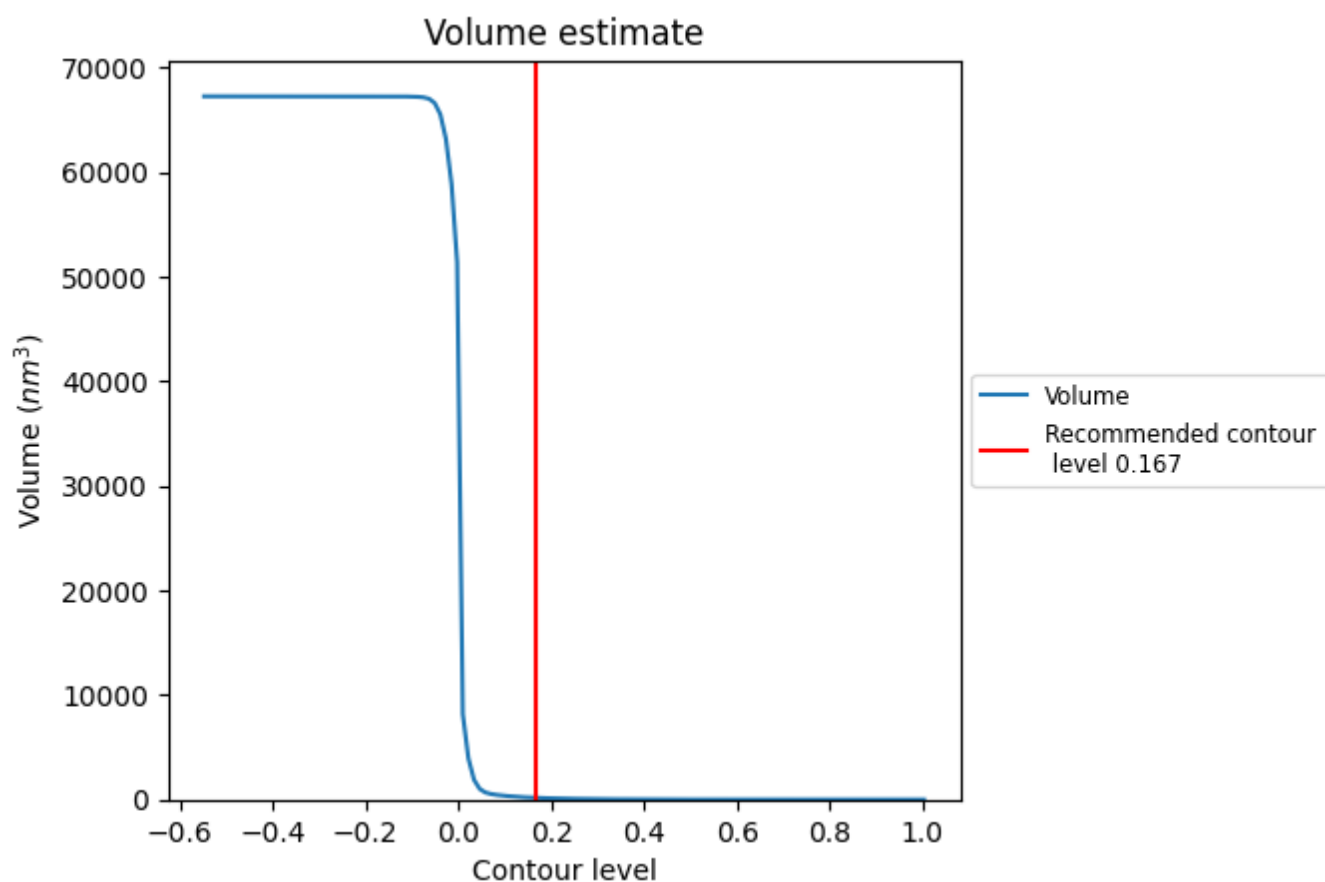
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

