



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 12:30 PM UTC

PDB ID : 9V6R / pdb_00009v6r
EMDB ID : EMD-64805
Title : Hexameric RVFV GnGc-Fab140 complex
Authors : Zhang, L.; Meng, K.; Xiang, Y.
Deposited on : 2025-05-27
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

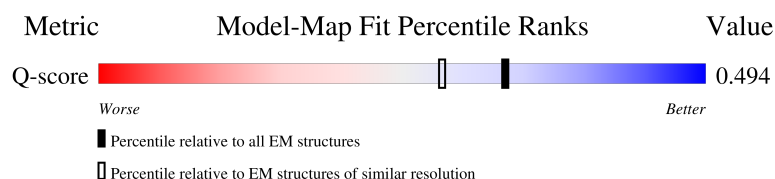
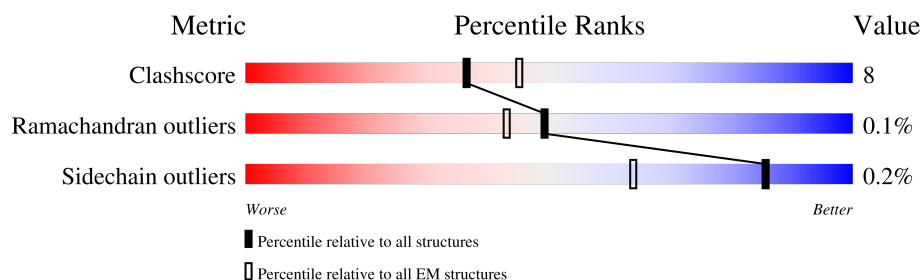
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 3.10 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.



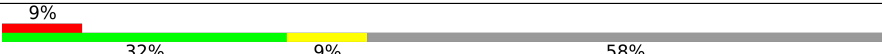
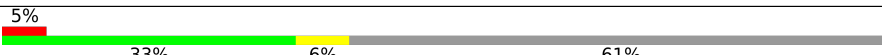
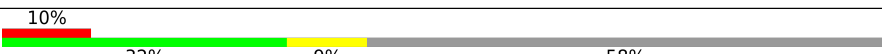
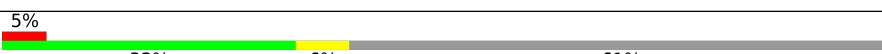
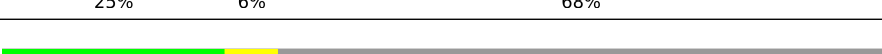
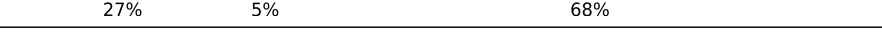
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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

Mol	Chain	Length	Quality of chain
1	A	1064	 10% 33% 6% 61%
1	B	1064	 10% 32% 9% 58%
1	C	1064	 5% 33% 6% 61%
1	H	1064	 10% 33% 9% 58%

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Mol	Chain	Length	Quality of chain
1	I	1064	
1	L	1064	
1	M	1064	
1	P	1064	
1	Q	1064	
1	T	1064	
1	V	1064	
1	Y	1064	
2	D	224	
2	F	224	
2	J	224	
2	N	224	
2	R	224	
2	W	224	
3	E	248	
3	G	248	
3	K	248	
3	O	248	
3	S	248	
3	X	248	
4	U	3	
4	Z	3	
4	a	3	
4	b	3	
4	c	3	

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Mol	Chain	Length	Quality of chain
4	d	3	67% 67% 33%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 45636 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 Envelopment polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	412	Total	C	N	O	S	0	0
			3119	1941	544	600	34		
1	B	444	Total	C	N	O	S	0	0
			3374	2093	582	671	28		
1	C	412	Total	C	N	O	S	0	0
			3119	1941	544	600	34		
1	H	444	Total	C	N	O	S	0	0
			3374	2093	582	671	28		
1	I	412	Total	C	N	O	S	0	0
			3119	1941	544	600	34		
1	L	444	Total	C	N	O	S	0	0
			3374	2093	582	671	28		
1	M	412	Total	C	N	O	S	0	0
			3119	1941	544	600	34		
1	P	444	Total	C	N	O	S	0	0
			3374	2093	582	671	28		
1	Q	412	Total	C	N	O	S	0	0
			3119	1941	544	600	34		
1	T	444	Total	C	N	O	S	0	0
			3374	2093	582	671	28		
1	V	412	Total	C	N	O	S	0	0
			3119	1941	544	600	34		
1	Y	444	Total	C	N	O	S	0	0
			3374	2093	582	671	28		

There are 264 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1198	ASP	-	expression tag	UNP A2T069
A	1199	TYR	-	expression tag	UNP A2T069
A	1200	LYS	-	expression tag	UNP A2T069
A	1201	ASP	-	expression tag	UNP A2T069
A	1202	HIS	-	expression tag	UNP A2T069
A	1203	ASP	-	expression tag	UNP A2T069

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1204	GLY	-	expression tag	UNP A2T069
A	1205	ASP	-	expression tag	UNP A2T069
A	1206	TYR	-	expression tag	UNP A2T069
A	1207	LYS	-	expression tag	UNP A2T069
A	1208	ASP	-	expression tag	UNP A2T069
A	1209	HIS	-	expression tag	UNP A2T069
A	1210	ASP	-	expression tag	UNP A2T069
A	1211	ILE	-	expression tag	UNP A2T069
A	1212	ASP	-	expression tag	UNP A2T069
A	1213	TYR	-	expression tag	UNP A2T069
A	1214	LYS	-	expression tag	UNP A2T069
A	1215	ASP	-	expression tag	UNP A2T069
A	1216	ASP	-	expression tag	UNP A2T069
A	1217	ASP	-	expression tag	UNP A2T069
A	1218	ASP	-	expression tag	UNP A2T069
A	1219	LYS	-	expression tag	UNP A2T069
B	1198	ASP	-	expression tag	UNP A2T069
B	1199	TYR	-	expression tag	UNP A2T069
B	1200	LYS	-	expression tag	UNP A2T069
B	1201	ASP	-	expression tag	UNP A2T069
B	1202	HIS	-	expression tag	UNP A2T069
B	1203	ASP	-	expression tag	UNP A2T069
B	1204	GLY	-	expression tag	UNP A2T069
B	1205	ASP	-	expression tag	UNP A2T069
B	1206	TYR	-	expression tag	UNP A2T069
B	1207	LYS	-	expression tag	UNP A2T069
B	1208	ASP	-	expression tag	UNP A2T069
B	1209	HIS	-	expression tag	UNP A2T069
B	1210	ASP	-	expression tag	UNP A2T069
B	1211	ILE	-	expression tag	UNP A2T069
B	1212	ASP	-	expression tag	UNP A2T069
B	1213	TYR	-	expression tag	UNP A2T069
B	1214	LYS	-	expression tag	UNP A2T069
B	1215	ASP	-	expression tag	UNP A2T069
B	1216	ASP	-	expression tag	UNP A2T069
B	1217	ASP	-	expression tag	UNP A2T069
B	1218	ASP	-	expression tag	UNP A2T069
B	1219	LYS	-	expression tag	UNP A2T069
C	1198	ASP	-	expression tag	UNP A2T069
C	1199	TYR	-	expression tag	UNP A2T069
C	1200	LYS	-	expression tag	UNP A2T069
C	1201	ASP	-	expression tag	UNP A2T069

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1202	HIS	-	expression tag	UNP A2T069
C	1203	ASP	-	expression tag	UNP A2T069
C	1204	GLY	-	expression tag	UNP A2T069
C	1205	ASP	-	expression tag	UNP A2T069
C	1206	TYR	-	expression tag	UNP A2T069
C	1207	LYS	-	expression tag	UNP A2T069
C	1208	ASP	-	expression tag	UNP A2T069
C	1209	HIS	-	expression tag	UNP A2T069
C	1210	ASP	-	expression tag	UNP A2T069
C	1211	ILE	-	expression tag	UNP A2T069
C	1212	ASP	-	expression tag	UNP A2T069
C	1213	TYR	-	expression tag	UNP A2T069
C	1214	LYS	-	expression tag	UNP A2T069
C	1215	ASP	-	expression tag	UNP A2T069
C	1216	ASP	-	expression tag	UNP A2T069
C	1217	ASP	-	expression tag	UNP A2T069
C	1218	ASP	-	expression tag	UNP A2T069
C	1219	LYS	-	expression tag	UNP A2T069
H	1198	ASP	-	expression tag	UNP A2T069
H	1199	TYR	-	expression tag	UNP A2T069
H	1200	LYS	-	expression tag	UNP A2T069
H	1201	ASP	-	expression tag	UNP A2T069
H	1202	HIS	-	expression tag	UNP A2T069
H	1203	ASP	-	expression tag	UNP A2T069
H	1204	GLY	-	expression tag	UNP A2T069
H	1205	ASP	-	expression tag	UNP A2T069
H	1206	TYR	-	expression tag	UNP A2T069
H	1207	LYS	-	expression tag	UNP A2T069
H	1208	ASP	-	expression tag	UNP A2T069
H	1209	HIS	-	expression tag	UNP A2T069
H	1210	ASP	-	expression tag	UNP A2T069
H	1211	ILE	-	expression tag	UNP A2T069
H	1212	ASP	-	expression tag	UNP A2T069
H	1213	TYR	-	expression tag	UNP A2T069
H	1214	LYS	-	expression tag	UNP A2T069
H	1215	ASP	-	expression tag	UNP A2T069
H	1216	ASP	-	expression tag	UNP A2T069
H	1217	ASP	-	expression tag	UNP A2T069
H	1218	ASP	-	expression tag	UNP A2T069
H	1219	LYS	-	expression tag	UNP A2T069
I	1198	ASP	-	expression tag	UNP A2T069
I	1199	TYR	-	expression tag	UNP A2T069

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Chain	Residue	Modelled	Actual	Comment	Reference
I	1200	LYS	-	expression tag	UNP A2T069
I	1201	ASP	-	expression tag	UNP A2T069
I	1202	HIS	-	expression tag	UNP A2T069
I	1203	ASP	-	expression tag	UNP A2T069
I	1204	GLY	-	expression tag	UNP A2T069
I	1205	ASP	-	expression tag	UNP A2T069
I	1206	TYR	-	expression tag	UNP A2T069
I	1207	LYS	-	expression tag	UNP A2T069
I	1208	ASP	-	expression tag	UNP A2T069
I	1209	HIS	-	expression tag	UNP A2T069
I	1210	ASP	-	expression tag	UNP A2T069
I	1211	ILE	-	expression tag	UNP A2T069
I	1212	ASP	-	expression tag	UNP A2T069
I	1213	TYR	-	expression tag	UNP A2T069
I	1214	LYS	-	expression tag	UNP A2T069
I	1215	ASP	-	expression tag	UNP A2T069
I	1216	ASP	-	expression tag	UNP A2T069
I	1217	ASP	-	expression tag	UNP A2T069
I	1218	ASP	-	expression tag	UNP A2T069
I	1219	LYS	-	expression tag	UNP A2T069
L	1198	ASP	-	expression tag	UNP A2T069
L	1199	TYR	-	expression tag	UNP A2T069
L	1200	LYS	-	expression tag	UNP A2T069
L	1201	ASP	-	expression tag	UNP A2T069
L	1202	HIS	-	expression tag	UNP A2T069
L	1203	ASP	-	expression tag	UNP A2T069
L	1204	GLY	-	expression tag	UNP A2T069
L	1205	ASP	-	expression tag	UNP A2T069
L	1206	TYR	-	expression tag	UNP A2T069
L	1207	LYS	-	expression tag	UNP A2T069
L	1208	ASP	-	expression tag	UNP A2T069
L	1209	HIS	-	expression tag	UNP A2T069
L	1210	ASP	-	expression tag	UNP A2T069
L	1211	ILE	-	expression tag	UNP A2T069
L	1212	ASP	-	expression tag	UNP A2T069
L	1213	TYR	-	expression tag	UNP A2T069
L	1214	LYS	-	expression tag	UNP A2T069
L	1215	ASP	-	expression tag	UNP A2T069
L	1216	ASP	-	expression tag	UNP A2T069
L	1217	ASP	-	expression tag	UNP A2T069
L	1218	ASP	-	expression tag	UNP A2T069
L	1219	LYS	-	expression tag	UNP A2T069

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Chain	Residue	Modelled	Actual	Comment	Reference
M	1198	ASP	-	expression tag	UNP A2T069
M	1199	TYR	-	expression tag	UNP A2T069
M	1200	LYS	-	expression tag	UNP A2T069
M	1201	ASP	-	expression tag	UNP A2T069
M	1202	HIS	-	expression tag	UNP A2T069
M	1203	ASP	-	expression tag	UNP A2T069
M	1204	GLY	-	expression tag	UNP A2T069
M	1205	ASP	-	expression tag	UNP A2T069
M	1206	TYR	-	expression tag	UNP A2T069
M	1207	LYS	-	expression tag	UNP A2T069
M	1208	ASP	-	expression tag	UNP A2T069
M	1209	HIS	-	expression tag	UNP A2T069
M	1210	ASP	-	expression tag	UNP A2T069
M	1211	ILE	-	expression tag	UNP A2T069
M	1212	ASP	-	expression tag	UNP A2T069
M	1213	TYR	-	expression tag	UNP A2T069
M	1214	LYS	-	expression tag	UNP A2T069
M	1215	ASP	-	expression tag	UNP A2T069
M	1216	ASP	-	expression tag	UNP A2T069
M	1217	ASP	-	expression tag	UNP A2T069
M	1218	ASP	-	expression tag	UNP A2T069
M	1219	LYS	-	expression tag	UNP A2T069
P	1198	ASP	-	expression tag	UNP A2T069
P	1199	TYR	-	expression tag	UNP A2T069
P	1200	LYS	-	expression tag	UNP A2T069
P	1201	ASP	-	expression tag	UNP A2T069
P	1202	HIS	-	expression tag	UNP A2T069
P	1203	ASP	-	expression tag	UNP A2T069
P	1204	GLY	-	expression tag	UNP A2T069
P	1205	ASP	-	expression tag	UNP A2T069
P	1206	TYR	-	expression tag	UNP A2T069
P	1207	LYS	-	expression tag	UNP A2T069
P	1208	ASP	-	expression tag	UNP A2T069
P	1209	HIS	-	expression tag	UNP A2T069
P	1210	ASP	-	expression tag	UNP A2T069
P	1211	ILE	-	expression tag	UNP A2T069
P	1212	ASP	-	expression tag	UNP A2T069
P	1213	TYR	-	expression tag	UNP A2T069
P	1214	LYS	-	expression tag	UNP A2T069
P	1215	ASP	-	expression tag	UNP A2T069
P	1216	ASP	-	expression tag	UNP A2T069
P	1217	ASP	-	expression tag	UNP A2T069

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Chain	Residue	Modelled	Actual	Comment	Reference
P	1218	ASP	-	expression tag	UNP A2T069
P	1219	LYS	-	expression tag	UNP A2T069
Q	1198	ASP	-	expression tag	UNP A2T069
Q	1199	TYR	-	expression tag	UNP A2T069
Q	1200	LYS	-	expression tag	UNP A2T069
Q	1201	ASP	-	expression tag	UNP A2T069
Q	1202	HIS	-	expression tag	UNP A2T069
Q	1203	ASP	-	expression tag	UNP A2T069
Q	1204	GLY	-	expression tag	UNP A2T069
Q	1205	ASP	-	expression tag	UNP A2T069
Q	1206	TYR	-	expression tag	UNP A2T069
Q	1207	LYS	-	expression tag	UNP A2T069
Q	1208	ASP	-	expression tag	UNP A2T069
Q	1209	HIS	-	expression tag	UNP A2T069
Q	1210	ASP	-	expression tag	UNP A2T069
Q	1211	ILE	-	expression tag	UNP A2T069
Q	1212	ASP	-	expression tag	UNP A2T069
Q	1213	TYR	-	expression tag	UNP A2T069
Q	1214	LYS	-	expression tag	UNP A2T069
Q	1215	ASP	-	expression tag	UNP A2T069
Q	1216	ASP	-	expression tag	UNP A2T069
Q	1217	ASP	-	expression tag	UNP A2T069
Q	1218	ASP	-	expression tag	UNP A2T069
Q	1219	LYS	-	expression tag	UNP A2T069
T	1198	ASP	-	expression tag	UNP A2T069
T	1199	TYR	-	expression tag	UNP A2T069
T	1200	LYS	-	expression tag	UNP A2T069
T	1201	ASP	-	expression tag	UNP A2T069
T	1202	HIS	-	expression tag	UNP A2T069
T	1203	ASP	-	expression tag	UNP A2T069
T	1204	GLY	-	expression tag	UNP A2T069
T	1205	ASP	-	expression tag	UNP A2T069
T	1206	TYR	-	expression tag	UNP A2T069
T	1207	LYS	-	expression tag	UNP A2T069
T	1208	ASP	-	expression tag	UNP A2T069
T	1209	HIS	-	expression tag	UNP A2T069
T	1210	ASP	-	expression tag	UNP A2T069
T	1211	ILE	-	expression tag	UNP A2T069
T	1212	ASP	-	expression tag	UNP A2T069
T	1213	TYR	-	expression tag	UNP A2T069
T	1214	LYS	-	expression tag	UNP A2T069
T	1215	ASP	-	expression tag	UNP A2T069

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Chain	Residue	Modelled	Actual	Comment	Reference
T	1216	ASP	-	expression tag	UNP A2T069
T	1217	ASP	-	expression tag	UNP A2T069
T	1218	ASP	-	expression tag	UNP A2T069
T	1219	LYS	-	expression tag	UNP A2T069
V	1198	ASP	-	expression tag	UNP A2T069
V	1199	TYR	-	expression tag	UNP A2T069
V	1200	LYS	-	expression tag	UNP A2T069
V	1201	ASP	-	expression tag	UNP A2T069
V	1202	HIS	-	expression tag	UNP A2T069
V	1203	ASP	-	expression tag	UNP A2T069
V	1204	GLY	-	expression tag	UNP A2T069
V	1205	ASP	-	expression tag	UNP A2T069
V	1206	TYR	-	expression tag	UNP A2T069
V	1207	LYS	-	expression tag	UNP A2T069
V	1208	ASP	-	expression tag	UNP A2T069
V	1209	HIS	-	expression tag	UNP A2T069
V	1210	ASP	-	expression tag	UNP A2T069
V	1211	ILE	-	expression tag	UNP A2T069
V	1212	ASP	-	expression tag	UNP A2T069
V	1213	TYR	-	expression tag	UNP A2T069
V	1214	LYS	-	expression tag	UNP A2T069
V	1215	ASP	-	expression tag	UNP A2T069
V	1216	ASP	-	expression tag	UNP A2T069
V	1217	ASP	-	expression tag	UNP A2T069
V	1218	ASP	-	expression tag	UNP A2T069
V	1219	LYS	-	expression tag	UNP A2T069
Y	1198	ASP	-	expression tag	UNP A2T069
Y	1199	TYR	-	expression tag	UNP A2T069
Y	1200	LYS	-	expression tag	UNP A2T069
Y	1201	ASP	-	expression tag	UNP A2T069
Y	1202	HIS	-	expression tag	UNP A2T069
Y	1203	ASP	-	expression tag	UNP A2T069
Y	1204	GLY	-	expression tag	UNP A2T069
Y	1205	ASP	-	expression tag	UNP A2T069
Y	1206	TYR	-	expression tag	UNP A2T069
Y	1207	LYS	-	expression tag	UNP A2T069
Y	1208	ASP	-	expression tag	UNP A2T069
Y	1209	HIS	-	expression tag	UNP A2T069
Y	1210	ASP	-	expression tag	UNP A2T069
Y	1211	ILE	-	expression tag	UNP A2T069
Y	1212	ASP	-	expression tag	UNP A2T069
Y	1213	TYR	-	expression tag	UNP A2T069

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	1214	LYS	-	expression tag	UNP A2T069
Y	1215	ASP	-	expression tag	UNP A2T069
Y	1216	ASP	-	expression tag	UNP A2T069
Y	1217	ASP	-	expression tag	UNP A2T069
Y	1218	ASP	-	expression tag	UNP A2T069
Y	1219	LYS	-	expression tag	UNP A2T069

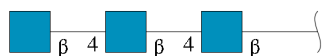
- Molecule 2 is a protein called Fab140 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	71	Total	C	N	O	S	0	0
			530	331	87	110	2		
2	F	71	Total	C	N	O	S	0	0
			530	331	87	110	2		
2	J	71	Total	C	N	O	S	0	0
			530	331	87	110	2		
2	N	71	Total	C	N	O	S	0	0
			530	331	87	110	2		
2	R	71	Total	C	N	O	S	0	0
			530	331	87	110	2		
2	W	71	Total	C	N	O	S	0	0
			530	331	87	110	2		

- Molecule 3 is a protein called Fab140 heavy chain.

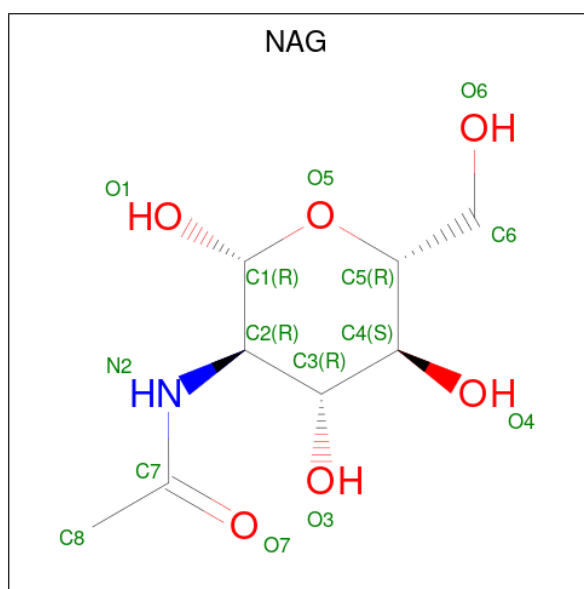
Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	58	Total	C	N	O	S	0	0
			513	346	73	93	1		
3	G	58	Total	C	N	O	S	0	0
			513	346	73	93	1		
3	K	58	Total	C	N	O	S	0	0
			513	346	73	93	1		
3	O	58	Total	C	N	O	S	0	0
			513	346	73	93	1		
3	S	58	Total	C	N	O	S	0	0
			513	346	73	93	1		
3	X	58	Total	C	N	O	S	0	0
			513	346	73	93	1		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	U	3	Total	C	N	O	0	0
			42	24	3	15		
4	Z	3	Total	C	N	O	0	0
			42	24	3	15		
4	a	3	Total	C	N	O	0	0
			42	24	3	15		
4	b	3	Total	C	N	O	0	0
			42	24	3	15		
4	c	3	Total	C	N	O	0	0
			42	24	3	15		
4	d	3	Total	C	N	O	0	0
			42	24	3	15		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



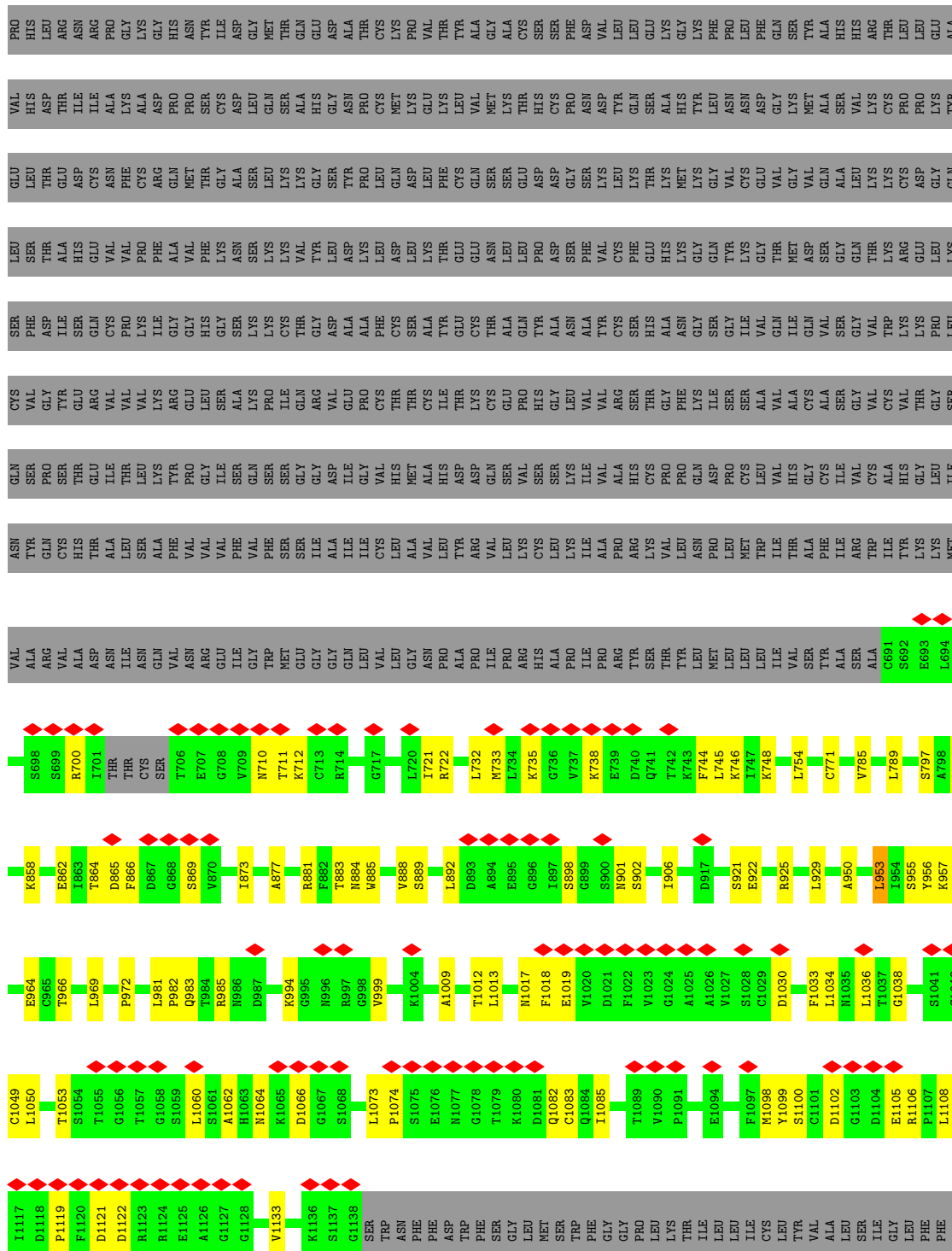
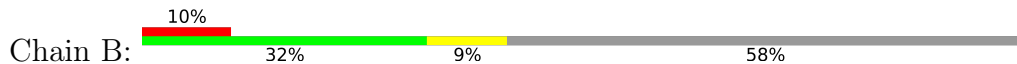
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	

