



Full wwPDB EM Validation Report ⓘ

Sep 8, 2026 – 02:46 pm BST

PDB ID : 30XT / pdb_000030xt
EMDB ID : EMD-58134
Title : Structre of ANDV spike in complex with EC1 domain of human PCDH1
Authors : Battini, L.; Guardado-Calvo, P.
Deposited on : 2026-05-17
Resolution : 2.55 Å(reported)
Based on initial models : ., 9P3I

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.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
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) : 2.50

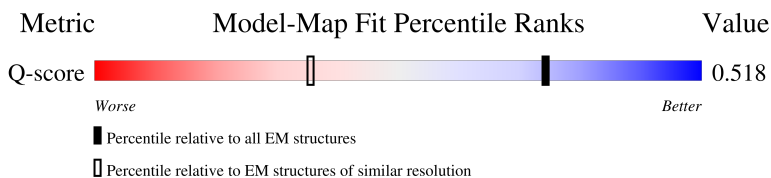
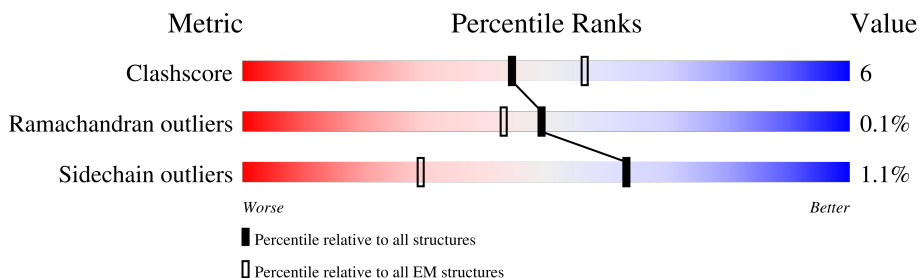
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.55 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	7475 (2.05 - 3.05)

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	517	 79% 10% 11%
1	C	517	 82% 7% 11%
1	E	517	 78% 10% 11%
1	G	517	 80% 8% 11%

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Mol	Chain	Length	Quality of chain
2	B	532	
2	D	532	
2	F	532	
2	H	532	
3	Y	486	
4	I	4	
4	J	4	
4	M	4	
4	N	4	
4	Q	4	
4	R	4	
4	U	4	
4	V	4	
5	K	2	
5	L	2	
5	O	2	
5	P	2	
5	S	2	
5	T	2	
5	W	2	
5	X	2	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28749 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Envelopment polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	460	Total	C	N	O	S	0	0
			3523	2227	583	683	30		
1	C	460	Total	C	N	O	S	0	0
			3523	2227	583	683	30		
1	E	460	Total	C	N	O	S	0	0
			3523	2227	583	683	30		
1	G	460	Total	C	N	O	S	0	0
			3523	2227	583	683	30		

There are 212 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	485	GLY	-	expression tag	UNP Q9E006
A	486	GLY	-	expression tag	UNP Q9E006
A	487	GLY	-	expression tag	UNP Q9E006
A	488	SER	-	expression tag	UNP Q9E006
A	489	GLY	-	expression tag	UNP Q9E006
A	490	MET	-	expression tag	UNP Q9E006
A	491	SER	-	expression tag	UNP Q9E006
A	492	PRO	-	expression tag	UNP Q9E006
A	493	TYR	-	expression tag	UNP Q9E006
A	494	LYS	-	expression tag	UNP Q9E006
A	495	LYS	-	expression tag	UNP Q9E006
A	496	ALA	-	expression tag	UNP Q9E006
A	497	ILE	-	expression tag	UNP Q9E006
A	498	GLU	-	expression tag	UNP Q9E006
A	499	ILE	-	expression tag	UNP Q9E006
A	500	THR	-	expression tag	UNP Q9E006
A	501	LYS	-	expression tag	UNP Q9E006
A	502	ARG	-	expression tag	UNP Q9E006
A	503	LEU	-	expression tag	UNP Q9E006
A	504	LEU	-	expression tag	UNP Q9E006
A	505	GLU	-	expression tag	UNP Q9E006
A	506	LEU	-	expression tag	UNP Q9E006

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Chain	Residue	Modelled	Actual	Comment	Reference
A	507	LEU	-	expression tag	UNP Q9E006
A	508	LEU	-	expression tag	UNP Q9E006
A	509	SER	-	expression tag	UNP Q9E006
A	510	ASN	-	expression tag	UNP Q9E006
A	511	PRO	-	expression tag	UNP Q9E006
A	512	GLU	-	expression tag	UNP Q9E006
A	513	LEU	-	expression tag	UNP Q9E006
A	514	ALA	-	expression tag	UNP Q9E006
A	515	LYS	-	expression tag	UNP Q9E006
A	516	LYS	-	expression tag	UNP Q9E006
A	517	ASN	-	expression tag	UNP Q9E006
A	518	LEU	-	expression tag	UNP Q9E006
A	519	GLY	-	expression tag	UNP Q9E006
A	520	GLY	-	expression tag	UNP Q9E006
A	521	ILE	-	expression tag	UNP Q9E006
A	522	ALA	-	expression tag	UNP Q9E006
A	523	THR	-	expression tag	UNP Q9E006
A	524	LEU	-	expression tag	UNP Q9E006
A	525	ILE	-	expression tag	UNP Q9E006
A	526	SER	-	expression tag	UNP Q9E006
A	527	LEU	-	expression tag	UNP Q9E006
A	528	LEU	-	expression tag	UNP Q9E006
A	529	ALA	-	expression tag	UNP Q9E006
A	530	LEU	-	expression tag	UNP Q9E006
A	531	ILE	-	expression tag	UNP Q9E006
A	532	SER	-	expression tag	UNP Q9E006
A	533	ALA	-	expression tag	UNP Q9E006
A	534	LEU	-	expression tag	UNP Q9E006
A	535	ASP	-	expression tag	UNP Q9E006
A	536	GLY	-	expression tag	UNP Q9E006
A	537	CYS	-	expression tag	UNP Q9E006
C	485	GLY	-	expression tag	UNP Q9E006
C	486	GLY	-	expression tag	UNP Q9E006
C	487	GLY	-	expression tag	UNP Q9E006
C	488	SER	-	expression tag	UNP Q9E006
C	489	GLY	-	expression tag	UNP Q9E006
C	490	MET	-	expression tag	UNP Q9E006
C	491	SER	-	expression tag	UNP Q9E006
C	492	PRO	-	expression tag	UNP Q9E006
C	493	TYR	-	expression tag	UNP Q9E006
C	494	LYS	-	expression tag	UNP Q9E006
C	495	LYS	-	expression tag	UNP Q9E006

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Chain	Residue	Modelled	Actual	Comment	Reference
C	496	ALA	-	expression tag	UNP Q9E006
C	497	ILE	-	expression tag	UNP Q9E006
C	498	GLU	-	expression tag	UNP Q9E006
C	499	ILE	-	expression tag	UNP Q9E006
C	500	THR	-	expression tag	UNP Q9E006
C	501	LYS	-	expression tag	UNP Q9E006
C	502	ARG	-	expression tag	UNP Q9E006
C	503	LEU	-	expression tag	UNP Q9E006
C	504	LEU	-	expression tag	UNP Q9E006
C	505	GLU	-	expression tag	UNP Q9E006
C	506	LEU	-	expression tag	UNP Q9E006
C	507	LEU	-	expression tag	UNP Q9E006
C	508	LEU	-	expression tag	UNP Q9E006
C	509	SER	-	expression tag	UNP Q9E006
C	510	ASN	-	expression tag	UNP Q9E006
C	511	PRO	-	expression tag	UNP Q9E006
C	512	GLU	-	expression tag	UNP Q9E006
C	513	LEU	-	expression tag	UNP Q9E006
C	514	ALA	-	expression tag	UNP Q9E006
C	515	LYS	-	expression tag	UNP Q9E006
C	516	LYS	-	expression tag	UNP Q9E006
C	517	ASN	-	expression tag	UNP Q9E006
C	518	LEU	-	expression tag	UNP Q9E006
C	519	GLY	-	expression tag	UNP Q9E006
C	520	GLY	-	expression tag	UNP Q9E006
C	521	ILE	-	expression tag	UNP Q9E006
C	522	ALA	-	expression tag	UNP Q9E006
C	523	THR	-	expression tag	UNP Q9E006
C	524	LEU	-	expression tag	UNP Q9E006
C	525	ILE	-	expression tag	UNP Q9E006
C	526	SER	-	expression tag	UNP Q9E006
C	527	LEU	-	expression tag	UNP Q9E006
C	528	LEU	-	expression tag	UNP Q9E006
C	529	ALA	-	expression tag	UNP Q9E006
C	530	LEU	-	expression tag	UNP Q9E006
C	531	ILE	-	expression tag	UNP Q9E006
C	532	SER	-	expression tag	UNP Q9E006
C	533	ALA	-	expression tag	UNP Q9E006
C	534	LEU	-	expression tag	UNP Q9E006
C	535	ASP	-	expression tag	UNP Q9E006
C	536	GLY	-	expression tag	UNP Q9E006
C	537	CYS	-	expression tag	UNP Q9E006

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Chain	Residue	Modelled	Actual	Comment	Reference
E	485	GLY	-	expression tag	UNP Q9E006
E	486	GLY	-	expression tag	UNP Q9E006
E	487	GLY	-	expression tag	UNP Q9E006
E	488	SER	-	expression tag	UNP Q9E006
E	489	GLY	-	expression tag	UNP Q9E006
E	490	MET	-	expression tag	UNP Q9E006
E	491	SER	-	expression tag	UNP Q9E006
E	492	PRO	-	expression tag	UNP Q9E006
E	493	TYR	-	expression tag	UNP Q9E006
E	494	LYS	-	expression tag	UNP Q9E006
E	495	LYS	-	expression tag	UNP Q9E006
E	496	ALA	-	expression tag	UNP Q9E006
E	497	ILE	-	expression tag	UNP Q9E006
E	498	GLU	-	expression tag	UNP Q9E006
E	499	ILE	-	expression tag	UNP Q9E006
E	500	THR	-	expression tag	UNP Q9E006
E	501	LYS	-	expression tag	UNP Q9E006
E	502	ARG	-	expression tag	UNP Q9E006
E	503	LEU	-	expression tag	UNP Q9E006
E	504	LEU	-	expression tag	UNP Q9E006
E	505	GLU	-	expression tag	UNP Q9E006
E	506	LEU	-	expression tag	UNP Q9E006
E	507	LEU	-	expression tag	UNP Q9E006
E	508	LEU	-	expression tag	UNP Q9E006
E	509	SER	-	expression tag	UNP Q9E006
E	510	ASN	-	expression tag	UNP Q9E006
E	511	PRO	-	expression tag	UNP Q9E006
E	512	GLU	-	expression tag	UNP Q9E006
E	513	LEU	-	expression tag	UNP Q9E006
E	514	ALA	-	expression tag	UNP Q9E006
E	515	LYS	-	expression tag	UNP Q9E006
E	516	LYS	-	expression tag	UNP Q9E006
E	517	ASN	-	expression tag	UNP Q9E006
E	518	LEU	-	expression tag	UNP Q9E006
E	519	GLY	-	expression tag	UNP Q9E006
E	520	GLY	-	expression tag	UNP Q9E006
E	521	ILE	-	expression tag	UNP Q9E006
E	522	ALA	-	expression tag	UNP Q9E006
E	523	THR	-	expression tag	UNP Q9E006
E	524	LEU	-	expression tag	UNP Q9E006
E	525	ILE	-	expression tag	UNP Q9E006
E	526	SER	-	expression tag	UNP Q9E006

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Chain	Residue	Modelled	Actual	Comment	Reference
E	527	LEU	-	expression tag	UNP Q9E006
E	528	LEU	-	expression tag	UNP Q9E006
E	529	ALA	-	expression tag	UNP Q9E006
E	530	LEU	-	expression tag	UNP Q9E006
E	531	ILE	-	expression tag	UNP Q9E006
E	532	SER	-	expression tag	UNP Q9E006
E	533	ALA	-	expression tag	UNP Q9E006
E	534	LEU	-	expression tag	UNP Q9E006
E	535	ASP	-	expression tag	UNP Q9E006
E	536	GLY	-	expression tag	UNP Q9E006
E	537	CYS	-	expression tag	UNP Q9E006
G	485	GLY	-	expression tag	UNP Q9E006
G	486	GLY	-	expression tag	UNP Q9E006
G	487	GLY	-	expression tag	UNP Q9E006
G	488	SER	-	expression tag	UNP Q9E006
G	489	GLY	-	expression tag	UNP Q9E006
G	490	MET	-	expression tag	UNP Q9E006
G	491	SER	-	expression tag	UNP Q9E006
G	492	PRO	-	expression tag	UNP Q9E006
G	493	TYR	-	expression tag	UNP Q9E006
G	494	LYS	-	expression tag	UNP Q9E006
G	495	LYS	-	expression tag	UNP Q9E006
G	496	ALA	-	expression tag	UNP Q9E006
G	497	ILE	-	expression tag	UNP Q9E006
G	498	GLU	-	expression tag	UNP Q9E006
G	499	ILE	-	expression tag	UNP Q9E006
G	500	THR	-	expression tag	UNP Q9E006
G	501	LYS	-	expression tag	UNP Q9E006
G	502	ARG	-	expression tag	UNP Q9E006
G	503	LEU	-	expression tag	UNP Q9E006
G	504	LEU	-	expression tag	UNP Q9E006
G	505	GLU	-	expression tag	UNP Q9E006
G	506	LEU	-	expression tag	UNP Q9E006
G	507	LEU	-	expression tag	UNP Q9E006
G	508	LEU	-	expression tag	UNP Q9E006
G	509	SER	-	expression tag	UNP Q9E006
G	510	ASN	-	expression tag	UNP Q9E006
G	511	PRO	-	expression tag	UNP Q9E006
G	512	GLU	-	expression tag	UNP Q9E006
G	513	LEU	-	expression tag	UNP Q9E006
G	514	ALA	-	expression tag	UNP Q9E006
G	515	LYS	-	expression tag	UNP Q9E006

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Chain	Residue	Modelled	Actual	Comment	Reference
G	516	LYS	-	expression tag	UNP Q9E006
G	517	ASN	-	expression tag	UNP Q9E006
G	518	LEU	-	expression tag	UNP Q9E006
G	519	GLY	-	expression tag	UNP Q9E006
G	520	GLY	-	expression tag	UNP Q9E006
G	521	ILE	-	expression tag	UNP Q9E006
G	522	ALA	-	expression tag	UNP Q9E006
G	523	THR	-	expression tag	UNP Q9E006
G	524	LEU	-	expression tag	UNP Q9E006
G	525	ILE	-	expression tag	UNP Q9E006
G	526	SER	-	expression tag	UNP Q9E006
G	527	LEU	-	expression tag	UNP Q9E006
G	528	LEU	-	expression tag	UNP Q9E006
G	529	ALA	-	expression tag	UNP Q9E006
G	530	LEU	-	expression tag	UNP Q9E006
G	531	ILE	-	expression tag	UNP Q9E006
G	532	SER	-	expression tag	UNP Q9E006
G	533	ALA	-	expression tag	UNP Q9E006
G	534	LEU	-	expression tag	UNP Q9E006
G	535	ASP	-	expression tag	UNP Q9E006
G	536	GLY	-	expression tag	UNP Q9E006
G	537	CYS	-	expression tag	UNP Q9E006

- Molecule 2 is a protein called Envelopment polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	433	Total	C	N	O	S	0	0
			3308	2073	555	646	34		
2	D	433	Total	C	N	O	S	0	0
			3308	2073	555	646	34		
2	F	433	Total	C	N	O	S	0	0
			3308	2073	555	646	34		
2	H	433	Total	C	N	O	S	0	0
			3308	2073	555	646	34		

There are 320 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1089	ALA	PHE	conflict	UNP Q9E006
B	1093	ALA	PHE	conflict	UNP Q9E006
B	1100	ALA	LEU	conflict	UNP Q9E006
B	1104	ALA	LEU	conflict	UNP Q9E006

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1108	GLY	-	expression tag	UNP Q9E006
B	1109	GLY	-	expression tag	UNP Q9E006
B	1110	GLY	-	expression tag	UNP Q9E006
B	1111	SER	-	expression tag	UNP Q9E006
B	1112	CYS	-	expression tag	UNP Q9E006
B	1113	THR	-	expression tag	UNP Q9E006
B	1114	LEU	-	expression tag	UNP Q9E006
B	1115	ASP	-	expression tag	UNP Q9E006
B	1116	GLU	-	expression tag	UNP Q9E006
B	1117	LYS	-	expression tag	UNP Q9E006
B	1118	ASP	-	expression tag	UNP Q9E006
B	1119	ILE	-	expression tag	UNP Q9E006
B	1120	GLU	-	expression tag	UNP Q9E006
B	1121	PRO	-	expression tag	UNP Q9E006
B	1122	TYR	-	expression tag	UNP Q9E006
B	1123	ILE	-	expression tag	UNP Q9E006
B	1124	LYS	-	expression tag	UNP Q9E006
B	1125	LYS	-	expression tag	UNP Q9E006
B	1126	LEU	-	expression tag	UNP Q9E006
B	1127	GLU	-	expression tag	UNP Q9E006
B	1128	GLU	-	expression tag	UNP Q9E006
B	1129	SER	-	expression tag	UNP Q9E006
B	1130	LEU	-	expression tag	UNP Q9E006
B	1131	GLY	-	expression tag	UNP Q9E006
B	1132	SER	-	expression tag	UNP Q9E006
B	1133	GLY	-	expression tag	UNP Q9E006
B	1134	GLY	-	expression tag	UNP Q9E006
B	1135	GLY	-	expression tag	UNP Q9E006
B	1136	SER	-	expression tag	UNP Q9E006
B	1137	LEU	-	expression tag	UNP Q9E006
B	1138	VAL	-	expression tag	UNP Q9E006
B	1139	PRO	-	expression tag	UNP Q9E006
B	1140	ARG	-	expression tag	UNP Q9E006
B	1141	GLY	-	expression tag	UNP Q9E006
B	1142	SER	-	expression tag	UNP Q9E006
B	1143	GLY	-	expression tag	UNP Q9E006
B	1144	SER	-	expression tag	UNP Q9E006
B	1145	GLY	-	expression tag	UNP Q9E006
B	1146	SER	-	expression tag	UNP Q9E006
B	1147	ALA	-	expression tag	UNP Q9E006
B	1148	TRP	-	expression tag	UNP Q9E006
B	1149	SER	-	expression tag	UNP Q9E006

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1150	HIS	-	expression tag	UNP Q9E006
B	1151	PRO	-	expression tag	UNP Q9E006
B	1152	GLN	-	expression tag	UNP Q9E006
B	1153	PHE	-	expression tag	UNP Q9E006
B	1154	GLU	-	expression tag	UNP Q9E006
B	1155	LYS	-	expression tag	UNP Q9E006
B	1156	GLY	-	expression tag	UNP Q9E006
B	1157	SER	-	expression tag	UNP Q9E006
B	1158	GLY	-	expression tag	UNP Q9E006
B	1159	SER	-	expression tag	UNP Q9E006
B	1160	ALA	-	expression tag	UNP Q9E006
B	1161	TRP	-	expression tag	UNP Q9E006
B	1162	SER	-	expression tag	UNP Q9E006
B	1163	HIS	-	expression tag	UNP Q9E006
B	1164	PRO	-	expression tag	UNP Q9E006
B	1165	GLN	-	expression tag	UNP Q9E006
B	1166	PHE	-	expression tag	UNP Q9E006
B	1167	GLU	-	expression tag	UNP Q9E006
B	1168	LYS	-	expression tag	UNP Q9E006
B	1169	GLY	-	expression tag	UNP Q9E006
B	1170	LEU	-	expression tag	UNP Q9E006
B	1171	ASN	-	expression tag	UNP Q9E006
B	1172	ASP	-	expression tag	UNP Q9E006
B	1173	ILE	-	expression tag	UNP Q9E006
B	1174	PHE	-	expression tag	UNP Q9E006
B	1175	GLU	-	expression tag	UNP Q9E006
B	1176	ALA	-	expression tag	UNP Q9E006
B	1177	GLN	-	expression tag	UNP Q9E006
B	1178	LYS	-	expression tag	UNP Q9E006
B	1179	ILE	-	expression tag	UNP Q9E006
B	1180	GLU	-	expression tag	UNP Q9E006
B	1181	TRP	-	expression tag	UNP Q9E006
B	1182	HIS	-	expression tag	UNP Q9E006
B	1183	GLU	-	expression tag	UNP Q9E006
D	1089	ALA	PHE	conflict	UNP Q9E006
D	1093	ALA	PHE	conflict	UNP Q9E006
D	1100	ALA	LEU	conflict	UNP Q9E006
D	1104	ALA	LEU	conflict	UNP Q9E006
D	1108	GLY	-	expression tag	UNP Q9E006
D	1109	GLY	-	expression tag	UNP Q9E006
D	1110	GLY	-	expression tag	UNP Q9E006
D	1111	SER	-	expression tag	UNP Q9E006

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1112	CYS	-	expression tag	UNP Q9E006
D	1113	THR	-	expression tag	UNP Q9E006
D	1114	LEU	-	expression tag	UNP Q9E006
D	1115	ASP	-	expression tag	UNP Q9E006
D	1116	GLU	-	expression tag	UNP Q9E006
D	1117	LYS	-	expression tag	UNP Q9E006
D	1118	ASP	-	expression tag	UNP Q9E006
D	1119	ILE	-	expression tag	UNP Q9E006
D	1120	GLU	-	expression tag	UNP Q9E006
D	1121	PRO	-	expression tag	UNP Q9E006
D	1122	TYR	-	expression tag	UNP Q9E006
D	1123	ILE	-	expression tag	UNP Q9E006
D	1124	LYS	-	expression tag	UNP Q9E006
D	1125	LYS	-	expression tag	UNP Q9E006
D	1126	LEU	-	expression tag	UNP Q9E006
D	1127	GLU	-	expression tag	UNP Q9E006
D	1128	GLU	-	expression tag	UNP Q9E006
D	1129	SER	-	expression tag	UNP Q9E006
D	1130	LEU	-	expression tag	UNP Q9E006
D	1131	GLY	-	expression tag	UNP Q9E006
D	1132	SER	-	expression tag	UNP Q9E006
D	1133	GLY	-	expression tag	UNP Q9E006
D	1134	GLY	-	expression tag	UNP Q9E006
D	1135	GLY	-	expression tag	UNP Q9E006
D	1136	SER	-	expression tag	UNP Q9E006
D	1137	LEU	-	expression tag	UNP Q9E006
D	1138	VAL	-	expression tag	UNP Q9E006
D	1139	PRO	-	expression tag	UNP Q9E006
D	1140	ARG	-	expression tag	UNP Q9E006
D	1141	GLY	-	expression tag	UNP Q9E006
D	1142	SER	-	expression tag	UNP Q9E006
D	1143	GLY	-	expression tag	UNP Q9E006
D	1144	SER	-	expression tag	UNP Q9E006
D	1145	GLY	-	expression tag	UNP Q9E006
D	1146	SER	-	expression tag	UNP Q9E006
D	1147	ALA	-	expression tag	UNP Q9E006
D	1148	TRP	-	expression tag	UNP Q9E006
D	1149	SER	-	expression tag	UNP Q9E006
D	1150	HIS	-	expression tag	UNP Q9E006
D	1151	PRO	-	expression tag	UNP Q9E006
D	1152	GLN	-	expression tag	UNP Q9E006
D	1153	PHE	-	expression tag	UNP Q9E006

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1154	GLU	-	expression tag	UNP Q9E006
D	1155	LYS	-	expression tag	UNP Q9E006
D	1156	GLY	-	expression tag	UNP Q9E006
D	1157	SER	-	expression tag	UNP Q9E006
D	1158	GLY	-	expression tag	UNP Q9E006
D	1159	SER	-	expression tag	UNP Q9E006
D	1160	ALA	-	expression tag	UNP Q9E006
D	1161	TRP	-	expression tag	UNP Q9E006
D	1162	SER	-	expression tag	UNP Q9E006
D	1163	HIS	-	expression tag	UNP Q9E006
D	1164	PRO	-	expression tag	UNP Q9E006
D	1165	GLN	-	expression tag	UNP Q9E006
D	1166	PHE	-	expression tag	UNP Q9E006
D	1167	GLU	-	expression tag	UNP Q9E006
D	1168	LYS	-	expression tag	UNP Q9E006
D	1169	GLY	-	expression tag	UNP Q9E006
D	1170	LEU	-	expression tag	UNP Q9E006
D	1171	ASN	-	expression tag	UNP Q9E006
D	1172	ASP	-	expression tag	UNP Q9E006
D	1173	ILE	-	expression tag	UNP Q9E006
D	1174	PHE	-	expression tag	UNP Q9E006
D	1175	GLU	-	expression tag	UNP Q9E006
D	1176	ALA	-	expression tag	UNP Q9E006
D	1177	GLN	-	expression tag	UNP Q9E006
D	1178	LYS	-	expression tag	UNP Q9E006
D	1179	ILE	-	expression tag	UNP Q9E006
D	1180	GLU	-	expression tag	UNP Q9E006
D	1181	TRP	-	expression tag	UNP Q9E006
D	1182	HIS	-	expression tag	UNP Q9E006
D	1183	GLU	-	expression tag	UNP Q9E006
F	1089	ALA	PHE	conflict	UNP Q9E006
F	1093	ALA	PHE	conflict	UNP Q9E006
F	1100	ALA	LEU	conflict	UNP Q9E006
F	1104	ALA	LEU	conflict	UNP Q9E006
F	1108	GLY	-	expression tag	UNP Q9E006
F	1109	GLY	-	expression tag	UNP Q9E006
F	1110	GLY	-	expression tag	UNP Q9E006
F	1111	SER	-	expression tag	UNP Q9E006
F	1112	CYS	-	expression tag	UNP Q9E006
F	1113	THR	-	expression tag	UNP Q9E006
F	1114	LEU	-	expression tag	UNP Q9E006
F	1115	ASP	-	expression tag	UNP Q9E006

