



wwPDB EM Validation Summary Report ⓘ

Nov 15, 2022 – 11:49 AM JST

PDB ID : 6KXS
EMDB ID : EMD-0782
Title : Cryo-EM structure of human IgM-Fc in complex with the J chain and the ectodomain of pIgR
Authors : Li, Y.; Wang, G.; Xiao, J.
Deposited on : 2019-09-12
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

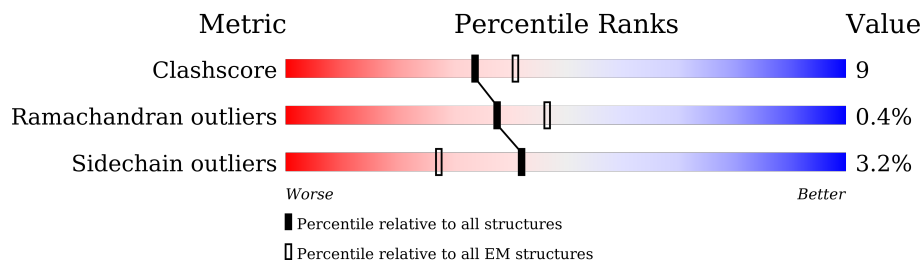
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



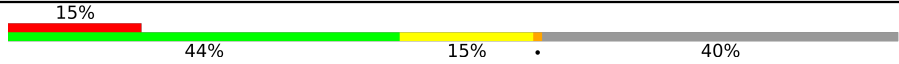
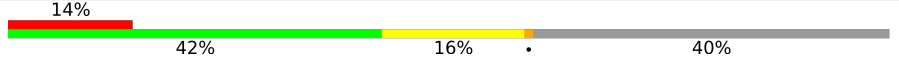
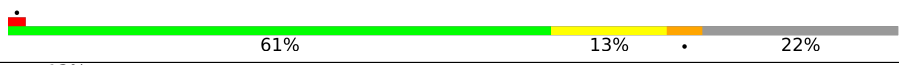

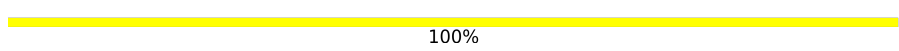
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	383	
1	B	383	
1	C	383	
1	D	383	
1	E	383	
1	F	383	
1	G	383	
1	H	383	

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Mol	Chain	Length	Quality of chain
1	K	383	
1	L	383	
2	J	136	
3	P	555	
4	I	2	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 22499 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 Immunoglobulin heavy constant mu.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	232	Total 1798	C 1132	N 304	O 353	S 9	0	0
1	B	227	Total 1764	C 1111	N 299	O 346	S 8	0	0
1	C	225	Total 1748	C 1103	N 297	O 340	S 8	0	0
1	D	224	Total 1743	C 1100	N 296	O 339	S 8	0	0
1	E	224	Total 1743	C 1100	N 296	O 339	S 8	0	0
1	F	221	Total 1723	C 1087	N 292	O 336	S 8	0	0
1	G	224	Total 1742	C 1100	N 296	O 338	S 8	0	0
1	H	230	Total 1785	C 1124	N 301	O 351	S 9	0	0
1	K	230	Total 1786	C 1124	N 302	O 351	S 9	0	0
1	L	228	Total 1773	C 1116	N 299	O 349	S 9	0	0

There are 350 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	194	ALA	-	expression tag	UNP P01871
A	195	SER	-	expression tag	UNP P01871
A	196	ALA	-	expression tag	UNP P01871
A	197	TRP	-	expression tag	UNP P01871
A	198	SER	-	expression tag	UNP P01871
A	199	HIS	-	expression tag	UNP P01871
A	200	PRO	-	expression tag	UNP P01871
A	201	GLN	-	expression tag	UNP P01871
A	202	PHE	-	expression tag	UNP P01871
A	203	GLU	-	expression tag	UNP P01871

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Chain	Residue	Modelled	Actual	Comment	Reference
A	204	LYS	-	expression tag	UNP P01871
A	205	GLY	-	expression tag	UNP P01871
A	206	GLY	-	expression tag	UNP P01871
A	207	GLY	-	expression tag	UNP P01871
A	208	SER	-	expression tag	UNP P01871
A	209	GLY	-	expression tag	UNP P01871
A	210	GLY	-	expression tag	UNP P01871
A	211	GLY	-	expression tag	UNP P01871
A	212	SER	-	expression tag	UNP P01871
A	213	GLY	-	expression tag	UNP P01871
A	214	GLY	-	expression tag	UNP P01871
A	215	SER	-	expression tag	UNP P01871
A	216	ALA	-	expression tag	UNP P01871
A	217	TRP	-	expression tag	UNP P01871
A	218	SER	-	expression tag	UNP P01871
A	219	HIS	-	expression tag	UNP P01871
A	220	PRO	-	expression tag	UNP P01871
A	221	GLN	-	expression tag	UNP P01871
A	222	PHE	-	expression tag	UNP P01871
A	223	GLU	-	expression tag	UNP P01871
A	224	LYS	-	expression tag	UNP P01871
A	225	ILE	-	expression tag	UNP P01871
A	226	ASP	-	expression tag	UNP P01871
A	227	THR	-	expression tag	UNP P01871
A	228	THR	-	expression tag	UNP P01871
B	194	ALA	-	expression tag	UNP P01871
B	195	SER	-	expression tag	UNP P01871
B	196	ALA	-	expression tag	UNP P01871
B	197	TRP	-	expression tag	UNP P01871
B	198	SER	-	expression tag	UNP P01871
B	199	HIS	-	expression tag	UNP P01871
B	200	PRO	-	expression tag	UNP P01871
B	201	GLN	-	expression tag	UNP P01871
B	202	PHE	-	expression tag	UNP P01871
B	203	GLU	-	expression tag	UNP P01871
B	204	LYS	-	expression tag	UNP P01871
B	205	GLY	-	expression tag	UNP P01871
B	206	GLY	-	expression tag	UNP P01871
B	207	GLY	-	expression tag	UNP P01871
B	208	SER	-	expression tag	UNP P01871
B	209	GLY	-	expression tag	UNP P01871
B	210	GLY	-	expression tag	UNP P01871

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Chain	Residue	Modelled	Actual	Comment	Reference
B	211	GLY	-	expression tag	UNP P01871
B	212	SER	-	expression tag	UNP P01871
B	213	GLY	-	expression tag	UNP P01871
B	214	GLY	-	expression tag	UNP P01871
B	215	SER	-	expression tag	UNP P01871
B	216	ALA	-	expression tag	UNP P01871
B	217	TRP	-	expression tag	UNP P01871
B	218	SER	-	expression tag	UNP P01871
B	219	HIS	-	expression tag	UNP P01871
B	220	PRO	-	expression tag	UNP P01871
B	221	GLN	-	expression tag	UNP P01871
B	222	PHE	-	expression tag	UNP P01871
B	223	GLU	-	expression tag	UNP P01871
B	224	LYS	-	expression tag	UNP P01871
B	225	ILE	-	expression tag	UNP P01871
B	226	ASP	-	expression tag	UNP P01871
B	227	THR	-	expression tag	UNP P01871
B	228	THR	-	expression tag	UNP P01871
C	194	ALA	-	expression tag	UNP P01871
C	195	SER	-	expression tag	UNP P01871
C	196	ALA	-	expression tag	UNP P01871
C	197	TRP	-	expression tag	UNP P01871
C	198	SER	-	expression tag	UNP P01871
C	199	HIS	-	expression tag	UNP P01871
C	200	PRO	-	expression tag	UNP P01871
C	201	GLN	-	expression tag	UNP P01871
C	202	PHE	-	expression tag	UNP P01871
C	203	GLU	-	expression tag	UNP P01871
C	204	LYS	-	expression tag	UNP P01871
C	205	GLY	-	expression tag	UNP P01871
C	206	GLY	-	expression tag	UNP P01871
C	207	GLY	-	expression tag	UNP P01871
C	208	SER	-	expression tag	UNP P01871
C	209	GLY	-	expression tag	UNP P01871
C	210	GLY	-	expression tag	UNP P01871
C	211	GLY	-	expression tag	UNP P01871
C	212	SER	-	expression tag	UNP P01871
C	213	GLY	-	expression tag	UNP P01871
C	214	GLY	-	expression tag	UNP P01871
C	215	SER	-	expression tag	UNP P01871
C	216	ALA	-	expression tag	UNP P01871
C	217	TRP	-	expression tag	UNP P01871

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Chain	Residue	Modelled	Actual	Comment	Reference
C	218	SER	-	expression tag	UNP P01871
C	219	HIS	-	expression tag	UNP P01871
C	220	PRO	-	expression tag	UNP P01871
C	221	GLN	-	expression tag	UNP P01871
C	222	PHE	-	expression tag	UNP P01871
C	223	GLU	-	expression tag	UNP P01871
C	224	LYS	-	expression tag	UNP P01871
C	225	ILE	-	expression tag	UNP P01871
C	226	ASP	-	expression tag	UNP P01871
C	227	THR	-	expression tag	UNP P01871
C	228	THR	-	expression tag	UNP P01871
D	194	ALA	-	expression tag	UNP P01871
D	195	SER	-	expression tag	UNP P01871
D	196	ALA	-	expression tag	UNP P01871
D	197	TRP	-	expression tag	UNP P01871
D	198	SER	-	expression tag	UNP P01871
D	199	HIS	-	expression tag	UNP P01871
D	200	PRO	-	expression tag	UNP P01871
D	201	GLN	-	expression tag	UNP P01871
D	202	PHE	-	expression tag	UNP P01871
D	203	GLU	-	expression tag	UNP P01871
D	204	LYS	-	expression tag	UNP P01871
D	205	GLY	-	expression tag	UNP P01871
D	206	GLY	-	expression tag	UNP P01871
D	207	GLY	-	expression tag	UNP P01871
D	208	SER	-	expression tag	UNP P01871
D	209	GLY	-	expression tag	UNP P01871
D	210	GLY	-	expression tag	UNP P01871
D	211	GLY	-	expression tag	UNP P01871
D	212	SER	-	expression tag	UNP P01871
D	213	GLY	-	expression tag	UNP P01871
D	214	GLY	-	expression tag	UNP P01871
D	215	SER	-	expression tag	UNP P01871
D	216	ALA	-	expression tag	UNP P01871
D	217	TRP	-	expression tag	UNP P01871
D	218	SER	-	expression tag	UNP P01871
D	219	HIS	-	expression tag	UNP P01871
D	220	PRO	-	expression tag	UNP P01871
D	221	GLN	-	expression tag	UNP P01871
D	222	PHE	-	expression tag	UNP P01871
D	223	GLU	-	expression tag	UNP P01871
D	224	LYS	-	expression tag	UNP P01871

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Chain	Residue	Modelled	Actual	Comment	Reference
D	225	ILE	-	expression tag	UNP P01871
D	226	ASP	-	expression tag	UNP P01871
D	227	THR	-	expression tag	UNP P01871
D	228	THR	-	expression tag	UNP P01871
E	194	ALA	-	expression tag	UNP P01871
E	195	SER	-	expression tag	UNP P01871
E	196	ALA	-	expression tag	UNP P01871
E	197	TRP	-	expression tag	UNP P01871
E	198	SER	-	expression tag	UNP P01871
E	199	HIS	-	expression tag	UNP P01871
E	200	PRO	-	expression tag	UNP P01871
E	201	GLN	-	expression tag	UNP P01871
E	202	PHE	-	expression tag	UNP P01871
E	203	GLU	-	expression tag	UNP P01871
E	204	LYS	-	expression tag	UNP P01871
E	205	GLY	-	expression tag	UNP P01871
E	206	GLY	-	expression tag	UNP P01871
E	207	GLY	-	expression tag	UNP P01871
E	208	SER	-	expression tag	UNP P01871
E	209	GLY	-	expression tag	UNP P01871
E	210	GLY	-	expression tag	UNP P01871
E	211	GLY	-	expression tag	UNP P01871
E	212	SER	-	expression tag	UNP P01871
E	213	GLY	-	expression tag	UNP P01871
E	214	GLY	-	expression tag	UNP P01871
E	215	SER	-	expression tag	UNP P01871
E	216	ALA	-	expression tag	UNP P01871
E	217	TRP	-	expression tag	UNP P01871
E	218	SER	-	expression tag	UNP P01871
E	219	HIS	-	expression tag	UNP P01871
E	220	PRO	-	expression tag	UNP P01871
E	221	GLN	-	expression tag	UNP P01871
E	222	PHE	-	expression tag	UNP P01871
E	223	GLU	-	expression tag	UNP P01871
E	224	LYS	-	expression tag	UNP P01871
E	225	ILE	-	expression tag	UNP P01871
E	226	ASP	-	expression tag	UNP P01871
E	227	THR	-	expression tag	UNP P01871
E	228	THR	-	expression tag	UNP P01871
F	194	ALA	-	expression tag	UNP P01871
F	195	SER	-	expression tag	UNP P01871
F	196	ALA	-	expression tag	UNP P01871

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Chain	Residue	Modelled	Actual	Comment	Reference
F	197	TRP	-	expression tag	UNP P01871
F	198	SER	-	expression tag	UNP P01871
F	199	HIS	-	expression tag	UNP P01871
F	200	PRO	-	expression tag	UNP P01871
F	201	GLN	-	expression tag	UNP P01871
F	202	PHE	-	expression tag	UNP P01871
F	203	GLU	-	expression tag	UNP P01871
F	204	LYS	-	expression tag	UNP P01871
F	205	GLY	-	expression tag	UNP P01871
F	206	GLY	-	expression tag	UNP P01871
F	207	GLY	-	expression tag	UNP P01871
F	208	SER	-	expression tag	UNP P01871
F	209	GLY	-	expression tag	UNP P01871
F	210	GLY	-	expression tag	UNP P01871
F	211	GLY	-	expression tag	UNP P01871
F	212	SER	-	expression tag	UNP P01871
F	213	GLY	-	expression tag	UNP P01871
F	214	GLY	-	expression tag	UNP P01871
F	215	SER	-	expression tag	UNP P01871
F	216	ALA	-	expression tag	UNP P01871
F	217	TRP	-	expression tag	UNP P01871
F	218	SER	-	expression tag	UNP P01871
F	219	HIS	-	expression tag	UNP P01871
F	220	PRO	-	expression tag	UNP P01871
F	221	GLN	-	expression tag	UNP P01871
F	222	PHE	-	expression tag	UNP P01871
F	223	GLU	-	expression tag	UNP P01871
F	224	LYS	-	expression tag	UNP P01871
F	225	ILE	-	expression tag	UNP P01871
F	226	ASP	-	expression tag	UNP P01871
F	227	THR	-	expression tag	UNP P01871
F	228	THR	-	expression tag	UNP P01871
G	194	ALA	-	expression tag	UNP P01871
G	195	SER	-	expression tag	UNP P01871
G	196	ALA	-	expression tag	UNP P01871
G	197	TRP	-	expression tag	UNP P01871
G	198	SER	-	expression tag	UNP P01871
G	199	HIS	-	expression tag	UNP P01871
G	200	PRO	-	expression tag	UNP P01871
G	201	GLN	-	expression tag	UNP P01871
G	202	PHE	-	expression tag	UNP P01871
G	203	GLU	-	expression tag	UNP P01871