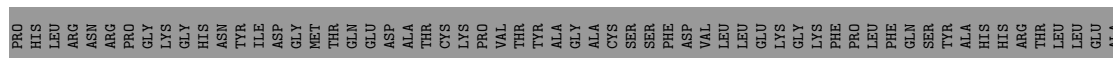
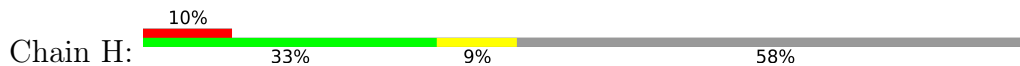
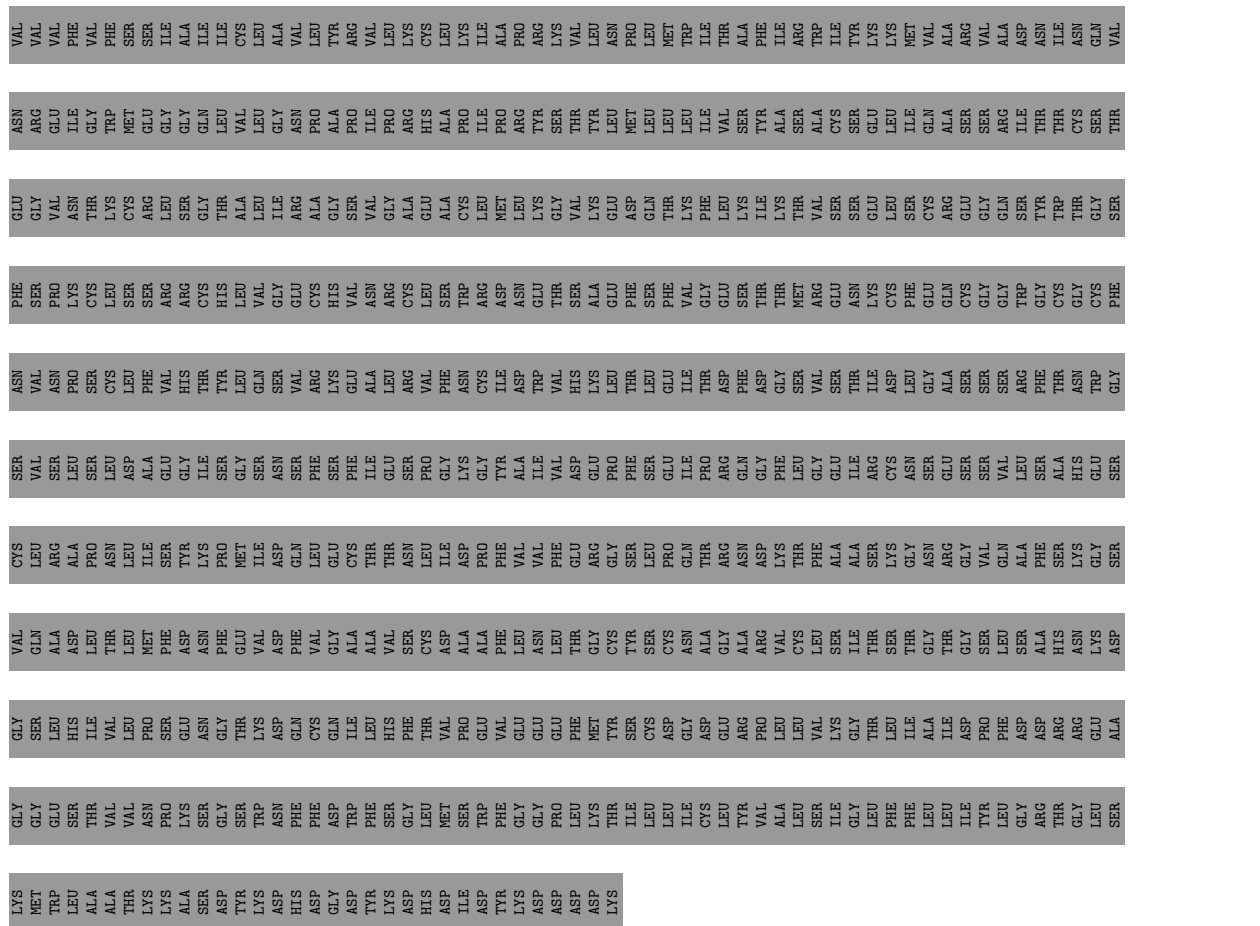
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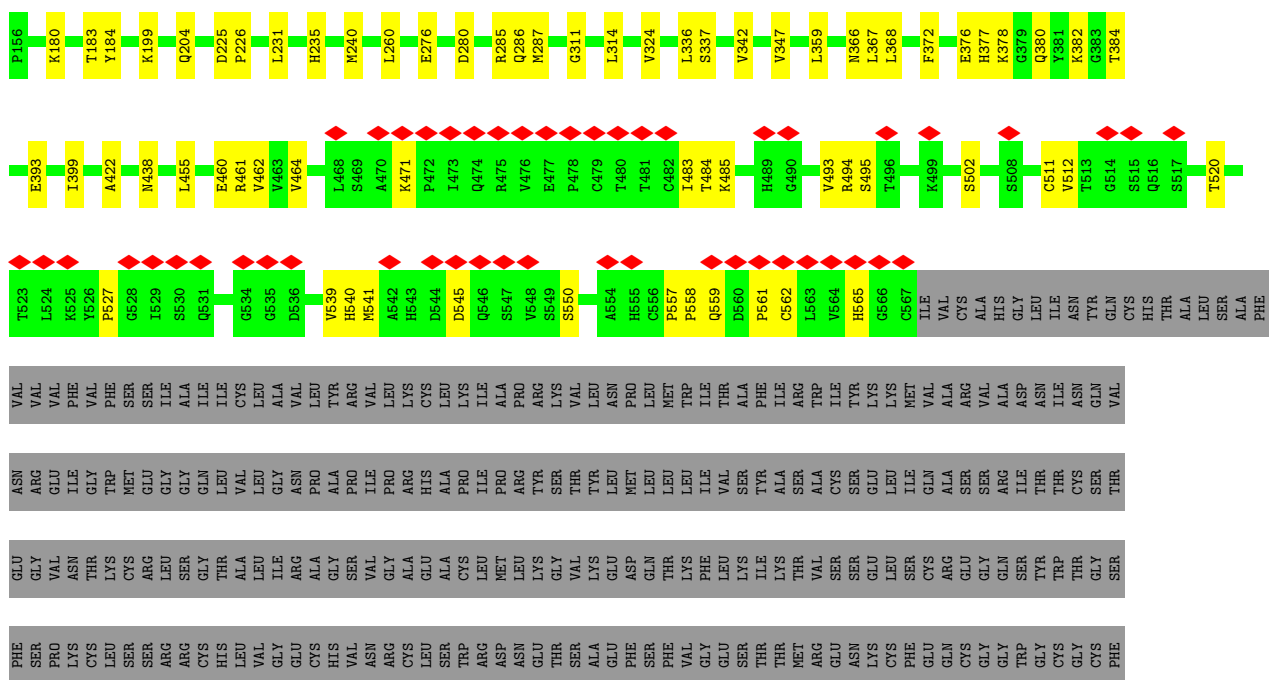
Mol	Chain	Residues	Atoms				AltConf
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	I	1	Total	C	N	O	0
			14	8	1	5	
5	L	1	Total	C	N	O	0
			14	8	1	5	
5	M	1	Total	C	N	O	0
			14	8	1	5	
5	P	1	Total	C	N	O	0
			14	8	1	5	
5	Q	1	Total	C	N	O	0
			14	8	1	5	
5	T	1	Total	C	N	O	0
			14	8	1	5	
5	V	1	Total	C	N	O	0
			14	8	1	5	
5	Y	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 1: Envelopment polyprotein







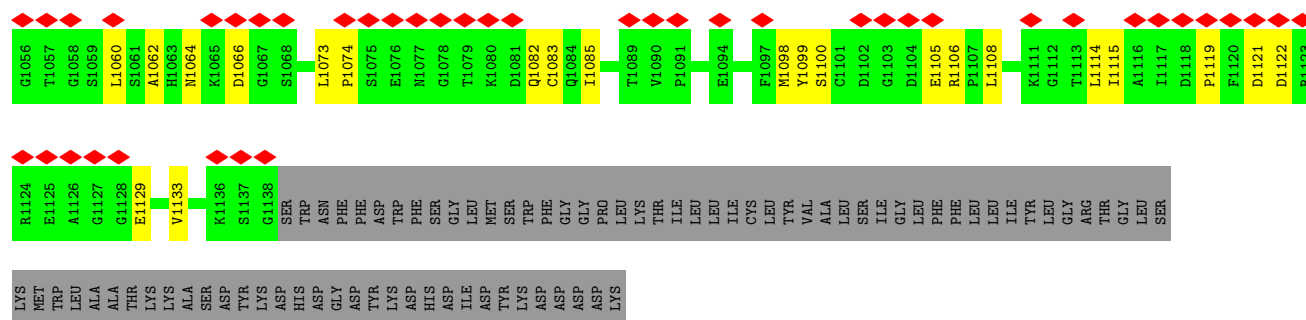


[illegible]

- Molecule 1: Envelopment polypotein

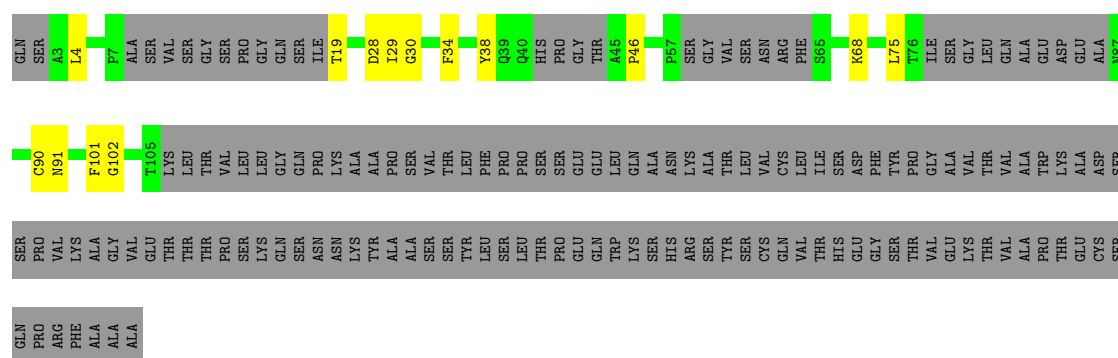
[illegible]





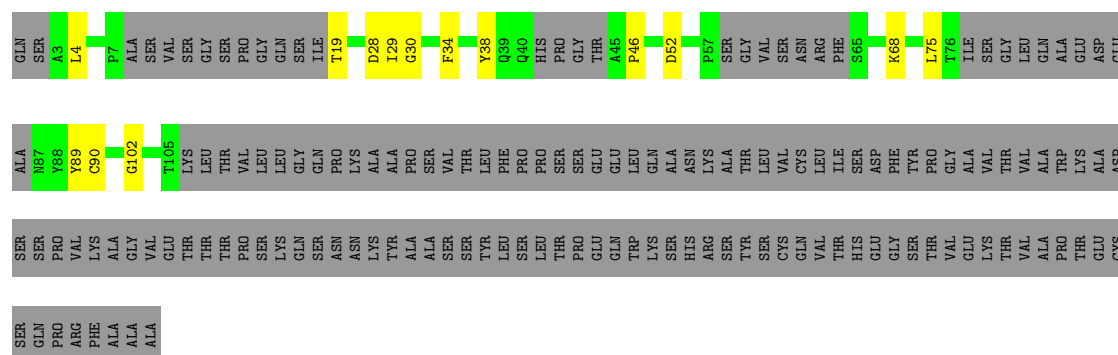
• Molecule 2: Fab140 light chain

Chain D: 25% 6% 68%



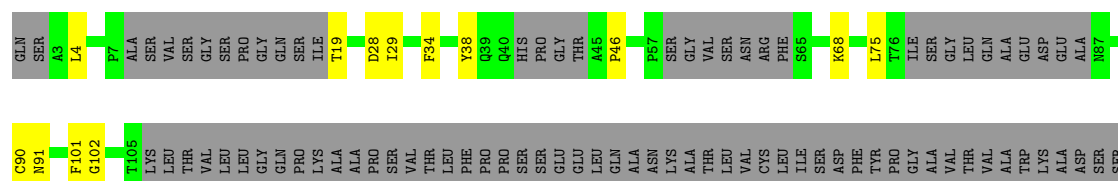
• Molecule 2: Fab140 light chain

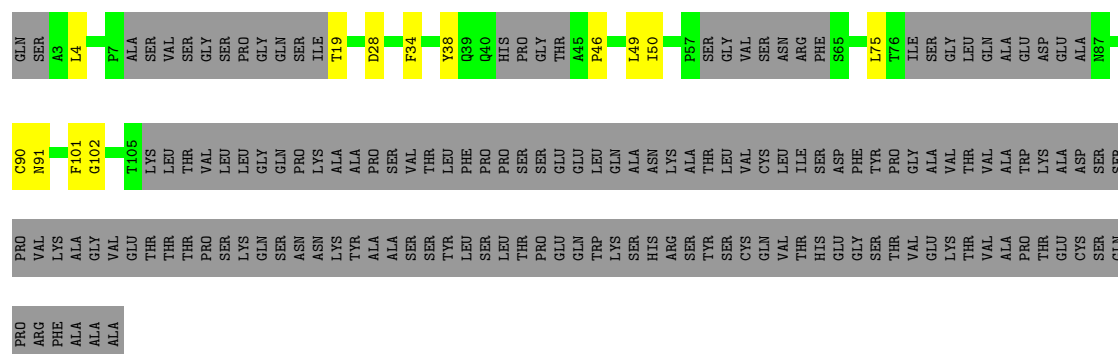
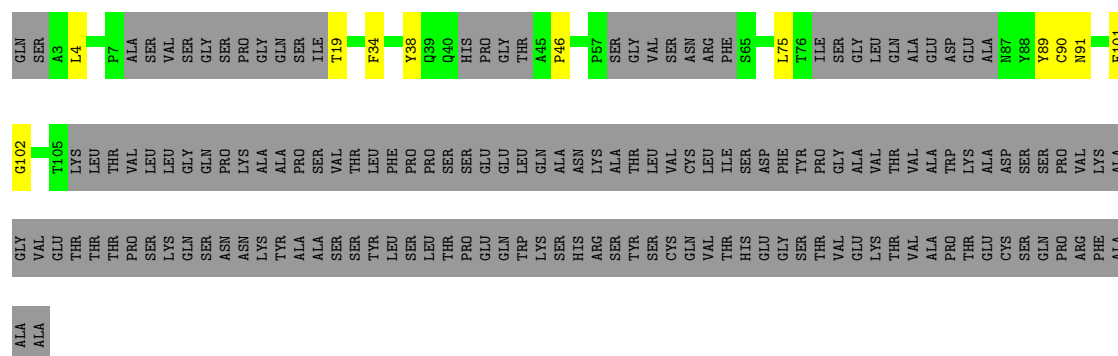
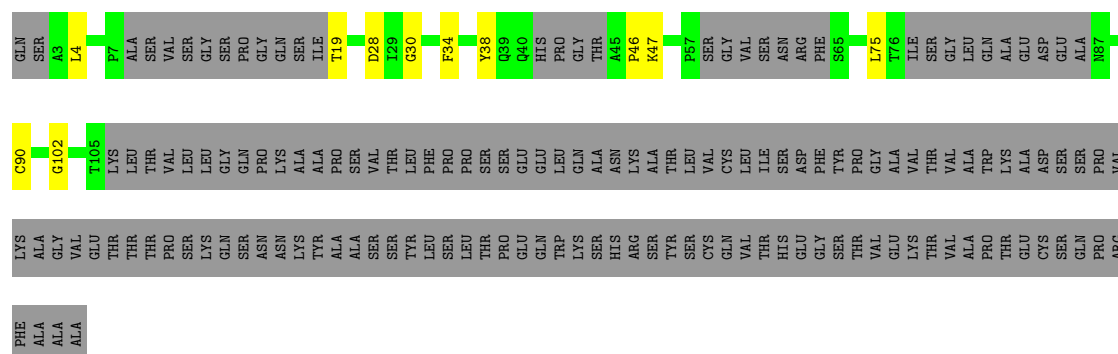
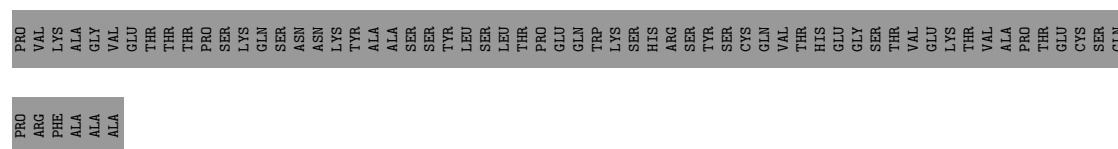
Chain F: 25% 6% 68%

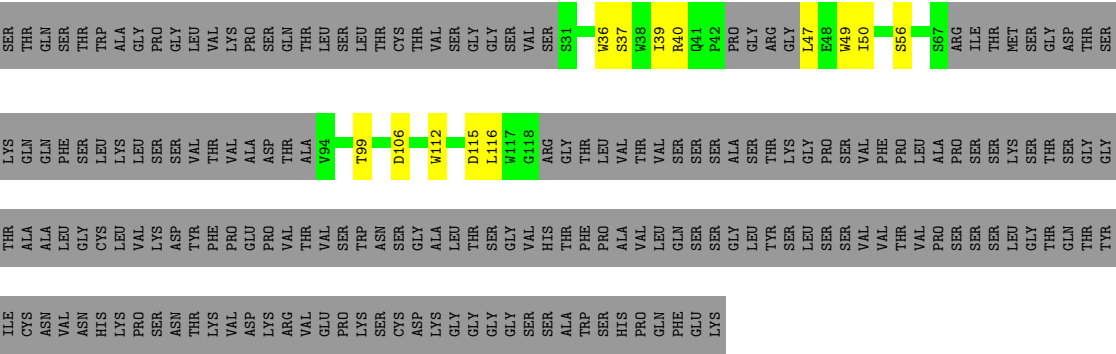


• Molecule 2: Fab140 light chain

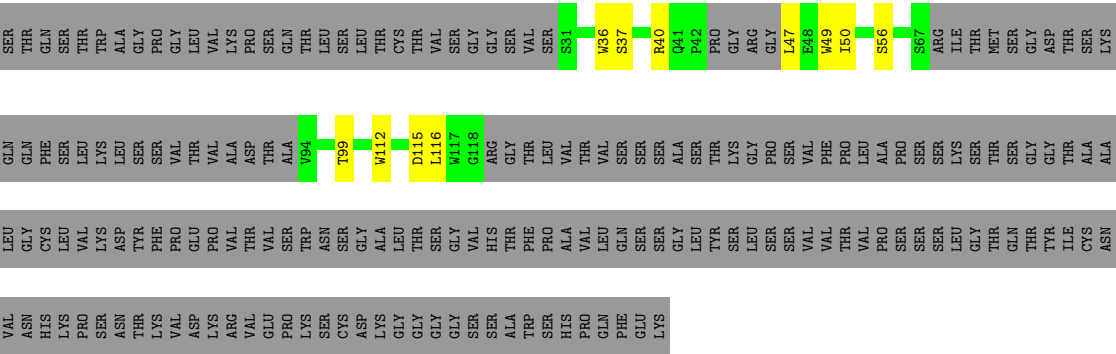
Chain J: 26% 6% 68%



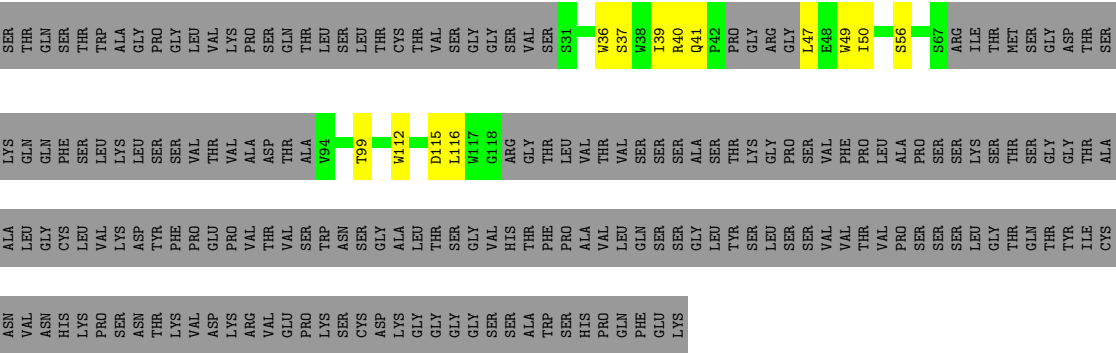




● Molecule 3: Fab140 heavy chain



● Molecule 3: Fab140 heavy chain



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



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

Chain Z: 



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

Chain a: 



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

Chain b: 



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

Chain c: 



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

Chain d: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	640793	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.103	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0156	Depositor
Map size (Å)	307.41202, 307.41202, 307.41202	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0979, 1.0979, 1.0979	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.16	0/3186	0.30	0/4300
1	B	0.14	0/3435	0.34	0/4640
1	C	0.16	0/3186	0.32	0/4300
1	H	0.13	0/3435	0.33	0/4640
1	I	0.16	0/3186	0.32	0/4300
1	L	0.13	0/3435	0.32	0/4640
1	M	0.16	0/3186	0.30	0/4300
1	P	0.13	0/3435	0.34	0/4640
1	Q	0.16	0/3186	0.32	0/4300
1	T	0.13	0/3435	0.34	0/4640
1	V	0.16	0/3186	0.32	0/4300
1	Y	0.13	0/3435	0.32	0/4640
2	D	0.11	0/539	0.28	0/730
2	F	0.10	0/539	0.28	0/730
2	J	0.11	0/539	0.28	0/730
2	N	0.11	0/539	0.28	0/730
2	R	0.10	0/539	0.27	0/730
2	W	0.10	0/539	0.28	0/730
3	E	0.13	0/538	0.35	0/736
3	G	0.13	0/538	0.34	0/736
3	K	0.13	0/538	0.37	0/736
3	O	0.13	0/538	0.35	0/736
3	S	0.14	0/538	0.35	0/736
3	X	0.13	0/538	0.36	0/736
All	All	0.14	0/46188	0.32	0/62436

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
1	I	0	2
1	M	0	2
1	Q	0	2
1	V	0	2
All	All	0	12

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	180	LYS	Peptide
1	A	225	ASP	Peptide
1	C	180	LYS	Peptide
1	C	225	ASP	Peptide
1	I	180	LYS	Peptide
1	I	225	ASP	Peptide
1	M	180	LYS	Peptide
1	M	225	ASP	Peptide
1	Q	180	LYS	Peptide
1	Q	225	ASP	Peptide
1	V	180	LYS	Peptide
1	V	225	ASP	Peptide