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1116	GLU	-	expression tag	UNP Q9E006
F	1117	LYS	-	expression tag	UNP Q9E006
F	1118	ASP	-	expression tag	UNP Q9E006
F	1119	ILE	-	expression tag	UNP Q9E006
F	1120	GLU	-	expression tag	UNP Q9E006
F	1121	PRO	-	expression tag	UNP Q9E006
F	1122	TYR	-	expression tag	UNP Q9E006
F	1123	ILE	-	expression tag	UNP Q9E006
F	1124	LYS	-	expression tag	UNP Q9E006
F	1125	LYS	-	expression tag	UNP Q9E006
F	1126	LEU	-	expression tag	UNP Q9E006
F	1127	GLU	-	expression tag	UNP Q9E006
F	1128	GLU	-	expression tag	UNP Q9E006
F	1129	SER	-	expression tag	UNP Q9E006
F	1130	LEU	-	expression tag	UNP Q9E006
F	1131	GLY	-	expression tag	UNP Q9E006
F	1132	SER	-	expression tag	UNP Q9E006
F	1133	GLY	-	expression tag	UNP Q9E006
F	1134	GLY	-	expression tag	UNP Q9E006
F	1135	GLY	-	expression tag	UNP Q9E006
F	1136	SER	-	expression tag	UNP Q9E006
F	1137	LEU	-	expression tag	UNP Q9E006
F	1138	VAL	-	expression tag	UNP Q9E006
F	1139	PRO	-	expression tag	UNP Q9E006
F	1140	ARG	-	expression tag	UNP Q9E006
F	1141	GLY	-	expression tag	UNP Q9E006
F	1142	SER	-	expression tag	UNP Q9E006
F	1143	GLY	-	expression tag	UNP Q9E006
F	1144	SER	-	expression tag	UNP Q9E006
F	1145	GLY	-	expression tag	UNP Q9E006
F	1146	SER	-	expression tag	UNP Q9E006
F	1147	ALA	-	expression tag	UNP Q9E006
F	1148	TRP	-	expression tag	UNP Q9E006
F	1149	SER	-	expression tag	UNP Q9E006
F	1150	HIS	-	expression tag	UNP Q9E006
F	1151	PRO	-	expression tag	UNP Q9E006
F	1152	GLN	-	expression tag	UNP Q9E006
F	1153	PHE	-	expression tag	UNP Q9E006
F	1154	GLU	-	expression tag	UNP Q9E006
F	1155	LYS	-	expression tag	UNP Q9E006
F	1156	GLY	-	expression tag	UNP Q9E006
F	1157	SER	-	expression tag	UNP Q9E006

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1158	GLY	-	expression tag	UNP Q9E006
F	1159	SER	-	expression tag	UNP Q9E006
F	1160	ALA	-	expression tag	UNP Q9E006
F	1161	TRP	-	expression tag	UNP Q9E006
F	1162	SER	-	expression tag	UNP Q9E006
F	1163	HIS	-	expression tag	UNP Q9E006
F	1164	PRO	-	expression tag	UNP Q9E006
F	1165	GLN	-	expression tag	UNP Q9E006
F	1166	PHE	-	expression tag	UNP Q9E006
F	1167	GLU	-	expression tag	UNP Q9E006
F	1168	LYS	-	expression tag	UNP Q9E006
F	1169	GLY	-	expression tag	UNP Q9E006
F	1170	LEU	-	expression tag	UNP Q9E006
F	1171	ASN	-	expression tag	UNP Q9E006
F	1172	ASP	-	expression tag	UNP Q9E006
F	1173	ILE	-	expression tag	UNP Q9E006
F	1174	PHE	-	expression tag	UNP Q9E006
F	1175	GLU	-	expression tag	UNP Q9E006
F	1176	ALA	-	expression tag	UNP Q9E006
F	1177	GLN	-	expression tag	UNP Q9E006
F	1178	LYS	-	expression tag	UNP Q9E006
F	1179	ILE	-	expression tag	UNP Q9E006
F	1180	GLU	-	expression tag	UNP Q9E006
F	1181	TRP	-	expression tag	UNP Q9E006
F	1182	HIS	-	expression tag	UNP Q9E006
F	1183	GLU	-	expression tag	UNP Q9E006
H	1089	ALA	PHE	conflict	UNP Q9E006
H	1093	ALA	PHE	conflict	UNP Q9E006
H	1100	ALA	LEU	conflict	UNP Q9E006
H	1104	ALA	LEU	conflict	UNP Q9E006
H	1108	GLY	-	expression tag	UNP Q9E006
H	1109	GLY	-	expression tag	UNP Q9E006
H	1110	GLY	-	expression tag	UNP Q9E006
H	1111	SER	-	expression tag	UNP Q9E006
H	1112	CYS	-	expression tag	UNP Q9E006
H	1113	THR	-	expression tag	UNP Q9E006
H	1114	LEU	-	expression tag	UNP Q9E006
H	1115	ASP	-	expression tag	UNP Q9E006
H	1116	GLU	-	expression tag	UNP Q9E006
H	1117	LYS	-	expression tag	UNP Q9E006
H	1118	ASP	-	expression tag	UNP Q9E006
H	1119	ILE	-	expression tag	UNP Q9E006

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Chain	Residue	Modelled	Actual	Comment	Reference
H	1120	GLU	-	expression tag	UNP Q9E006
H	1121	PRO	-	expression tag	UNP Q9E006
H	1122	TYR	-	expression tag	UNP Q9E006
H	1123	ILE	-	expression tag	UNP Q9E006
H	1124	LYS	-	expression tag	UNP Q9E006
H	1125	LYS	-	expression tag	UNP Q9E006
H	1126	LEU	-	expression tag	UNP Q9E006
H	1127	GLU	-	expression tag	UNP Q9E006
H	1128	GLU	-	expression tag	UNP Q9E006
H	1129	SER	-	expression tag	UNP Q9E006
H	1130	LEU	-	expression tag	UNP Q9E006
H	1131	GLY	-	expression tag	UNP Q9E006
H	1132	SER	-	expression tag	UNP Q9E006
H	1133	GLY	-	expression tag	UNP Q9E006
H	1134	GLY	-	expression tag	UNP Q9E006
H	1135	GLY	-	expression tag	UNP Q9E006
H	1136	SER	-	expression tag	UNP Q9E006
H	1137	LEU	-	expression tag	UNP Q9E006
H	1138	VAL	-	expression tag	UNP Q9E006
H	1139	PRO	-	expression tag	UNP Q9E006
H	1140	ARG	-	expression tag	UNP Q9E006
H	1141	GLY	-	expression tag	UNP Q9E006
H	1142	SER	-	expression tag	UNP Q9E006
H	1143	GLY	-	expression tag	UNP Q9E006
H	1144	SER	-	expression tag	UNP Q9E006
H	1145	GLY	-	expression tag	UNP Q9E006
H	1146	SER	-	expression tag	UNP Q9E006
H	1147	ALA	-	expression tag	UNP Q9E006
H	1148	TRP	-	expression tag	UNP Q9E006
H	1149	SER	-	expression tag	UNP Q9E006
H	1150	HIS	-	expression tag	UNP Q9E006
H	1151	PRO	-	expression tag	UNP Q9E006
H	1152	GLN	-	expression tag	UNP Q9E006
H	1153	PHE	-	expression tag	UNP Q9E006
H	1154	GLU	-	expression tag	UNP Q9E006
H	1155	LYS	-	expression tag	UNP Q9E006
H	1156	GLY	-	expression tag	UNP Q9E006
H	1157	SER	-	expression tag	UNP Q9E006
H	1158	GLY	-	expression tag	UNP Q9E006
H	1159	SER	-	expression tag	UNP Q9E006
H	1160	ALA	-	expression tag	UNP Q9E006
H	1161	TRP	-	expression tag	UNP Q9E006

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Chain	Residue	Modelled	Actual	Comment	Reference
H	1162	SER	-	expression tag	UNP Q9E006
H	1163	HIS	-	expression tag	UNP Q9E006
H	1164	PRO	-	expression tag	UNP Q9E006
H	1165	GLN	-	expression tag	UNP Q9E006
H	1166	PHE	-	expression tag	UNP Q9E006
H	1167	GLU	-	expression tag	UNP Q9E006
H	1168	LYS	-	expression tag	UNP Q9E006
H	1169	GLY	-	expression tag	UNP Q9E006
H	1170	LEU	-	expression tag	UNP Q9E006
H	1171	ASN	-	expression tag	UNP Q9E006
H	1172	ASP	-	expression tag	UNP Q9E006
H	1173	ILE	-	expression tag	UNP Q9E006
H	1174	PHE	-	expression tag	UNP Q9E006
H	1175	GLU	-	expression tag	UNP Q9E006
H	1176	ALA	-	expression tag	UNP Q9E006
H	1177	GLN	-	expression tag	UNP Q9E006
H	1178	LYS	-	expression tag	UNP Q9E006
H	1179	ILE	-	expression tag	UNP Q9E006
H	1180	GLU	-	expression tag	UNP Q9E006
H	1181	TRP	-	expression tag	UNP Q9E006
H	1182	HIS	-	expression tag	UNP Q9E006
H	1183	GLU	-	expression tag	UNP Q9E006

- Molecule 3 is a protein called Protocadherin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Y	103	Total	C	N	O	S	0	0
			801	505	132	162	2		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	56	ARG	-	expression tag	UNP Q08174
Y	57	SER	-	expression tag	UNP Q08174
Y	504	GLY	-	expression tag	UNP Q08174
Y	505	PRO	-	expression tag	UNP Q08174
Y	506	GLY	-	expression tag	UNP Q08174
Y	507	GLY	-	expression tag	UNP Q08174
Y	508	GLY	-	expression tag	UNP Q08174
Y	509	SER	-	expression tag	UNP Q08174
Y	510	HIS	-	expression tag	UNP Q08174
Y	511	HIS	-	expression tag	UNP Q08174

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	512	HIS	-	expression tag	UNP Q08174
Y	513	HIS	-	expression tag	UNP Q08174
Y	514	HIS	-	expression tag	UNP Q08174
Y	515	HIS	-	expression tag	UNP Q08174
Y	516	HIS	-	expression tag	UNP Q08174
Y	517	HIS	-	expression tag	UNP Q08174
Y	518	GLY	-	expression tag	UNP Q08174
Y	519	GLY	-	expression tag	UNP Q08174
Y	520	GLY	-	expression tag	UNP Q08174
Y	521	SER	-	expression tag	UNP Q08174
Y	522	GLY	-	expression tag	UNP Q08174
Y	523	GLY	-	expression tag	UNP Q08174
Y	524	SER	-	expression tag	UNP Q08174
Y	525	LEU	-	expression tag	UNP Q08174
Y	526	VAL	-	expression tag	UNP Q08174
Y	527	PRO	-	expression tag	UNP Q08174
Y	528	ARG	-	expression tag	UNP Q08174
Y	529	GLY	-	expression tag	UNP Q08174
Y	530	SER	-	expression tag	UNP Q08174
Y	531	GLY	-	expression tag	UNP Q08174
Y	532	GLY	-	expression tag	UNP Q08174
Y	533	THR	-	expression tag	UNP Q08174
Y	534	TRP	-	expression tag	UNP Q08174
Y	535	SER	-	expression tag	UNP Q08174
Y	536	HIS	-	expression tag	UNP Q08174
Y	537	PRO	-	expression tag	UNP Q08174
Y	538	GLN	-	expression tag	UNP Q08174
Y	539	PHE	-	expression tag	UNP Q08174
Y	540	GLU	-	expression tag	UNP Q08174
Y	541	LYS	-	expression tag	UNP Q08174

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	I	4	Total	C	N	O	0	0
			50	28	2	20		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	J	4	Total	C	N	O	0	0
			50	28	2	20		
4	M	4	Total	C	N	O	0	0
			50	28	2	20		
4	N	4	Total	C	N	O	0	0
			50	28	2	20		
4	Q	4	Total	C	N	O	0	0
			50	28	2	20		
4	R	4	Total	C	N	O	0	0
			50	28	2	20		
4	U	4	Total	C	N	O	0	0
			50	28	2	20		
4	V	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



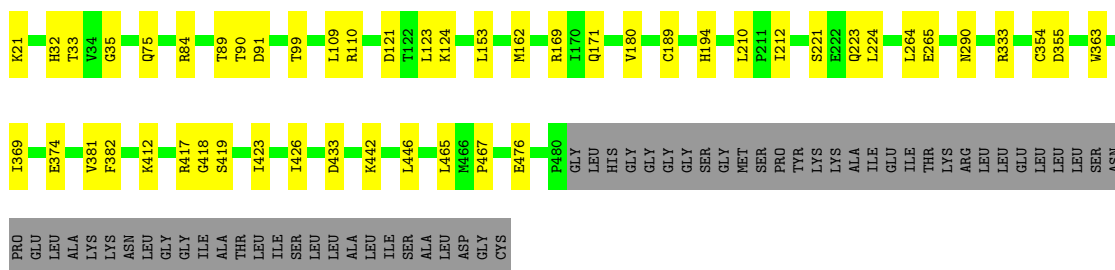
Mol	Chain	Residues	Atoms				AltConf	Trace
5	K	2	Total	C	N	O	0	0
			28	16	2	10		
5	L	2	Total	C	N	O	0	0
			28	16	2	10		
5	O	2	Total	C	N	O	0	0
			28	16	2	10		
5	P	2	Total	C	N	O	0	0
			28	16	2	10		
5	S	2	Total	C	N	O	0	0
			28	16	2	10		
5	T	2	Total	C	N	O	0	0
			28	16	2	10		
5	W	2	Total	C	N	O	0	0
			28	16	2	10		
5	X	2	Total	C	N	O	0	0
			28	16	2	10		

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.

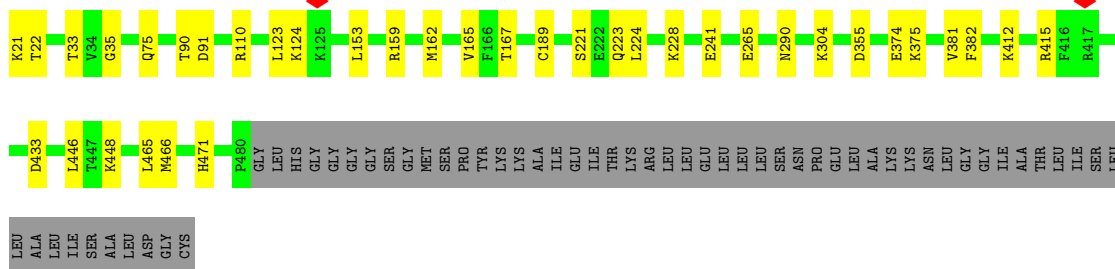
- Molecule 1: Envelopment polyprotein

Chain A: 



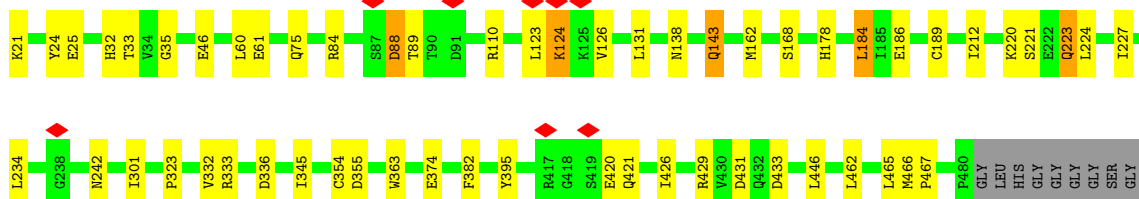
- Molecule 1: Envelopment polyprotein

Chain C: 

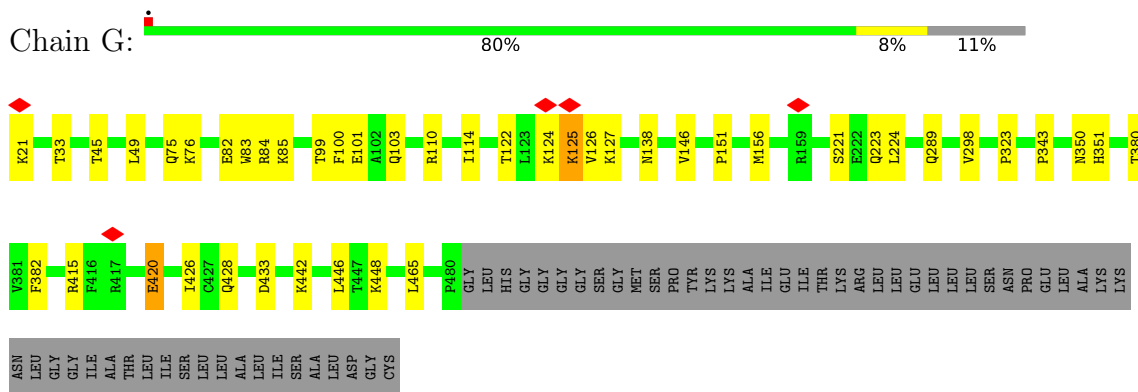


- Molecule 1: Envelopment polyprotein

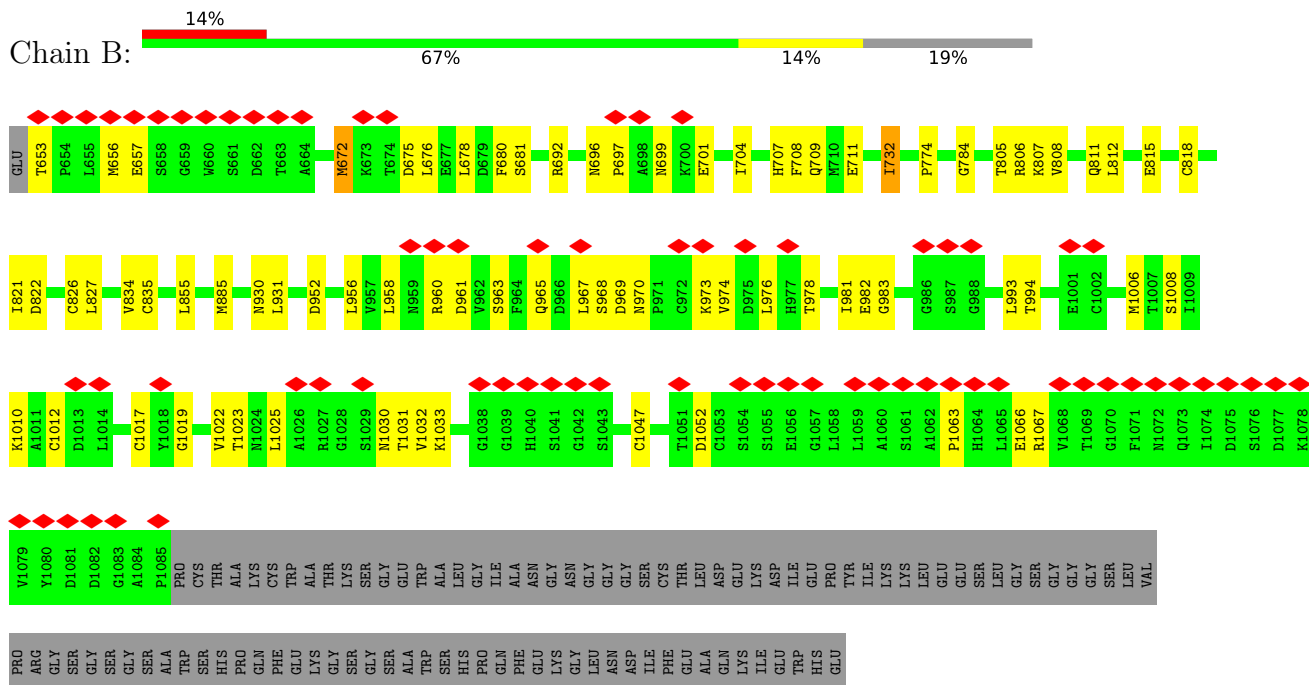
Chain E: 