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Chain	Residue	Modelled	Actual	Comment	Reference
G	204	LYS	-	expression tag	UNP P01871
G	205	GLY	-	expression tag	UNP P01871
G	206	GLY	-	expression tag	UNP P01871
G	207	GLY	-	expression tag	UNP P01871
G	208	SER	-	expression tag	UNP P01871
G	209	GLY	-	expression tag	UNP P01871
G	210	GLY	-	expression tag	UNP P01871
G	211	GLY	-	expression tag	UNP P01871
G	212	SER	-	expression tag	UNP P01871
G	213	GLY	-	expression tag	UNP P01871
G	214	GLY	-	expression tag	UNP P01871
G	215	SER	-	expression tag	UNP P01871
G	216	ALA	-	expression tag	UNP P01871
G	217	TRP	-	expression tag	UNP P01871
G	218	SER	-	expression tag	UNP P01871
G	219	HIS	-	expression tag	UNP P01871
G	220	PRO	-	expression tag	UNP P01871
G	221	GLN	-	expression tag	UNP P01871
G	222	PHE	-	expression tag	UNP P01871
G	223	GLU	-	expression tag	UNP P01871
G	224	LYS	-	expression tag	UNP P01871
G	225	ILE	-	expression tag	UNP P01871
G	226	ASP	-	expression tag	UNP P01871
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G	228	THR	-	expression tag	UNP P01871
H	194	ALA	-	expression tag	UNP P01871
H	195	SER	-	expression tag	UNP P01871
H	196	ALA	-	expression tag	UNP P01871
H	197	TRP	-	expression tag	UNP P01871
H	198	SER	-	expression tag	UNP P01871
H	199	HIS	-	expression tag	UNP P01871
H	200	PRO	-	expression tag	UNP P01871
H	201	GLN	-	expression tag	UNP P01871
H	202	PHE	-	expression tag	UNP P01871
H	203	GLU	-	expression tag	UNP P01871
H	204	LYS	-	expression tag	UNP P01871
H	205	GLY	-	expression tag	UNP P01871
H	206	GLY	-	expression tag	UNP P01871
H	207	GLY	-	expression tag	UNP P01871
H	208	SER	-	expression tag	UNP P01871
H	209	GLY	-	expression tag	UNP P01871
H	210	GLY	-	expression tag	UNP P01871

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Chain	Residue	Modelled	Actual	Comment	Reference
H	211	GLY	-	expression tag	UNP P01871
H	212	SER	-	expression tag	UNP P01871
H	213	GLY	-	expression tag	UNP P01871
H	214	GLY	-	expression tag	UNP P01871
H	215	SER	-	expression tag	UNP P01871
H	216	ALA	-	expression tag	UNP P01871
H	217	TRP	-	expression tag	UNP P01871
H	218	SER	-	expression tag	UNP P01871
H	219	HIS	-	expression tag	UNP P01871
H	220	PRO	-	expression tag	UNP P01871
H	221	GLN	-	expression tag	UNP P01871
H	222	PHE	-	expression tag	UNP P01871
H	223	GLU	-	expression tag	UNP P01871
H	224	LYS	-	expression tag	UNP P01871
H	225	ILE	-	expression tag	UNP P01871
H	226	ASP	-	expression tag	UNP P01871
H	227	THR	-	expression tag	UNP P01871
H	228	THR	-	expression tag	UNP P01871
K	194	ALA	-	expression tag	UNP P01871
K	195	SER	-	expression tag	UNP P01871
K	196	ALA	-	expression tag	UNP P01871
K	197	TRP	-	expression tag	UNP P01871
K	198	SER	-	expression tag	UNP P01871
K	199	HIS	-	expression tag	UNP P01871
K	200	PRO	-	expression tag	UNP P01871
K	201	GLN	-	expression tag	UNP P01871
K	202	PHE	-	expression tag	UNP P01871
K	203	GLU	-	expression tag	UNP P01871
K	204	LYS	-	expression tag	UNP P01871
K	205	GLY	-	expression tag	UNP P01871
K	206	GLY	-	expression tag	UNP P01871
K	207	GLY	-	expression tag	UNP P01871
K	208	SER	-	expression tag	UNP P01871
K	209	GLY	-	expression tag	UNP P01871
K	210	GLY	-	expression tag	UNP P01871
K	211	GLY	-	expression tag	UNP P01871
K	212	SER	-	expression tag	UNP P01871
K	213	GLY	-	expression tag	UNP P01871
K	214	GLY	-	expression tag	UNP P01871
K	215	SER	-	expression tag	UNP P01871
K	216	ALA	-	expression tag	UNP P01871
K	217	TRP	-	expression tag	UNP P01871

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Chain	Residue	Modelled	Actual	Comment	Reference
K	218	SER	-	expression tag	UNP P01871
K	219	HIS	-	expression tag	UNP P01871
K	220	PRO	-	expression tag	UNP P01871
K	221	GLN	-	expression tag	UNP P01871
K	222	PHE	-	expression tag	UNP P01871
K	223	GLU	-	expression tag	UNP P01871
K	224	LYS	-	expression tag	UNP P01871
K	225	ILE	-	expression tag	UNP P01871
K	226	ASP	-	expression tag	UNP P01871
K	227	THR	-	expression tag	UNP P01871
K	228	THR	-	expression tag	UNP P01871
L	194	ALA	-	expression tag	UNP P01871
L	195	SER	-	expression tag	UNP P01871
L	196	ALA	-	expression tag	UNP P01871
L	197	TRP	-	expression tag	UNP P01871
L	198	SER	-	expression tag	UNP P01871
L	199	HIS	-	expression tag	UNP P01871
L	200	PRO	-	expression tag	UNP P01871
L	201	GLN	-	expression tag	UNP P01871
L	202	PHE	-	expression tag	UNP P01871
L	203	GLU	-	expression tag	UNP P01871
L	204	LYS	-	expression tag	UNP P01871
L	205	GLY	-	expression tag	UNP P01871
L	206	GLY	-	expression tag	UNP P01871
L	207	GLY	-	expression tag	UNP P01871
L	208	SER	-	expression tag	UNP P01871
L	209	GLY	-	expression tag	UNP P01871
L	210	GLY	-	expression tag	UNP P01871
L	211	GLY	-	expression tag	UNP P01871
L	212	SER	-	expression tag	UNP P01871
L	213	GLY	-	expression tag	UNP P01871
L	214	GLY	-	expression tag	UNP P01871
L	215	SER	-	expression tag	UNP P01871
L	216	ALA	-	expression tag	UNP P01871
L	217	TRP	-	expression tag	UNP P01871
L	218	SER	-	expression tag	UNP P01871
L	219	HIS	-	expression tag	UNP P01871
L	220	PRO	-	expression tag	UNP P01871
L	221	GLN	-	expression tag	UNP P01871
L	222	PHE	-	expression tag	UNP P01871
L	223	GLU	-	expression tag	UNP P01871
L	224	LYS	-	expression tag	UNP P01871

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Chain	Residue	Modelled	Actual	Comment	Reference
L	225	ILE	-	expression tag	UNP P01871
L	226	ASP	-	expression tag	UNP P01871
L	227	THR	-	expression tag	UNP P01871
L	228	THR	-	expression tag	UNP P01871

- Molecule 2 is a protein called Immunoglobulin J chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	J	106	851	528	150	166	7	0	0

- Molecule 3 is a protein called Polymeric immunoglobulin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	P	498	3875	2448	674	734	19	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	548	HIS	-	expression tag	UNP P01833
P	549	HIS	-	expression tag	UNP P01833
P	550	HIS	-	expression tag	UNP P01833
P	551	HIS	-	expression tag	UNP P01833
P	552	HIS	-	expression tag	UNP P01833
P	553	HIS	-	expression tag	UNP P01833
P	554	HIS	-	expression tag	UNP P01833
P	555	HIS	-	expression tag	UNP P01833

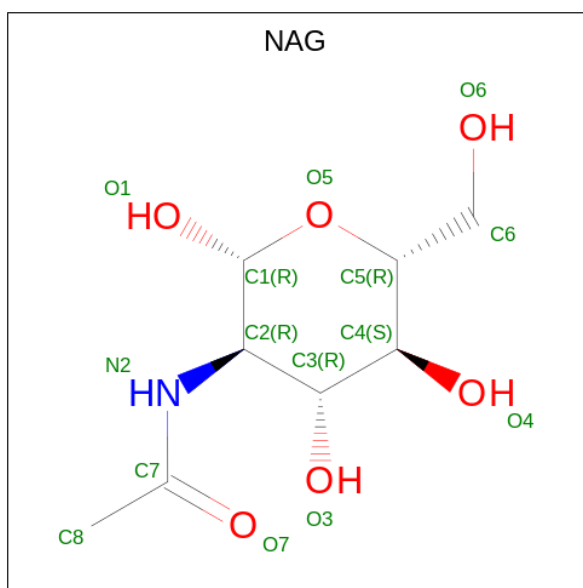
- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	I	2	28	16	2	10	0	0

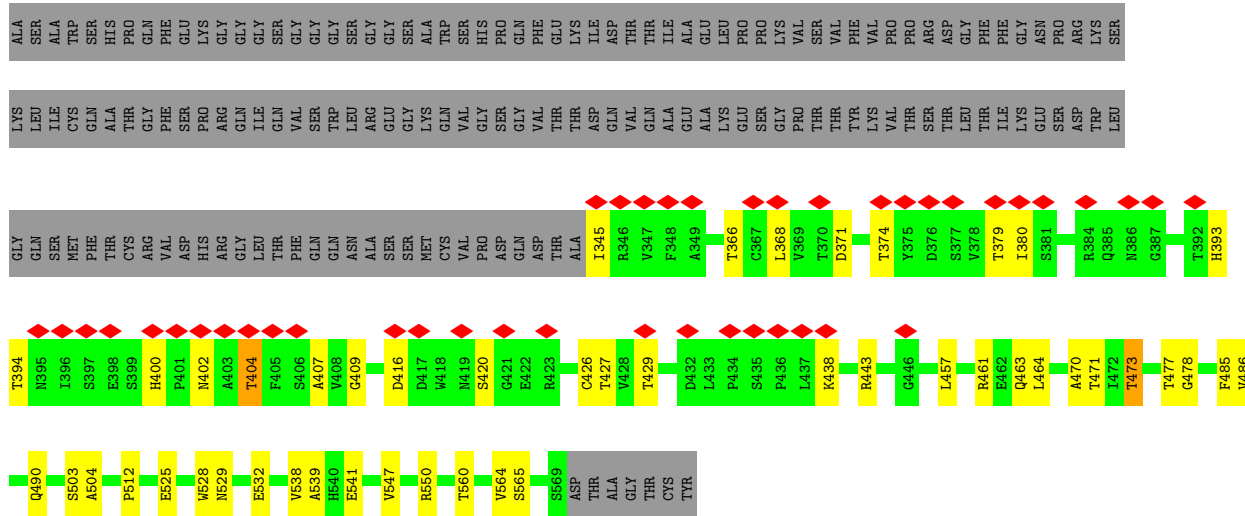
- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

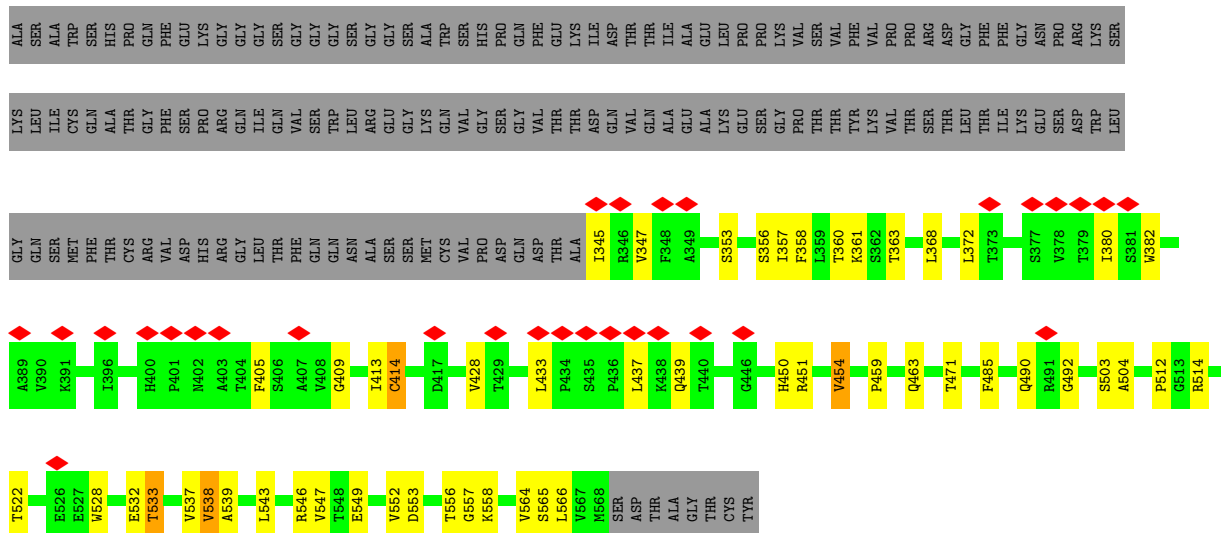


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	Total 14	8	1	5	0
5	B	1	Total 14	8	1	5	0
5	C	1	Total 14	8	1	5	0
5	D	1	Total 14	8	1	5	0
5	E	1	Total 14	8	1	5	0
5	F	1	Total 14	8	1	5	0
5	G	1	Total 14	8	1	5	0
5	H	1	Total 14	8	1	5	0
5	K	1	Total 14	8	1	5	0
5	L	1	Total 14	8	1	5	0

