



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 10:57 PM UTC

PDB ID : 6KXS / pdb_00006kxs
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 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

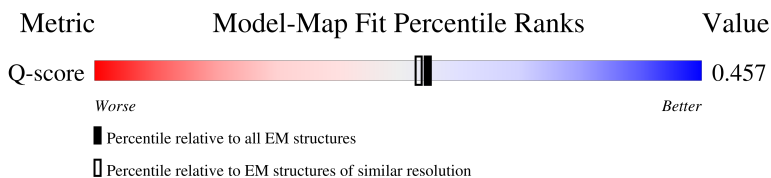
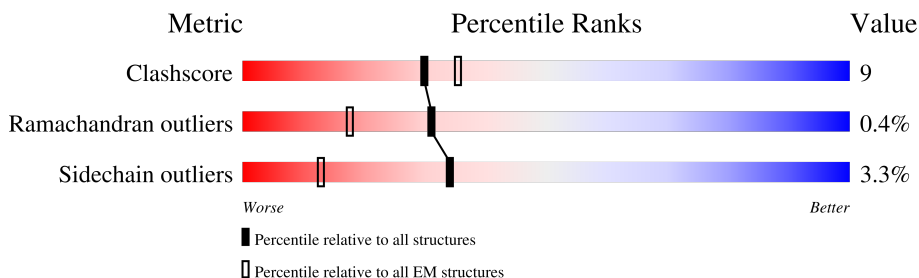
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

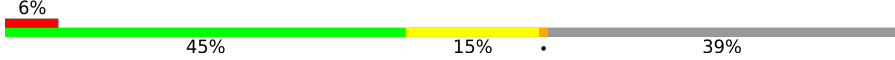
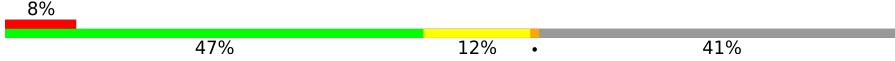
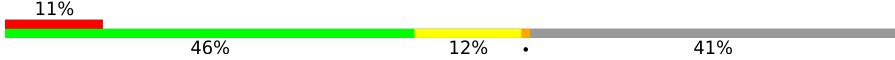
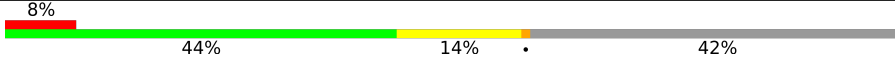
The reported resolution of this entry is 3.40 Å.

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	

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Mol	Chain	Length	Quality of chain
1	E	383	
1	F	383	
1	G	383	
1	H	383	
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
1	A	232	Total	C	N	O	S	0	0
			1798	1132	304	353	9		
1	B	227	Total	C	N	O	S	0	0
			1764	1111	299	346	8		
1	C	225	Total	C	N	O	S	0	0
			1748	1103	297	340	8		
1	D	224	Total	C	N	O	S	0	0
			1743	1100	296	339	8		
1	E	224	Total	C	N	O	S	0	0
			1743	1100	296	339	8		
1	F	221	Total	C	N	O	S	0	0
			1723	1087	292	336	8		
1	G	224	Total	C	N	O	S	0	0
			1742	1100	296	338	8		
1	H	230	Total	C	N	O	S	0	0
			1785	1124	301	351	9		
1	K	230	Total	C	N	O	S	0	0
			1786	1124	302	351	9		
1	L	228	Total	C	N	O	S	0	0
			1773	1116	299	349	9		

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
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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
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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
2	J	106	Total	C	N	O	S	0	0
			851	528	150	166	7		

- Molecule 3 is a protein called Polymeric immunoglobulin receptor.

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

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

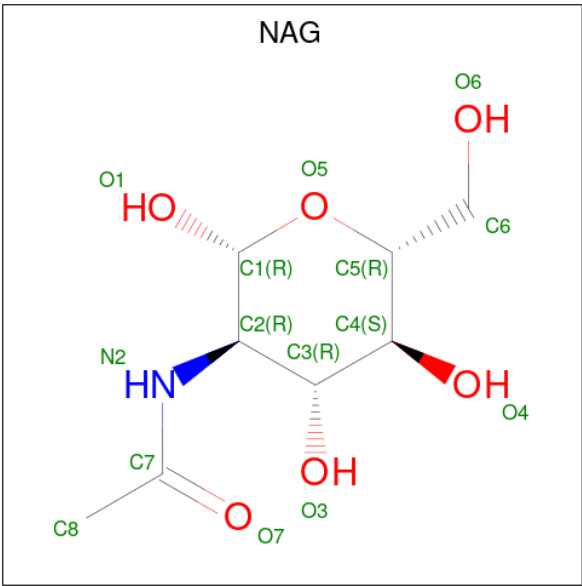
- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

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

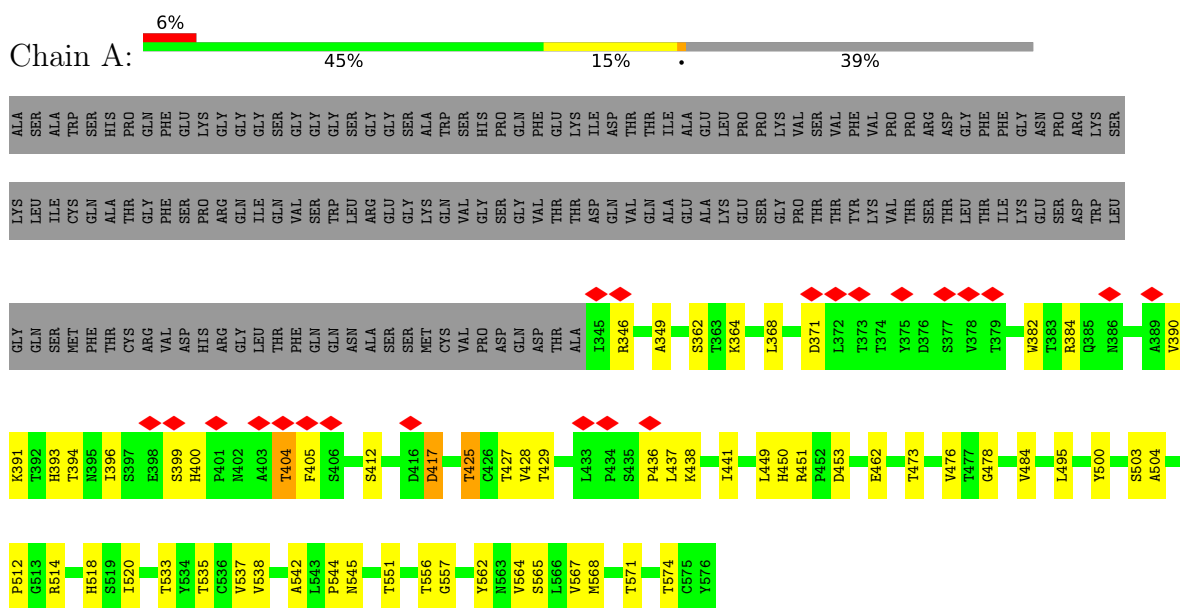


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	
5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

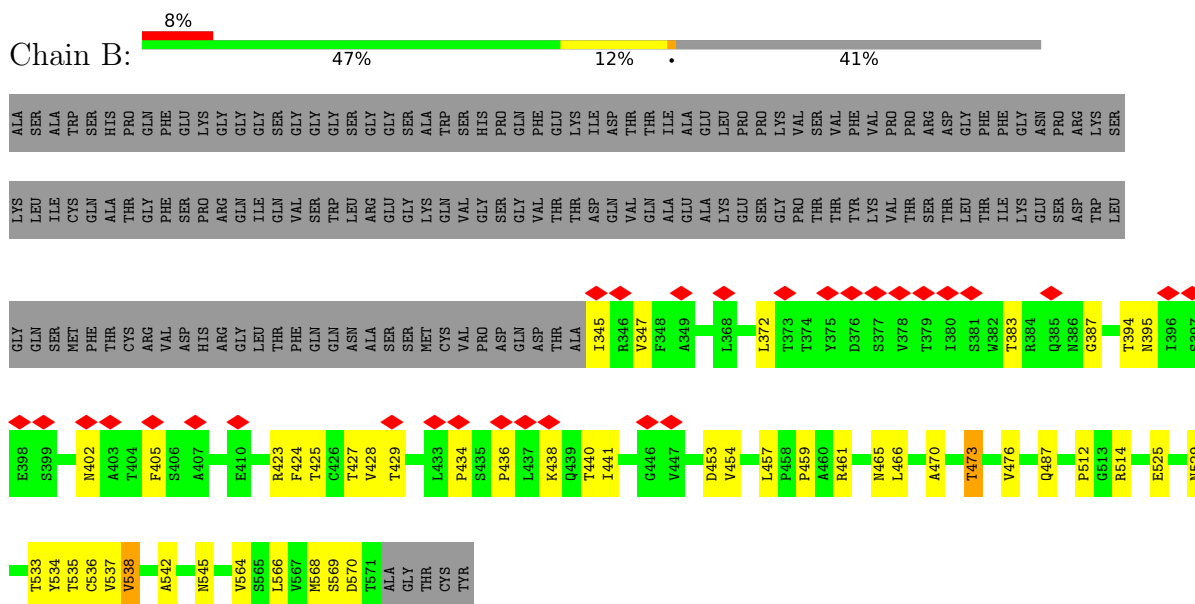
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Immunoglobulin heavy constant mu



• Molecule 1: Immunoglobulin heavy constant mu



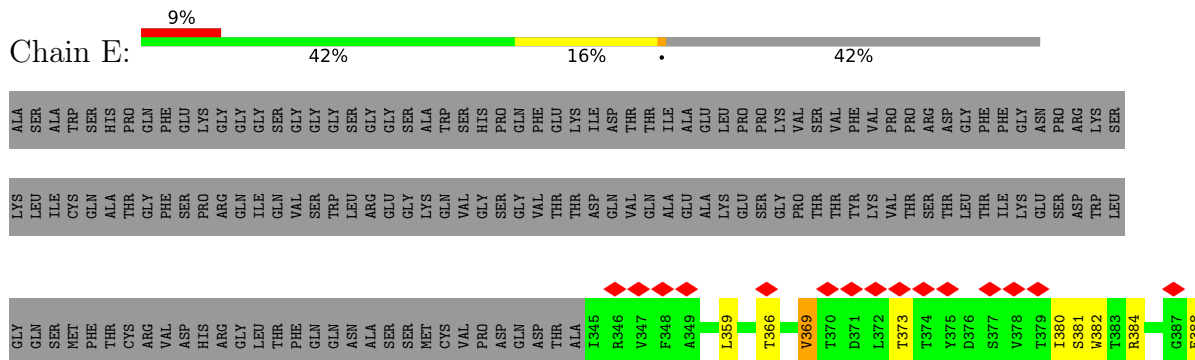
Chain C:

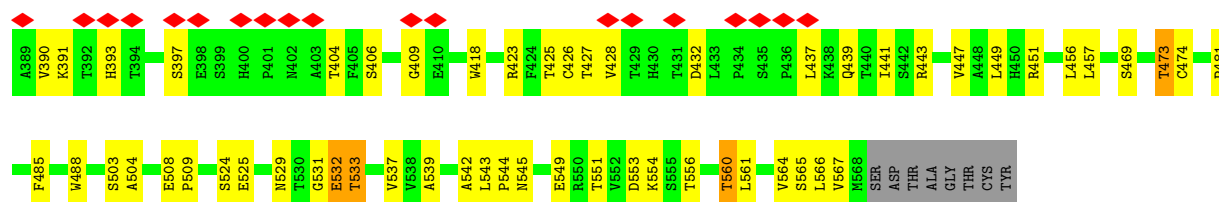


Chain D:

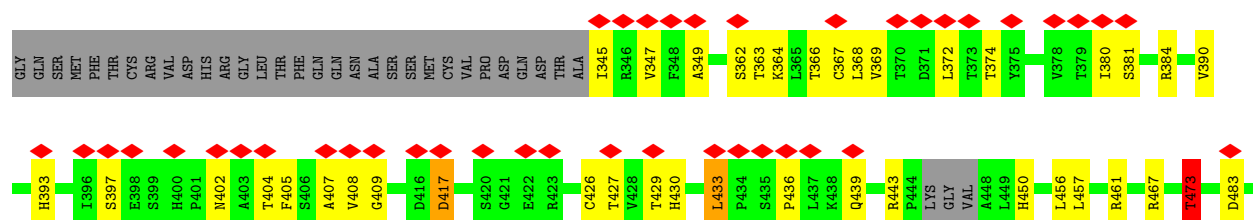
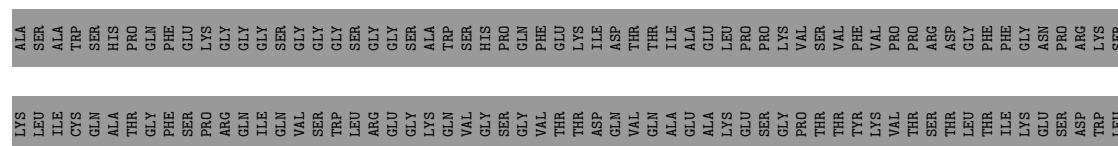


Chain E:

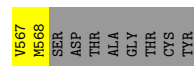
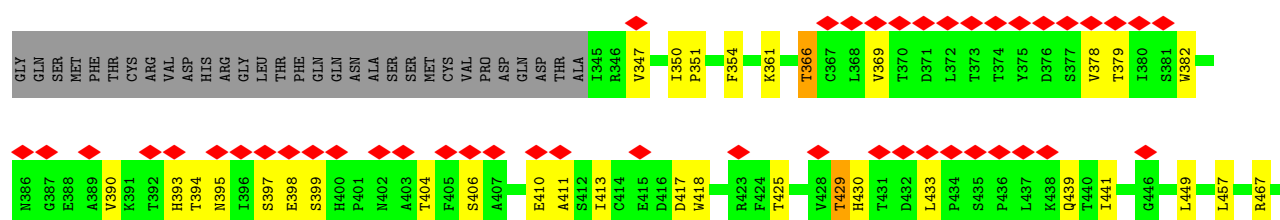
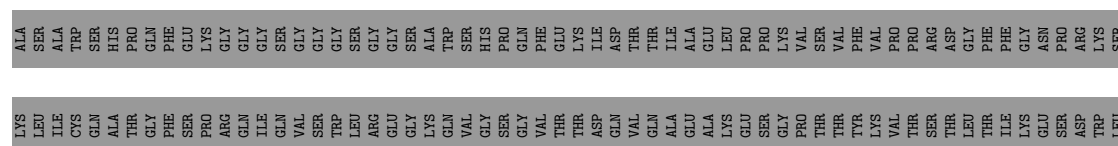




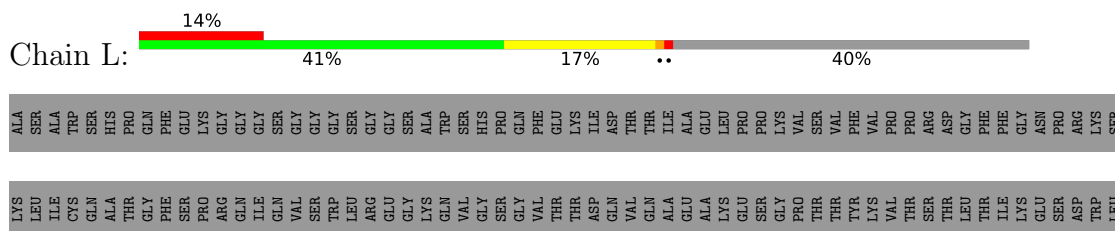
• Molecule 1: Immunoglobulin heavy constant mu