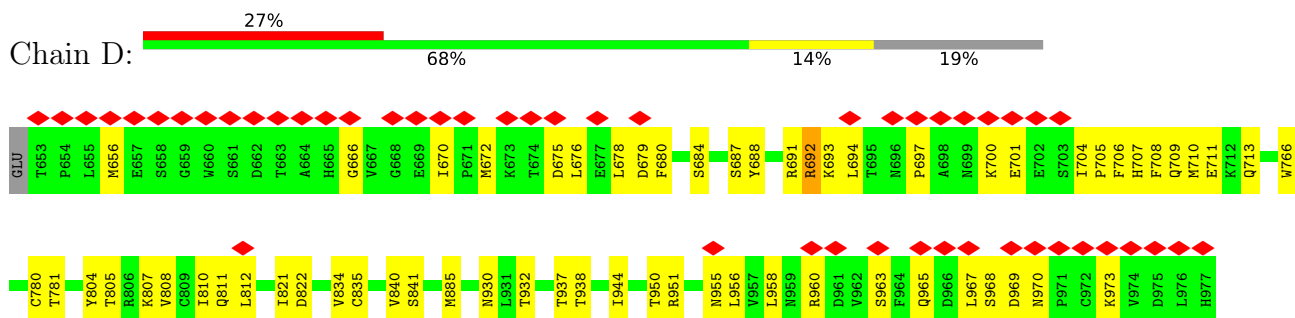
- Molecule 1: Envelopment polypeptide



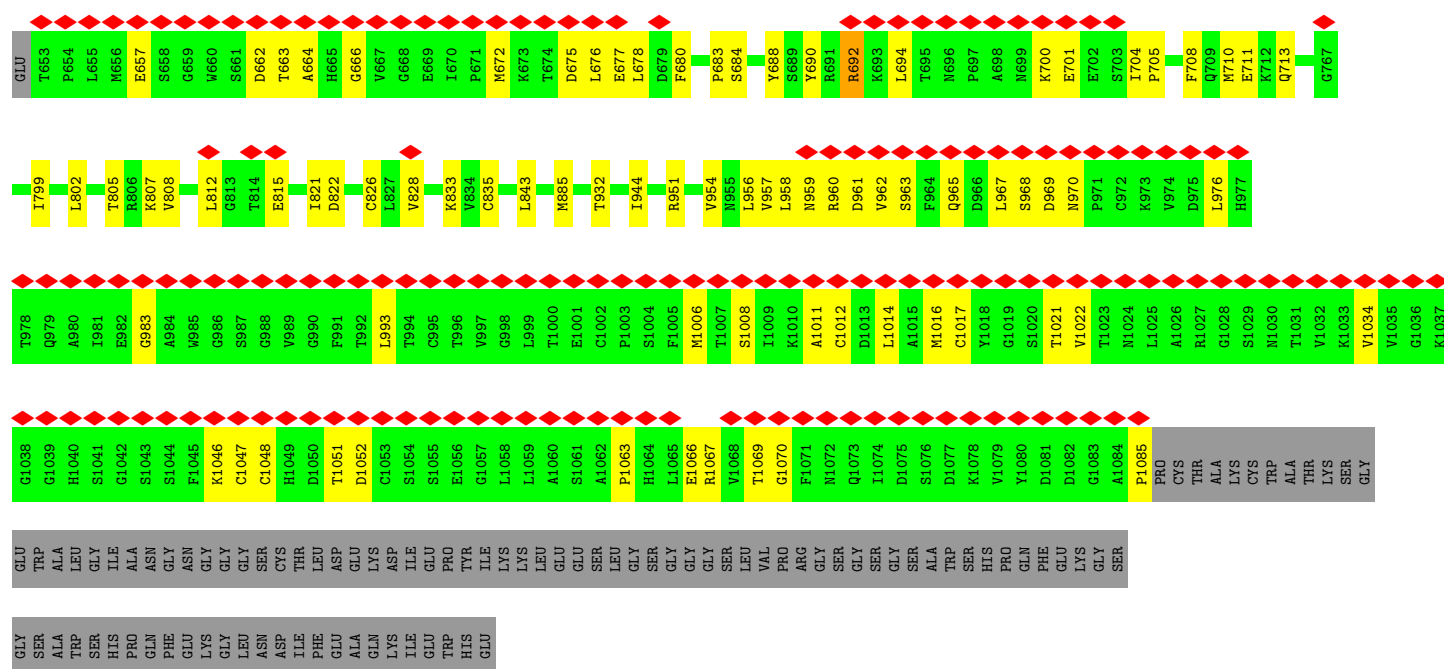
- Molecule 2: Envelopment polyprotein



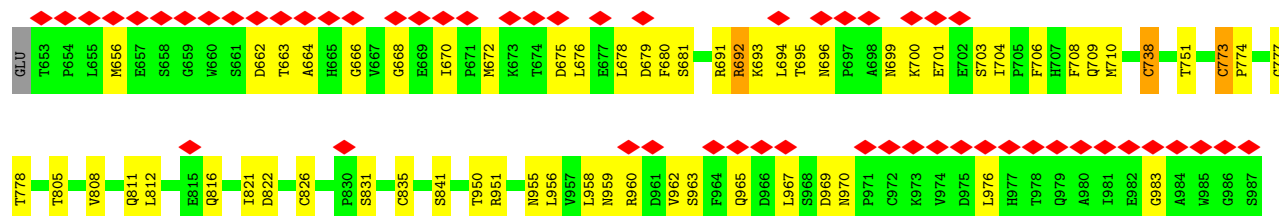
- Molecule 2: Envelopment polyprotein

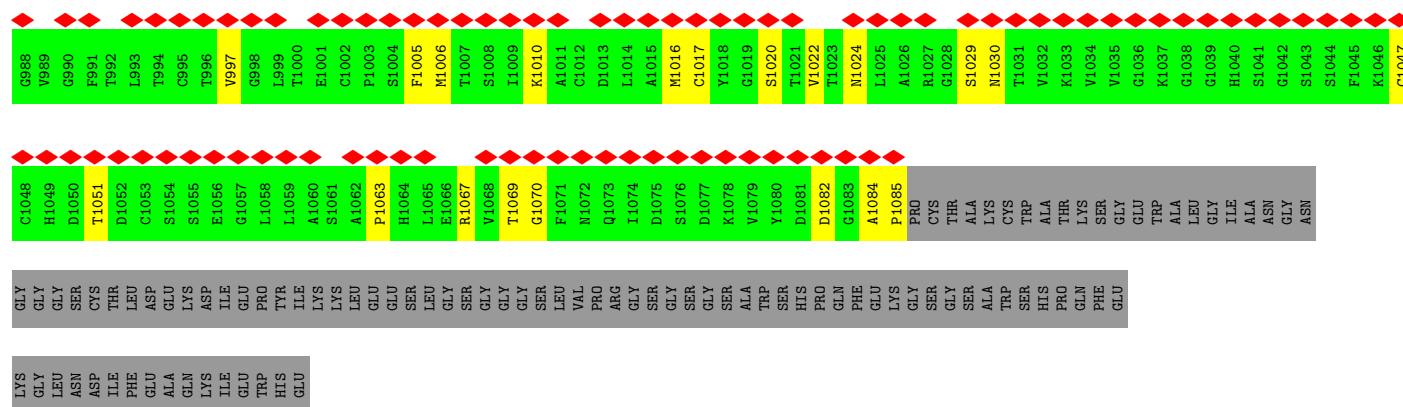


- Molecule 2: Envelopment polyprotein

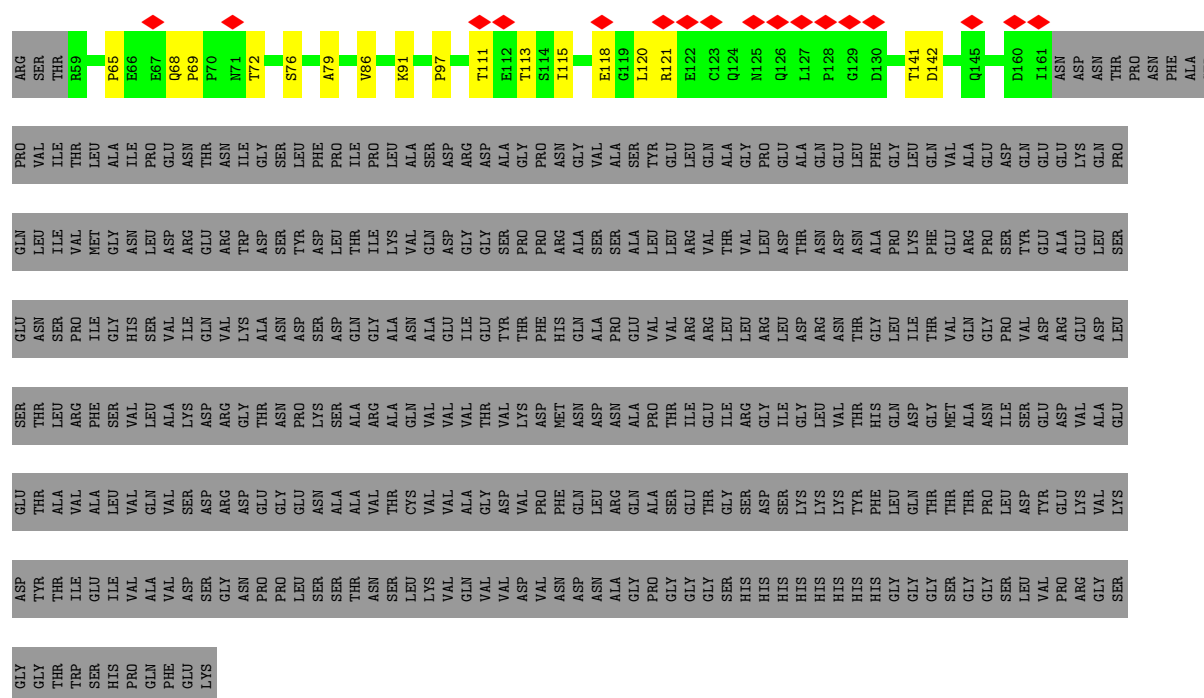


- Molecule 2: Envelopment polyprotein





• Molecule 3: Protocadherin-1



• Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  50% 50%

HA01
HA02

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  50% 50%

HA01
HA02

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	267242	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.498	Depositor
Minimum map value	-0.228	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	310.12802, 310.12802, 310.12802	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7455, 0.7455, 0.7455	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, BMA, 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	0.17	0/3593	0.43	0/4887
1	C	0.16	0/3593	0.42	0/4887
1	E	0.17	0/3593	0.44	0/4887
1	G	0.16	0/3593	0.46	0/4887
2	B	0.15	0/3388	0.42	0/4595
2	D	0.15	0/3388	0.43	0/4595
2	F	0.15	0/3388	0.41	0/4595
2	H	0.15	0/3388	0.45	2/4595 (0.0%)
3	Y	0.12	0/816	0.31	0/1111
All	All	0.16	0/28740	0.43	2/39039 (0.0%)

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
2	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	738	CYS	CA-CB-SG	7.04	130.59	114.40
2	H	773	CYS	CA-CB-SG	6.65	129.70	114.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	692	ARG	Sidechain
2	D	692	ARG	Sidechain
2	F	692	ARG	Sidechain
2	H	692	ARG	Sidechain

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	3523	0	3517	38	0
1	C	3523	0	3517	25	0
1	E	3523	0	3517	37	0
1	G	3523	0	3517	37	0
2	B	3308	0	3165	58	0
2	D	3308	0	3165	56	0
2	F	3308	0	3165	58	0
2	H	3308	0	3165	60	0
3	Y	801	0	781	13	0
4	I	50	0	43	0	0
4	J	50	0	43	0	0
4	M	50	0	43	0	0
4	N	50	0	43	0	0
4	Q	50	0	43	0	0
4	R	50	0	43	0	0
4	U	50	0	43	0	0
4	V	50	0	43	1	0
5	K	28	0	25	0	0
5	L	28	0	25	1	0
5	O	28	0	25	1	0
5	P	28	0	25	1	0
5	S	28	0	24	1	0
5	T	28	0	25	0	0
5	W	28	0	24	0	0
5	X	28	0	25	0	0
All	All	28749	0	28051	362	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 6.

All (362) 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:G:75:GLN:HG2	1:G:110:ARG:HB2	1.59	0.82
2:F:1011:ALA:HB2	2:F:1034:VAL:HG11	1.61	0.82
2:B:1031:THR:HB	2:B:1033:LYS:HZ1	1.44	0.81
2:B:930:ASN:OD1	5:L:1:NAG:N2	2.16	0.79
1:A:333:ARG:NH2	1:A:355:ASP:OD1	2.16	0.78
2:D:679:ASP:OD2	2:D:955:ASN:ND2	2.17	0.78
1:E:88:ASP:OD1	1:E:88:ASP:N	2.17	0.78
1:E:242:ASN:HB3	1:E:332:VAL:HG22	1.66	0.77
2:B:1010:LYS:NZ	2:B:1012:CYS:SG	2.57	0.76
2:F:1021:THR:HG23	2:F:1034:VAL:HG23	1.65	0.76
2:D:805:THR:HG22	2:D:822:ASP:HB3	1.69	0.75
2:B:1067:ARG:NH1	1:C:381:VAL:O	2.21	0.74
1:A:446:LEU:HD11	2:H:1063:PRO:HB2	1.68	0.73
1:E:333:ARG:NH2	1:E:355:ASP:OD1	2.21	0.73
1:G:223:GLN:N	1:G:223:GLN:OE1	2.22	0.72
3:Y:118:GLU:N	3:Y:118:GLU:OE1	2.22	0.72
2:B:657:GLU:N	2:B:657:GLU:OE1	2.23	0.71
2:D:1063:PRO:HB2	1:E:446:LEU:HD11	1.72	0.71
2:F:657:GLU:N	2:F:657:GLU:OE1	2.24	0.71
2:H:679:ASP:OD2	2:H:955:ASN:ND2	2.24	0.71
2:H:694:LEU:HD23	2:H:704:ILE:HD11	1.74	0.70
1:C:221:SER:OG	1:C:223:GLN:OE1	2.09	0.70
1:E:138:ASN:HB3	1:E:323:PRO:HG3	1.72	0.70
1:E:124:LYS:NZ	1:E:126:VAL:O	2.23	0.69
1:A:75:GLN:HG2	1:A:110:ARG:HB2	1.74	0.69
1:E:223:GLN:N	1:E:223:GLN:OE1	2.26	0.68
2:F:951:ARG:HH11	2:F:951:ARG:HG2	1.58	0.67
2:H:738:CYS:O	2:H:778:THR:N	2.23	0.67
2:B:1032:VAL:C	2:B:1033:LYS:HE2	2.20	0.66
2:H:681:SER:OG	2:H:951:ARG:HD2	1.96	0.66
2:D:670:ILE:HG13	2:D:692:ARG:HD2	1.78	0.66
2:D:704:ILE:HD13	2:D:968:SER:HB3	1.77	0.66
2:H:805:THR:HG22	2:H:822:ASP:HB3	1.78	0.65
2:F:1063:PRO:HB2	1:G:446:LEU:HD11	1.79	0.65
1:C:221:SER:HB3	1:C:224:LEU:HD22	1.78	0.64
2:B:805:THR:HG22	2:B:822:ASP:HB3	1.77	0.64
2:D:692:ARG:HA	2:D:692:ARG:HH11	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:672:MET:HE1	2:F:960:ARG:HG2	1.80	0.64
1:E:46:GLU:OE2	1:E:143:GLN:NE2	2.29	0.63
2:F:684:SER:OG	2:F:713:GLN:OE1	2.17	0.63
1:A:265:GLU:OE1	1:A:265:GLU:N	2.32	0.63
1:A:381:VAL:O	2:H:1067:ARG:NH1	2.32	0.63
1:A:189:CYS:HB2	1:A:374:GLU:HB2	1.80	0.62
1:A:89:THR:HG21	1:A:99:THR:HG23	1.80	0.62
2:D:992:THR:HG22	2:D:1035:VAL:HG22	1.82	0.62
2:H:1029:SER:C	2:H:1030:ASN:HD22	2.07	0.62
2:B:672:MET:HE1	2:B:960:ARG:HA	1.82	0.62
1:C:75:GLN:HG2	1:C:110:ARG:HB2	1.80	0.62
2:H:831:SER:HA	2:H:959:ASN:HD21	1.64	0.62
2:F:678:LEU:HB2	2:F:956:LEU:HB3	1.82	0.62
1:A:221:SER:HB3	1:A:224:LEU:HD22	1.82	0.61
1:E:75:GLN:HG2	1:E:110:ARG:HB2	1.82	0.61
2:F:805:THR:HG22	2:F:822:ASP:HB3	1.82	0.61
1:G:420:GLU:N	1:G:420:GLU:OE1	2.34	0.61
1:G:49:LEU:HD11	1:G:289:GLN:NE2	2.16	0.61
2:B:806:ARG:NH1	2:B:952:ASP:OD2	2.34	0.60
2:B:960:ARG:HH22	2:B:961:ASP:HB2	1.66	0.60
2:F:688:TYR:HB3	2:F:710:MET:HB3	1.83	0.60
2:F:993:LEU:HB3	2:F:1034:VAL:HG12	1.81	0.60
2:H:951:ARG:HG2	2:H:951:ARG:HH11	1.65	0.60
2:H:710:MET:HG2	2:H:808:VAL:HG12	1.83	0.60
1:G:101:GLU:OE1	1:G:101:GLU:N	2.35	0.60
2:D:676:LEU:HB3	2:D:958:LEU:HB3	1.82	0.60
2:F:1016:MET:SD	2:F:1017:CYS:N	2.73	0.59
2:D:930:ASN:OD1	5:P:1:NAG:N2	2.36	0.59
2:B:821:ILE:HG21	2:B:827:LEU:HB2	1.85	0.58
2:H:738:CYS:HB2	2:H:777:GLY:HA2	1.83	0.58
2:D:672:MET:HE2	2:D:694:LEU:HG	1.86	0.58
1:E:60:LEU:HD21	1:E:131:LEU:HG	1.84	0.58
2:B:678:LEU:HB2	2:B:956:LEU:HB3	1.85	0.58
2:B:656:MET:HE3	2:B:680:PHE:HB2	1.86	0.58
2:D:707:HIS:HB3	2:D:811:GLN:HB3	1.85	0.58
1:E:420:GLU:OE1	1:E:420:GLU:N	2.35	0.58
5:S:1:NAG:H61	5:S:2:NAG:C7	2.34	0.58
2:D:841:SER:HB3	2:D:950:THR:HG23	1.87	0.57
2:H:663:THR:H	2:H:1016:MET:HE1	1.68	0.57
2:H:692:ARG:NH1	2:H:1082:ASP:O	2.25	0.57
2:D:810:ILE:O	2:D:810:ILE:HD12	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:LEU:HD12	1:E:124:LYS:N	2.20	0.57
2:H:959:ASN:O	2:H:962:VAL:HG23	2.05	0.56
1:G:49:LEU:HD11	1:G:289:GLN:HE22	1.68	0.56
2:D:932:THR:HG22	2:D:944:ILE:O	2.05	0.56
2:B:994:THR:HG23	2:B:1033:LYS:HZ2	1.72	0.55
2:H:670:ILE:HG13	2:H:692:ARG:HD2	1.88	0.55
1:A:412:LYS:HE3	1:A:423:ILE:HD12	1.89	0.55
1:E:24:TYR:HE2	1:E:168:SER:HG	1.54	0.55
1:G:85:LYS:HB2	2:H:774:PRO:HB3	1.89	0.55
2:H:709:GLN:HE21	2:H:1022:VAL:HG11	1.72	0.55
2:H:1016:MET:HE3	2:H:1017:CYS:O	2.06	0.55
2:D:709:GLN:HE22	2:D:1022:VAL:HG21	1.71	0.54
2:H:826:CYS:HA	2:H:835:CYS:HB3	1.89	0.54
1:C:159:ARG:NH2	5:O:1:NAG:O3	2.40	0.54
2:H:841:SER:HB3	2:H:950:THR:HG23	1.89	0.54
2:H:664:ALA:HB3	2:H:1085:PRO:HG2	1.89	0.54
2:B:709:GLN:HE21	2:B:1022:VAL:HG11	1.72	0.54
2:F:1070:GLY:C	1:G:442:LYS:HD3	2.33	0.54
2:D:1016:MET:SD	2:D:1017:CYS:N	2.81	0.54
2:H:678:LEU:HB2	2:H:956:LEU:HB3	1.90	0.54
1:C:189:CYS:HB2	1:C:374:GLU:HB2	1.90	0.54
1:E:84:ARG:HG3	1:E:84:ARG:HH11	1.72	0.54
2:F:663:THR:H	2:F:1016:MET:HE1	1.72	0.53
2:F:704:ILE:HG13	2:F:705:PRO:HD2	1.91	0.53
1:C:265:GLU:OE2	1:C:265:GLU:N	2.42	0.53
1:A:417:ARG:C	1:A:419:SER:H	2.17	0.52
2:B:1063:PRO:HB2	1:C:446:LEU:HD11	1.92	0.52
2:H:699:ASN:ND2	2:H:701:GLU:OE2	2.43	0.52
2:H:811:GLN:HB2	2:H:1006:MET:HB3	1.92	0.52
2:D:692:ARG:HA	2:D:692:ARG:NH1	2.24	0.52
2:B:1031:THR:HB	2:B:1033:LYS:NZ	2.22	0.52
2:D:684:SER:OG	2:D:713:GLN:OE1	2.18	0.52
1:G:138:ASN:HB3	1:G:323:PRO:HG3	1.92	0.52
2:F:708:PHE:HE1	2:F:808:VAL:HG23	1.73	0.52
1:G:45:THR:HG22	1:G:146:VAL:HG22	1.92	0.51
3:Y:69:PRO:O	3:Y:72:THR:OG1	2.26	0.51
2:B:994:THR:HG23	2:B:1033:LYS:NZ	2.26	0.51
2:F:976:LEU:HD11	2:F:1047:CYS:O	2.10	0.51
2:B:707:HIS:CD2	2:B:1006:MET:HE3	2.46	0.51
3:Y:68:GLN:HG3	3:Y:69:PRO:HD2	1.93	0.51
2:F:821:ILE:HD12	2:F:835:CYS:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:969:ASP:OD1	2:F:970:ASN:N	2.43	0.51
2:D:937:THR:HG22	2:D:938:THR:N	2.25	0.51
2:F:808:VAL:HG11	2:F:821:ILE:HD13	1.93	0.51
1:G:221:SER:HB3	1:G:224:LEU:HD12	1.93	0.51
2:H:676:LEU:HB3	2:H:958:LEU:HB3	1.93	0.51
1:E:186:GLU:OE1	1:E:186:GLU:N	2.44	0.50
1:A:417:ARG:HG2	1:A:417:ARG:HH11	1.76	0.50
2:D:937:THR:HG22	2:D:938:THR:H	1.75	0.50
2:F:826:CYS:HA	2:F:835:CYS:HB3	1.93	0.50
1:G:125:LYS:H	1:G:125:LYS:HD2	1.75	0.50
2:D:656:MET:HE3	2:D:680:PHE:CD2	2.46	0.50
1:E:189:CYS:HB2	1:E:374:GLU:HB2	1.92	0.50
2:F:711:GLU:OE1	2:F:807:LYS:HB3	2.11	0.50
2:H:983:GLY:HA2	2:H:1069:THR:O	2.10	0.50
2:B:675:ASP:OD1	2:B:960:ARG:HB2	2.10	0.50
1:C:90:THR:OG1	1:C:91:ASP:N	2.45	0.50
1:E:221:SER:HB3	1:E:224:LEU:HD12	1.93	0.50
1:A:123:LEU:O	1:A:124:LYS:HB2	2.11	0.50
2:B:1010:LYS:HG3	2:B:1019:GLY:O	2.12	0.50
2:F:662:ASP:HB3	2:F:1016:MET:HE2	1.93	0.50
1:G:82:GLU:HG3	1:G:83:TRP:N	2.27	0.50
1:C:375:LYS:HA	1:C:375:LYS:HE3	1.94	0.49
1:A:467:PRO:HB2	1:C:448:LYS:HG3	1.94	0.49
2:F:683:PRO:HA	2:F:951:ARG:HD3	1.94	0.49
2:F:1066:GLU:HB3	2:F:1067:ARG:CZ	2.42	0.49
2:B:978:THR:HG22	2:B:1047:CYS:SG	2.52	0.49
2:D:672:MET:HG2	2:D:697:PRO:HD3	1.93	0.49
2:H:656:MET:HE2	2:H:680:PHE:HB2	1.93	0.49
1:G:124:LYS:HG2	1:G:126:VAL:O	2.13	0.49
2:D:969:ASP:OD1	2:D:970:ASN:N	2.45	0.49
2:B:1025:LEU:HB3	2:B:1030:ASN:ND2	2.28	0.49
2:B:1066:GLU:HB3	2:B:1067:ARG:HE	1.76	0.49
1:C:355:ASP:OD1	1:C:355:ASP:N	2.46	0.48
2:D:701:GLU:N	2:D:701:GLU:OE1	2.46	0.48
2:F:690:TYR:HE1	2:F:692:ARG:CZ	2.27	0.48
2:D:687:SER:O	2:D:1079:VAL:HG22	2.13	0.48
2:D:937:THR:CG2	2:D:938:THR:H	2.26	0.48
2:F:676:LEU:HB3	2:F:958:LEU:HB3	1.95	0.48
2:B:701:GLU:N	2:B:701:GLU:OE1	2.47	0.48
2:D:666:GLY:HA2	2:D:1051:THR:HG22	1.94	0.48
2:H:969:ASP:OD1	2:H:970:ASN:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:THR:HG22	1:A:35:GLY:H	1.79	0.48
2:D:656:MET:HE3	2:D:680:PHE:CG	2.48	0.48
2:F:828:VAL:HG22	2:F:833:LYS:HG3	1.96	0.48
2:B:711:GLU:OE2	2:B:807:LYS:HD3	2.14	0.47
2:B:969:ASP:OD1	2:B:970:ASN:N	2.45	0.47
1:E:467:PRO:HB2	1:G:448:LYS:HG3	1.96	0.47
2:H:701:GLU:OE1	2:H:701:GLU:N	2.47	0.47
1:A:418:GLY:HA3	3:Y:86:VAL:HG23	1.97	0.47
2:B:1010:LYS:HG2	2:B:1012:CYS:SG	2.53	0.47
3:Y:115:ILE:HD11	3:Y:120:LEU:HD11	1.95	0.47
2:H:951:ARG:HH11	2:H:951:ARG:CG	2.28	0.47
1:E:227:ILE:CD1	1:E:332:VAL:HG23	2.45	0.47
1:E:433:ASP:OD2	1:E:446:LEU:HD22	2.15	0.47
1:G:82:GLU:HG3	1:G:83:TRP:H	1.80	0.47
2:D:678:LEU:HB2	2:D:956:LEU:HB3	1.97	0.47
1:E:33:THR:HG22	1:E:35:GLY:H	1.79	0.47
2:D:704:ILE:HD12	2:D:705:PRO:HD2	1.97	0.47
1:A:412:LYS:HB2	1:A:412:LYS:HE2	1.61	0.47
2:D:1067:ARG:NH1	1:G:428:GLN:OE1	2.48	0.47
2:F:1012:CYS:HA	2:F:1017:CYS:HA	1.96	0.47
2:B:885:MET:HE2	2:B:885:MET:HB2	1.75	0.46
2:F:960:ARG:HH22	2:F:961:ASP:HB3	1.80	0.46
1:A:162:MET:HE1	1:A:169:ARG:HB3	1.95	0.46
1:E:220:LYS:NZ	1:E:336:ASP:OD2	2.48	0.46
2:F:1011:ALA:HB2	2:F:1034:VAL:CG1	2.41	0.46
1:G:100:PHE:CE1	1:G:298:VAL:HG12	2.50	0.46
2:B:1010:LYS:HB3	2:B:1010:LYS:HE3	1.67	0.46
3:Y:91:LYS:HE2	3:Y:91:LYS:HB2	1.66	0.46
1:A:21:LYS:HA	1:A:21:LYS:HD2	1.58	0.46
2:D:713:GLN:HE21	2:D:804:TYR:HB3	1.81	0.46
2:B:960:ARG:NH2	2:B:961:ASP:HB2	2.31	0.46
2:F:812:LEU:HB3	2:F:815:GLU:OE2	2.15	0.46
2:H:692:ARG:HH12	2:H:1082:ASP:C	2.19	0.46
1:A:90:THR:OG1	1:A:91:ASP:N	2.48	0.46
2:B:675:ASP:CG	2:B:960:ARG:HB2	2.41	0.46
2:B:981:ILE:HD12	2:B:993:LEU:HD13	1.98	0.46
2:H:821:ILE:HD12	2:H:835:CYS:HA	1.97	0.46
2:D:951:ARG:HB2	2:D:951:ARG:CZ	2.46	0.46
1:A:162:MET:HE3	1:A:162:MET:HB3	1.74	0.46
1:A:442:LYS:HD3	2:H:1070:GLY:C	2.41	0.46
2:H:751:THR:HG22	4:V:1:NAG:H81	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:THR:HG22	1:A:35:GLY:N	2.31	0.45
2:B:707:HIS:HB3	2:B:811:GLN:HB3	1.98	0.45
2:F:1067:ARG:HD2	1:G:380:THR:HG23	1.98	0.45
1:C:412:LYS:HB2	1:C:412:LYS:HE2	1.62	0.45
2:F:677:GLU:OE1	2:F:957:VAL:HG22	2.16	0.45
2:D:691:ARG:NH1	2:D:707:HIS:HB2	2.32	0.45
2:H:704:ILE:HD12	2:H:812:LEU:HD11	1.98	0.45
2:H:816:GLN:HE22	2:H:1024:ASN:CG	2.20	0.45
2:B:826:CYS:HA	2:B:835:CYS:HB3	1.99	0.45
3:Y:76:SER:HB3	3:Y:79:ALA:HB3	1.99	0.45
2:F:1014:LEU:HD23	2:F:1046:LYS:NZ	2.32	0.45
1:G:82:GLU:HB3	1:G:103:GLN:HG3	1.98	0.45
2:H:666:GLY:HA2	2:H:1051:THR:HG22	1.99	0.45
1:E:21:LYS:HA	1:E:21:LYS:HD2	1.70	0.44
1:A:433:ASP:OD2	1:A:446:LEU:HD22	2.17	0.44
2:D:812:LEU:HG	2:D:967:LEU:HD22	1.98	0.44
2:B:653:THR:OG1	2:B:681:SER:HB2	2.18	0.44
2:B:732:ILE:HD12	2:B:784:GLY:O	2.18	0.44
2:B:696:ASN:HB3	2:B:699:ASN:O	2.18	0.44
2:D:691:ARG:O	2:D:692:ARG:NH1	2.51	0.44
2:F:675:ASP:OD1	2:F:960:ARG:HB2	2.17	0.44
2:H:672:MET:HE2	2:H:960:ARG:HA	1.99	0.44
1:A:426:ILE:HD13	1:G:382:PHE:CD2	2.53	0.44
1:E:465:LEU:HD23	1:E:465:LEU:HA	1.85	0.44
2:F:678:LEU:HD11	2:F:690:TYR:CE2	2.52	0.44
3:Y:97:PRO:O	3:Y:111:THR:OG1	2.28	0.44
2:F:983:GLY:HA2	2:F:1069:THR:O	2.17	0.44
1:G:82:GLU:OE1	1:G:343:PRO:HG2	2.17	0.44
3:Y:142:ASP:OD1	3:Y:142:ASP:N	2.36	0.44
3:Y:120:LEU:HA	3:Y:121:ARG:NH1	2.33	0.43
2:D:937:THR:CG2	2:D:938:THR:N	2.82	0.43
2:F:1008:SER:HB3	2:F:1022:VAL:HG22	2.00	0.43
2:F:1016:MET:HE3	2:F:1017:CYS:O	2.18	0.43
1:A:121:ASP:OD1	1:A:124:LYS:HE2	2.18	0.43
2:B:672:MET:HB3	2:B:697:PRO:HD3	1.99	0.43
1:C:162:MET:HE2	1:C:162:MET:HB2	1.76	0.43
2:H:963:SER:O	2:H:967:LEU:HD12	2.17	0.43
2:H:976:LEU:HD12	2:H:997:VAL:HG13	2.00	0.43
1:C:228:LYS:NZ	1:C:241:GLU:HA	2.33	0.43
1:C:433:ASP:OD2	1:C:446:LEU:HD22	2.18	0.43
2:D:808:VAL:HG11	2:D:821:ILE:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:672:MET:HB2	2:H:694:LEU:HD11	1.99	0.43
2:F:672:MET:HB2	2:F:694:LEU:HD11	2.01	0.43
2:B:973:LYS:HB3	2:B:973:LYS:HE3	1.76	0.43
2:D:965:GLN:N	2:D:965:GLN:CD	2.77	0.43
2:F:965:GLN:N	2:F:965:GLN:CD	2.77	0.43
1:G:433:ASP:OD2	1:G:446:LEU:HD22	2.18	0.43
2:H:662:ASP:HB3	2:H:1016:MET:HE2	2.01	0.43
2:D:780:CYS:SG	2:D:781:THR:N	2.91	0.43
1:E:84:ARG:HG3	1:E:84:ARG:NH1	2.33	0.43
2:F:951:ARG:HG2	2:F:951:ARG:NH1	2.28	0.43
2:H:695:THR:HG22	2:H:703:SER:OG	2.19	0.43
2:B:1006:MET:HE2	2:B:1006:MET:HB3	1.83	0.43
1:C:382:PHE:CD2	1:E:426:ILE:HD13	2.54	0.43
2:D:706:PHE:CD1	2:D:812:LEU:HD13	2.54	0.43
1:A:32:HIS:HB2	1:A:180:VAL:HA	2.01	0.43
1:A:382:PHE:CD2	1:C:426:ILE:HD13	2.54	0.43
2:B:812:LEU:HB3	2:B:815:GLU:OE2	2.19	0.43
1:C:33:THR:HG22	1:C:35:GLY:H	1.84	0.43
2:D:937:THR:HG23	1:E:61:GLU:OE1	2.19	0.43
2:H:691:ARG:HB3	2:H:691:ARG:CZ	2.48	0.43
2:H:965:GLN:CD	2:H:965:GLN:N	2.77	0.43
1:A:417:ARG:HH11	1:A:417:ARG:CG	2.32	0.42
1:G:21:LYS:HD2	1:G:21:LYS:HA	1.80	0.42
1:G:465:LEU:HD23	1:G:465:LEU:HA	1.86	0.42
2:B:808:VAL:HG21	2:B:834:VAL:HG11	2.00	0.42
2:B:965:GLN:N	2:B:965:GLN:CD	2.77	0.42
2:B:1052:ASP:OD1	2:B:1052:ASP:C	2.61	0.42
1:E:162:MET:HE2	1:E:162:MET:HB2	1.83	0.42
1:E:234:LEU:HD23	1:E:234:LEU:HA	1.82	0.42
2:D:1052:ASP:OD1	2:D:1052:ASP:C	2.62	0.42
1:E:301:ILE:HG21	1:E:345:ILE:HD13	2.01	0.42
1:E:466:MET:HE2	1:E:466:MET:HB2	1.81	0.42
1:G:33:THR:HG23	1:G:415:ARG:O	2.19	0.42
1:G:76:LYS:HZ3	1:G:114:ILE:HB	1.84	0.42
1:G:127:LYS:HB3	1:G:151:PRO:CG	2.49	0.42
2:H:668:GLY:C	2:H:692:ARG:HD3	2.45	0.42
2:B:982:GLU:OE1	2:B:983:GLY:N	2.53	0.42
1:E:382:PHE:CD2	1:G:426:ILE:HD13	2.53	0.42
1:G:156:MET:CE	1:G:415:ARG:HB3	2.50	0.42
2:F:701:GLU:N	2:F:701:GLU:OE1	2.52	0.42
1:G:122:THR:O	1:G:124:LYS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:706:PHE:CE2	2:H:812:LEU:HD13	2.55	0.42
2:B:1066:GLU:HB3	2:B:1067:ARG:HH21	1.85	0.42
2:H:811:GLN:OE1	2:H:1005:PHE:HA	2.18	0.42
2:D:688:TYR:CD1	2:D:1079:VAL:HG23	2.54	0.42
2:H:675:ASP:OD1	2:H:960:ARG:HB2	2.20	0.42
3:Y:121:ARG:H	3:Y:121:ARG:HD2	1.85	0.42
2:F:680:PHE:O	2:F:954:VAL:HG12	2.20	0.42
1:G:156:MET:HE3	1:G:415:ARG:HB3	2.01	0.42
2:H:663:THR:N	2:H:1016:MET:HE1	2.34	0.42
1:A:99:THR:HG21	2:B:774:PRO:O	2.20	0.42
2:B:961:ASP:O	2:B:961:ASP:CG	2.63	0.42
2:F:1012:CYS:HB2	2:F:1048:CYS:SG	2.60	0.42
2:F:1052:ASP:OD1	2:F:1052:ASP:C	2.62	0.42
2:H:976:LEU:HD23	2:H:1047:CYS:O	2.20	0.42
2:F:932:THR:OG1	2:F:944:ILE:O	2.32	0.42
1:G:82:GLU:HB3	1:G:103:GLN:HE21	1.84	0.42
2:H:706:PHE:CD2	2:H:812:LEU:HD13	2.54	0.42
2:B:963:SER:O	2:B:967:LEU:HD12	2.20	0.41
2:D:963:SER:O	2:D:967:LEU:HD12	2.20	0.41
2:F:963:SER:O	2:F:967:LEU:HD12	2.19	0.41
2:B:708:PHE:HE1	2:B:808:VAL:HG23	1.85	0.41
2:B:807:LYS:NZ	2:B:818:CYS:HB3	2.34	0.41
1:C:471:HIS:NE2	1:E:431:ASP:OD1	2.54	0.41
2:D:708:PHE:HD1	2:D:810:ILE:HG22	1.85	0.41
2:D:840:VAL:HG23	2:D:951:ARG:HB3	2.02	0.41
2:F:799:ILE:HG21	2:F:802:LEU:HD11	2.01	0.41
2:H:1010:LYS:HA	2:H:1020:SER:HA	2.02	0.41
3:Y:120:LEU:HD23	3:Y:121:ARG:NH1	2.35	0.41
1:A:123:LEU:HD23	1:A:123:LEU:HA	1.81	0.41
2:B:676:LEU:HB3	2:B:958:LEU:HB3	2.01	0.41
1:C:33:THR:HG22	1:C:35:GLY:N	2.35	0.41
2:B:855:LEU:O	2:B:931:LEU:HD12	2.21	0.41
2:B:1010:LYS:HD2	2:B:1017:CYS:SG	2.60	0.41
2:F:704:ILE:CD1	2:F:968:SER:HB3	2.50	0.41
1:G:125:LYS:HD2	1:G:125:LYS:N	2.35	0.41
2:H:692:ARG:HG3	2:H:693:LYS:N	2.35	0.41
1:A:194:HIS:HB3	1:A:369:ILE:HD11	2.02	0.41
1:A:465:LEU:HD23	1:A:465:LEU:HA	1.88	0.41
1:E:212:ILE:HD11	1:E:363:TRP:HZ3	1.85	0.41
2:F:666:GLY:HA2	2:F:1051:THR:HG22	2.01	0.41
2:F:885:MET:HE2	2:F:885:MET:HB2	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:THR:O	1:A:99:THR:HG22	2.21	0.41
2:B:1023:THR:HG21	2:B:1032:VAL:HG11	2.02	0.41
1:E:178:HIS:CE1	1:E:184:LEU:HD11	2.56	0.41
2:B:704:ILE:HG22	2:B:968:SER:HB3	2.03	0.41
2:F:959:ASN:O	2:F:962:VAL:HG13	2.20	0.41
2:H:708:PHE:CZ	2:H:710:MET:HG3	2.56	0.41
1:A:210:LEU:HD12	1:A:369:ILE:HG21	2.03	0.41
1:E:33:THR:HG22	1:E:35:GLY:N	2.36	0.41
2:F:664:ALA:HB3	2:F:1085:PRO:HG2	2.03	0.41
2:F:700:LYS:NZ	2:F:700:LYS:HB3	2.35	0.41
2:F:710:MET:HE3	2:F:808:VAL:HB	2.02	0.41
1:G:350:ASN:O	1:G:351:HIS:HB2	2.20	0.41
2:H:664:ALA:O	2:H:1084:ALA:HB1	2.20	0.41
2:H:812:LEU:HG	2:H:967:LEU:HD22	2.02	0.41
1:A:153:LEU:HD12	1:A:153:LEU:HA	1.89	0.41
1:A:212:ILE:HD11	1:A:363:TRP:HZ3	1.86	0.41
2:B:1008:SER:HB3	2:B:1022:VAL:HG22	2.03	0.41
2:D:885:MET:HE2	2:D:885:MET:HB2	1.79	0.41
2:H:700:LYS:NZ	2:H:700:LYS:HB3	2.35	0.41
1:C:21:LYS:HB2	1:C:167:THR:O	2.21	0.40
1:C:465:LEU:HD23	1:C:465:LEU:HA	1.87	0.40
1:A:264:LEU:HD23	1:A:264:LEU:HA	1.87	0.40
1:C:33:THR:HG23	1:C:415:ARG:O	2.21	0.40
1:C:304:LYS:HE2	1:C:304:LYS:HB3	1.97	0.40
2:D:675:ASP:OD1	2:D:960:ARG:HB2	2.21	0.40
2:D:834:VAL:O	2:D:835:CYS:SG	2.79	0.40
1:E:395:TYR:CE1	1:E:421:GLN:HB3	2.55	0.40
1:G:99:THR:O	1:G:99:THR:HG22	2.21	0.40
3:Y:65:PRO:HD2	3:Y:68:GLN:OE1	2.21	0.40
2:D:700:LYS:NZ	2:D:700:LYS:HB3	2.35	0.40
2:D:973:LYS:HE3	2:D:973:LYS:HB3	1.96	0.40
2:F:704:ILE:HD13	2:F:968:SER:HB3	2.04	0.40
1:A:109:LEU:HD23	1:A:109:LEU:HA	1.92	0.40
2:D:656:MET:HE1	2:D:688:TYR:CZ	2.56	0.40
2:D:711:GLU:OE2	2:D:807:LYS:HD3	2.22	0.40
2:D:688:TYR:HB3	2:D:710:MET:HB3	2.03	0.40
2:D:692:ARG:HG3	2:D:693:LYS:N	2.36	0.40
2:H:696:ASN:HB3	2:H:699:ASN:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	458/517 (89%)	448 (98%)	10 (2%)	0	100	100
1	C	458/517 (89%)	447 (98%)	10 (2%)	1 (0%)	43	56
1	E	458/517 (89%)	447 (98%)	10 (2%)	1 (0%)	43	56
1	G	458/517 (89%)	447 (98%)	11 (2%)	0	100	100
2	B	431/532 (81%)	421 (98%)	10 (2%)	0	100	100
2	D	431/532 (81%)	422 (98%)	9 (2%)	0	100	100
2	F	431/532 (81%)	421 (98%)	10 (2%)	0	100	100
2	H	431/532 (81%)	421 (98%)	10 (2%)	0	100	100
3	Y	101/486 (21%)	100 (99%)	1 (1%)	0	100	100
All	All	3657/4682 (78%)	3574 (98%)	81 (2%)	2 (0%)	49	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	124	LYS
1	E	124	LYS

