



Full wwPDB EM Validation Report ⓘ

Mar 16, 2025 – 12:38 AM JST

PDB ID : 8ZGH
EMDB ID : EMD-60079
Title : Human lysine O-link glycosylation complex, LH3/ColGalT1 in its apo state
Authors : Peng, J.; Li, W.; Yao, D.; Xia, Y.; Wang, Q.; Cai, Y.; Li, S.; Cao, M.; Shen, Y.; Ma, P.; Liao, R.; Qin, A.; Cao, Y.
Deposited on : 2024-05-09
Resolution : 3.93 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.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

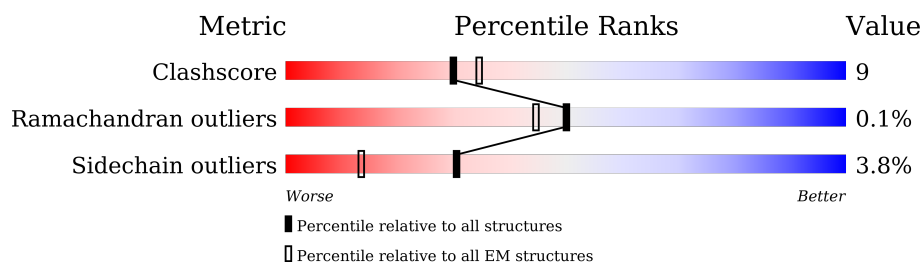
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.93 Å.

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




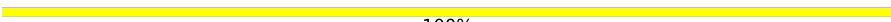
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	778	
1	B	778	
1	C	778	
1	D	778	
2	U	653	
2	V	653	
2	W	653	
2	X	653	

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Mol	Chain	Length	Quality of chain
3	E	2	 100%
3	F	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	AKG	A	802	-	X	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 34092 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 Multifunctional procollagen lysine hydroxylase and glycosyl-transferase LH3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	706	Total	C	N	O	S	0	0
			5756	3680	999	1053	24		
1	B	706	Total	C	N	O	S	0	0
			5756	3680	999	1053	24		
1	C	706	Total	C	N	O		0	0
			3476	2064	706	706			
1	D	706	Total	C	N	O		0	0
			3476	2064	706	706			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	739	ALA	-	expression tag	UNP O60568
A	740	ALA	-	expression tag	UNP O60568
A	741	ALA	-	expression tag	UNP O60568
A	742	GLU	-	expression tag	UNP O60568
A	743	ASN	-	expression tag	UNP O60568
A	744	LEU	-	expression tag	UNP O60568
A	745	TYR	-	expression tag	UNP O60568
A	746	PHE	-	expression tag	UNP O60568
A	747	GLN	-	expression tag	UNP O60568
A	748	GLY	-	expression tag	UNP O60568
A	749	ASP	-	expression tag	UNP O60568
A	750	TYR	-	expression tag	UNP O60568
A	751	LYS	-	expression tag	UNP O60568
A	752	ASP	-	expression tag	UNP O60568
A	753	HIS	-	expression tag	UNP O60568
A	754	ASP	-	expression tag	UNP O60568
A	755	GLY	-	expression tag	UNP O60568
A	756	ASP	-	expression tag	UNP O60568
A	757	TYR	-	expression tag	UNP O60568
A	758	LYS	-	expression tag	UNP O60568
A	759	ASP	-	expression tag	UNP O60568

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Chain	Residue	Modelled	Actual	Comment	Reference
A	760	HIS	-	expression tag	UNP O60568
A	761	ASP	-	expression tag	UNP O60568
A	762	ILE	-	expression tag	UNP O60568
A	763	ASP	-	expression tag	UNP O60568
A	764	TYR	-	expression tag	UNP O60568
A	765	LYS	-	expression tag	UNP O60568
A	766	ASP	-	expression tag	UNP O60568
A	767	ASP	-	expression tag	UNP O60568
A	768	ASP	-	expression tag	UNP O60568
A	769	ASP	-	expression tag	UNP O60568
A	770	LYS	-	expression tag	UNP O60568
A	771	HIS	-	expression tag	UNP O60568
A	772	HIS	-	expression tag	UNP O60568
A	773	HIS	-	expression tag	UNP O60568
A	774	HIS	-	expression tag	UNP O60568
A	775	HIS	-	expression tag	UNP O60568
A	776	HIS	-	expression tag	UNP O60568
A	777	HIS	-	expression tag	UNP O60568
A	778	HIS	-	expression tag	UNP O60568
B	739	ALA	-	expression tag	UNP O60568
B	740	ALA	-	expression tag	UNP O60568
B	741	ALA	-	expression tag	UNP O60568
B	742	GLU	-	expression tag	UNP O60568
B	743	ASN	-	expression tag	UNP O60568
B	744	LEU	-	expression tag	UNP O60568
B	745	TYR	-	expression tag	UNP O60568
B	746	PHE	-	expression tag	UNP O60568
B	747	GLN	-	expression tag	UNP O60568
B	748	GLY	-	expression tag	UNP O60568
B	749	ASP	-	expression tag	UNP O60568
B	750	TYR	-	expression tag	UNP O60568
B	751	LYS	-	expression tag	UNP O60568
B	752	ASP	-	expression tag	UNP O60568
B	753	HIS	-	expression tag	UNP O60568
B	754	ASP	-	expression tag	UNP O60568
B	755	GLY	-	expression tag	UNP O60568
B	756	ASP	-	expression tag	UNP O60568
B	757	TYR	-	expression tag	UNP O60568
B	758	LYS	-	expression tag	UNP O60568
B	759	ASP	-	expression tag	UNP O60568
B	760	HIS	-	expression tag	UNP O60568
B	761	ASP	-	expression tag	UNP O60568

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Chain	Residue	Modelled	Actual	Comment	Reference
B	762	ILE	-	expression tag	UNP O60568
B	763	ASP	-	expression tag	UNP O60568
B	764	TYR	-	expression tag	UNP O60568
B	765	LYS	-	expression tag	UNP O60568
B	766	ASP	-	expression tag	UNP O60568
B	767	ASP	-	expression tag	UNP O60568
B	768	ASP	-	expression tag	UNP O60568
B	769	ASP	-	expression tag	UNP O60568
B	770	LYS	-	expression tag	UNP O60568
B	771	HIS	-	expression tag	UNP O60568
B	772	HIS	-	expression tag	UNP O60568
B	773	HIS	-	expression tag	UNP O60568
B	774	HIS	-	expression tag	UNP O60568
B	775	HIS	-	expression tag	UNP O60568
B	776	HIS	-	expression tag	UNP O60568
B	777	HIS	-	expression tag	UNP O60568
B	778	HIS	-	expression tag	UNP O60568
C	739	ALA	-	expression tag	UNP O60568
C	740	ALA	-	expression tag	UNP O60568
C	741	ALA	-	expression tag	UNP O60568
C	742	GLU	-	expression tag	UNP O60568
C	743	ASN	-	expression tag	UNP O60568
C	744	LEU	-	expression tag	UNP O60568
C	745	TYR	-	expression tag	UNP O60568
C	746	PHE	-	expression tag	UNP O60568
C	747	GLN	-	expression tag	UNP O60568
C	748	GLY	-	expression tag	UNP O60568
C	749	ASP	-	expression tag	UNP O60568
C	750	TYR	-	expression tag	UNP O60568
C	751	LYS	-	expression tag	UNP O60568
C	752	ASP	-	expression tag	UNP O60568
C	753	HIS	-	expression tag	UNP O60568
C	754	ASP	-	expression tag	UNP O60568
C	755	GLY	-	expression tag	UNP O60568
C	756	ASP	-	expression tag	UNP O60568
C	757	TYR	-	expression tag	UNP O60568
C	758	LYS	-	expression tag	UNP O60568
C	759	ASP	-	expression tag	UNP O60568
C	760	HIS	-	expression tag	UNP O60568
C	761	ASP	-	expression tag	UNP O60568
C	762	ILE	-	expression tag	UNP O60568
C	763	ASP	-	expression tag	UNP O60568

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Chain	Residue	Modelled	Actual	Comment	Reference
C	764	TYR	-	expression tag	UNP O60568
C	765	LYS	-	expression tag	UNP O60568
C	766	ASP	-	expression tag	UNP O60568
C	767	ASP	-	expression tag	UNP O60568
C	768	ASP	-	expression tag	UNP O60568
C	769	ASP	-	expression tag	UNP O60568
C	770	LYS	-	expression tag	UNP O60568
C	771	HIS	-	expression tag	UNP O60568
C	772	HIS	-	expression tag	UNP O60568
C	773	HIS	-	expression tag	UNP O60568
C	774	HIS	-	expression tag	UNP O60568
C	775	HIS	-	expression tag	UNP O60568
C	776	HIS	-	expression tag	UNP O60568
C	777	HIS	-	expression tag	UNP O60568
C	778	HIS	-	expression tag	UNP O60568
D	739	ALA	-	expression tag	UNP O60568
D	740	ALA	-	expression tag	UNP O60568
D	741	ALA	-	expression tag	UNP O60568
D	742	GLU	-	expression tag	UNP O60568
D	743	ASN	-	expression tag	UNP O60568
D	744	LEU	-	expression tag	UNP O60568
D	745	TYR	-	expression tag	UNP O60568
D	746	PHE	-	expression tag	UNP O60568
D	747	GLN	-	expression tag	UNP O60568
D	748	GLY	-	expression tag	UNP O60568
D	749	ASP	-	expression tag	UNP O60568
D	750	TYR	-	expression tag	UNP O60568
D	751	LYS	-	expression tag	UNP O60568
D	752	ASP	-	expression tag	UNP O60568
D	753	HIS	-	expression tag	UNP O60568
D	754	ASP	-	expression tag	UNP O60568
D	755	GLY	-	expression tag	UNP O60568
D	756	ASP	-	expression tag	UNP O60568
D	757	TYR	-	expression tag	UNP O60568
D	758	LYS	-	expression tag	UNP O60568
D	759	ASP	-	expression tag	UNP O60568
D	760	HIS	-	expression tag	UNP O60568
D	761	ASP	-	expression tag	UNP O60568
D	762	ILE	-	expression tag	UNP O60568
D	763	ASP	-	expression tag	UNP O60568
D	764	TYR	-	expression tag	UNP O60568
D	765	LYS	-	expression tag	UNP O60568

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Chain	Residue	Modelled	Actual	Comment	Reference
D	766	ASP	-	expression tag	UNP O60568
D	767	ASP	-	expression tag	UNP O60568
D	768	ASP	-	expression tag	UNP O60568
D	769	ASP	-	expression tag	UNP O60568
D	770	LYS	-	expression tag	UNP O60568
D	771	HIS	-	expression tag	UNP O60568
D	772	HIS	-	expression tag	UNP O60568
D	773	HIS	-	expression tag	UNP O60568
D	774	HIS	-	expression tag	UNP O60568
D	775	HIS	-	expression tag	UNP O60568
D	776	HIS	-	expression tag	UNP O60568
D	777	HIS	-	expression tag	UNP O60568
D	778	HIS	-	expression tag	UNP O60568

- Molecule 2 is a protein called Procollagen galactosyltransferase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	587	Total	C	N	O	S	0	0
			4801	3053	850	872	26		
2	V	587	Total	C	N	O	S	0	0
			4801	3053	850	872	26		
2	W	587	Total	C	N	O		0	0
			2916	1742	587	587			
2	X	587	Total	C	N	O		0	0
			2916	1742	587	587			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	-27	MET	-	initiating methionine	UNP Q8NBJ5
U	-26	LYS	-	expression tag	UNP Q8NBJ5
U	-25	THR	-	expression tag	UNP Q8NBJ5
U	-24	ILE	-	expression tag	UNP Q8NBJ5
U	-23	ILE	-	expression tag	UNP Q8NBJ5
U	-22	ALA	-	expression tag	UNP Q8NBJ5
U	-21	LEU	-	expression tag	UNP Q8NBJ5
U	-20	SER	-	expression tag	UNP Q8NBJ5
U	-19	TYR	-	expression tag	UNP Q8NBJ5
U	-18	ILE	-	expression tag	UNP Q8NBJ5
U	-17	PHE	-	expression tag	UNP Q8NBJ5
U	-16	CYS	-	expression tag	UNP Q8NBJ5
U	-15	LEU	-	expression tag	UNP Q8NBJ5