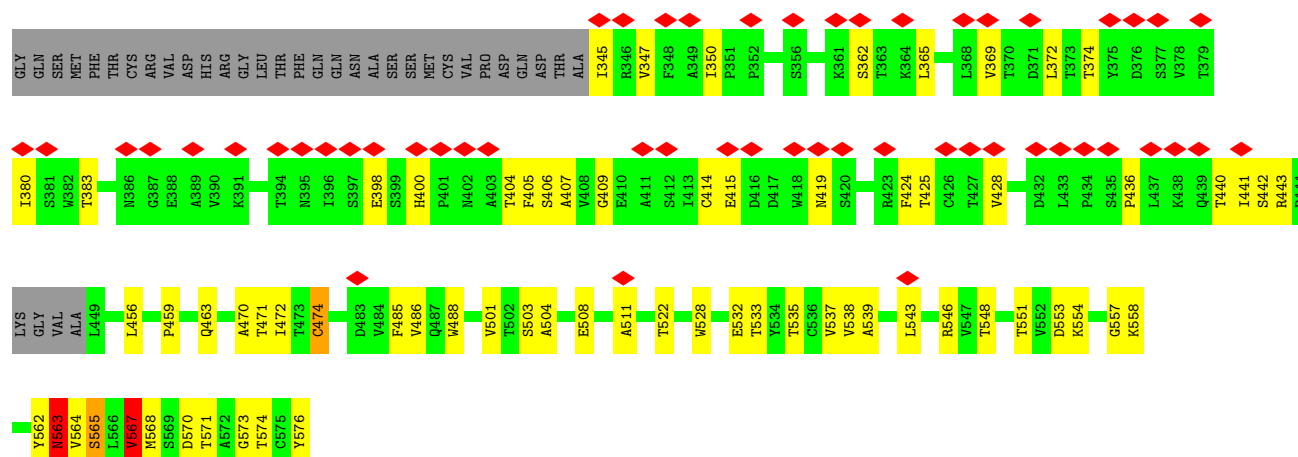


• Molecule 1: Immunoglobulin heavy constant mu

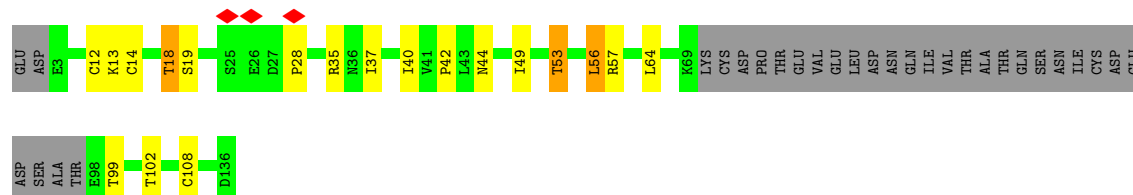


• Molecule 1: Immunoglobulin heavy constant mu

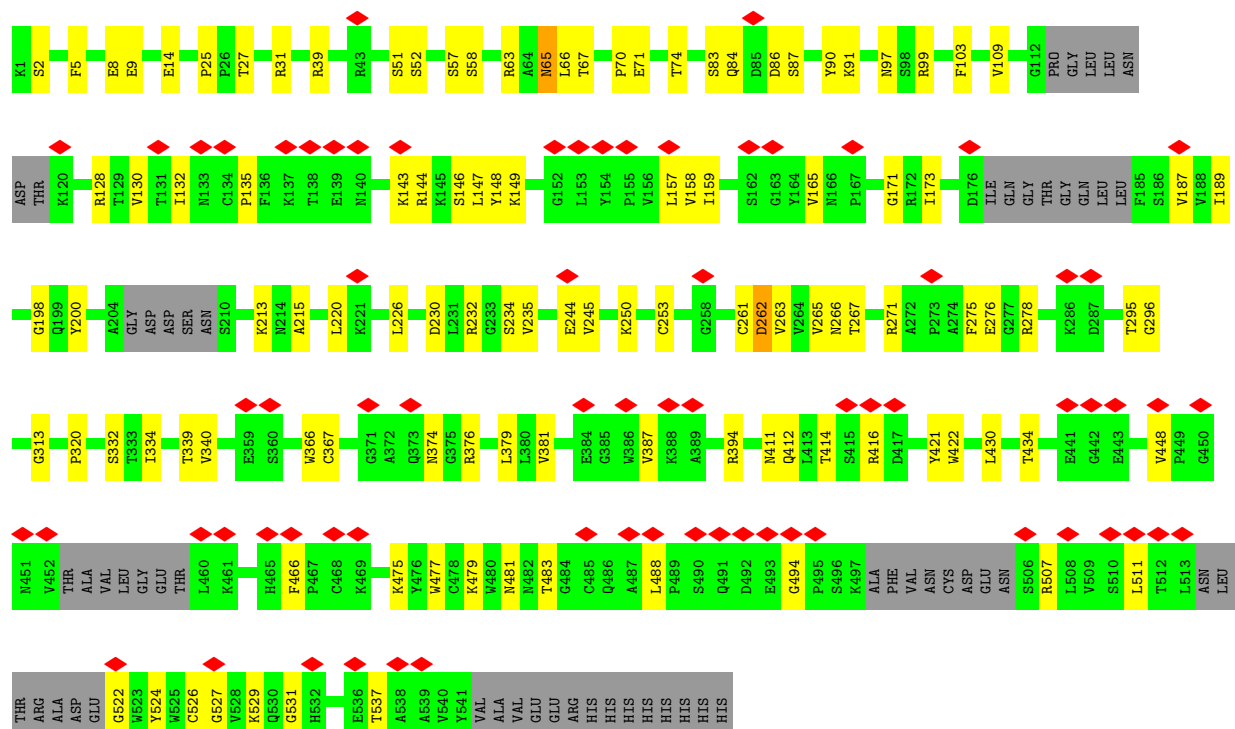




• Molecule 2: Immunoglobulin J chain



• 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

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	0.85	0/1844	0.86	2/2526 (0.1%)
1	B	0.86	1/1809 (0.1%)	0.91	3/2478 (0.1%)
1	C	0.72	0/1793	0.84	1/2455 (0.0%)
1	D	0.71	1/1788 (0.1%)	0.81	0/2449
1	E	0.67	0/1788	0.83	0/2449
1	F	0.71	0/1767	0.86	1/2420 (0.0%)
1	G	0.67	0/1787	0.80	2/2447 (0.1%)
1	H	0.70	0/1830	0.78	0/2507
1	K	0.63	0/1831	0.77	2/2506 (0.1%)
1	L	0.67	3/1818 (0.2%)	0.86	7/2490 (0.3%)
2	J	1.13	0/864	1.14	4/1173 (0.3%)
3	P	0.75	0/3959	0.83	2/5365 (0.0%)
All	All	0.75	5/22878 (0.0%)	0.85	24/31265 (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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	563	ASN	CB-CG	-5.80	1.37	1.52
1	L	567	VAL	CB-CG2	-5.15	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	542	ALA	C-N	-5.10	1.25	1.33
1	D	542	ALA	C-N	-5.05	1.26	1.33
1	L	565	SER	CA-C	-5.03	1.47	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	507	PRO	CA-C-N	8.39	132.06	120.39
1	G	507	PRO	C-N-CA	8.39	132.06	120.39
3	P	448	VAL	N-CA-C	-6.92	103.52	109.19
2	J	13	LYS	CA-C-N	6.73	134.29	123.93
2	J	13	LYS	C-N-CA	6.73	134.29	123.93
3	P	99	ARG	CB-CA-C	-6.63	103.00	111.22
1	L	573	GLY	CA-C-N	-6.18	112.62	122.08
1	L	573	GLY	C-N-CA	-6.18	112.62	122.08
1	L	456	LEU	CA-C-N	5.88	136.08	122.31
1	L	456	LEU	C-N-CA	5.88	136.08	122.31
1	A	545	ASN	CA-C-N	5.86	132.74	121.54
1	A	545	ASN	C-N-CA	5.86	132.74	121.54
2	J	12	CYS	CA-CB-SG	5.74	127.59	114.40
1	L	532	GLU	CA-C-N	5.70	132.43	121.54
1	L	532	GLU	C-N-CA	5.70	132.43	121.54
1	B	534	TYR	N-CA-C	5.65	118.08	111.02
2	J	57	ARG	CA-CB-CG	5.55	125.20	114.10
1	B	545	ASN	CA-C-N	5.55	132.14	121.54
1	B	545	ASN	C-N-CA	5.55	132.14	121.54
1	K	531	GLY	CA-C-N	5.52	132.09	121.54
1	K	531	GLY	C-N-CA	5.52	132.09	121.54
1	L	563	ASN	N-CA-C	5.19	116.36	107.28
1	F	473	THR	N-CA-C	5.06	117.85	107.37
1	C	530	THR	N-CA-C	-5.03	108.42	114.75

There are no chirality outliers.

All (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
1	L	562	TYR	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	1798	0	1752	33	0
1	B	1764	0	1723	27	0
1	C	1748	0	1712	26	0
1	D	1743	0	1707	34	0
1	E	1743	0	1707	42	0
1	F	1723	0	1681	38	0
1	G	1742	0	1706	39	0
1	H	1785	0	1734	34	0
1	K	1786	0	1735	40	0
1	L	1773	0	1721	41	0
2	J	851	0	842	11	0
3	P	3875	0	3789	66	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	404	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.