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	411/454 (90%)	405 (98%)	6 (2%)	57	74
1	C	411/454 (90%)	405 (98%)	6 (2%)	57	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	411/454 (90%)	401 (98%)	10 (2%)	43	61
1	G	411/454 (90%)	408 (99%)	3 (1%)	76	85
2	B	373/449 (83%)	369 (99%)	4 (1%)	65	79
2	D	373/449 (83%)	372 (100%)	1 (0%)	86	92
2	F	373/449 (83%)	371 (100%)	2 (0%)	81	88
2	H	373/449 (83%)	372 (100%)	1 (0%)	86	92
3	Y	90/411 (22%)	88 (98%)	2 (2%)	45	64
All	All	3226/4023 (80%)	3191 (99%)	35 (1%)	63	79

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ARG
1	A	171	GLN
1	A	223	GLN
1	A	290	ASN
1	A	354	CYS
1	A	476	GLU
2	B	672	MET
2	B	732	ILE
2	B	974	VAL
2	B	976	LEU
1	C	22	THR
1	C	123	LEU
1	C	153	LEU
1	C	165	VAL
1	C	290	ASN
1	C	466	MET
2	D	766	TRP
1	E	25	GLU
1	E	32	HIS
1	E	88	ASP
1	E	89	THR
1	E	143	GLN
1	E	184	LEU
1	E	223	GLN
1	E	354	CYS
1	E	429	ARG
1	E	462	LEU
2	F	843	LEU

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Mol	Chain	Res	Type
2	F	1006	MET
1	G	84	ARG
1	G	125	LYS
1	G	420	GLU
2	H	773	CYS
3	Y	113	THR
3	Y	141	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	80	GLN
1	A	94	ASN
1	A	143	GLN
2	B	707	HIS
2	B	709	GLN
2	B	716	HIS
2	B	816	GLN
2	B	820	HIS
2	B	955	ASN
1	C	38	GLN
1	C	80	GLN
1	C	108	ASN
1	C	143	GLN
1	C	242	ASN
1	C	421	GLN
2	D	716	HIS
2	D	820	HIS
2	D	1049	HIS
2	D	1073	GLN
1	E	38	GLN
1	E	421	GLN
2	F	824	ASN
2	F	955	ASN
2	F	1073	GLN
1	G	38	GLN
1	G	108	ASN
1	G	289	GLN
1	G	351	HIS
2	H	716	HIS
2	H	844	GLN

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Mol	Chain	Res	Type
2	H	1049	HIS
2	H	1072	ASN
2	H	1073	GLN
3	Y	124	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 ⓘ

48 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	4,1	14,14,15	0.41	0	17,19,21	0.77	1 (5%)
4	NAG	I	2	4	14,14,15	0.71	1 (7%)	17,19,21	0.61	0
4	BMA	I	3	4	11,11,12	0.66	0	15,15,17	0.78	0
4	MAN	I	4	4	11,11,12	0.58	0	15,15,17	0.94	2 (13%)
4	NAG	J	1	4,1	14,14,15	0.29	0	17,19,21	0.58	0
4	NAG	J	2	4	14,14,15	0.21	0	17,19,21	0.54	0
4	BMA	J	3	4	11,11,12	0.63	0	15,15,17	0.77	0
4	MAN	J	4	4	11,11,12	0.61	0	15,15,17	0.97	2 (13%)
5	NAG	K	1	1,5	14,14,15	1.20	2 (14%)	17,19,21	0.68	1 (5%)
5	NAG	K	2	5	14,14,15	0.20	0	17,19,21	0.41	0
5	NAG	L	1	2,5	14,14,15	1.64	2 (14%)	17,19,21	0.67	1 (5%)
5	NAG	L	2	5	14,14,15	0.20	0	17,19,21	0.53	0
4	NAG	M	1	4,1	14,14,15	0.35	0	17,19,21	0.74	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	M	2	4	14,14,15	0.73	1 (7%)	17,19,21	0.56	0
4	BMA	M	3	4	11,11,12	0.70	0	15,15,17	0.82	0
4	MAN	M	4	4	11,11,12	0.60	0	15,15,17	0.95	2 (13%)
4	NAG	N	1	4,1	14,14,15	0.29	0	17,19,21	0.57	0
4	NAG	N	2	4	14,14,15	0.19	0	17,19,21	0.53	0
4	BMA	N	3	4	11,11,12	0.60	0	15,15,17	0.76	0
4	MAN	N	4	4	11,11,12	0.66	0	15,15,17	0.97	2 (13%)
5	NAG	O	1	1,5	14,14,15	1.00	2 (14%)	17,19,21	0.84	1 (5%)
5	NAG	O	2	5	14,14,15	0.25	0	17,19,21	0.44	0
5	NAG	P	1	2,5	14,14,15	1.28	2 (14%)	17,19,21	0.71	1 (5%)
5	NAG	P	2	5	14,14,15	0.30	0	17,19,21	0.51	0
4	NAG	Q	1	4,1	14,14,15	0.18	0	17,19,21	0.76	1 (5%)
4	NAG	Q	2	4	14,14,15	0.53	0	17,19,21	0.47	0
4	BMA	Q	3	4	11,11,12	0.64	0	15,15,17	0.79	0
4	MAN	Q	4	4	11,11,12	0.63	0	15,15,17	0.97	2 (13%)
4	NAG	R	1	4,1	14,14,15	0.41	0	17,19,21	0.59	0
4	NAG	R	2	4	14,14,15	0.17	0	17,19,21	0.55	0
4	BMA	R	3	4	11,11,12	0.61	0	15,15,17	0.78	0
4	MAN	R	4	4	11,11,12	0.62	0	15,15,17	0.94	2 (13%)
5	NAG	S	1	1,5	14,14,15	1.20	2 (14%)	17,19,21	0.85	1 (5%)
5	NAG	S	2	5	14,14,15	0.70	1 (7%)	17,19,21	0.66	0
5	NAG	T	1	2,5	14,14,15	1.09	2 (14%)	17,19,21	0.75	1 (5%)
5	NAG	T	2	5	14,14,15	0.29	0	17,19,21	0.55	0
4	NAG	U	1	4,1	14,14,15	0.14	0	17,19,21	0.75	1 (5%)
4	NAG	U	2	4	14,14,15	0.55	0	17,19,21	0.52	0
4	BMA	U	3	4	11,11,12	0.63	0	15,15,17	0.79	0
4	MAN	U	4	4	11,11,12	0.61	0	15,15,17	0.94	2 (13%)
4	NAG	V	1	4,1	14,14,15	0.41	0	17,19,21	0.59	0
4	NAG	V	2	4	14,14,15	0.18	0	17,19,21	0.58	0
4	BMA	V	3	4	11,11,12	0.63	0	15,15,17	0.75	0
4	MAN	V	4	4	11,11,12	0.65	0	15,15,17	0.96	2 (13%)
5	NAG	W	1	1,5	14,14,15	1.10	2 (14%)	17,19,21	0.67	1 (5%)
5	NAG	W	2	5	14,14,15	0.34	0	17,19,21	0.44	0
5	NAG	X	1	2,5	14,14,15	1.06	2 (14%)	17,19,21	0.71	1 (5%)
5	NAG	X	2	5	14,14,15	0.24	0	17,19,21	0.52	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	I	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	1/6/23/26	0/1/1/1
4	BMA	I	3	4	-	2/2/19/22	0/1/1/1
4	MAN	I	4	4	-	0/2/19/22	0/1/1/1
4	NAG	J	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	4/6/23/26	0/1/1/1
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1
4	MAN	J	4	4	-	1/2/19/22	0/1/1/1
5	NAG	K	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	4/6/23/26	0/1/1/1
5	NAG	L	1	2,5	-	1/6/23/26	0/1/1/1
5	NAG	L	2	5	-	4/6/23/26	0/1/1/1
4	NAG	M	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	BMA	M	3	4	-	2/2/19/22	0/1/1/1
4	MAN	M	4	4	-	0/2/19/22	0/1/1/1
4	NAG	N	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	N	2	4	-	4/6/23/26	0/1/1/1
4	BMA	N	3	4	-	0/2/19/22	0/1/1/1
4	MAN	N	4	4	-	1/2/19/22	0/1/1/1
5	NAG	O	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	4/6/23/26	0/1/1/1
5	NAG	P	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	P	2	5	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	1/6/23/26	0/1/1/1
4	BMA	Q	3	4	-	0/2/19/22	0/1/1/1
4	MAN	Q	4	4	-	0/2/19/22	0/1/1/1
4	NAG	R	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	R	2	4	-	4/6/23/26	0/1/1/1
4	BMA	R	3	4	-	0/2/19/22	0/1/1/1
4	MAN	R	4	4	-	2/2/19/22	0/1/1/1
5	NAG	S	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	S	2	5	-	4/6/23/26	0/1/1/1
5	NAG	T	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	T	2	5	-	3/6/23/26	0/1/1/1
4	NAG	U	1	4,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	U	2	4	-	1/6/23/26	0/1/1/1
4	BMA	U	3	4	-	0/2/19/22	0/1/1/1
4	MAN	U	4	4	-	0/2/19/22	0/1/1/1
4	NAG	V	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	4/6/23/26	0/1/1/1
4	BMA	V	3	4	-	0/2/19/22	0/1/1/1
4	MAN	V	4	4	-	1/2/19/22	0/1/1/1
5	NAG	W	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	W	2	5	-	2/6/23/26	0/1/1/1
5	NAG	X	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	X	2	5	-	1/6/23/26	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1	NAG	C1-C2	5.24	1.60	1.52
5	P	1	NAG	C1-C2	3.64	1.57	1.52
5	K	1	NAG	O5-C1	3.51	1.49	1.43
5	T	1	NAG	C1-C2	3.11	1.57	1.52
5	S	1	NAG	C1-C2	3.10	1.57	1.52
5	S	1	NAG	O5-C1	3.08	1.48	1.43
5	L	1	NAG	O5-C1	3.05	1.48	1.43
5	X	1	NAG	C1-C2	2.99	1.56	1.52
5	P	1	NAG	O5-C1	2.98	1.48	1.43
5	W	1	NAG	C1-C2	2.85	1.56	1.52
5	O	1	NAG	C1-C2	2.81	1.56	1.52
5	W	1	NAG	O5-C1	2.76	1.48	1.43
5	K	1	NAG	C1-C2	2.62	1.56	1.52
5	T	1	NAG	O5-C1	2.38	1.47	1.43
5	X	1	NAG	O5-C1	2.35	1.47	1.43
5	S	2	NAG	O5-C1	-2.35	1.40	1.43
4	M	2	NAG	O5-C1	2.35	1.47	1.43
4	I	2	NAG	O5-C1	2.25	1.47	1.43
5	O	1	NAG	O5-C1	2.16	1.47	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	1	NAG	C1-O5-C5	2.82	116.01	112.19
4	Q	1	NAG	C1-O5-C5	2.60	115.72	112.19
4	U	1	NAG	C1-O5-C5	2.57	115.67	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	T	1	NAG	C1-O5-C5	2.49	115.57	112.19
5	S	1	NAG	C1-O5-C5	2.43	115.49	112.19
4	J	4	MAN	O2-C2-C3	-2.41	105.31	110.14
4	M	1	NAG	C1-O5-C5	2.37	115.41	112.19
4	N	4	MAN	O2-C2-C3	-2.36	105.41	110.14
4	M	4	MAN	O2-C2-C3	-2.35	105.42	110.14
4	Q	4	MAN	O2-C2-C3	-2.35	105.42	110.14
4	V	4	MAN	O2-C2-C3	-2.34	105.45	110.14
5	X	1	NAG	C1-O5-C5	2.29	115.29	112.19
4	I	1	NAG	C1-O5-C5	2.29	115.29	112.19
4	I	4	MAN	O2-C2-C3	-2.25	105.63	110.14
4	U	4	MAN	O2-C2-C3	-2.24	105.64	110.14
4	R	4	MAN	O2-C2-C3	-2.24	105.64	110.14
5	P	1	NAG	C1-O5-C5	2.17	115.13	112.19
4	N	4	MAN	C1-O5-C5	2.15	115.11	112.19
5	W	1	NAG	C1-O5-C5	2.15	115.10	112.19
4	Q	4	MAN	C1-O5-C5	2.13	115.08	112.19
4	J	4	MAN	C1-O5-C5	2.12	115.06	112.19
4	I	4	MAN	C1-O5-C5	2.10	115.04	112.19
4	U	4	MAN	C1-O5-C5	2.10	115.03	112.19
4	M	4	MAN	C1-O5-C5	2.09	115.03	112.19
4	R	4	MAN	C1-O5-C5	2.08	115.00	112.19
5	K	1	NAG	C1-O5-C5	2.05	114.97	112.19
4	V	4	MAN	C1-O5-C5	2.03	114.94	112.19
5	L	1	NAG	C1-O5-C5	2.00	114.91	112.19