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	3119	0	3055	38	0
1	B	3374	0	3243	65	0
1	C	3119	0	3055	45	0
1	H	3374	0	3243	66	0
1	I	3119	0	3055	43	0
1	L	3374	0	3243	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	3119	0	3055	36	0
1	P	3374	0	3243	64	0
1	Q	3119	0	3055	43	0
1	T	3374	0	3243	68	0
1	V	3119	0	3055	40	0
1	Y	3374	0	3243	62	0
2	D	530	0	491	8	0
2	F	530	0	491	9	0
2	J	530	0	491	7	0
2	N	530	0	491	7	0
2	R	530	0	491	7	0
2	W	530	0	491	7	0
3	E	513	0	433	9	0
3	G	513	0	433	9	0
3	K	513	0	433	10	0
3	O	513	0	433	9	0
3	S	513	0	433	8	0
3	X	513	0	433	9	0
4	U	42	0	37	1	0
4	Z	42	0	37	1	0
4	a	42	0	37	1	0
4	b	42	0	37	1	0
4	c	42	0	37	1	0
4	d	42	0	37	1	0
5	A	14	0	13	1	0
5	B	14	0	13	0	0
5	C	14	0	13	2	0
5	H	14	0	13	0	0
5	I	14	0	13	2	0
5	L	14	0	13	0	0
5	M	14	0	13	1	0
5	P	14	0	13	0	0
5	Q	14	0	13	2	0
5	T	14	0	13	0	0
5	V	14	0	13	2	0
5	Y	14	0	13	0	0
All	All	45636	0	43710	684	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 (684) 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:T:922:GLU:OE2	1:T:922:GLU:N	2.20	0.75
1:Y:957:LYS:HB3	1:Y:964:GLU:HB2	1.70	0.74
1:B:957:LYS:HB3	1:B:964:GLU:HB2	1.70	0.73
1:C:460:GLU:HG2	1:C:462:VAL:HG13	1.70	0.73
1:P:957:LYS:HB3	1:P:964:GLU:HB2	1.71	0.73
1:T:957:LYS:HB3	1:T:964:GLU:HB2	1.70	0.73
1:L:957:LYS:HB3	1:L:964:GLU:HB2	1.72	0.72
1:T:1031:ALA:HB1	1:T:1050:LEU:HD11	1.71	0.72
1:H:957:LYS:HB3	1:H:964:GLU:HB2	1.72	0.72
1:H:1031:ALA:HB1	1:H:1050:LEU:HD11	1.71	0.71
1:Q:460:GLU:HG2	1:Q:462:VAL:HG13	1.72	0.71
1:H:922:GLU:OE2	1:H:922:GLU:N	2.20	0.71
2:N:4:LEU:HB2	2:N:102:GLY:HA2	1.73	0.69
1:H:746:LYS:HB2	1:H:864:THR:HB	1.75	0.68
1:Y:746:LYS:HB2	1:Y:864:THR:HB	1.75	0.68
1:B:746:LYS:HB2	1:B:864:THR:HB	1.76	0.68
1:T:746:LYS:HB2	1:T:864:THR:HB	1.75	0.68
2:D:4:LEU:HB2	2:D:102:GLY:HA2	1.73	0.67
1:L:746:LYS:HB2	1:L:864:THR:HB	1.75	0.67
1:P:748:LYS:HB3	1:P:862:GLU:HB3	1.77	0.66
1:P:746:LYS:HB2	1:P:864:THR:HB	1.76	0.66
1:V:378:LYS:HD3	1:V:393:GLU:HB2	1.78	0.66
1:T:748:LYS:HB3	1:T:862:GLU:HB3	1.78	0.66
2:R:4:LEU:HB2	2:R:102:GLY:HA2	1.78	0.65
1:B:748:LYS:HB3	1:B:862:GLU:HB3	1.77	0.65
2:F:4:LEU:HB2	2:F:102:GLY:HA2	1.78	0.65
1:Y:748:LYS:HB3	1:Y:862:GLU:HB3	1.78	0.65
1:M:495:SER:N	1:M:520:THR:O	2.29	0.65
1:I:378:LYS:HD3	1:I:393:GLU:HB2	1.78	0.64
1:L:748:LYS:HB3	1:L:862:GLU:HB3	1.78	0.64
1:H:748:LYS:HB3	1:H:862:GLU:HB3	1.78	0.64
1:A:495:SER:N	1:A:520:THR:O	2.29	0.63
1:Y:1029:CYS:O	1:Y:1106:ARG:NH1	2.31	0.63
1:L:981:LEU:O	1:L:983:GLN:N	2.31	0.63
1:T:771:CYS:HB3	1:T:837:THR:HG22	1.80	0.63
1:L:735:LYS:HZ1	1:L:738:LYS:HA	1.64	0.63
1:H:735:LYS:HZ1	1:H:738:LYS:HA	1.63	0.63
1:Y:981:LEU:O	1:Y:983:GLN:N	2.31	0.63
1:L:1029:CYS:O	1:L:1106:ARG:NH1	2.31	0.63
1:B:771:CYS:HB3	1:B:837:THR:HG22	1.80	0.63
1:T:735:LYS:HZ1	1:T:738:LYS:HA	1.63	0.62
1:B:955:SER:OG	1:B:966:THR:O	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:981:LEU:O	1:P:983:GLN:N	2.32	0.62
1:P:771:CYS:HB3	1:P:837:THR:HG22	1.81	0.62
1:Y:771:CYS:HB3	1:Y:837:THR:HG22	1.81	0.62
1:C:495:SER:N	1:C:520:THR:O	2.31	0.62
1:A:391:LYS:NZ	1:A:393:GLU:OE2	2.29	0.62
1:V:495:SER:N	1:V:520:THR:O	2.32	0.62
1:I:495:SER:N	1:I:520:THR:O	2.32	0.61
1:B:981:LEU:O	1:B:983:GLN:N	2.32	0.61
1:Q:495:SER:N	1:Q:520:THR:O	2.31	0.61
1:H:797:SER:OG	1:H:799:GLU:OE1	2.19	0.61
1:I:502:SER:OG	1:L:982:PRO:O	2.18	0.61
1:L:771:CYS:HB3	1:L:837:THR:HG22	1.81	0.61
1:P:735:LYS:HZ1	1:P:738:LYS:HA	1.66	0.61
1:L:797:SER:OG	1:L:799:GLU:OE1	2.19	0.61
1:L:1100:SER:HB2	1:L:1105:GLU:HA	1.84	0.60
1:H:771:CYS:HB3	1:H:837:THR:HG22	1.83	0.60
1:V:502:SER:OG	1:Y:982:PRO:O	2.18	0.60
1:Y:955:SER:OG	1:Y:966:THR:O	2.15	0.60
1:A:367:LEU:HD13	1:A:422:ALA:HB2	1.84	0.60
1:B:1047:ARG:HD2	1:B:1083:CYS:HB3	1.84	0.60
1:P:785:VAL:O	1:P:789:LEU:HD12	2.01	0.60
1:T:1100:SER:HA	1:T:1106:ARG:HH21	1.66	0.60
1:B:922:GLU:OE2	1:B:922:GLU:N	2.25	0.60
1:Y:1100:SER:HB2	1:Y:1105:GLU:HA	1.84	0.60
1:B:785:VAL:O	1:B:789:LEU:HD12	2.01	0.60
1:P:1047:ARG:HD2	1:P:1083:CYS:HB3	1.84	0.60
1:B:735:LYS:HZ1	1:B:738:LYS:HA	1.66	0.59
1:T:797:SER:OG	1:T:799:GLU:OE1	2.19	0.59
1:Y:797:SER:OG	1:Y:799:GLU:OE1	2.19	0.59
1:Y:735:LYS:HZ1	1:Y:738:LYS:HA	1.66	0.59
1:H:981:LEU:O	1:H:983:GLN:N	2.34	0.59
1:P:797:SER:OG	1:P:799:GLU:OE1	2.20	0.59
1:Y:901:ASN:OD1	1:Y:902:SER:N	2.36	0.59
1:B:901:ASN:OD1	1:B:902:SER:N	2.36	0.59
1:H:901:ASN:OD1	1:H:902:SER:N	2.35	0.59
1:M:367:LEU:HD13	1:M:422:ALA:HB2	1.84	0.59
1:H:1100:SER:HA	1:H:1106:ARG:HH21	1.66	0.59
1:M:502:SER:OG	1:P:982:PRO:O	2.19	0.59
1:T:889:SER:OG	1:T:1012:THR:OG1	2.20	0.59
1:H:1060:LEU:HD13	1:H:1062:ALA:H	1.67	0.59
1:P:1100:SER:HA	1:P:1106:ARG:HH21	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:797:SER:OG	1:B:799:GLU:OE1	2.20	0.58
1:C:378:LYS:HD3	1:C:393:GLU:HB2	1.85	0.58
1:L:889:SER:OG	1:L:1012:THR:OG1	2.20	0.58
1:P:955:SER:OG	1:P:966:THR:O	2.12	0.58
1:A:502:SER:OG	1:B:982:PRO:O	2.19	0.58
1:I:511:CYS:HB2	1:L:1133:VAL:HG11	1.84	0.58
1:L:1047:ARG:HD2	1:L:1083:CYS:HB3	1.85	0.58
1:Y:785:VAL:O	1:Y:789:LEU:HD12	2.04	0.58
1:H:981:LEU:HD11	1:H:999:VAL:HG12	1.86	0.58
1:Q:378:LYS:HD3	1:Q:393:GLU:HB2	1.84	0.58
1:T:981:LEU:O	1:T:983:GLN:N	2.34	0.58
1:H:889:SER:OG	1:H:1012:THR:OG1	2.20	0.58
1:L:901:ASN:OD1	1:L:902:SER:N	2.36	0.58
1:M:391:LYS:NZ	1:M:393:GLU:OE2	2.29	0.58
1:V:511:CYS:HB2	1:Y:1133:VAL:HG11	1.84	0.58
2:F:29:ILE:O	2:F:68:LYS:NZ	2.31	0.58
1:Y:1047:ARG:HD2	1:Y:1083:CYS:HB3	1.85	0.58
1:L:785:VAL:O	1:L:789:LEU:HD12	2.04	0.57
1:T:1073:LEU:HD22	1:T:1082:GLN:HB3	1.86	0.57
1:V:183:THR:HG22	1:V:184:TYR:H	1.69	0.57
1:B:953:LEU:HD23	1:B:969:LEU:HD21	1.86	0.57
1:C:502:SER:OG	1:H:982:PRO:O	2.21	0.57
1:B:889:SER:OG	1:B:1012:THR:OG1	2.22	0.57
1:B:1100:SER:HB2	1:B:1105:GLU:HA	1.87	0.57
1:C:286:GLN:OE1	3:G:56:SER:OG	2.22	0.57
1:T:1060:LEU:HD13	1:T:1062:ALA:H	1.68	0.57
1:P:1100:SER:HB2	1:P:1105:GLU:HA	1.87	0.57
1:M:276:GLU:OE2	1:M:285:ARG:NH1	2.38	0.57
1:T:981:LEU:HD11	1:T:999:VAL:HG12	1.85	0.57
1:P:901:ASN:OD1	1:P:902:SER:N	2.36	0.57
1:P:1073:LEU:HD22	1:P:1082:GLN:HB3	1.86	0.57
1:B:906:ILE:HD11	1:B:929:LEU:HD21	1.87	0.57
1:B:1100:SER:HA	1:B:1106:ARG:HH21	1.68	0.57
1:L:1060:LEU:HD13	1:L:1062:ALA:H	1.69	0.57
1:P:922:GLU:OE2	1:P:922:GLU:N	2.25	0.56
1:A:276:GLU:OE2	1:A:285:ARG:NH1	2.38	0.56
1:Q:367:LEU:HD13	1:Q:422:ALA:HB2	1.87	0.56
1:Q:502:SER:OG	1:T:982:PRO:O	2.21	0.56
1:Y:1060:LEU:HD13	1:Y:1062:ALA:H	1.69	0.56
1:I:183:THR:HG22	1:I:184:TYR:H	1.69	0.56
1:B:847:LEU:HD12	1:B:972:PRO:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:367:LEU:HD13	1:V:422:ALA:HB2	1.87	0.56
2:J:4:LEU:HB2	2:J:102:GLY:HA2	1.88	0.56
1:C:367:LEU:HD13	1:C:422:ALA:HB2	1.87	0.56
1:L:1100:SER:HA	1:L:1106:ARG:HH21	1.70	0.56
1:T:901:ASN:OD1	1:T:902:SER:N	2.36	0.56
1:H:1100:SER:HB2	1:H:1105:GLU:HA	1.87	0.56
1:I:367:LEU:HD13	1:I:422:ALA:HB2	1.87	0.56
1:B:1073:LEU:HD22	1:B:1082:GLN:HB3	1.87	0.56
1:H:1073:LEU:HD22	1:H:1082:GLN:HB3	1.87	0.56
3:K:41:GLN:HB2	3:K:47:LEU:HD13	1.88	0.56
1:P:889:SER:OG	1:P:1012:THR:OG1	2.21	0.56
1:Q:286:GLN:OE1	3:S:56:SER:OG	2.24	0.56
1:Y:1045:GLY:HA3	1:Y:1085:ILE:HD11	1.88	0.56
1:Y:1100:SER:HA	1:Y:1106:ARG:HH21	1.70	0.56
2:D:34:PHE:HB3	3:E:112:TRP:HE1	1.71	0.55
3:G:36:TRP:CE3	3:G:99:THR:HG21	2.41	0.55
1:A:183:THR:HG22	1:A:184:TYR:H	1.71	0.55
1:M:183:THR:HG22	1:M:184:TYR:H	1.71	0.55
1:M:286:GLN:OE1	3:O:56:SER:OG	2.24	0.55
1:Q:511:CYS:HB2	1:T:1133:VAL:HG11	1.88	0.55
3:S:36:TRP:CE3	3:S:99:THR:HG21	2.41	0.55
1:T:1100:SER:HB2	1:T:1105:GLU:HA	1.89	0.55
1:I:286:GLN:OE1	3:K:56:SER:OG	2.24	0.55
2:J:34:PHE:HB3	3:K:112:TRP:HE1	1.72	0.55
1:P:1060:LEU:HD13	1:P:1062:ALA:H	1.71	0.55
1:Y:847:LEU:HD12	1:Y:972:PRO:HB2	1.89	0.55
1:M:511:CYS:HB2	1:P:1133:VAL:HG11	1.88	0.55
1:B:1045:GLY:HA3	1:B:1085:ILE:HD11	1.89	0.55
1:B:1060:LEU:HD13	1:B:1062:ALA:H	1.71	0.55
3:O:106:ASP:OD1	3:O:106:ASP:N	2.35	0.55
1:P:906:ILE:HD11	1:P:929:LEU:HD21	1.87	0.55
1:C:511:CYS:HB2	1:H:1133:VAL:HG11	1.88	0.55
2:D:29:ILE:O	2:D:68:LYS:NZ	2.32	0.55
1:L:955:SER:OG	1:L:966:THR:O	2.13	0.55
1:L:1045:GLY:HA3	1:L:1085:ILE:HD11	1.89	0.55
1:T:847:LEU:HD12	1:T:972:PRO:HB2	1.87	0.55
1:Y:981:LEU:HD11	1:Y:999:VAL:HG12	1.89	0.55
1:A:511:CYS:HB2	1:B:1133:VAL:HG11	1.88	0.55
3:K:36:TRP:CE3	3:K:99:THR:HG21	2.42	0.55
3:O:36:TRP:CE3	3:O:99:THR:HG21	2.42	0.55
1:H:1036:LEU:HD13	1:H:1048:VAL:HG12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:745:LEU:HD12	1:B:865:ASP:HA	1.89	0.54
1:C:183:THR:HG22	1:C:184:TYR:H	1.72	0.54
2:N:34:PHE:HB3	3:O:112:TRP:HE1	1.71	0.54
1:Y:1073:LEU:HD22	1:Y:1082:GLN:HB3	1.89	0.54
1:L:981:LEU:HD11	1:L:999:VAL:HG12	1.89	0.54
3:O:116:LEU:HD23	3:O:116:LEU:O	2.08	0.54
1:Q:183:THR:HG22	1:Q:184:TYR:H	1.72	0.54
1:Y:745:LEU:HD12	1:Y:865:ASP:HA	1.90	0.54
1:A:286:GLN:OE1	3:E:56:SER:OG	2.24	0.54
1:P:745:LEU:HD12	1:P:865:ASP:HA	1.89	0.54
1:P:1045:GLY:HA3	1:P:1085:ILE:HD11	1.89	0.54
2:W:34:PHE:HB3	3:X:112:TRP:HE1	1.71	0.54
1:Y:1064:ASN:ND2	1:Y:1066:ASP:OD1	2.41	0.54
3:E:36:TRP:CE3	3:E:99:THR:HG21	2.42	0.54
1:B:877:ALA:HB2	1:B:892:LEU:HD22	1.89	0.54
1:B:981:LEU:HD11	1:B:999:VAL:HG12	1.90	0.54
1:P:877:ALA:HB2	1:P:892:LEU:HD22	1.89	0.54
1:B:700:ARG:O	1:B:711:THR:OG1	2.26	0.54
1:T:885:TRP:HB2	1:T:1017:ASN:H	1.73	0.54
1:L:877:ALA:HB2	1:L:892:LEU:HD22	1.89	0.54
1:P:981:LEU:HD11	1:P:999:VAL:HG12	1.90	0.54
1:Y:885:TRP:HB2	1:Y:1017:ASN:H	1.72	0.54
1:B:710:ASN:HD21	1:B:1019:GLU:HB3	1.72	0.54
1:H:906:ILE:HD11	1:H:929:LEU:HD21	1.89	0.54
3:K:115:ASP:N	3:K:115:ASP:OD1	2.41	0.54
1:L:1064:ASN:ND2	1:L:1066:ASP:OD1	2.41	0.54
1:L:1073:LEU:HD22	1:L:1082:GLN:HB3	1.88	0.54
1:T:906:ILE:HD11	1:T:929:LEU:HD21	1.89	0.54
3:E:116:LEU:HD23	3:E:116:LEU:O	2.08	0.54
2:F:34:PHE:HB3	3:G:112:TRP:HE1	1.73	0.54
1:H:847:LEU:HD12	1:H:972:PRO:HB2	1.89	0.54
1:P:847:LEU:HD12	1:P:972:PRO:HB2	1.88	0.54
1:P:885:TRP:HB2	1:P:1017:ASN:H	1.73	0.54
1:T:745:LEU:HD12	1:T:865:ASP:HA	1.90	0.54
3:X:36:TRP:CE3	3:X:99:THR:HG21	2.42	0.54
1:H:1047:ARG:HD2	1:H:1083:CYS:HB3	1.90	0.53
1:L:885:TRP:HB2	1:L:1017:ASN:H	1.73	0.53
1:Y:877:ALA:HB2	1:Y:892:LEU:HD22	1.89	0.53
1:M:541:MET:SD	1:M:541:MET:N	2.81	0.53
1:V:541:MET:SD	1:V:541:MET:N	2.81	0.53
1:L:745:LEU:HD12	1:L:865:ASP:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:847:LEU:HD12	1:L:972:PRO:HB2	1.89	0.53
1:L:898:SER:O	1:L:898:SER:OG	2.26	0.53
1:T:1036:LEU:HD13	1:T:1048:VAL:HG12	1.89	0.53
1:T:1047:ARG:HD2	1:T:1083:CYS:HB3	1.90	0.53
3:G:116:LEU:HD23	3:G:116:LEU:O	2.09	0.53
1:B:1064:ASN:ND2	1:B:1066:ASP:OD1	2.41	0.53
3:K:116:LEU:O	3:K:116:LEU:HD23	2.09	0.53
3:S:115:ASP:OD1	3:S:115:ASP:N	2.41	0.53
1:T:1064:ASN:ND2	1:T:1066:ASP:OD1	2.42	0.53
1:P:1064:ASN:ND2	1:P:1066:ASP:OD1	2.41	0.53
1:V:286:GLN:OE1	3:X:56:SER:OG	2.25	0.53
1:H:745:LEU:HD12	1:H:865:ASP:HA	1.90	0.53
1:H:1064:ASN:ND2	1:H:1066:ASP:OD1	2.42	0.52
1:A:541:MET:SD	1:A:541:MET:N	2.81	0.52
1:B:885:TRP:HB2	1:B:1017:ASN:H	1.72	0.52
1:Q:276:GLU:OE2	1:Q:285:ARG:NH1	2.42	0.52
1:H:898:SER:O	1:H:898:SER:OG	2.25	0.52
1:B:957:LYS:HE3	1:Y:997:ARG:HH22	1.75	0.52
3:S:116:LEU:O	3:S:116:LEU:HD23	2.09	0.52
2:W:4:LEU:HB2	2:W:102:GLY:HA2	1.90	0.52
1:I:541:MET:SD	1:I:541:MET:N	2.82	0.52
1:C:276:GLU:OE2	1:C:285:ARG:NH1	2.42	0.52
1:H:885:TRP:HB2	1:H:1017:ASN:H	1.73	0.52
3:G:115:ASP:OD1	3:G:115:ASP:N	2.40	0.52
3:X:116:LEU:HD23	3:X:116:LEU:O	2.09	0.52
1:H:953:LEU:HD23	1:H:969:LEU:HD21	1.91	0.52
1:V:512:VAL:HG22	1:V:527:PRO:HB3	1.92	0.52
1:Y:898:SER:O	1:Y:898:SER:OG	2.26	0.52
1:H:955:SER:OG	1:H:966:THR:O	2.14	0.51
1:H:1045:GLY:HA3	1:H:1085:ILE:HD11	1.92	0.51
1:B:898:SER:O	1:B:898:SER:OG	2.25	0.51
1:I:342:VAL:HG22	1:I:461:ARG:HG2	1.93	0.51
1:T:953:LEU:HD23	1:T:969:LEU:HD21	1.91	0.51
1:V:438:ASN:HB3	5:V:1301:NAG:O5	2.10	0.51
1:T:785:VAL:O	1:T:789:LEU:HD12	2.10	0.51
1:V:342:VAL:HG22	1:V:461:ARG:HG2	1.93	0.51
1:T:997:ARG:HH22	1:Y:957:LYS:HE3	1.75	0.51
3:E:106:ASP:OD1	3:E:106:ASP:N	2.35	0.51
1:H:785:VAL:O	1:H:789:LEU:HD12	2.10	0.51
1:P:997:ARG:HH22	1:T:957:LYS:HE3	1.75	0.51
3:X:115:ASP:OD1	3:X:115:ASP:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:906:ILE:HD11	1:Y:929:LEU:HD21	1.92	0.51
1:I:438:ASN:HD21	5:I:1301:NAG:H83	1.76	0.51
1:M:378:LYS:HD3	1:M:393:GLU:HB2	1.92	0.51
1:Q:541:MET:SD	1:Q:541:MET:N	2.84	0.51
1:A:378:LYS:HD3	1:A:393:GLU:HB2	1.92	0.51
1:Q:438:ASN:HD21	5:Q:1301:NAG:H83	1.76	0.51
1:T:1045:GLY:HA3	1:T:1085:ILE:HD11	1.92	0.51
1:L:700:ARG:O	1:L:711:THR:OG1	2.27	0.50
1:L:921:SER:OG	1:L:925:ARG:NH2	2.43	0.50
2:R:19:THR:HA	2:R:75:LEU:O	2.11	0.50
1:P:883:THR:OG1	1:P:884:ASN:N	2.44	0.50
1:Q:438:ASN:HB3	5:Q:1301:NAG:O5	2.11	0.50
1:I:512:VAL:HG22	1:I:527:PRO:HB3	1.93	0.50
1:C:541:MET:SD	1:C:541:MET:N	2.85	0.50
2:F:19:THR:HA	2:F:75:LEU:O	2.10	0.50
1:Q:287:MET:HE2	1:V:392:ARG:HG2	1.93	0.50
1:C:342:VAL:HG22	1:C:461:ARG:HG2	1.94	0.50
1:Y:873:ILE:HD11	1:Y:881:ARG:HG2	1.94	0.50
1:I:438:ASN:HB3	5:I:1301:NAG:O5	2.10	0.50
1:Q:512:VAL:HG22	1:Q:527:PRO:HB3	1.94	0.50
2:R:34:PHE:HB3	3:S:112:TRP:HE1	1.76	0.50
1:A:342:VAL:HG22	1:A:461:ARG:HG2	1.94	0.50
1:M:342:VAL:HG22	1:M:461:ARG:HG2	1.94	0.50
3:O:37:SER:OG	3:O:49:TRP:NE1	2.41	0.50
1:T:873:ILE:HD11	1:T:881:ARG:HG2	1.94	0.50
1:H:922:GLU:H	1:H:922:GLU:CD	2.18	0.50
1:L:906:ILE:HD11	1:L:929:LEU:HD21	1.92	0.50
1:T:893:ASP:OD1	1:T:893:ASP:N	2.44	0.50
1:M:512:VAL:HG22	1:M:527:PRO:HB3	1.94	0.49
1:Q:342:VAL:HG22	1:Q:461:ARG:HG2	1.94	0.49
1:C:512:VAL:HG22	1:C:527:PRO:HB3	1.94	0.49
1:P:921:SER:OG	1:P:925:ARG:NH2	2.45	0.49
1:T:883:THR:OG1	1:T:884:ASN:N	2.45	0.49
1:L:873:ILE:HD11	1:L:881:ARG:HG2	1.94	0.49
1:M:438:ASN:HB3	5:M:1301:NAG:O5	2.13	0.49
1:A:438:ASN:HB3	5:A:1301:NAG:O5	2.13	0.49
1:V:438:ASN:HD21	5:V:1301:NAG:H83	1.76	0.49
1:C:438:ASN:HD21	5:C:1301:NAG:H83	1.77	0.49
1:Y:1034:LEU:HB2	1:Y:1049:CYS:O	2.13	0.49
1:B:883:THR:OG1	1:B:884:ASN:N	2.44	0.49
1:A:512:VAL:HG22	1:A:527:PRO:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:MET:HE2	1:I:392:ARG:HG2	1.93	0.49
3:K:37:SER:OG	3:K:49:TRP:NE1	2.43	0.49
3:X:41:GLN:HB2	3:X:47:LEU:HD13	1.94	0.49
2:N:19:THR:HA	2:N:75:LEU:O	2.13	0.49
2:N:90:CYS:O	2:N:102:GLY:N	2.45	0.49
2:D:19:THR:HA	2:D:75:LEU:O	2.13	0.49
2:D:90:CYS:O	2:D:102:GLY:N	2.45	0.49
1:Y:883:THR:OG1	1:Y:884:ASN:N	2.45	0.49
1:H:873:ILE:HD11	1:H:881:ARG:HG2	1.94	0.48
1:I:359:LEU:HD12	1:I:445:ILE:HD11	1.94	0.48
1:L:706:THR:HB	1:L:709:VAL:HG22	1.95	0.48
1:C:228:SER:O	1:C:228:SER:OG	2.31	0.48
1:Q:199:LYS:O	1:Q:204:GLN:NE2	2.46	0.48
1:C:199:LYS:O	1:C:204:GLN:NE2	2.46	0.48
1:H:700:ARG:O	1:H:711:THR:OG1	2.27	0.48
1:Y:921:SER:OG	1:Y:925:ARG:NH2	2.43	0.48
1:B:828:VAL:HG11	1:V:337:SER:HB2	1.96	0.48
1:H:1098:MET:HE2	1:H:1098:MET:HA	1.95	0.48
1:L:1034:LEU:HB2	1:L:1049:CYS:O	2.13	0.48
1:Q:485:LYS:HB3	1:Q:485:LYS:HE2	1.61	0.48
1:L:883:THR:OG1	1:L:884:ASN:N	2.45	0.48
1:P:873:ILE:HD11	1:P:881:ARG:HG2	1.96	0.48
1:Y:1074:PRO:O	1:Y:1082:GLN:NE2	2.47	0.48
1:L:1033:PHE:HA	1:L:1050:LEU:HD13	1.96	0.48
1:H:883:THR:OG1	1:H:884:ASN:N	2.45	0.48
1:L:893:ASP:OD1	1:L:893:ASP:N	2.44	0.48
1:Y:957:LYS:HG2	1:Y:959:MET:HG2	1.96	0.48
1:Y:1033:PHE:HA	1:Y:1050:LEU:HD13	1.96	0.48
1:A:557:PRO:O	1:A:559:GLN:NE2	2.40	0.48
1:B:873:ILE:HD11	1:B:881:ARG:HG2	1.96	0.48
1:L:1074:PRO:O	1:L:1082:GLN:NE2	2.46	0.47
1:H:921:SER:OG	1:H:925:ARG:NH2	2.46	0.47
1:H:950:ALA:HB3	1:H:953:LEU:HD11	1.96	0.47
1:P:893:ASP:OD1	1:P:893:ASP:N	2.45	0.47
1:T:921:SER:OG	1:T:925:ARG:NH2	2.46	0.47
1:P:953:LEU:HD23	1:P:969:LEU:HD21	1.96	0.47
1:B:957:LYS:HG2	1:B:959:MET:HG2	1.95	0.47
1:M:557:PRO:O	1:M:559:GLN:NE2	2.40	0.47
1:A:228:SER:O	1:A:228:SER:OG	2.32	0.47
1:H:706:THR:HB	1:H:709:VAL:HG22	1.96	0.47
1:T:720:LEU:HG	1:V:545:ASP:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:955:SER:OG	1:T:966:THR:O	2.11	0.47
3:E:115:ASP:OD1	3:E:115:ASP:N	2.47	0.47
3:K:53:ILE:HG13	3:K:59:THR:HG22	1.96	0.47
1:H:1074:PRO:O	1:H:1082:GLN:NE2	2.48	0.47
1:I:199:LYS:O	1:I:204:GLN:NE2	2.48	0.47
1:I:337:SER:HB2	1:P:828:VAL:HG11	1.96	0.47
3:S:37:SER:OG	3:S:49:TRP:NE1	2.42	0.47
1:T:700:ARG:O	1:T:711:THR:OG1	2.27	0.47
1:T:1074:PRO:O	1:T:1082:GLN:NE2	2.48	0.47
1:Y:706:THR:HB	1:Y:709:VAL:HG22	1.96	0.47
1:B:921:SER:OG	1:B:925:ARG:NH2	2.45	0.47
1:I:376:GLU:OE2	1:I:384:THR:OG1	2.30	0.47
1:M:199:LYS:O	1:M:204:GLN:NE2	2.48	0.47
3:G:37:SER:OG	3:G:49:TRP:NE1	2.42	0.47
1:I:557:PRO:O	1:I:559:GLN:NE2	2.39	0.47
2:J:29:ILE:O	2:J:68:LYS:NZ	2.33	0.47
1:P:1074:PRO:O	1:P:1082:GLN:NE2	2.48	0.47
1:T:922:GLU:H	1:T:922:GLU:CD	2.18	0.47
1:T:1030:ASP:N	1:T:1053:THR:O	2.48	0.47
1:A:485:LYS:HB3	1:A:485:LYS:HE2	1.62	0.47
1:M:347:VAL:O	1:M:455:LEU:N	2.48	0.47
1:P:732:LEU:HD23	1:P:732:LEU:HA	1.78	0.46
1:Y:1108:LEU:HD12	1:Y:1108:LEU:HA	1.85	0.46
1:A:372:PHE:HB2	1:A:399:ILE:HD12	1.97	0.46
1:C:438:ASN:HB3	5:C:1301:NAG:O5	2.15	0.46
1:I:300:GLN:NE2	1:I:460:GLU:OE2	2.48	0.46
1:I:311:GLY:HA2	1:I:314:LEU:HD23	1.97	0.46
1:M:260:LEU:HD21	1:M:347:VAL:HG21	1.97	0.46
1:M:471:LYS:HD2	1:M:471:LYS:HA	1.67	0.46
1:V:199:LYS:O	1:V:204:GLN:NE2	2.48	0.46
1:Y:889:SER:OG	1:Y:1012:THR:OG1	2.29	0.46
1:I:561:PRO:HG2	1:L:1115:ILE:HG21	1.97	0.46
1:P:1030:ASP:N	1:P:1053:THR:O	2.49	0.46
1:Q:280:ASP:OD1	1:Q:280:ASP:N	2.49	0.46
1:T:738:LYS:HA	1:T:738:LYS:HD2	1.77	0.46
2:D:28:ASP:O	2:D:30:GLY:N	2.42	0.46
1:B:721:ILE:HD12	1:B:721:ILE:C	2.41	0.46
1:C:280:ASP:OD1	1:C:280:ASP:N	2.49	0.46
1:C:311:GLY:HA2	1:C:314:LEU:HD23	1.96	0.46
1:C:562:CYS:HA	1:C:565:HIS:CE1	2.51	0.46
2:F:90:CYS:O	2:F:102:GLY:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:311:GLY:HA2	1:M:314:LEU:HD23	1.97	0.46
1:V:311:GLY:HA2	1:V:314:LEU:HD23	1.97	0.46
1:B:1074:PRO:O	1:B:1082:GLN:NE2	2.48	0.46
1:Y:700:ARG:O	1:Y:711:THR:OG1	2.28	0.46
1:A:260:LEU:HD21	1:A:347:VAL:HG21	1.97	0.46
1:H:858:LYS:HB2	1:H:858:LYS:HE3	1.65	0.46
1:M:372:PHE:HB2	1:M:399:ILE:HD12	1.97	0.46
1:A:199:LYS:O	1:A:204:GLN:NE2	2.48	0.46
1:I:562:CYS:HA	1:I:565:HIS:CE1	2.51	0.46
1:M:280:ASP:OD1	1:M:280:ASP:N	2.49	0.46
2:R:90:CYS:O	2:R:102:GLY:N	2.48	0.46
1:V:542:ALA:HB2	1:Y:982:PRO:HB2	1.98	0.46
1:P:1033:PHE:HA	1:P:1050:LEU:HD13	1.98	0.46
1:Q:311:GLY:HA2	1:Q:314:LEU:HD23	1.97	0.46
1:T:706:THR:HB	1:T:709:VAL:HG22	1.96	0.46
1:B:712:LYS:HE2	1:B:712:LYS:HB2	1.75	0.46
1:P:700:ARG:O	1:P:711:THR:OG1	2.28	0.46
1:Y:953:LEU:HD23	1:Y:969:LEU:HD21	1.98	0.46
1:Y:1040:TYR:HD2	1:Y:1114:LEU:HB2	1.81	0.46
1:A:347:VAL:O	1:A:455:LEU:N	2.48	0.45
3:E:37:SER:OG	3:E:49:TRP:NE1	2.41	0.45
1:B:981:LEU:HD23	1:B:981:LEU:HA	1.81	0.45
1:L:1040:TYR:HD2	1:L:1114:LEU:HB2	1.81	0.45
1:P:733:MET:HE1	1:P:744:PHE:CE2	2.52	0.45
1:V:561:PRO:HG2	1:Y:1115:ILE:HG21	1.98	0.45
1:A:311:GLY:HA2	1:A:314:LEU:HD23	1.97	0.45
1:B:1030:ASP:N	1:B:1053:THR:O	2.49	0.45
1:B:1033:PHE:HA	1:B:1050:LEU:HD13	1.98	0.45
1:I:540:HIS:HA	1:I:550:SER:O	2.17	0.45
1:L:722:ARG:NH1	1:L:1009:ALA:H	2.15	0.45
1:L:712:LYS:HB2	1:L:712:LYS:HE2	1.75	0.45
1:Q:240:MET:HE2	1:Q:240:MET:HB3	1.81	0.45
1:Q:558:PRO:HG3	4:c:1:NAG:H83	1.97	0.45
1:V:231:LEU:O	1:V:235:HIS:HB3	2.17	0.45
1:L:866:PHE:HD2	1:L:1018:PHE:HB3	1.82	0.45
1:M:540:HIS:HA	1:M:550:SER:O	2.16	0.45
1:Y:722:ARG:NH1	1:Y:1009:ALA:H	2.15	0.45
3:K:106:ASP:OD1	3:K:106:ASP:N	2.47	0.45
1:P:1036:LEU:HD13	1:P:1048:VAL:HG12	1.98	0.45
1:Q:562:CYS:HA	1:Q:565:HIS:CE1	2.51	0.45
1:Y:738:LYS:HA	1:Y:738:LYS:HD2	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:GLU:OE2	1:C:384:THR:OG1	2.29	0.45
1:I:280:ASP:OD1	1:I:280:ASP:N	2.49	0.45
1:L:858:LYS:HB2	1:L:858:LYS:HE3	1.65	0.45
1:A:376:GLU:OE2	1:A:384:THR:OG1	2.31	0.45
1:B:733:MET:HE1	1:B:744:PHE:CE2	2.52	0.45
1:Q:471:LYS:HD2	1:Q:471:LYS:HA	1.67	0.45
1:A:562:CYS:HA	1:A:565:HIS:CE1	2.52	0.45
1:C:561:PRO:HG2	1:H:1115:ILE:HG21	1.98	0.45
1:I:231:LEU:O	1:I:235:HIS:HB3	2.17	0.45
1:Q:483:ILE:HD11	1:Q:494:ARG:HE	1.81	0.45
1:A:561:PRO:HG2	1:B:1115:ILE:HG21	1.99	0.45
1:B:837:THR:HG21	1:B:956:TYR:HE1	1.82	0.45
1:C:540:HIS:HA	1:C:550:SER:O	2.17	0.45
1:M:562:CYS:HA	1:M:565:HIS:CE1	2.51	0.45
1:Q:336:LEU:HD23	1:Q:336:LEU:HA	1.86	0.45
1:Q:561:PRO:HG2	1:T:1115:ILE:HG21	1.98	0.45
1:V:484:THR:HG22	1:V:493:VAL:HG23	1.99	0.45
1:V:562:CYS:HA	1:V:565:HIS:CE1	2.51	0.45
1:A:359:LEU:HD12	1:A:359:LEU:HA	1.87	0.45
1:B:1036:LEU:HD13	1:B:1048:VAL:HG12	1.97	0.45
1:C:377:HIS:HB2	1:C:380:GLN:HB2	1.99	0.45
1:H:1030:ASP:N	1:H:1053:THR:O	2.48	0.45
1:H:1108:LEU:HD12	1:H:1108:LEU:HA	1.85	0.45
1:P:720:LEU:HG	1:Q:545:ASP:HA	1.98	0.45
1:P:837:THR:HG21	1:P:956:TYR:HE1	1.82	0.45
1:P:1034:LEU:HB2	1:P:1049:CYS:O	2.17	0.45
1:A:540:HIS:HA	1:A:550:SER:O	2.16	0.44
2:D:38:TYR:HB3	2:D:46:PRO:HB2	1.99	0.44
1:H:722:ARG:NH1	1:H:1009:ALA:H	2.15	0.44
1:I:485:LYS:HE2	1:I:485:LYS:HB3	1.62	0.44
1:M:561:PRO:HG2	1:P:1115:ILE:HG21	1.99	0.44
2:N:38:TYR:HB3	2:N:46:PRO:HB2	1.99	0.44
1:T:1098:MET:HE2	1:T:1098:MET:HA	1.99	0.44
1:H:712:LYS:HE2	1:H:712:LYS:HB2	1.75	0.44
1:L:1098:MET:HE2	1:L:1098:MET:HA	2.00	0.44
1:Q:382:LYS:HD2	1:Q:382:LYS:HA	1.87	0.44
1:A:382:LYS:HD2	1:A:382:LYS:HA	1.88	0.44
1:C:471:LYS:HD2	1:C:471:LYS:HA	1.67	0.44
1:H:837:THR:HG21	1:H:956:TYR:HE1	1.82	0.44
3:O:115:ASP:OD1	3:O:115:ASP:N	2.47	0.44
1:P:722:ARG:NH1	1:P:1009:ALA:H	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:865:ASP:OD1	1:B:866:PHE:N	2.48	0.44
1:B:950:ALA:HB3	1:B:953:LEU:HD11	1.99	0.44
1:C:558:PRO:HG3	4:Z:1:NAG:H83	2.00	0.44
1:H:864:THR:HG23	1:H:869:SER:HB3	1.99	0.44
1:I:471:LYS:HD2	1:I:471:LYS:HA	1.67	0.44
1:P:898:SER:O	1:P:898:SER:OG	2.25	0.44
1:Q:337:SER:HB2	1:Y:828:VAL:HG11	2.00	0.44
1:Q:539:VAL:HG12	1:Q:541:MET:HE3	2.00	0.44
1:T:734:LEU:HD23	1:T:743:LYS:HB2	2.00	0.44
1:Y:866:PHE:HD2	1:Y:1018:PHE:HB3	1.82	0.44
1:Y:953:LEU:O	1:Y:967:THR:OG1	2.33	0.44
1:C:557:PRO:O	1:C:559:GLN:NE2	2.40	0.44
1:H:866:PHE:HD2	1:H:1018:PHE:HB3	1.83	0.44
1:M:366:ASN:HD22	1:M:368:LEU:HD23	1.83	0.44
1:P:866:PHE:HD2	1:P:1018:PHE:HB3	1.83	0.44
1:I:366:ASN:HD22	1:I:368:LEU:HD23	1.82	0.44
1:I:542:ALA:HB2	1:L:982:PRO:HB2	1.98	0.44
1:L:864:THR:HG23	1:L:869:SER:HB3	2.00	0.44
2:F:38:TYR:HB3	2:F:46:PRO:HB2	2.00	0.44
1:H:981:LEU:HA	1:H:981:LEU:HD23	1.78	0.44
1:L:950:ALA:HB3	1:L:953:LEU:HD11	2.00	0.44
1:Q:377:HIS:HB2	1:Q:380:GLN:HB2	1.99	0.44
1:Q:484:THR:HG22	1:Q:493:VAL:HG23	2.00	0.44
1:Q:540:HIS:HA	1:Q:550:SER:O	2.18	0.44
1:T:712:LYS:HB2	1:T:712:LYS:HE2	1.75	0.44
3:X:37:SER:OG	3:X:49:TRP:NE1	2.43	0.44
1:T:722:ARG:NH1	1:T:1009:ALA:H	2.15	0.44
1:T:898:SER:O	1:T:898:SER:OG	2.25	0.44
1:A:366:ASN:HD22	1:A:368:LEU:HD23	1.83	0.44
1:H:953:LEU:O	1:H:967:THR:OG1	2.30	0.44
1:Q:231:LEU:O	1:Q:235:HIS:HB3	2.18	0.44
1:V:228:SER:O	1:V:228:SER:OG	2.30	0.44
1:V:540:HIS:HA	1:V:550:SER:O	2.18	0.44
1:A:280:ASP:OD1	1:A:280:ASP:N	2.49	0.43
1:C:539:VAL:HG12	1:C:541:MET:HE3	2.00	0.43
1:I:484:THR:HG22	1:I:493:VAL:HG23	1.99	0.43
1:M:558:PRO:HG3	4:b:1:NAG:H83	2.00	0.43
2:N:28:ASP:O	2:N:30:GLY:N	2.42	0.43
1:Q:260:LEU:HD21	1:Q:347:VAL:HG21	2.00	0.43
1:T:866:PHE:HD2	1:T:1018:PHE:HB3	1.83	0.43
1:T:1111:LYS:HE2	1:T:1111:LYS:HB2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1034:LEU:HB2	1:B:1049:CYS:O	2.17	0.43
1:B:1119:PRO:C	1:B:1121:ASP:H	2.26	0.43
1:C:231:LEU:O	1:C:235:HIS:HB3	2.18	0.43
1:Q:347:VAL:O	1:Q:455:LEU:N	2.51	0.43
1:T:994:LYS:HA	1:T:994:LYS:HD3	1.82	0.43
3:G:40:ARG:HB3	3:G:50:ILE:HD11	2.00	0.43
3:S:40:ARG:HB3	3:S:50:ILE:HD11	2.00	0.43
1:V:300:GLN:NE2	1:V:460:GLU:OE2	2.51	0.43
1:Y:1119:PRO:C	1:Y:1121:ASP:H	2.26	0.43
1:B:866:PHE:HD2	1:B:1018:PHE:HB3	1.83	0.43
1:H:1029:CYS:O	1:H:1106:ARG:NH1	2.51	0.43
1:I:558:PRO:HG3	4:a:1:NAG:H83	2.01	0.43
1:P:957:LYS:HG2	1:P:959:MET:HG2	1.99	0.43
1:V:280:ASP:OD1	1:V:280:ASP:N	2.49	0.43
1:C:260:LEU:HD21	1:C:347:VAL:HG21	2.00	0.43
1:L:733:MET:HE3	1:L:734:LEU:H	1.83	0.43
1:V:366:ASN:HD22	1:V:368:LEU:HD23	1.81	0.43
1:Y:864:THR:HG23	1:Y:869:SER:HB3	2.00	0.43
1:B:722:ARG:NH1	1:B:1009:ALA:H	2.16	0.43
1:B:858:LYS:HB2	1:B:858:LYS:HE3	1.65	0.43
1:C:347:VAL:O	1:C:455:LEU:N	2.51	0.43
2:F:89:TYR:CD1	3:G:47:LEU:HD22	2.54	0.43
1:I:505:ALA:O	1:I:511:CYS:HA	2.19	0.43
1:M:391:LYS:HB2	1:M:391:LYS:HE3	1.80	0.43
1:P:1119:PRO:C	1:P:1121:ASP:H	2.27	0.43
2:R:38:TYR:HB3	2:R:46:PRO:HB2	1.99	0.43
2:R:89:TYR:CD2	3:S:47:LEU:HD22	2.54	0.43
3:E:40:ARG:HB3	3:E:50:ILE:HD11	2.00	0.43
1:I:359:LEU:HD12	1:I:359:LEU:HA	1.90	0.43
1:I:372:PHE:HB2	1:I:399:ILE:HD12	2.01	0.43
1:B:888:VAL:HG22	1:B:1013:LEU:HD13	2.00	0.43
2:F:28:ASP:O	2:F:30:GLY:N	2.46	0.43
1:L:873:ILE:HD12	1:L:873:ILE:HA	1.86	0.43
1:P:811:GLU:OE2	1:P:956:TYR:OH	2.29	0.43
1:V:471:LYS:HA	1:V:471:LYS:HD2	1.67	0.43
1:C:483:ILE:HD11	1:C:494:ARG:HE	1.84	0.43
1:H:865:ASP:OD1	1:H:866:PHE:N	2.50	0.43
1:H:892:LEU:HD23	1:H:892:LEU:O	2.19	0.43
1:T:892:LEU:HD23	1:T:892:LEU:O	2.19	0.43
1:Y:865:ASP:OD1	1:Y:866:PHE:N	2.49	0.43
1:Y:1098:MET:HE2	1:Y:1098:MET:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1122:ASP:N	1:B:1122:ASP:OD1	2.52	0.43
1:C:183:THR:HG22	1:C:184:TYR:N	2.34	0.43
1:I:347:VAL:O	1:I:455:LEU:N	2.51	0.43
1:L:1119:PRO:C	1:L:1121:ASP:H	2.27	0.43
3:O:40:ARG:HB3	3:O:50:ILE:HD11	2.00	0.43
1:T:837:THR:HG21	1:T:956:TYR:HE1	1.83	0.43
1:V:336:LEU:HD23	1:V:336:LEU:HA	1.85	0.43
1:C:337:SER:HB2	1:L:828:VAL:HG11	2.00	0.42
1:H:1122:ASP:OD1	1:H:1122:ASP:N	2.51	0.42
1:I:228:SER:O	1:I:228:SER:OG	2.30	0.42
1:I:276:GLU:OE2	1:I:285:ARG:NH1	2.52	0.42
1:V:485:LYS:HE2	1:V:485:LYS:HB3	1.62	0.42
1:Y:1122:ASP:OD1	1:Y:1122:ASP:N	2.52	0.42
1:A:336:LEU:HD23	1:A:336:LEU:HA	1.83	0.42
1:H:994:LYS:HD3	1:H:994:LYS:HA	1.82	0.42
2:J:19:THR:HA	2:J:75:LEU:O	2.19	0.42
1:Q:376:GLU:OE2	1:Q:384:THR:OG1	2.31	0.42
1:T:864:THR:HG23	1:T:869:SER:HB3	2.00	0.42
1:V:372:PHE:HB2	1:V:399:ILE:HD12	2.01	0.42
1:Y:716:SER:HA	1:Y:1015:PHE:HA	2.01	0.42
1:M:487:GLU:O	1:M:526:TYR:OH	2.35	0.42
1:T:811:GLU:OE2	1:T:956:TYR:OH	2.27	0.42
1:B:864:THR:HG23	1:B:869:SER:HB3	2.01	0.42
1:P:888:VAL:HG22	1:P:1013:LEU:HD13	2.00	0.42
1:T:1029:CYS:O	1:T:1106:ARG:NH1	2.50	0.42
3:X:40:ARG:HB3	3:X:50:ILE:HD11	2.00	0.42
1:A:558:PRO:HG3	4:U:1:NAG:H83	2.00	0.42
1:M:485:LYS:HE2	1:M:485:LYS:HB3	1.62	0.42
1:Q:557:PRO:O	1:Q:559:GLN:NE2	2.42	0.42
1:T:950:ALA:HB3	1:T:953:LEU:HD11	2.01	0.42
1:V:558:PRO:HG3	4:d:1:NAG:H83	2.01	0.42
2:W:38:TYR:HB3	2:W:46:PRO:HB2	2.01	0.42
1:A:544:ASP:OD1	1:A:544:ASP:N	2.52	0.42
3:K:40:ARG:HB3	3:K:50:ILE:HD11	2.00	0.42
1:L:716:SER:HA	1:L:1015:PHE:HA	2.01	0.42
1:T:1122:ASP:OD1	1:T:1122:ASP:N	2.51	0.42
1:V:376:GLU:OE2	1:V:384:THR:OG1	2.30	0.42
1:V:382:LYS:HD2	1:V:382:LYS:HA	1.88	0.42
2:W:19:THR:HA	2:W:75:LEU:O	2.19	0.42
1:M:231:LEU:O	1:M:235:HIS:HB3	2.19	0.42
1:P:950:ALA:HB3	1:P:953:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:981:LEU:HD23	1:P:981:LEU:HA	1.81	0.42
1:T:865:ASP:OD1	1:T:866:PHE:N	2.50	0.42
1:V:505:ALA:O	1:V:511:CYS:HA	2.19	0.42
1:L:1122:ASP:N	1:L:1122:ASP:OD1	2.52	0.42
1:V:347:VAL:O	1:V:455:LEU:N	2.51	0.42
2:W:90:CYS:O	2:W:102:GLY:N	2.48	0.42
1:B:983:GLN:OE1	1:B:985:ARG:NH1	2.39	0.42
1:C:485:LYS:HE2	1:C:485:LYS:HB3	1.60	0.42
1:L:981:LEU:HD23	1:L:981:LEU:HA	1.80	0.42
1:P:994:LYS:HA	1:P:994:LYS:HD3	1.83	0.42
1:A:231:LEU:O	1:A:235:HIS:HB3	2.19	0.41
1:A:324:VAL:HG23	1:A:464:VAL:HG12	2.02	0.41
1:B:754:LEU:HD12	1:B:754:LEU:HA	1.90	0.41
1:B:994:LYS:HA	1:B:994:LYS:HD3	1.84	0.41
1:C:336:LEU:HD23	1:C:336:LEU:HA	1.85	0.41
1:M:324:VAL:HG23	1:M:464:VAL:HG12	2.02	0.41
1:P:1111:LYS:HB2	1:P:1111:LYS:HE2	1.85	0.41
1:Q:366:ASN:HD22	1:Q:368:LEU:HD23	1.85	0.41
2:R:91:ASN:HB3	2:R:101:PHE:CE1	2.55	0.41
1:C:372:PHE:HB2	1:C:399:ILE:HD12	2.02	0.41
1:H:1029:CYS:N	1:H:1101:CYS:SG	2.93	0.41
1:H:1119:PRO:C	1:H:1121:ASP:H	2.27	0.41
2:J:91:ASN:HB3	2:J:101:PHE:CE1	2.55	0.41
1:L:837:THR:HG21	1:L:956:TYR:HE1	1.84	0.41
1:L:1030:ASP:N	1:L:1053:THR:O	2.50	0.41
1:M:359:LEU:HD12	1:M:359:LEU:HA	1.88	0.41
1:T:716:SER:HA	1:T:1015:PHE:HA	2.02	0.41
2:W:91:ASN:HB3	2:W:101:PHE:CE1	2.55	0.41
1:Y:893:ASP:OD1	1:Y:893:ASP:N	2.43	0.41
2:J:38:TYR:HB3	2:J:46:PRO:HB2	2.01	0.41
1:L:754:LEU:HD12	1:L:754:LEU:HA	1.89	0.41
3:O:39:ILE:HG22	3:O:47:LEU:HB3	2.02	0.41
1:A:455:LEU:HD23	1:A:455:LEU:HA	1.93	0.41
3:E:39:ILE:HG22	3:E:47:LEU:HB3	2.02	0.41
1:C:484:THR:HG22	1:C:493:VAL:HG23	2.02	0.41
1:H:981:LEU:HD13	1:H:991:ALA:C	2.45	0.41
1:L:950:ALA:O	1:L:953:LEU:HD13	2.20	0.41
1:T:1065:LYS:H	1:T:1065:LYS:HG3	1.68	0.41
1:Y:837:THR:HG21	1:Y:956:TYR:HE1	1.84	0.41
2:F:52:ASP:OD1	3:G:113:TYR:OH	2.26	0.41
1:I:544:ASP:OD1	1:I:544:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1122:ASP:N	1:P:1122:ASP:OD1	2.52	0.41
1:T:981:LEU:HD13	1:T:991:ALA:C	2.45	0.41
1:B:1098:MET:HE2	1:B:1098:MET:HA	2.03	0.41
1:C:240:MET:HB3	1:C:240:MET:HE2	1.80	0.41
1:C:366:ASN:HD22	1:C:368:LEU:HD23	1.85	0.41
1:H:1038:GLY:O	1:H:1115:ILE:HG12	2.21	0.41
1:P:858:LYS:HE3	1:P:858:LYS:HB2	1.65	0.41
1:V:276:GLU:OE2	1:V:285:ARG:NH1	2.52	0.41
1:I:294:LYS:HE3	1:I:294:LYS:HB3	1.90	0.41
1:M:544:ASP:OD1	1:M:544:ASP:N	2.51	0.41
1:T:1038:GLY:O	1:T:1115:ILE:HG12	2.20	0.41
1:T:1119:PRO:C	1:T:1121:ASP:H	2.27	0.41
1:Y:931:GLU:H	1:Y:931:GLU:HG2	1.71	0.41
1:Y:1099:TYR:CE1	1:Y:1108:LEU:HD13	2.56	0.41
1:C:391:LYS:HE3	1:C:391:LYS:HB2	1.83	0.41
1:L:865:ASP:OD1	1:L:866:PHE:N	2.49	0.41
1:L:957:LYS:HG2	1:L:959:MET:HG2	2.02	0.41
1:L:1099:TYR:CE1	1:L:1108:LEU:HD13	2.56	0.41
1:P:864:THR:HG23	1:P:869:SER:HB3	2.01	0.41
1:T:733:MET:HE1	1:T:744:PHE:CE2	2.56	0.41
1:V:183:THR:HG22	1:V:184:TYR:N	2.35	0.41
1:V:260:LEU:HD21	1:V:347:VAL:HG21	2.03	0.41
1:B:1099:TYR:CE1	1:B:1108:LEU:HD13	2.56	0.41
1:I:260:LEU:HD21	1:I:347:VAL:HG21	2.02	0.41
1:L:734:LEU:HD23	1:L:743:LYS:HB2	2.02	0.41
1:L:994:LYS:HA	1:L:994:LYS:HD3	1.82	0.41
2:D:91:ASN:HB3	2:D:101:PHE:CD1	2.56	0.41
1:B:1038:GLY:O	1:B:1115:ILE:HG12	2.21	0.41
1:C:324:VAL:HG23	1:C:464:VAL:HG12	2.02	0.41
1:H:716:SER:HA	1:H:1015:PHE:HA	2.02	0.41
1:H:733:MET:HE1	1:H:744:PHE:CE1	2.56	0.41
1:I:487:GLU:HG3	1:I:489:HIS:H	1.86	0.41
1:M:376:GLU:OE2	1:M:384:THR:OG1	2.31	0.41
2:N:47:LYS:HE3	2:N:47:LYS:HB3	1.99	0.41
1:P:1099:TYR:CE1	1:P:1108:LEU:HD13	2.56	0.41
1:Q:372:PHE:HB2	1:Q:399:ILE:HD12	2.02	0.41
1:Y:722:ARG:HH21	1:Y:1129:GLU:HA	1.86	0.41
1:L:1111:LYS:HB2	1:L:1111:LYS:HE2	1.85	0.40
1:T:722:ARG:HH21	1:T:1129:GLU:HA	1.86	0.40
3:X:39:ILE:HG22	3:X:47:LEU:HB3	2.03	0.40
1:H:734:LEU:HD23	1:H:743:LYS:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:892:LEU:HA	1:H:1008:GLN:O	2.22	0.40
1:I:183:THR:HG22	1:I:184:TYR:N	2.35	0.40
1:L:995:GLY:O	1:L:997:ARG:HD2	2.21	0.40
1:P:722:ARG:HH21	1:P:1129:GLU:HA	1.86	0.40
2:W:50:ILE:HD13	2:W:50:ILE:HA	1.90	0.40
1:A:377:HIS:HB2	1:A:380:GLN:HB2	2.03	0.40
1:A:487:GLU:HG3	1:A:489:HIS:H	1.87	0.40
1:C:511:CYS:O	1:H:1133:VAL:HG13	2.22	0.40
1:H:748:LYS:HD2	1:H:748:LYS:HA	1.95	0.40
1:H:1099:TYR:CE1	1:H:1108:LEU:HD13	2.56	0.40
2:J:90:CYS:O	2:J:102:GLY:N	2.47	0.40
1:M:511:CYS:O	1:P:1133:VAL:HG13	2.21	0.40
1:V:324:VAL:HG23	1:V:464:VAL:HG12	2.04	0.40
1:Y:950:ALA:HB3	1:Y:953:LEU:HD11	2.03	0.40
1:Y:994:LYS:HD3	1:Y:994:LYS:HA	1.83	0.40
1:B:732:LEU:HD23	1:B:732:LEU:HA	1.79	0.40
1:C:225:ASP:OD2	1:C:225:ASP:C	2.65	0.40
1:I:377:HIS:HB2	1:I:380:GLN:HB2	2.03	0.40
1:M:491:LEU:O	1:M:523:THR:HA	2.21	0.40
1:Q:359:LEU:HD12	1:Q:359:LEU:HA	1.87	0.40
1:A:511:CYS:O	1:B:1133:VAL:HG13	2.22	0.40
1:C:231:LEU:HD23	1:C:231:LEU:HA	1.94	0.40
1:P:913:TYR:HB2	1:P:981:LEU:CD1	2.51	0.40
1:P:1098:MET:HE2	1:P:1098:MET:HA	2.03	0.40
1:Q:324:VAL:HG23	1:Q:464:VAL:HG12	2.02	0.40
1:Q:511:CYS:O	1:T:1133:VAL:HG13	2.21	0.40
1:T:1029:CYS:N	1:T:1101:CYS:SG	2.94	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	410/1064 (38%)	397 (97%)	12 (3%)	1 (0%)	43	73
1	B	440/1064 (41%)	413 (94%)	27 (6%)	0	100	100
1	C	410/1064 (38%)	398 (97%)	11 (3%)	1 (0%)	43	73
1	H	440/1064 (41%)	412 (94%)	28 (6%)	0	100	100
1	I	410/1064 (38%)	398 (97%)	11 (3%)	1 (0%)	43	73
1	L	440/1064 (41%)	415 (94%)	25 (6%)	0	100	100
1	M	410/1064 (38%)	397 (97%)	12 (3%)	1 (0%)	43	73
1	P	440/1064 (41%)	413 (94%)	27 (6%)	0	100	100
1	Q	410/1064 (38%)	400 (98%)	9 (2%)	1 (0%)	43	73
1	T	440/1064 (41%)	411 (93%)	29 (7%)	0	100	100
1	V	410/1064 (38%)	398 (97%)	11 (3%)	1 (0%)	43	73
1	Y	440/1064 (41%)	414 (94%)	26 (6%)	0	100	100
2	D	61/224 (27%)	58 (95%)	3 (5%)	0	100	100
2	F	61/224 (27%)	58 (95%)	3 (5%)	0	100	100
2	J	61/224 (27%)	58 (95%)	3 (5%)	0	100	100
2	N	61/224 (27%)	58 (95%)	3 (5%)	0	100	100
2	R	61/224 (27%)	58 (95%)	3 (5%)	0	100	100
2	W	61/224 (27%)	58 (95%)	3 (5%)	0	100	100
3	E	52/248 (21%)	47 (90%)	5 (10%)	0	100	100
3	G	52/248 (21%)	49 (94%)	3 (6%)	0	100	100
3	K	52/248 (21%)	49 (94%)	3 (6%)	0	100	100
3	O	52/248 (21%)	47 (90%)	5 (10%)	0	100	100
3	S	52/248 (21%)	48 (92%)	4 (8%)	0	100	100
3	X	52/248 (21%)	49 (94%)	3 (6%)	0	100	100
All	All	5778/15600 (37%)	5503 (95%)	269 (5%)	6 (0%)	49	78