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Chain	Residue	Modelled	Actual	Comment	Reference
U	-14	VAL	-	expression tag	UNP Q8NBJ5
U	-13	PHE	-	expression tag	UNP Q8NBJ5
U	-12	ALA	-	expression tag	UNP Q8NBJ5
U	-11	TRP	-	expression tag	UNP Q8NBJ5
U	-10	SER	-	expression tag	UNP Q8NBJ5
U	-9	HIS	-	expression tag	UNP Q8NBJ5
U	-8	PRO	-	expression tag	UNP Q8NBJ5
U	-7	GLN	-	expression tag	UNP Q8NBJ5
U	-6	PHE	-	expression tag	UNP Q8NBJ5
U	-5	GLU	-	expression tag	UNP Q8NBJ5
U	-4	LYS	-	expression tag	UNP Q8NBJ5
U	-3	GLY	-	expression tag	UNP Q8NBJ5
U	-2	GLY	-	expression tag	UNP Q8NBJ5
U	-1	GLY	-	expression tag	UNP Q8NBJ5
U	0	SER	-	expression tag	UNP Q8NBJ5
U	1	GLY	-	expression tag	UNP Q8NBJ5
U	2	GLY	-	expression tag	UNP Q8NBJ5
U	3	GLY	-	expression tag	UNP Q8NBJ5
U	4	SER	-	expression tag	UNP Q8NBJ5
U	5	GLY	-	expression tag	UNP Q8NBJ5
U	6	GLY	-	expression tag	UNP Q8NBJ5
U	7	SER	-	expression tag	UNP Q8NBJ5
U	8	ALA	-	expression tag	UNP Q8NBJ5
U	9	TRP	-	expression tag	UNP Q8NBJ5
U	10	SER	-	expression tag	UNP Q8NBJ5
U	11	HIS	-	expression tag	UNP Q8NBJ5
U	12	PRO	-	expression tag	UNP Q8NBJ5
U	13	GLN	-	expression tag	UNP Q8NBJ5
U	14	PHE	-	expression tag	UNP Q8NBJ5
U	15	GLU	-	expression tag	UNP Q8NBJ5
U	16	LYS	-	expression tag	UNP Q8NBJ5
U	17	SER	-	expression tag	UNP Q8NBJ5
U	18	ALA	-	expression tag	UNP Q8NBJ5
U	19	LEU	-	expression tag	UNP Q8NBJ5
U	20	GLU	-	expression tag	UNP Q8NBJ5
U	21	VAL	-	expression tag	UNP Q8NBJ5
U	22	LEU	-	expression tag	UNP Q8NBJ5
U	23	PHE	-	expression tag	UNP Q8NBJ5
U	24	GLN	-	expression tag	UNP Q8NBJ5
U	25	GLY	-	expression tag	UNP Q8NBJ5
U	26	PRO	-	expression tag	UNP Q8NBJ5
U	27	GLY	-	expression tag	UNP Q8NBJ5

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Chain	Residue	Modelled	Actual	Comment	Reference
U	28	ARG	-	expression tag	UNP Q8NBJ5
U	29	ALA	-	expression tag	UNP Q8NBJ5
U	623	ALA	-	expression tag	UNP Q8NBJ5
U	624	ALA	-	expression tag	UNP Q8NBJ5
U	625	ALA	-	expression tag	UNP Q8NBJ5
V	-27	MET	-	initiating methionine	UNP Q8NBJ5
V	-26	LYS	-	expression tag	UNP Q8NBJ5
V	-25	THR	-	expression tag	UNP Q8NBJ5
V	-24	ILE	-	expression tag	UNP Q8NBJ5
V	-23	ILE	-	expression tag	UNP Q8NBJ5
V	-22	ALA	-	expression tag	UNP Q8NBJ5
V	-21	LEU	-	expression tag	UNP Q8NBJ5
V	-20	SER	-	expression tag	UNP Q8NBJ5
V	-19	TYR	-	expression tag	UNP Q8NBJ5
V	-18	ILE	-	expression tag	UNP Q8NBJ5
V	-17	PHE	-	expression tag	UNP Q8NBJ5
V	-16	CYS	-	expression tag	UNP Q8NBJ5
V	-15	LEU	-	expression tag	UNP Q8NBJ5
V	-14	VAL	-	expression tag	UNP Q8NBJ5
V	-13	PHE	-	expression tag	UNP Q8NBJ5
V	-12	ALA	-	expression tag	UNP Q8NBJ5
V	-11	TRP	-	expression tag	UNP Q8NBJ5
V	-10	SER	-	expression tag	UNP Q8NBJ5
V	-9	HIS	-	expression tag	UNP Q8NBJ5
V	-8	PRO	-	expression tag	UNP Q8NBJ5
V	-7	GLN	-	expression tag	UNP Q8NBJ5
V	-6	PHE	-	expression tag	UNP Q8NBJ5
V	-5	GLU	-	expression tag	UNP Q8NBJ5
V	-4	LYS	-	expression tag	UNP Q8NBJ5
V	-3	GLY	-	expression tag	UNP Q8NBJ5
V	-2	GLY	-	expression tag	UNP Q8NBJ5
V	-1	GLY	-	expression tag	UNP Q8NBJ5
V	0	SER	-	expression tag	UNP Q8NBJ5
V	1	GLY	-	expression tag	UNP Q8NBJ5
V	2	GLY	-	expression tag	UNP Q8NBJ5
V	3	GLY	-	expression tag	UNP Q8NBJ5
V	4	SER	-	expression tag	UNP Q8NBJ5
V	5	GLY	-	expression tag	UNP Q8NBJ5
V	6	GLY	-	expression tag	UNP Q8NBJ5
V	7	SER	-	expression tag	UNP Q8NBJ5
V	8	ALA	-	expression tag	UNP Q8NBJ5
V	9	TRP	-	expression tag	UNP Q8NBJ5

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Chain	Residue	Modelled	Actual	Comment	Reference
V	10	SER	-	expression tag	UNP Q8NBJ5
V	11	HIS	-	expression tag	UNP Q8NBJ5
V	12	PRO	-	expression tag	UNP Q8NBJ5
V	13	GLN	-	expression tag	UNP Q8NBJ5
V	14	PHE	-	expression tag	UNP Q8NBJ5
V	15	GLU	-	expression tag	UNP Q8NBJ5
V	16	LYS	-	expression tag	UNP Q8NBJ5
V	17	SER	-	expression tag	UNP Q8NBJ5
V	18	ALA	-	expression tag	UNP Q8NBJ5
V	19	LEU	-	expression tag	UNP Q8NBJ5
V	20	GLU	-	expression tag	UNP Q8NBJ5
V	21	VAL	-	expression tag	UNP Q8NBJ5
V	22	LEU	-	expression tag	UNP Q8NBJ5
V	23	PHE	-	expression tag	UNP Q8NBJ5
V	24	GLN	-	expression tag	UNP Q8NBJ5
V	25	GLY	-	expression tag	UNP Q8NBJ5
V	26	PRO	-	expression tag	UNP Q8NBJ5
V	27	GLY	-	expression tag	UNP Q8NBJ5
V	28	ARG	-	expression tag	UNP Q8NBJ5
V	29	ALA	-	expression tag	UNP Q8NBJ5
V	623	ALA	-	expression tag	UNP Q8NBJ5
V	624	ALA	-	expression tag	UNP Q8NBJ5
V	625	ALA	-	expression tag	UNP Q8NBJ5
W	-27	MET	-	initiating methionine	UNP Q8NBJ5
W	-26	LYS	-	expression tag	UNP Q8NBJ5
W	-25	THR	-	expression tag	UNP Q8NBJ5
W	-24	ILE	-	expression tag	UNP Q8NBJ5
W	-23	ILE	-	expression tag	UNP Q8NBJ5
W	-22	ALA	-	expression tag	UNP Q8NBJ5
W	-21	LEU	-	expression tag	UNP Q8NBJ5
W	-20	SER	-	expression tag	UNP Q8NBJ5
W	-19	TYR	-	expression tag	UNP Q8NBJ5
W	-18	ILE	-	expression tag	UNP Q8NBJ5
W	-17	PHE	-	expression tag	UNP Q8NBJ5
W	-16	CYS	-	expression tag	UNP Q8NBJ5
W	-15	LEU	-	expression tag	UNP Q8NBJ5
W	-14	VAL	-	expression tag	UNP Q8NBJ5
W	-13	PHE	-	expression tag	UNP Q8NBJ5
W	-12	ALA	-	expression tag	UNP Q8NBJ5
W	-11	TRP	-	expression tag	UNP Q8NBJ5
W	-10	SER	-	expression tag	UNP Q8NBJ5
W	-9	HIS	-	expression tag	UNP Q8NBJ5

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Chain	Residue	Modelled	Actual	Comment	Reference
W	-8	PRO	-	expression tag	UNP Q8NBJ5
W	-7	GLN	-	expression tag	UNP Q8NBJ5
W	-6	PHE	-	expression tag	UNP Q8NBJ5
W	-5	GLU	-	expression tag	UNP Q8NBJ5
W	-4	LYS	-	expression tag	UNP Q8NBJ5
W	-3	GLY	-	expression tag	UNP Q8NBJ5
W	-2	GLY	-	expression tag	UNP Q8NBJ5
W	-1	GLY	-	expression tag	UNP Q8NBJ5
W	0	SER	-	expression tag	UNP Q8NBJ5
W	1	GLY	-	expression tag	UNP Q8NBJ5
W	2	GLY	-	expression tag	UNP Q8NBJ5
W	3	GLY	-	expression tag	UNP Q8NBJ5
W	4	SER	-	expression tag	UNP Q8NBJ5
W	5	GLY	-	expression tag	UNP Q8NBJ5
W	6	GLY	-	expression tag	UNP Q8NBJ5
W	7	SER	-	expression tag	UNP Q8NBJ5
W	8	ALA	-	expression tag	UNP Q8NBJ5
W	9	TRP	-	expression tag	UNP Q8NBJ5
W	10	SER	-	expression tag	UNP Q8NBJ5
W	11	HIS	-	expression tag	UNP Q8NBJ5
W	12	PRO	-	expression tag	UNP Q8NBJ5
W	13	GLN	-	expression tag	UNP Q8NBJ5
W	14	PHE	-	expression tag	UNP Q8NBJ5
W	15	GLU	-	expression tag	UNP Q8NBJ5
W	16	LYS	-	expression tag	UNP Q8NBJ5
W	17	SER	-	expression tag	UNP Q8NBJ5
W	18	ALA	-	expression tag	UNP Q8NBJ5
W	19	LEU	-	expression tag	UNP Q8NBJ5
W	20	GLU	-	expression tag	UNP Q8NBJ5
W	21	VAL	-	expression tag	UNP Q8NBJ5
W	22	LEU	-	expression tag	UNP Q8NBJ5
W	23	PHE	-	expression tag	UNP Q8NBJ5
W	24	GLN	-	expression tag	UNP Q8NBJ5
W	25	GLY	-	expression tag	UNP Q8NBJ5
W	26	PRO	-	expression tag	UNP Q8NBJ5
W	27	GLY	-	expression tag	UNP Q8NBJ5
W	28	ARG	-	expression tag	UNP Q8NBJ5
W	29	ALA	-	expression tag	UNP Q8NBJ5
W	623	ALA	-	expression tag	UNP Q8NBJ5
W	624	ALA	-	expression tag	UNP Q8NBJ5
W	625	ALA	-	expression tag	UNP Q8NBJ5
X	-27	MET	-	initiating methionine	UNP Q8NBJ5

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Chain	Residue	Modelled	Actual	Comment	Reference
X	-26	LYS	-	expression tag	UNP Q8NBJ5
X	-25	THR	-	expression tag	UNP Q8NBJ5
X	-24	ILE	-	expression tag	UNP Q8NBJ5
X	-23	ILE	-	expression tag	UNP Q8NBJ5
X	-22	ALA	-	expression tag	UNP Q8NBJ5
X	-21	LEU	-	expression tag	UNP Q8NBJ5
X	-20	SER	-	expression tag	UNP Q8NBJ5
X	-19	TYR	-	expression tag	UNP Q8NBJ5
X	-18	ILE	-	expression tag	UNP Q8NBJ5
X	-17	PHE	-	expression tag	UNP Q8NBJ5
X	-16	CYS	-	expression tag	UNP Q8NBJ5
X	-15	LEU	-	expression tag	UNP Q8NBJ5
X	-14	VAL	-	expression tag	UNP Q8NBJ5
X	-13	PHE	-	expression tag	UNP Q8NBJ5
X	-12	ALA	-	expression tag	UNP Q8NBJ5
X	-11	TRP	-	expression tag	UNP Q8NBJ5
X	-10	SER	-	expression tag	UNP Q8NBJ5
X	-9	HIS	-	expression tag	UNP Q8NBJ5
X	-8	PRO	-	expression tag	UNP Q8NBJ5
X	-7	GLN	-	expression tag	UNP Q8NBJ5
X	-6	PHE	-	expression tag	UNP Q8NBJ5
X	-5	GLU	-	expression tag	UNP Q8NBJ5
X	-4	LYS	-	expression tag	UNP Q8NBJ5
X	-3	GLY	-	expression tag	UNP Q8NBJ5
X	-2	GLY	-	expression tag	UNP Q8NBJ5
X	-1	GLY	-	expression tag	UNP Q8NBJ5
X	0	SER	-	expression tag	UNP Q8NBJ5
X	1	GLY	-	expression tag	UNP Q8NBJ5
X	2	GLY	-	expression tag	UNP Q8NBJ5
X	3	GLY	-	expression tag	UNP Q8NBJ5
X	4	SER	-	expression tag	UNP Q8NBJ5
X	5	GLY	-	expression tag	UNP Q8NBJ5
X	6	GLY	-	expression tag	UNP Q8NBJ5
X	7	SER	-	expression tag	UNP Q8NBJ5
X	8	ALA	-	expression tag	UNP Q8NBJ5
X	9	TRP	-	expression tag	UNP Q8NBJ5
X	10	SER	-	expression tag	UNP Q8NBJ5
X	11	HIS	-	expression tag	UNP Q8NBJ5
X	12	PRO	-	expression tag	UNP Q8NBJ5
X	13	GLN	-	expression tag	UNP Q8NBJ5
X	14	PHE	-	expression tag	UNP Q8NBJ5
X	15	GLU	-	expression tag	UNP Q8NBJ5

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Chain	Residue	Modelled	Actual	Comment	Reference
X	16	LYS	-	expression tag	UNP Q8NBJ5
X	17	SER	-	expression tag	UNP Q8NBJ5
X	18	ALA	-	expression tag	UNP Q8NBJ5
X	19	LEU	-	expression tag	UNP Q8NBJ5
X	20	GLU	-	expression tag	UNP Q8NBJ5
X	21	VAL	-	expression tag	UNP Q8NBJ5
X	22	LEU	-	expression tag	UNP Q8NBJ5
X	23	PHE	-	expression tag	UNP Q8NBJ5
X	24	GLN	-	expression tag	UNP Q8NBJ5
X	25	GLY	-	expression tag	UNP Q8NBJ5
X	26	PRO	-	expression tag	UNP Q8NBJ5
X	27	GLY	-	expression tag	UNP Q8NBJ5
X	28	ARG	-	expression tag	UNP Q8NBJ5
X	29	ALA	-	expression tag	UNP Q8NBJ5
X	623	ALA	-	expression tag	UNP Q8NBJ5
X	624	ALA	-	expression tag	UNP Q8NBJ5
X	625	ALA	-	expression tag	UNP Q8NBJ5

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



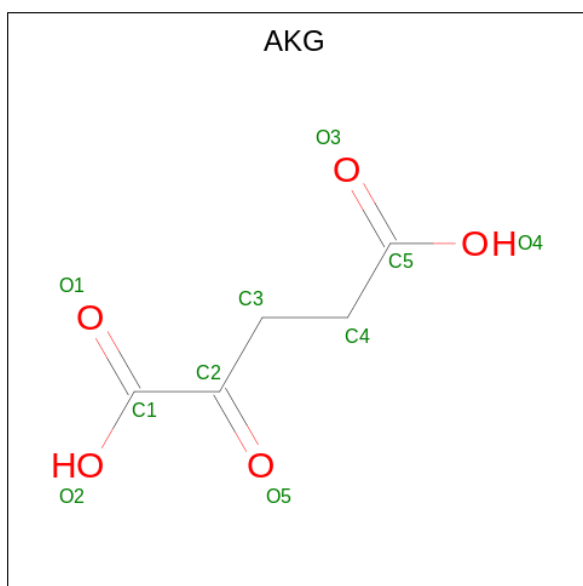
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$) (labeled as "Ligand of Interest" by depositor).