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	2	NAG	C4-C5-C6-O6
4	R	1	NAG	O5-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
5	X	1	NAG	O5-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
4	I	3	BMA	C4-C5-C6-O6
4	M	3	BMA	O5-C5-C6-O6
5	P	1	NAG	O5-C5-C6-O6
4	R	4	MAN	C4-C5-C6-O6
5	L	2	NAG	C4-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	J	2	NAG	O5-C5-C6-O6
5	L	2	NAG	O5-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
4	R	4	MAN	O5-C5-C6-O6
4	M	3	BMA	C4-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
5	X	1	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	J	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
4	N	1	NAG	C8-C7-N2-C2
4	N	1	NAG	O7-C7-N2-C2
4	N	2	NAG	C8-C7-N2-C2
4	N	2	NAG	O7-C7-N2-C2
4	R	1	NAG	C8-C7-N2-C2
4	R	1	NAG	O7-C7-N2-C2
4	R	2	NAG	C8-C7-N2-C2
4	R	2	NAG	O7-C7-N2-C2
4	V	1	NAG	C8-C7-N2-C2
4	V	1	NAG	O7-C7-N2-C2
4	V	2	NAG	C8-C7-N2-C2
4	V	2	NAG	O7-C7-N2-C2
5	K	1	NAG	C8-C7-N2-C2
5	K	1	NAG	O7-C7-N2-C2
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
5	O	1	NAG	C8-C7-N2-C2
5	O	1	NAG	O7-C7-N2-C2
5	O	2	NAG	C8-C7-N2-C2
5	O	2	NAG	O7-C7-N2-C2
5	S	1	NAG	C8-C7-N2-C2
5	S	1	NAG	O7-C7-N2-C2
5	S	2	NAG	C8-C7-N2-C2
5	S	2	NAG	O7-C7-N2-C2
5	W	1	NAG	C8-C7-N2-C2
5	W	1	NAG	O7-C7-N2-C2
5	W	2	NAG	C8-C7-N2-C2
5	W	2	NAG	O7-C7-N2-C2
4	V	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	P	1	NAG	C4-C5-C6-O6
4	I	3	BMA	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6
5	S	2	NAG	O5-C5-C6-O6
5	T	2	NAG	C4-C5-C6-O6
5	O	2	NAG	C4-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
5	S	2	NAG	C4-C5-C6-O6
4	V	4	MAN	O5-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
4	N	4	MAN	O5-C5-C6-O6
4	J	4	MAN	O5-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
5	W	1	NAG	C4-C5-C6-O6
4	I	1	NAG	C1-C2-N2-C7
5	L	1	NAG	O5-C5-C6-O6
5	L	2	NAG	C1-C2-N2-C7
5	T	2	NAG	C3-C2-N2-C7
5	X	2	NAG	C3-C2-N2-C7
4	I	1	NAG	C3-C2-N2-C7
5	L	2	NAG	C3-C2-N2-C7
5	P	2	NAG	C3-C2-N2-C7
5	W	1	NAG	O5-C5-C6-O6
5	P	2	NAG	C1-C2-N2-C7

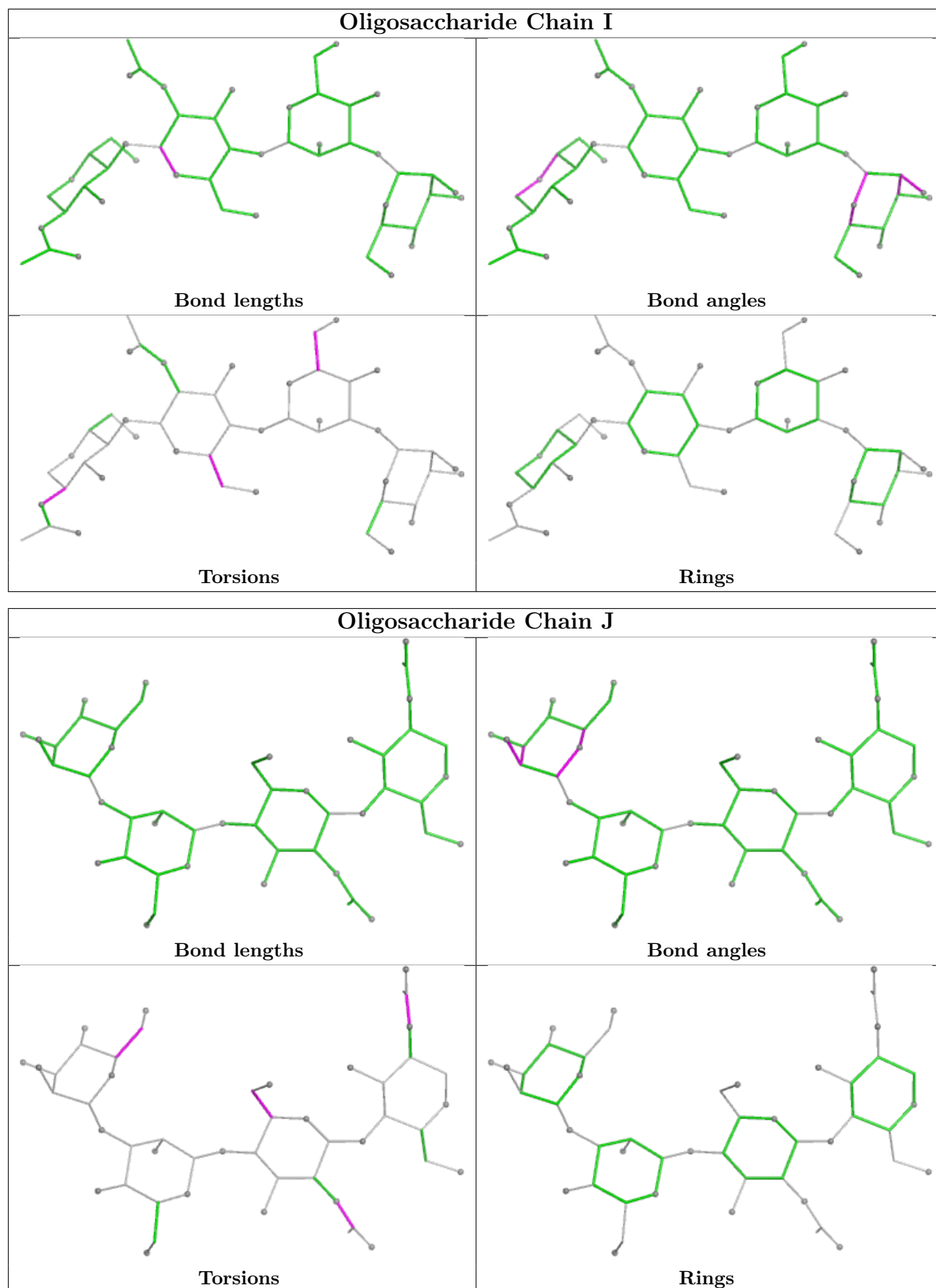
There are no ring outliers.

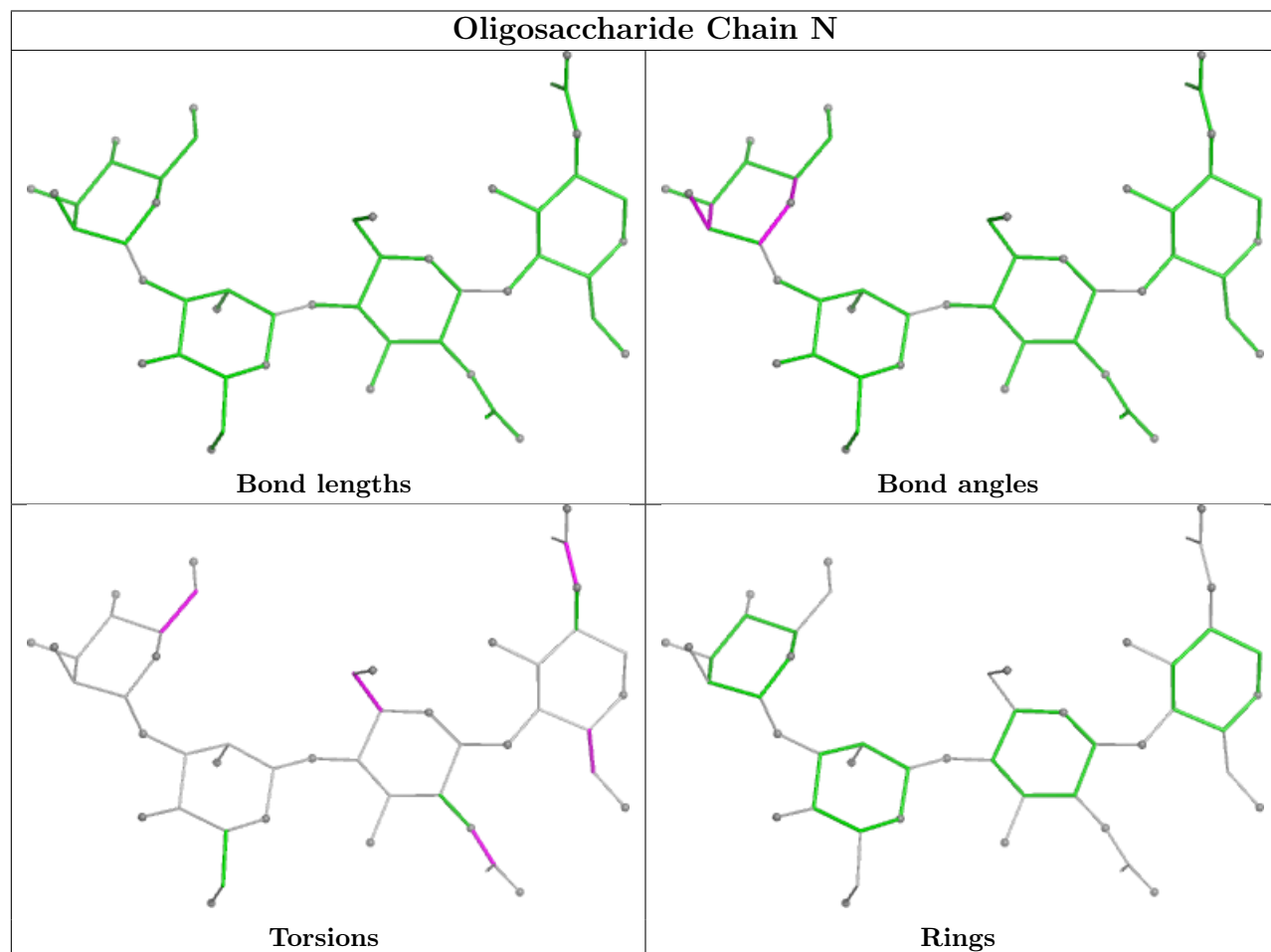
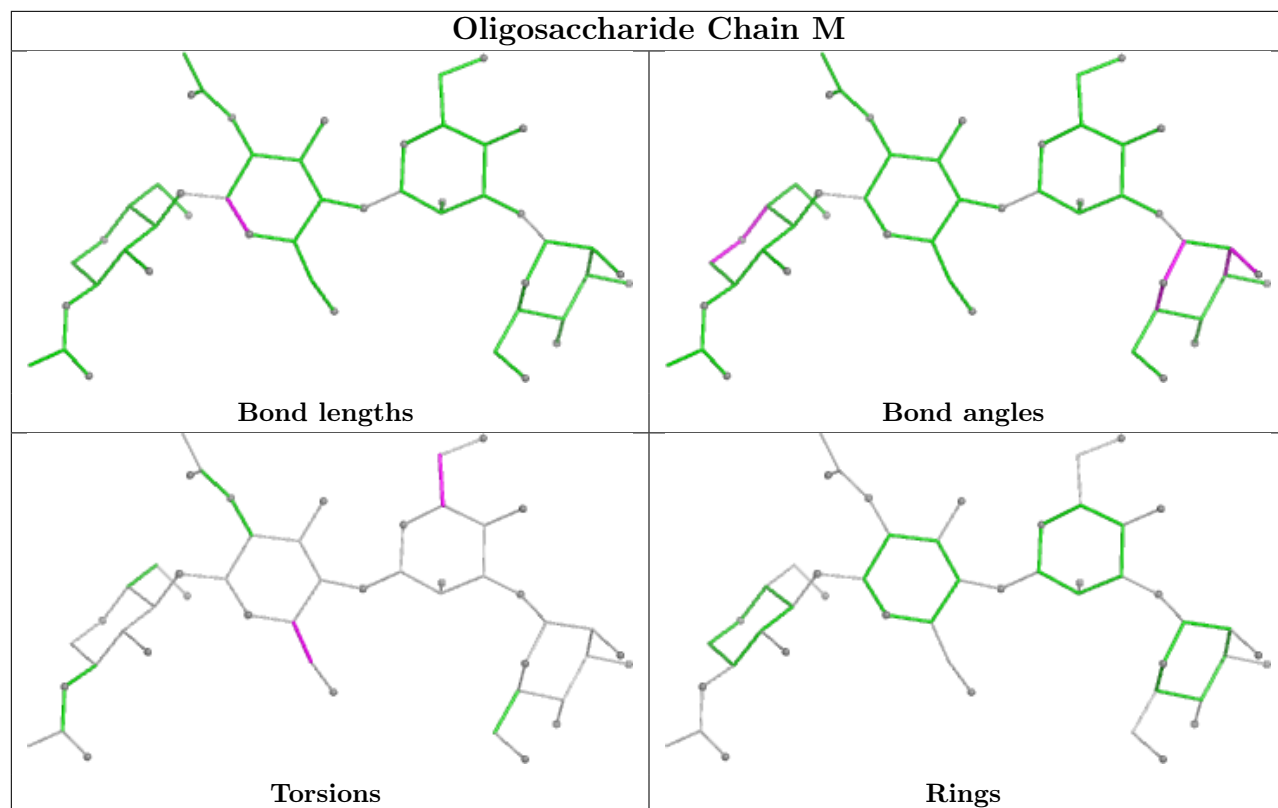
6 monomers are involved in 5 short contacts:

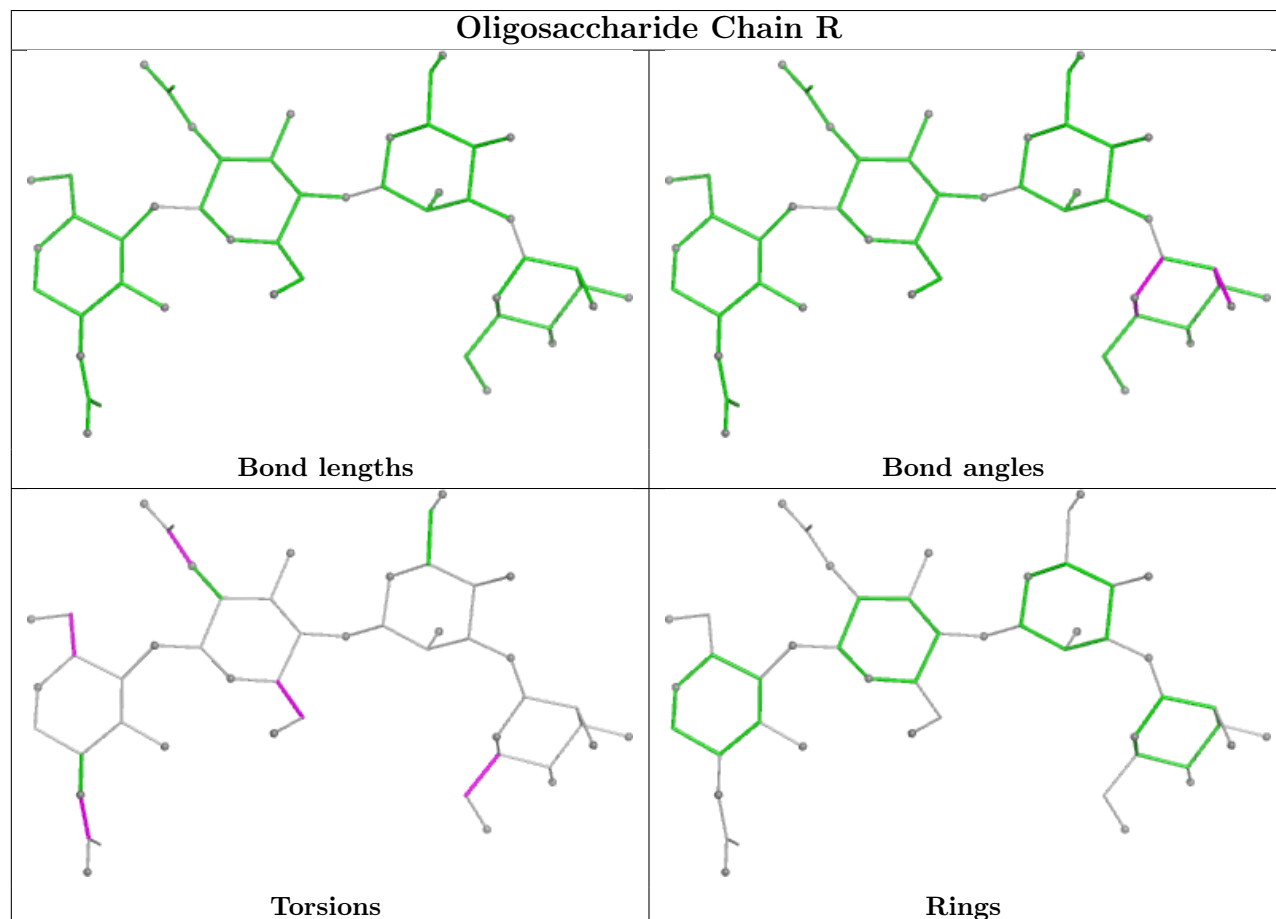
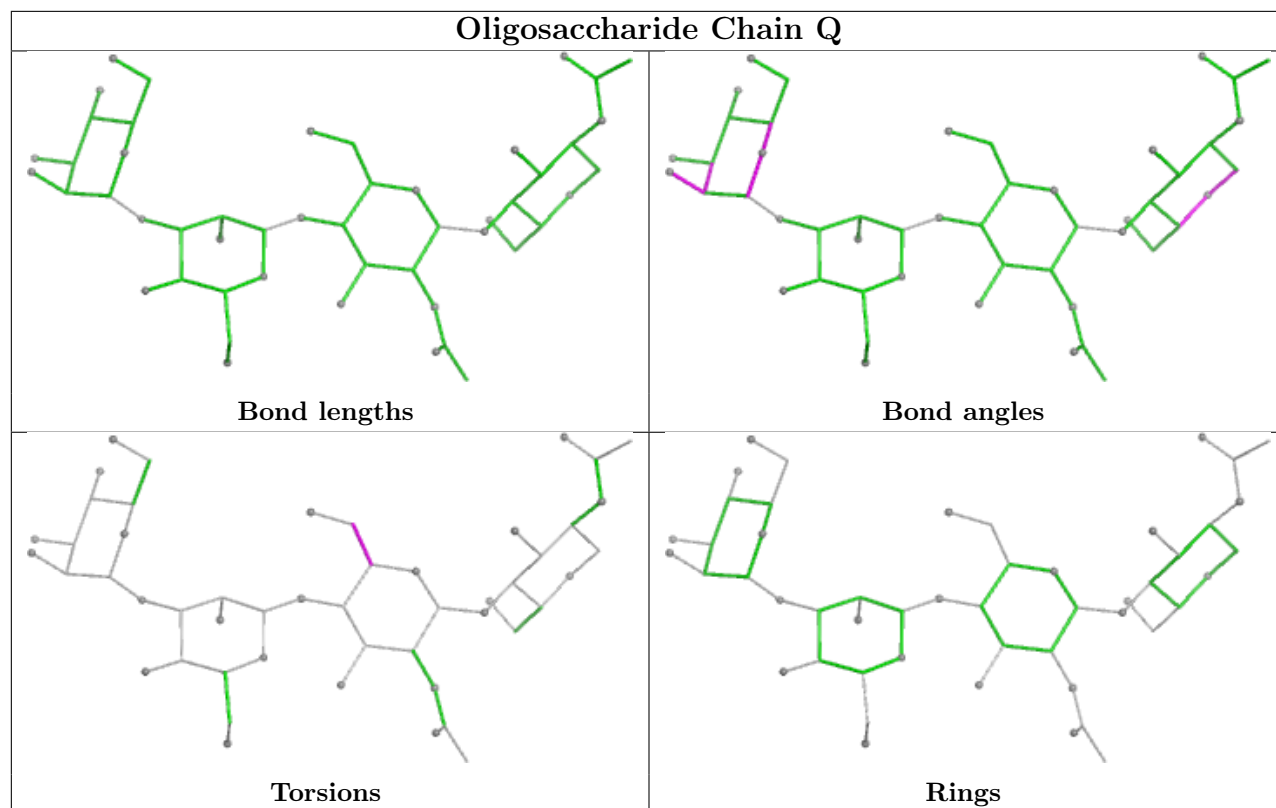
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	S	1	NAG	1	0
5	S	2	NAG	1	0
5	P	1	NAG	1	0
5	L	1	NAG	1	0
4	V	1	NAG	1	0
5	O	1	NAG	1	0

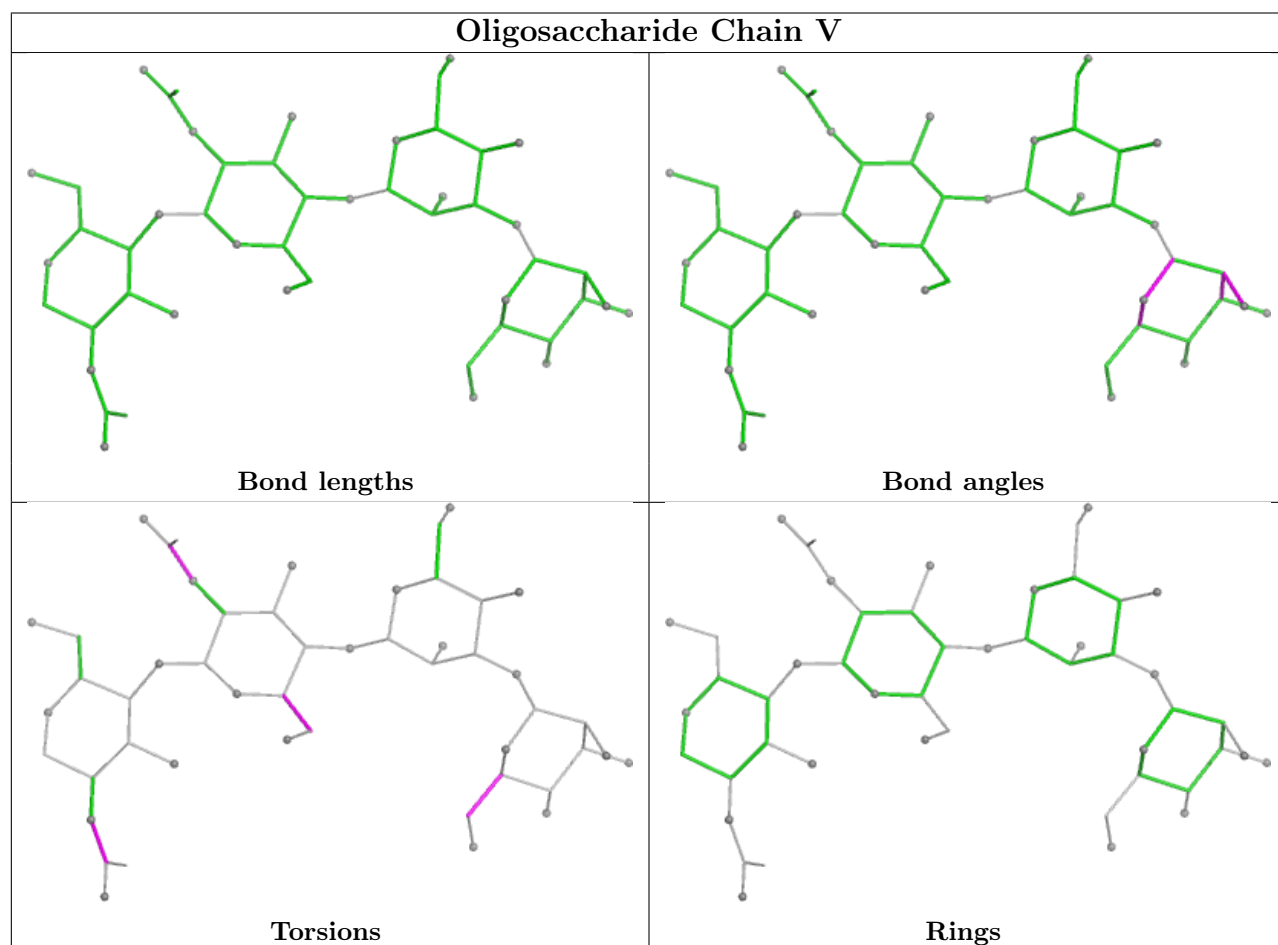
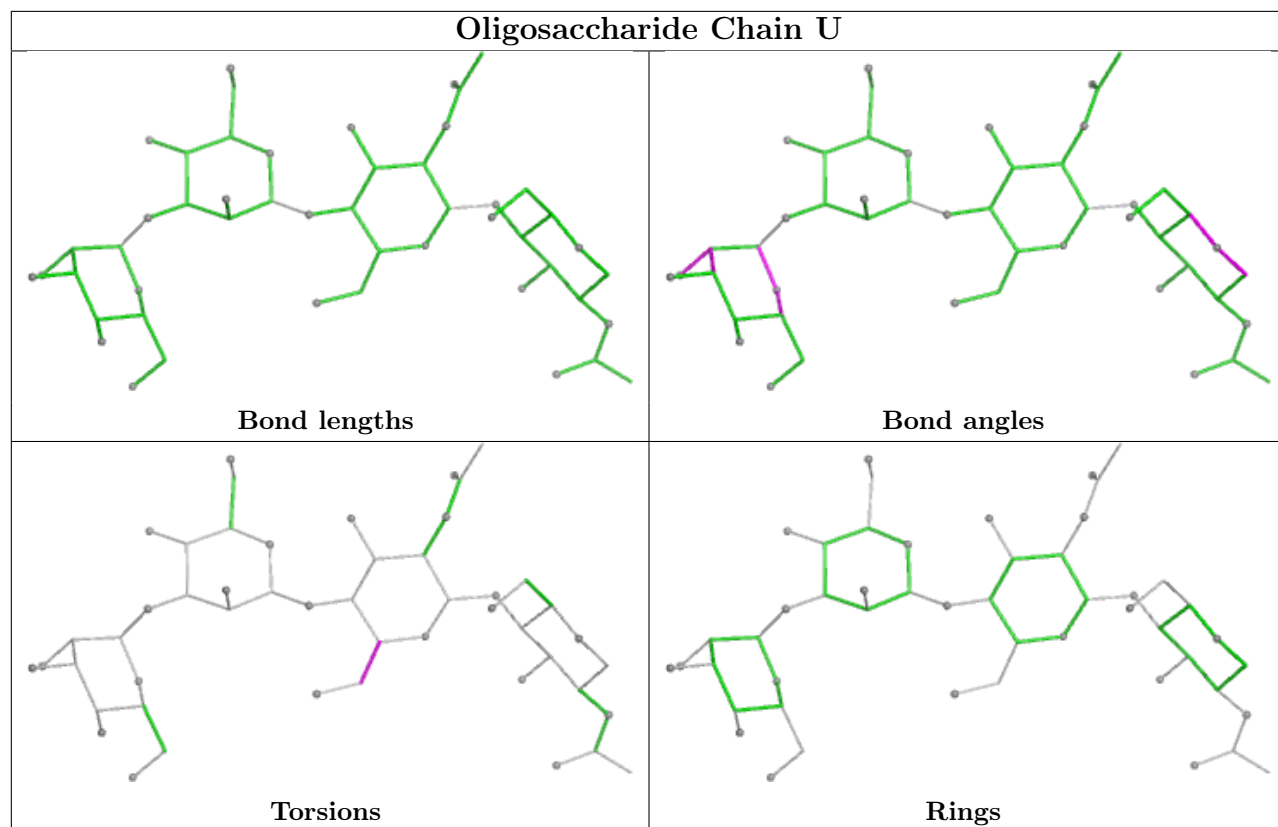
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