• Molecule 1: Immunoglobulin heavy constant mu

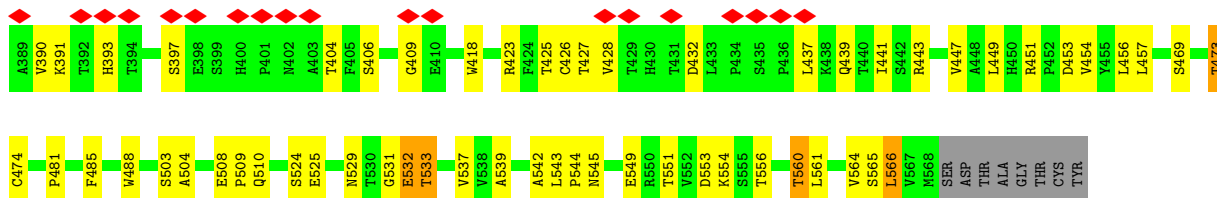


• Molecule 1: Immunoglobulin heavy constant mu

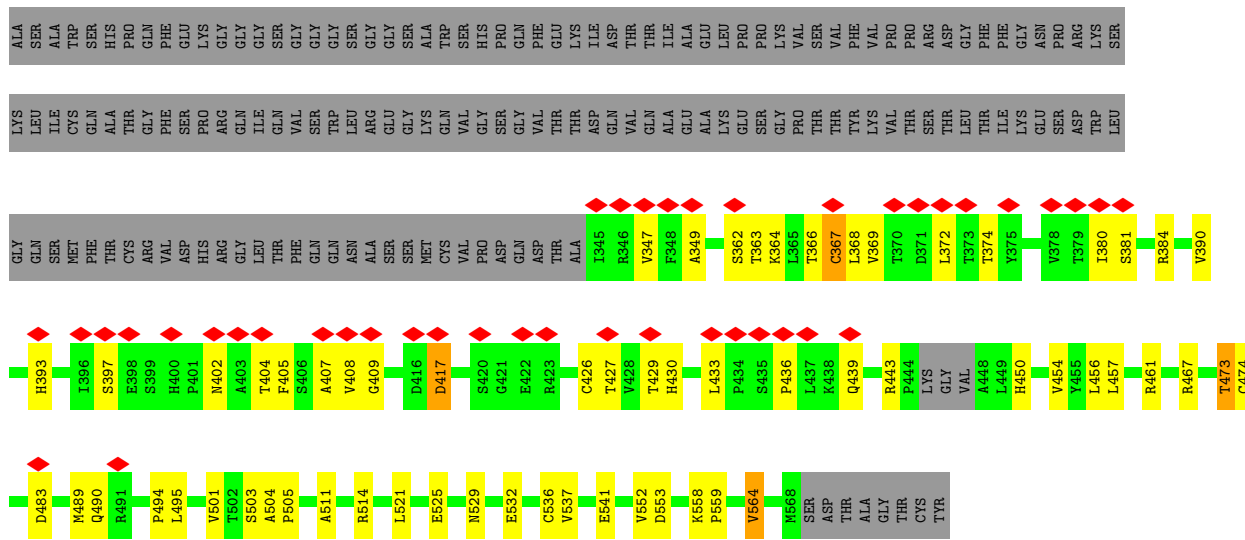


• Molecule 1: Immunoglobulin heavy constant mu

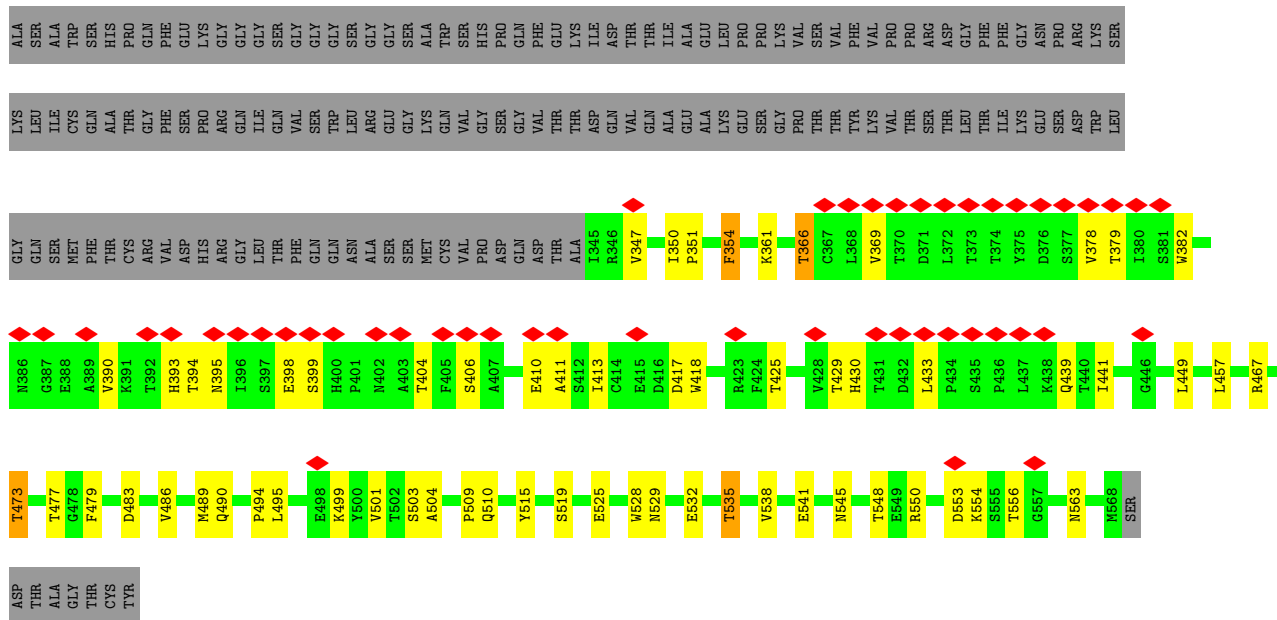
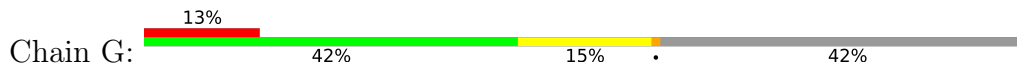




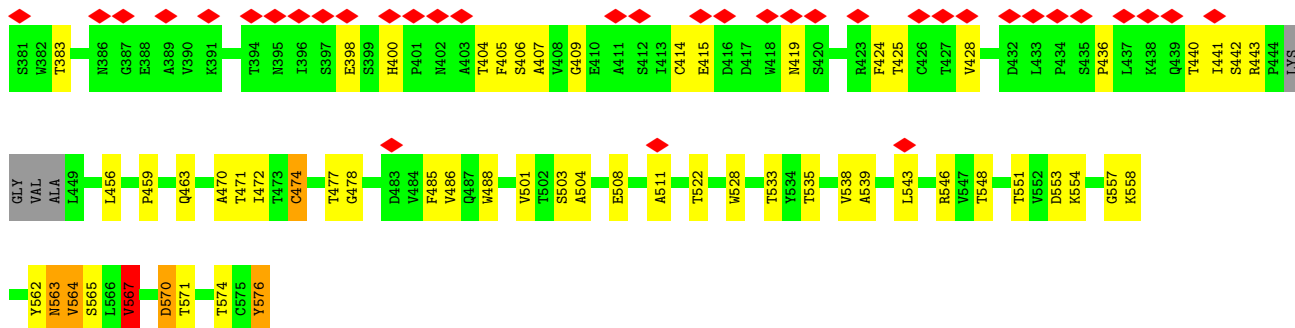
• Molecule 1: Immunoglobulin heavy constant mu



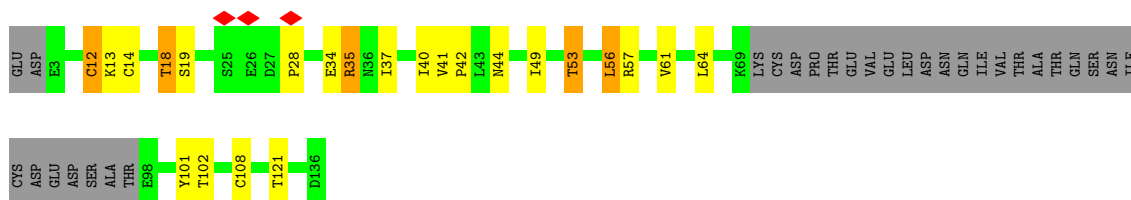
• Molecule 1: Immunoglobulin heavy constant mu



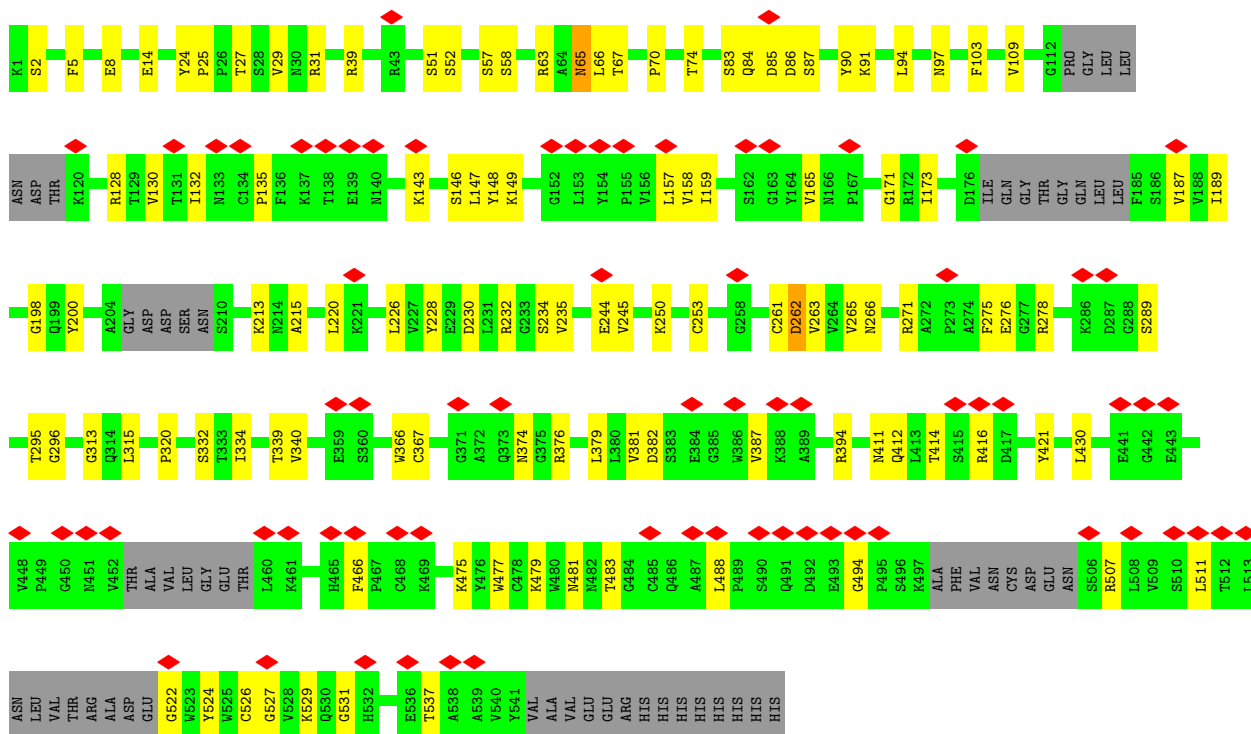
• Molecule 1: Immunoglobulin heavy constant mu




• Molecule 2: Immunoglobulin J chain



• Molecule 3: Polymeric immunoglobulin receptor



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

Chain I:  100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1183008	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59.74	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.119	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	264.96, 264.96, 264.96	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82799995, 0.82799995, 0.82799995	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	0.94	3/1844 (0.2%)	0.80	4/2526 (0.2%)
1	B	0.92	2/1809 (0.1%)	0.81	4/2478 (0.2%)
1	C	0.79	1/1793 (0.1%)	0.73	0/2455
1	D	0.78	2/1788 (0.1%)	0.73	0/2449
1	E	0.75	2/1788 (0.1%)	0.74	2/2449 (0.1%)
1	F	0.78	3/1767 (0.2%)	0.74	1/2420 (0.0%)
1	G	0.72	0/1787	0.68	0/2447
1	H	0.80	3/1830 (0.2%)	0.72	2/2507 (0.1%)
1	K	0.71	1/1831 (0.1%)	0.71	2/2506 (0.1%)
1	L	0.73	5/1818 (0.3%)	0.75	2/2490 (0.1%)
2	J	1.24	5/864 (0.6%)	1.01	3/1173 (0.3%)
3	P	0.84	4/3959 (0.1%)	0.75	2/5365 (0.0%)
All	All	0.83	31/22878 (0.1%)	0.76	22/31265 (0.1%)

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	D	0	1
1	G	0	1
1	K	0	2
1	L	0	2
All	All	0	6

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	567	VAL	CB-CG2	-8.23	1.35	1.52
1	L	576	TYR	CD1-CE1	-7.26	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	567	VAL	CB-CG1	-6.87	1.38	1.52
2	J	34	GLU	CB-CG	-6.40	1.40	1.52
1	C	547	VAL	CB-CG2	-6.13	1.40	1.52

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	12	CYS	CA-CB-SG	7.55	127.59	114.00
1	A	566	LEU	CB-CG-CD1	-6.99	99.12	111.00
1	A	456	LEU	CB-CG-CD1	-6.44	100.05	111.00
1	H	566	LEU	CB-CG-CD1	-6.36	100.19	111.00
3	P	94	LEU	CB-CG-CD2	-6.24	100.39	111.00

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	414	CYS	Peptide
1	G	483	ASP	Peptide
1	K	530	THR	Peptide
1	K	531	GLY	Peptide
1	L	528	TRP	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1798	0	1752	33	0
1	B	1764	0	1723	27	0
1	C	1748	0	1712	26	0
1	D	1743	0	1707	33	0
1	E	1743	0	1707	42	0
1	F	1723	0	1681	38	0
1	G	1742	0	1706	37	0
1	H	1785	0	1734	33	0
1	K	1786	0	1735	38	0
1	L	1773	0	1721	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	851	0	842	11	0
3	P	3875	0	3789	65	0
4	I	28	0	25	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	C	14	0	13	0	0
5	D	14	0	13	0	0
5	E	14	0	13	0	0
5	F	14	0	13	1	0
5	G	14	0	13	1	0
5	H	14	0	13	0	0
5	K	14	0	13	0	0
5	L	14	0	13	0	0
All	All	22499	0	21964	399	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 9.