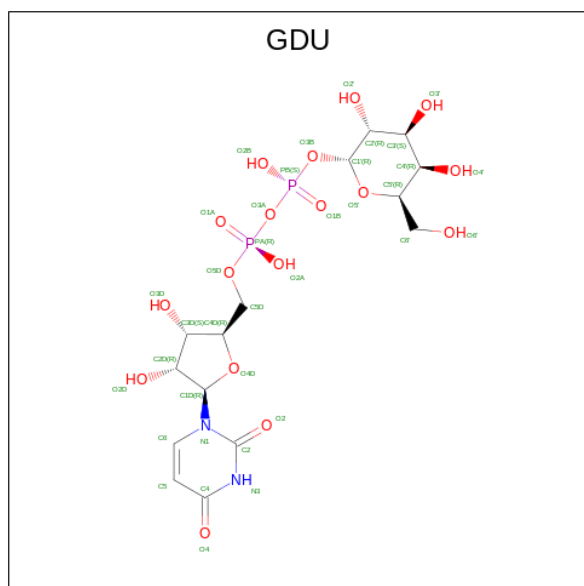


Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			10	5	5	
5	B	1	Total	C	O	0
			10	5	5	

- Molecule 6 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Fe	0
			1	1	
6	B	1	Total	Fe	0
			1	1	

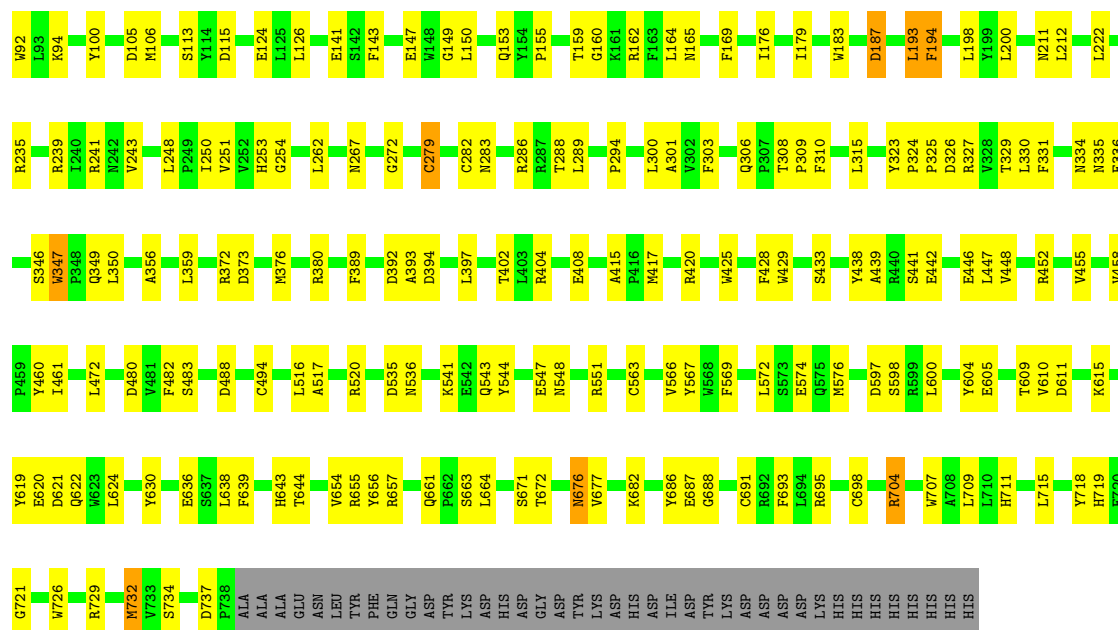
- Molecule 7 is GALACTOSE-URIDINE-5'-DIPHOSPHATE (three-letter code: GDU) (formula: C₁₅H₂₄N₂O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



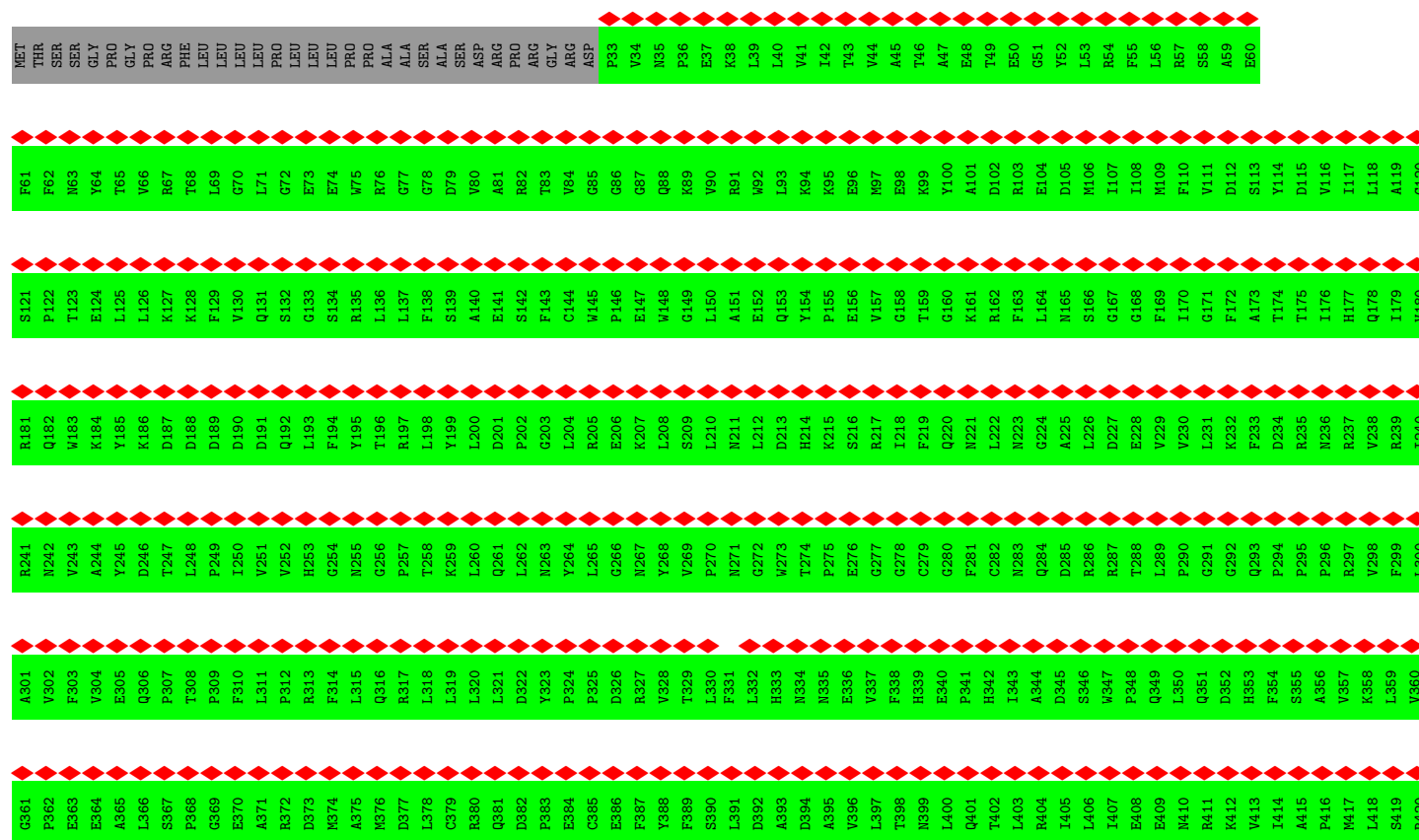
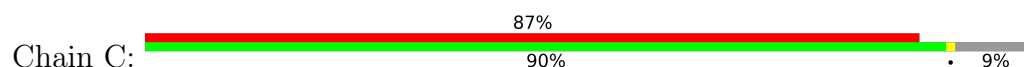
Mol	Chain	Residues	Atoms					AltConf
7	U	1	Total	C	N	O	P	0
			36	15	2	17	2	
7	V	1	Total	C	N	O	P	0
			36	15	2	17	2	

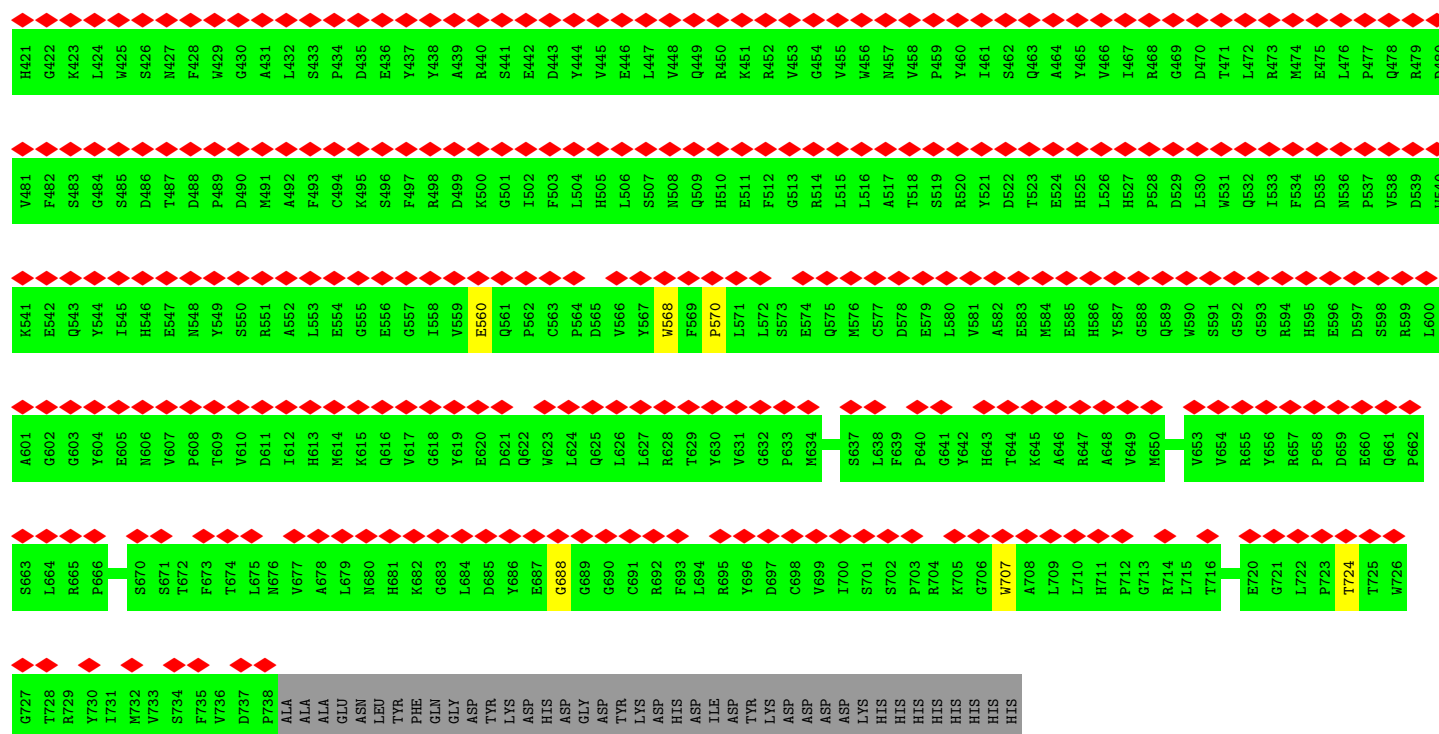
- Molecule 8 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	U	1	Total 1	Mn 1	0
8	V	1	Total 1	Mn 1	0