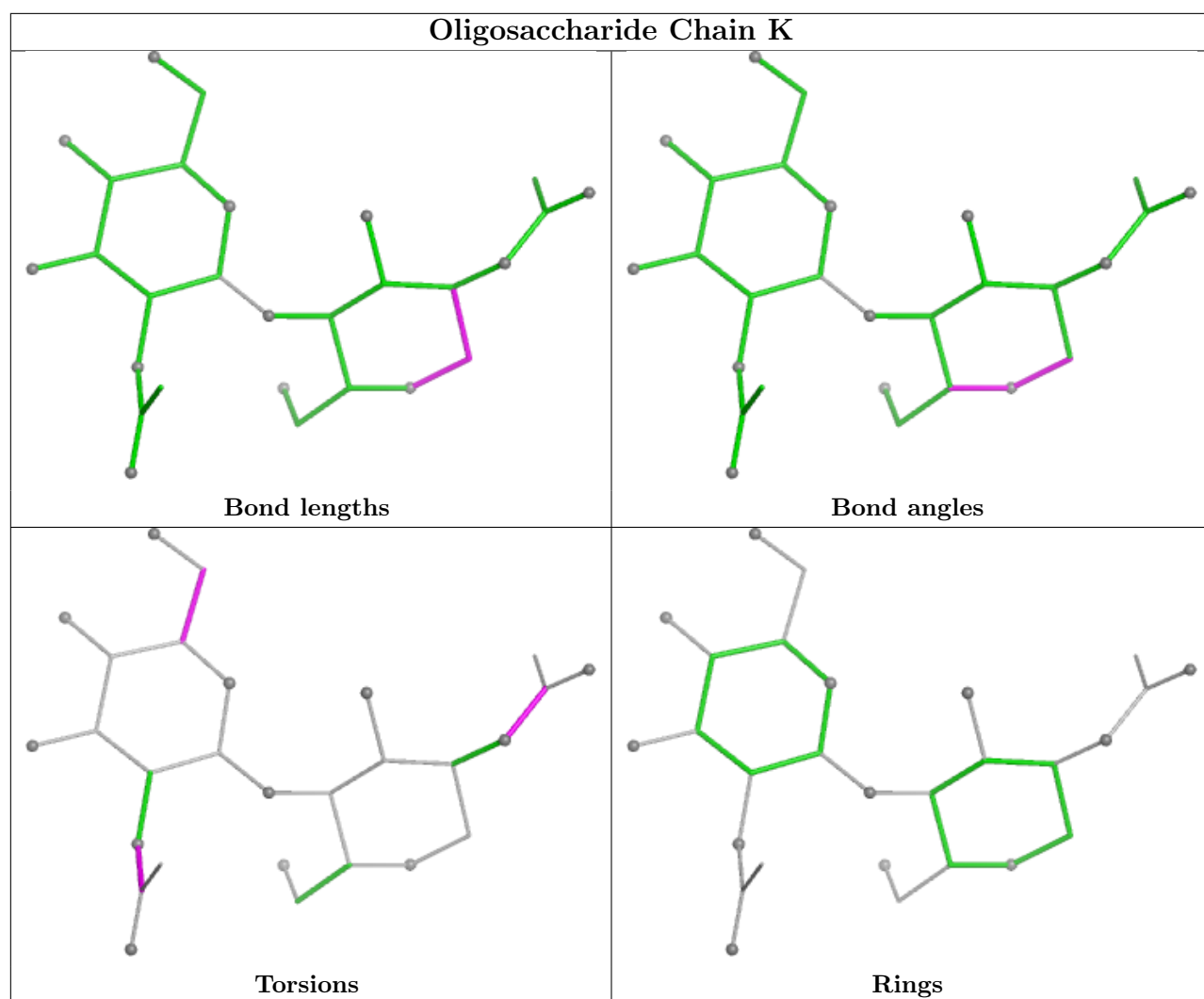
bond angles, torsion angles, and ring geometry for oligosaccharide.