The worst 5 of 399 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:C:366:THR:HA	1:C:409:GLY:O	1.84	0.77
1:B:454:VAL:HG21	1:B:538:VAL:HG11	1.67	0.76
1:H:454:VAL:HG21	1:H:538:VAL:HG11	1.68	0.75
1:H:562:TYR:HB3	1:K:562:TYR:HB2	1.68	0.74
1:E:423:ARG:HA	1:E:441:ILE:O	1.89	0.72

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	230/383 (60%)	195 (85%)	33 (14%)	2 (1%)	17	49
1	B	225/383 (59%)	186 (83%)	39 (17%)	0	100	100
1	C	223/383 (58%)	182 (82%)	40 (18%)	1 (0%)	34	67
1	D	222/383 (58%)	188 (85%)	32 (14%)	2 (1%)	17	49
1	E	222/383 (58%)	180 (81%)	39 (18%)	3 (1%)	11	37
1	F	217/383 (57%)	192 (88%)	25 (12%)	0	100	100
1	G	222/383 (58%)	190 (86%)	32 (14%)	0	100	100
1	H	226/383 (59%)	195 (86%)	31 (14%)	0	100	100
1	K	226/383 (59%)	189 (84%)	36 (16%)	1 (0%)	34	67
1	L	224/383 (58%)	188 (84%)	36 (16%)	0	100	100
2	J	102/136 (75%)	69 (68%)	31 (30%)	2 (2%)	7	30
3	P	484/555 (87%)	429 (89%)	55 (11%)	0	100	100
All	All	2823/4521 (62%)	2383 (84%)	429 (15%)	11 (0%)	38	67

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	560	THR
1	D	532	GLU
2	J	56	LEU
1	K	532	GLU
2	J	28	PRO

5.3.2 Protein sidechains [i](#)

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	206/331 (62%)	196 (95%)	10 (5%)	25	55
1	B	203/331 (61%)	198 (98%)	5 (2%)	47	72
1	C	201/331 (61%)	194 (96%)	7 (4%)	36	65
1	D	200/331 (60%)	194 (97%)	6 (3%)	41	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	200/331 (60%)	194 (97%)	6 (3%)	41	68
1	F	198/331 (60%)	191 (96%)	7 (4%)	36	65
1	G	200/331 (60%)	193 (96%)	7 (4%)	36	65
1	H	205/331 (62%)	194 (95%)	11 (5%)	22	52
1	K	205/331 (62%)	204 (100%)	1 (0%)	88	94
1	L	204/331 (62%)	199 (98%)	5 (2%)	47	72
2	J	100/128 (78%)	94 (94%)	6 (6%)	19	49
3	P	426/474 (90%)	416 (98%)	10 (2%)	50	74
All	All	2548/3912 (65%)	2467 (97%)	81 (3%)	42	67

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	575	CYS
3	P	65	ASN
1	K	551	THR
2	J	12	CYS
3	P	262	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
2	J	45	ASN
3	P	97	ASN
3	P	411	ASN
1	D	493	GLN
1	D	490	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates i

2 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	I	1	2,4	14,14,15	1.67	2 (14%)	17,19,21	1.43	3 (17%)
4	NAG	I	2	4	14,14,15	0.50	0	17,19,21	0.92	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
4	NAG	I	1	2,4	-	4/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	1	NAG	O5-C1	-4.33	1.36	1.43
4	I	1	NAG	C1-C2	4.27	1.58	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1	NAG	C4-C3-C2	4.18	117.15	111.02
4	I	2	NAG	C1-O5-C5	3.17	116.48	112.19
4	I	1	NAG	O5-C5-C4	-2.47	104.83	110.83
4	I	1	NAG	C2-N2-C7	2.10	125.90	122.90

There are no chirality outliers.

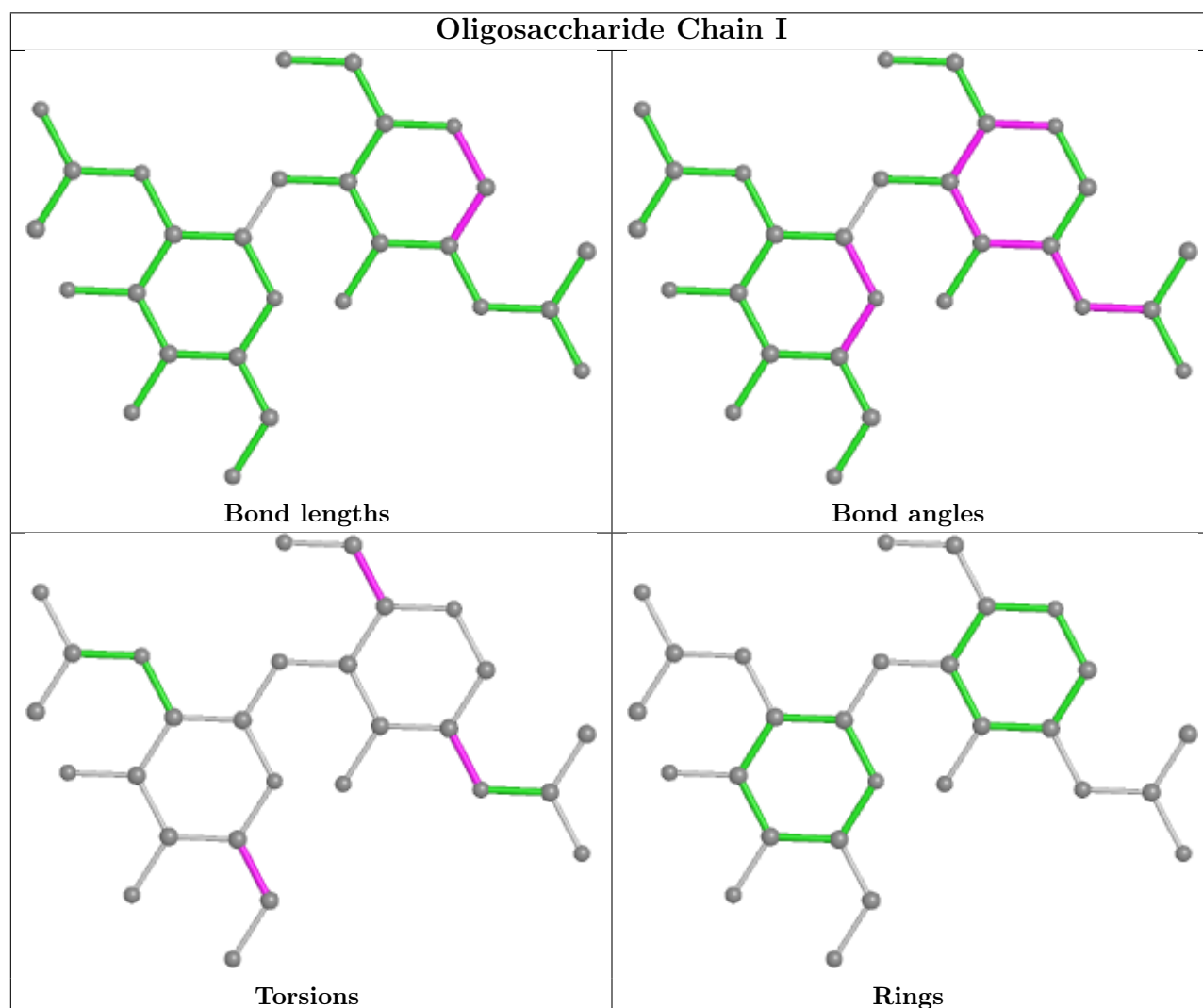
5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	1	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	I	1	NAG	C1-C2-N2-C7
4	I	2	NAG	O5-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](#)

10 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	A	601	1	14,14,15	0.75	1 (7%)	17,19,21	0.80	1 (5%)
5	NAG	B	601	1	14,14,15	0.26	0	17,19,21	0.75	1 (5%)
5	NAG	F	601	1	14,14,15	0.35	0	17,19,21	0.60	0
5	NAG	E	601	1	14,14,15	0.59	0	17,19,21	0.78	0
5	NAG	L	601	1	14,14,15	0.80	1 (7%)	17,19,21	0.63	0
5	NAG	K	601	1	14,14,15	1.46	2 (14%)	17,19,21	1.00	1 (5%)
5	NAG	C	601	1	14,14,15	0.44	0	17,19,21	0.95	1 (5%)
5	NAG	H	601	1	14,14,15	0.87	1 (7%)	17,19,21	1.01	2 (11%)
5	NAG	G	601	1	14,14,15	0.88	1 (7%)	17,19,21	0.63	0
5	NAG	D	601	1	14,14,15	0.72	0	17,19,21	0.74	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	601	1	-	0/6/23/26	0/1/1/1
5	NAG	B	601	1	-	0/6/23/26	0/1/1/1
5	NAG	F	601	1	-	2/6/23/26	0/1/1/1
5	NAG	E	601	1	-	2/6/23/26	0/1/1/1
5	NAG	L	601	1	-	2/6/23/26	0/1/1/1
5	NAG	K	601	1	-	4/6/23/26	0/1/1/1
5	NAG	C	601	1	-	4/6/23/26	0/1/1/1
5	NAG	H	601	1	-	2/6/23/26	0/1/1/1
5	NAG	G	601	1	-	3/6/23/26	0/1/1/1
5	NAG	D	601	1	-	2/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	601	NAG	O5-C1	-4.78	1.36	1.43
5	H	601	NAG	O5-C1	-3.06	1.38	1.43
5	G	601	NAG	O5-C1	-3.02	1.38	1.43
5	L	601	NAG	O5-C1	-2.49	1.39	1.43
5	A	601	NAG	O5-C1	2.27	1.47	1.43

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	601	NAG	C2-N2-C7	2.70	126.74	122.90
5	H	601	NAG	C1-O5-C5	2.65	115.78	112.19
5	C	601	NAG	C2-N2-C7	2.24	126.09	122.90
5	B	601	NAG	C1-O5-C5	2.23	115.21	112.19
5	A	601	NAG	C1-O5-C5	2.11	115.05	112.19

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	601	NAG	C4-C5-C6-O6
5	E	601	NAG	C4-C5-C6-O6
5	D	601	NAG	O5-C5-C6-O6
5	H	601	NAG	O5-C5-C6-O6
5	K	601	NAG	O5-C5-C6-O6

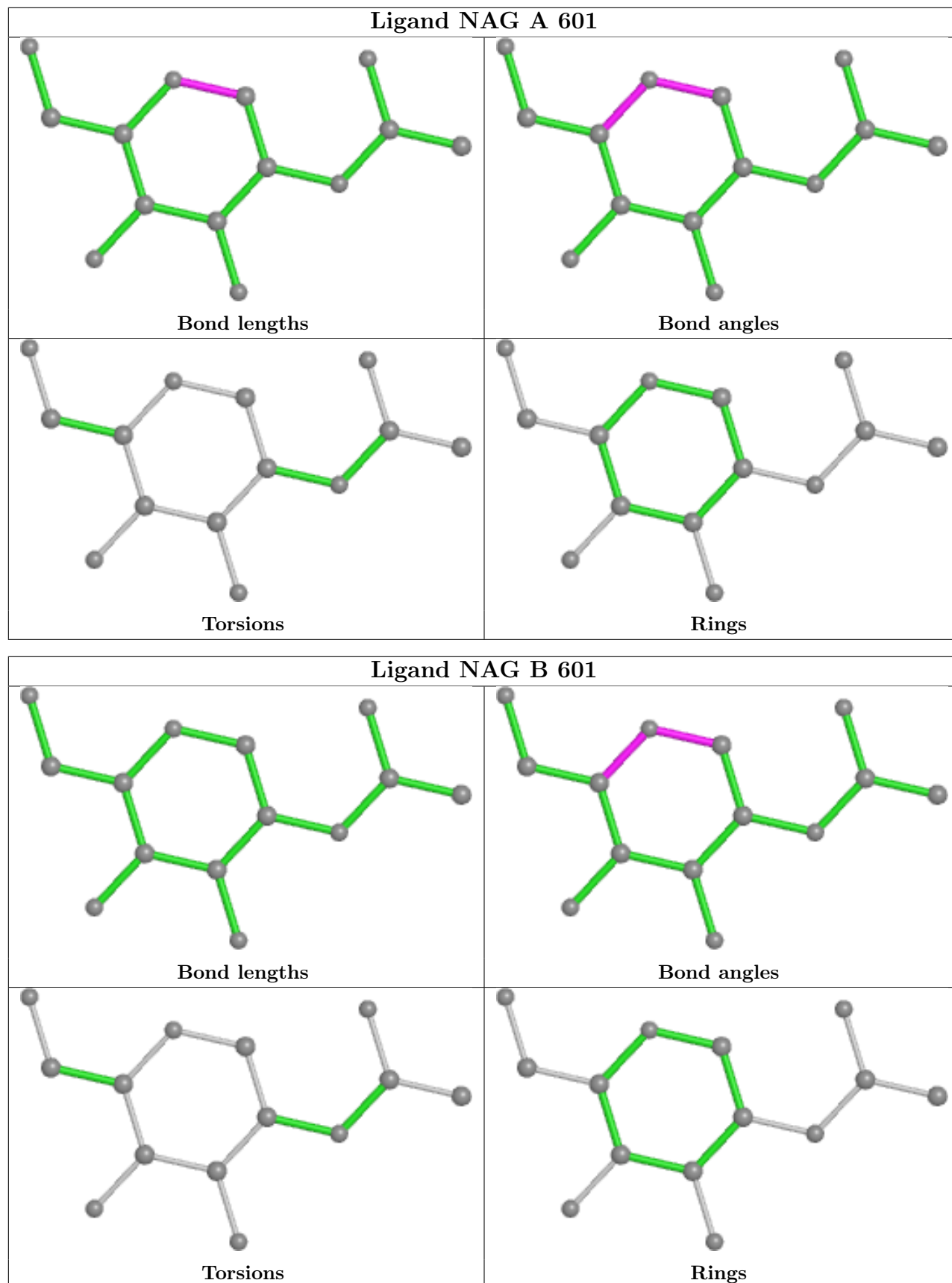
There are no ring outliers.