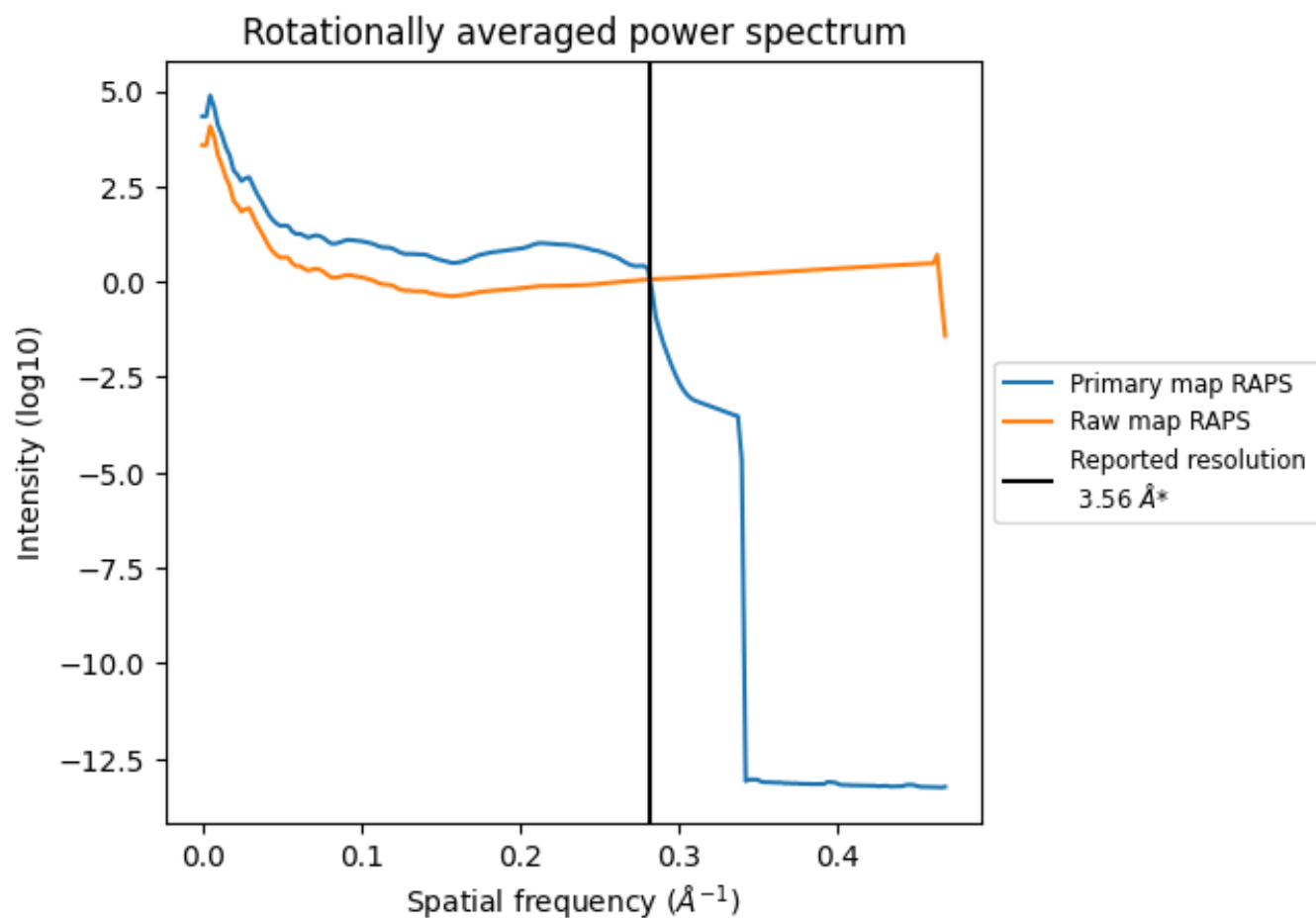
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 168 nm<sup>3</sup>; this corresponds to an approximate mass of 152 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 ⓘ