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	PRO
1	C	226	PRO
1	I	226	PRO
1	M	226	PRO
1	Q	226	PRO
1	V	226	PRO

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	352/912 (39%)	352 (100%)	0	100	100
1	B	381/912 (42%)	379 (100%)	2 (0%)	81	85
1	C	352/912 (39%)	352 (100%)	0	100	100
1	H	381/912 (42%)	380 (100%)	1 (0%)	86	87
1	I	352/912 (39%)	350 (99%)	2 (1%)	78	83
1	L	381/912 (42%)	381 (100%)	0	100	100
1	M	352/912 (39%)	352 (100%)	0	100	100
1	P	381/912 (42%)	379 (100%)	2 (0%)	81	85
1	Q	352/912 (39%)	352 (100%)	0	100	100
1	T	381/912 (42%)	381 (100%)	0	100	100
1	V	352/912 (39%)	352 (100%)	0	100	100
1	Y	381/912 (42%)	380 (100%)	1 (0%)	86	87
2	D	60/187 (32%)	60 (100%)	0	100	100
2	F	60/187 (32%)	60 (100%)	0	100	100
2	J	60/187 (32%)	59 (98%)	1 (2%)	53	74
2	N	60/187 (32%)	60 (100%)	0	100	100
2	R	60/187 (32%)	60 (100%)	0	100	100
2	W	60/187 (32%)	58 (97%)	2 (3%)	33	63
3	E	52/212 (24%)	52 (100%)	0	100	100
3	G	52/212 (24%)	52 (100%)	0	100	100
3	K	52/212 (24%)	52 (100%)	0	100	100
3	O	52/212 (24%)	52 (100%)	0	100	100
3	S	52/212 (24%)	52 (100%)	0	100	100
3	X	52/212 (24%)	52 (100%)	0	100	100
All	All	5070/13338 (38%)	5059 (100%)	11 (0%)	85	89

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	953	LEU
1	B	1102	ASP
1	H	1085	ILE
1	I	239	CYS
1	I	513	THR
2	J	28	ASP
1	P	809	MET
1	P	1102	ASP
2	W	28	ASP
2	W	49	LEU
1	Y	1012	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	HIS
1	A	204	GLN
1	A	209	HIS
1	A	350	ASN
1	A	380	GLN
1	A	444	GLN
1	B	710	ASN
1	B	817	GLN
1	C	166	HIS
1	C	204	GLN
1	C	350	ASN
1	C	377	HIS
1	C	380	GLN
1	C	444	GLN
1	H	817	GLN
1	I	166	HIS
1	I	204	GLN
1	I	209	HIS
1	I	377	HIS
1	I	380	GLN
1	I	408	HIS
1	I	444	GLN
3	K	41	GLN
1	L	817	GLN
1	L	986	ASN
1	L	996	ASN
1	M	166	HIS
1	M	204	GLN

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Mol	Chain	Res	Type
1	M	209	HIS
1	M	350	ASN
1	M	380	GLN
1	M	444	GLN
1	P	817	GLN
1	Q	166	HIS
1	Q	204	GLN
1	Q	350	ASN
1	Q	377	HIS
1	Q	380	GLN
1	Q	444	GLN
1	T	817	GLN
1	T	986	ASN
1	V	166	HIS
1	V	204	GLN
1	V	209	HIS
1	V	350	ASN
1	V	377	HIS
1	V	380	GLN
1	V	408	HIS
1	V	444	GLN
3	X	41	GLN
1	Y	817	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