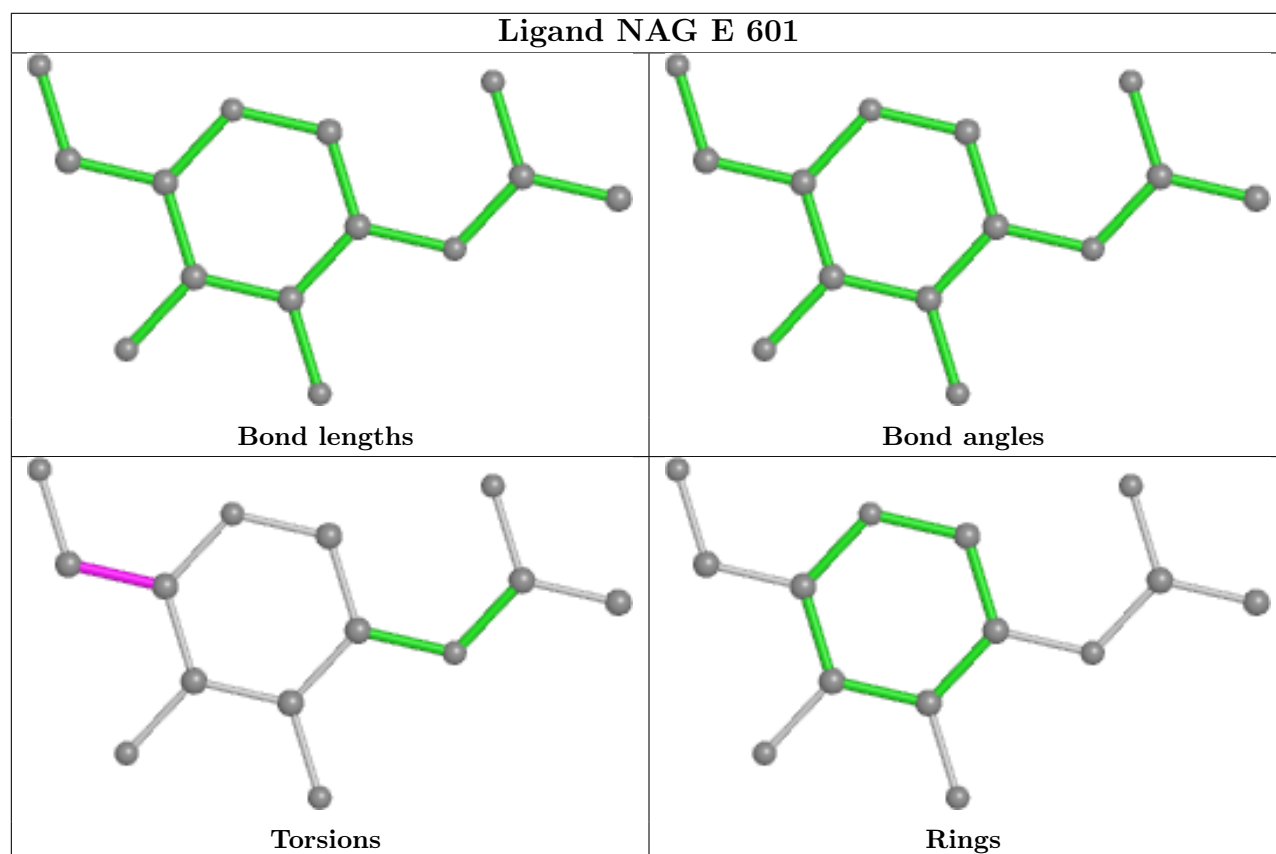
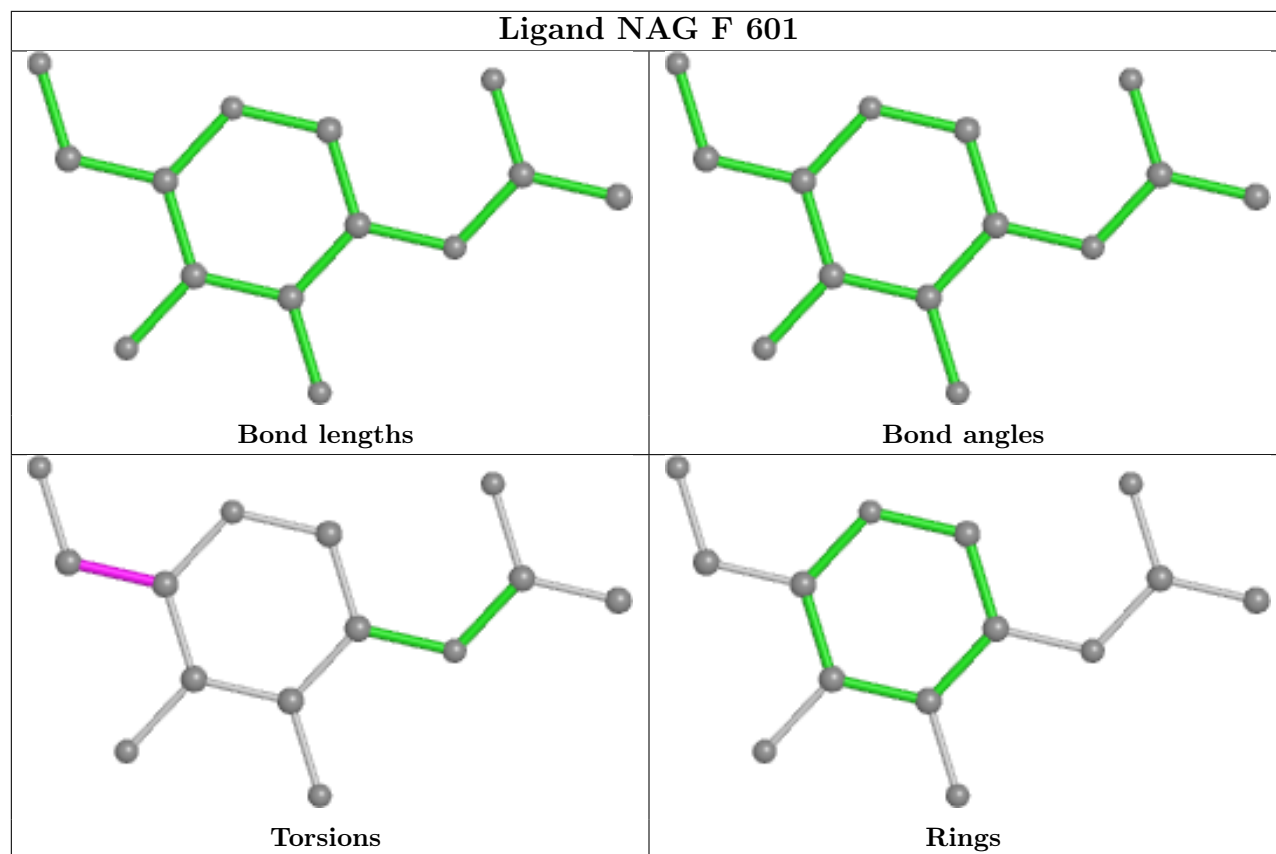
2 monomers are involved in 1 short contact:

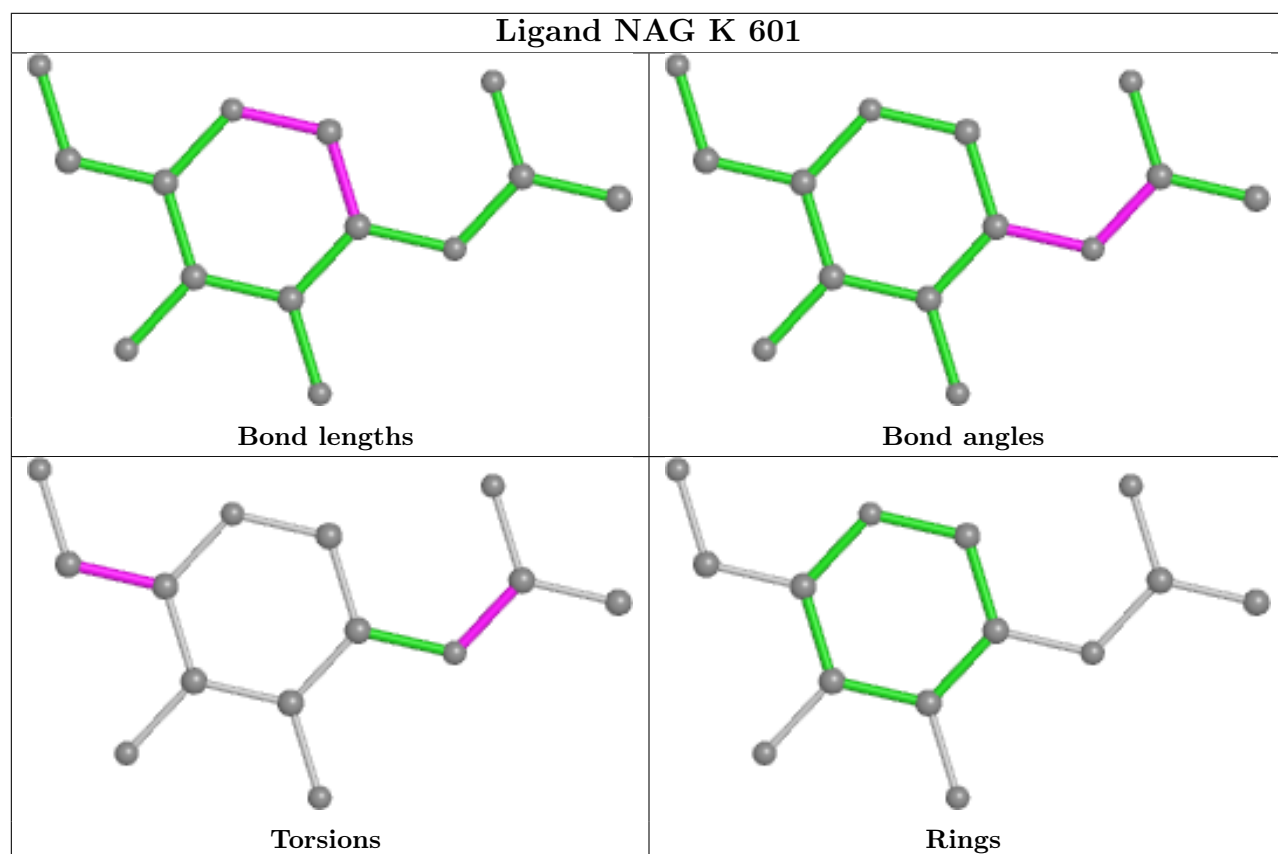
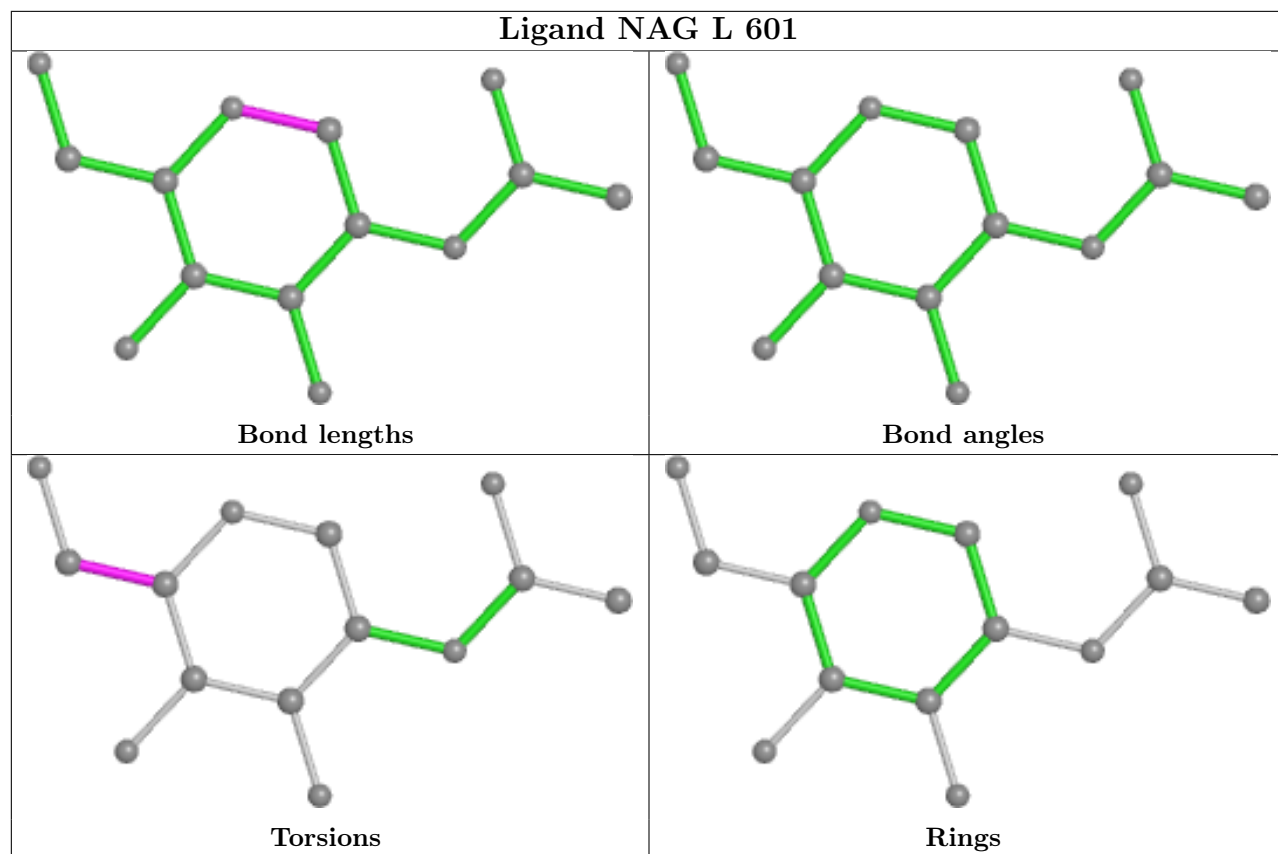
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	601	NAG	1	0
5	G	601	NAG	1	0