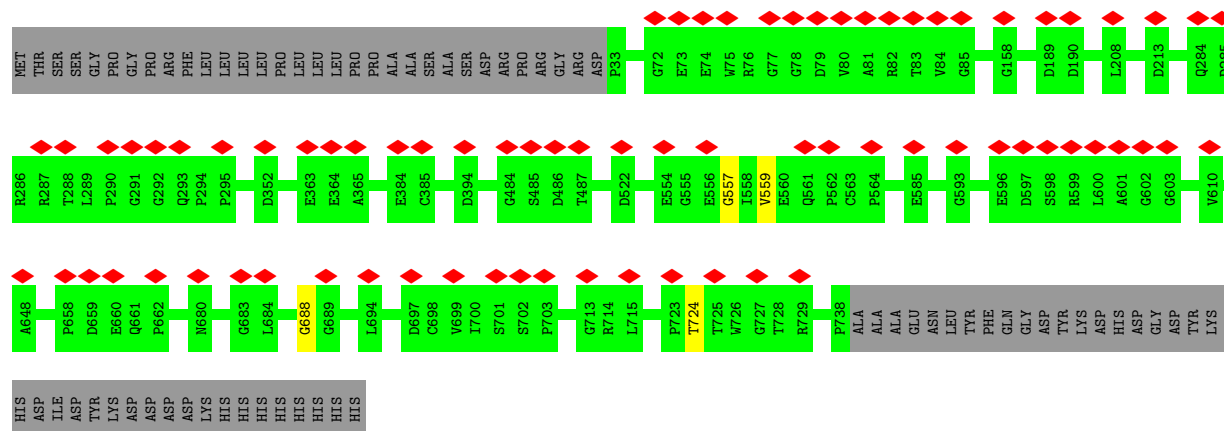
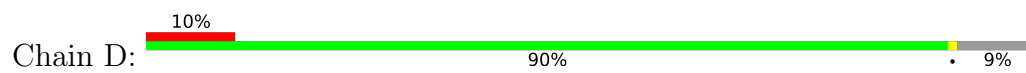


- Molecule 1: Multifunctional procollagen lysine hydroxylase and glycosyltransferase LH3

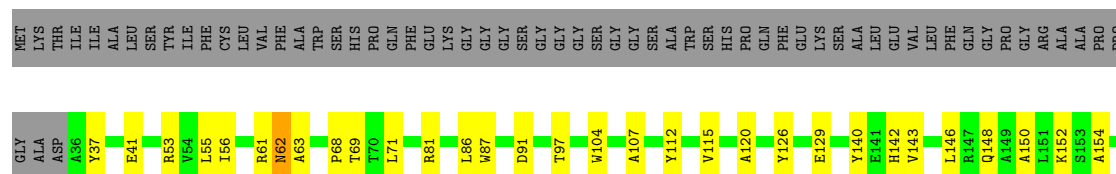


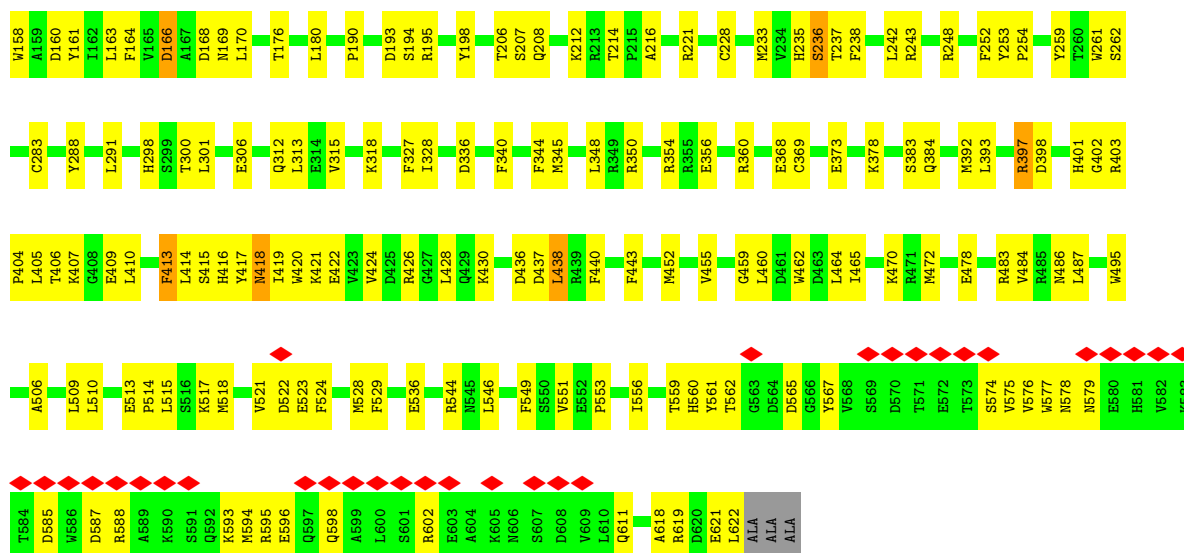


- Molecule 1: Multifunctional procollagen lysine hydroxylase and glycosyltransferase LH3

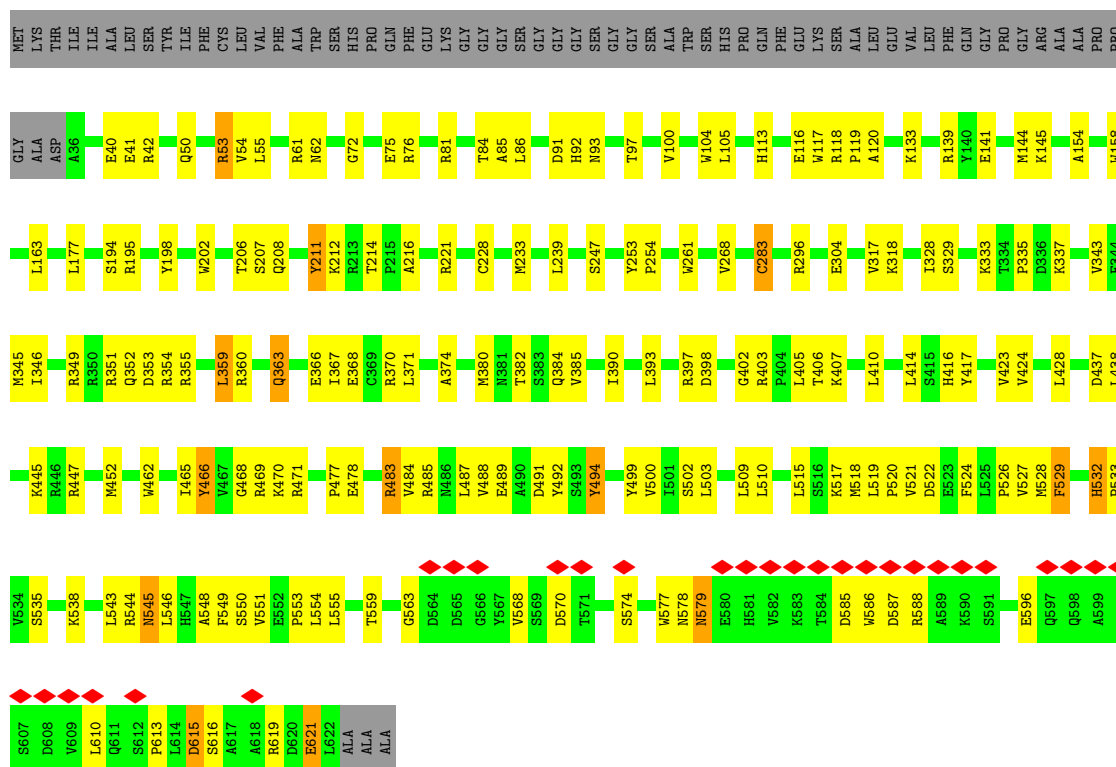


- Molecule 2: Procollagen galactosyltransferase 1

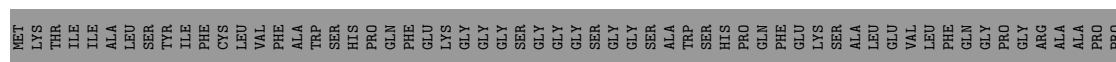
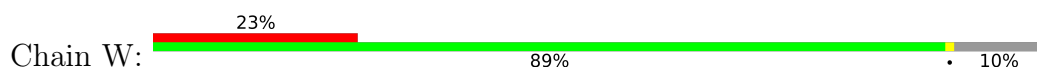


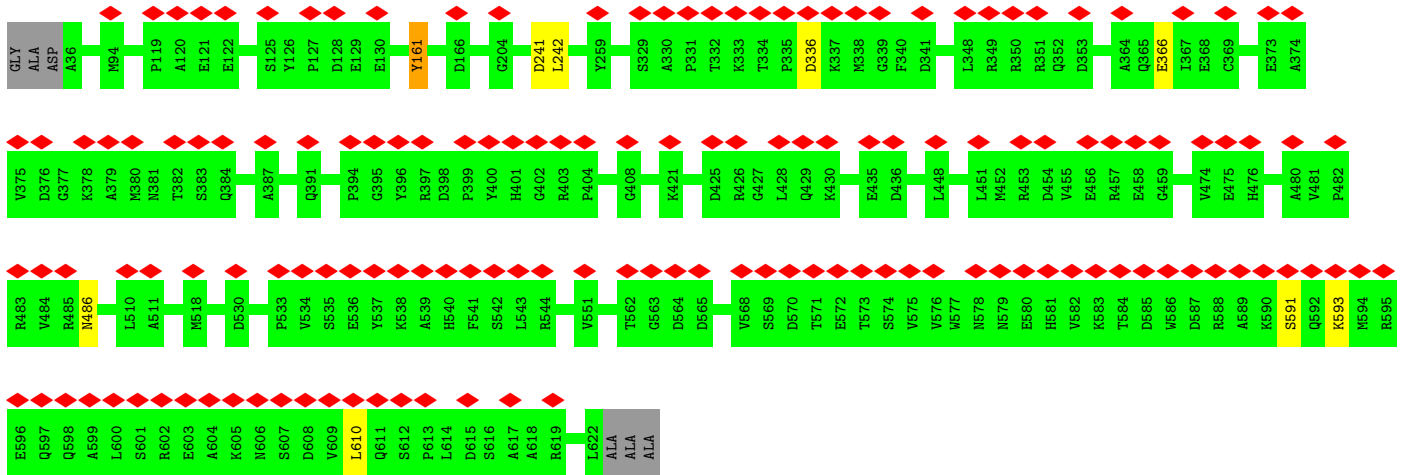


• Molecule 2: Procollagen galactosyltransferase 1

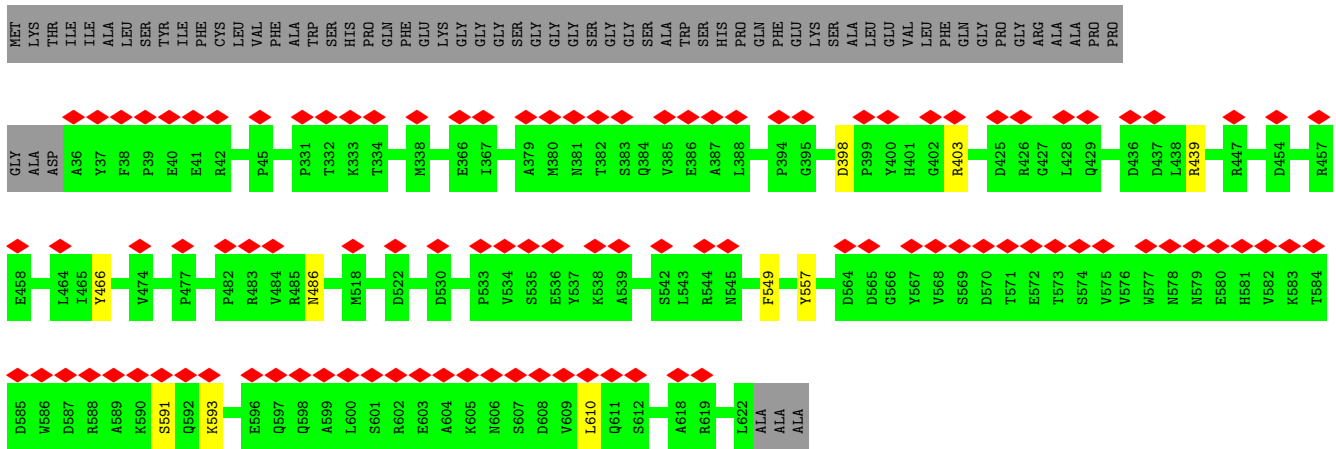
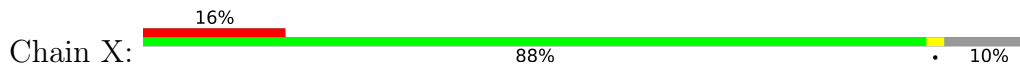


• Molecule 2: Procollagen galactosyltransferase 1





- Molecule 2: Procollagen galactosyltransferase 1



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	635839	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.743	Depositor
Minimum map value	-3.316	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.216	Depositor
Map size (\AA)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MN, FE2, GDU, AKG