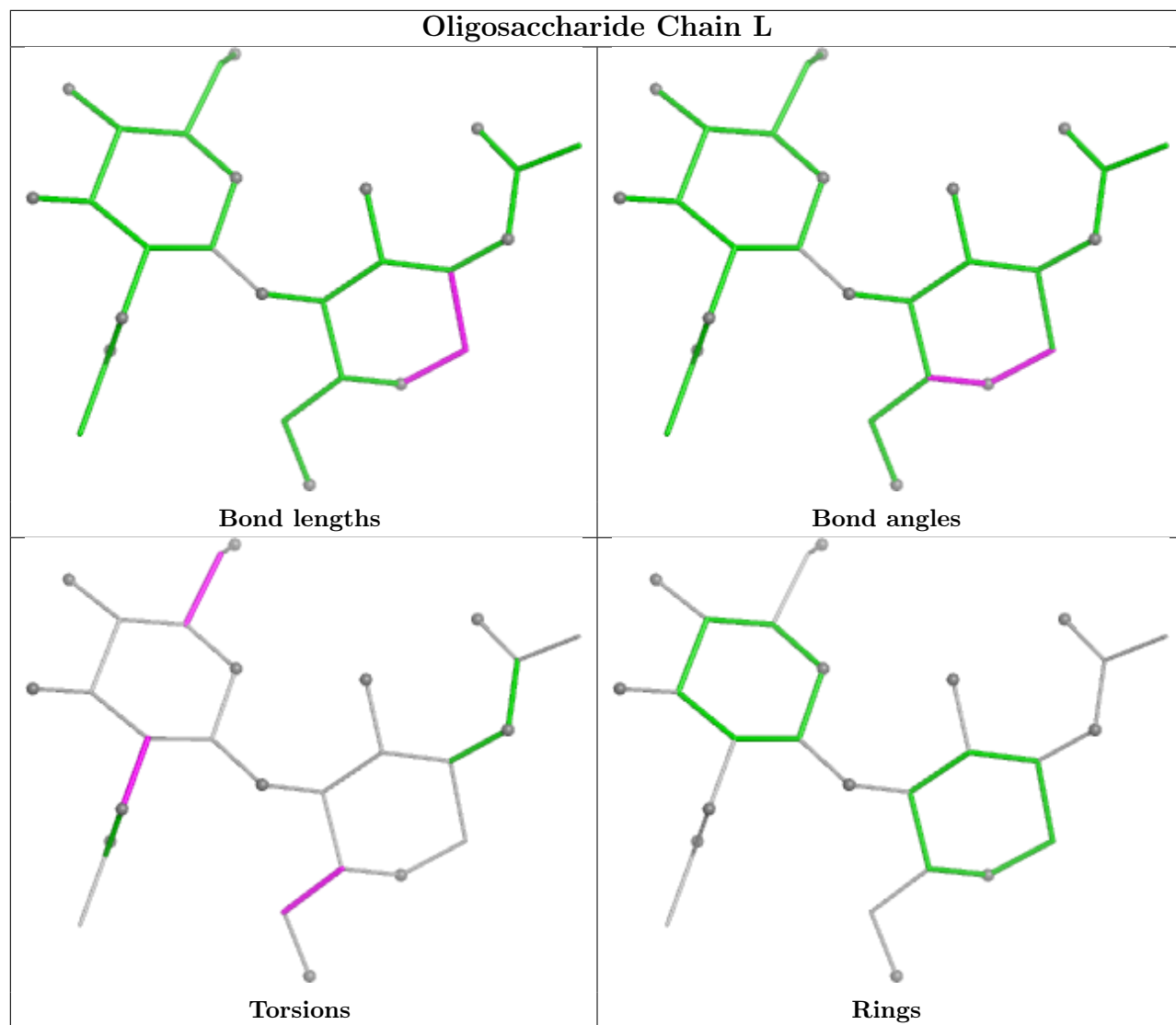


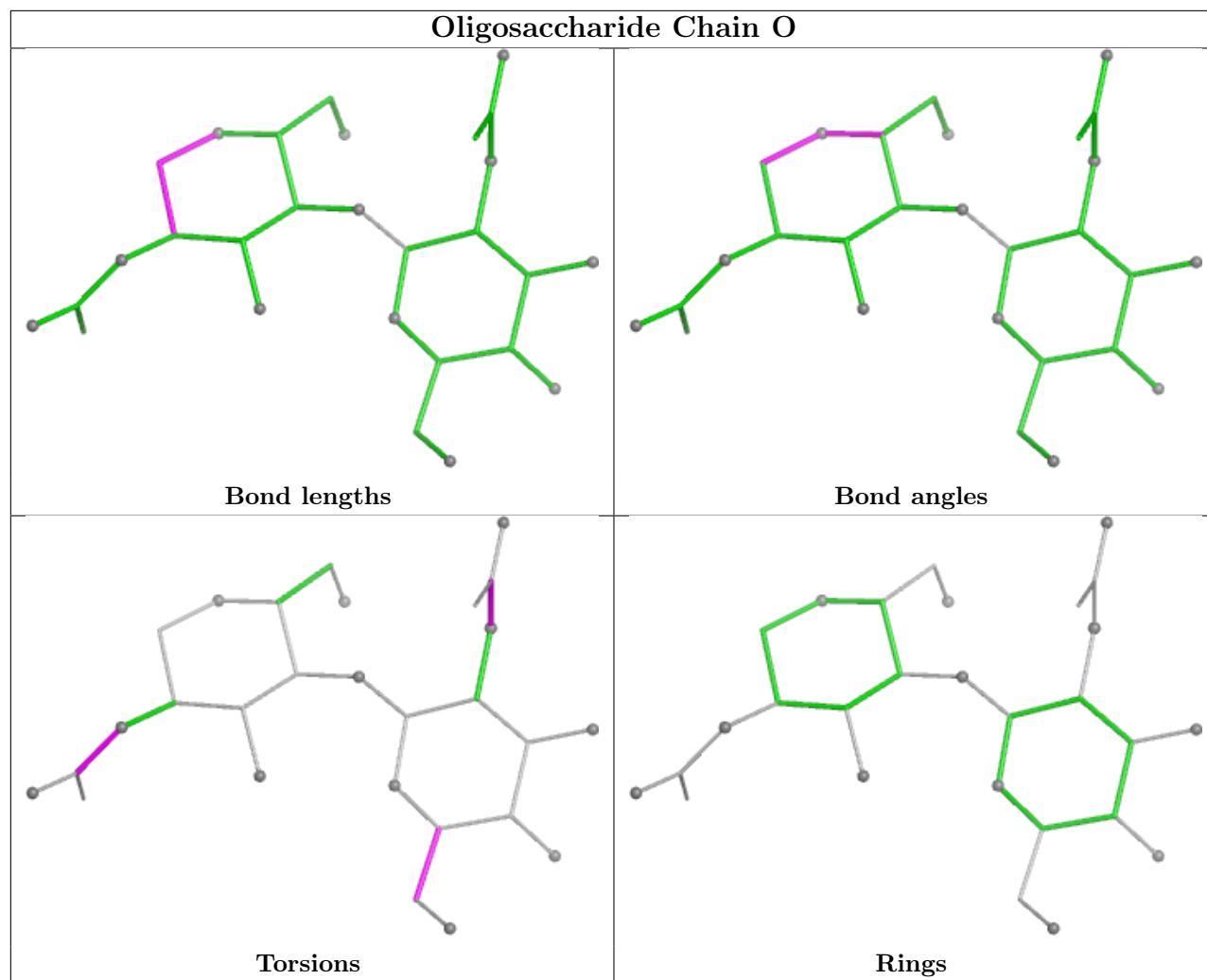


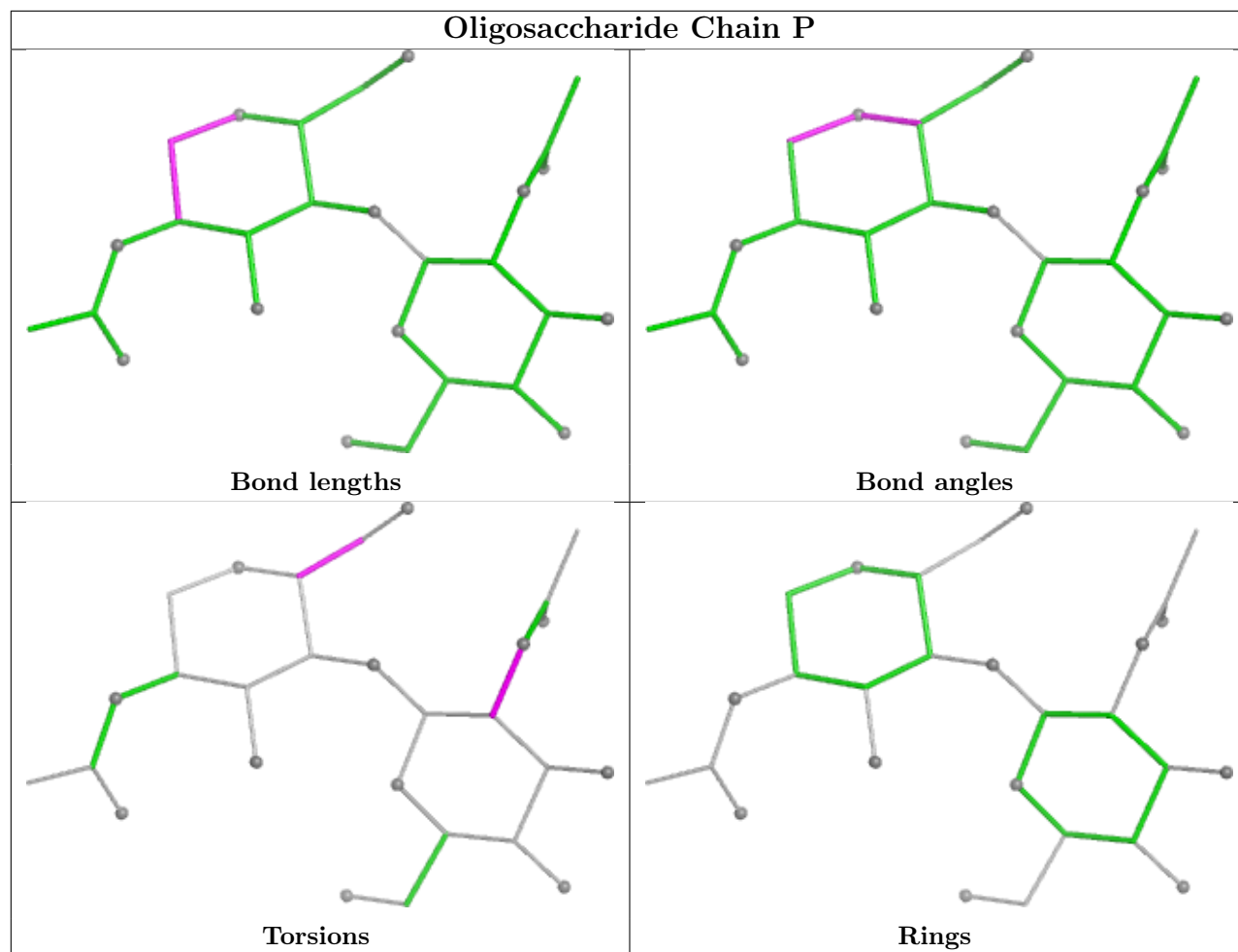


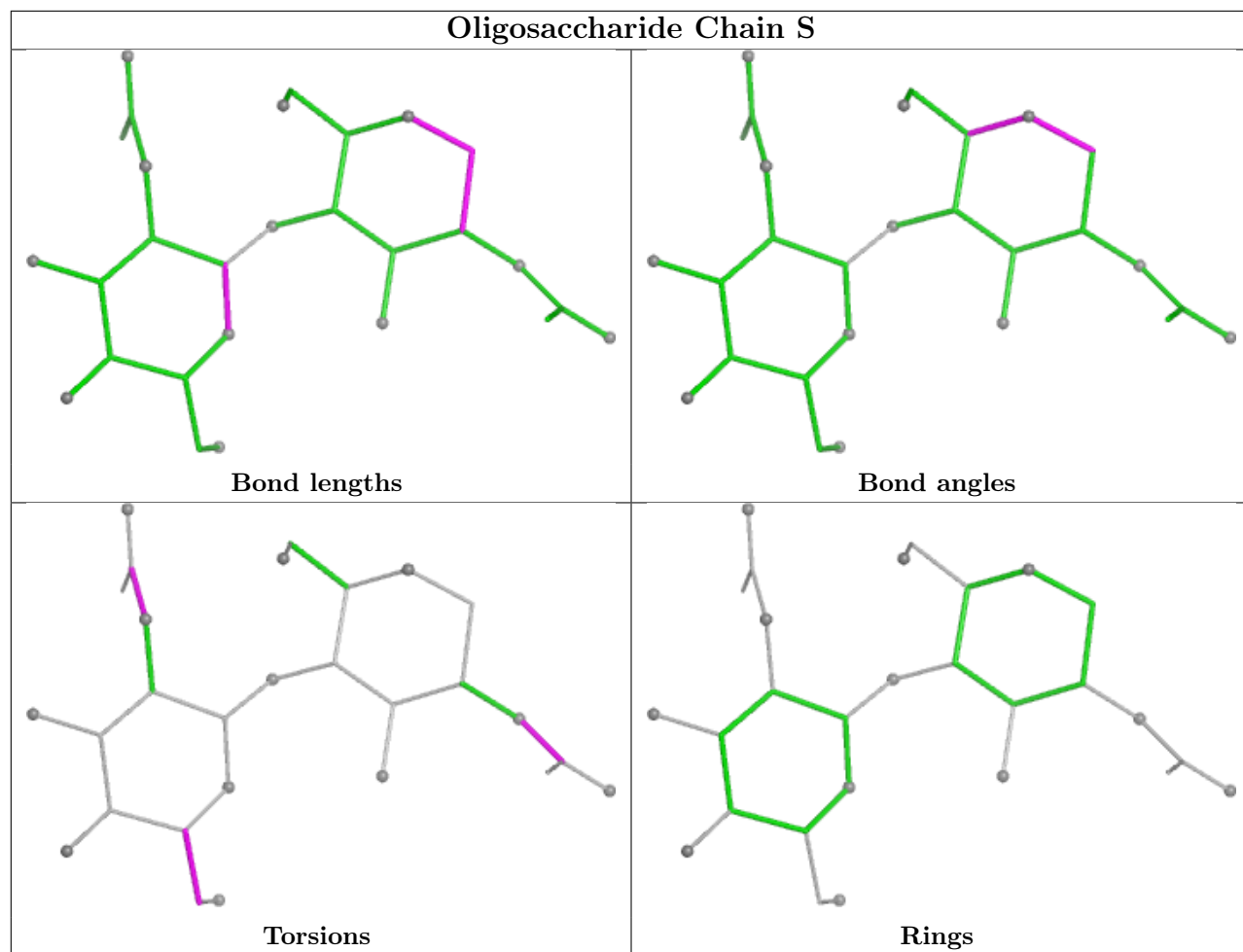


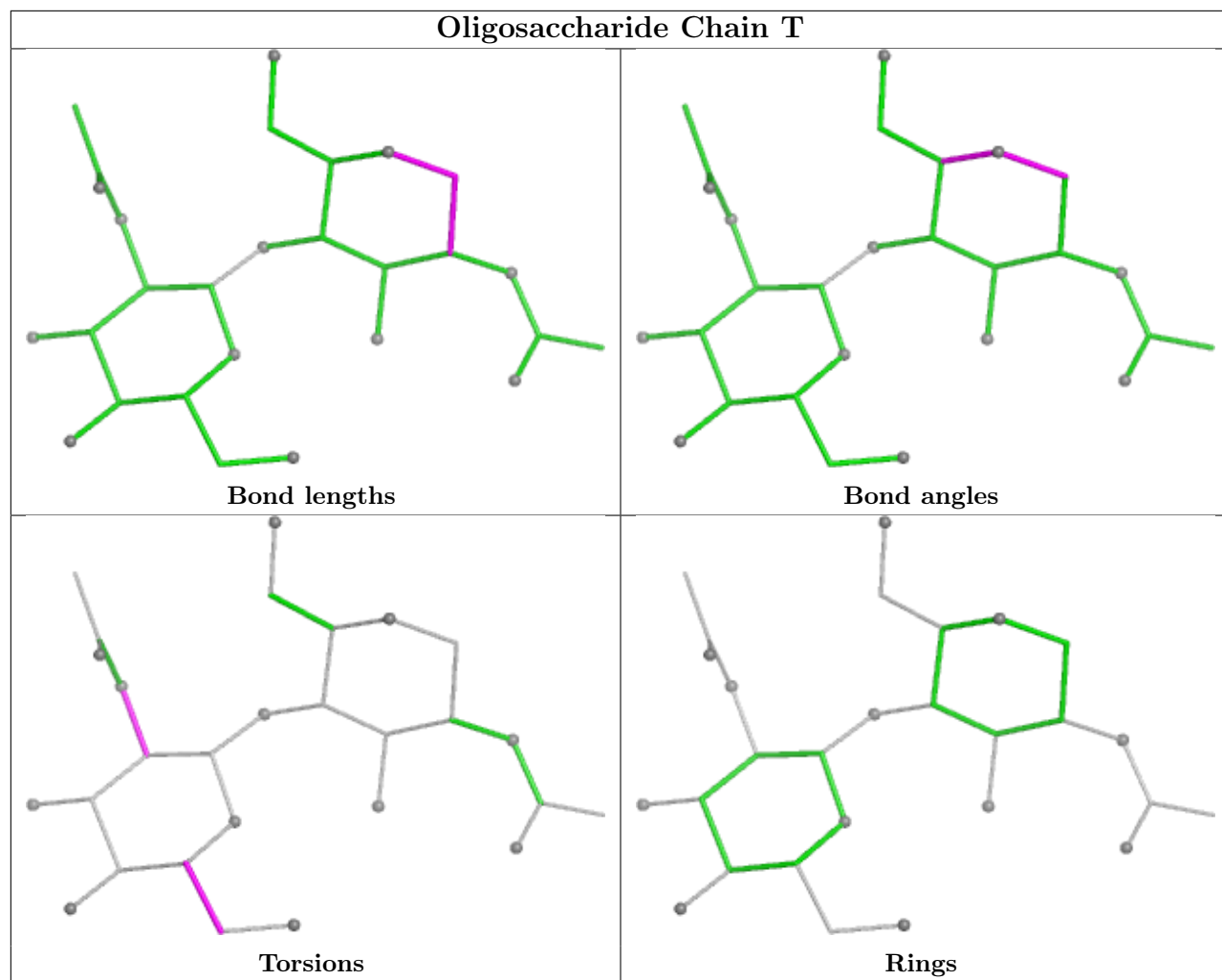


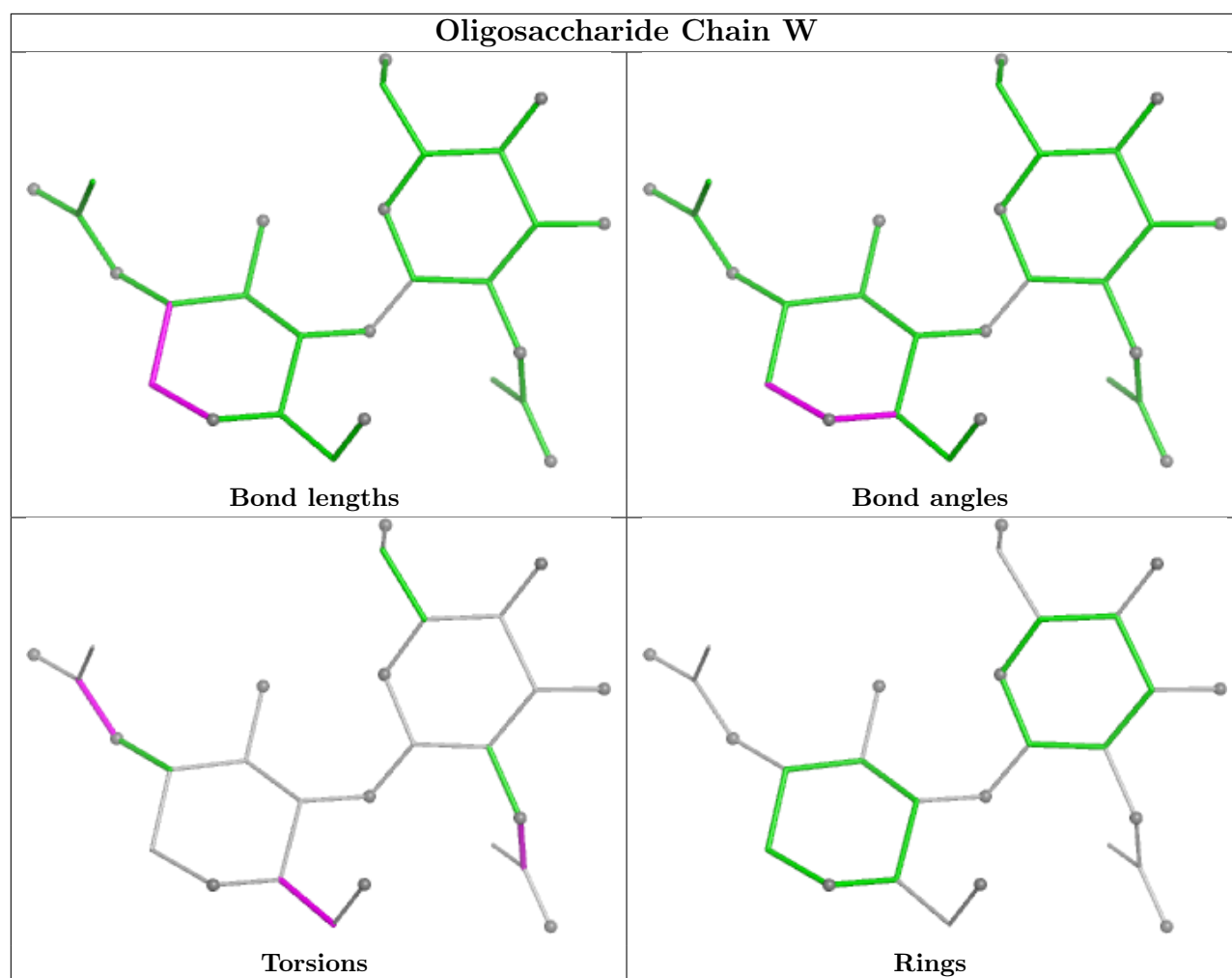


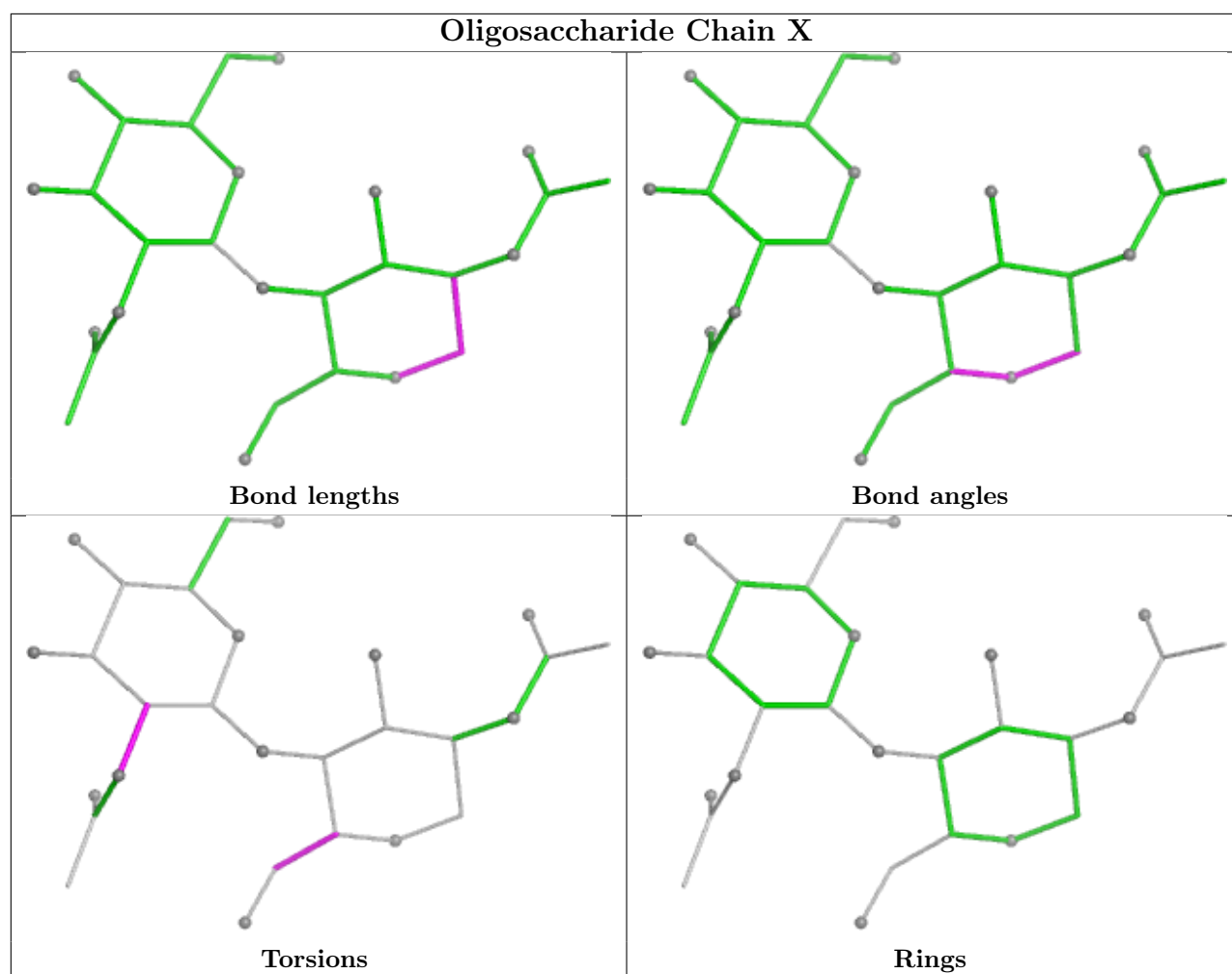












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

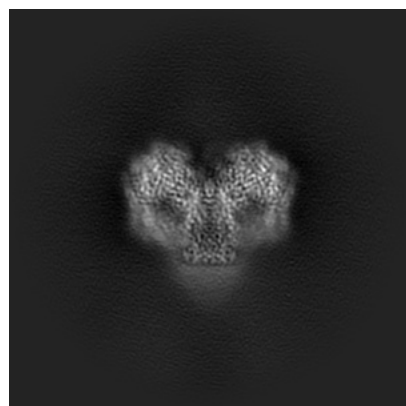
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-58134. These allow visual inspection of the internal detail of the map and identification of artifacts.

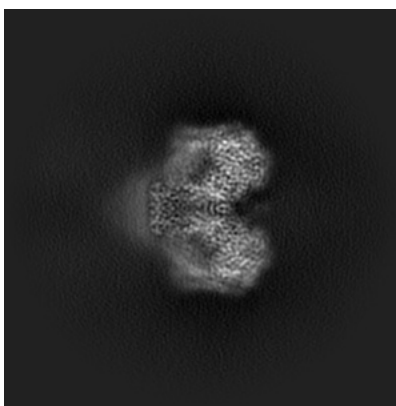
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

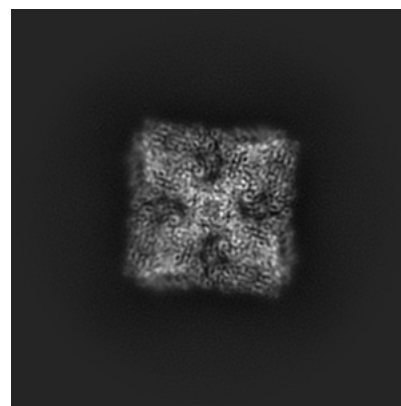
6.1.1 Primary map



X

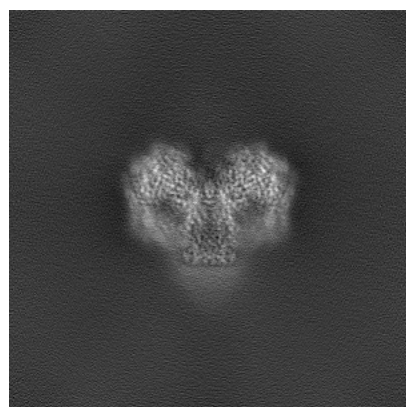


Y

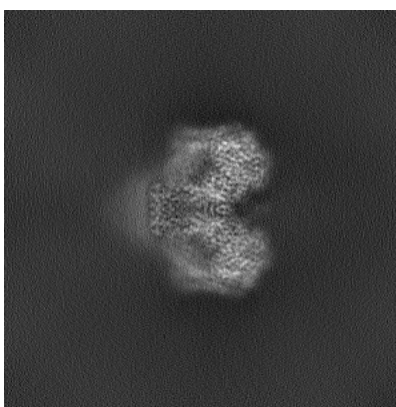


Z

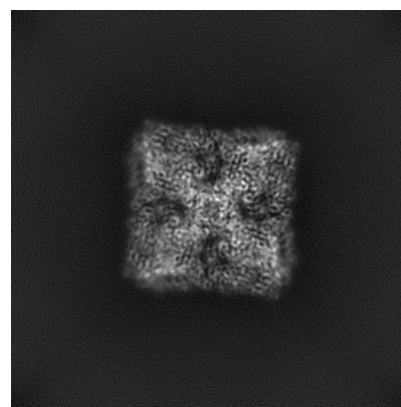
6.1.2 Raw map



X



Y

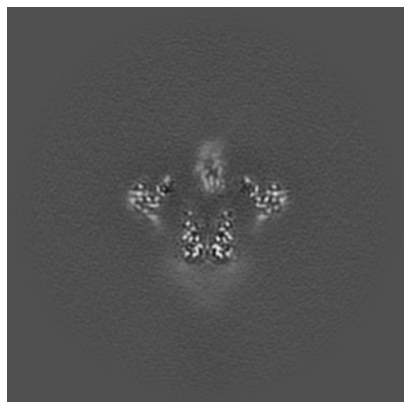


Z

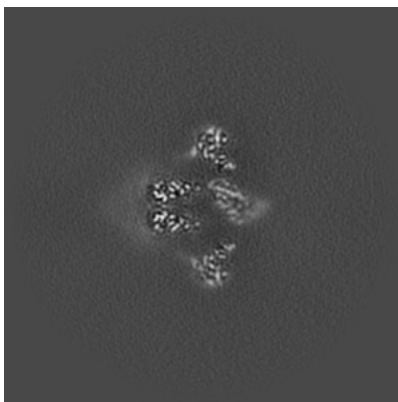
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

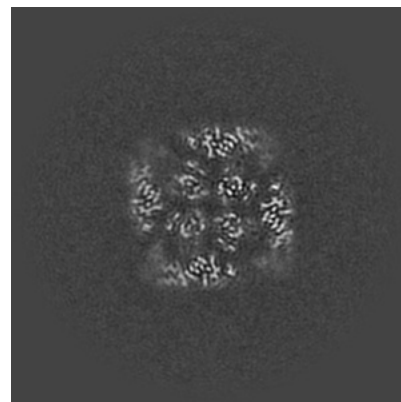
6.2.1 Primary map



X Index: 208

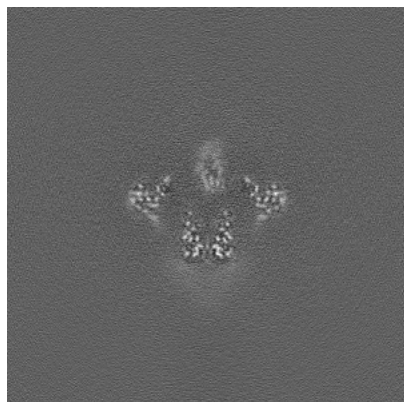


Y Index: 208

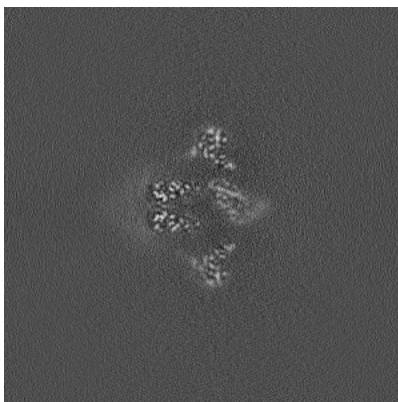


Z Index: 208

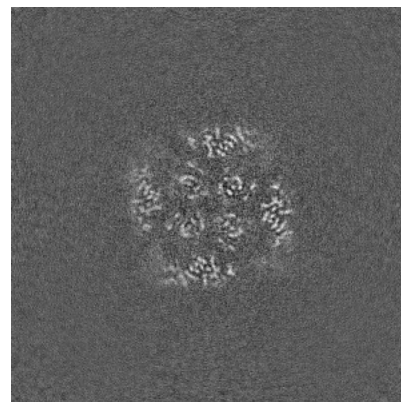
6.2.2 Raw map



X Index: 208



Y Index: 208

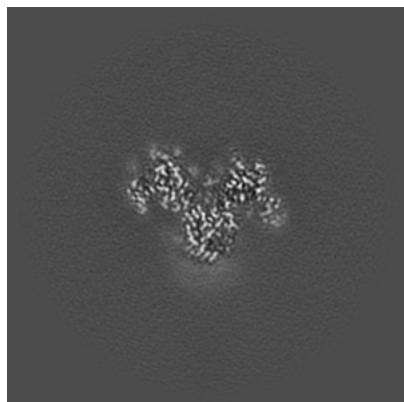


Z Index: 208

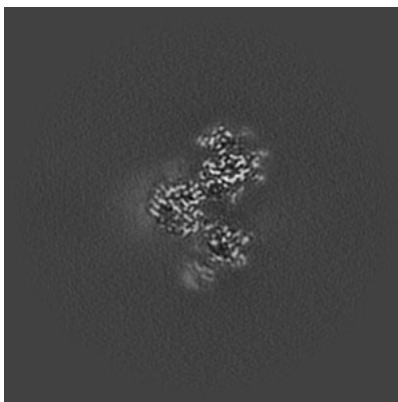
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

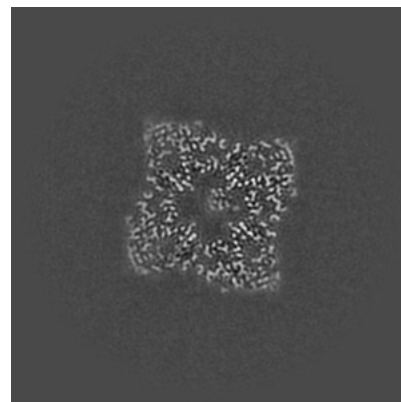
6.3.1 Primary map



X Index: 230

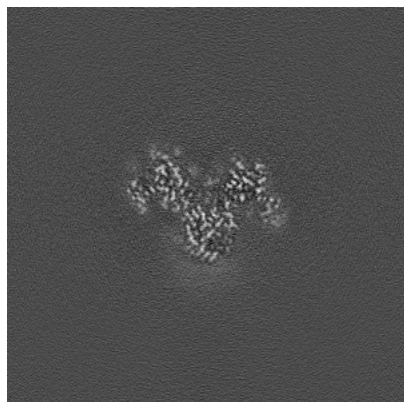


Y Index: 230

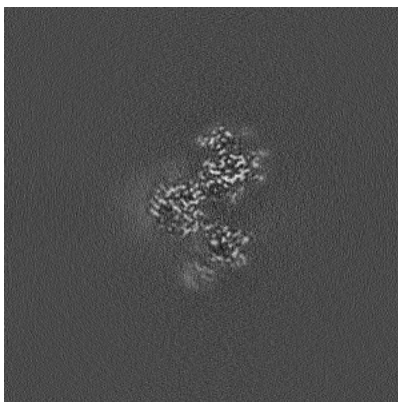


Z Index: 229

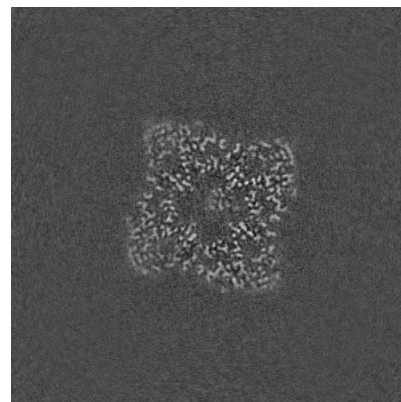
6.3.2 Raw map



X Index: 230



Y Index: 230

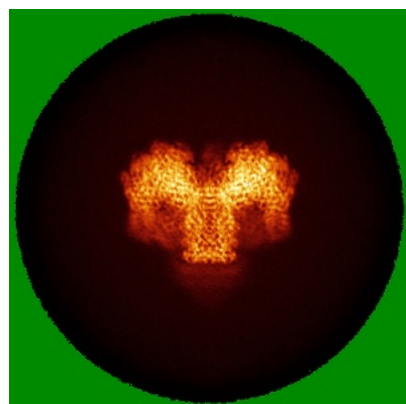


Z Index: 229

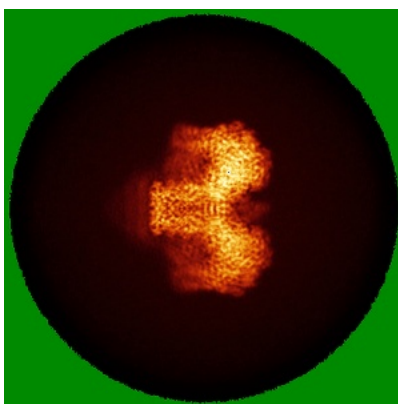
The images above show the largest variance slices of the map in three orthogonal directions.

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

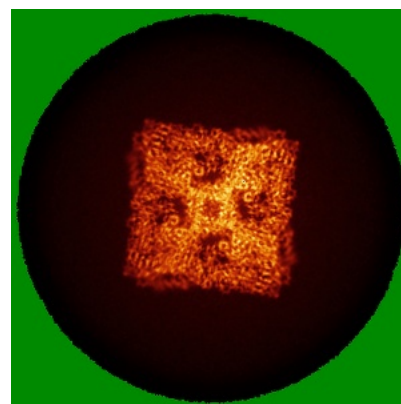
6.4.1 Primary map



X

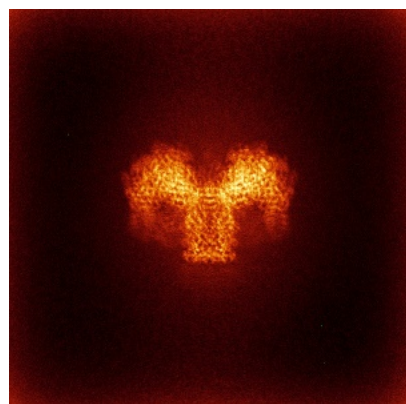


Y

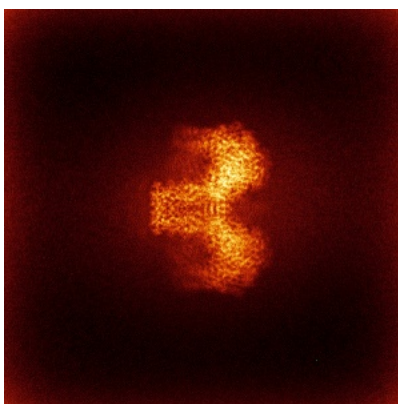


Z

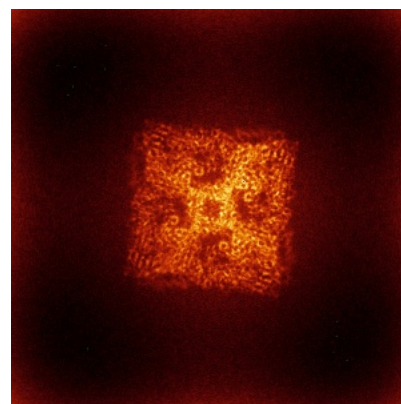
6.4.2 Raw map



X



Y

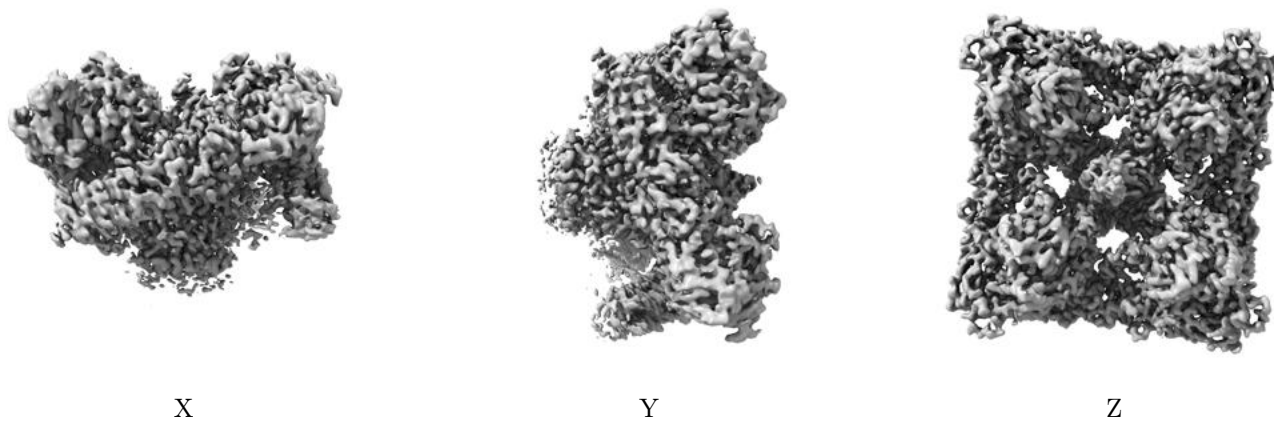


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

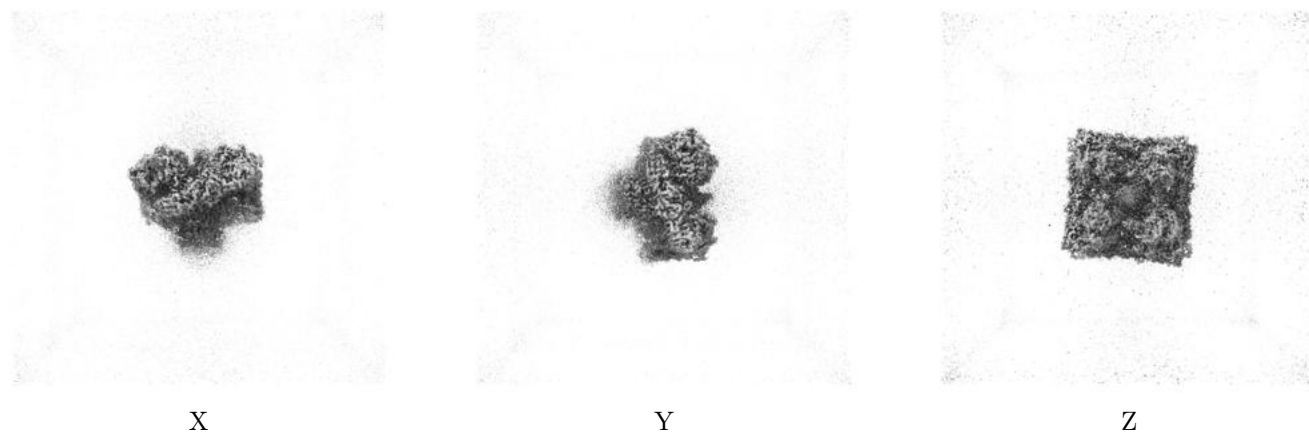
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