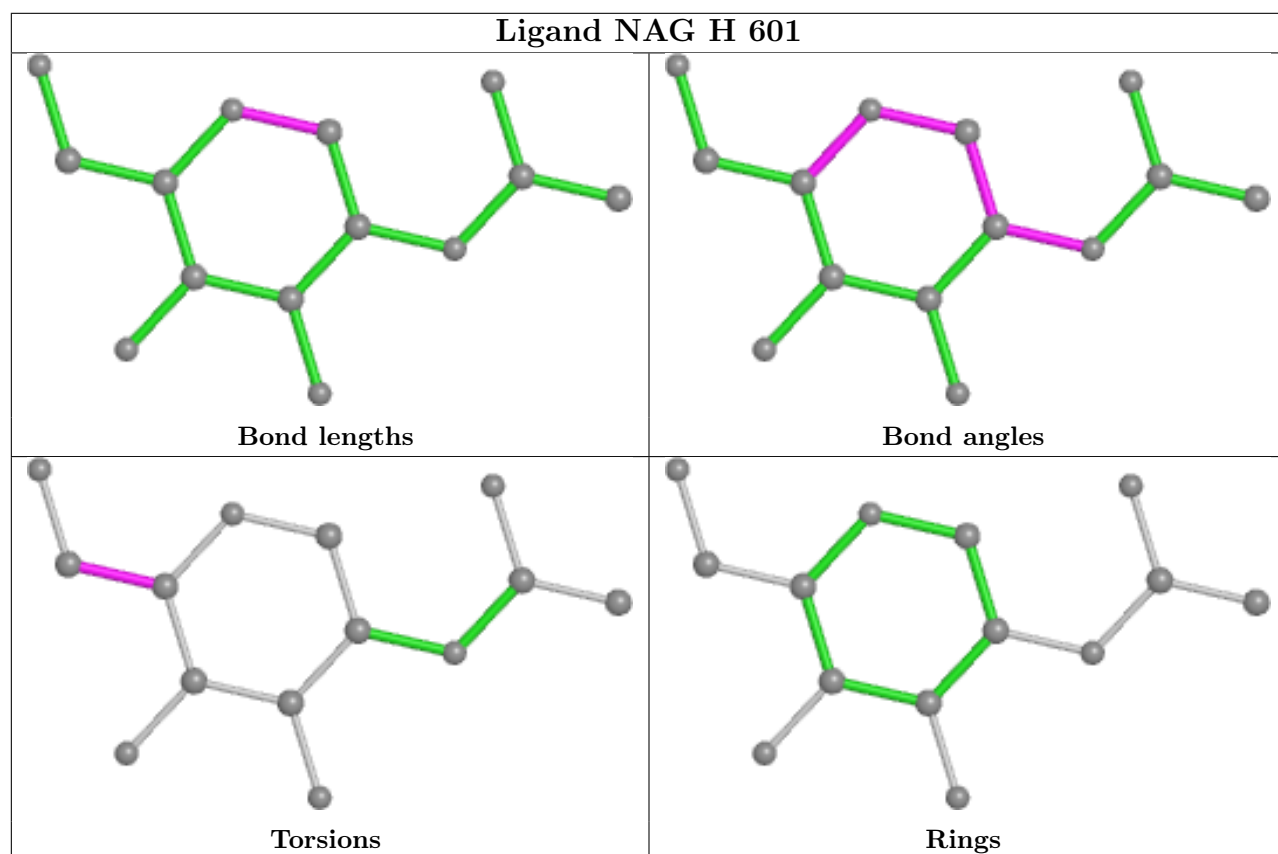
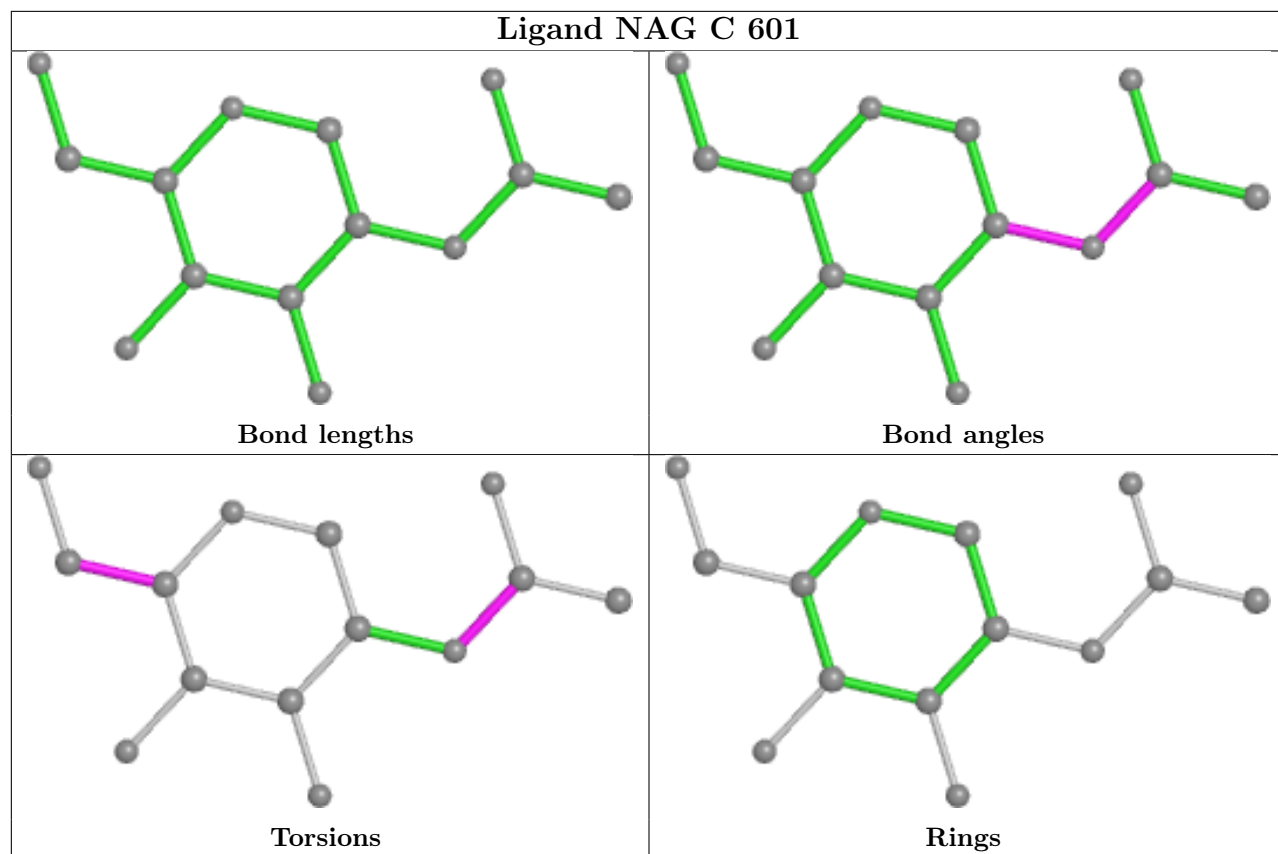
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

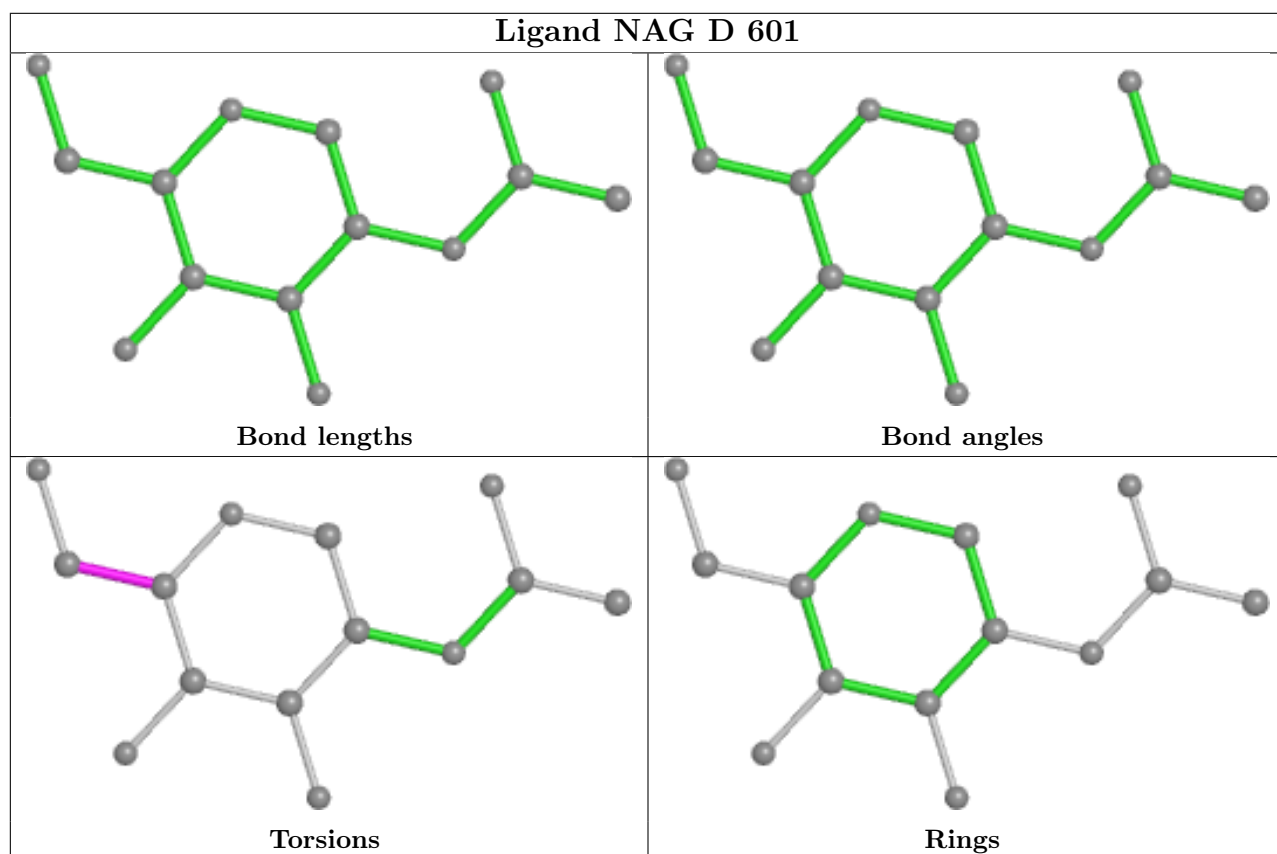
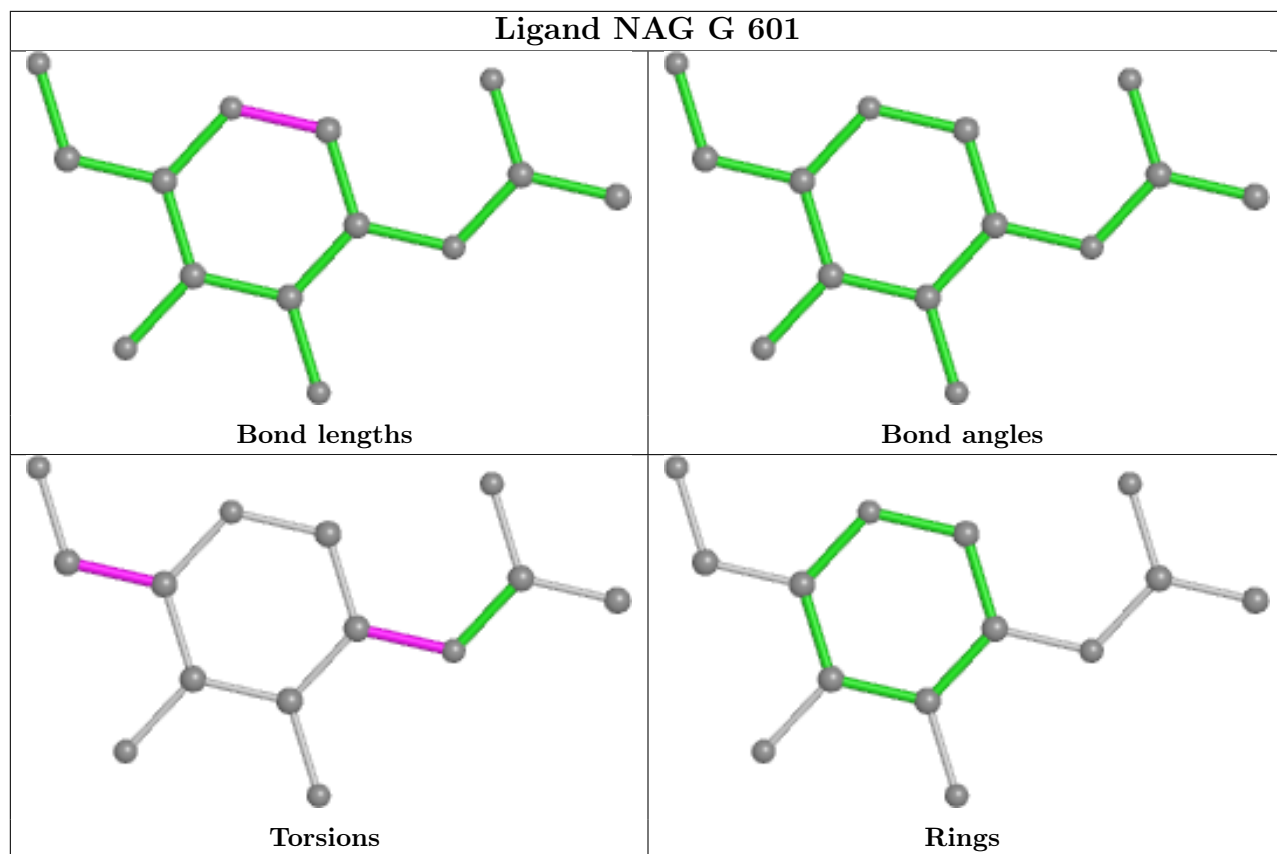
equivalents in the CSD to analyse the geometry.











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.

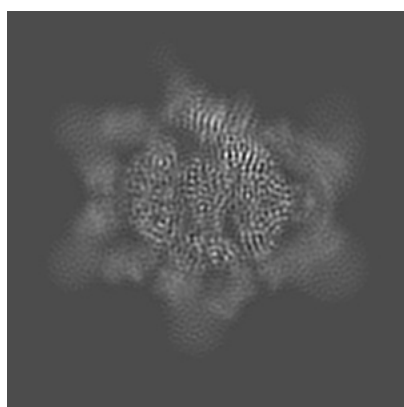
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0782. These allow visual inspection of the internal detail of the map and identification of artifacts.