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	0.27	0/5924	0.53	0/8050
1	B	0.34	0/5924	0.55	0/8050
1	C	0.24	0/3475	0.43	0/4831
1	D	0.24	0/3475	0.43	0/4831
2	U	0.30	0/4929	0.57	0/6688
2	V	0.32	0/4929	0.58	1/6688 (0.0%)
2	W	0.24	0/2915	0.43	0/4068
2	X	0.24	0/2915	0.43	0/4068
All	All	0.29	0/34486	0.51	1/47274 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	359	LEU	CA-CB-CG	8.81	135.57	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5756	0	5543	130	0
1	B	5756	0	5542	123	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3476	0	1518	3	0
1	D	3476	0	1518	2	0
2	U	4801	0	4717	137	0
2	V	4801	0	4717	141	0
2	W	2916	0	1305	5	0
2	X	2916	0	1305	5	0
3	E	28	0	25	0	0
3	F	28	0	25	1	0
4	A	14	0	13	0	0
4	B	28	0	26	0	0
5	A	10	0	4	0	0
5	B	10	0	4	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	U	36	0	22	0	0
7	V	36	0	22	0	0
8	U	1	0	0	0	0
8	V	1	0	0	0	0
All	All	34092	0	26306	537	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 (537) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:228:CYS:HA	2:V:283:CYS:HB3	1.56	0.88
2:V:487:LEU:HD11	2:V:549:PHE:HB3	1.58	0.84
2:U:407:LYS:HA	2:U:410:LEU:HD12	1.59	0.84
1:B:179:ILE:HD11	1:B:198:LEU:HD21	1.56	0.84
2:U:228:CYS:HA	2:U:283:CYS:HB3	1.59	0.83
2:U:618:ALA:HB1	2:U:622:LEU:HD21	1.63	0.79
1:B:150:LEU:HD23	1:B:200:LEU:HD13	1.65	0.78
2:V:483:ARG:O	2:V:483:ARG:NE	2.17	0.77
2:U:393:LEU:HD12	2:U:517:LYS:HB2	1.65	0.76
2:V:317:VAL:HG13	2:V:318:LYS:HG2	1.67	0.76
2:V:447:ARG:NH1	2:V:615:ASP:OD2	2.19	0.76
2:V:578:ASN:O	2:V:579:ASN:ND2	2.20	0.75
2:V:398:ASP:HB3	2:V:402:GLY:H	1.49	0.75
1:B:43:THR:HB	1:B:113:SER:HB2	1.68	0.75
1:B:566:VAL:HG23	1:B:711:HIS:HB3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:100:VAL:HG23	2:V:328:ILE:HG12	1.69	0.74
2:U:86:LEU:HB2	2:U:115:VAL:HG12	1.67	0.74
1:B:397:LEU:HD22	1:B:402:THR:HG21	1.70	0.73
2:U:198:TYR:HA	2:U:621:GLU:HG2	1.69	0.73
2:U:55:LEU:HD22	2:U:154:ALA:HB2	1.71	0.72
1:A:469:GLY:HA2	1:A:472:LEU:HD12	1.71	0.72
1:B:334:ASN:OD1	1:B:335:ASN:N	2.22	0.72
2:U:166:ASP:OD1	2:U:169:ASN:ND2	2.21	0.72
2:V:355:ARG:O	2:V:359:LEU:HD12	1.89	0.71
1:A:380:ARG:NH1	1:A:478:GLN:O	2.24	0.70
1:B:250:ILE:HG22	1:B:251:VAL:HG23	1.74	0.69
2:V:551:VAL:HG12	2:V:553:PRO:HD2	1.75	0.69
1:A:334:ASN:OD1	1:A:335:ASN:N	2.26	0.68
2:U:414:LEU:O	2:U:418:ASN:ND2	2.26	0.68
1:A:190:ASP:HB3	1:A:193:LEU:HD22	1.75	0.68
2:U:398:ASP:HB3	2:U:402:GLY:H	1.58	0.68
2:U:248:ARG:NH2	2:V:50:GLN:OE1	2.26	0.67
2:V:206:THR:HG22	2:V:212:LYS:HB2	1.74	0.67
1:A:672:THR:HG22	1:B:715:LEU:HD22	1.76	0.67
1:B:574:GLU:N	1:B:574:GLU:OE2	2.26	0.67
1:B:415:ALA:HB2	1:B:461:ILE:HD12	1.75	0.67
2:V:117:TRP:HE1	2:V:119:PRO:HB3	1.59	0.66
2:V:406:THR:OG1	2:V:574:SER:OG	2.12	0.66
2:U:354:ARG:HB3	2:U:436:ASP:OD1	1.96	0.66
1:A:410:ASN:O	1:A:410:ASN:ND2	2.28	0.66
1:A:392:ASP:OD1	1:A:393:ALA:N	2.27	0.66
1:B:94:LYS:NZ	1:B:183:TRP:O	2.30	0.65
2:V:602:ARG:HG2	2:V:603:GLU:N	2.11	0.65
1:B:547:GLU:OE1	1:B:547:GLU:N	2.29	0.65
2:V:602:ARG:HG2	2:V:603:GLU:H	1.61	0.65
2:V:221:ARG:O	2:V:221:ARG:NH1	2.30	0.64
2:U:578:ASN:O	2:U:579:ASN:ND2	2.30	0.64
1:B:392:ASP:OD1	1:B:393:ALA:N	2.30	0.64
2:U:378:LYS:HZ1	2:U:575:VAL:HG12	1.62	0.64
2:U:422:GLU:HG2	2:U:426:ARG:HH12	1.62	0.64
2:V:75:GLU:OE2	2:V:104:TRP:NE1	2.30	0.64
2:U:378:LYS:HE3	2:U:378:LYS:HA	1.80	0.64
1:B:301:ALA:HB1	1:B:303:PHE:HE1	1.63	0.63
1:B:283:ASN:HA	1:B:286:ARG:HH21	1.62	0.63
2:U:61:ARG:HG2	2:U:62:ASN:OD1	1.99	0.62
2:V:469:ARG:NH1	2:V:550:SER:OG	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:PHE:CE2	1:B:372:ARG:HG2	2.34	0.62
2:V:206:THR:OG1	2:V:207:SER:N	2.33	0.62
2:U:392:MET:HA	2:U:518:MET:HB3	1.82	0.62
2:U:483:ARG:O	2:U:483:ARG:NE	2.30	0.62
1:A:379:CYS:O	1:A:473:ARG:NH2	2.31	0.62
2:U:430:LYS:HB3	2:U:462:TRP:HH2	1.64	0.62
2:W:161:TYR:HA	2:W:241:ASP:HA	1.81	0.62
1:B:329:THR:HG22	1:B:330:LEU:H	1.65	0.62
1:A:499:ASP:OD1	1:A:499:ASP:N	2.33	0.62
2:U:206:THR:OG1	2:U:207:SER:N	2.31	0.62
1:A:42:ILE:HG23	1:A:69:LEU:HD23	1.82	0.61
1:B:417:MET:HE1	1:B:448:VAL:HA	1.82	0.61
1:B:433:SER:HB3	1:B:439:ALA:HB2	1.82	0.61
2:V:526:PRO:HA	2:V:529:PHE:CE1	2.35	0.61
1:A:199:TYR:O	1:A:205:ARG:NH1	2.32	0.61
2:U:438:LEU:HD22	2:U:556:ILE:HD12	1.82	0.61
2:U:318:LYS:HE2	2:U:318:LYS:HA	1.83	0.61
1:A:693:PHE:HB2	1:A:698:CYS:HB3	1.81	0.61
2:V:354:ARG:NH2	2:V:568:VAL:O	2.34	0.61
1:A:176:ILE:O	1:A:180:VAL:HG12	2.00	0.60
2:U:180:LEU:HD11	2:U:190:PRO:HD3	1.83	0.60
2:U:464:LEU:HD23	2:U:546:LEU:HD11	1.81	0.60
2:V:91:ASP:HB2	2:V:92:HIS:HD2	1.65	0.60
2:U:161:TYR:OH	2:U:243:ARG:NH2	2.34	0.60
2:U:598:GLN:O	2:U:602:ARG:NH2	2.34	0.60
1:C:688:GLY:HA3	1:C:724:THR:HA	1.83	0.60
2:U:522:ASP:OD1	2:U:523:GLU:N	2.34	0.60
2:V:335:PRO:HA	2:V:366:GLU:HB2	1.83	0.60
1:B:656:TYR:HB2	1:B:729:ARG:HG2	1.84	0.60
1:B:687:GLU:HG3	1:B:726:TRP:HD1	1.66	0.59
2:V:370:ARG:NH1	2:V:371:LEU:O	2.35	0.59
2:V:53:ARG:H	2:V:53:ARG:HD2	1.67	0.59
2:V:228:CYS:CA	2:V:283:CYS:HB3	2.29	0.59
2:V:328:ILE:HD12	2:V:329:SER:H	1.67	0.59
1:B:597:ASP:HB2	1:B:605:GLU:HG2	1.84	0.59
1:A:656:TYR:HB3	1:A:724:THR:HG21	1.85	0.59
2:U:514:PRO:HA	2:U:517:LYS:HE2	1.85	0.59
2:U:206:THR:HG22	2:U:212:LYS:HB2	1.84	0.59
1:B:153:GLN:HB2	1:B:200:LEU:HD11	1.84	0.58
1:B:155:PRO:O	1:B:162:ARG:NH1	2.36	0.58
1:C:570:PRO:HA	1:C:707:TRP:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:228:CYS:HA	2:U:283:CYS:CB	2.33	0.58
2:V:535:SER:HA	2:V:538:LYS:HD3	1.84	0.58
2:V:208:GLN:HA	2:V:261:TRP:CD1	2.39	0.58
2:V:538:LYS:O	2:V:544:ARG:NH2	2.37	0.58
1:A:307:PRO:HG3	1:A:336:GLU:HG2	1.85	0.58
1:A:589:GLN:HE22	1:A:591:SER:HB3	1.69	0.58
1:A:566:VAL:HG22	1:A:711:HIS:HB3	1.85	0.57
1:B:235:ARG:HG3	1:B:235:ARG:HH11	1.69	0.57
2:U:398:ASP:N	2:U:403:ARG:O	2.37	0.57
2:U:403:ARG:CZ	2:U:406:THR:HG22	2.34	0.57
1:A:625:GLN:OE1	1:A:629:THR:OG1	2.22	0.57
1:B:91:ARG:NH2	1:B:187:ASP:OD2	2.35	0.57
2:U:588:ARG:O	2:U:588:ARG:NH1	2.36	0.57
1:A:136:LEU:HD23	1:A:210:LEU:HD22	1.84	0.57
1:A:478:GLN:NE2	1:A:480:ASP:O	2.36	0.57
1:B:693:PHE:HB2	1:B:698:CYS:HB3	1.85	0.57
1:B:329:THR:HG23	1:B:356:ALA:HB3	1.85	0.57
2:V:194:SER:OG	2:V:195:ARG:N	2.36	0.57
1:A:193:LEU:HG	1:A:197:ARG:HH22	1.70	0.57
1:B:677:VAL:HB	1:B:732:MET:HB3	1.86	0.57
2:U:486:ASN:ND2	2:U:611:GLN:OE1	2.35	0.57
2:U:470:LYS:HG3	2:U:596:GLU:HG3	1.85	0.57
2:V:382:THR:HA	2:V:385:VAL:HB	1.86	0.57
1:A:480:ASP:OD1	1:A:483:SER:OG	2.18	0.56
2:U:529:PHE:HB3	2:U:546:LEU:HB3	1.87	0.56
2:U:561:TYR:HB3	2:U:595:ARG:HH21	1.69	0.56
1:A:441:SER:OG	1:A:442:GLU:N	2.39	0.56
2:V:296:ARG:NE	2:V:616:SER:O	2.38	0.56
1:A:686:TYR:HA	1:A:727:GLY:HA3	1.87	0.56
1:A:557:GLY:O	1:A:559:VAL:N	2.38	0.56
1:A:389:PHE:CZ	1:A:391:LEU:HD12	2.40	0.56
2:V:40:GLU:OE1	2:V:42:ARG:NH1	2.38	0.56
2:U:236:SER:OG	2:U:237:THR:N	2.36	0.56
2:V:494:TYR:HA	2:V:522:ASP:HB2	1.87	0.56
2:U:410:LEU:O	2:U:414:LEU:HG	2.06	0.56
2:V:85:ALA:O	2:V:86:LEU:HD22	2.06	0.56
2:U:306:GLU:HG2	2:U:443:PHE:CD1	2.40	0.56
2:V:380:MET:HG3	2:V:385:VAL:HG23	1.88	0.56
2:U:207:SER:O	2:U:261:TRP:NE1	2.40	0.55
1:B:622:GLN:N	1:B:622:GLN:OE1	2.39	0.55
1:A:93:LEU:O	1:A:97:MET:HG3	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:528:MET:HB3	2:V:546:LEU:HD12	1.88	0.55
2:U:437:ASP:OD1	2:U:559:THR:HG22	2.06	0.55
2:V:502:SER:OG	2:V:503:LEU:N	2.38	0.55
1:A:147:GLU:HG3	1:A:150:LEU:HD13	1.88	0.55
2:V:468:GLY:HA2	2:V:554:LEU:HD22	1.89	0.55
1:A:461:ILE:HD11	1:A:504:LEU:HB3	1.88	0.55
2:U:176:THR:HG1	2:U:288:TYR:HD1	1.53	0.55
1:B:169:PHE:CE1	1:B:176:ILE:HD11	2.42	0.54
2:V:543:LEU:HD12	2:V:545:ASN:HD21	1.72	0.54
2:U:214:THR:HG22	2:U:216:ALA:H	1.72	0.54
2:V:133:LYS:NZ	2:V:304:GLU:OE1	2.33	0.54
1:A:99:LYS:H	1:A:99:LYS:HD2	1.72	0.54
1:A:191:ASP:OD1	1:A:191:ASP:N	2.34	0.54
2:V:438:LEU:O	2:V:559:THR:OG1	2.25	0.54
1:A:303:PHE:CE2	1:A:372:ARG:HG2	2.42	0.54
2:U:415:SER:O	2:U:419:ILE:HG12	2.08	0.54
2:U:430:LYS:HB3	2:U:462:TRP:CH2	2.43	0.54
1:A:302:VAL:HG21	1:A:318:LEU:HD11	1.89	0.53
1:A:76:ARG:N	1:A:88:GLN:OE1	2.35	0.53
1:A:389:PHE:CE2	1:A:403:LEU:HD21	2.44	0.53
2:U:345:MET:SD	2:U:345:MET:N	2.82	0.53
2:V:484:VAL:HG11	2:V:487:LEU:HD23	1.90	0.53
2:V:520:PRO:HB2	2:V:522:ASP:OD1	2.08	0.53
1:A:382:ASP:O	1:A:473:ARG:NH2	2.42	0.53
1:B:420:ARG:HD2	1:B:425:TRP:HB3	1.91	0.53
2:U:344:PHE:HD2	2:U:419:ILE:HD12	1.73	0.53
2:W:486:ASN:N	2:W:610:LEU:O	2.42	0.53
1:A:370:GLU:O	1:A:374:MET:HG2	2.09	0.53
1:A:692:ARG:N	1:A:720:GLU:O	2.42	0.53
1:B:428:PHE:HB2	1:B:458:VAL:HG11	1.91	0.53
1:A:141:GLU:HB2	1:A:165:ASN:HB2	1.91	0.52
1:B:480:ASP:OD1	1:B:483:SER:OG	2.19	0.52
2:U:253:TYR:HB3	2:U:254:PRO:HD3	1.91	0.52
1:A:522:ASP:OD2	1:A:525:HIS:NE2	2.42	0.52
1:B:334:ASN:OD1	1:B:336:GLU:N	2.29	0.52
1:A:137:LEU:HB3	1:A:170:ILE:HG22	1.90	0.52
1:B:458:VAL:HG12	1:B:460:TYR:H	1.74	0.52
2:U:378:LYS:HZ3	2:U:575:VAL:H	1.56	0.52
2:V:91:ASP:OD1	2:V:91:ASP:N	2.42	0.52
1:B:124:GLU:OE2	1:B:239:ARG:NH2	2.39	0.52
2:V:359:LEU:HB3	2:V:363:GLN:HE22	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:SER:OG	1:B:442:GLU:N	2.42	0.52
2:U:300:THR:OG1	2:U:301:LEU:N	2.43	0.52
2:W:161:TYR:H	2:W:242:LEU:H	1.57	0.52
1:A:238:VAL:HG12	1:A:239:ARG:H	1.74	0.52
1:A:572:LEU:HD22	1:A:576:MET:HG2	1.91	0.52
2:V:116:GLU:OE1	2:V:117:TRP:N	2.43	0.52
1:A:548:ASN:OD1	1:A:551:ARG:NH2	2.43	0.51
2:U:521:VAL:HA	2:U:524:PHE:HB3	1.91	0.51
1:B:147:GLU:OE2	1:B:149:GLY:N	2.43	0.51
1:B:600:LEU:HD23	1:B:604:TYR:H	1.76	0.51
2:U:420:TRP:HB3	2:U:510:LEU:HD21	1.92	0.51
1:A:289:LEU:HD11	1:A:404:ARG:HH11	1.76	0.51
1:B:46:THR:OG1	1:B:47:ALA:N	2.44	0.51
1:A:627:LEU:HD23	1:A:631:VAL:HG21	1.92	0.51
2:V:437:ASP:O	2:V:438:LEU:HD23	2.10	0.51
2:U:69:THR:HG22	2:U:170:LEU:HD11	1.93	0.51
1:A:154:TYR:O	1:A:162:ARG:NH1	2.43	0.51
1:B:294:PRO:HB2	1:B:327:ARG:NH1	2.26	0.51
1:B:446:GLU:OE2	1:B:452:ARG:NH2	2.44	0.51
2:U:416:HIS:CE1	2:U:521:VAL:HG21	2.46	0.51
2:V:471:ARG:NH1	2:V:606:ASN:OD1	2.43	0.51
2:V:585:ASP:OD1	2:V:585:ASP:N	2.44	0.51
1:A:680:ASN:HD21	1:A:729:ARG:HA	1.76	0.50
1:B:548:ASN:OD1	1:B:551:ARG:NH1	2.43	0.50
2:X:398:ASP:N	2:X:403:ARG:O	2.43	0.50
1:A:584:MET:SD	1:A:612:ILE:HD12	2.51	0.50
1:B:429:TRP:CD2	1:B:460:TYR:HD2	2.30	0.50
2:U:348:LEU:HD21	2:U:350:ARG:HE	1.77	0.50
1:A:205:ARG:HA	1:A:210:LEU:HG	1.94	0.50
1:A:164:LEU:HD12	1:A:212:LEU:HD21	1.94	0.50
1:B:141:GLU:OE1	1:B:165:ASN:ND2	2.45	0.50
2:U:53:ARG:NH1	2:U:160:ASP:OD2	2.44	0.50
2:U:312:GLN:O	2:U:315:VAL:HG12	2.12	0.50
1:A:389:PHE:HZ	1:A:391:LEU:HD12	1.76	0.49
1:B:267:ASN:O	1:B:272:GLY:HA3	2.11	0.49
1:B:330:LEU:HD23	1:B:331:PHE:N	2.27	0.49
2:U:383:SER:OG	2:U:384:GLN:OE1	2.30	0.49
2:V:477:PRO:HB3	2:V:606:ASN:H	1.77	0.49
2:U:536:GLU:N	2:U:536:GLU:OE1	2.45	0.49
1:B:37:GLU:N	1:B:37:GLU:OE1	2.45	0.49
2:V:211:TYR:HD1	2:V:212:LYS:N	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:509:LEU:HD11	2:V:524:PHE:HE2	1.78	0.49
2:V:471:ARG:HH22	2:V:606:ASN:HD21	1.60	0.49
2:V:84:THR:O	2:V:113:HIS:HB3	2.12	0.49
1:A:663:SER:OG	1:A:722:LEU:O	2.29	0.49
1:B:655:ARG:CZ	1:B:657:ARG:HH21	2.26	0.49
2:U:68:PRO:HA	2:U:328:ILE:HD11	1.94	0.49
2:U:470:LYS:HG2	2:U:472:MET:SD	2.52	0.49
2:V:211:TYR:CD2	2:V:621:GLU:HA	2.47	0.49
2:V:247:SER:O	2:V:247:SER:OG	2.30	0.49
2:V:407:LYS:HD3	2:V:577:TRP:HA	1.95	0.49
1:B:704:ARG:HB3	1:B:707:TRP:CD1	2.47	0.49
2:U:378:LYS:NZ	2:U:575:VAL:H	2.11	0.49
1:D:688:GLY:HA3	1:D:724:THR:HA	1.95	0.49
1:B:179:ILE:HD11	1:B:198:LEU:CD2	2.37	0.48
2:V:447:ARG:NH2	2:V:555:LEU:HD21	2.27	0.48
1:A:461:ILE:HG22	1:A:462:SER:H	1.78	0.48
1:B:243:VAL:HB	2:V:216:ALA:HB2	1.96	0.48
1:B:663:SER:OG	1:B:664:LEU:N	2.44	0.48
1:B:147:GLU:OE2	1:B:150:LEU:N	2.27	0.48
1:B:682:LYS:NZ	1:B:688:GLY:O	2.43	0.48
2:U:193:ASP:OD1	2:U:221:ARG:NH1	2.44	0.48
2:V:214:THR:O	2:V:216:ALA:N	2.47	0.48
1:A:75:TRP:HE1	1:A:78:GLY:H	1.60	0.48
1:B:719:HIS:NE2	5:B:803:AKG:O2	2.38	0.48
2:U:63:ALA:H	2:U:97:THR:HG21	1.79	0.48
1:A:300:LEU:HD23	1:A:301:ALA:N	2.29	0.48
2:U:472:MET:SD	2:U:472:MET:N	2.86	0.48
1:A:295:PRO:O	1:A:327:ARG:HD3	2.14	0.48
2:U:148:GLN:HB2	2:U:252:PHE:HB2	1.95	0.48
2:V:423:VAL:HG23	2:V:428:LEU:HB2	1.96	0.48
1:A:111:VAL:HG21	1:A:116:VAL:HG11	1.96	0.48
1:B:309:PRO:HB2	1:B:310:PHE:HD1	1.79	0.48
2:V:417:TYR:CE2	2:V:515:LEU:HD21	2.48	0.48
1:A:176:ILE:HA	1:A:179:ILE:HG22	1.95	0.47
1:B:682:LYS:HA	1:B:686:TYR:CE1	2.49	0.47
2:U:235:HIS:O	2:U:236:SER:OG	2.31	0.47
2:V:202:TRP:HB2	2:V:233:MET:HB3	1.96	0.47
2:V:359:LEU:HB3	2:V:363:GLN:NE2	2.29	0.47
2:U:91:ASP:OD2	2:U:142:HIS:NE2	2.32	0.47
1:B:105:ASP:OD1	1:B:105:ASP:N	2.39	0.47
2:U:426:ARG:HD2	2:U:428:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:484:VAL:HB	2:U:487:LEU:HD13	1.95	0.47
2:V:91:ASP:HB3	2:V:120:ALA:HB3	1.96	0.47