All (404) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:423:ARG:HA	1:E:441:ILE:O	1.89	0.72
1:L:345:ILE:HG13	1:L:372:LEU:HA	1.76	0.68
1:L:485:PHE:HB3	1:L:539:ALA:HB3	1.77	0.66
1:B:383:THR:HB	1:B:387:GLY:HA2	1.78	0.65
1:E:457:LEU:HB2	1:E:473:THR:HG23	1.77	0.65
1:F:490:GLN:NE2	1:F:532:GLU:OE1	2.29	0.65
1:F:368:LEU:HA	1:F:407:ALA:O	1.97	0.64
1:L:570:ASP:OD1	2:J:44:ASN:ND2	2.30	0.64
1:A:427:THR:HA	1:A:437:LEU:O	1.98	0.63
1:D:503:SER:OG	1:D:504:ALA:N	2.30	0.63
1:B:424:PHE:HB2	1:B:441:ILE:HG22	1.81	0.63
3:P:39:ARG:NH2	3:P:87:SER:O	2.32	0.63
1:L:533:THR:O	1:L:551:THR:OG1	2.16	0.63
3:P:173:ILE:HB	3:P:189:ILE:HG13	1.79	0.63
1:C:461:ARG:HH22	1:D:557:GLY:HA2	1.64	0.62
1:C:485:PHE:HB3	1:C:539:ALA:HB3	1.81	0.62
3:P:271:ARG:NH2	3:P:275:PHE:O	2.32	0.62
1:D:463:GLN:HE22	1:D:471:THR:HG23	1.65	0.62
1:A:478:GLY:O	1:A:514:ARG:NH1	2.32	0.62
1:H:463:GLN:HE22	1:H:471:THR:HG23	1.65	0.62
1:L:414:CYS:SG	1:L:415:GLU:N	2.73	0.62
3:P:475:LYS:HE3	3:P:507:ARG:HG2	1.81	0.62
1:C:503:SER:OG	1:C:504:ALA:N	2.31	0.62
1:K:529:ASN:HA	1:K:554:LYS:HD2	1.82	0.61
1:H:369:VAL:O	1:H:406:SER:HA	2.00	0.61
1:C:525:GLU:OE2	1:C:529:ASN:ND2	2.32	0.61
1:A:400:HIS:HD2	1:A:404:THR:HG23	1.66	0.61
1:C:463:GLN:HE22	1:C:471:THR:HG23	1.66	0.61
1:E:380:ILE:O	1:E:393:HIS:NE2	2.34	0.60
3:P:481:ASN:HB3	3:P:483:THR:HG22	1.83	0.60
3:P:522:GLY:N	3:P:524:TYR:HH	1.98	0.60
3:P:245:VAL:O	3:P:250:LYS:NZ	2.34	0.60
1:G:503:SER:OG	1:G:504:ALA:N	2.34	0.60
1:B:465:ASN:ND2	1:L:571:THR:OG1	2.34	0.60
1:L:503:SER:OG	1:L:504:ALA:N	2.34	0.60
2:J:18:THR:OG1	2:J:19:SER:N	2.35	0.60
1:C:379:THR:HB	1:C:429:THR:HB	1.83	0.60
1:D:454:VAL:HG21	1:D:538:VAL:HG11	1.83	0.59
1:F:374:THR:HA	1:F:405:PHE:HB2	1.84	0.59
3:P:51:SER:OG	3:P:52:SER:N	2.35	0.59
3:P:374:ASN:HB3	3:P:376:ARG:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:MET:HE3	2:J:64:LEU:HD11	1.85	0.58
1:F:443:ARG:NH2	1:F:541:GLU:OE1	2.37	0.58
1:A:428:VAL:O	1:A:436:PRO:HA	2.02	0.58
1:A:473:THR:O	1:A:473:THR:OG1	2.20	0.58
1:D:372:LEU:H	1:D:405:PHE:HB2	1.69	0.58
1:G:457:LEU:HB2	1:G:473:THR:HG23	1.85	0.58
3:P:63:ARG:NH2	3:P:86:ASP:OD2	2.36	0.58
1:A:533:THR:HG21	2:J:53:THR:HA	1.86	0.58
3:P:262:ASP:OD1	3:P:262:ASP:N	2.33	0.58
2:J:42:PRO:HG3	2:J:102:THR:HG22	1.85	0.58
3:P:14:GLU:OE2	3:P:84:GLN:NE2	2.37	0.58
3:P:422:TRP:CD1	3:P:434:THR:HG1	2.22	0.58
1:B:525:GLU:OE2	1:B:529:ASN:ND2	2.37	0.57
1:L:567:VAL:HG22	2:J:40:ILE:HG12	1.85	0.57
3:P:87:SER:HB2	3:P:109:VAL:HG22	1.86	0.57
1:A:384:ARG:HE	1:A:390:VAL:HG12	1.70	0.57
1:B:428:VAL:O	1:B:436:PRO:HA	2.03	0.57
1:F:347:VAL:HB	1:F:439:GLN:HG3	1.85	0.57
3:P:339:THR:HG23	3:P:340:VAL:HG23	1.85	0.57
1:G:489:MET:O	1:G:535:THR:OG1	2.23	0.57
3:P:232:ARG:NH2	3:P:334:ILE:O	2.37	0.57
1:K:383:THR:HG1	1:K:425:THR:HG1	1.52	0.57
1:A:346:ARG:H	1:A:371:ASP:HB3	1.70	0.57
1:C:564:VAL:HG21	1:H:566:LEU:HD13	1.87	0.57
3:P:494:GLY:O	3:P:507:ARG:NH1	2.38	0.56
1:E:381:SER:O	1:E:426:CYS:HA	2.04	0.56
1:C:490:GLN:NE2	1:C:532:GLU:OE2	2.38	0.56
1:G:413:ILE:HD12	1:G:417:ASP:HB2	1.86	0.56
1:B:427:THR:HG22	1:B:438:LYS:HG2	1.88	0.56
1:C:400:HIS:HB2	1:C:404:THR:H	1.71	0.56
1:D:553:ASP:OD1	1:D:553:ASP:N	2.38	0.56
1:A:556:THR:HG22	2:J:56:LEU:HD13	1.88	0.56
1:E:369:VAL:O	1:E:406:SER:HA	2.06	0.56
1:L:415:GLU:HG2	1:L:419:ASN:HD21	1.69	0.56
1:G:379:THR:HB	1:G:429:THR:O	2.06	0.56
1:H:381:SER:HG	1:H:427:THR:HG1	1.54	0.56
3:P:57:SER:OG	3:P:58:SER:N	2.38	0.56
1:F:457:LEU:HB2	1:F:473:THR:HG23	1.88	0.56
1:K:563:ASN:HB3	1:L:563:ASN:HB3	1.87	0.56
1:A:476:VAL:HG11	1:A:484:VAL:HG21	1.87	0.56
1:H:503:SER:OG	1:H:504:ALA:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:HIS:HD2	1:A:396:ILE:HD11	1.71	0.56
1:E:553:ASP:N	1:E:553:ASP:OD1	2.38	0.56
3:P:31:ARG:NH1	3:P:70:PRO:O	2.39	0.56
3:P:381:VAL:HG12	3:P:387:VAL:HG13	1.86	0.56
1:E:485:PHE:HB3	1:E:539:ALA:HB3	1.88	0.55
1:K:457:LEU:HB2	1:K:473:THR:HG23	1.87	0.55
1:D:358:PHE:HA	1:D:361:LYS:HE3	1.87	0.55
1:D:380:ILE:HG22	1:D:428:VAL:HG22	1.89	0.55
3:P:278:ARG:NH1	3:P:296:GLY:O	2.40	0.55
1:A:556:THR:OG1	1:A:557:GLY:N	2.37	0.55
1:B:425:THR:HG22	1:B:440:THR:HG22	1.88	0.55
1:B:457:LEU:HB2	1:B:473:THR:HG23	1.88	0.55
1:B:487:GLN:HG3	1:B:537:VAL:HG23	1.89	0.55
1:D:356:SER:O	1:D:360:THR:OG1	2.22	0.55
3:P:130:VAL:HG12	3:P:189:ILE:HG22	1.88	0.55
1:L:374:THR:HA	1:L:405:PHE:HB2	1.89	0.55
1:E:451:ARG:HH21	1:E:544:PRO:HD3	1.72	0.54
1:D:537:VAL:HG21	1:E:545:ASN:HD21	1.73	0.54
1:L:383:THR:OG1	1:L:425:THR:OG1	2.22	0.54
3:P:245:VAL:HG11	3:P:320:PRO:HG2	1.89	0.54
1:F:372:LEU:O	1:F:405:PHE:N	2.39	0.54
3:P:39:ARG:NH1	3:P:90:TYR:OH	2.40	0.54
3:P:65:ASN:N	3:P:65:ASN:OD1	2.41	0.54
1:K:354:PHE:N	1:K:483:ASP:OD1	2.40	0.54
1:G:393:HIS:HB3	1:G:411:ALA:HB2	1.90	0.54
3:P:394:ARG:NH1	3:P:412:GLN:O	2.40	0.54
1:G:430:HIS:HB3	1:G:433:LEU:HD13	1.89	0.54
1:L:563:ASN:OD1	1:L:563:ASN:N	2.37	0.54
1:D:347:VAL:O	1:D:439:GLN:NE2	2.41	0.53
1:D:450:HIS:HD2	1:D:514:ARG:HE	1.55	0.53
1:F:349:ALA:HA	1:F:367:CYS:HA	1.91	0.53
1:G:509:PRO:HB2	1:G:510:GLN:HE21	1.72	0.53
1:C:477:THR:OG1	1:C:478:GLY:N	2.41	0.53
1:D:553:ASP:OD1	1:D:556:THR:OG1	2.25	0.53
1:G:347:VAL:HG23	1:G:369:VAL:HG22	1.91	0.53
1:K:384:ARG:H	1:K:390:VAL:HG21	1.73	0.53
1:K:397:SER:OG	1:K:398:GLU:N	2.40	0.53
1:D:490:GLN:NE2	1:D:533:THR:OG1	2.41	0.53
3:P:83:SER:OG	3:P:84:GLN:N	2.41	0.53
1:C:380:ILE:HD13	1:C:407:ALA:HB1	1.91	0.53
1:E:533:THR:O	1:E:551:THR:OG1	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:537:VAL:HG12	1:E:549:GLU:HB3	1.90	0.53
1:F:456:LEU:HD22	1:F:552:VAL:HG22	1.90	0.53
5:F:601:NAG:H5	5:G:601:NAG:H2	1.91	0.53
1:H:499:LYS:NZ	1:H:522:THR:O	2.39	0.53
1:L:463:GLN:HE22	1:L:471:THR:HG23	1.73	0.53
3:P:149:LYS:HE3	3:P:198:GLY:HA3	1.91	0.53
1:K:485:PHE:HB3	1:K:539:ALA:HB3	1.90	0.52
1:B:453:ASP:N	1:B:453:ASP:OD1	2.39	0.52
3:P:466:PHE:HB2	3:P:507:ARG:HB3	1.90	0.52
1:B:566:LEU:HD11	1:B:568:MET:HG3	1.91	0.52
1:G:378:VAL:HG13	1:G:430:HIS:HB2	1.91	0.52
1:A:503:SER:OG	1:A:504:ALA:N	2.42	0.52
1:B:423:ARG:HA	1:B:441:ILE:O	2.10	0.52
1:F:367:CYS:O	1:F:408:VAL:HA	2.10	0.52
1:G:563:ASN:HB3	1:H:563:ASN:HB3	1.91	0.52
1:K:459:PRO:HD3	1:K:472:ILE:HG12	1.90	0.52
1:D:485:PHE:HB3	1:D:539:ALA:HB3	1.92	0.52
1:G:413:ILE:HD11	1:G:418:TRP:HB2	1.92	0.52
1:H:381:SER:OG	1:H:427:THR:OG1	2.24	0.51
1:G:467:ARG:HA	1:G:525:GLU:HG3	1.92	0.51
1:K:413:ILE:HD12	1:K:417:ASP:HB2	1.92	0.51
1:L:424:PHE:O	1:L:440:THR:HA	2.10	0.51
1:C:457:LEU:HB2	1:C:473:THR:HG23	1.91	0.51
1:H:425:THR:HA	1:H:439:GLN:O	2.10	0.51
1:D:543:LEU:HB2	1:D:546:ARG:HA	1.93	0.51
1:K:478:GLY:O	1:K:514:ARG:NH1	2.43	0.51
1:C:426:CYS:O	1:C:438:LYS:HA	2.11	0.51
3:P:200:TYR:N	3:P:215:ALA:O	2.43	0.51
1:E:556:THR:O	1:F:461:ARG:NH1	2.33	0.51
1:F:366:THR:HA	1:F:409:GLY:O	2.10	0.51
1:F:429:THR:HG22	1:F:436:PRO:HB3	1.93	0.51
3:P:135:PRO:HD2	3:P:213:LYS:HD3	1.91	0.51
1:E:508:GLU:HG2	1:E:509:PRO:HD2	1.92	0.51
1:L:543:LEU:HB2	1:L:546:ARG:HA	1.91	0.51
3:P:295:THR:OG1	3:P:296:GLY:N	2.42	0.51
1:D:428:VAL:HB	1:D:437:LEU:HB3	1.92	0.50
1:D:564:VAL:HB	1:E:564:VAL:HG22	1.94	0.50
1:D:565:SER:O	1:D:565:SER:OG	2.28	0.50
1:F:402:ASN:OD1	1:F:404:THR:OG1	2.30	0.50
1:A:349:ALA:HB1	1:A:441:ILE:HD11	1.93	0.50
1:E:382:TRP:HB2	1:E:390:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:230:ASP:OD1	3:P:332:SER:OG	2.17	0.50
1:H:414:CYS:SG	1:H:415:GLU:N	2.84	0.50
1:F:362:SER:OG	1:F:364:LYS:NZ	2.44	0.50
1:C:380:ILE:HA	1:C:427:THR:O	2.12	0.50
3:P:411:ASN:ND2	3:P:537:THR:OG1	2.45	0.50
1:G:553:ASP:OD1	1:G:556:THR:OG1	2.29	0.49
3:P:52:SER:HB2	3:P:66:LEU:HD22	1.94	0.49
1:E:369:VAL:HG11	1:E:428:VAL:HG21	1.94	0.49
1:E:529:ASN:HA	1:E:554:LYS:HD2	1.94	0.49
1:G:398:GLU:O	1:G:406:SER:OG	2.28	0.49
1:G:529:ASN:HA	1:G:554:LYS:HD2	1.95	0.49
3:P:477:TRP:CE2	3:P:526:CYS:HB3	2.47	0.49
3:P:488:LEU:HD23	3:P:511:LEU:HD11	1.94	0.49
1:B:512:PRO:O	1:B:514:ARG:N	2.44	0.49
1:G:399:SER:OG	1:G:404:THR:O	2.26	0.49
1:C:565:SER:O	1:C:565:SER:OG	2.27	0.49
1:A:391:LYS:HD3	1:A:412:SER:HB3	1.94	0.49
1:E:447:VAL:HG21	1:E:481:PRO:HB3	1.95	0.49
1:A:399:SER:HA	1:A:405:PHE:HA	1.95	0.49
1:G:394:THR:OG1	1:G:395:ASN:N	2.44	0.49
1:G:479:PHE:O	1:G:515:TYR:N	2.44	0.49
1:G:490:GLN:HE22	1:G:532:GLU:HG3	1.78	0.49
3:P:84:GLN:HA	3:P:109:VAL:HG21	1.95	0.49
1:H:530:THR:OG1	1:H:532:GLU:OE1	2.31	0.48
1:G:501:VAL:O	1:G:519:SER:HA	2.13	0.48
1:H:487:GLN:HG3	1:H:537:VAL:HG13	1.95	0.48
3:P:266:ASN:HD21	3:P:313:GLY:HA3	1.77	0.48
1:D:363:THR:OG1	1:D:413:ILE:O	2.30	0.48
1:H:545:ASN:OD1	1:H:545:ASN:N	2.44	0.48
1:D:451:ARG:HG3	1:D:543:LEU:HD23	1.96	0.48
1:L:398:GLU:O	1:L:406:SER:OG	2.31	0.48
1:H:459:PRO:HG3	1:H:470:ALA:HB1	1.95	0.48
1:L:535:THR:HG22	1:L:551:THR:HB	1.95	0.48
1:D:492:GLY:O	1:E:451:ARG:NH1	2.47	0.48
1:E:469:SER:HA	1:E:524:SER:HA	1.95	0.48
1:F:489:MET:HA	1:F:494:PRO:HA	1.96	0.48
1:G:418:TRP:HH2	1:G:441:ILE:HG13	1.79	0.48
1:H:553:ASP:N	1:H:553:ASP:OD1	2.46	0.48
1:L:486:VAL:HG22	1:L:538:VAL:HG23	1.96	0.48
1:A:393:HIS:CD2	1:A:396:ILE:HD11	2.49	0.48
1:F:347:VAL:HG22	1:F:369:VAL:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:525:GLU:OE2	1:F:529:ASN:ND2	2.47	0.48
1:K:487:GLN:HG3	1:K:537:VAL:HG13	1.95	0.48
3:P:253:CYS:HB2	3:P:261:CYS:HB3	1.43	0.48
1:D:357:ILE:HG12	1:D:363:THR:HG22	1.96	0.47
1:E:397:SER:OG	1:E:406:SER:O	2.31	0.47
1:H:368:LEU:HA	1:H:407:ALA:O	2.14	0.47
1:K:484:VAL:HG12	1:K:540:HIS:HB2	1.96	0.47
1:E:564:VAL:HG21	1:F:564:VAL:HG21	1.95	0.47
1:H:354:PHE:HA	1:H:357:ILE:HD12	1.96	0.47
1:H:400:HIS:CD2	1:H:406:SER:HB3	2.49	0.47
3:P:479:LYS:HA	3:P:524:TYR:HD1	1.78	0.47
1:K:417:ASP:O	1:K:420:SER:OG	2.28	0.47
1:K:565:SER:O	1:K:565:SER:OG	2.23	0.47
1:L:442:SER:OG	1:L:443:ARG:N	2.47	0.47
3:P:2:SER:O	3:P:2:SER:OG	2.33	0.47
1:A:429:THR:HG22	1:A:436:PRO:HB3	1.95	0.47
3:P:366:TRP:CZ3	3:P:421:TYR:HB3	2.50	0.47
1:G:495:LEU:HD23	1:G:499:LYS:HD3	1.97	0.47
1:K:461:ARG:HD3	1:L:558:LYS:HD3	1.97	0.47
1:K:526:GLU:O	1:K:530:THR:OG1	2.27	0.47
1:L:428:VAL:O	1:L:436:PRO:HA	2.15	0.47
1:B:394:THR:HG22	1:B:395:ASN:H	1.79	0.47
1:L:347:VAL:HG22	1:L:369:VAL:HG12	1.97	0.47
1:L:380:ILE:HG21	1:L:409:GLY:HA3	1.97	0.47
3:P:527:GLY:HA3	3:P:537:THR:HG22	1.97	0.47
1:G:350:ILE:HB	1:G:366:THR:HG23	1.95	0.46
3:P:271:ARG:HH22	3:P:276:GLU:HA	1.80	0.46
1:A:535:THR:HG22	1:A:551:THR:HB	1.96	0.46
1:B:454:VAL:HG22	1:B:476:VAL:HG13	1.96	0.46
1:F:483:ASP:H	1:F:505:PRO:HG2	1.80	0.46
3:P:158:VAL:HG12	3:P:159:ILE:HG12	1.97	0.46
1:L:369:VAL:HG23	1:L:407:ALA:HB3	1.97	0.46
1:L:565:SER:O	1:L:565:SER:OG	2.22	0.46
3:P:128:ARG:NH1	3:P:244:GLU:OE2	2.43	0.46
1:C:416:ASP:O	1:C:420:SER:CB	2.64	0.46
1:F:362:SER:O	1:F:364:LYS:NZ	2.39	0.46
1:G:366:THR:HB	1:G:410:GLU:HG2	1.96	0.46
1:K:527:GLU:O	1:K:534:TYR:OH	2.30	0.46
1:A:495:LEU:HD23	1:A:495:LEU:HA	1.80	0.46
1:B:372:LEU:O	1:B:405:PHE:N	2.49	0.46
1:L:474:CYS:HB2	1:L:488:TRP:HZ2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:THR:HA	2:J:64:LEU:HD12	1.98	0.46
1:K:354:PHE:HA	1:K:357:ILE:HG12	1.98	0.46
1:H:495:LEU:HD22	1:H:499:LYS:HD3	1.97	0.46
1:A:565:SER:O	1:A:565:SER:OG	2.30	0.45
1:F:503:SER:OG	1:F:504:ALA:O	2.31	0.45
1:G:489:MET:HA	1:G:494:PRO:HA	1.97	0.45
1:H:369:VAL:HG11	1:H:428:VAL:HG11	1.97	0.45
1:K:394:THR:OG1	1:K:395:ASN:N	2.49	0.45
1:K:486:VAL:HG22	1:K:538:VAL:HG12	1.98	0.45
3:P:165:VAL:HG21	3:P:171:GLY:H	1.81	0.45
1:F:553:ASP:OD1	1:F:553:ASP:N	2.39	0.45
1:L:459:PRO:HD3	1:L:472:ILE:HG13	1.97	0.45
3:P:132:ILE:HB	3:P:187:VAL:HG13	1.98	0.45
1:L:362:SER:O	1:L:362:SER:OG	2.31	0.45
1:B:535:THR:OG1	1:B:536:CYS:N	2.49	0.45
1:C:443:ARG:NH2	1:C:541:GLU:OE1	2.50	0.45
1:D:562:TYR:OH	1:G:568:MET:SD	2.70	0.45
1:F:558:LYS:HA	1:F:559:PRO:HD3	1.81	0.45
1:G:351:PRO:HB3	1:G:441:ILE:HD11	1.98	0.45
1:K:383:THR:OG1	1:K:425:THR:OG1	2.26	0.45
1:E:449:LEU:HD22	1:E:542:ALA:HB2	1.99	0.45
1:E:524:SER:OG	1:E:525:GLU:N	2.49	0.45
1:L:553:ASP:OD1	1:L:554:LYS:N	2.37	0.45
3:P:25:PRO:O	3:P:27:THR:N	2.50	0.45
1:D:382:TRP:NE1	1:D:409:GLY:O	2.47	0.45
1:B:459:PRO:HG3	1:B:470:ALA:HB1	1.99	0.45
1:L:400:HIS:HB2	1:L:404:THR:H	1.82	0.45
3:P:529:LYS:NZ	3:P:531:GLY:O	2.49	0.45
1:C:464:LEU:HD21	1:C:470:ALA:HB2	1.99	0.44
1:E:373:THR:OG1	1:E:432:ASP:OD2	2.30	0.44
1:F:362:SER:OG	1:F:362:SER:O	2.34	0.44
1:F:467:ARG:HA	1:F:525:GLU:HG3	1.99	0.44
1:K:419:ASN:OD1	1:K:443:ARG:NH1	2.49	0.44
1:F:495:LEU:HD23	1:F:495:LEU:HA	1.83	0.44
1:H:508:GLU:HG2	1:H:511:ALA:HB3	1.98	0.44
1:L:459:PRO:HG3	1:L:470:ALA:HB1	1.99	0.44
1:D:347:VAL:HG21	1:D:428:VAL:HG21	1.98	0.44
1:G:486:VAL:HG12	1:G:538:VAL:HG23	1.99	0.44
1:H:345:ILE:HG23	1:H:372:LEU:HD23	2.00	0.44
1:L:508:GLU:HG2	1:L:511:ALA:HB3	2.00	0.44
1:H:471:THR:O	1:H:471:THR:OG1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:563:ASN:OD1	1:H:563:ASN:N	2.44	0.44
1:L:474:CYS:HB2	1:L:488:TRP:CZ2	2.53	0.44
1:H:420:SER:O	1:H:420:SER:OG	2.30	0.44
3:P:143:LYS:HB3	3:P:143:LYS:HE2	1.71	0.44
1:F:381:SER:HB3	1:F:427:THR:HB	1.99	0.44
1:G:361:LYS:HA	1:G:361:LYS:HD3	1.71	0.44
1:B:347:VAL:HG21	1:B:428:VAL:HG21	2.00	0.44
1:A:382:TRP:HH2	1:A:441:ILE:HD12	1.82	0.43
1:G:553:ASP:OD1	1:G:553:ASP:N	2.40	0.43
1:H:474:CYS:HB2	1:H:488:TRP:CZ2	2.53	0.43
1:H:575:CYS:HB2	1:K:575:CYS:HB3	1.60	0.43
3:P:144:ARG:HH12	3:P:148:TYR:HH	1.61	0.43
3:P:146:SER:OG	3:P:147:LEU:N	2.51	0.43
1:H:456:LEU:HD11	1:H:536:CYS:HB3	2.01	0.43
1:K:397:SER:HB3	1:K:407:ALA:HA	1.99	0.43
1:B:402:ASN:OD1	1:B:402:ASN:N	2.46	0.43
1:D:558:LYS:HE2	1:D:558:LYS:HB3	1.75	0.43
1:E:560:THR:O	1:E:560:THR:OG1	2.34	0.43
1:E:418:TRP:CD1	1:E:443:ARG:HB2	2.52	0.43
1:F:537:VAL:HG21	1:G:545:ASN:ND2	2.33	0.43
1:K:567:VAL:HB	1:L:567:VAL:HA	2.00	0.43
1:E:531:GLY:N	1:E:532:GLU:OE1	2.50	0.43
3:P:91:LYS:HA	3:P:103:PHE:O	2.18	0.43
1:F:511:ALA:HB1	1:F:514:ARG:HD3	2.00	0.43
1:K:359:LEU:HG	1:K:360:THR:HG23	2.00	0.43
1:K:509:PRO:HB3	1:L:501:VAL:HG23	2.01	0.43
1:A:417:ASP:OD1	1:A:417:ASP:N	2.51	0.43
1:B:466:LEU:O	3:P:97:ASN:ND2	2.52	0.43
1:D:345:ILE:HG12	1:D:433:LEU:HG	1.99	0.43
1:G:425:THR:HA	1:G:439:GLN:O	2.19	0.43
3:P:477:TRP:CD2	3:P:511:LEU:HD13	2.53	0.43
1:C:486:VAL:HG22	1:C:538:VAL:HG22	2.01	0.43
1:E:565:SER:OG	1:E:566:LEU:N	2.52	0.43
1:F:381:SER:O	1:F:426:CYS:HA	2.19	0.43
1:K:456:LEU:HA	1:K:456:LEU:HD12	1.82	0.43
1:G:449:LEU:HD12	1:G:449:LEU:HA	1.92	0.42
1:G:541:GLU:H	1:G:541:GLU:HG2	1.70	0.42
1:H:385:GLN:HG3	1:H:423:ARG:HG2	2.01	0.42
2:J:35:ARG:O	2:J:37:ILE:N	2.50	0.42
3:P:430:LEU:HD23	3:P:430:LEU:HA	1.84	0.42
1:C:416:ASP:O	1:C:420:SER:OG	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:543:LEU:HD23	1:E:543:LEU:HA	1.81	0.42
1:F:417:ASP:OD1	1:F:417:ASP:N	2.36	0.42
1:D:537:VAL:HG12	1:D:549:GLU:HG2	2.01	0.42
1:A:429:THR:O	1:A:429:THR:OG1	2.33	0.42
1:H:429:THR:HG22	1:H:436:PRO:HB3	2.01	0.42
1:D:450:HIS:CD2	1:D:514:ARG:HE	2.34	0.42
1:A:449:LEU:O	1:A:450:HIS:ND1	2.52	0.42
1:B:372:LEU:HD23	1:B:372:LEU:HA	1.84	0.42
1:E:474:CYS:HB2	1:E:488:TRP:CZ2	2.54	0.42
1:G:354:PHE:HE1	1:G:541:GLU:HB3	1.84	0.42
1:A:564:VAL:HG21	1:L:568:MET:HE3	2.02	0.42
1:D:368:LEU:HD12	1:D:368:LEU:HA	1.94	0.42
1:F:430:HIS:HB3	1:F:433:LEU:HG	2.02	0.42
1:L:365:LEU:HD23	1:L:441:ILE:HG13	2.01	0.42
1:G:382:TRP:HB2	1:G:390:VAL:HG21	2.01	0.42
1:G:535:THR:HA	1:G:550:ARG:O	2.19	0.42
1:B:569:SER:OG	1:B:570:ASP:N	2.48	0.42
1:K:474:CYS:HB2	1:K:488:TRP:CZ2	2.55	0.42
1:B:345:ILE:HG23	1:B:372:LEU:HG	2.02	0.42
1:C:380:ILE:HG13	1:C:393:HIS:HE1	1.84	0.42
3:P:8:GLU:HG3	3:P:103:PHE:HZ	1.84	0.42
1:A:449:LEU:HB3	1:A:542:ALA:HB2	2.02	0.41
1:E:366:THR:HA	1:E:409:GLY:O	2.20	0.41
1:H:400:HIS:CD2	1:H:404:THR:HG23	2.55	0.41
1:K:471:THR:O	1:K:471:THR:OG1	2.34	0.41
1:C:345:ILE:N	1:C:371:ASP:HB3	2.35	0.41
1:H:569:SER:O	1:H:569:SER:OG	2.31	0.41
1:K:489:MET:HA	1:K:494:PRO:HA	2.02	0.41
3:P:234:SER:OG	3:P:235:VAL:N	2.53	0.41
1:C:568:MET:HE2	1:C:568:MET:HB3	1.72	0.41
2:J:99:THR:O	2:J:99:THR:OG1	2.36	0.41
1:E:391:LYS:HA	1:E:391:LYS:HD3	1.88	0.41
1:F:397:SER:HB3	1:F:408:VAL:HG12	2.03	0.41
1:G:397:SER:OG	1:G:406:SER:O	2.36	0.41
3:P:148:TYR:HD1	3:P:157:LEU:HA	1.86	0.41
3:P:263:VAL:H	3:P:263:VAL:HG23	1.63	0.41
3:P:414:THR:HG22	3:P:416:ARG:H	1.86	0.41
1:B:429:THR:HG23	1:B:434:PRO:HA	2.02	0.41
1:E:427:THR:HA	1:E:437:LEU:O	2.21	0.41
1:E:561:LEU:HA	1:E:561:LEU:HD12	1.84	0.41
1:F:380:ILE:O	1:F:393:HIS:NE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:547:VAL:HG11	1:E:545:ASN:HD22	1.86	0.41
1:K:532:GLU:H	1:K:532:GLU:HG2	1.54	0.41
3:P:232:ARG:HE	3:P:232:ARG:HB2	1.68	0.41
1:D:353:SER:O	1:D:356:SER:OG	2.29	0.41
1:E:425:THR:HA	1:E:439:GLN:O	2.20	0.41
1:F:384:ARG:HE	1:F:390:VAL:HG12	1.86	0.41
1:K:386:ASN:N	1:K:422:GLU:OE2	2.54	0.41
2:J:49:ILE:HD12	2:J:49:ILE:HA	1.83	0.41
3:P:226:LEU:H	3:P:226:LEU:HG	1.45	0.41
1:C:374:THR:HG22	1:C:404:THR:HA	2.02	0.41
1:E:384:ARG:HD3	1:E:388:GLU:HB2	2.04	0.40
1:E:384:ARG:HE	1:E:390:VAL:HG12	1.86	0.40
1:E:531:GLY:O	1:E:533:THR:N	2.48	0.40
1:F:525:GLU:O	1:F:529:ASN:HB2	2.21	0.40
1:K:347:VAL:HG22	1:K:369:VAL:HG13	2.03	0.40
1:A:500:TYR:HA	1:A:520:ILE:O	2.21	0.40
1:B:461:ARG:HA	1:B:461:ARG:HD3	1.93	0.40
1:C:400:HIS:HB3	1:C:402:ASN:H	1.86	0.40
1:F:450:HIS:HD2	1:F:514:ARG:HG2	1.86	0.40
1:K:369:VAL:O	1:K:406:SER:HA	2.20	0.40
1:K:564:VAL:H	1:K:564:VAL:HG23	1.57	0.40
1:L:564:VAL:H	1:L:564:VAL:HG23	1.53	0.40
1:A:451:ARG:HH11	1:A:451:ARG:HD3	1.73	0.40
1:E:503:SER:OG	1:E:504:ALA:N	2.49	0.40
1:K:461:ARG:HH12	1:L:557:GLY:HA2	1.86	0.40
1:K:576:TYR:HD1	1:L:576:TYR:HB3	1.87	0.40
3:P:5:PHE:CE2	3:P:226:LEU:HB3	2.56	0.40
1:A:362:SER:O	1:A:364:LYS:N	2.48	0.40
1:A:425:THR:HB	1:A:438:LYS:HD2	2.04	0.40
1:D:471:THR:HG22	1:D:522:THR:HG22	2.04	0.40
1:E:456:LEU:HD12	1:E:456:LEU:HA	1.83	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	230/383 (60%)	195 (85%)	33 (14%)	2 (1%)	14	42
1	B	225/383 (59%)	186 (83%)	39 (17%)	0	100	100
1	C	223/383 (58%)	182 (82%)	40 (18%)	1 (0%)	30	59
1	D	222/383 (58%)	188 (85%)	32 (14%)	2 (1%)	14	42
1	E	222/383 (58%)	180 (81%)	39 (18%)	3 (1%)	9	31
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%)	30	59
1	L	224/383 (58%)	188 (84%)	36 (16%)	0	100	100
2	J	102/136 (75%)	69 (68%)	31 (30%)	2 (2%)	6	25
3	P	484/555 (87%)	429 (89%)	55 (11%)	0	100	100
All	All	2823/4521 (62%)	2383 (84%)	429 (15%)	11 (0%)	31	59