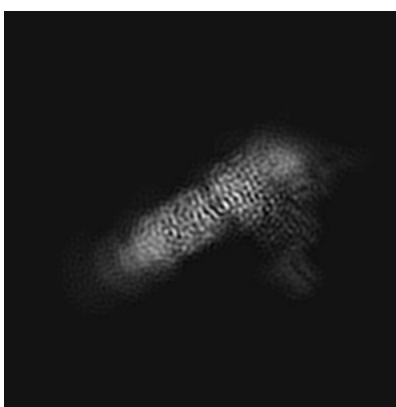
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

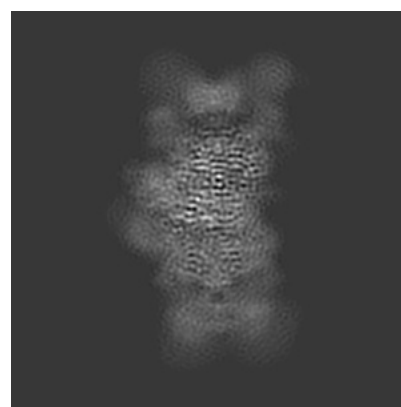
6.1.1 Primary map



X



Y

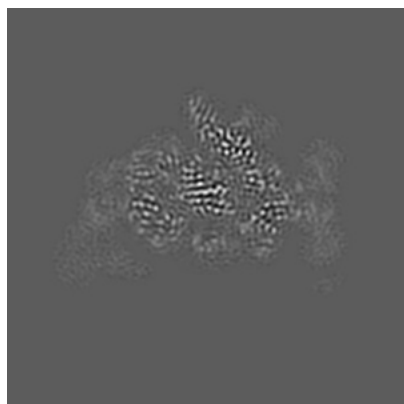


Z

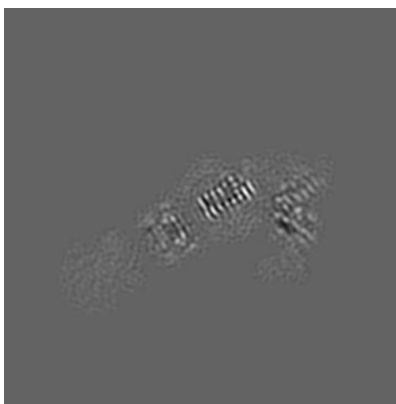
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

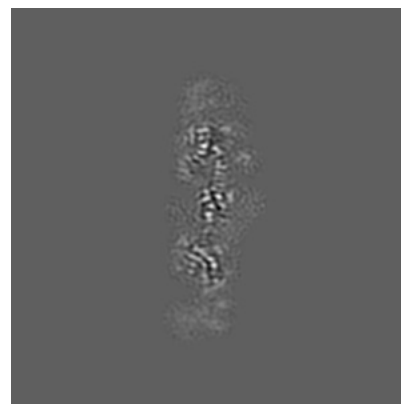
6.2.1 Primary map



X Index: 160



Y Index: 160

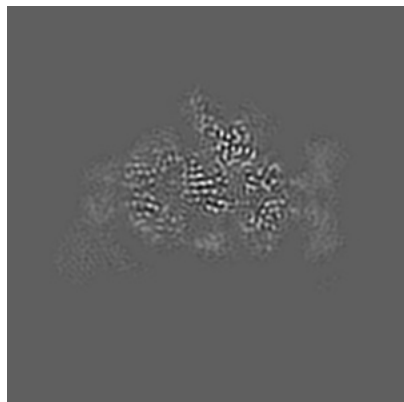


Z Index: 160

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

6.3 Largest variance slices [i](#)

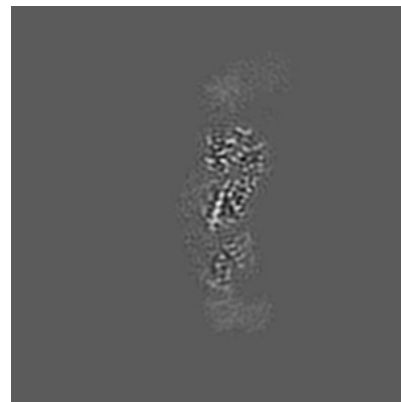
6.3.1 Primary map



X Index: 162



Y Index: 169

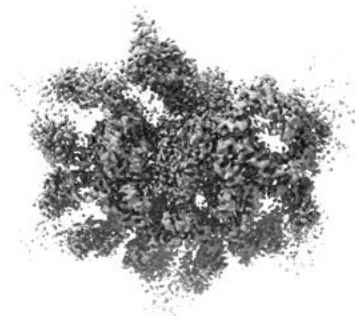


Z Index: 183

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

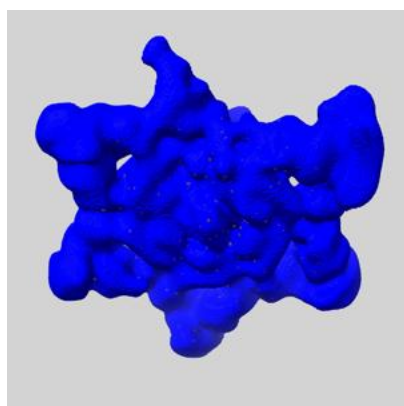
6.5 Mask visualisation [i](#)

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

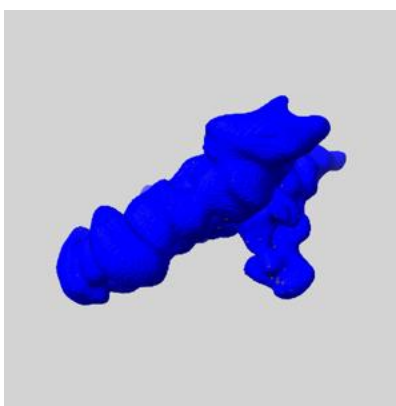
A mask typically either:

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

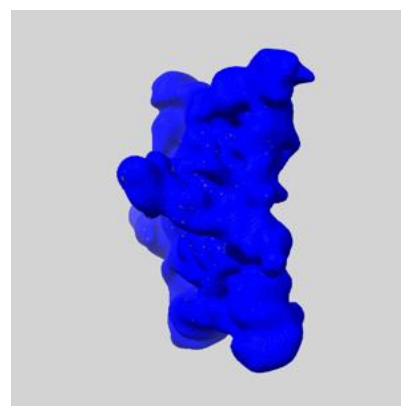
6.5.1 emd_0782_msk_1.map [i](#)



X



Y

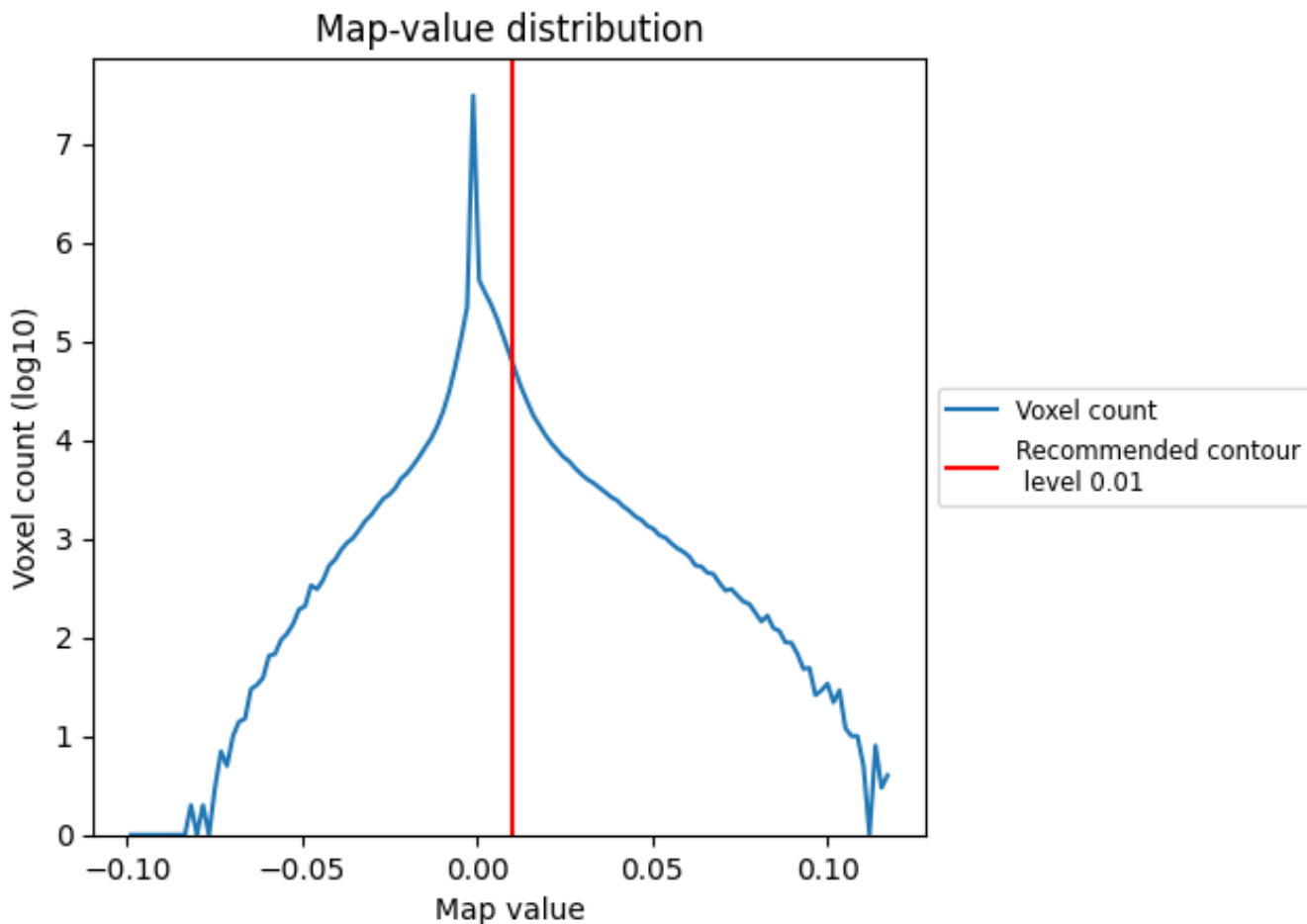


Z

7 Map analysis [i](#)

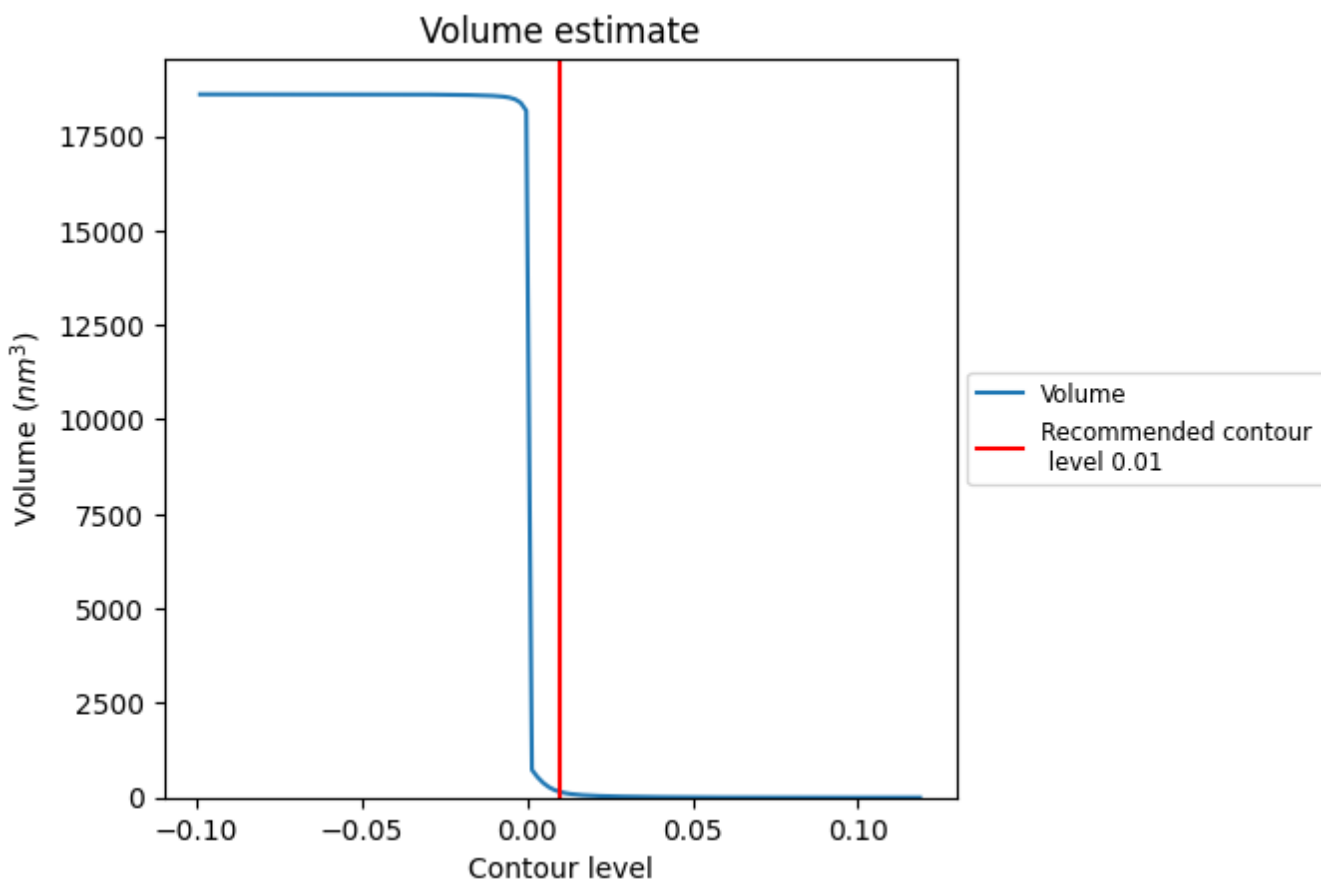
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

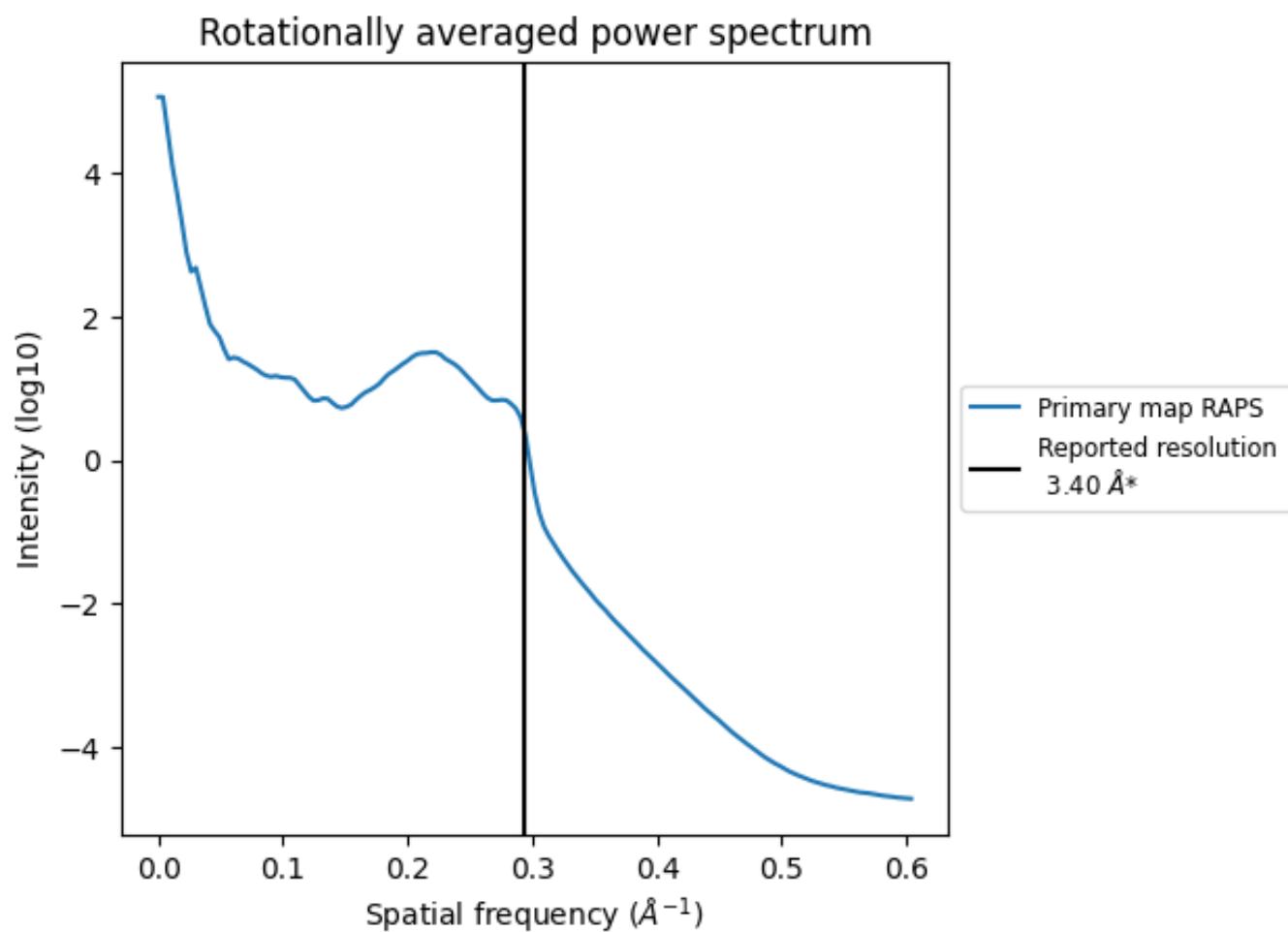
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 148 nm³; this corresponds to an approximate mass of 134 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 [i](#)