18 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	$\# Z > 2$
4	NAG	U	1	4,1	14,14,15	0.65	1 (7%)	17,19,21	0.73	0
4	NAG	U	2	4	14,14,15	0.23	0	17,19,21	0.57	0
4	NAG	U	3	4	14,14,15	0.26	0	17,19,21	0.59	0
4	NAG	Z	1	4,1	14,14,15	0.64	1 (7%)	17,19,21	0.72	0
4	NAG	Z	2	4	14,14,15	0.22	0	17,19,21	0.57	0
4	NAG	Z	3	4	14,14,15	0.25	0	17,19,21	0.59	0
4	NAG	a	1	4,1	14,14,15	0.65	1 (7%)	17,19,21	0.75	0
4	NAG	a	2	4	14,14,15	0.26	0	17,19,21	0.57	0
4	NAG	a	3	4	14,14,15	0.26	0	17,19,21	0.59	0
4	NAG	b	1	4,1	14,14,15	0.67	1 (7%)	17,19,21	0.72	0
4	NAG	b	2	4	14,14,15	0.25	0	17,19,21	0.58	0
4	NAG	b	3	4	14,14,15	0.25	0	17,19,21	0.59	0
4	NAG	c	1	4,1	14,14,15	0.64	1 (7%)	17,19,21	0.72	0
4	NAG	c	2	4	14,14,15	0.24	0	17,19,21	0.58	0
4	NAG	c	3	4	14,14,15	0.26	0	17,19,21	0.59	0
4	NAG	d	1	4,1	14,14,15	0.65	1 (7%)	17,19,21	0.74	0
4	NAG	d	2	4	14,14,15	0.24	0	17,19,21	0.57	0
4	NAG	d	3	4	14,14,15	0.27	0	17,19,21	0.59	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	U	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	U	2	4	-	4/6/23/26	0/1/1/1
4	NAG	U	3	4	-	4/6/23/26	0/1/1/1
4	NAG	Z	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	4/6/23/26	0/1/1/1
4	NAG	Z	3	4	-	4/6/23/26	0/1/1/1
4	NAG	a	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	a	2	4	-	4/6/23/26	0/1/1/1
4	NAG	a	3	4	-	4/6/23/26	0/1/1/1
4	NAG	b	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	b	2	4	-	4/6/23/26	0/1/1/1
4	NAG	b	3	4	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	c	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	c	2	4	-	4/6/23/26	0/1/1/1
4	NAG	c	3	4	-	4/6/23/26	0/1/1/1
4	NAG	d	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	d	2	4	-	4/6/23/26	0/1/1/1
4	NAG	d	3	4	-	4/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	b	1	NAG	O5-C1	-2.36	1.39	1.43
4	U	1	NAG	O5-C1	-2.31	1.39	1.43
4	a	1	NAG	O5-C1	-2.29	1.39	1.43
4	Z	1	NAG	O5-C1	-2.27	1.39	1.43
4	d	1	NAG	O5-C1	-2.27	1.39	1.43
4	c	1	NAG	O5-C1	-2.26	1.39	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	U	2	NAG	C8-C7-N2-C2
4	U	2	NAG	O7-C7-N2-C2
4	Z	2	NAG	C8-C7-N2-C2
4	Z	2	NAG	O7-C7-N2-C2
4	a	2	NAG	C8-C7-N2-C2
4	a	2	NAG	O7-C7-N2-C2
4	b	2	NAG	C8-C7-N2-C2
4	b	2	NAG	O7-C7-N2-C2
4	c	2	NAG	C8-C7-N2-C2
4	c	2	NAG	O7-C7-N2-C2
4	d	2	NAG	C8-C7-N2-C2
4	d	2	NAG	O7-C7-N2-C2
4	a	3	NAG	O5-C5-C6-O6
4	d	3	NAG	O5-C5-C6-O6
4	b	3	NAG	O5-C5-C6-O6
4	c	3	NAG	O5-C5-C6-O6
4	U	3	NAG	O5-C5-C6-O6
4	Z	3	NAG	O5-C5-C6-O6

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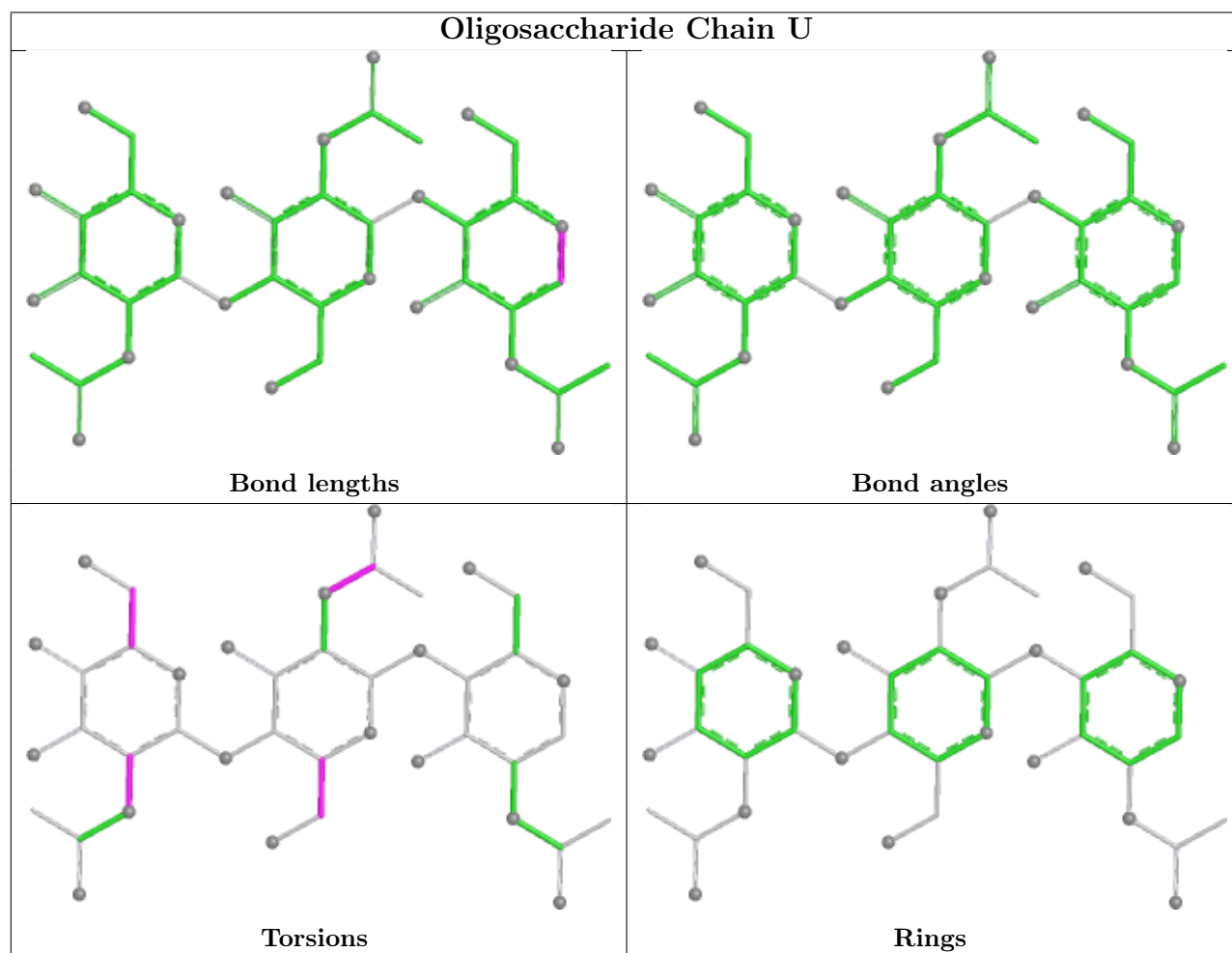
Mol	Chain	Res	Type	Atoms
4	a	2	NAG	O5-C5-C6-O6
4	d	2	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	b	2	NAG	O5-C5-C6-O6
4	c	2	NAG	O5-C5-C6-O6
4	Z	2	NAG	O5-C5-C6-O6
4	a	3	NAG	C4-C5-C6-O6
4	d	3	NAG	C4-C5-C6-O6
4	U	3	NAG	C1-C2-N2-C7
4	Z	3	NAG	C1-C2-N2-C7
4	a	3	NAG	C1-C2-N2-C7
4	b	3	NAG	C1-C2-N2-C7
4	c	3	NAG	C1-C2-N2-C7
4	d	3	NAG	C1-C2-N2-C7
4	b	3	NAG	C4-C5-C6-O6
4	c	3	NAG	C4-C5-C6-O6
4	U	3	NAG	C4-C5-C6-O6
4	Z	3	NAG	C4-C5-C6-O6
4	U	3	NAG	C3-C2-N2-C7
4	Z	3	NAG	C3-C2-N2-C7
4	a	3	NAG	C3-C2-N2-C7
4	b	3	NAG	C3-C2-N2-C7
4	c	3	NAG	C3-C2-N2-C7
4	d	3	NAG	C3-C2-N2-C7
4	a	2	NAG	C4-C5-C6-O6
4	d	2	NAG	C4-C5-C6-O6
4	b	2	NAG	C4-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
4	c	2	NAG	C4-C5-C6-O6
4	Z	2	NAG	C4-C5-C6-O6

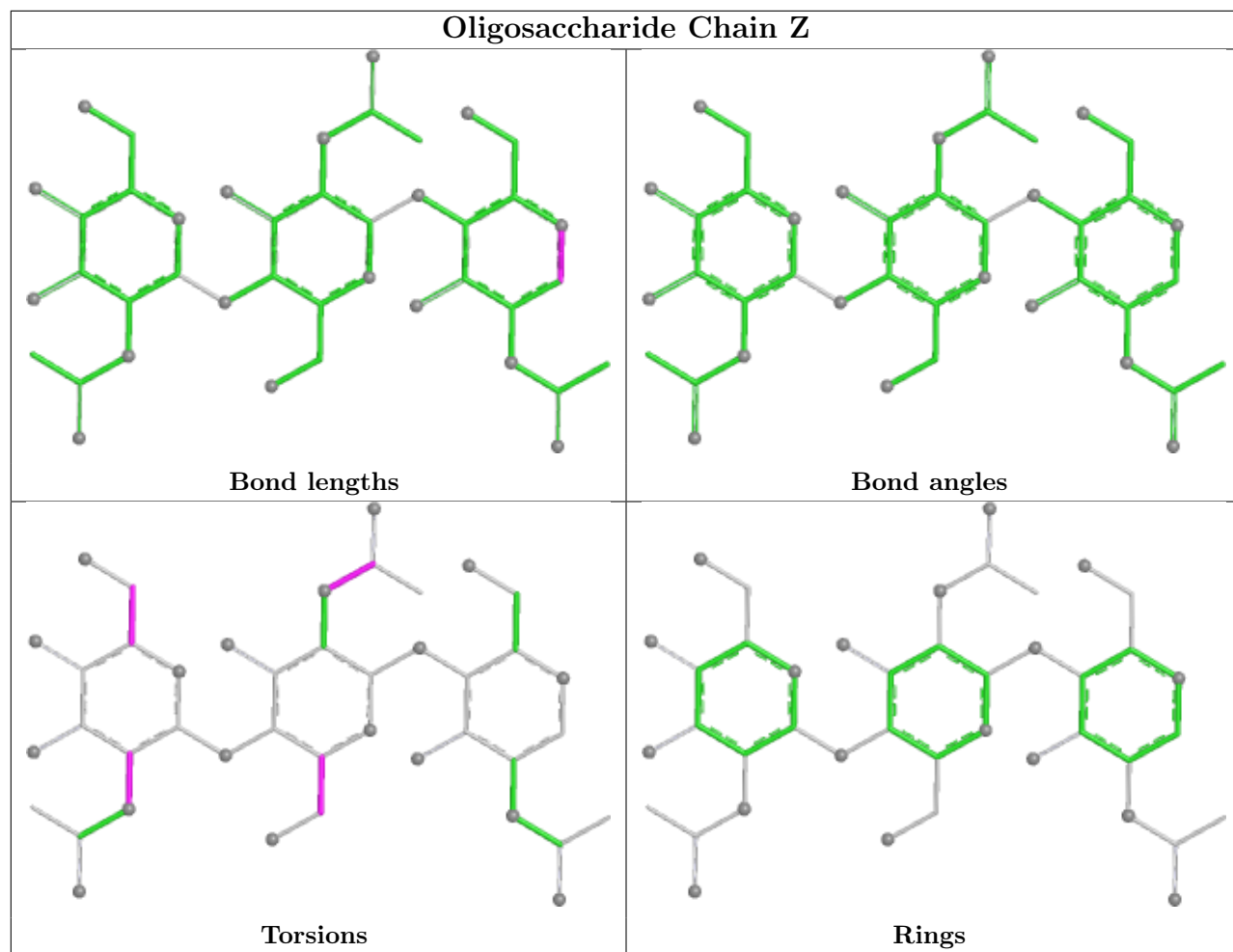
There are no ring outliers.

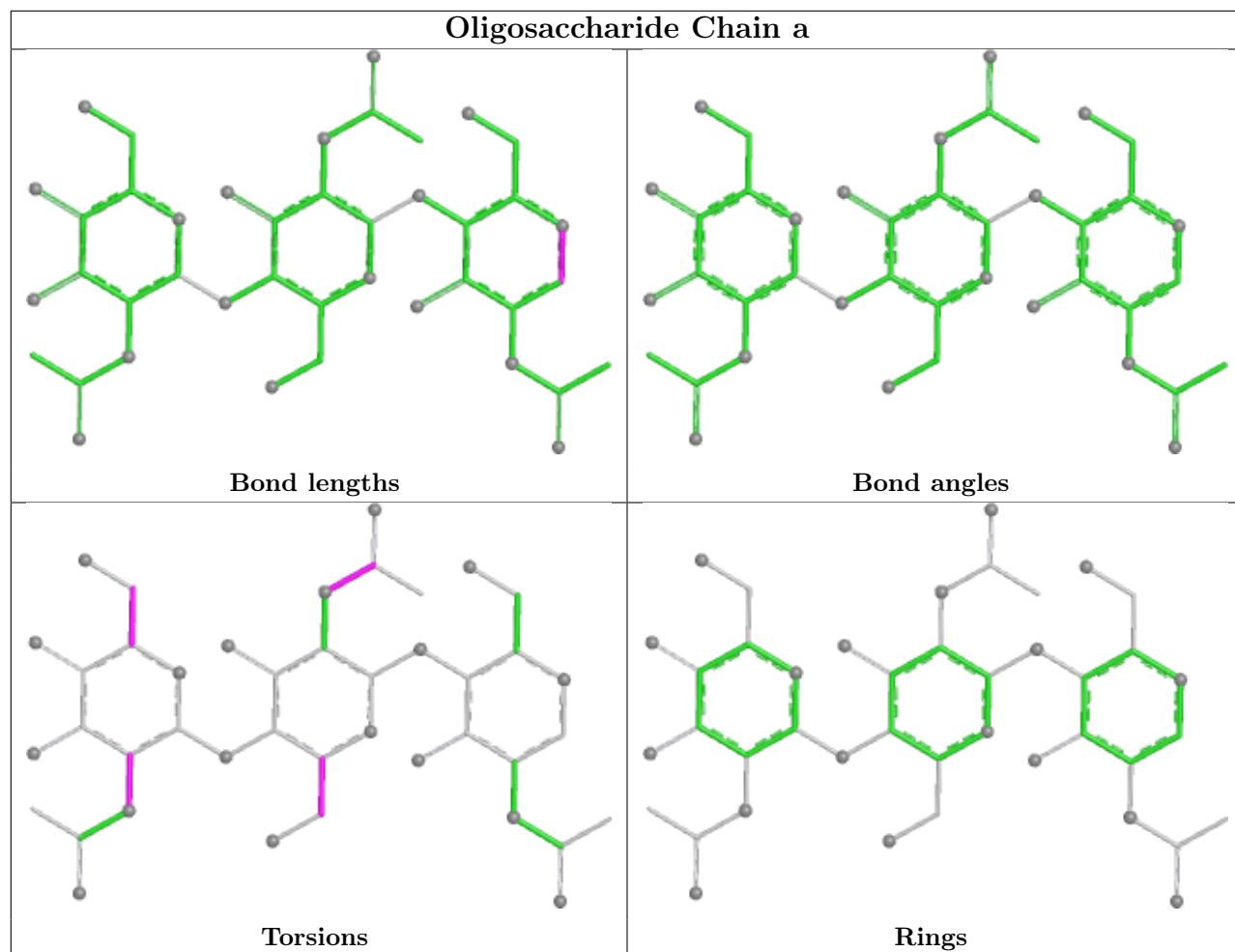
6 monomers are involved in 6 short contacts:

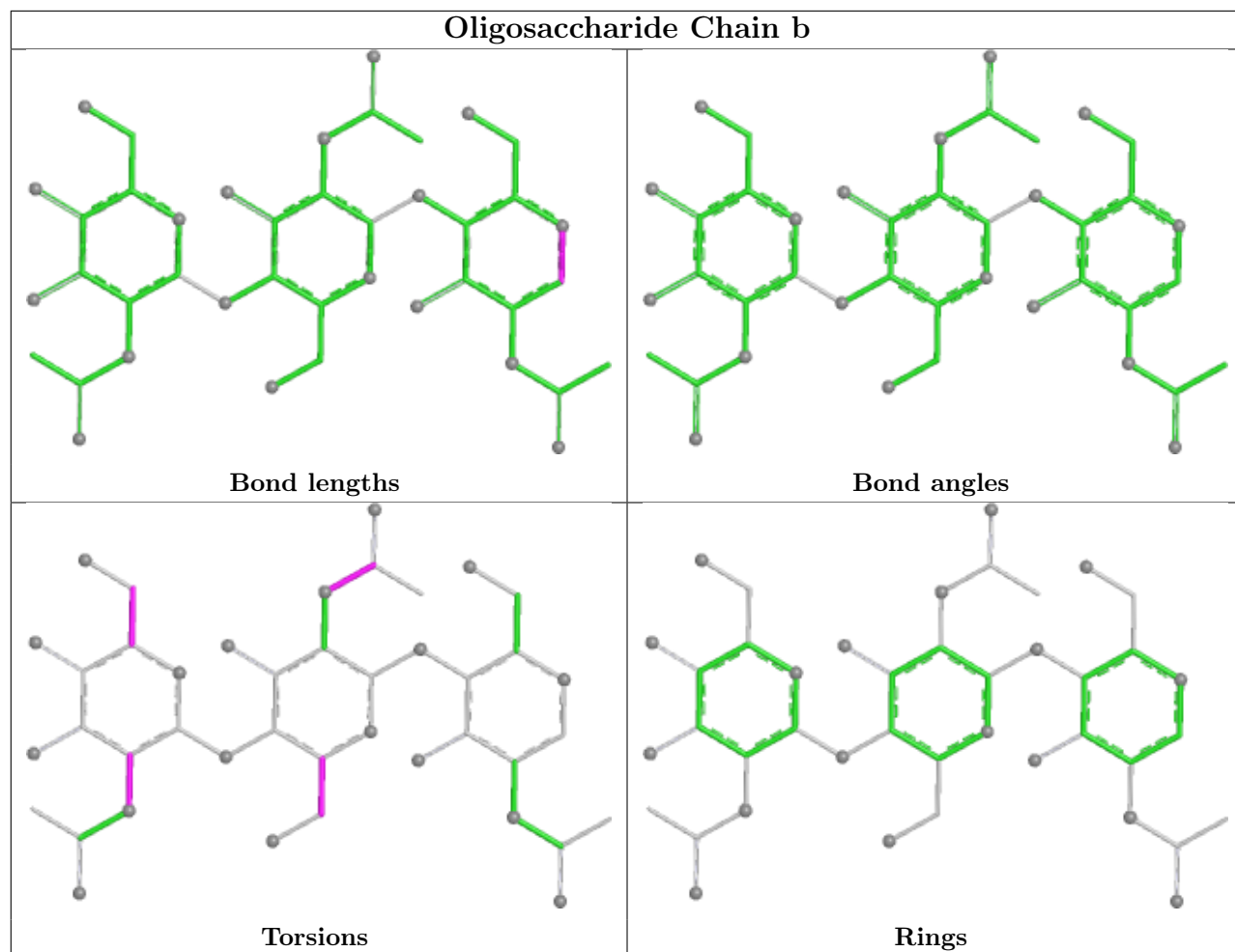
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Z	1	NAG	1	0
4	c	1	NAG	1	0
4	b	1	NAG	1	0
4	U	1	NAG	1	0
4	d	1	NAG	1	0
4	a	1	NAG	1	0

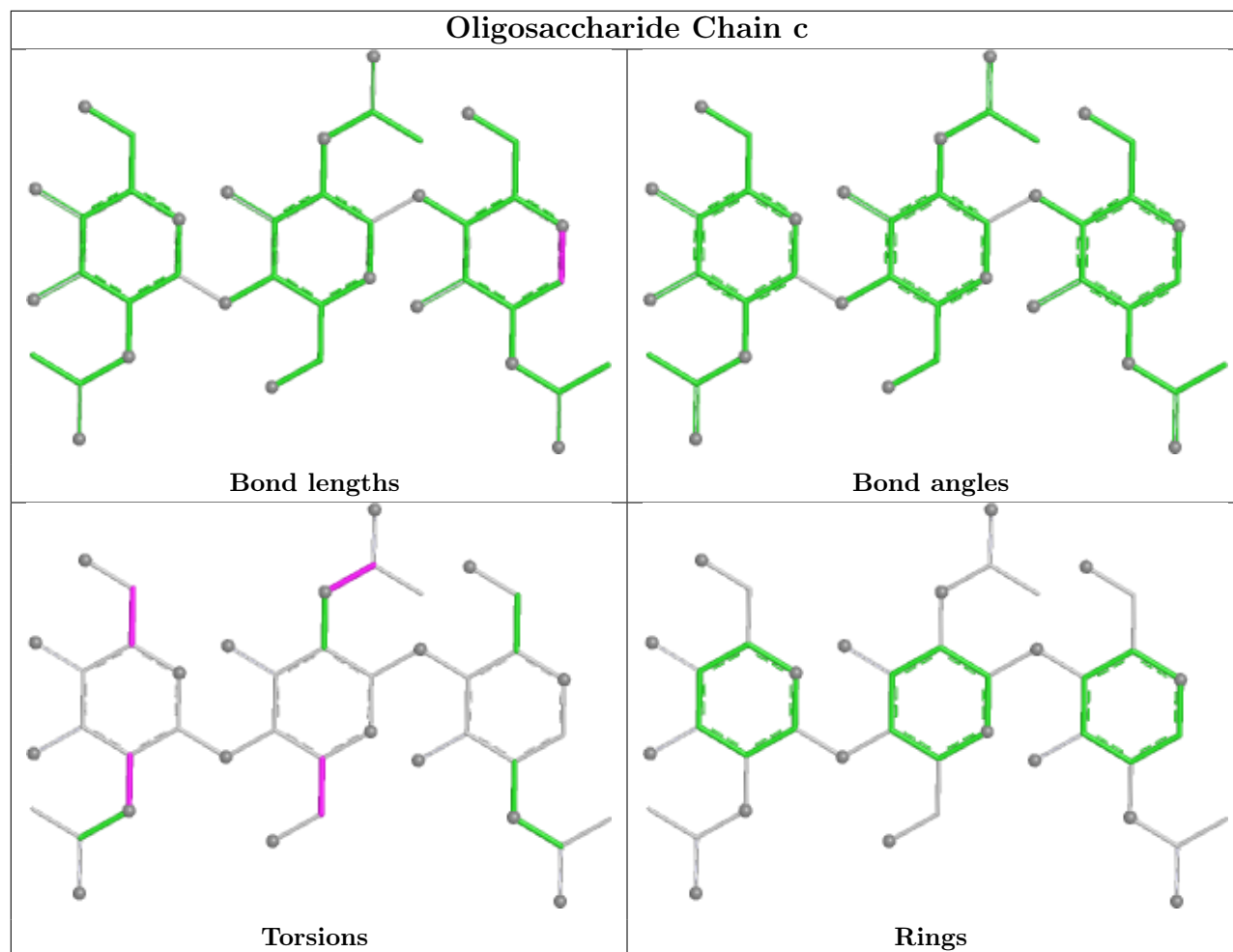
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

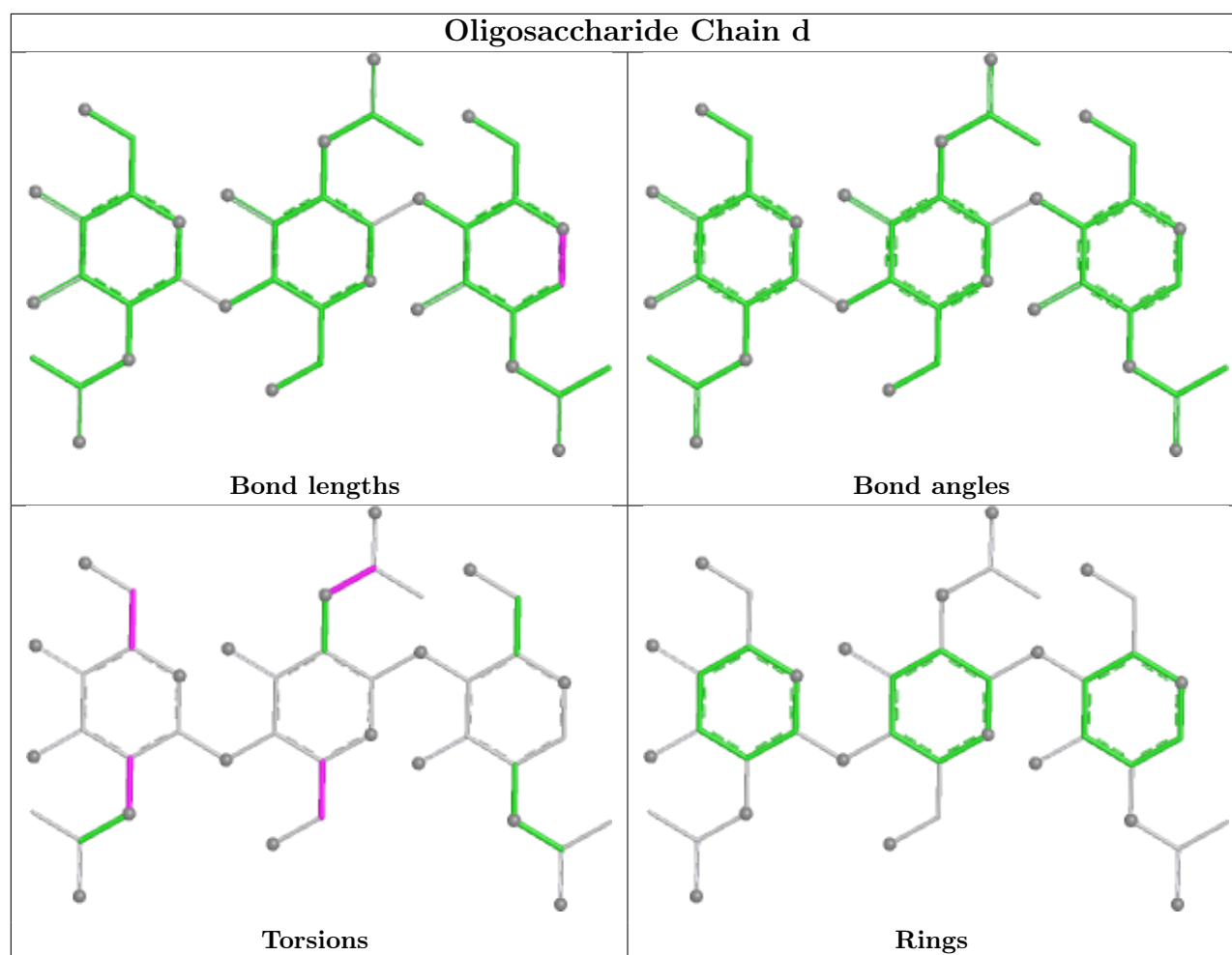












5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
5	NAG	M	1301	1	14,14,15	1.08	2 (14%)	17,19,21	1.37	1 (5%)
5	NAG	B	1301	1	14,14,15	0.23	0	17,19,21	0.42	0
5	NAG	T	1301	1	14,14,15	0.25	0	17,19,21	0.41	0
5	NAG	P	1301	1	14,14,15	0.24	0	17,19,21	0.41	0
5	NAG	Q	1301	1	14,14,15	0.55	0	17,19,21	0.84	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	H	1301	1	14,14,15	0.26	0	17,19,21	0.41	0
5	NAG	Y	1301	1	14,14,15	0.25	0	17,19,21	0.41	0
5	NAG	A	1301	1	14,14,15	1.07	2 (14%)	17,19,21	1.37	1 (5%)
5	NAG	L	1301	1	14,14,15	0.25	0	17,19,21	0.41	0
5	NAG	V	1301	1	14,14,15	0.54	0	17,19,21	0.84	1 (5%)
5	NAG	C	1301	1	14,14,15	0.57	0	17,19,21	0.83	1 (5%)
5	NAG	I	1301	1	14,14,15	0.55	0	17,19,21	0.85	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
5	NAG	M	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	4/6/23/26	0/1/1/1
5	NAG	T	1301	1	-	4/6/23/26	0/1/1/1
5	NAG	P	1301	1	-	4/6/23/26	0/1/1/1
5	NAG	Q	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	H	1301	1	-	4/6/23/26	0/1/1/1
5	NAG	Y	1301	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	L	1301	1	-	4/6/23/26	0/1/1/1
5	NAG	V	1301	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	I	1301	1	-	4/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1301	NAG	O5-C1	3.34	1.49	1.43
5	M	1301	NAG	O5-C1	3.34	1.49	1.43
5	M	1301	NAG	C1-C2	2.13	1.55	1.52
5	A	1301	NAG	C1-C2	2.10	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1301	NAG	C1-O5-C5	5.38	119.39	112.19
5	M	1301	NAG	C1-O5-C5	5.37	119.39	112.19
5	I	1301	NAG	C1-O5-C5	2.96	116.15	112.19
5	Q	1301	NAG	C1-O5-C5	2.91	116.09	112.19
5	V	1301	NAG	C1-O5-C5	2.90	116.08	112.19
5	C	1301	NAG	C1-O5-C5	2.87	116.03	112.19