All (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
1	E	532	GLU
1	E	533	THR
1	C	512	PRO
1	D	512	PRO
1	A	512	PRO
1	A	544	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	206/331 (62%)	193 (94%)	13 (6%)	16	42
1	B	203/331 (61%)	199 (98%)	4 (2%)	48	65
1	C	201/331 (61%)	194 (96%)	7 (4%)	32	56
1	D	200/331 (60%)	195 (98%)	5 (2%)	42	62
1	E	200/331 (60%)	195 (98%)	5 (2%)	42	62
1	F	198/331 (60%)	190 (96%)	8 (4%)	28	53
1	G	200/331 (60%)	192 (96%)	8 (4%)	28	53
1	H	205/331 (62%)	197 (96%)	8 (4%)	28	53
1	K	205/331 (62%)	202 (98%)	3 (2%)	57	69
1	L	204/331 (62%)	196 (96%)	8 (4%)	28	53
2	J	100/128 (78%)	96 (96%)	4 (4%)	28	53
3	P	426/474 (90%)	415 (97%)	11 (3%)	40	61
All	All	2548/3912 (65%)	2464 (97%)	84 (3%)	34	57

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	368	LEU
1	A	394	THR
1	A	404	THR
1	A	417	ASP
1	A	425	THR
1	A	453	ASP
1	A	462	GLU
1	A	518	HIS
1	A	537	VAL
1	A	538	VAL
1	A	562	TYR
1	A	567	VAL
1	A	574	THR
1	B	473	THR
1	B	533	THR
1	B	538	VAL
1	B	564	VAL
1	C	368	LEU
1	C	394	THR
1	C	404	THR

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Mol	Chain	Res	Type
1	C	453	ASP
1	C	473	THR
1	C	545	ASN
1	C	560	THR
1	D	456	LEU
1	D	533	THR
1	D	538	VAL
1	D	552	VAL
1	D	566	LEU
1	E	359	LEU
1	E	369	VAL
1	E	404	THR
1	E	473	THR
1	E	567	VAL
1	F	345	ILE
1	F	363	THR
1	F	417	ASP
1	F	433	LEU
1	F	473	THR
1	F	501	VAL
1	F	521	LEU
1	F	537	VAL
1	G	366	THR
1	G	429	THR
1	G	473	THR
1	G	477	THR
1	G	528	TRP
1	G	535	THR
1	G	548	THR
1	G	567	VAL
1	H	360	THR
1	H	533	THR
1	H	537	VAL
1	H	538	VAL
1	H	556	THR
1	H	562	TYR
1	H	563	ASN
1	H	567	VAL
1	K	547	VAL
1	K	551	THR
1	K	566	LEU
1	L	350	ILE

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Mol	Chain	Res	Type
1	L	474	CYS
1	L	522	THR
1	L	537	VAL
1	L	548	THR
1	L	563	ASN
1	L	567	VAL
1	L	574	THR
2	J	14	CYS
2	J	18	THR
2	J	53	THR
2	J	108	CYS
3	P	9	GLU
3	P	65	ASN
3	P	67	THR
3	P	71	GLU
3	P	74	THR
3	P	220	LEU
3	P	262	ASP
3	P	265	VAL
3	P	267	THR
3	P	367	CYS
3	P	379	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	393	HIS
1	A	400	HIS
1	A	402	ASN
1	A	510	GLN
1	B	419	ASN
1	B	465	ASN
1	B	490	GLN
1	B	518	HIS
1	C	518	HIS
1	D	439	GLN
1	D	450	HIS
1	D	463	GLN
1	D	490	GLN
1	D	493	GLN
1	D	529	ASN
1	D	545	ASN

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Mol	Chain	Res	Type
1	E	545	ASN
1	F	419	ASN
1	F	430	HIS
1	F	490	GLN
1	F	493	GLN
1	F	518	HIS
1	G	385	GLN
1	G	490	GLN
1	G	510	GLN
1	G	518	HIS
1	G	545	ASN
1	H	400	HIS
1	H	463	GLN
1	K	400	HIS
1	K	402	ASN
1	K	490	GLN
1	K	545	ASN
1	L	385	GLN
1	L	419	ASN
1	L	439	GLN
1	L	463	GLN
1	L	529	ASN
2	J	45	ASN
3	P	97	ASN
3	P	282	ASN
3	P	329	ASN
3	P	411	ASN
3	P	486	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 ⓘ

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	4,2	14,14,15	1.70	2 (14%)	17,19,21	1.44	3 (17%)
4	NAG	I	2	4	14,14,15	0.50	0	17,19,21	0.94	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	4,2	-	3/6/23/26	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	C1-C2	4.68	1.58	1.52
4	I	1	NAG	O5-C1	-4.10	1.36	1.43

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	3.20	116.48	112.19
4	I	1	NAG	O5-C5-C4	-2.47	104.83	110.83
4	I	1	NAG	C2-N2-C7	2.24	125.90	122.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	1	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6

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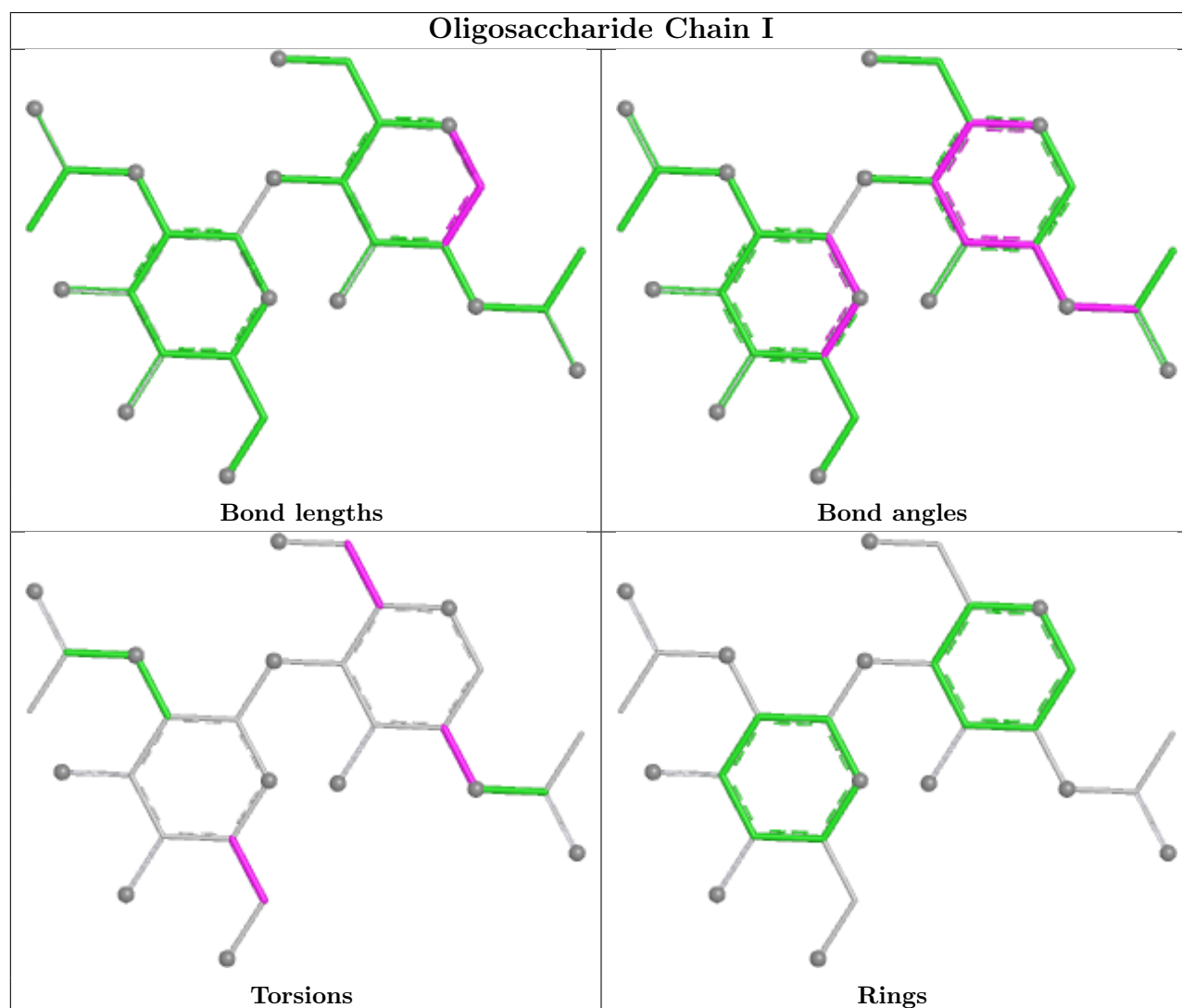
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Mol	Chain	Res	Type	Atoms
4	I	2	NAG	O5-C5-C6-O6
4	I	1	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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	L	601	1	14,14,15	0.79	1 (7%)	17,19,21	0.65	0
5	NAG	K	601	1	14,14,15	1.43	2 (14%)	17,19,21	1.03	1 (5%)
5	NAG	C	601	1	14,14,15	0.44	0	17,19,21	0.97	1 (5%)
5	NAG	A	601	1	14,14,15	0.75	1 (7%)	17,19,21	0.84	1 (5%)
5	NAG	G	601	1	14,14,15	0.84	1 (7%)	17,19,21	0.66	0
5	NAG	H	601	1	14,14,15	0.83	1 (7%)	17,19,21	1.05	2 (11%)
5	NAG	D	601	1	14,14,15	0.72	0	17,19,21	0.74	0
5	NAG	F	601	1	14,14,15	0.36	0	17,19,21	0.62	0
5	NAG	B	601	1	14,14,15	0.27	0	17,19,21	0.76	1 (5%)
5	NAG	E	601	1	14,14,15	0.63	1 (7%)	17,19,21	0.80	0

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

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	601	NAG	O5-C1	-4.54	1.36	1.43
5	H	601	NAG	O5-C1	-2.89	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	601	NAG	O5-C1	-2.86	1.38	1.43
5	L	601	NAG	O5-C1	-2.36	1.39	1.43
5	K	601	NAG	C1-C2	2.28	1.55	1.52
5	A	601	NAG	O5-C1	2.17	1.47	1.43
5	E	601	NAG	C1-C2	2.09	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	601	NAG	C2-N2-C7	2.87	126.74	122.90
5	H	601	NAG	C1-O5-C5	2.69	115.78	112.19
5	C	601	NAG	C2-N2-C7	2.38	126.09	122.90
5	H	601	NAG	C1-C2-N2	2.27	114.02	110.43
5	B	601	NAG	C1-O5-C5	2.25	115.21	112.19
5	A	601	NAG	C1-O5-C5	2.14	115.05	112.19

There are no chirality outliers.