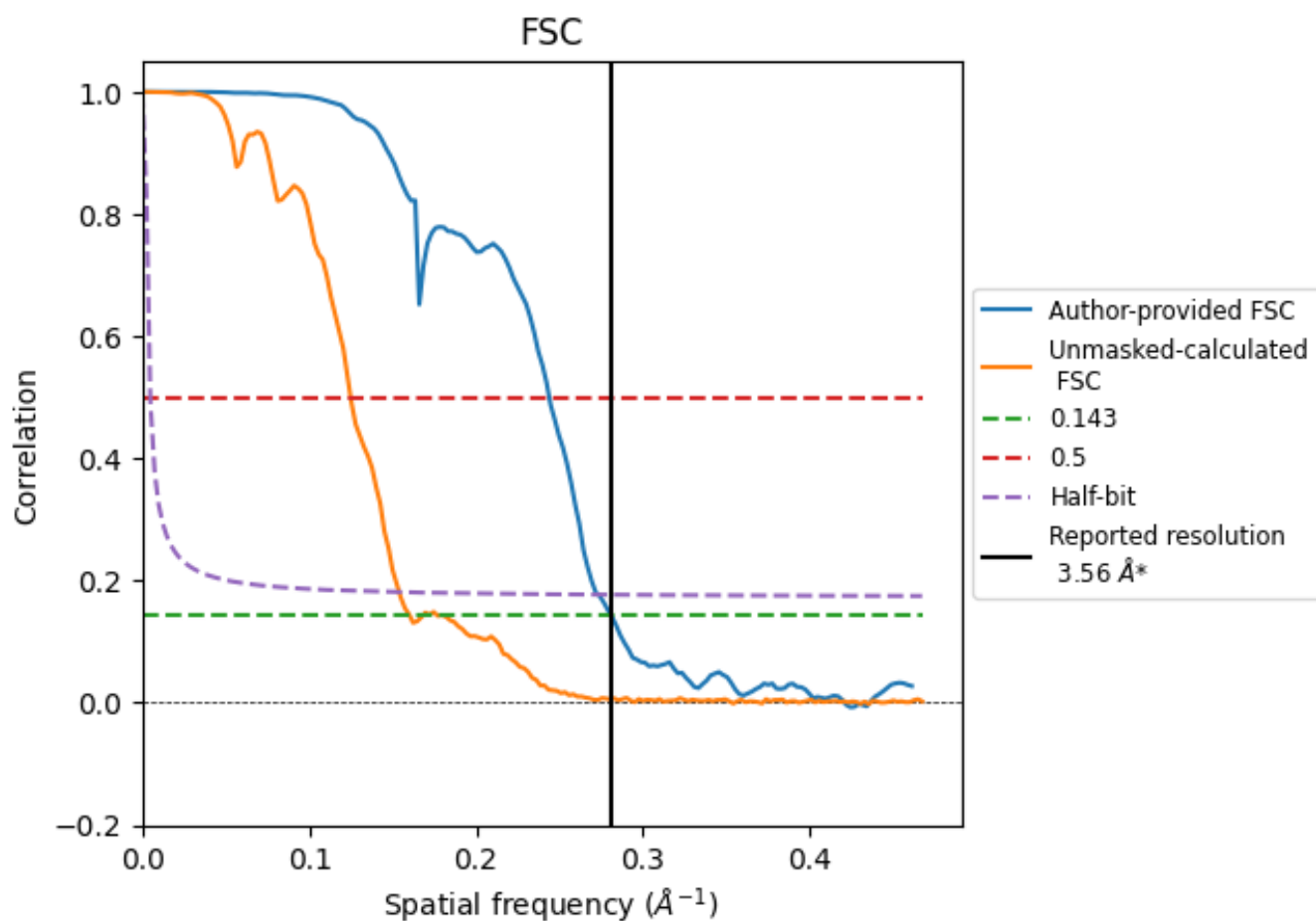


\*Reported resolution corresponds to spatial frequency of 0.281 Å<sup>-1</sup>

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



## 8.2 Resolution estimates [i](#)

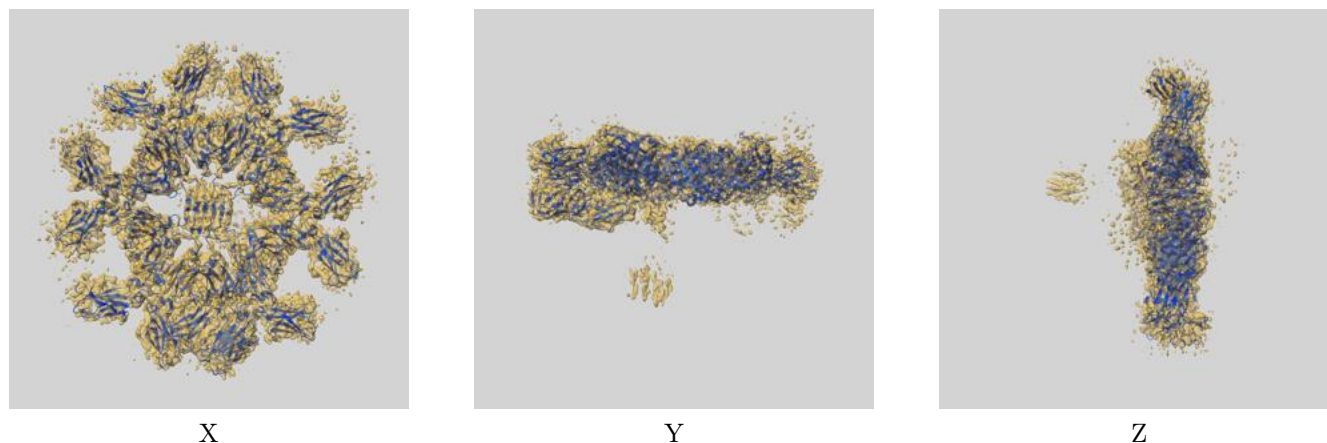
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.56	-	-
Author-provided FSC curve	3.56	4.10	3.66
Unmasked-calculated*	6.25	8.01	6.49