2:V:532:HIS:HD2	2:V:533:PRO:HD2	1.78	0.47
1:B:164:LEU:HD12	1:B:212:LEU:HD21	1.96	0.47
2:X:486:ASN:N	2:X:610:LEU:O	2.47	0.47
1:A:642:TYR:CD2	1:B:715:LEU:HD11	2.49	0.47
1:B:176:ILE:O	1:B:179:ILE:HG22	2.15	0.47
1:B:300:LEU:HD23	1:B:301:ALA:N	2.29	0.47
1:B:394:ASP:OD1	1:B:516:LEU:HB2	2.14	0.47
1:B:563:CYS:O	1:B:566:VAL:HG12	2.14	0.47
2:V:61:ARG:NE	2:V:62:ASN:OD1	2.48	0.47
2:V:211:TYR:CE2	2:V:621:GLU:HA	2.49	0.47
2:U:509:LEU:HD12	2:U:510:LEU:HD22	1.96	0.47
2:V:380:MET:SD	2:V:384:GLN:HB2	2.53	0.47
2:V:519:LEU:HD21	2:V:524:PHE:HD1	1.80	0.47
1:A:455:VAL:HG12	1:A:507:SER:HB2	1.97	0.47
2:U:164:PHE:HD2	2:U:238:PHE:HE1	1.61	0.47
2:U:587:ASP:OD1	2:U:587:ASP:N	2.47	0.47
2:V:117:TRP:HD1	2:V:119:PRO:HD3	1.78	0.47
1:A:529:ASP:OD1	1:A:529:ASP:N	2.33	0.47
1:A:678:ALA:HA	1:A:731:ILE:HD13	1.97	0.47
1:B:472:LEU:HD23	1:B:472:LEU:HA	1.76	0.47
2:V:207:SER:O	2:V:261:TRP:NE1	2.48	0.47
1:B:100:TYR:CD2	1:B:106:MET:HE1	2.50	0.47
1:A:39:LEU:HD12	1:A:40:LEU:N	2.29	0.46
1:A:715:LEU:HD22	1:B:672:THR:HG22	1.97	0.46
1:B:517:ALA:H	1:B:536:ASN:HD21	1.62	0.46
2:V:163:LEU:HD12	2:V:177:LEU:HD13	1.97	0.46
2:U:405:LEU:HB3	2:U:577:TRP:CD1	2.51	0.46
2:V:398:ASP:HB3	2:V:402:GLY:N	2.25	0.46
2:V:532:HIS:CD2	2:V:533:PRO:HD2	2.50	0.46
1:A:217:ARG:HG3	1:A:247:THR:HG21	1.96	0.46
1:B:346:SER:HA	1:B:349:GLN:HE22	1.80	0.46
2:U:340:PHE:CE1	2:U:452:MET:HG2	2.51	0.46
2:V:366:GLU:O	2:V:367:ILE:HD13	2.15	0.46
2:V:403:ARG:NH2	2:V:405:LEU:O	2.49	0.46
1:A:297:ARG:HH11	1:A:327:ARG:NH2	2.13	0.46
2:V:470:LYS:HE3	2:V:596:GLU:HB2	1.96	0.46
1:B:520:ARG:NH2	1:B:535:ASP:OD1	2.47	0.46
2:U:529:PHE:HD1	2:U:546:LEU:HD23	1.79	0.46
2:V:346:ILE:HG23	2:V:374:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:462:TRP:CZ3	2:V:502:SER:HB2	2.50	0.46
1:A:153:GLN:OE1	1:A:153:GLN:N	2.40	0.46
1:A:337:VAL:O	1:A:340:GLU:HG2	2.15	0.46
1:A:351:GLN:HA	1:A:357:VAL:HG21	1.98	0.46
1:A:650:MET:SD	1:A:735:PHE:HB2	2.55	0.46
2:X:466:TYR:N	2:X:549:PHE:O	2.37	0.46
1:A:41:VAL:HB	1:A:66:VAL:HA	1.97	0.46
2:V:133:LYS:HZ1	2:V:304:GLU:HB2	1.81	0.46
2:V:563:GLY:H	2:V:586:TRP:HZ2	1.63	0.46
1:B:279:CYS:HB3	1:B:282:CYS:HB2	1.75	0.46
1:B:303:PHE:HE2	1:B:372:ARG:HG2	1.79	0.46
1:B:347:TRP:CH2	1:B:359:LEU:HD12	2.51	0.46
2:U:344:PHE:CD2	2:U:419:ILE:HG23	2.51	0.46
2:U:413:PHE:HD1	2:U:413:PHE:O	1.99	0.46
2:V:105:LEU:HD23	2:V:117:TRP:HE3	1.81	0.46
2:V:337:LYS:HZ2	2:V:343:VAL:HG22	1.81	0.46
2:V:527:VAL:HG22	2:V:532:HIS:ND1	2.30	0.46
1:A:321:LEU:HD11	1:A:403:LEU:HD23	1.98	0.46
1:A:347:TRP:CH2	1:A:357:VAL:HG12	2.51	0.46
1:B:141:GLU:HG3	1:B:143:PHE:H	1.80	0.46
1:B:636:GLU:HG3	1:B:644:THR:HG22	1.97	0.46
2:V:54:VAL:HG11	2:V:177:LEU:HD21	1.97	0.46
1:A:141:GLU:CD	1:A:143:PHE:H	2.19	0.45
1:A:178:GLN:O	1:A:182:GLN:NE2	2.46	0.45
2:V:393:LEU:HD12	2:V:517:LYS:HB3	1.97	0.45
1:A:248:LEU:HD23	1:A:248:LEU:H	1.81	0.45
1:B:567:TYR:HE2	1:B:639:PHE:HE1	1.64	0.45
2:V:93:ASN:ND2	2:V:97:THR:OG1	2.48	0.45
1:B:624:LEU:HD12	1:B:624:LEU:HA	1.73	0.45
1:A:640:PRO:HD2	1:B:695:ARG:HD2	1.98	0.45
2:U:126:TYR:HB2	2:U:129:GLU:OE1	2.16	0.45
2:U:356:GLU:O	2:U:360:ARG:HG2	2.17	0.45
2:V:410:LEU:O	2:V:414:LEU:HG	2.16	0.45
2:U:107:ALA:HB1	2:U:327:PHE:HD2	1.82	0.45
2:V:202:TRP:CD2	2:V:233:MET:HG2	2.51	0.45
2:X:591:SER:O	2:X:593:LYS:N	2.49	0.45
1:A:359:LEU:HD23	1:A:360:VAL:N	2.31	0.45
1:B:543:GLN:HG2	1:B:544:TYR:CD1	2.51	0.45
2:U:470:LYS:HG3	2:U:596:GLU:HB2	1.98	0.45
2:W:591:SER:O	2:W:593:LYS:N	2.49	0.45
2:U:398:ASP:OD1	2:U:401:HIS:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:562:THR:HG22	2:U:567:TYR:CZ	2.51	0.45
2:V:351:ARG:HD3	2:V:351:ARG:HA	1.86	0.45
1:A:254:GLY:H	1:A:262:LEU:HD13	1.82	0.45
1:A:387:PHE:HE1	1:A:468:ARG:HD3	1.81	0.45
2:U:318:LYS:HE3	2:U:560:HIS:HE1	1.81	0.45
2:U:619:ARG:O	2:U:621:GLU:N	2.48	0.45
1:A:471:THR:HA	1:A:475:GLU:HB2	1.99	0.45
2:U:313:LEU:HD21	2:U:440:PHE:CD1	2.52	0.45
2:V:529:PHE:CE2	2:V:548:ALA:HB2	2.51	0.44
1:B:87:GLY:O	1:B:90:VAL:HG12	2.17	0.44
2:U:71:LEU:HD13	2:U:104:TRP:CD2	2.52	0.44
2:U:397:ARG:HG3	2:U:402:GLY:HA2	1.99	0.44
1:A:46:THR:OG1	1:A:47:ALA:N	2.49	0.44
1:A:53:LEU:HD23	1:A:53:LEU:HA	1.84	0.44
1:B:615:LYS:HZ2	1:B:620:GLU:HG3	1.83	0.44
2:U:318:LYS:HE3	2:U:560:HIS:CE1	2.52	0.44
2:V:447:ARG:NH2	2:V:553:PRO:HB2	2.32	0.44
1:A:41:VAL:C	1:A:42:ILE:HD13	2.38	0.44
1:A:329:THR:HG23	1:A:356:ALA:HB3	1.99	0.44
2:U:259:TYR:OH	2:U:262:SER:O	2.13	0.44
1:A:686:TYR:CG	1:A:729:ARG:HB3	2.53	0.44
1:A:702:SER:O	1:A:702:SER:OG	2.25	0.44
1:C:560:GLU:O	1:C:568:TRP:N	2.51	0.44
2:V:345:MET:HB3	2:V:345:MET:HE2	1.64	0.44
2:V:452:MET:HE1	2:V:500:VAL:HG11	1.99	0.44
2:V:487:LEU:HD12	2:V:488:VAL:N	2.32	0.44
1:A:267:ASN:O	1:A:272:GLY:HA3	2.17	0.44
1:B:176:ILE:HA	1:B:179:ILE:HG22	2.00	0.44
1:B:306:GLN:HB2	1:B:308:THR:HG22	1.98	0.44
2:U:140:TYR:O	2:U:143:VAL:N	2.45	0.44
2:U:513:GLU:HG3	2:U:515:LEU:CD2	2.47	0.44
2:U:551:VAL:HG12	2:U:553:PRO:HD2	1.99	0.44
2:V:84:THR:HG22	2:V:85:ALA:H	1.83	0.44
1:A:304:VAL:HA	1:A:393:ALA:HB2	1.99	0.44
1:B:417:MET:CE	1:B:448:VAL:HA	2.48	0.44
1:A:502:ILE:HD13	1:A:502:ILE:HA	1.83	0.44
1:B:294:PRO:HB2	1:B:327:ARG:HH11	1.81	0.44
1:A:330:LEU:HD21	1:A:332:LEU:HB2	2.00	0.44
1:A:339:HIS:O	1:A:343:ILE:HG13	2.17	0.44
1:B:326:ASP:OD1	1:B:326:ASP:N	2.44	0.44
2:V:538:LYS:HB3	2:V:544:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:336:ASP:N	2:W:366:GLU:O	2.49	0.44
1:B:611:ASP:HB3	1:B:654:VAL:HG12	1.99	0.43
2:U:152:LYS:HE2	2:U:152:LYS:HB2	1.76	0.43
2:U:208:GLN:HA	2:U:261:TRP:CD1	2.53	0.43
2:V:133:LYS:NZ	2:V:304:GLU:HB2	2.33	0.43
1:A:239:ARG:HG2	1:A:240:ILE:H	1.83	0.43
2:U:146:LEU:HD23	2:U:146:LEU:HA	1.78	0.43
2:U:336:ASP:C	2:U:368:GLU:HG2	2.38	0.43
1:A:326:ASP:OD1	1:A:326:ASP:N	2.51	0.43
1:A:676:ASN:HB3	1:A:709:LEU:HB2	1.99	0.43
1:A:715:LEU:HD11	1:B:639:PHE:HD2	1.82	0.43
2:U:393:LEU:N	2:U:518:MET:H	2.15	0.43
2:U:421:LYS:HA	2:U:424:VAL:HG22	2.01	0.43
2:V:485:ARG:HG2	2:V:610:LEU:HB3	2.00	0.43
2:V:485:ARG:HH21	2:V:613:PRO:HD2	1.83	0.43
1:B:315:LEU:HD12	1:B:350:LEU:HD11	2.01	0.43
1:B:347:TRP:CZ2	1:B:359:LEU:HB2	2.54	0.43
2:U:87:TRP:CZ3	2:U:150:ALA:HB2	2.53	0.43
2:U:126:TYR:HB2	2:U:129:GLU:CD	2.38	0.43
2:U:194:SER:OG	2:U:195:ARG:N	2.51	0.43
2:U:242:LEU:HD23	2:U:242:LEU:HA	1.73	0.43
2:U:398:ASP:HB3	2:U:402:GLY:N	2.31	0.43
2:V:72:GLY:O	2:V:76:ARG:NH1	2.51	0.43
2:V:117:TRP:CD1	2:V:118:ARG:N	2.87	0.43
2:V:465:ILE:HG23	2:V:500:VAL:HB	2.01	0.43
1:A:240:ILE:HG21	1:A:265:LEU:HD21	2.00	0.43
1:A:470:ASP:OD1	1:A:470:ASP:N	2.52	0.43
1:A:657:ARG:HD2	1:A:660:GLU:HG3	2.01	0.43
1:A:666:PRO:HG3	1:A:720:GLU:HG3	2.01	0.43
1:B:239:ARG:HE	1:B:248:LEU:HB3	1.82	0.43
1:B:638:LEU:HD23	1:B:638:LEU:HA	1.74	0.43
1:A:645:LYS:HE2	1:A:647:ARG:HE	1.84	0.43
1:B:615:LYS:HG2	1:B:620:GLU:HG3	2.00	0.43
2:U:565:ASP:OD1	2:U:565:ASP:N	2.45	0.43
2:V:105:LEU:HD23	2:V:117:TRP:CE3	2.54	0.43
2:V:352:GLN:HE22	2:V:355:ARG:HH11	1.67	0.43
2:U:166:ASP:O	2:U:168:ASP:N	2.43	0.43
2:V:163:LEU:CD1	2:V:177:LEU:HD13	2.49	0.43
1:A:389:PHE:CD1	1:A:466:VAL:HG22	2.54	0.43
1:B:460:TYR:HD1	1:B:494:CYS:SG	2.42	0.43
1:B:610:VAL:HG12	1:B:661:GLN:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:81:ARG:HG2	2:U:112:TYR:HE1	1.83	0.43
2:U:378:LYS:HZ2	2:U:574:SER:HB2	1.84	0.43
1:A:297:ARG:HH11	1:A:327:ARG:HH21	1.67	0.42
1:A:563:CYS:HB3	1:A:566:VAL:HB	2.01	0.42
2:U:478:GLU:OE1	2:U:478:GLU:N	2.50	0.42
1:A:347:TRP:CZ3	1:A:359:LEU:HD12	2.54	0.42
1:A:682:LYS:HE3	1:A:682:LYS:HB3	1.85	0.42
1:B:159:THR:OG1	1:B:160:GLY:N	2.52	0.42
1:B:324:PRO:HA	1:B:325:PRO:HD3	1.80	0.42
1:B:715:LEU:HD12	1:B:715:LEU:HA	1.70	0.42
2:V:351:ARG:NH2	2:V:570:ASP:OD1	2.52	0.42
1:A:88:GLN:HG2	1:A:92:TRP:CD1	2.53	0.42
1:A:584:MET:HG2	1:A:653:VAL:HG21	2.01	0.42
1:B:254:GLY:HA3	1:B:262:LEU:HD22	2.01	0.42
2:U:91:ASP:N	2:U:91:ASP:OD1	2.53	0.42
1:B:543:GLN:HG2	1:B:544:TYR:CE1	2.55	0.42
2:V:239:LEU:O	2:V:239:LEU:HD23	2.19	0.42
1:A:253:HIS:CE1	1:A:255:ASN:HB3	2.55	0.42
2:U:344:PHE:CD2	2:U:419:ILE:HD12	2.54	0.42
2:U:378:LYS:NZ	2:U:575:VAL:HG12	2.30	0.42
2:V:253:TYR:HB3	2:V:254:PRO:HD3	2.01	0.42
1:A:372:ARG:HD2	1:A:482:PHE:CD1	2.54	0.42
2:U:452:MET:HA	2:U:455:VAL:HG12	2.01	0.42
2:V:352:GLN:HE22	2:V:355:ARG:NH1	2.17	0.42
1:B:241:ARG:NH1	2:U:41:GLU:OE2	2.53	0.42
2:X:439:ARG:N	2:X:557:TYR:O	2.53	0.42
1:B:56:LEU:HD23	1:B:56:LEU:HA	1.70	0.42
2:V:105:LEU:HD12	2:V:105:LEU:HA	1.70	0.42
1:A:59:ALA:HA	1:A:118:LEU:HD12	2.01	0.42
1:A:215:LYS:HB2	1:A:217:ARG:NH2	2.35	0.42
1:B:222:LEU:HD23	1:B:222:LEU:HA	1.82	0.42
1:B:572:LEU:HG	1:B:576:MET:HG2	2.02	0.42
2:V:198:TYR:CD2	2:V:621:GLU:HG2	2.55	0.42
1:A:138:PHE:CD1	1:A:169:PHE:HB3	2.54	0.42
2:V:333:LYS:H	2:V:333:LYS:HG2	1.58	0.42
2:V:588:ARG:O	2:V:588:ARG:NH1	2.53	0.42
1:A:511:GLU:OE1	1:A:511:GLU:N	2.41	0.41
1:B:609:THR:HG22	1:B:664:LEU:HD21	2.01	0.41
2:V:416:HIS:ND1	2:V:499:TYR:OH	2.52	0.41
2:V:424:VAL:HG21	2:V:510:LEU:HD12	2.02	0.41
1:A:541:LYS:HB2	1:A:630:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:ILE:HD12	1:B:179:ILE:HA	1.64	0.41
2:U:313:LEU:HD12	2:U:313:LEU:O	2.19	0.41
2:U:528:MET:HG3	2:U:546:LEU:HD22	2.01	0.41
2:V:423:VAL:HG23	2:V:428:LEU:HD23	2.02	0.41
1:A:524:GLU:O	1:A:525:HIS:ND1	2.53	0.41
1:B:288:THR:H	1:B:408:GLU:CD	2.22	0.41
1:B:289:LEU:HD12	1:B:404:ARG:HD2	2.01	0.41
1:B:376:MET:HE3	1:B:482:PHE:HE1	1.86	0.41
1:B:676:ASN:O	1:B:709:LEU:N	2.53	0.41
2:U:506:ALA:O	2:U:510:LEU:HD23	2.20	0.41
2:U:619:ARG:HD2	2:U:619:ARG:HA	1.89	0.41
2:V:144:MET:SD	2:V:268:VAL:HG11	2.60	0.41
1:B:193:LEU:HD23	1:B:194:PHE:H	1.84	0.41
1:B:447:LEU:HD23	1:B:447:LEU:HA	1.77	0.41
2:U:56:ILE:HG12	2:U:163:LEU:HD23	2.02	0.41
2:U:397:ARG:HA	2:U:404:PRO:HA	2.03	0.41
2:V:390:ILE:HG23	2:V:518:MET:HE2	2.02	0.41
2:V:465:ILE:HD13	2:V:549:PHE:HB2	2.02	0.41
2:U:373:GLU:OE1	2:U:373:GLU:N	2.53	0.41
2:V:54:VAL:HG12	2:V:55:LEU:N	2.35	0.41
2:V:335:PRO:HB2	2:V:368:GLU:OE2	2.21	0.41
1:B:373:ASP:OD2	1:B:480:ASP:HA	2.20	0.41
2:V:55:LEU:HD22	2:V:154:ALA:HB2	2.02	0.41
2:V:447:ARG:CZ	2:V:555:LEU:HD21	2.50	0.41
2:V:619:ARG:HD2	2:V:619:ARG:HA	1.97	0.41
1:A:135:ARG:HB2	1:A:209:SER:HB2	2.03	0.41
1:B:541:LYS:HB2	1:B:630:TYR:OH	2.21	0.41
2:U:53:ARG:HD3	2:V:158:TRP:CE3	2.56	0.41
2:U:91:ASP:HB3	2:U:120:ALA:HB3	2.03	0.41
2:U:158:TRP:CD2	2:V:53:ARG:HG2	2.55	0.41
2:U:594:MET:HB3	2:U:595:ARG:NH1	2.36	0.41
2:V:491:ASP:OD1	2:V:492:TYR:N	2.44	0.41
2:V:521:VAL:HA	2:V:524:PHE:HB3	2.02	0.41
2:V:543:LEU:HB3	2:V:545:ASN:OD1	2.21	0.41
1:A:64:TYR:CE1	1:A:122:PRO:HG3	2.56	0.41
1:A:458:VAL:HG12	1:A:460:TYR:H	1.85	0.41
2:U:415:SER:HA	2:U:418:ASN:HD22	1.86	0.41
2:U:509:LEU:CD1	2:U:510:LEU:HD22	2.51	0.41
2:U:576:VAL:HB	2:U:579:ASN:HD21	1.85	0.41
2:V:54:VAL:HG12	2:V:55:LEU:H	1.85	0.41
3:F:1:NAG:O6	3:F:2:NAG:N2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:GLU:CD	1:B:150:LEU:HD13	2.41	0.41
2:U:180:LEU:HD23	2:U:180:LEU:HA	1.83	0.41
2:U:459:GLY:C	2:U:460:LEU:HD22	2.41	0.41
2:U:585:ASP:N	2:U:585:ASP:OD1	2.52	0.41
2:V:452:MET:CE	2:V:500:VAL:HG11	2.51	0.41
1:A:108:ILE:HD13	1:A:108:ILE:HA	1.87	0.40
1:A:134:SER:OG	1:A:209:SER:O	2.39	0.40
1:A:193:LEU:HD23	1:A:194:PHE:H	1.85	0.40
1:A:350:LEU:HG	1:A:354:PHE:HE1	1.86	0.40
1:A:432:LEU:HD11	1:A:459:PRO:HB2	2.04	0.40
2:V:367:ILE:HD11	2:V:445:LYS:HD3	2.03	0.40
1:A:235:ARG:HD3	1:A:235:ARG:HA	1.71	0.40
1:A:287:ARG:O	1:A:290:PRO:HD3	2.20	0.40
1:B:126:LEU:HD23	1:B:126:LEU:HA	1.92	0.40
1:B:376:MET:HE3	1:B:376:MET:HB2	1.96	0.40
1:B:691:CYS:HA	1:B:721:GLY:HA2	2.02	0.40
1:D:557:GLY:O	1:D:559:VAL:N	2.46	0.40
2:U:422:GLU:HG2	2:U:426:ARG:NH1	2.33	0.40
2:V:145:LYS:HD2	2:V:145:LYS:HA	1.82	0.40
1:A:170:ILE:HD12	1:A:170:ILE:HA	1.84	0.40
2:V:141:GLU:HG2	2:V:253:TYR:HE2	1.86	0.40
2:V:478:GLU:H	2:V:606:ASN:HD21	1.69	0.40
1:A:415:ALA:CB	1:A:461:ILE:HG21	2.51	0.40
1:A:450:ARG:NH2	1:A:508:ASN:O	2.48	0.40
1:B:455:VAL:HG23	1:B:455:VAL:O	2.21	0.40
2:V:465:ILE:HD12	2:V:466:TYR:N	2.36	0.40
1:B:115:ASP:OD1	1:B:115:ASP:N	2.52	0.40
1:B:303:PHE:N	1:B:303:PHE:CD1	2.89	0.40
2:U:344:PHE:HD2	2:U:419:ILE:HG23	1.87	0.40
2:U:465:ILE:H	2:U:465:ILE:HG13	1.58	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	704/778 (90%)	663 (94%)	41 (6%)	0	100	100
1	B	704/778 (90%)	639 (91%)	65 (9%)	0	100	100
1	C	704/778 (90%)	692 (98%)	12 (2%)	0	100	100
1	D	704/778 (90%)	682 (97%)	22 (3%)	0	100	100
2	U	585/653 (90%)	513 (88%)	71 (12%)	1 (0%)	44	75
2	V	585/653 (90%)	505 (86%)	78 (13%)	2 (0%)	37	70
2	W	585/653 (90%)	554 (95%)	30 (5%)	1 (0%)	44	75
2	X	585/653 (90%)	546 (93%)	39 (7%)	0	100	100
All	All	5156/5724 (90%)	4794 (93%)	358 (7%)	4 (0%)	50	81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	V	621	GLU
2	U	236	SER
2	W	161	TYR
2	V	579	ASN