All (20) torsion outliers are listed below:

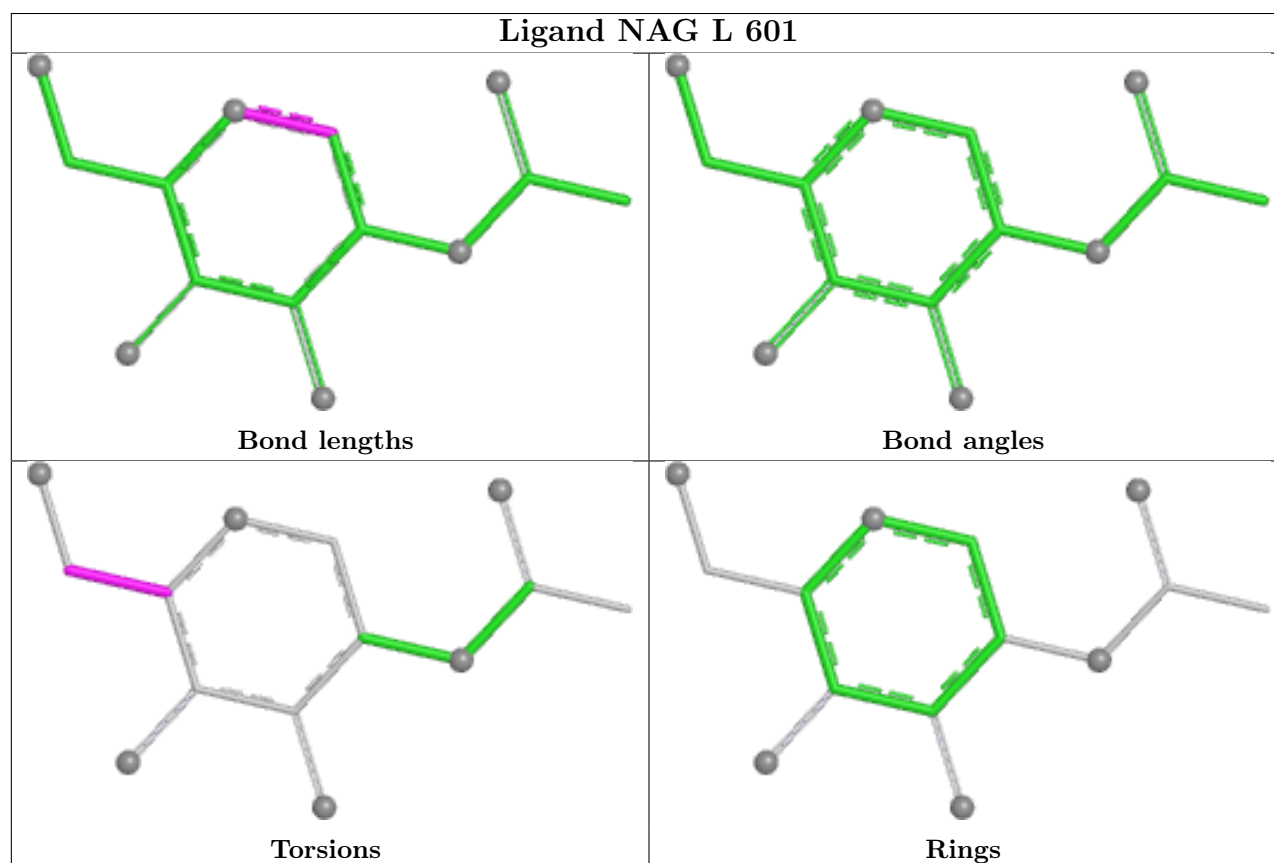
Mol	Chain	Res	Type	Atoms
5	D	601	NAG	C4-C5-C6-O6
5	E	601	NAG	C4-C5-C6-O6
5	D	601	NAG	O5-C5-C6-O6
5	K	601	NAG	O5-C5-C6-O6
5	H	601	NAG	O5-C5-C6-O6
5	F	601	NAG	O5-C5-C6-O6
5	E	601	NAG	O5-C5-C6-O6
5	G	601	NAG	O5-C5-C6-O6
5	H	601	NAG	C4-C5-C6-O6
5	K	601	NAG	C4-C5-C6-O6
5	F	601	NAG	C4-C5-C6-O6
5	G	601	NAG	C4-C5-C6-O6
5	C	601	NAG	C8-C7-N2-C2
5	C	601	NAG	O7-C7-N2-C2
5	K	601	NAG	C8-C7-N2-C2
5	K	601	NAG	O7-C7-N2-C2
5	L	601	NAG	O5-C5-C6-O6
5	L	601	NAG	C4-C5-C6-O6
5	C	601	NAG	O5-C5-C6-O6
5	C	601	NAG	C4-C5-C6-O6

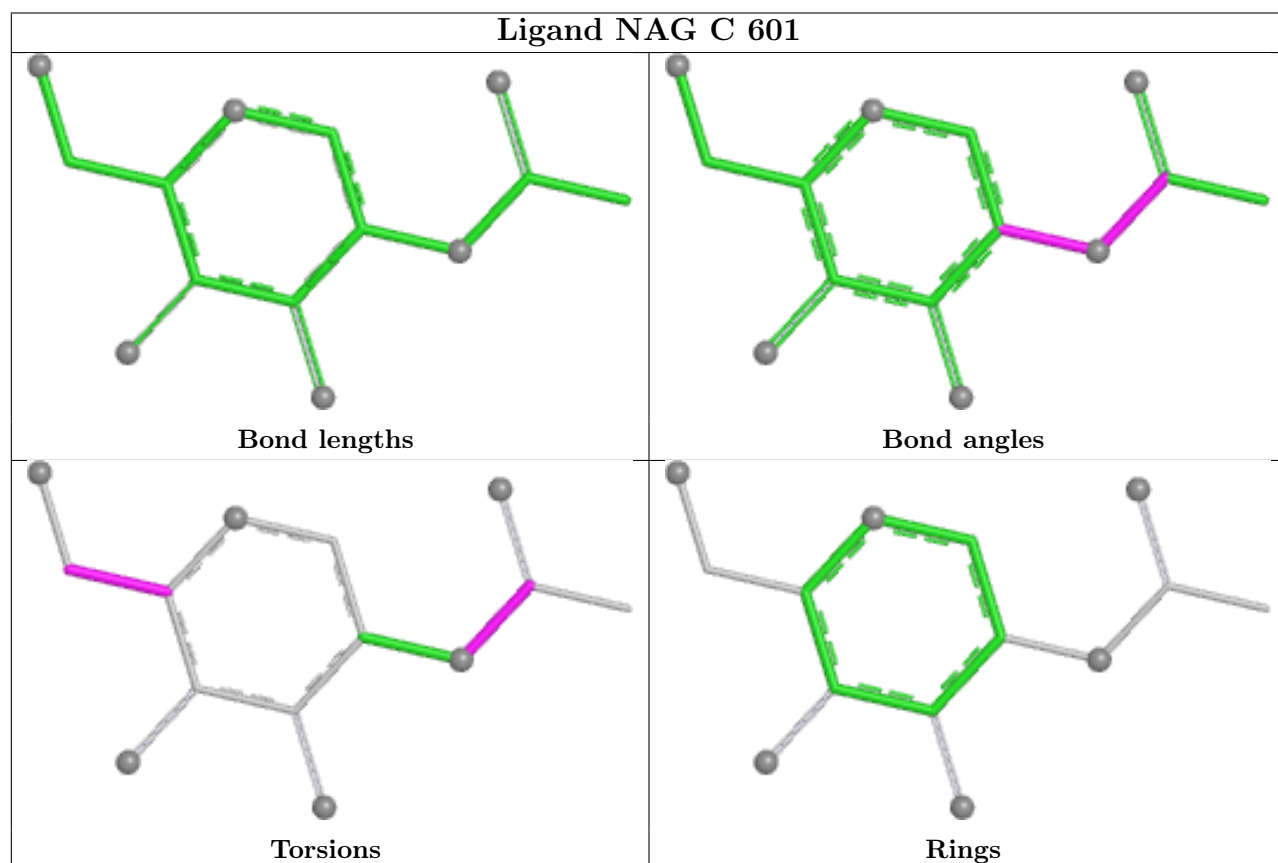
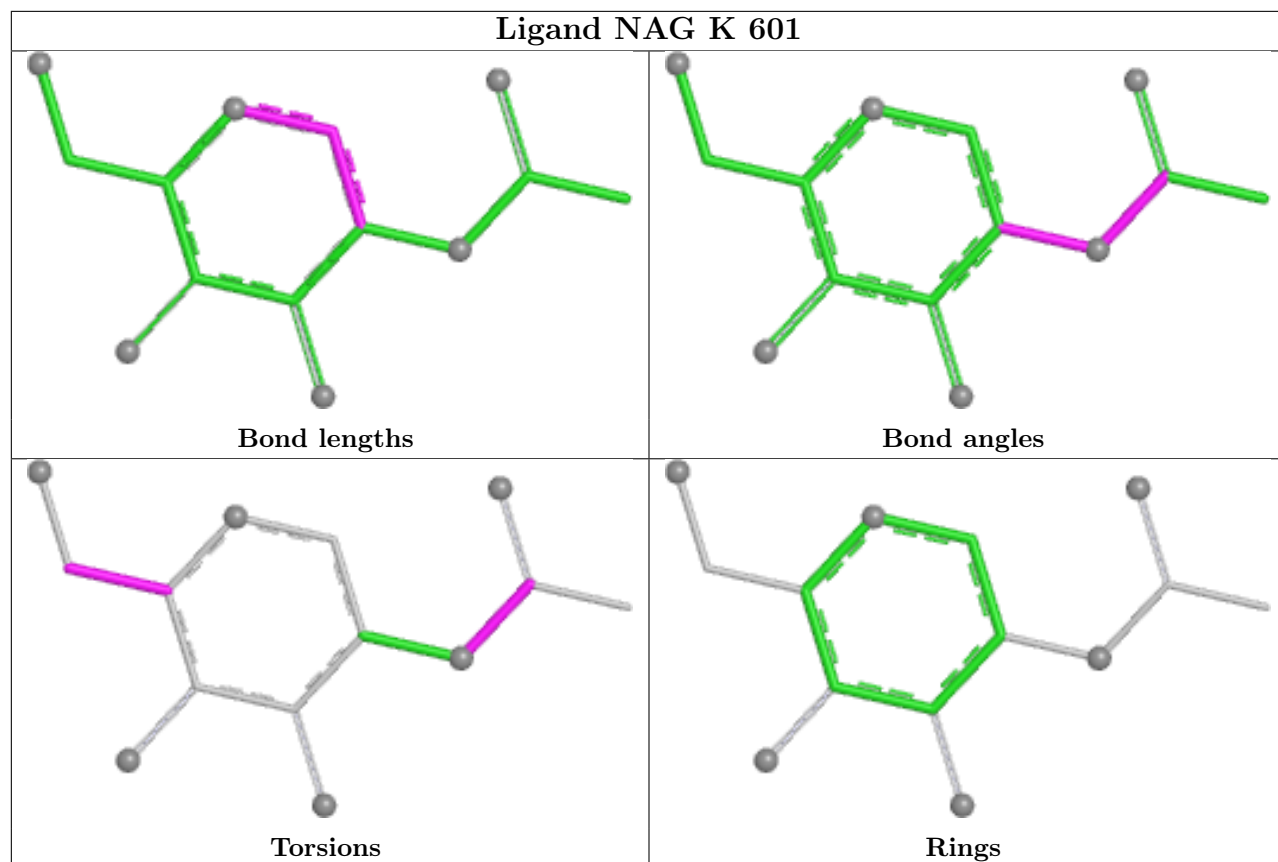
There are no ring outliers.

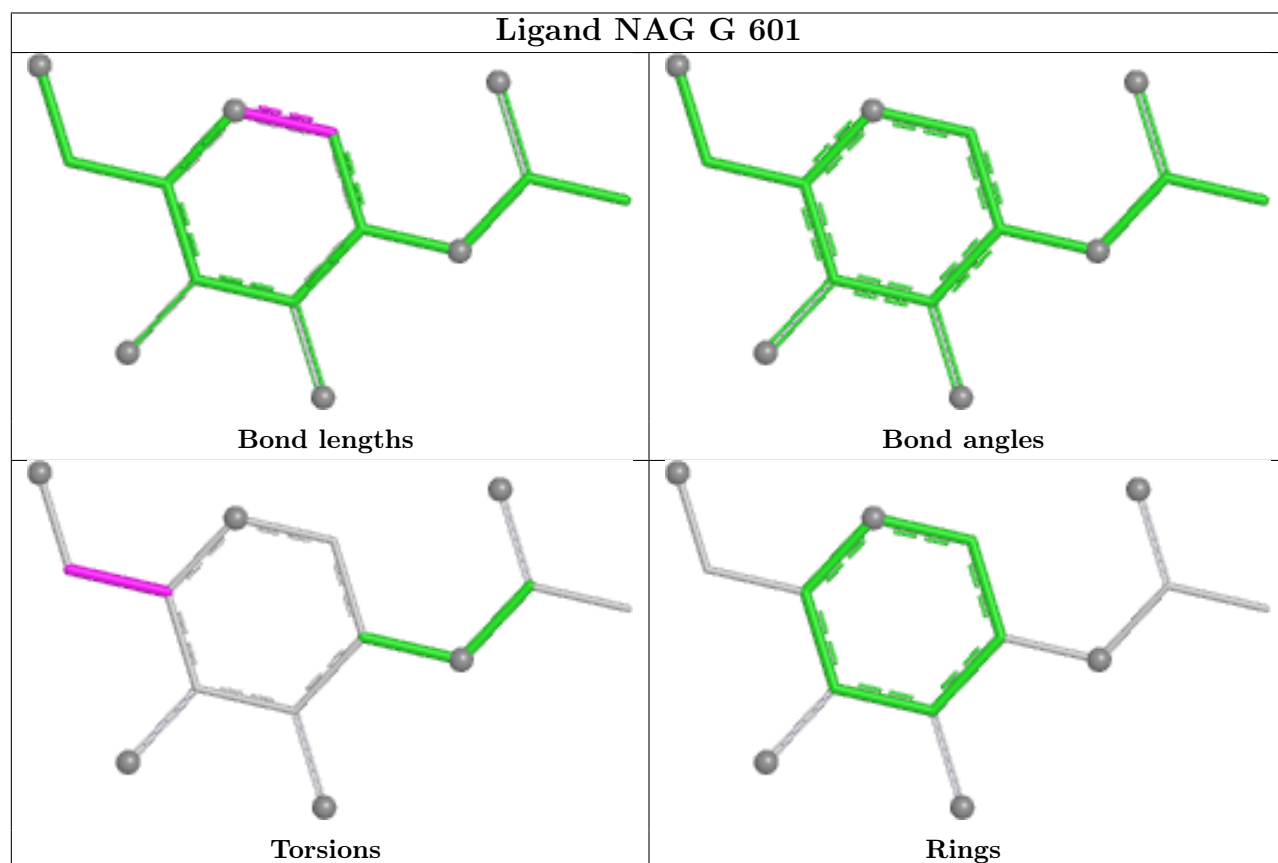
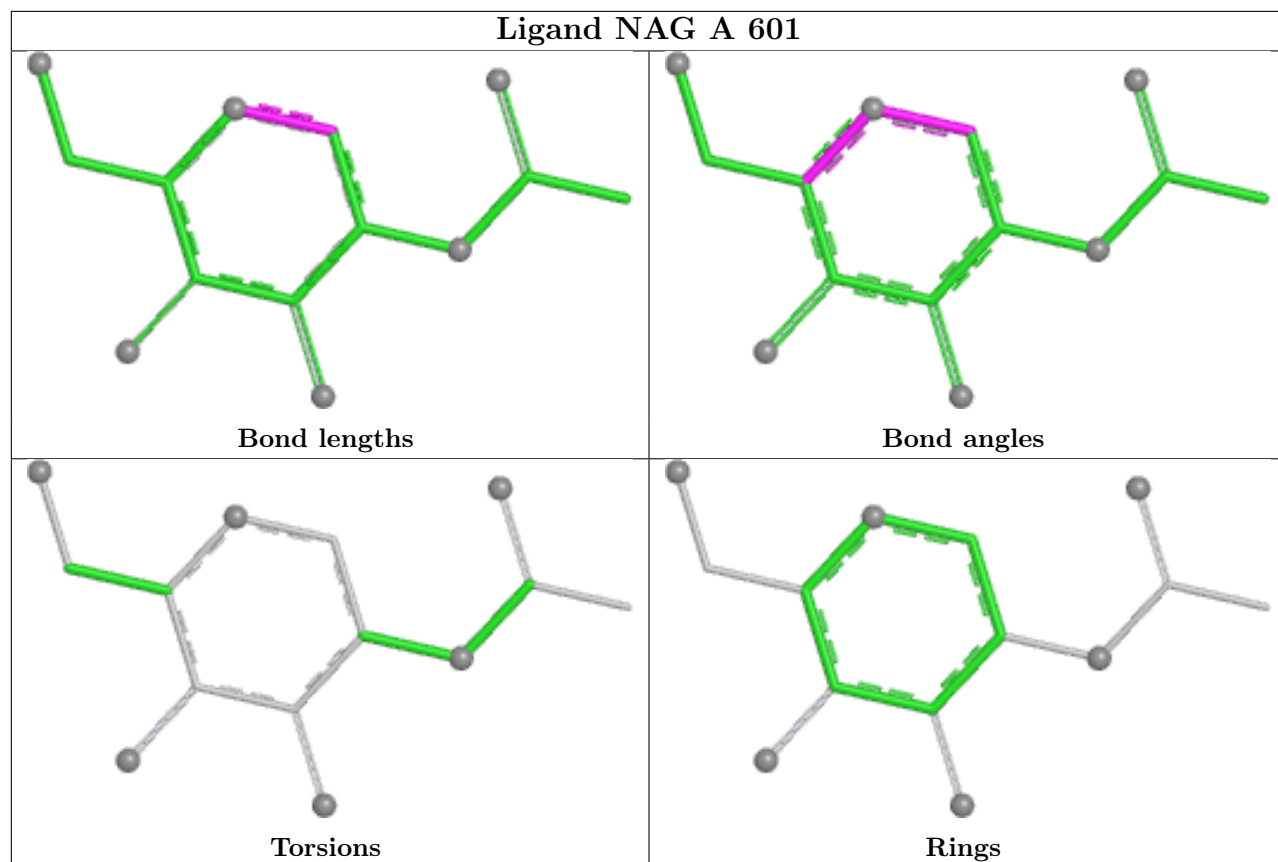
2 monomers are involved in 1 short contact:

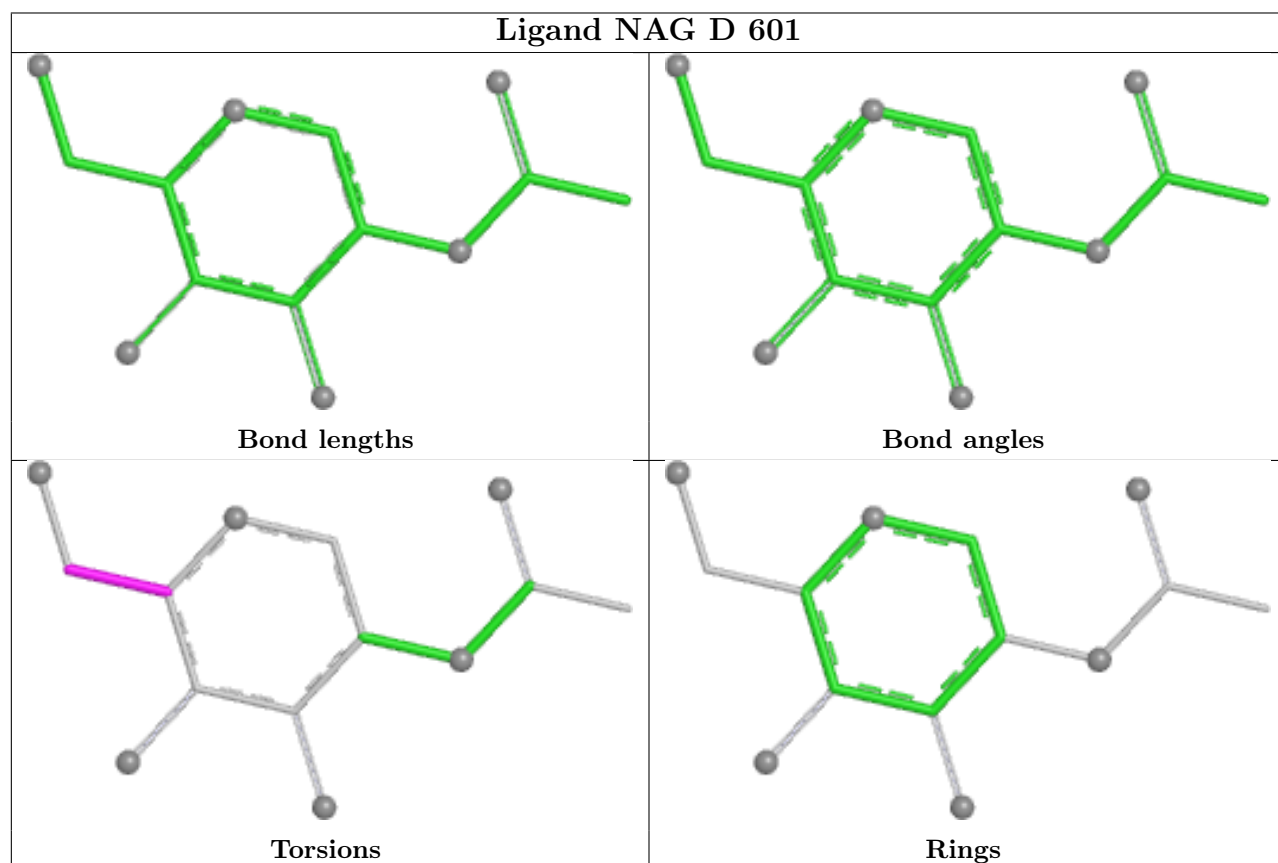
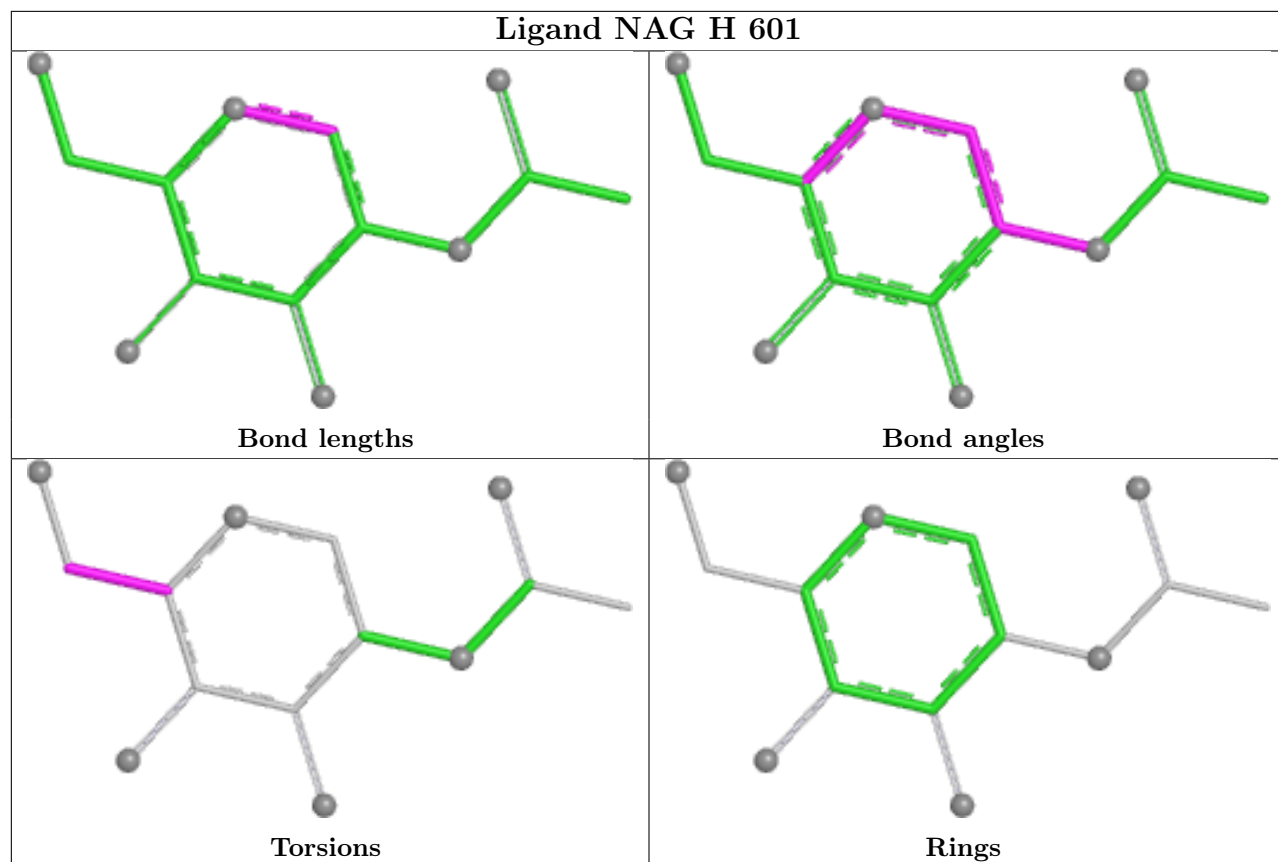
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	601	NAG	1	0
5	F	601	NAG	1	0

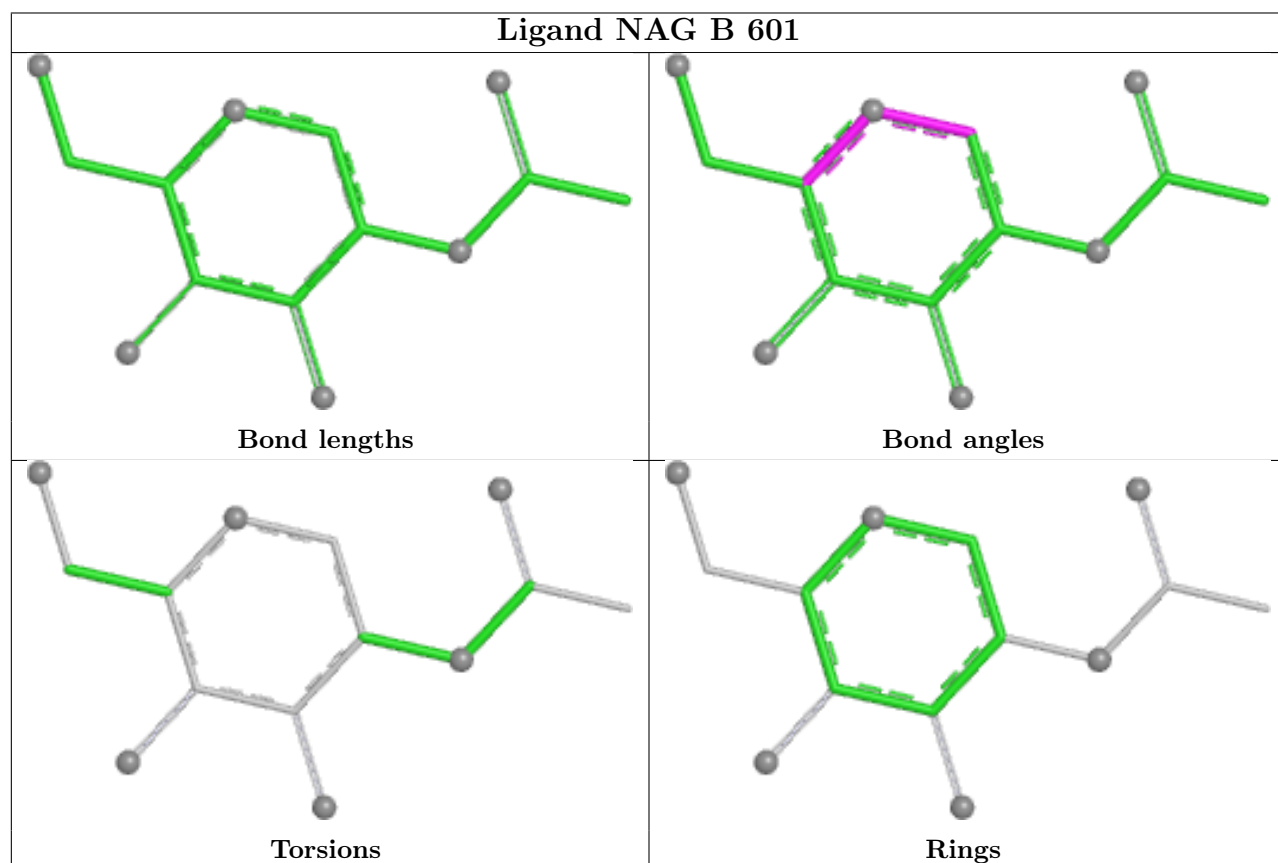
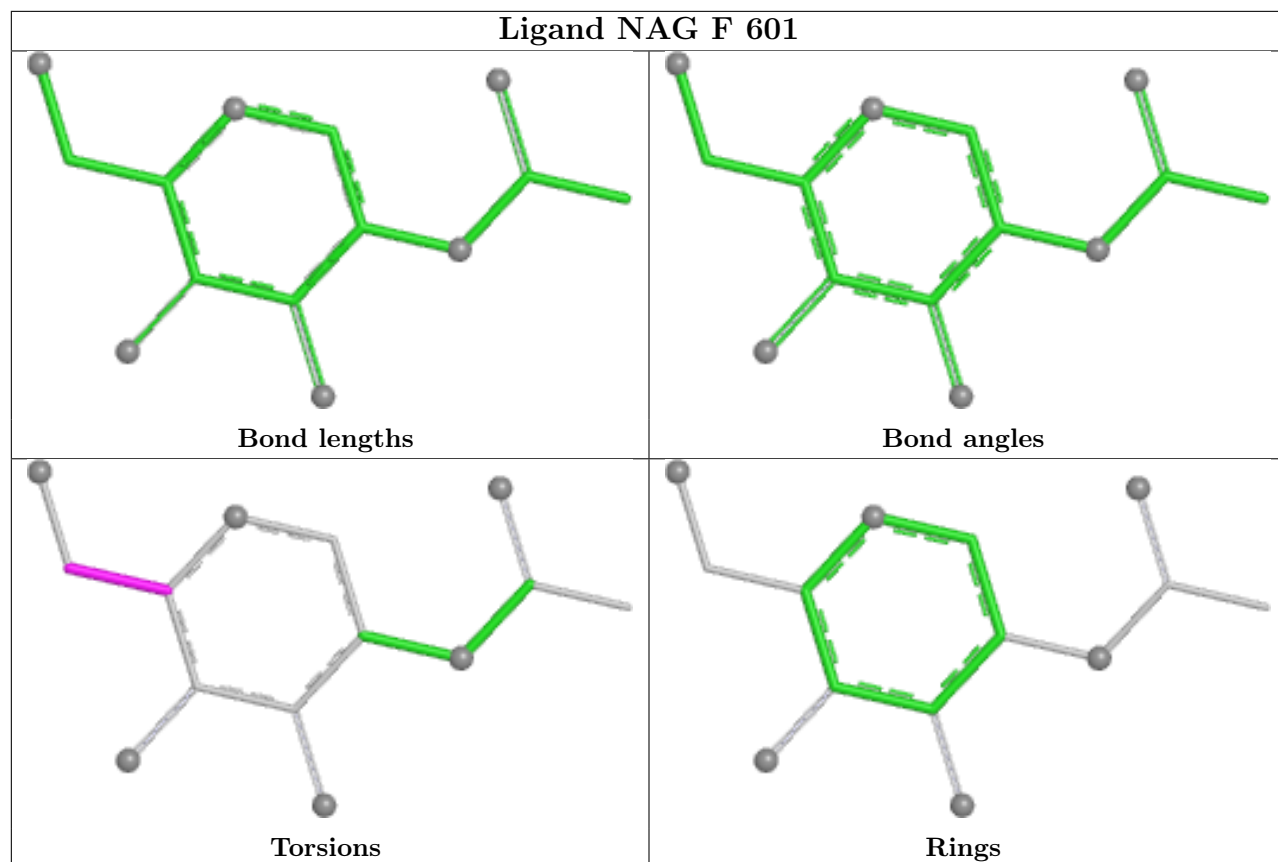
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

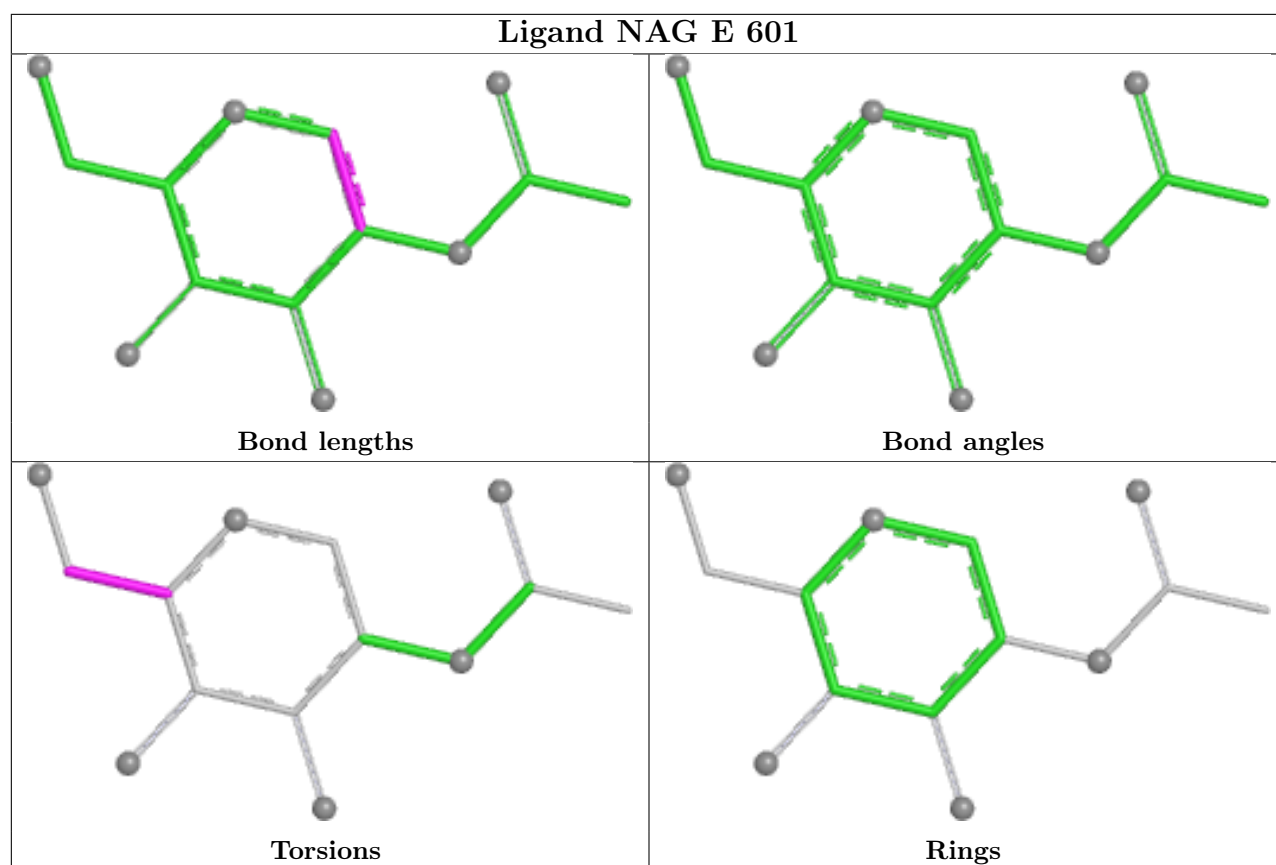












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

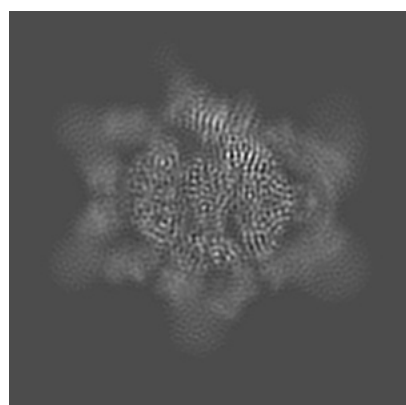
6 Map visualisation [i](#)

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.