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1301	NAG	O5-C5-C6-O6
5	P	1301	NAG	O5-C5-C6-O6
5	H	1301	NAG	O5-C5-C6-O6
5	L	1301	NAG	O5-C5-C6-O6
5	T	1301	NAG	O5-C5-C6-O6
5	Y	1301	NAG	O5-C5-C6-O6
5	L	1301	NAG	C4-C5-C6-O6
5	Y	1301	NAG	C4-C5-C6-O6
5	H	1301	NAG	C4-C5-C6-O6
5	T	1301	NAG	C4-C5-C6-O6
5	B	1301	NAG	C4-C5-C6-O6
5	P	1301	NAG	C4-C5-C6-O6
5	A	1301	NAG	C8-C7-N2-C2
5	A	1301	NAG	O7-C7-N2-C2
5	B	1301	NAG	C8-C7-N2-C2
5	B	1301	NAG	O7-C7-N2-C2
5	C	1301	NAG	C8-C7-N2-C2
5	C	1301	NAG	O7-C7-N2-C2
5	H	1301	NAG	C8-C7-N2-C2
5	H	1301	NAG	O7-C7-N2-C2
5	I	1301	NAG	C8-C7-N2-C2
5	I	1301	NAG	O7-C7-N2-C2
5	L	1301	NAG	C8-C7-N2-C2
5	L	1301	NAG	O7-C7-N2-C2
5	M	1301	NAG	C8-C7-N2-C2
5	M	1301	NAG	O7-C7-N2-C2
5	P	1301	NAG	C8-C7-N2-C2
5	P	1301	NAG	O7-C7-N2-C2
5	Q	1301	NAG	C8-C7-N2-C2
5	Q	1301	NAG	O7-C7-N2-C2
5	T	1301	NAG	C8-C7-N2-C2
5	T	1301	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	V	1301	NAG	C8-C7-N2-C2
5	V	1301	NAG	O7-C7-N2-C2
5	Y	1301	NAG	C8-C7-N2-C2
5	Y	1301	NAG	O7-C7-N2-C2
5	I	1301	NAG	C4-C5-C6-O6
5	V	1301	NAG	C4-C5-C6-O6
5	I	1301	NAG	O5-C5-C6-O6
5	V	1301	NAG	O5-C5-C6-O6

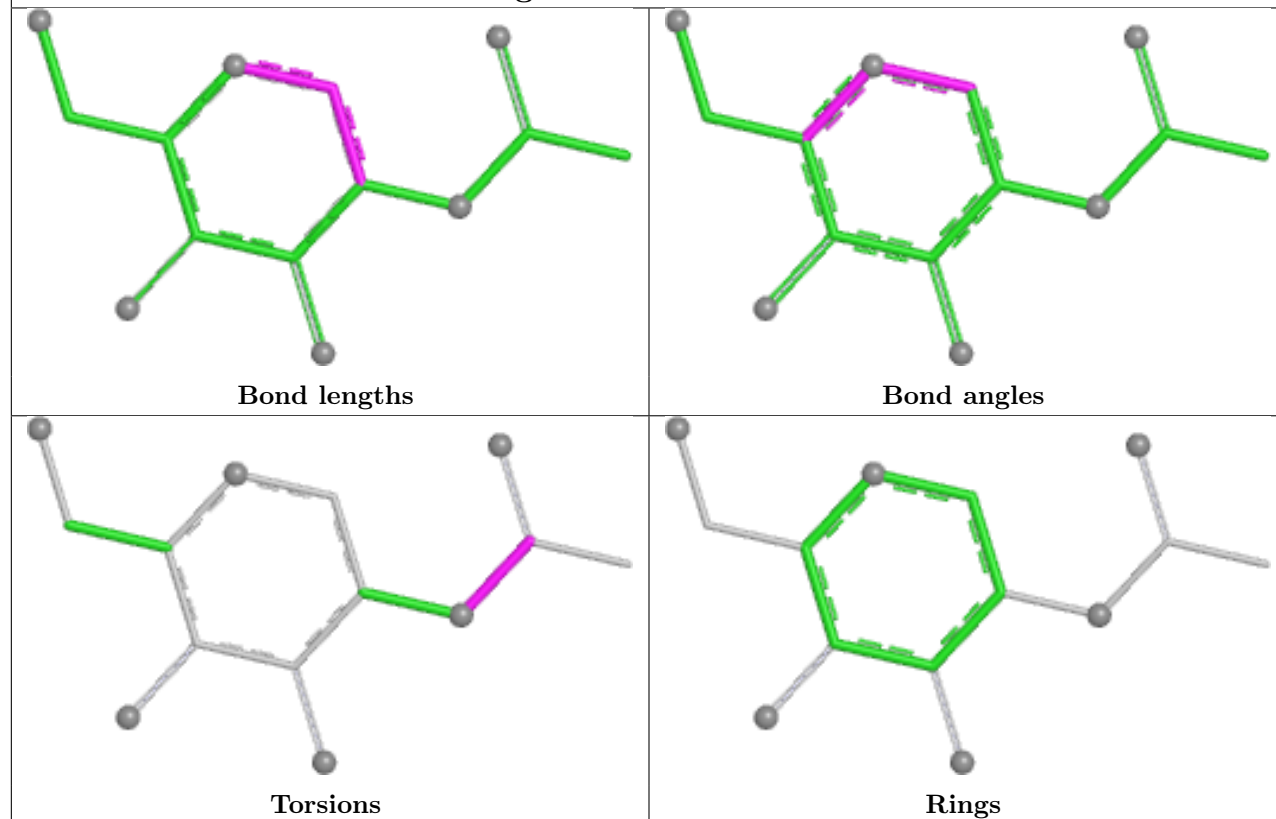
There are no ring outliers.

6 monomers are involved in 10 short contacts:

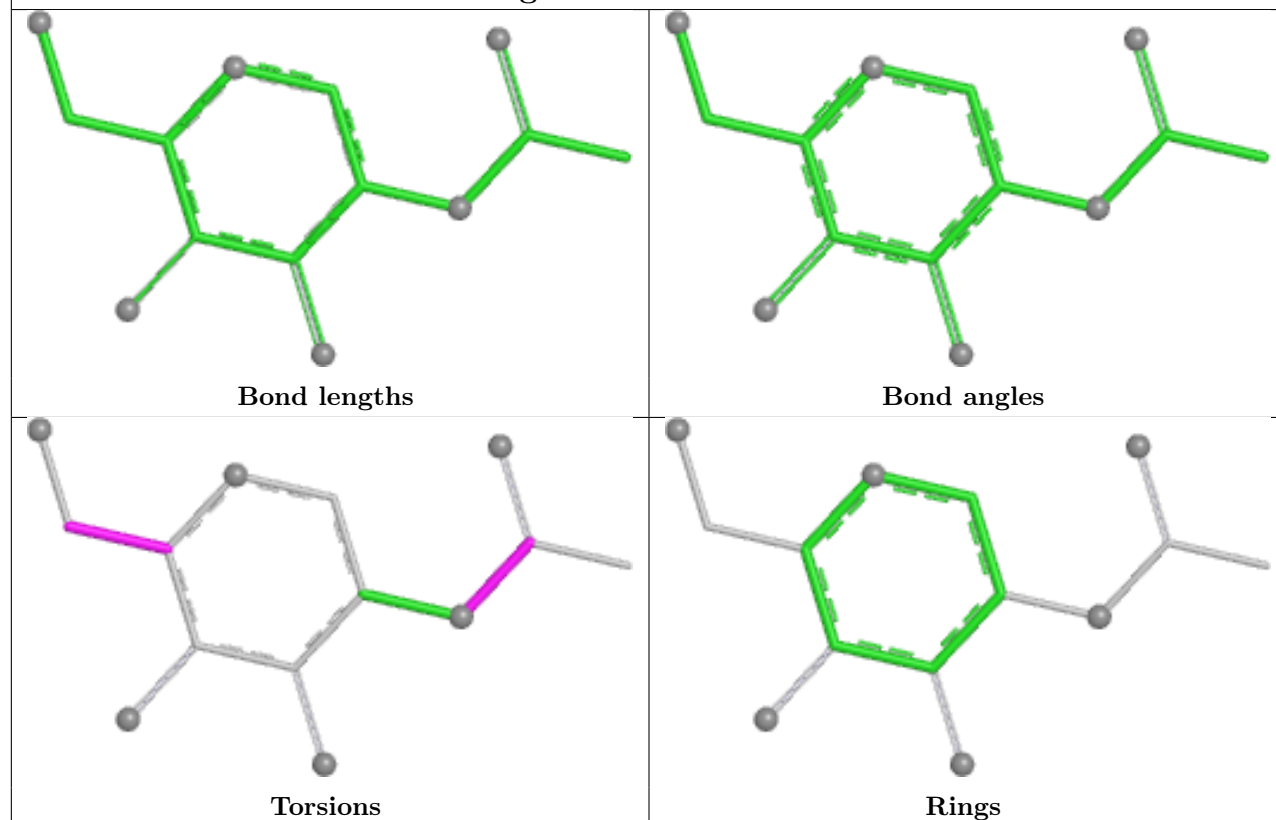
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	1301	NAG	1	0
5	Q	1301	NAG	2	0
5	A	1301	NAG	1	0
5	V	1301	NAG	2	0
5	C	1301	NAG	2	0
5	I	1301	NAG	2	0

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.

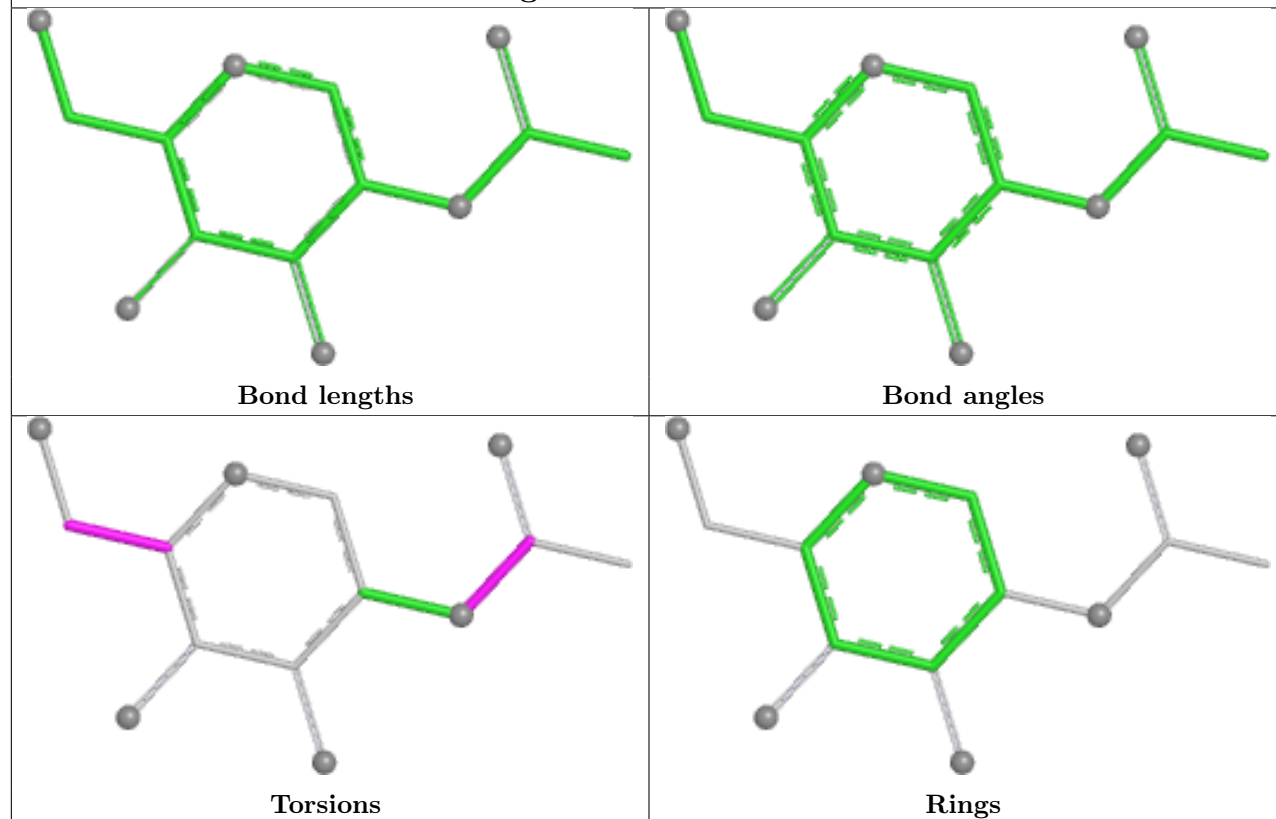
Ligand NAG M 1301



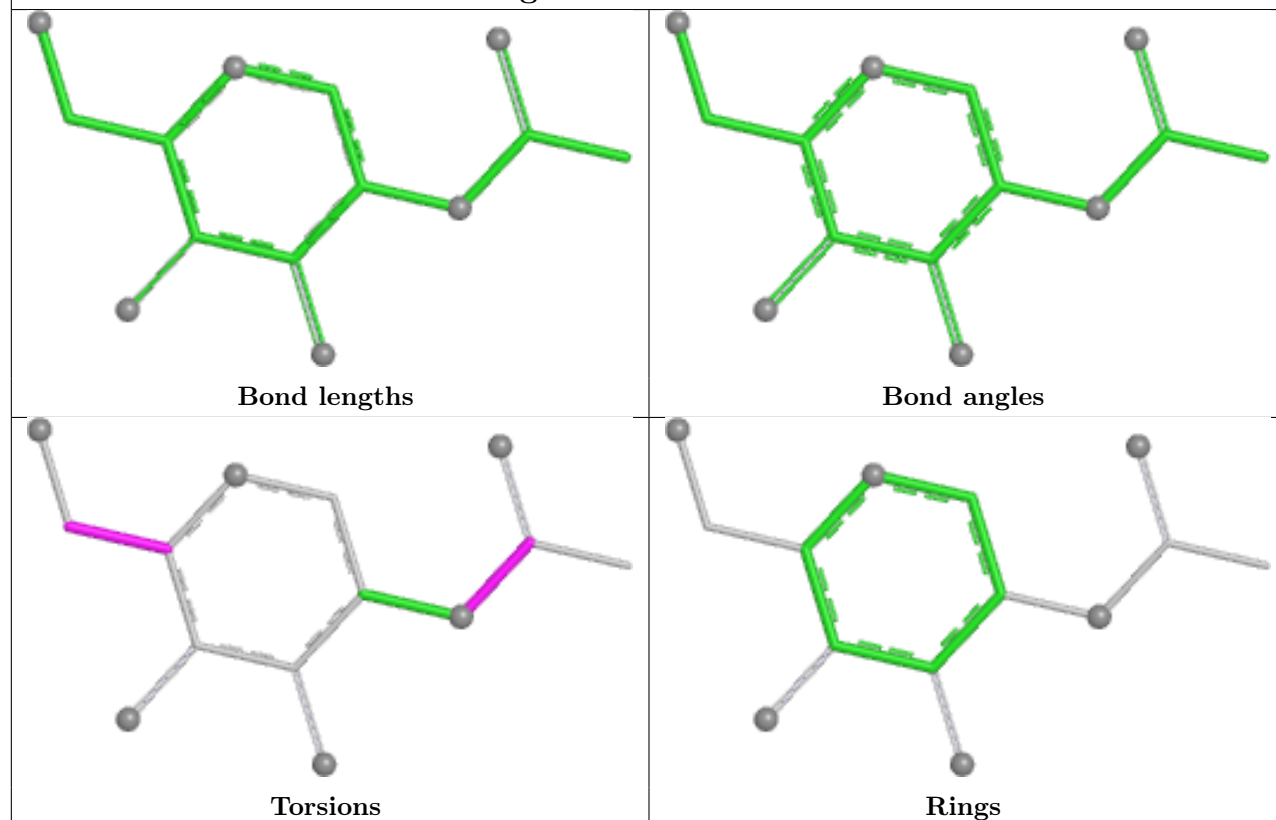
Ligand NAG B 1301

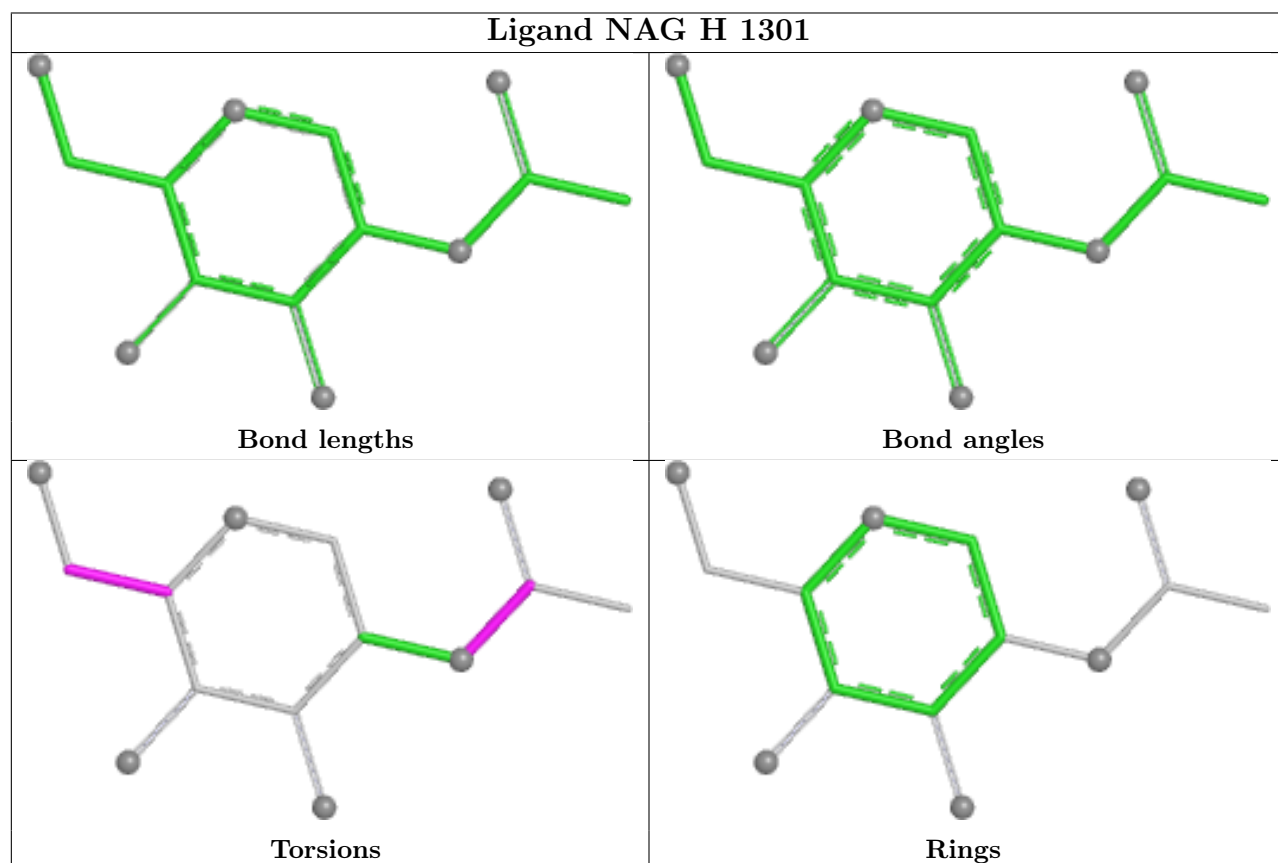
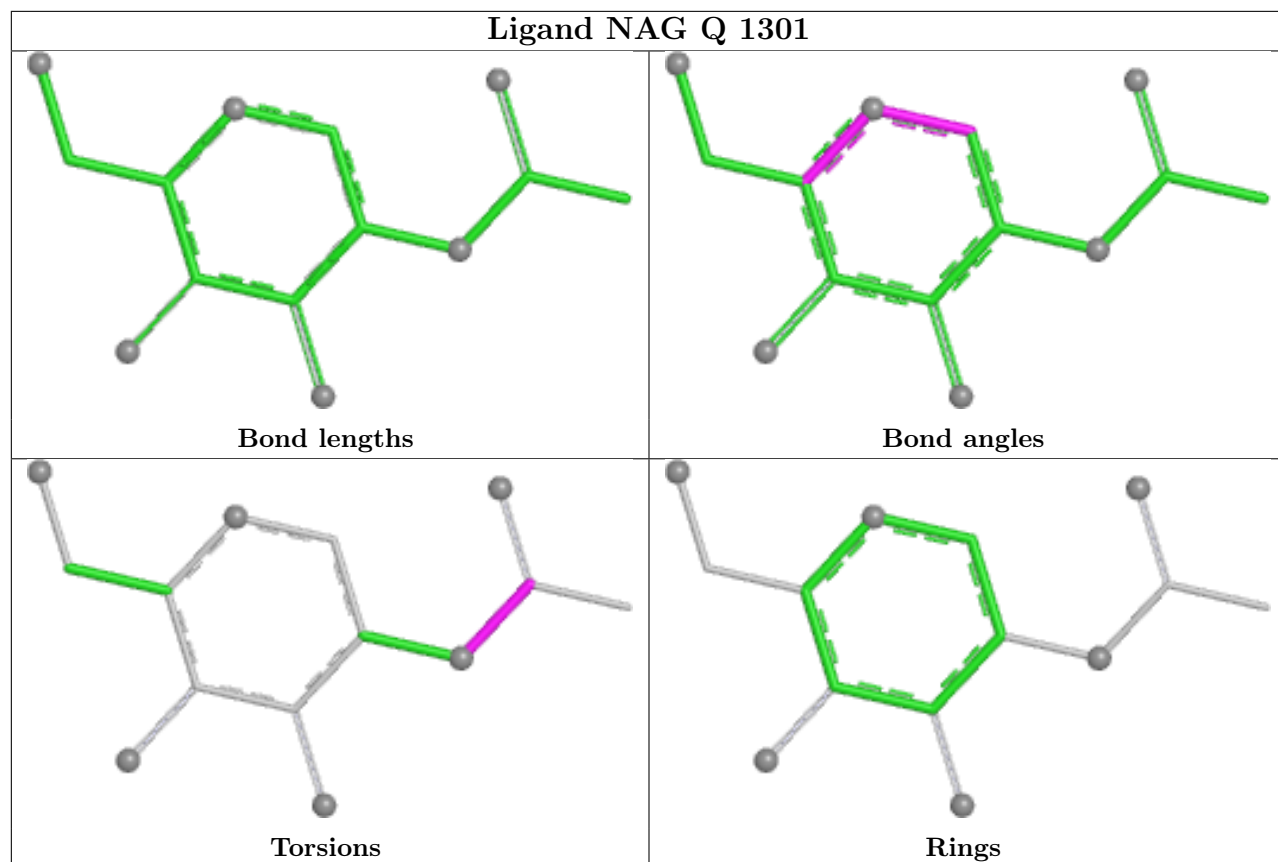