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	620/681 (91%)	596 (96%)	24 (4%)	27	50
1	B	620/681 (91%)	595 (96%)	25 (4%)	27	49
2	U	518/563 (92%)	501 (97%)	17 (3%)	33	55
2	V	518/563 (92%)	498 (96%)	20 (4%)	27	50
All	All	2276/2488 (92%)	2190 (96%)	86 (4%)	30	51

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	MET
1	A	106	MET
1	A	138	PHE
1	A	194	PHE
1	A	227	ASP
1	A	235	ARG
1	A	289	LEU
1	A	327	ARG
1	A	377	ASP
1	A	417	MET
1	A	437	TYR
1	A	468	ARG
1	A	474	MET
1	A	478	GLN
1	A	488	ASP
1	A	497	PHE
1	A	529	ASP
1	A	586	HIS
1	A	650	MET
1	A	665	ARG
1	A	697	ASP
1	A	704	ARG
1	A	718	TYR
1	A	737	ASP
1	B	92	TRP
1	B	187	ASP
1	B	193	LEU
1	B	194	PHE
1	B	211	ASN
1	B	253	HIS
1	B	279	CYS
1	B	323	TYR
1	B	347	TRP
1	B	380	ARG
1	B	389	PHE
1	B	438	TYR
1	B	488	ASP
1	B	569	PHE
1	B	598	SER
1	B	619	TYR
1	B	621	ASP
1	B	643	HIS
1	B	671	SER