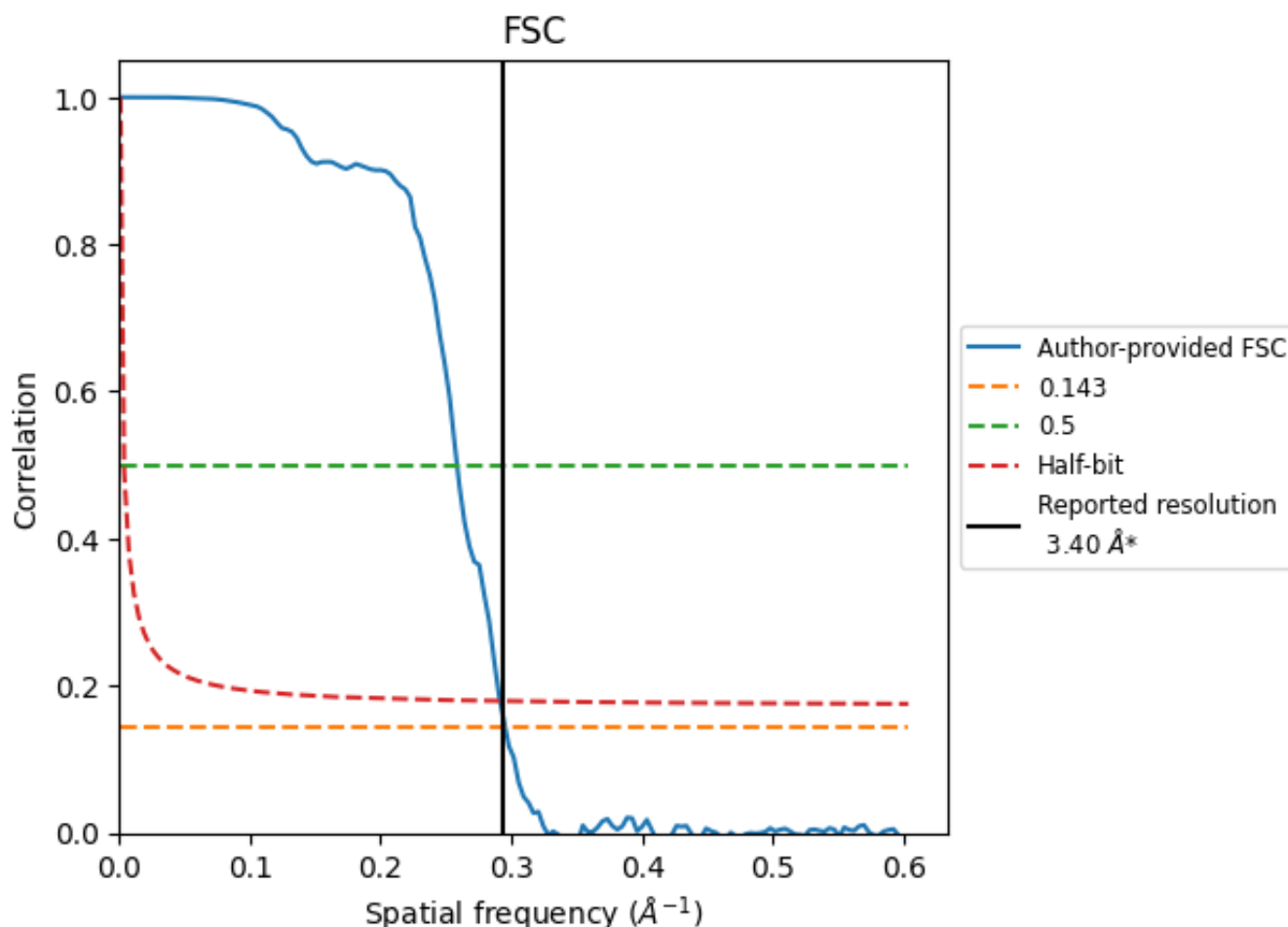


*Reported resolution corresponds to spatial frequency of 0.294\AA^{-1}

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

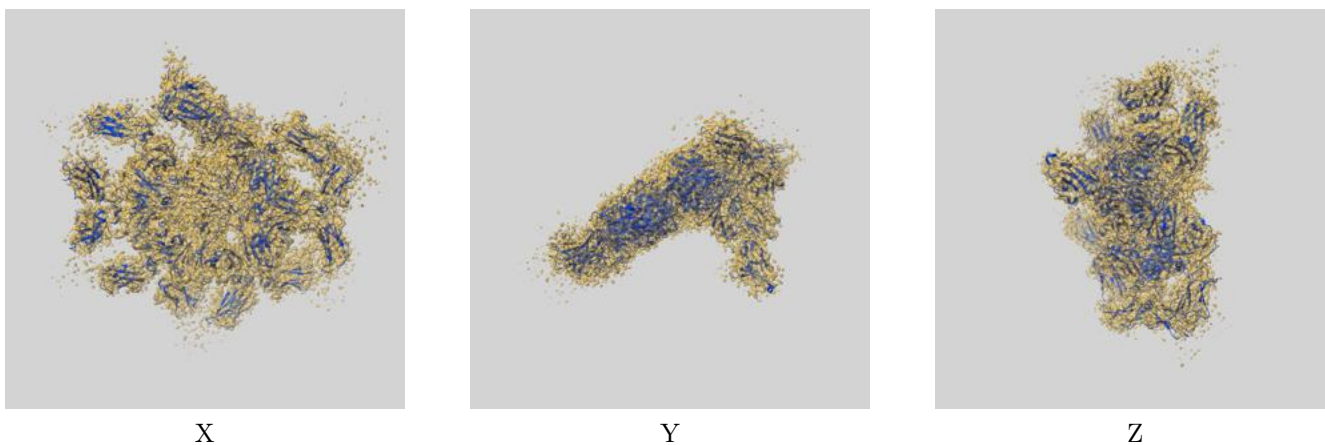
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	3.87	3.43
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

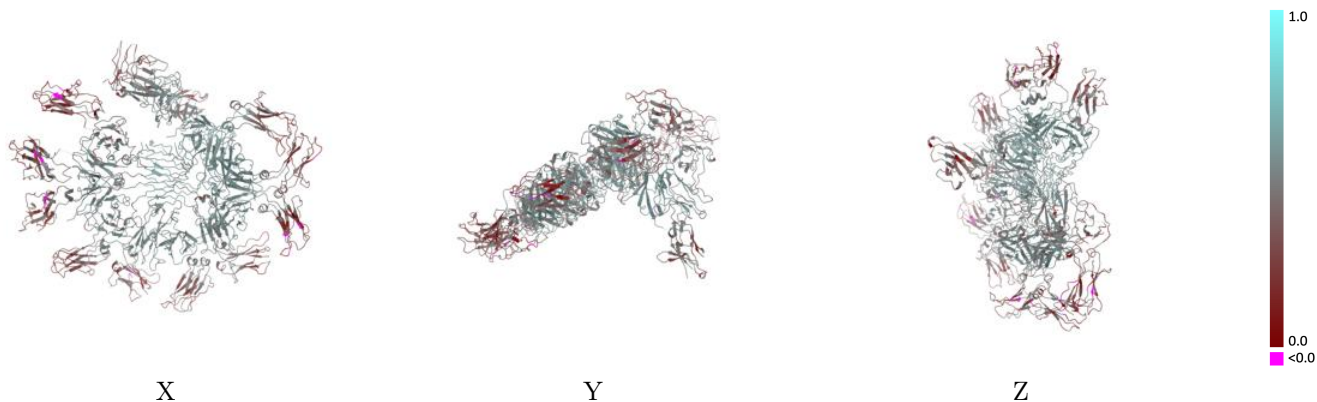
This section contains information regarding the fit between EMDB map EMD-0782 and PDB model 6KXS. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



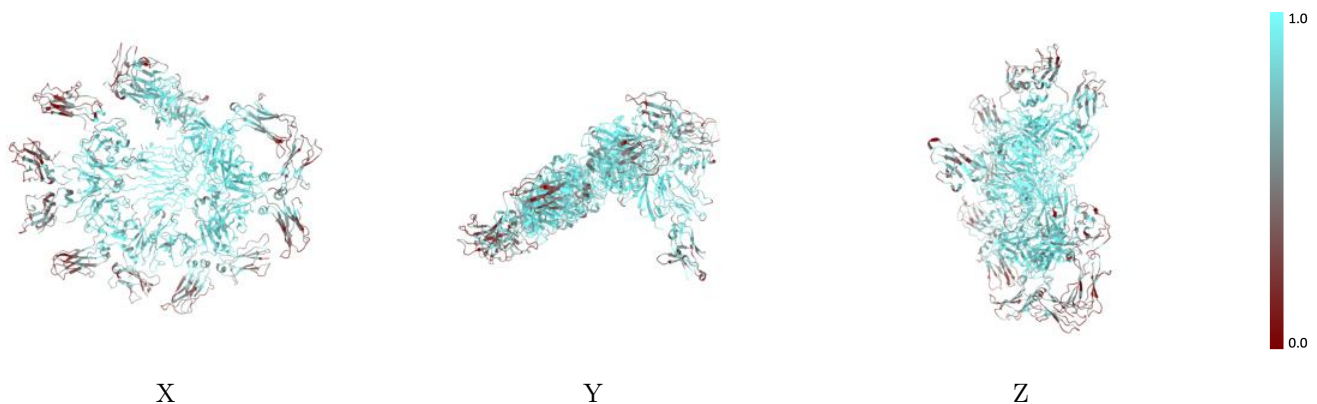
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



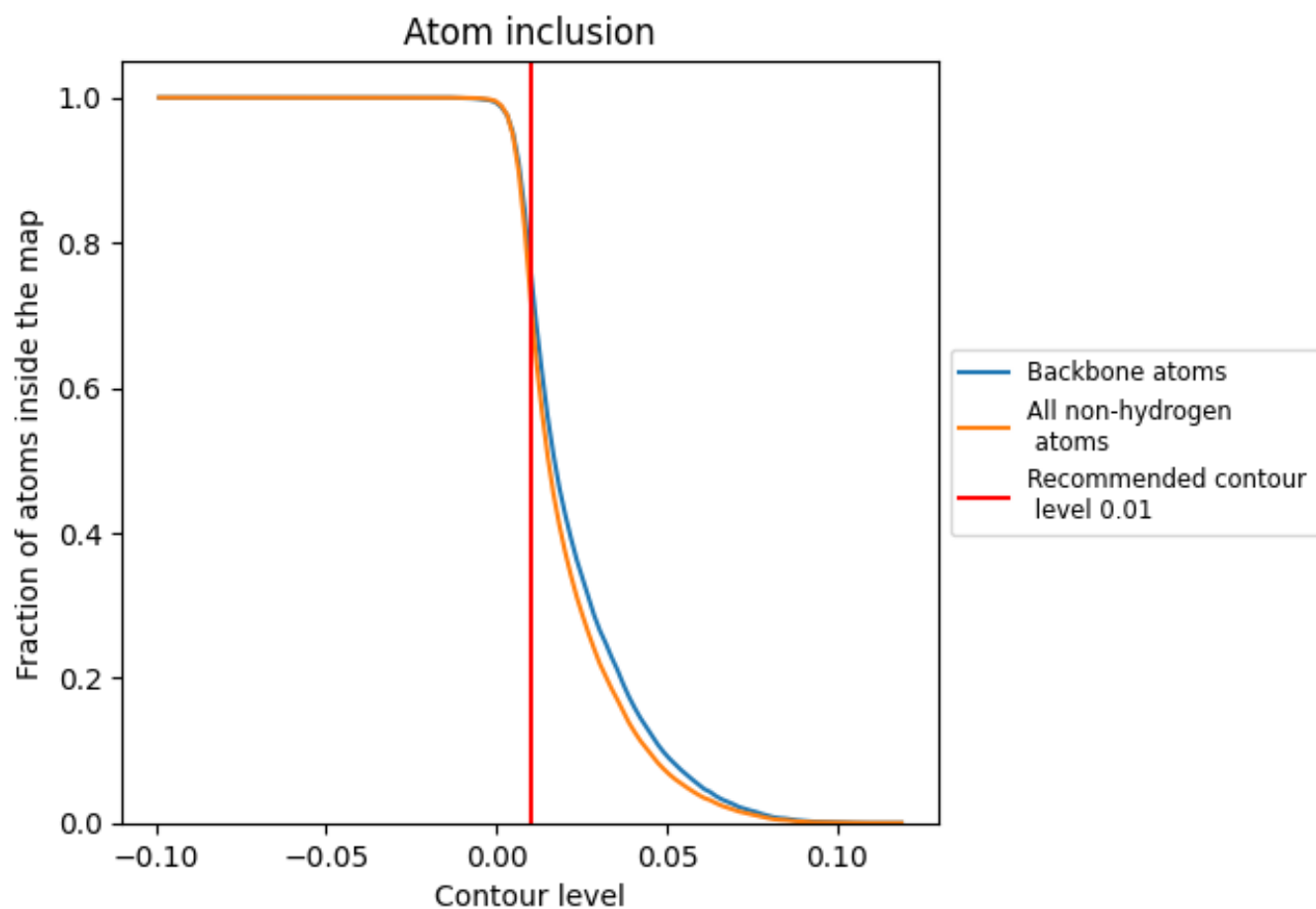
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 72% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7227	 0.4570
A	 0.7802	 0.4900
B	 0.7514	 0.4620
C	 0.7116	 0.4490
D	 0.7380	 0.4500
E	 0.7281	 0.4590
F	 0.7173	 0.4420
G	 0.6966	 0.4410
H	 0.7039	 0.4380
I	 0.8214	 0.4450
J	 0.8921	 0.5480
K	 0.6610	 0.4420
L	 0.6277	 0.4080
P	 0.7362	 0.4780