Ligand NAG T 1301

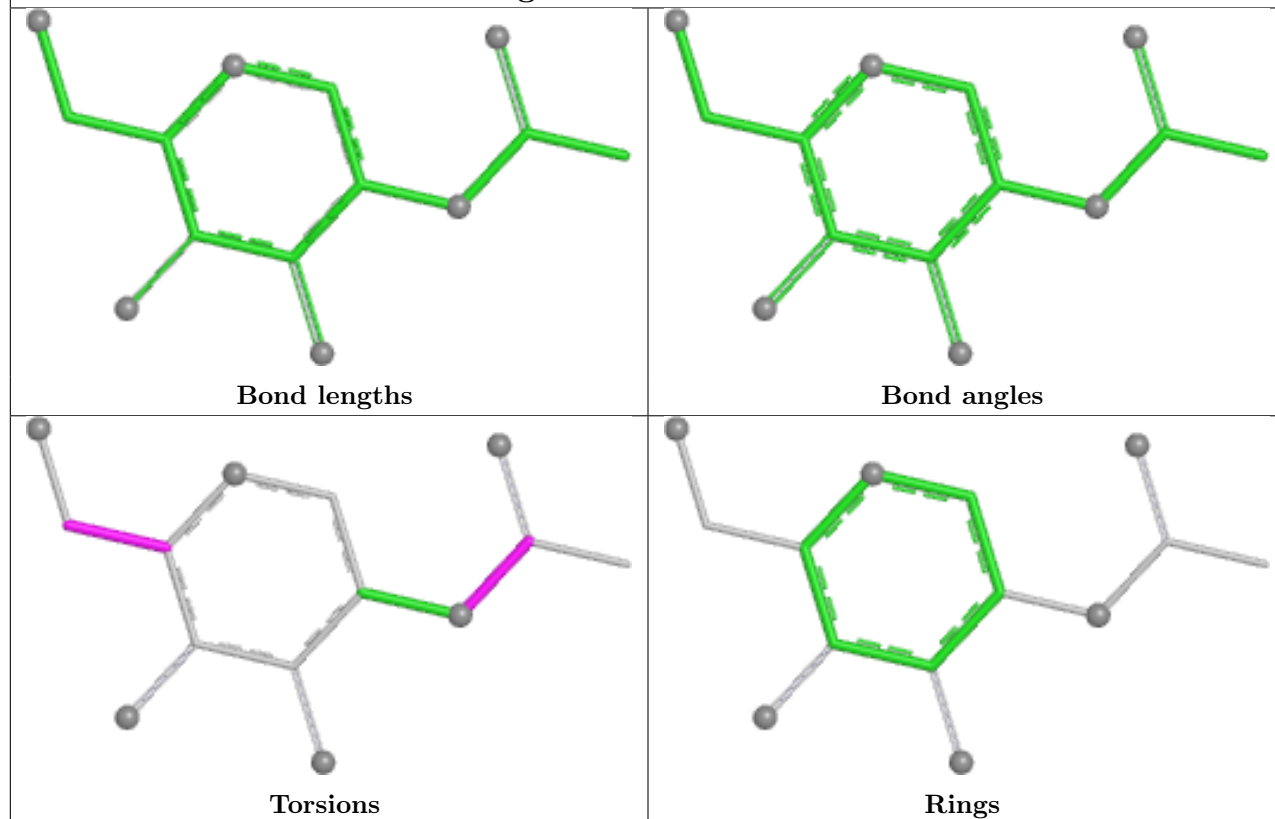


Ligand NAG P 1301

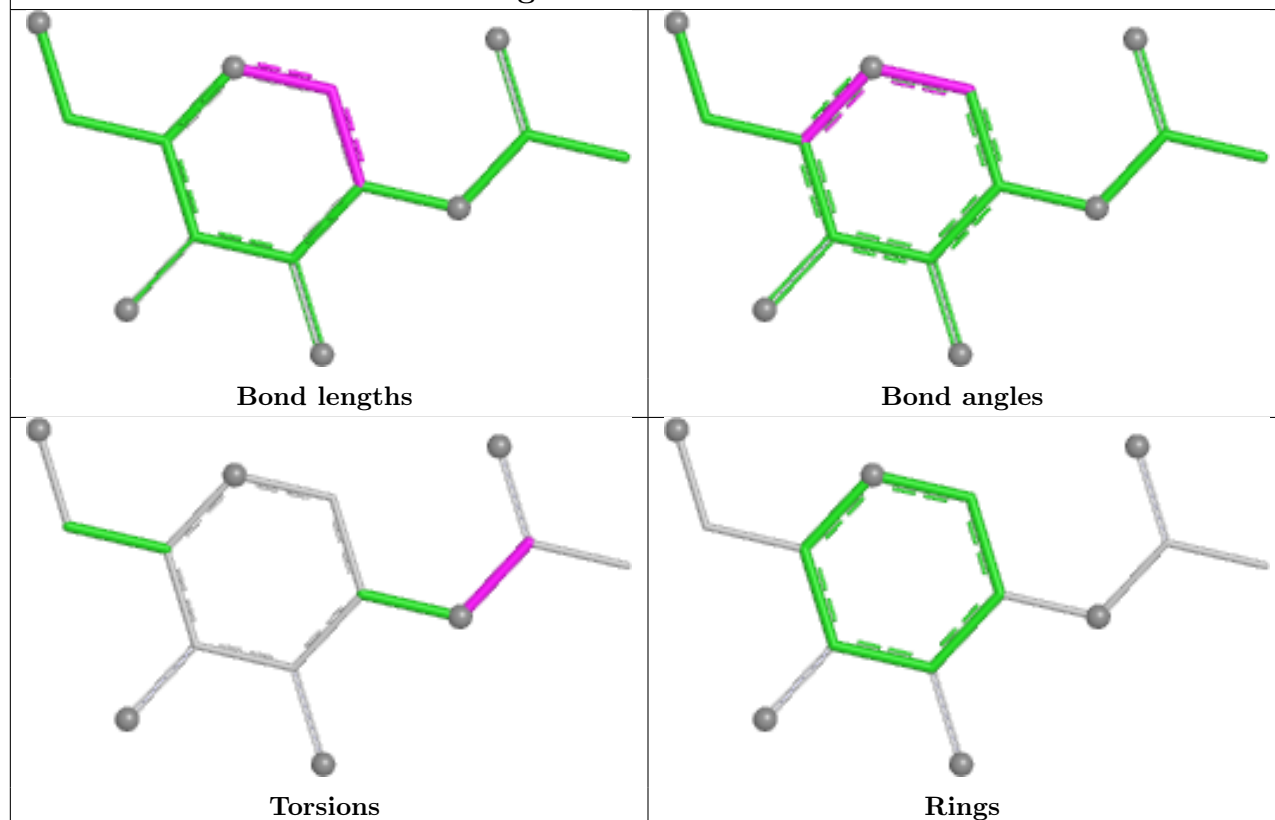


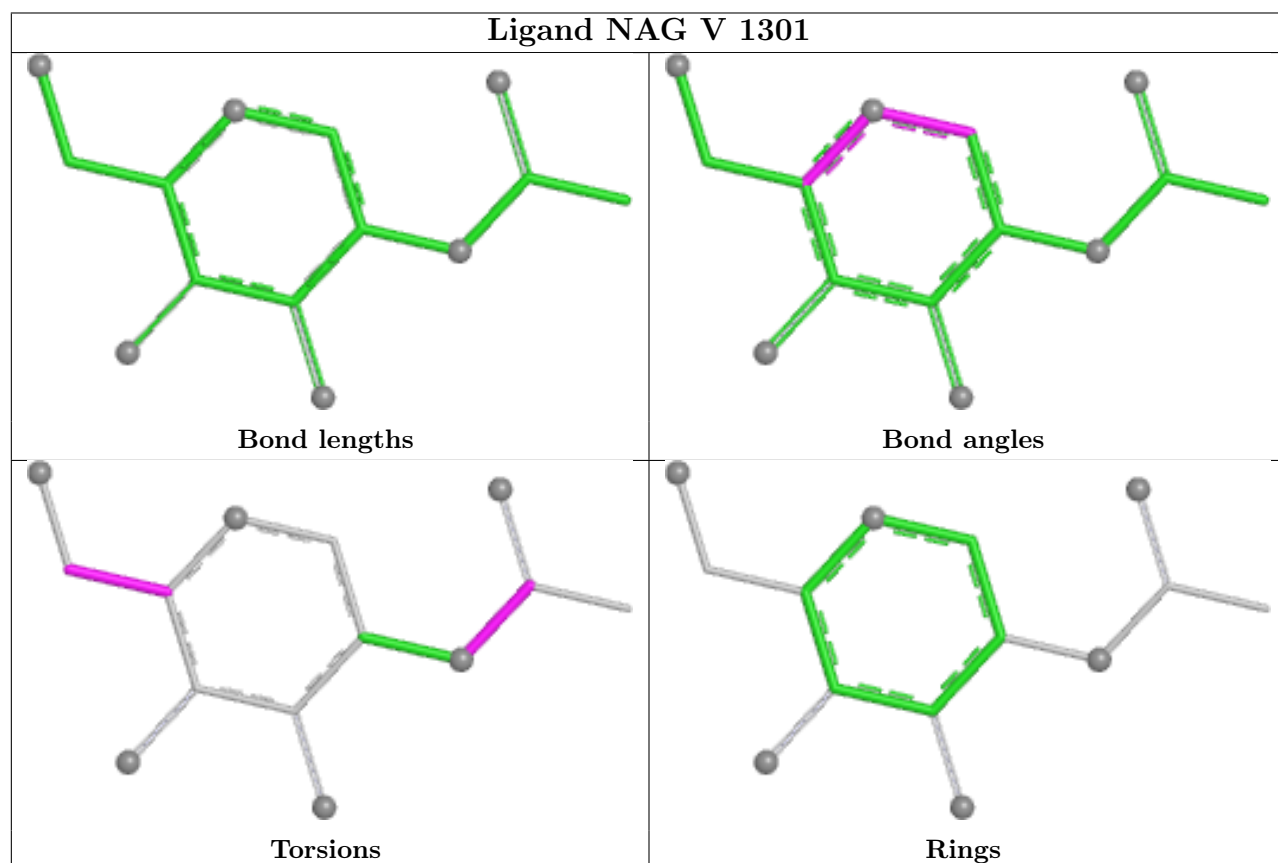
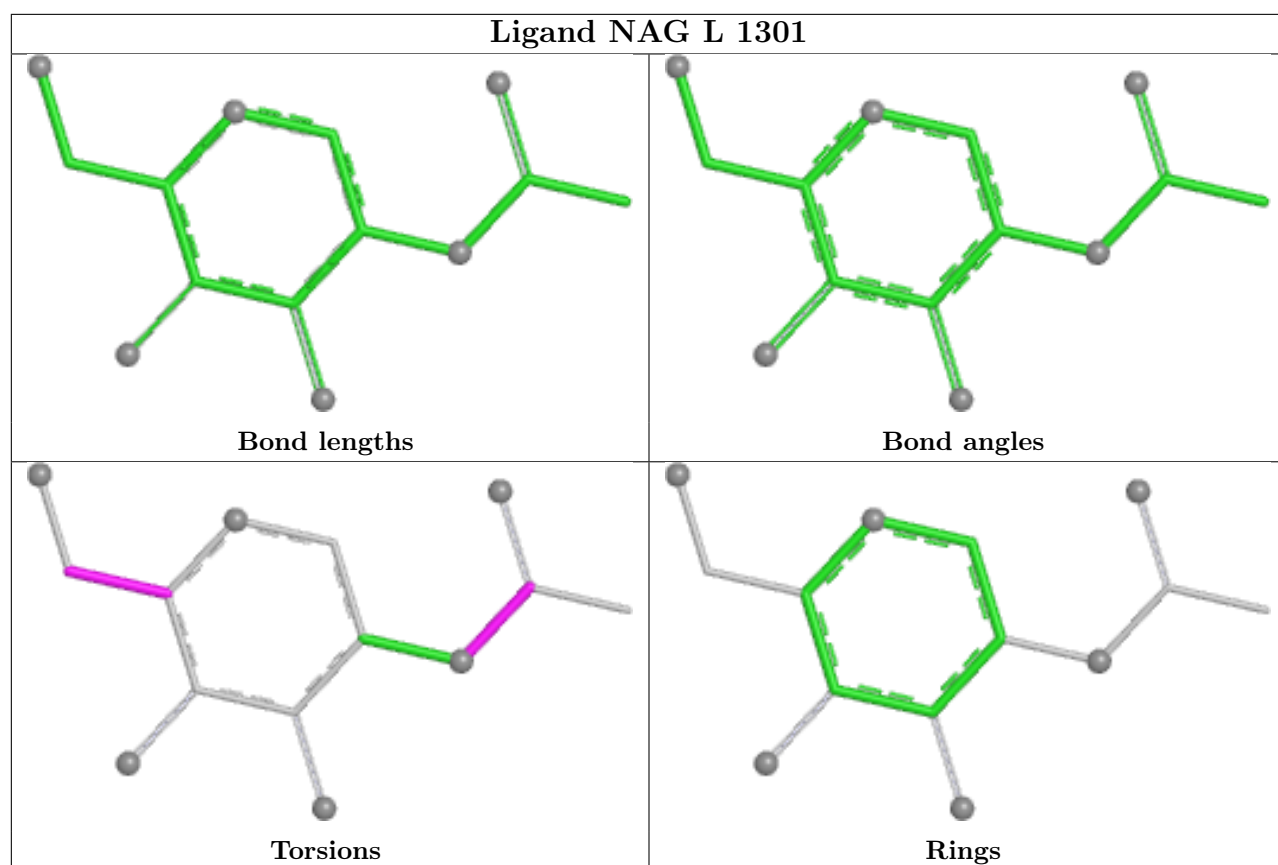


Ligand NAG Y 1301

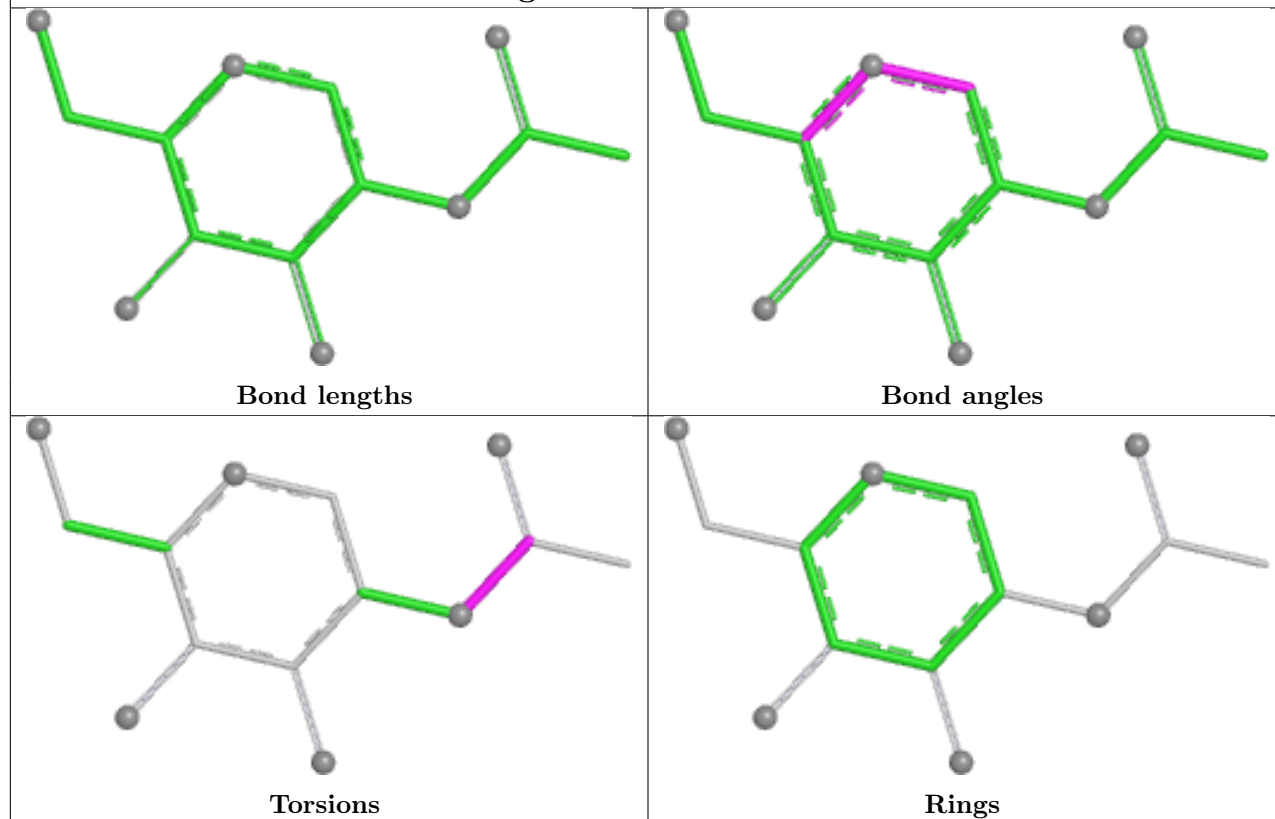


Ligand NAG A 1301

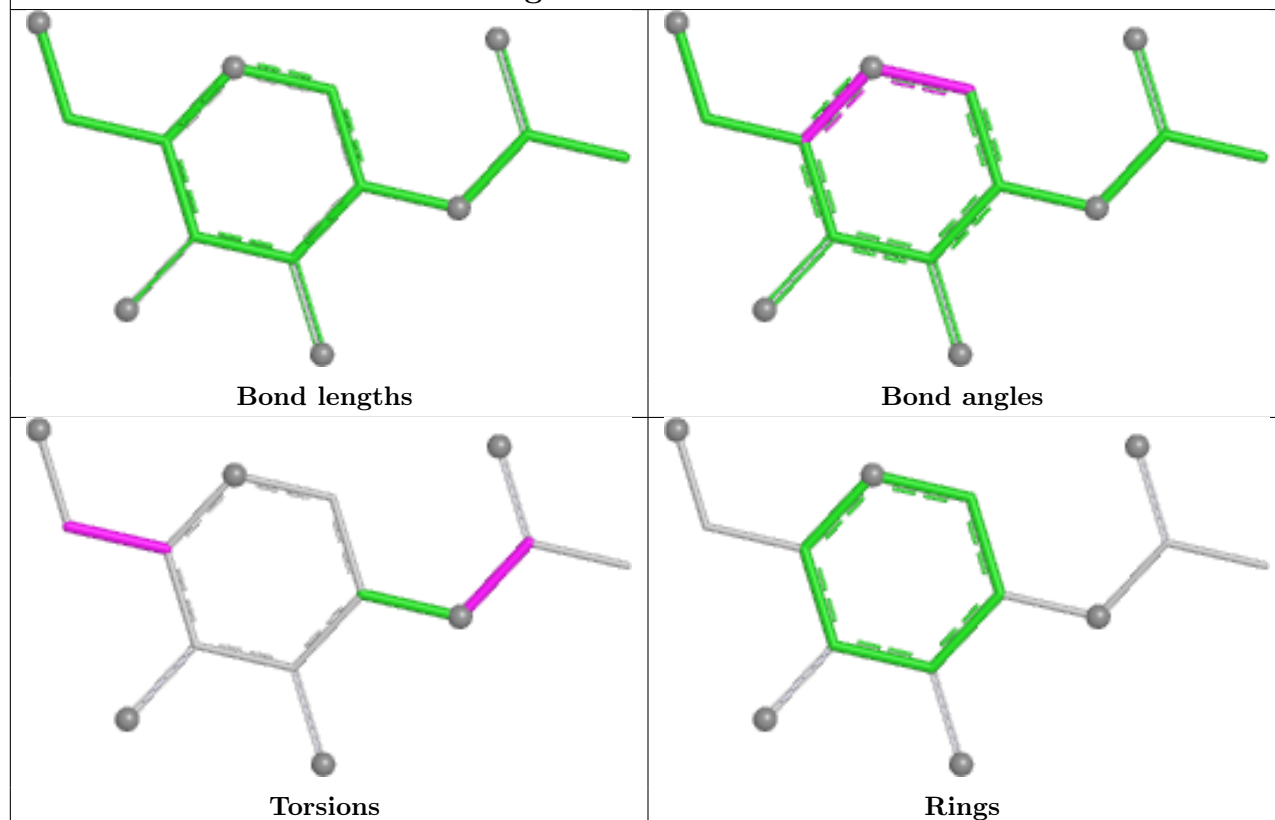




Ligand NAG C 1301



Ligand NAG I 1301



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.

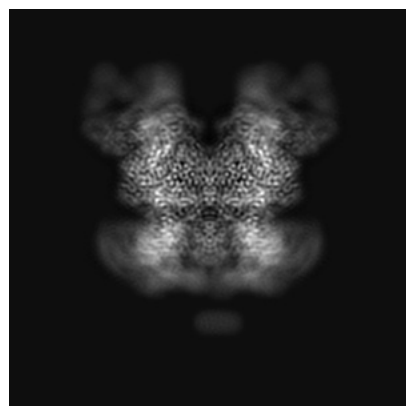
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64805. These allow visual inspection of the internal detail of the map and identification of artifacts.

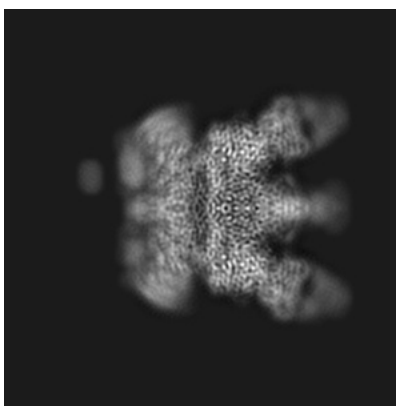
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

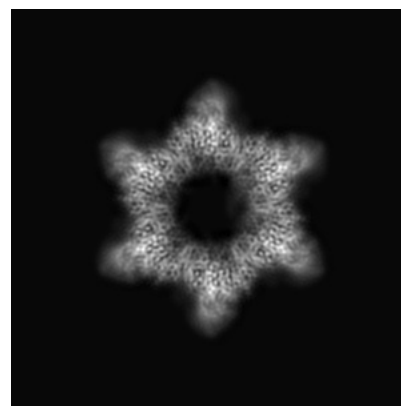
6.1.1 Primary map



X

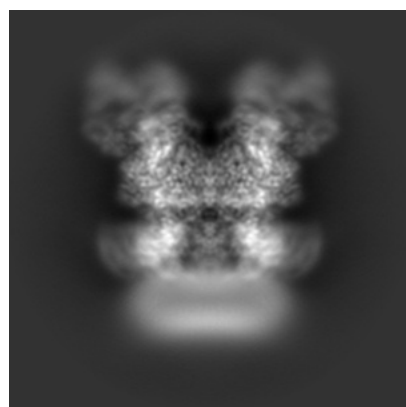


Y

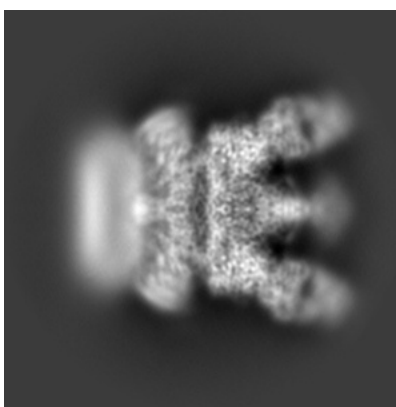


Z

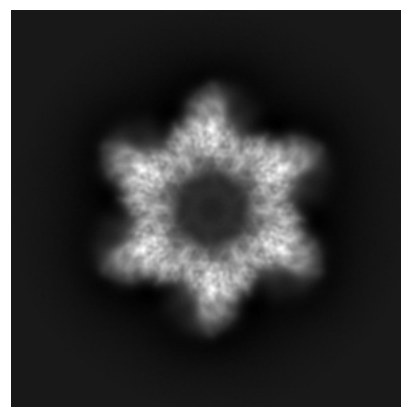
6.1.2 Raw map



X



Y

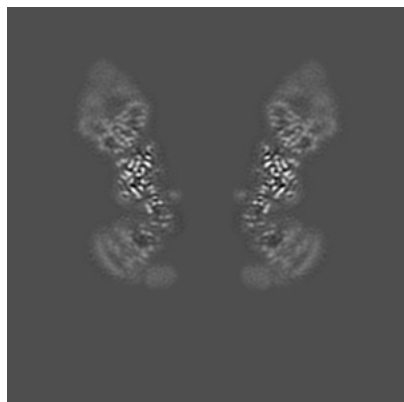


Z

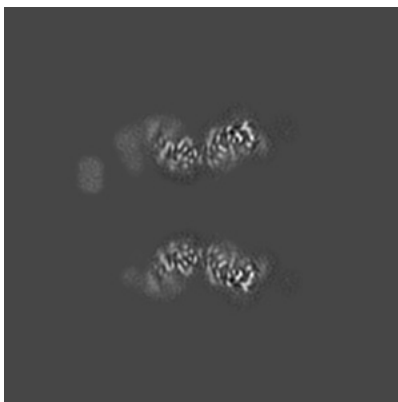
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

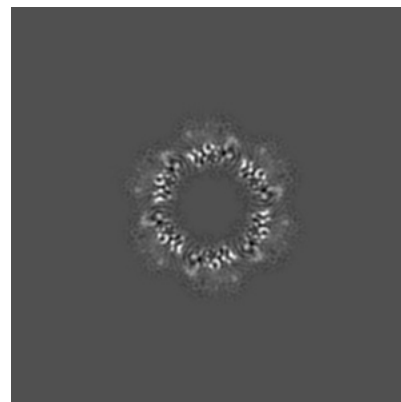
6.2.1 Primary map



X Index: 140

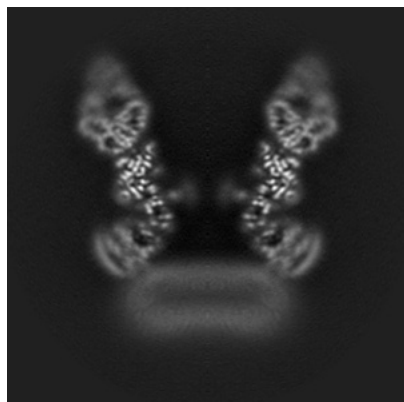


Y Index: 140

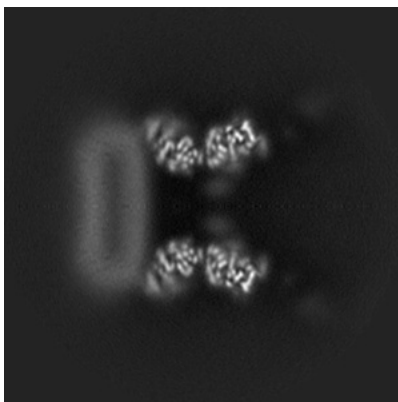


Z Index: 140

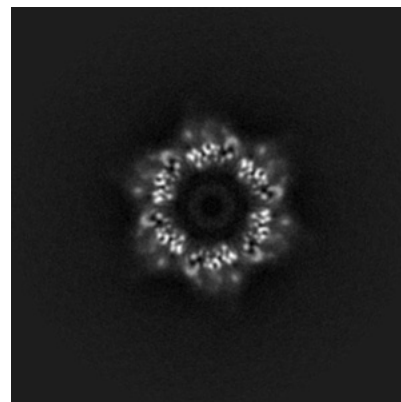
6.2.2 Raw map



X Index: 140



Y Index: 140

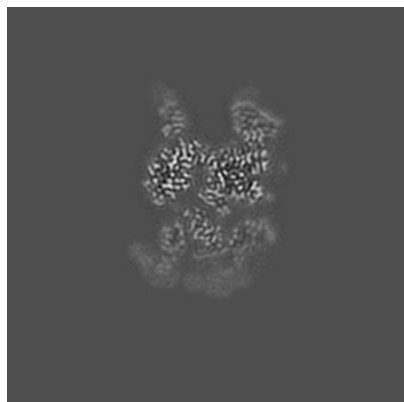


Z Index: 140

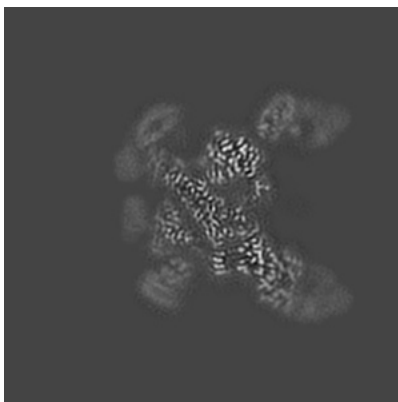
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

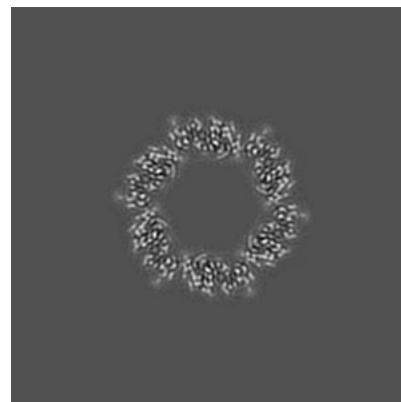
6.3.1 Primary map



X Index: 182

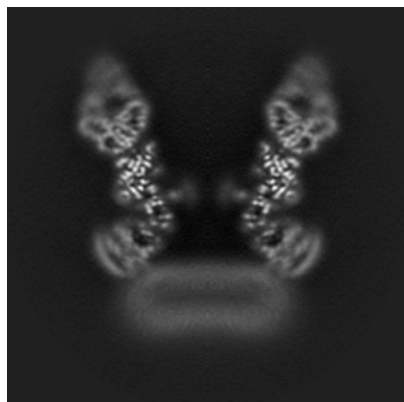


Y Index: 104

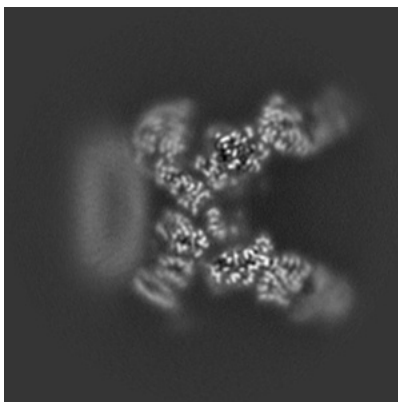


Z Index: 168

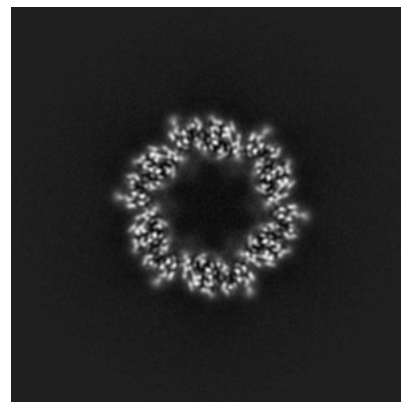
6.3.2 Raw map



X Index: 140



Y Index: 111

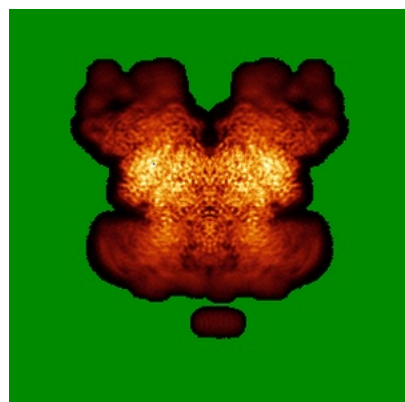


Z Index: 168

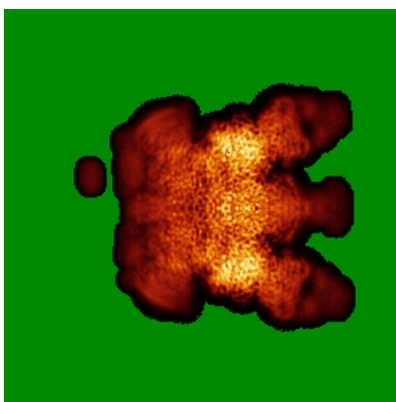
The images above show the largest variance slices of the map in three orthogonal directions.