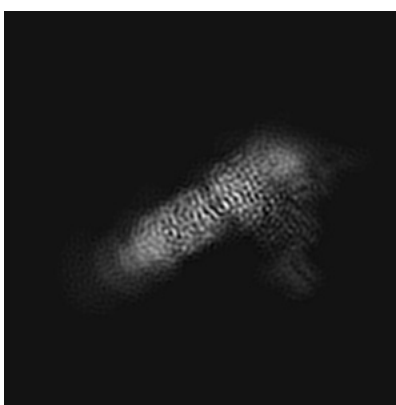
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

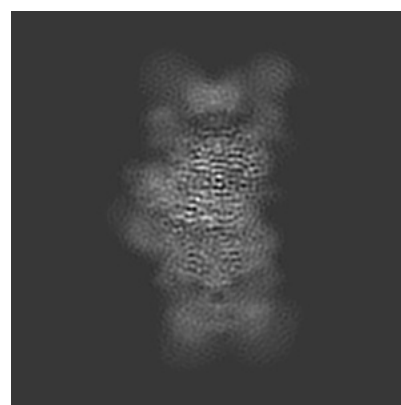
6.1.1 Primary map



X



Y

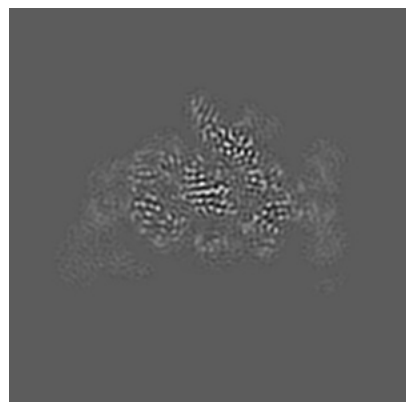


Z

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

6.2 Central slices [i](#)

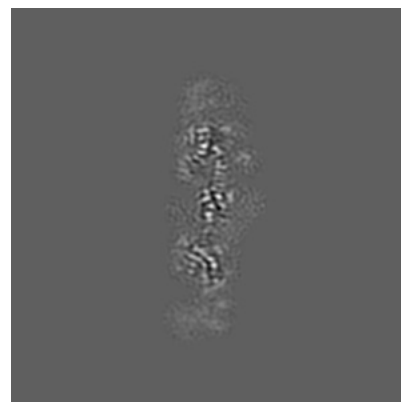
6.2.1 Primary map



X Index: 160



Y Index: 160

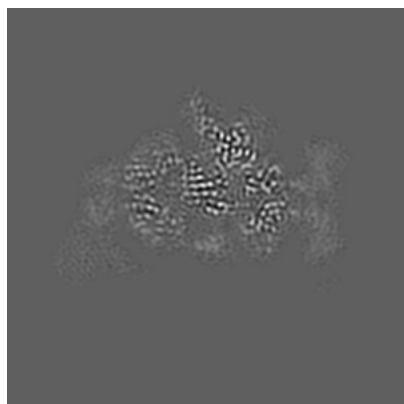


Z Index: 160

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

6.3 Largest variance slices [i](#)

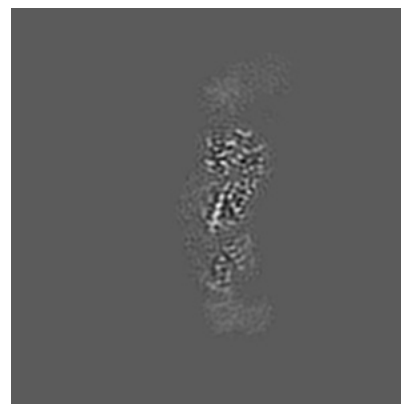
6.3.1 Primary map



X Index: 162



Y Index: 169

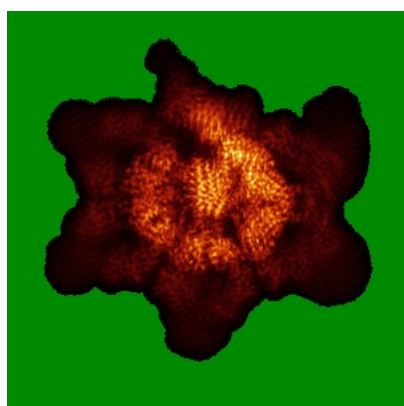


Z Index: 183

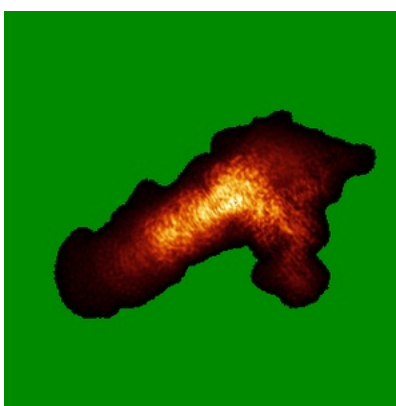
The images above show the largest variance slices of the map in three orthogonal directions.

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

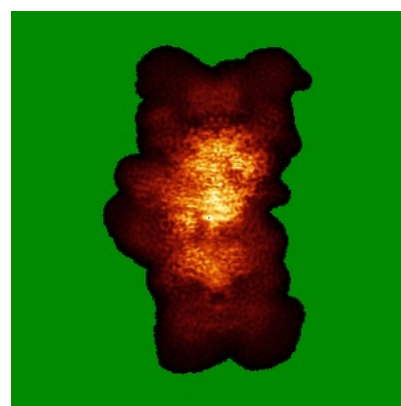
6.4.1 Primary map



X



Y

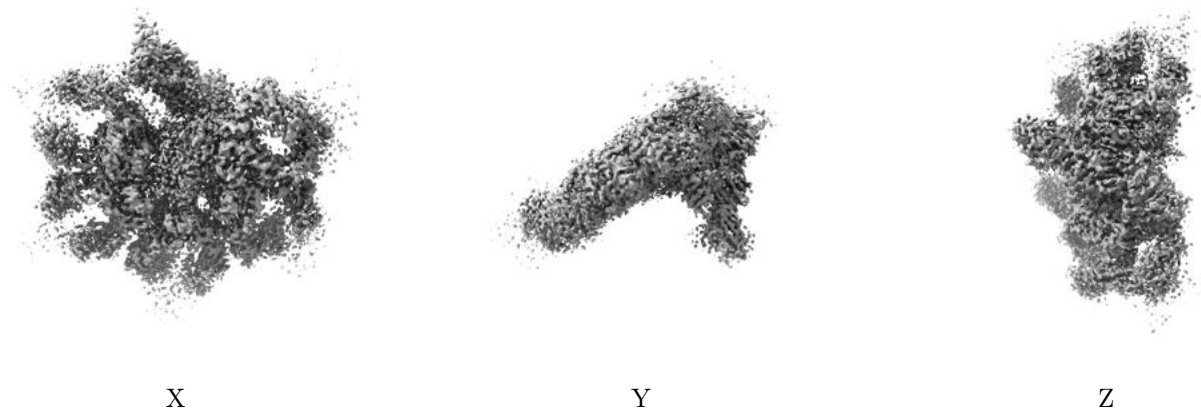


Z

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 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

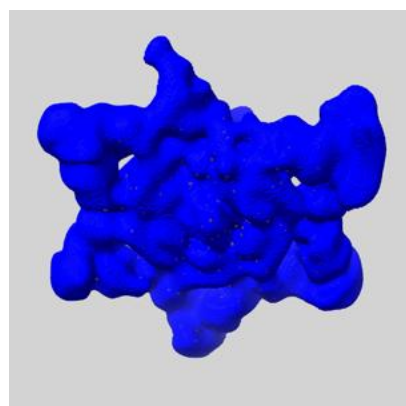
6.6 Mask visualisation [i](#)

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

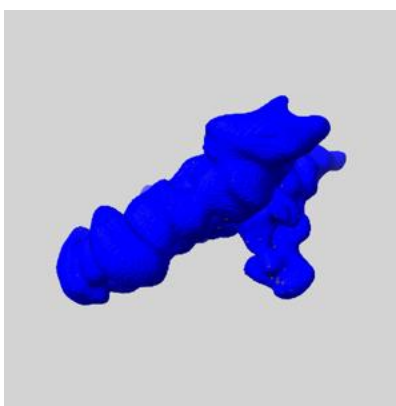
A mask typically either:

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

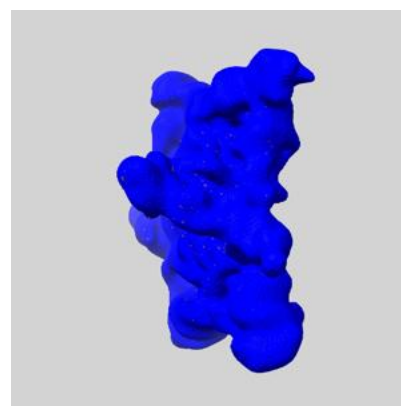
6.6.1 emd_0782_msk_1.map [i](#)



X



Y

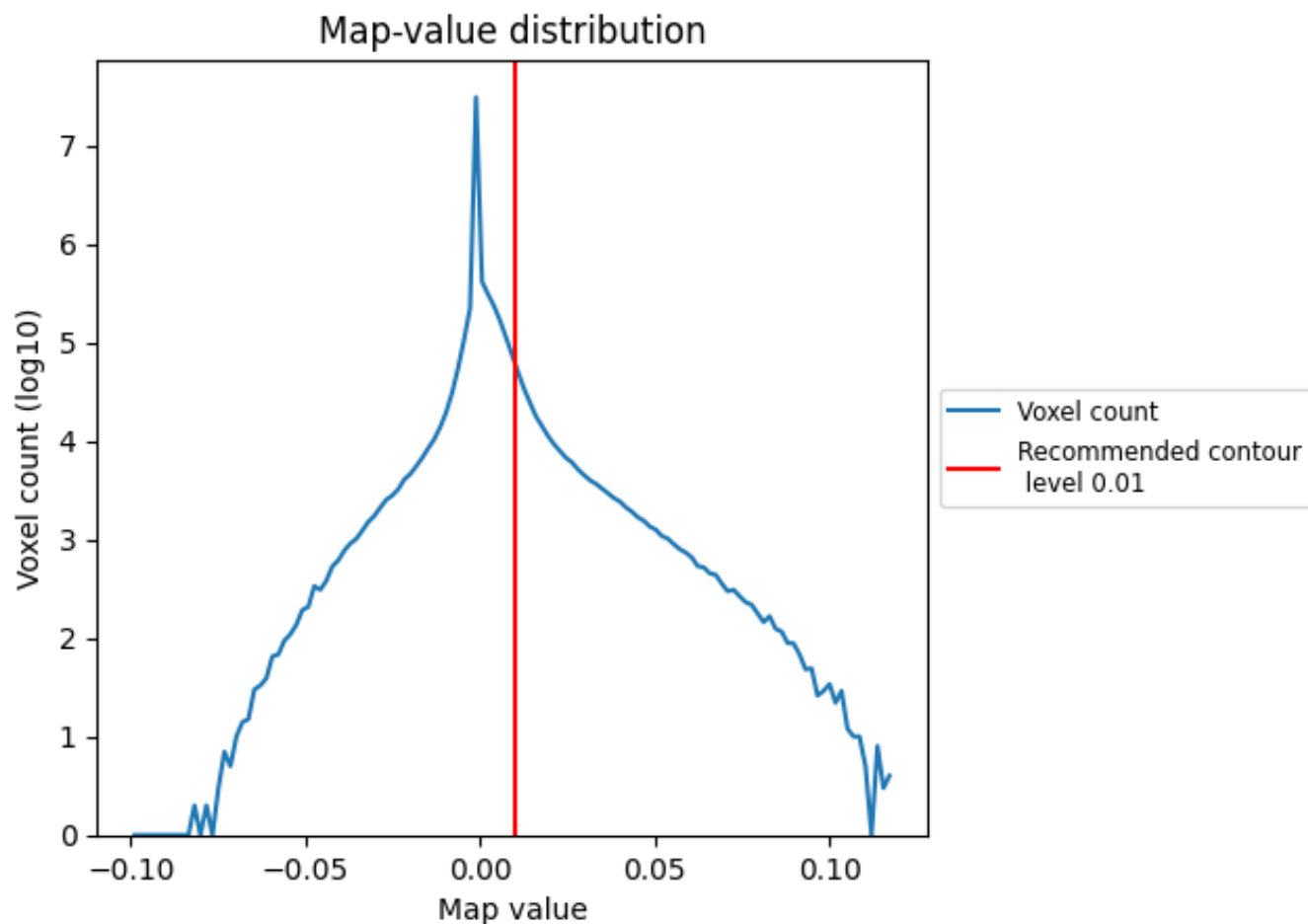


Z

7 Map analysis [i](#)

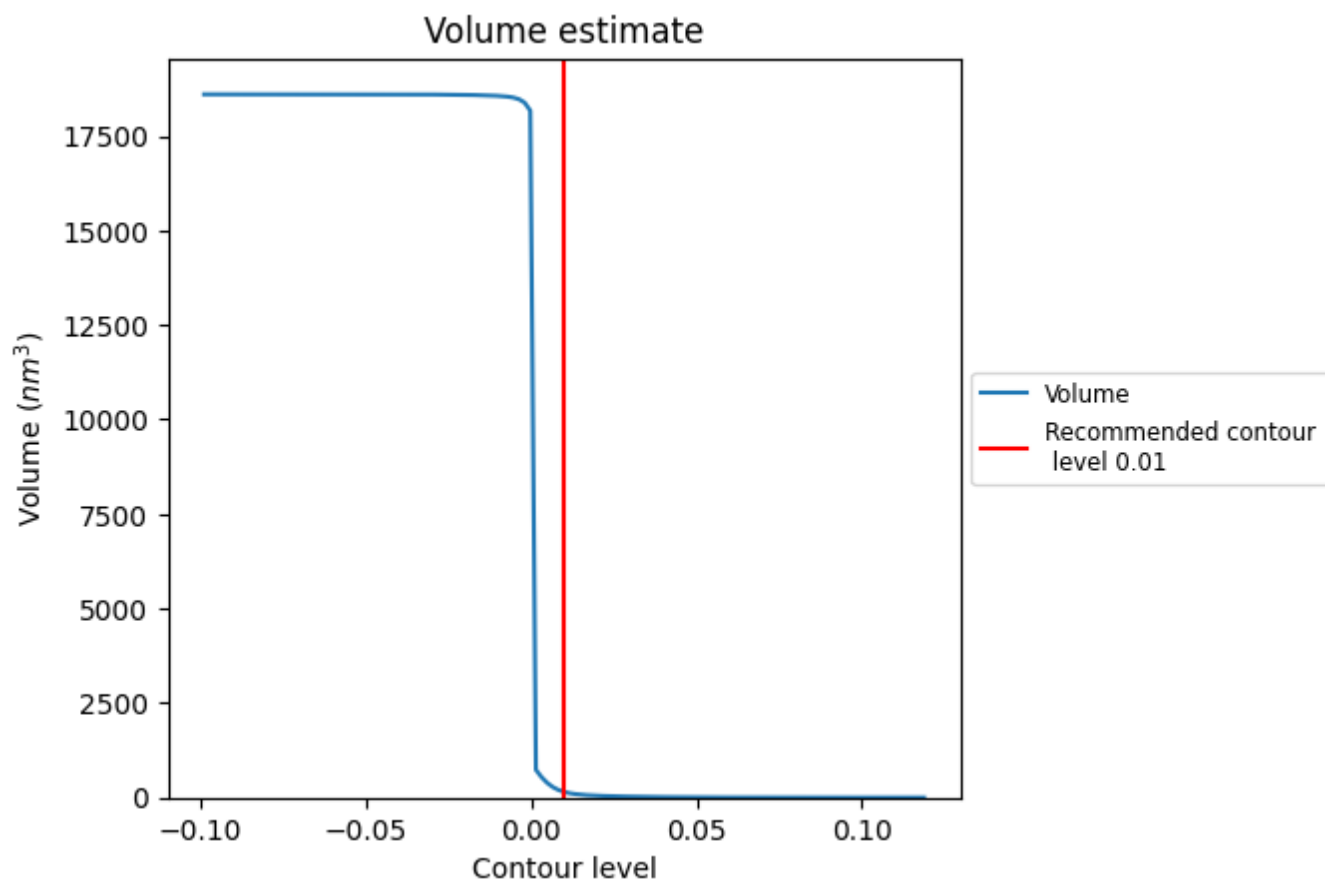
This section contains the results of statistical analysis of the map.