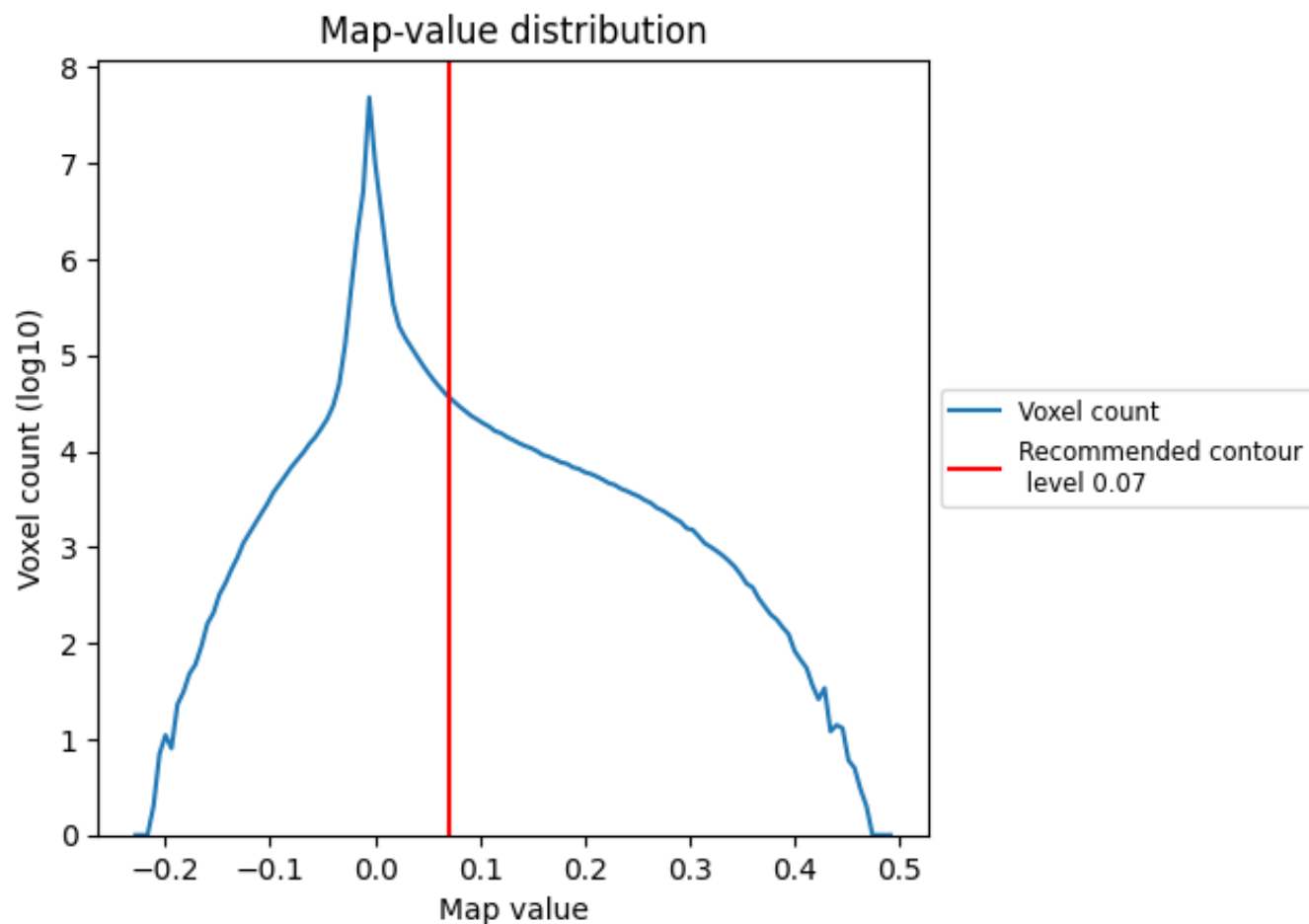
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

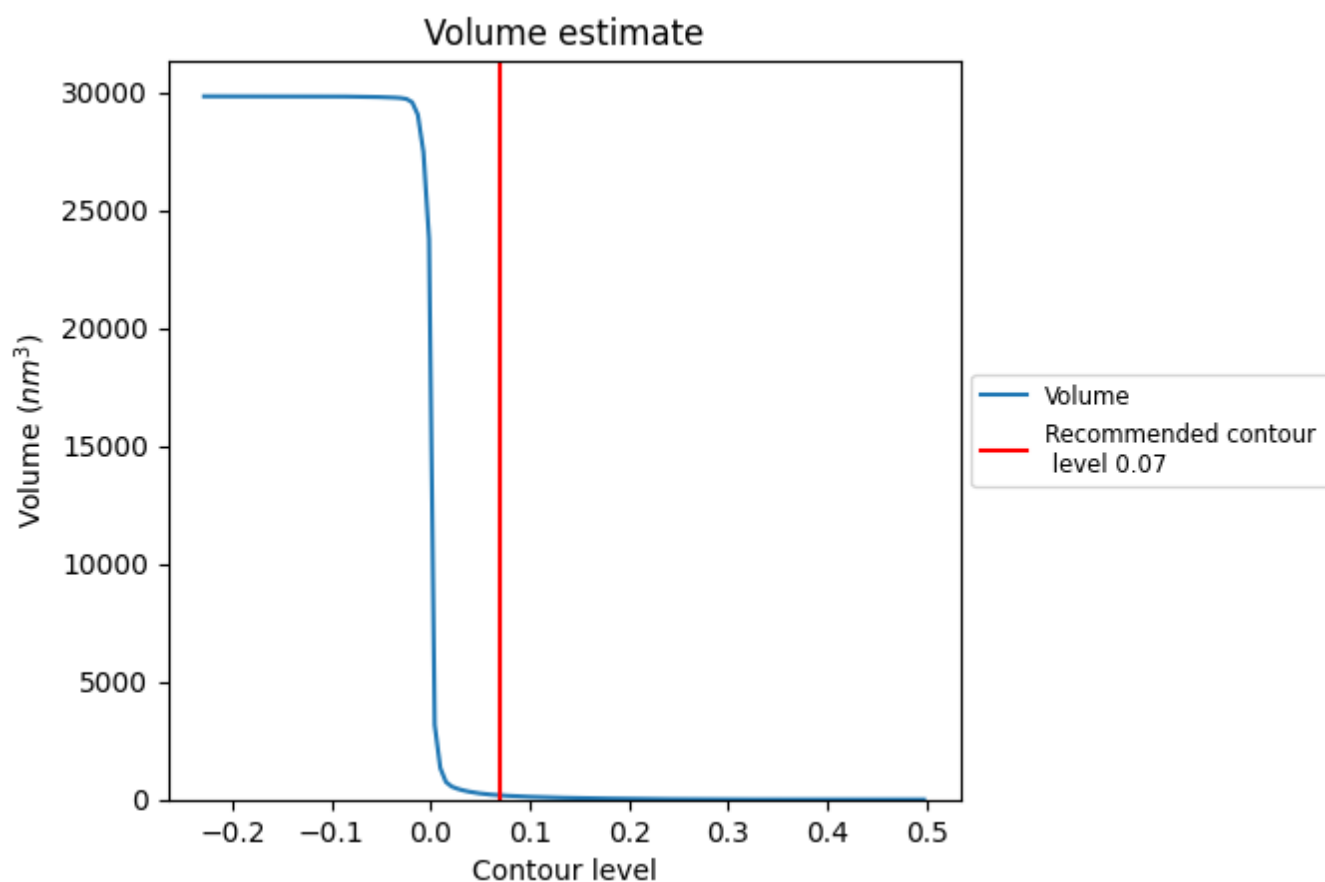
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

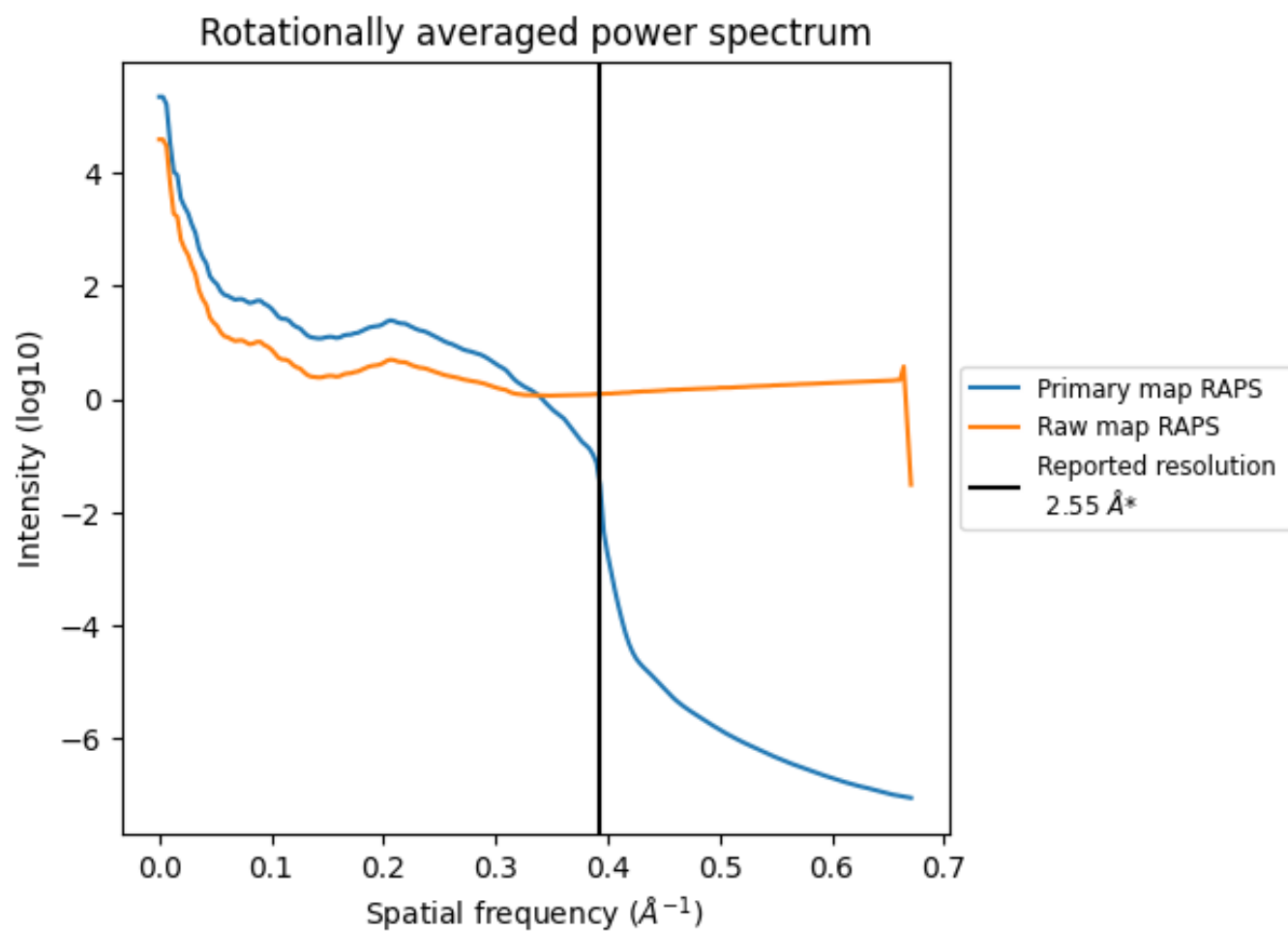
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 180 nm³; this corresponds to an approximate mass of 163 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 ⓘ

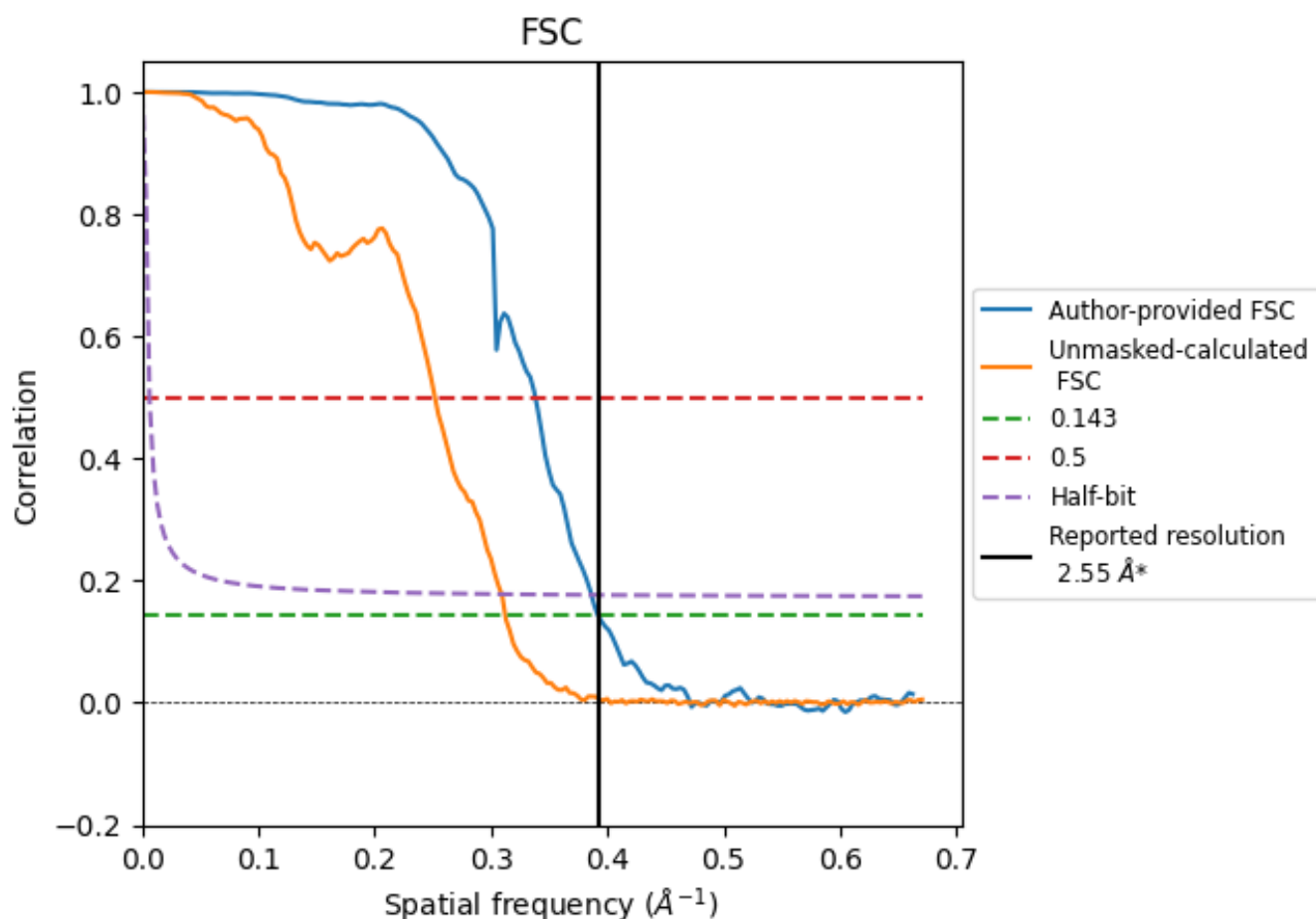


*Reported resolution corresponds to spatial frequency of 0.392 Å⁻¹

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 0.392 Å⁻¹

8.2 Resolution estimates [i](#)

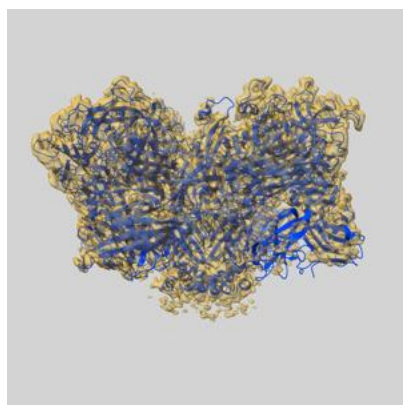
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.55	-	-
Author-provided FSC curve	2.55	2.96	2.59
Unmasked-calculated*	3.20	3.97	3.23

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.20 differs from the reported value 2.55 by more than 10 %

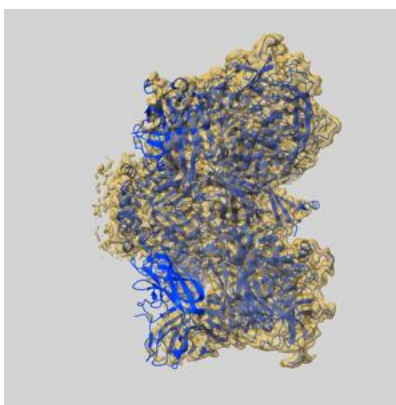
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-58134 and PDB model 30XT. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

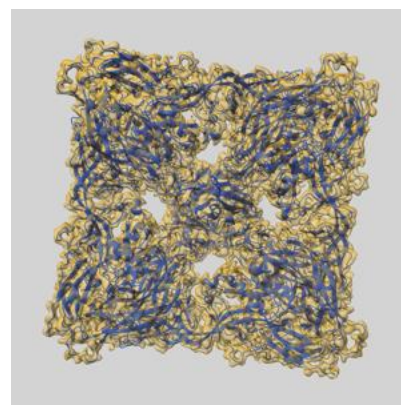
9.1 Map-model overlay [i](#)



X



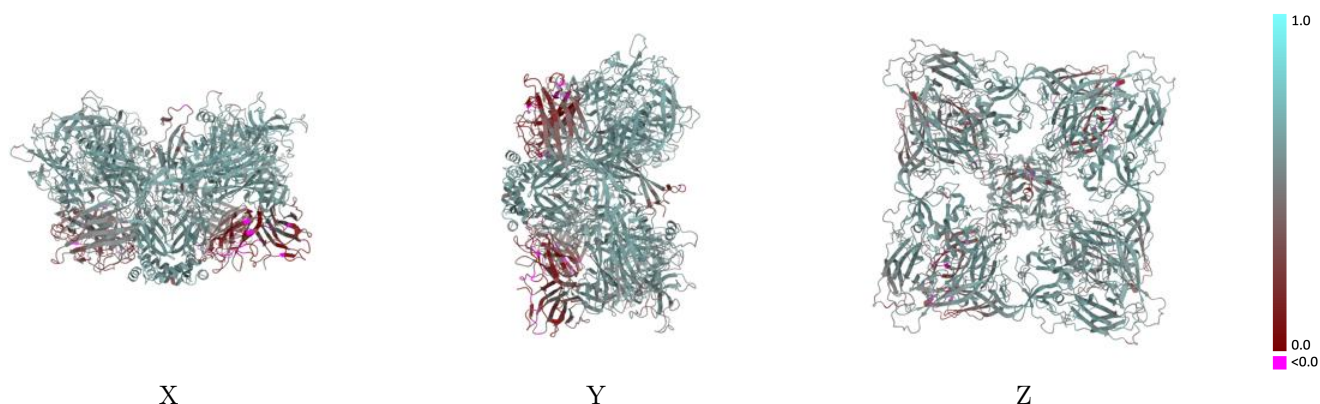
Y



Z

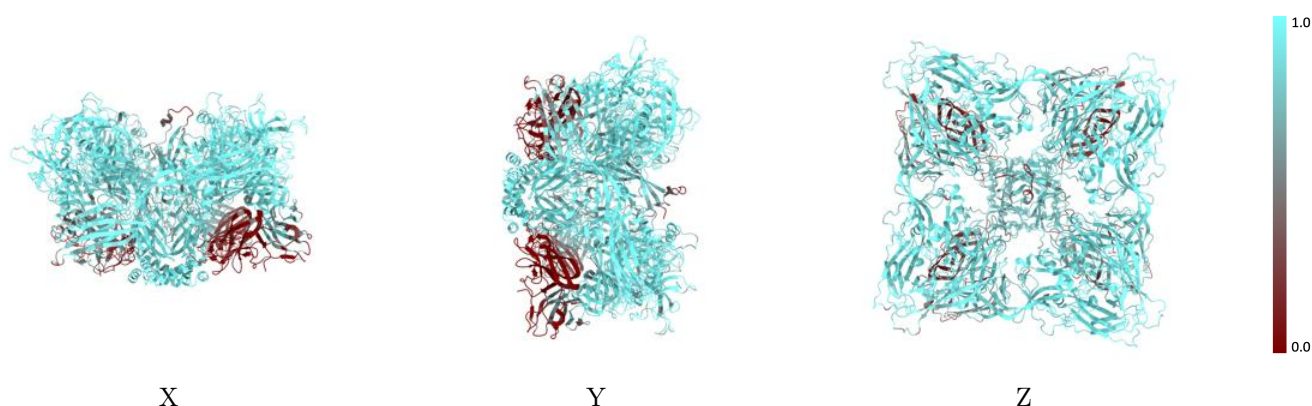
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



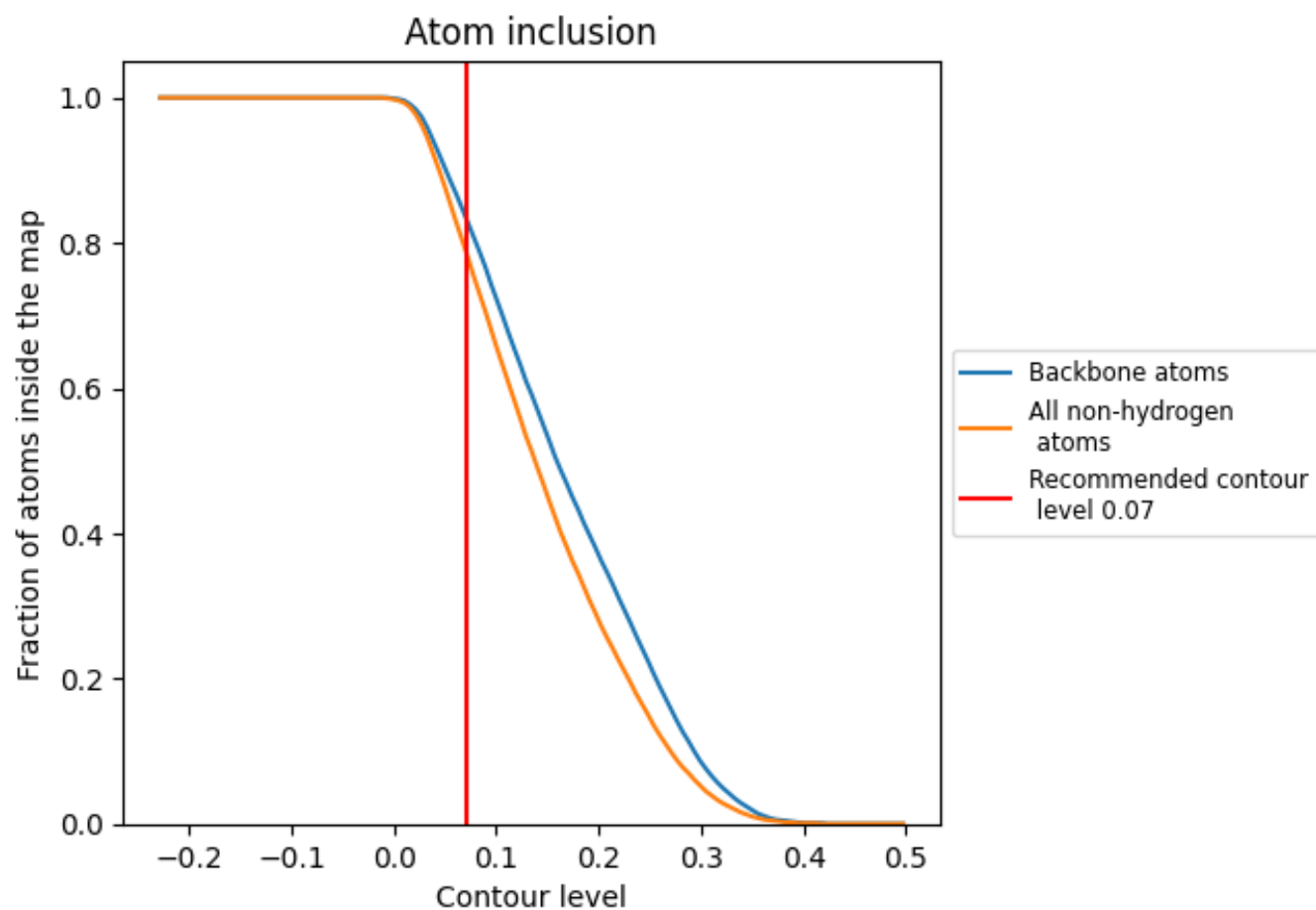
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7890	 0.5180
A	 0.9600	 0.6140
B	 0.7650	 0.5140
C	 0.9400	 0.5980
D	 0.6250	 0.4150
E	 0.9150	 0.5840
F	 0.5500	 0.4120
G	 0.9140	 0.5810
H	 0.6140	 0.4110
I	 1.0000	 0.5730
J	 1.0000	 0.5850
K	 0.9290	 0.5790
L	 0.6790	 0.4920
M	 0.9200	 0.5580
N	 0.9000	 0.5630
O	 0.8930	 0.5230
P	 0.6790	 0.4510
Q	 0.9200	 0.5120
R	 0.9800	 0.5500
S	 0.7860	 0.5010
T	 0.4640	 0.3340
U	 0.8600	 0.5160
V	 0.9200	 0.5370
W	 0.8570	 0.5030
X	 0.6790	 0.4860
Y	 0.6910	 0.4750