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

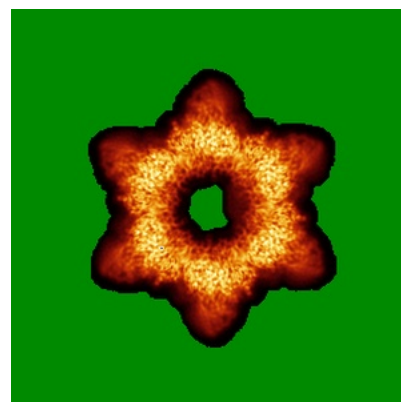
6.4.1 Primary map



X

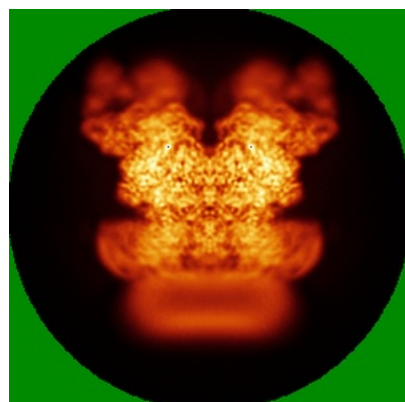


Y

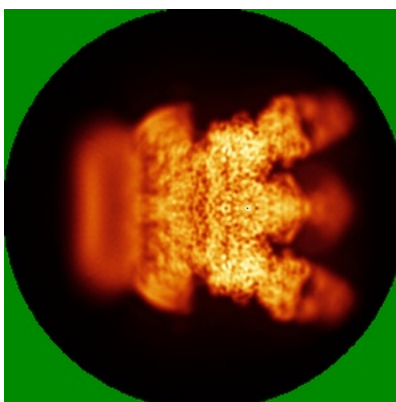


Z

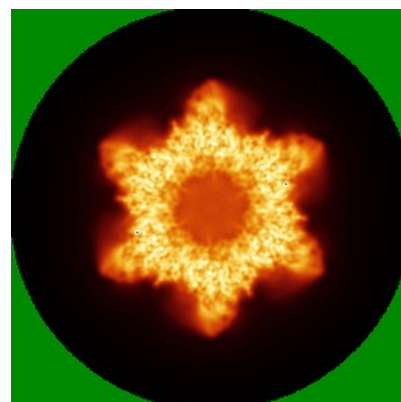
6.4.2 Raw map



X



Y

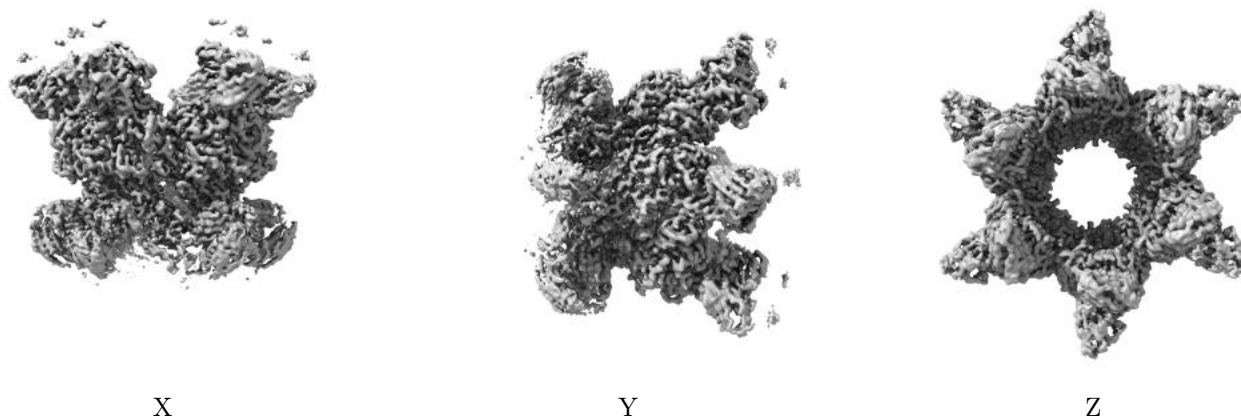


Z

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 0.0156. 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.

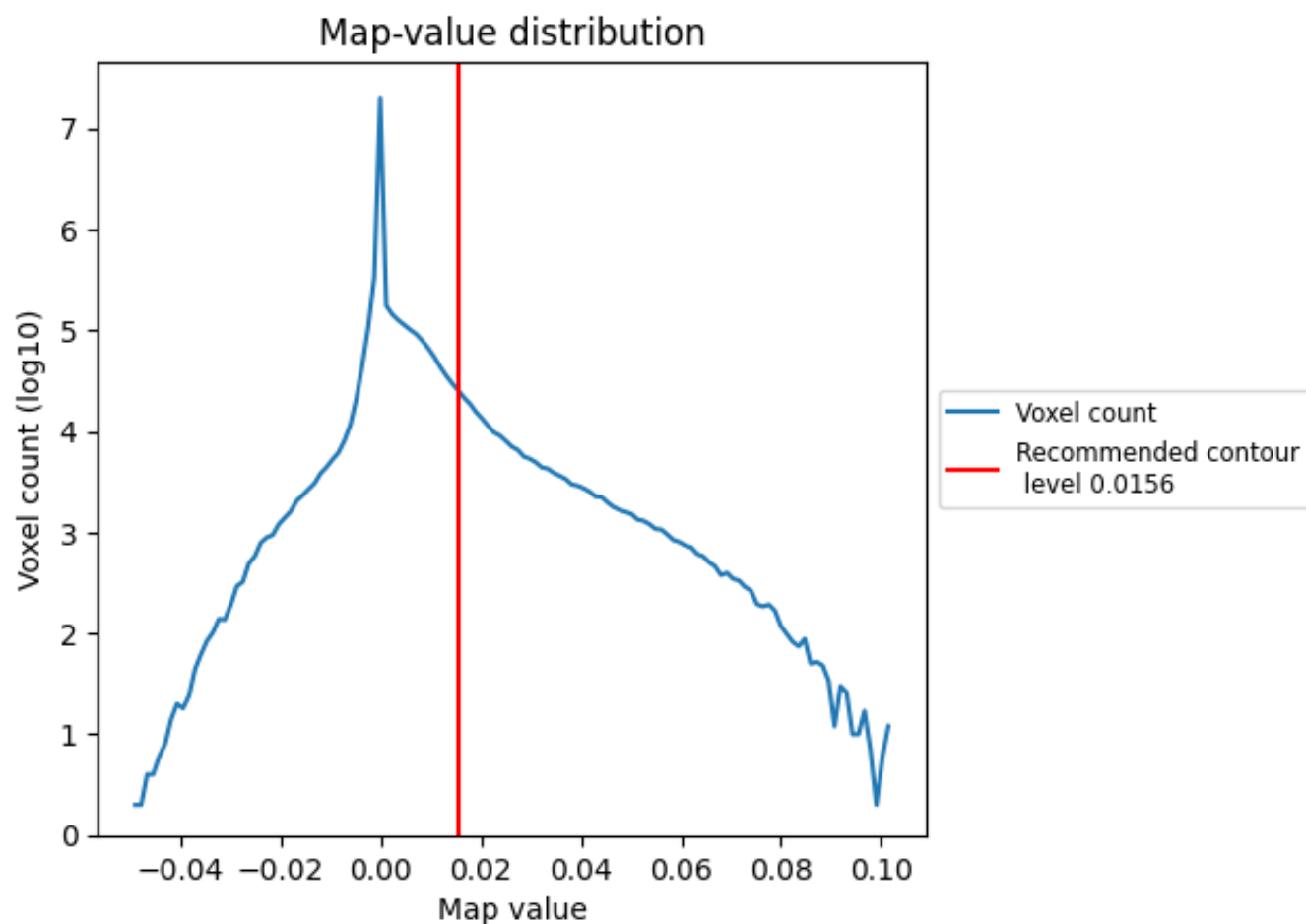
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

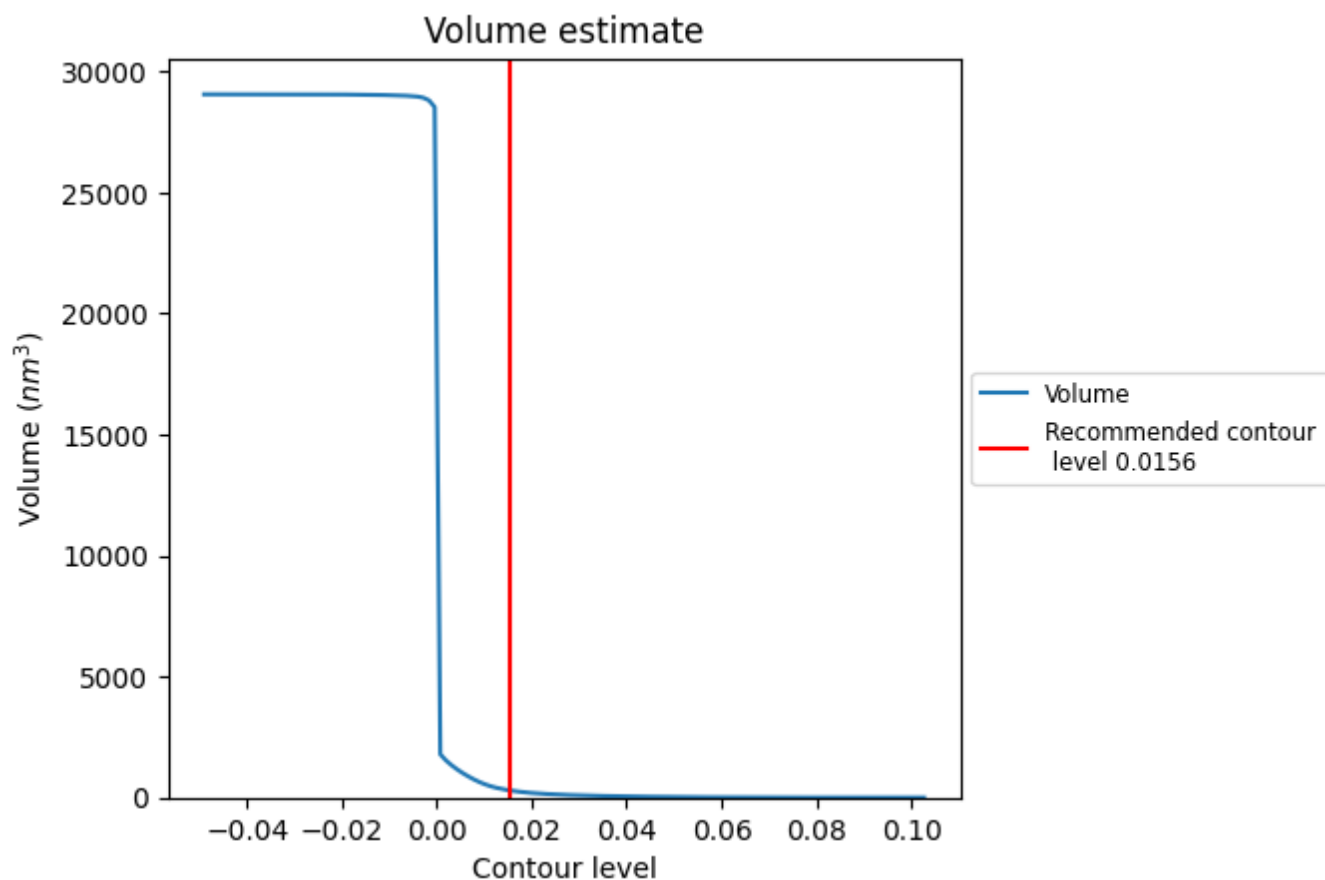
This section contains the results of statistical analysis of the map.

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.

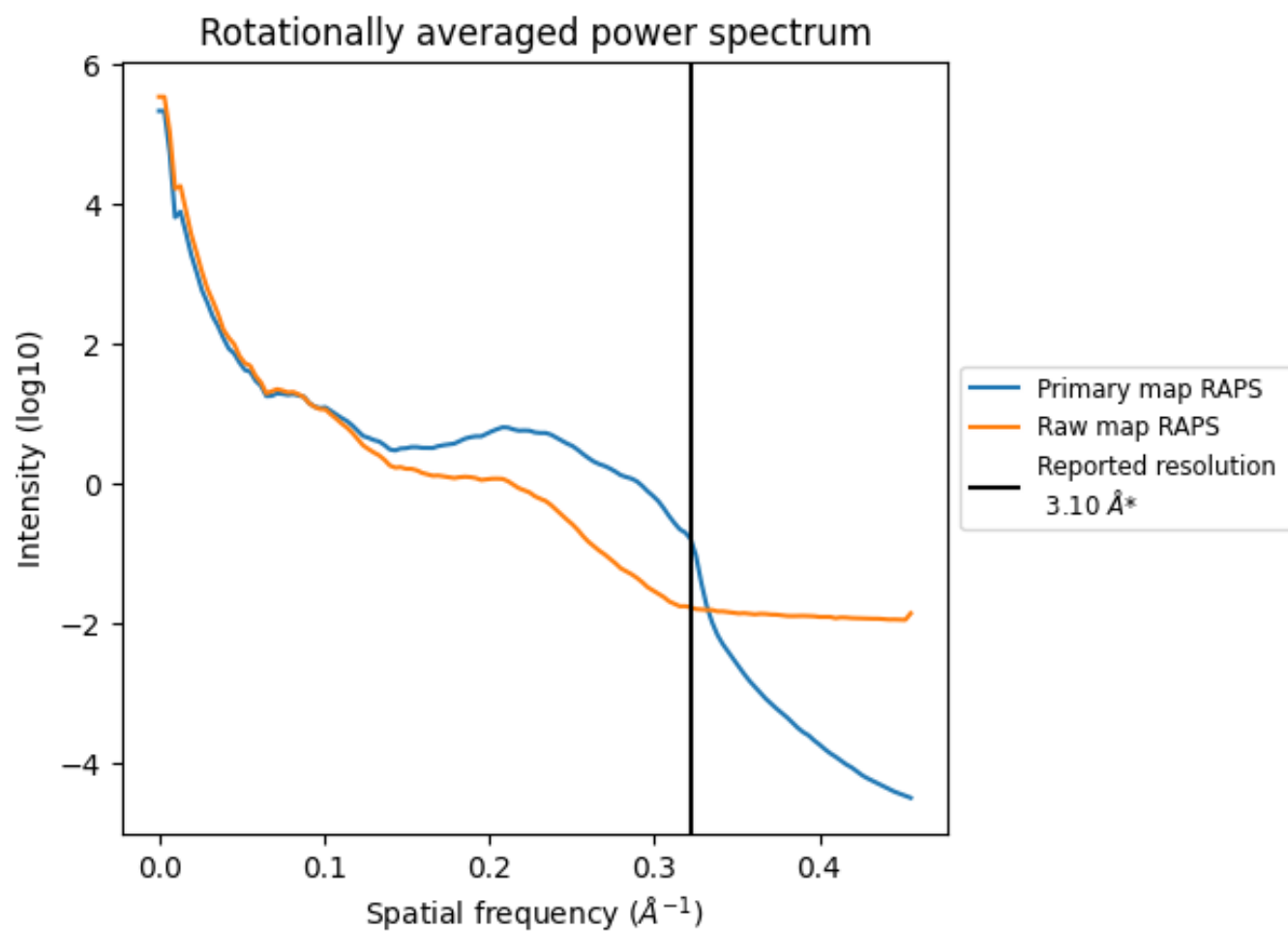
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 290 nm³; this corresponds to an approximate mass of 262 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 ⓘ

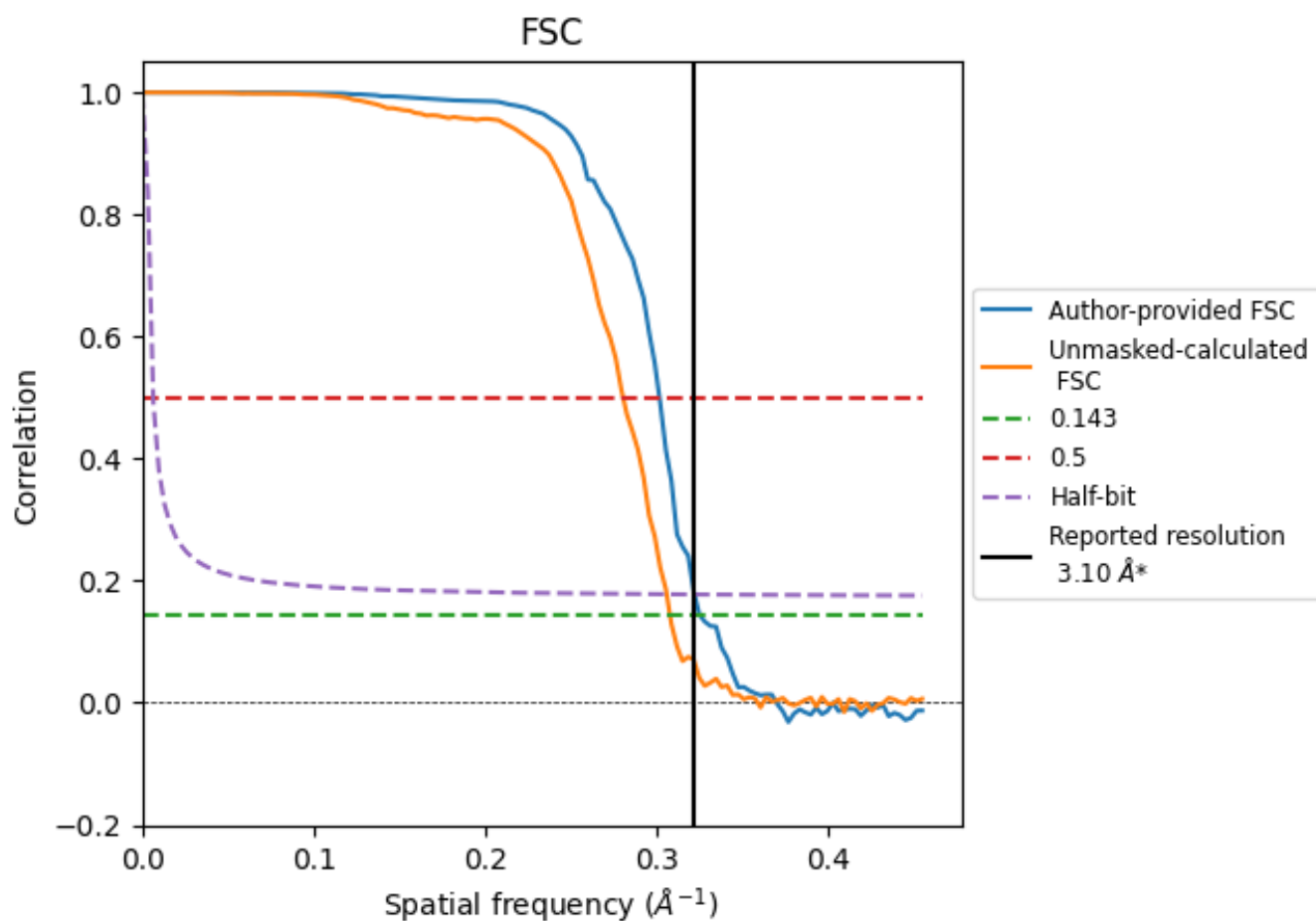


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

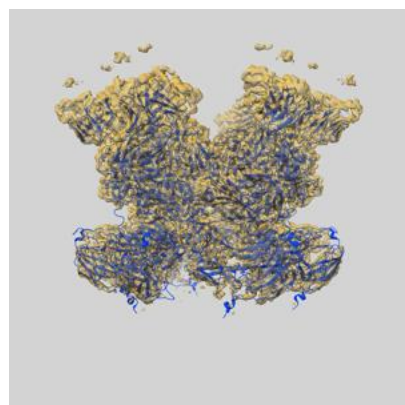
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.07	3.31	3.10
Unmasked-calculated*	3.24	3.56	3.27

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

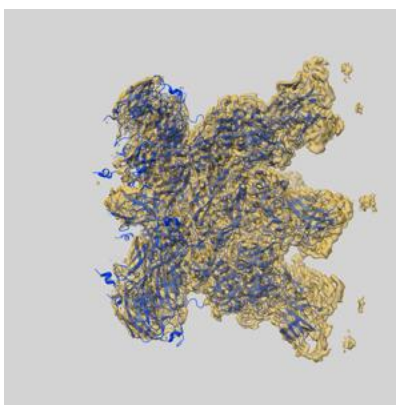
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-64805 and PDB model 9V6R. Per-residue inclusion information can be found in section [3](#) on page [15](#).

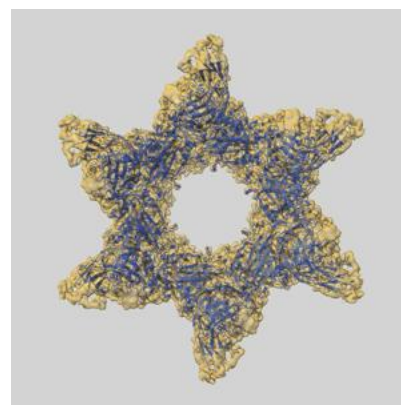
9.1 Map-model overlay [i](#)



X



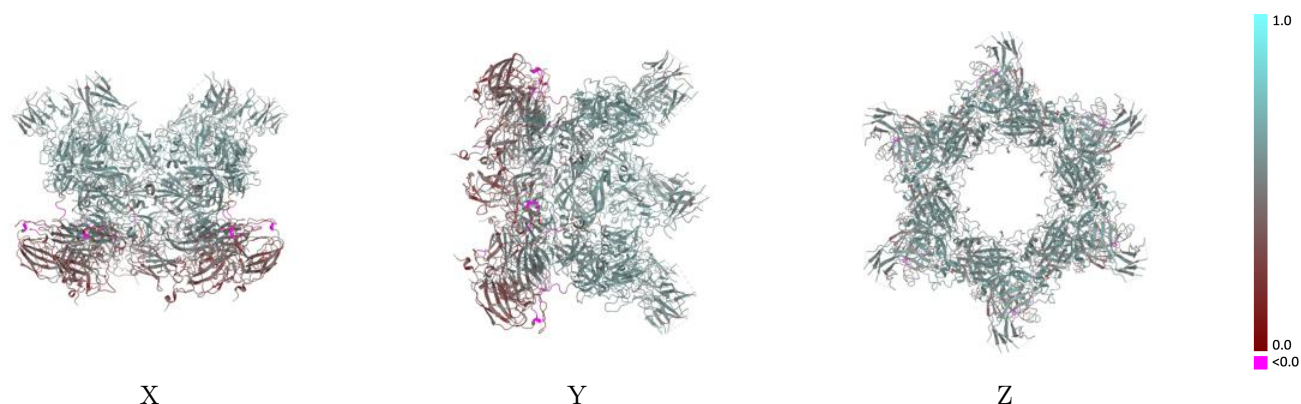
Y



Z

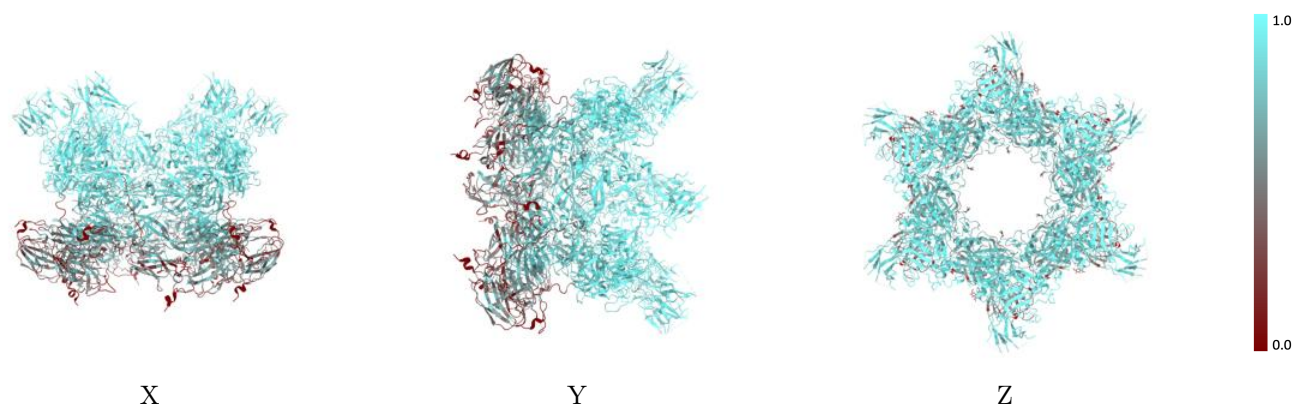
The images above show the 3D surface view of the map at the recommended contour level 0.0156 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



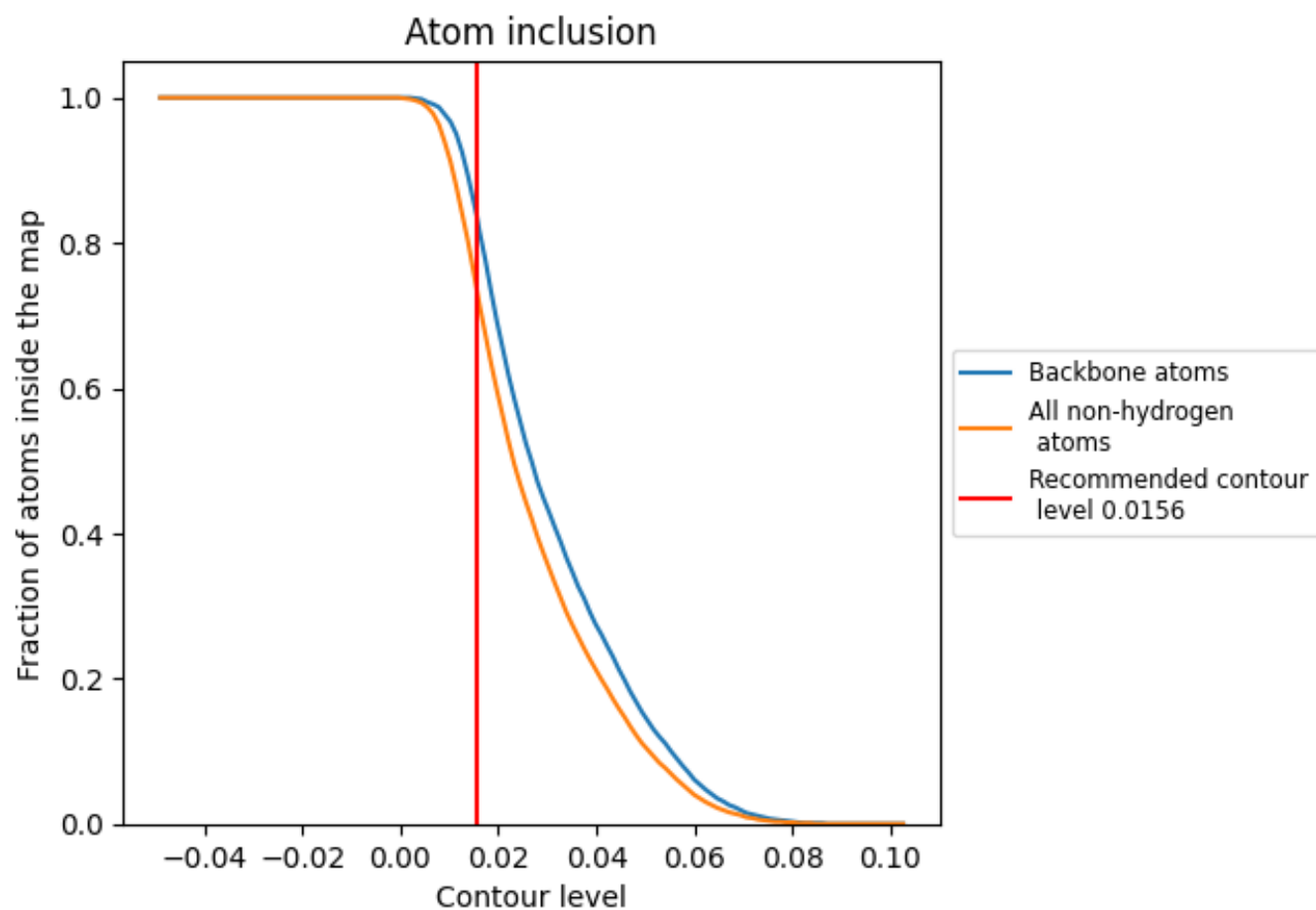
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0156).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 74% 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 (0.0156) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7350	 0.4940
A	 0.8010	 0.5340
B	 0.6340	 0.4460
C	 0.8000	 0.5330
D	 0.8580	 0.5290
E	 0.9130	 0.5480
F	 0.8560	 0.5280
G	 0.9170	 0.5520
H	 0.6350	 0.4470
I	 0.8030	 0.5330
J	 0.8620	 0.5240
K	 0.9150	 0.5510
L	 0.6360	 0.4470
M	 0.8010	 0.5340
N	 0.8580	 0.5260
O	 0.9130	 0.5490
P	 0.6350	 0.4460
Q	 0.8000	 0.5340
R	 0.8540	 0.5290
S	 0.9190	 0.5480
T	 0.6340	 0.4470
U	 0.1910	 0.2540
V	 0.8020	 0.5340
W	 0.8660	 0.5290
X	 0.9150	 0.5490
Y	 0.6350	 0.4480
Z	 0.1910	 0.2640
a	 0.2140	 0.2700
b	 0.1910	 0.2660
c	 0.1910	 0.2570
d	 0.2140	 0.2670