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.

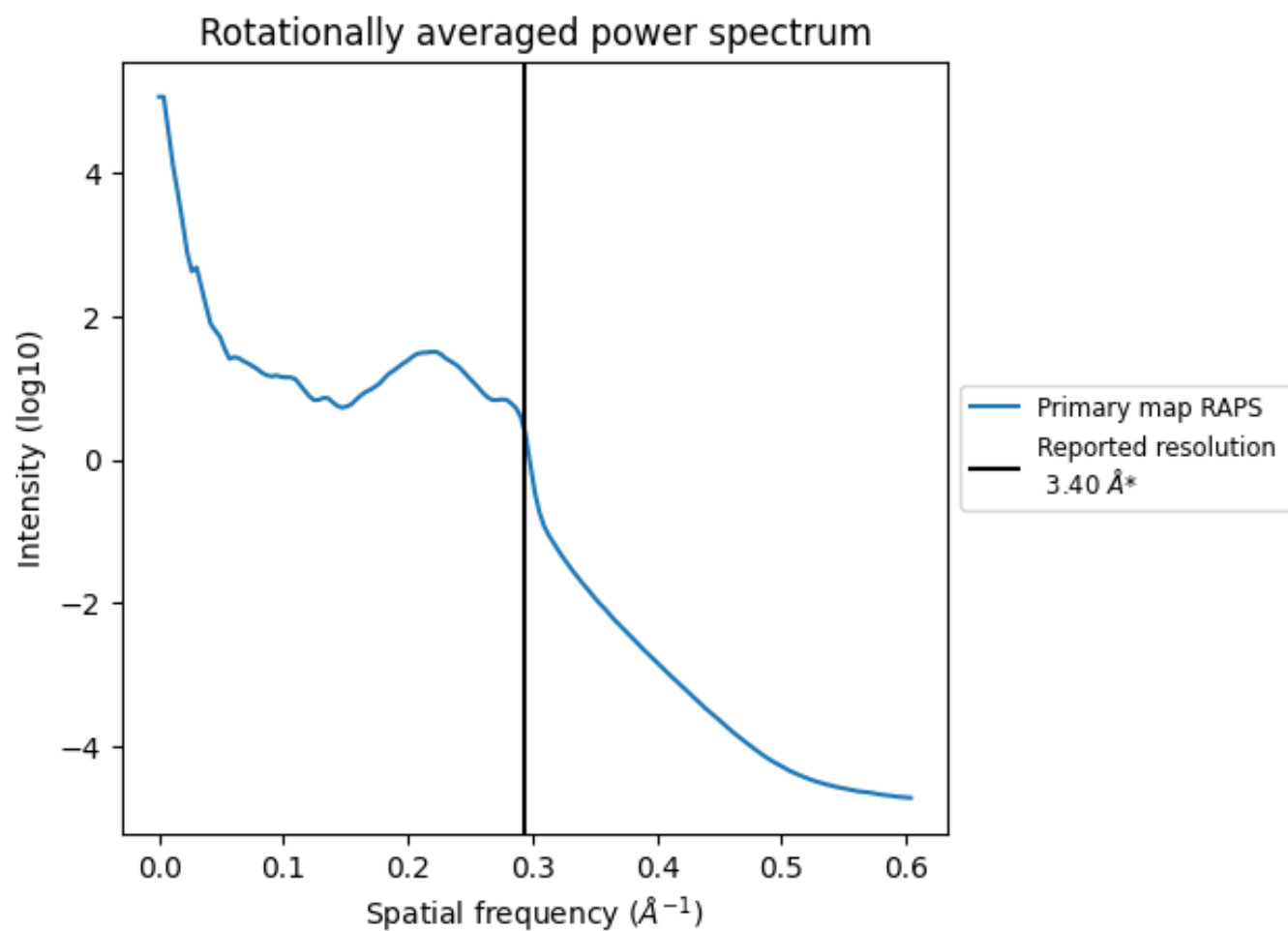
7.2 Volume estimate [i](#)



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 ⓘ

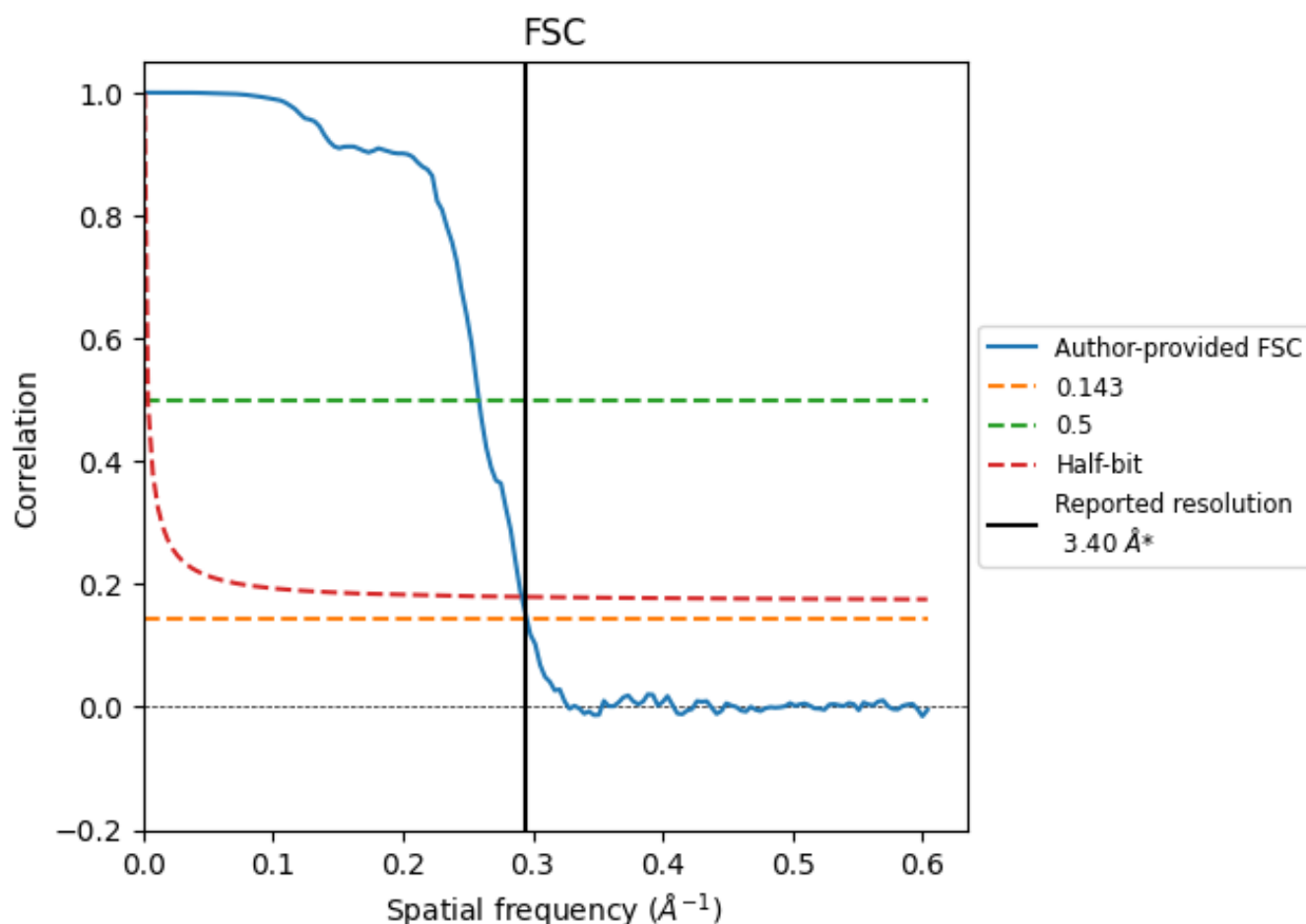


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

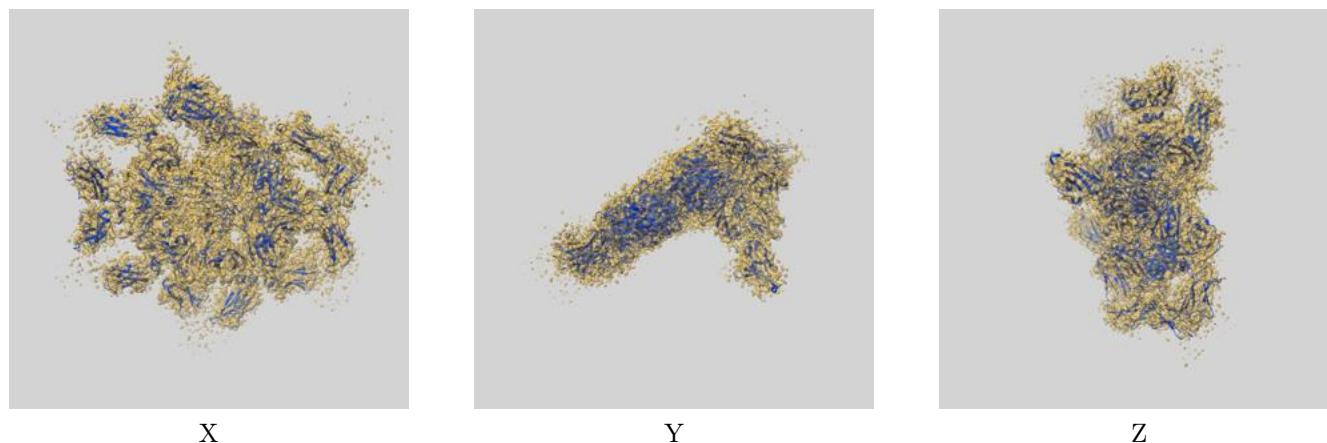
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	3.87	3.43
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

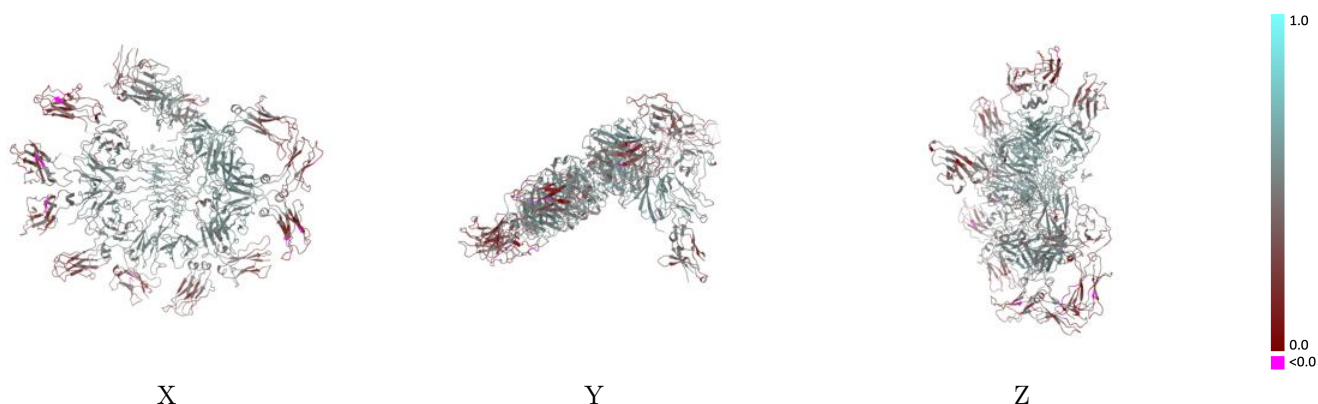
This section contains information regarding the fit between EMDB map EMD-0782 and PDB model 6KXS. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



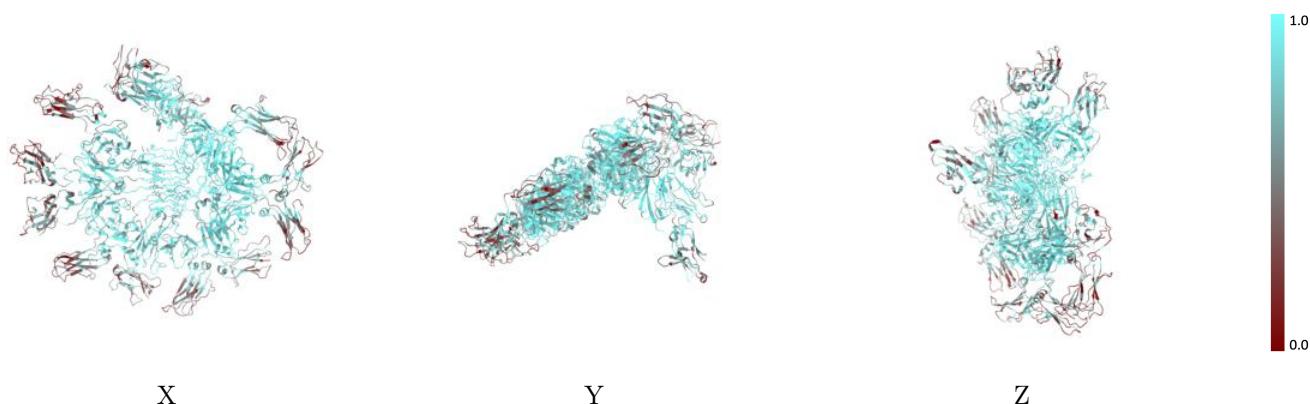
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



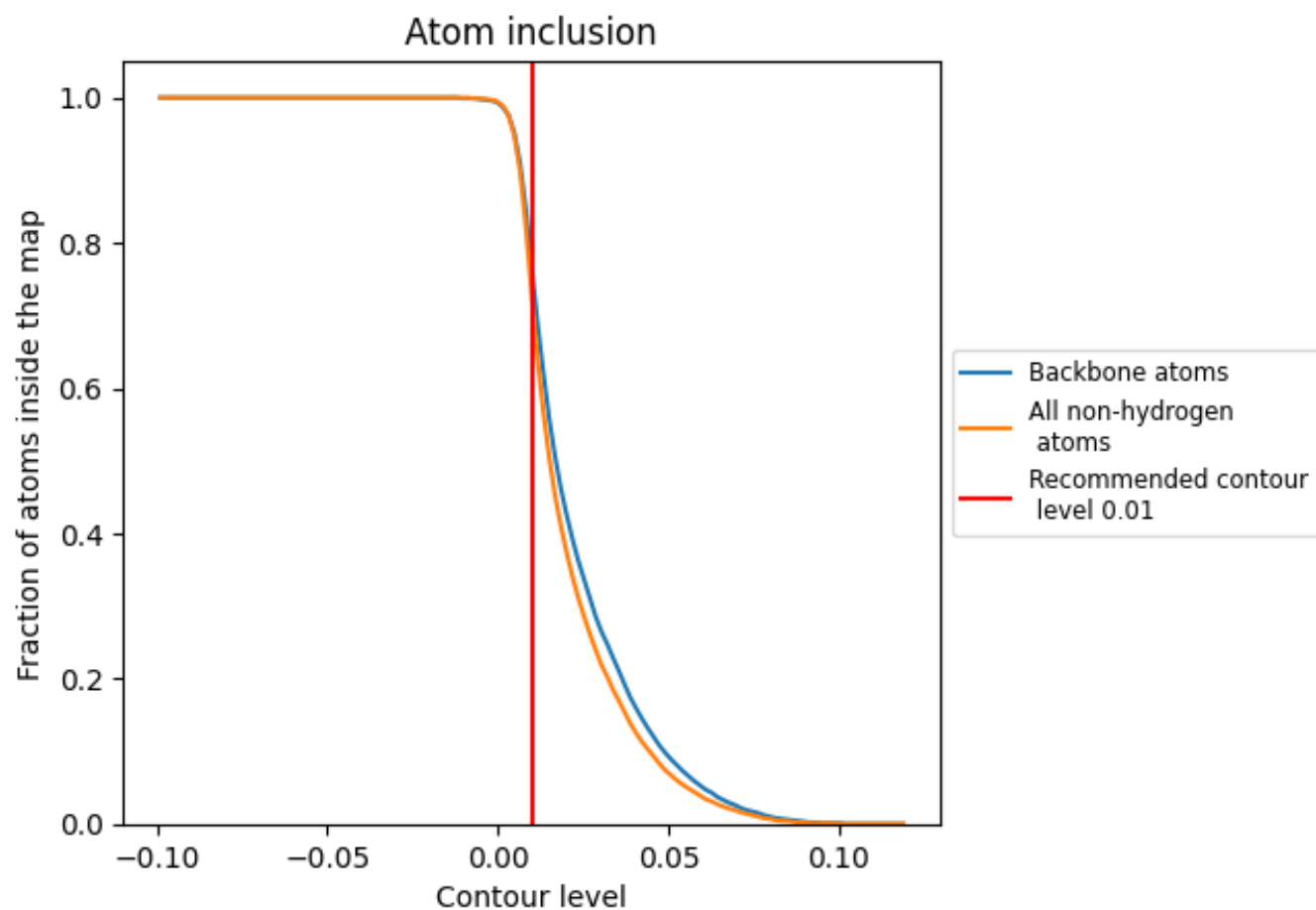
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.7230	0.4570
A	0.7800	0.4900
B	0.7510	0.4620
C	0.7120	0.4490
D	0.7380	0.4500
E	0.7280	0.4590
F	0.7170	0.4420
G	0.6970	0.4410
H	0.7040	0.4380
I	0.8210	0.4450
J	0.8920	0.5480
K	0.6610	0.4410
L	0.6280	0.4080
P	0.7360	0.4780

1.0

0.0

<0.0