\*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 6.25 differs from the reported value 3.56 by more than 10 %

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

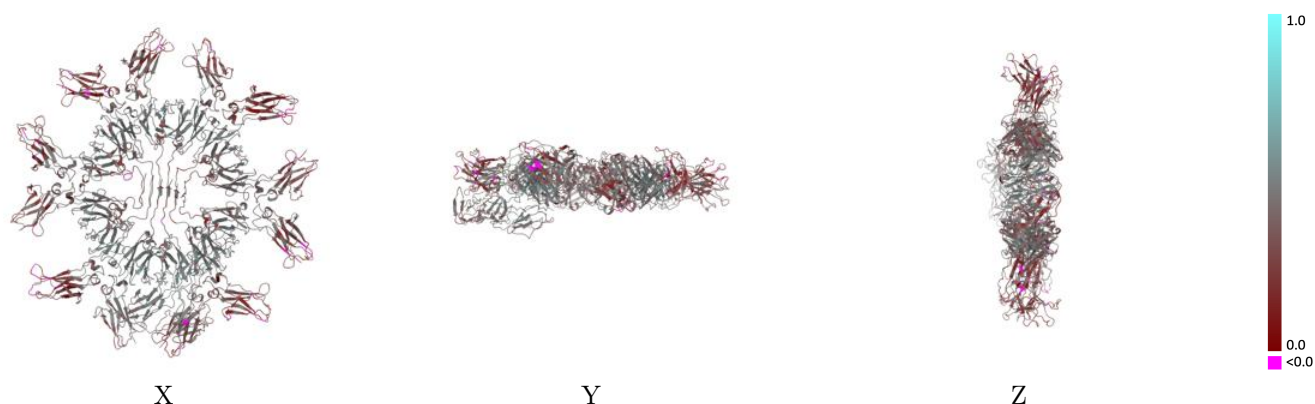
This section contains information regarding the fit between EMDB map EMD-63244 and PDB model 9LOC. Per-residue inclusion information can be found in section 3 on page 15.

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



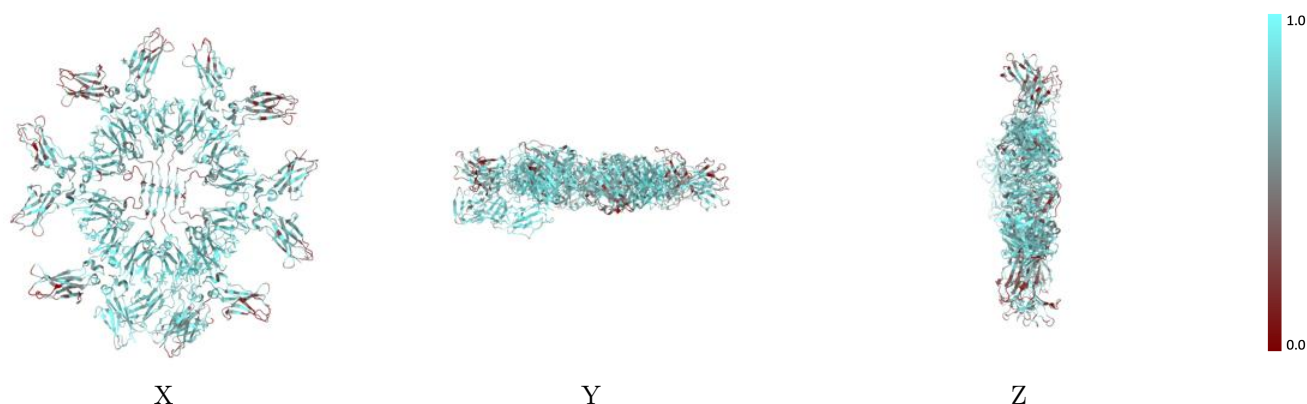
The images above show the 3D surface view of the map at the recommended contour level 0.167 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



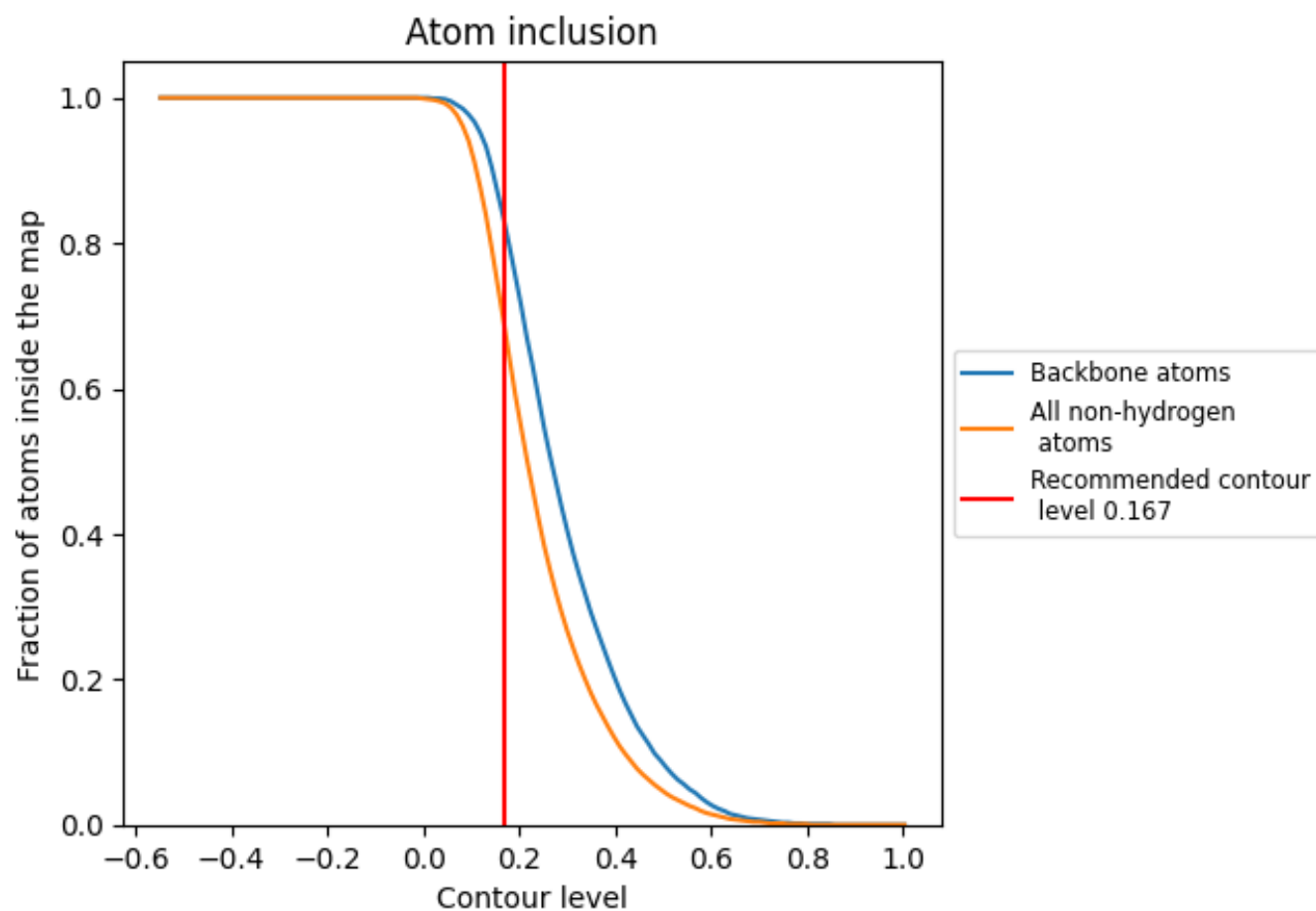
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.167).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% 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 (0.167) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6950	<div></div> 0.3980
A	<div></div> 0.7880	<div></div> 0.4300
B	<div></div> 0.8100	<div></div> 0.4580
C	<div></div> 0.7380	<div></div> 0.4230
D	<div></div> 0.6750	<div></div> 0.3900
E	<div></div> 0.6920	<div></div> 0.3900
F	<div></div> 0.6490	<div></div> 0.3800
G	<div></div> 0.6250	<div></div> 0.3580
H	<div></div> 0.7140	<div></div> 0.4080
I	<div></div> 0.6960	<div></div> 0.3970
J	<div></div> 0.6210	<div></div> 0.3710
K	<div></div> 0.6550	<div></div> 0.3740
L	<div></div> 0.6770	<div></div> 0.3930
M	<div></div> 0.6680	<div></div> 0.3870
N	<div></div> 0.7700	<div></div> 0.4870

1.0

0.0

<0.0