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Mol	Chain	Res	Type
1	B	676	ASN
1	B	704	ARG
1	B	718	TYR
1	B	732	MET
1	B	734	SER
1	B	737	ASP
2	U	37	TYR
2	U	62	ASN
2	U	166	ASP
2	U	233	MET
2	U	291	LEU
2	U	298	HIS
2	U	369	CYS
2	U	397	ARG
2	U	409	GLU
2	U	413	PHE
2	U	417	TYR
2	U	418	ASN
2	U	438	LEU
2	U	495	TRP
2	U	544	ARG
2	U	549	PHE
2	U	593	LYS
2	V	41	GLU
2	V	53	ARG
2	V	81	ARG
2	V	139	ARG
2	V	211	TYR
2	V	283	CYS
2	V	349	ARG
2	V	353	ASP
2	V	360	ARG
2	V	363	GLN
2	V	397	ARG
2	V	466	TYR
2	V	483	ARG
2	V	489	GLU
2	V	494	TYR
2	V	529	PHE
2	V	532	HIS
2	V	545	ASN
2	V	587	ASP

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Mol	Chain	Res	Type
2	V	615	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	HIS
1	A	589	GLN
1	A	719	HIS
1	B	532	GLN
1	B	536	ASN
2	U	418	ASN
2	V	92	HIS
2	V	93	ASN

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 ⓘ

4 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	E	1	2,3	14,14,15	0.23	0	17,19,21	0.44	0
3	NAG	E	2	3	14,14,15	0.30	0	17,19,21	0.47	0
3	NAG	F	1	2,3	14,14,15	0.25	0	17,19,21	0.41	0
3	NAG	F	2	3	14,14,15	0.24	0	17,19,21	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	2,3	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	3/6/23/26	0/1/1/1
3	NAG	F	1	2,3	-	1/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

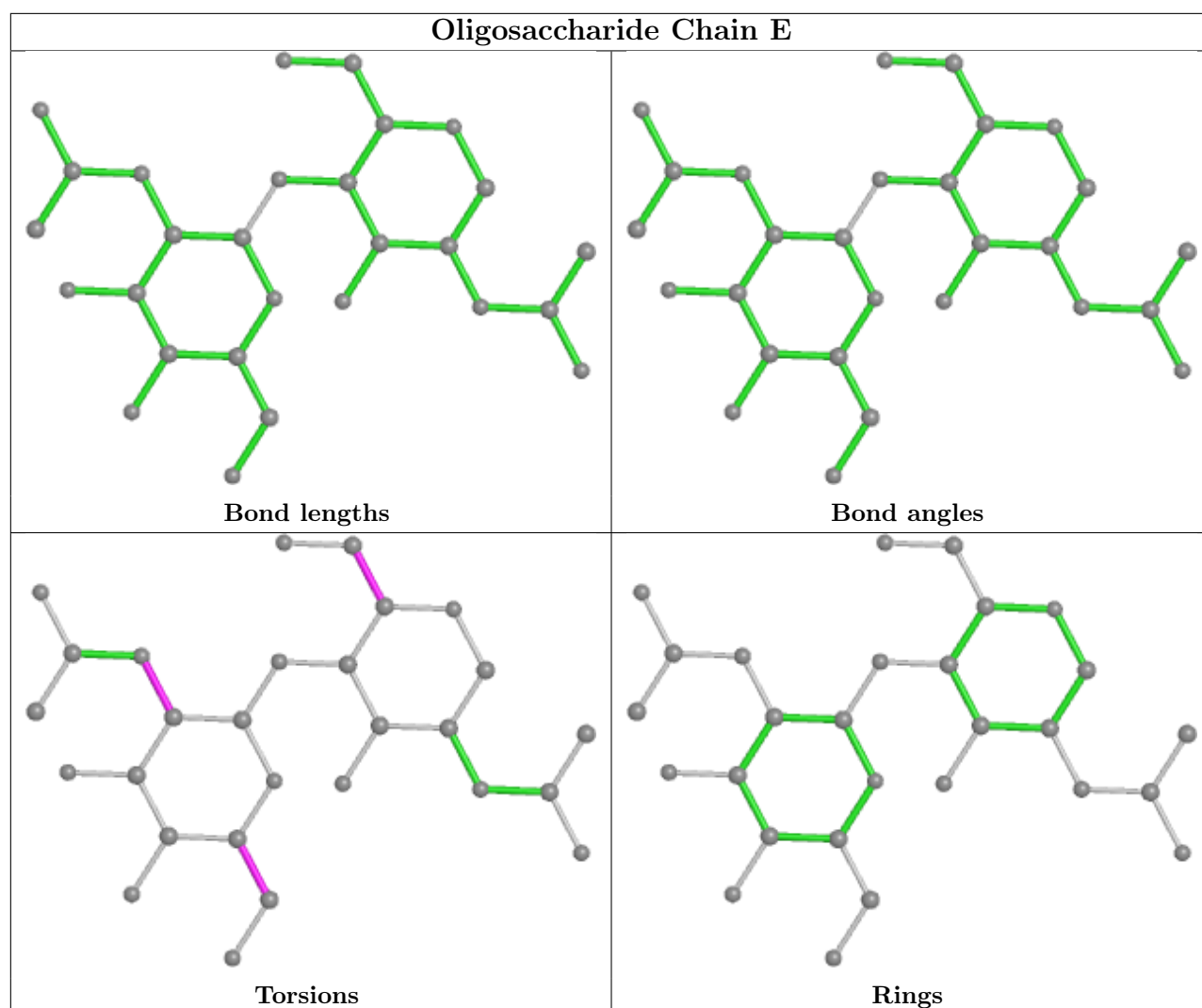
Mol	Chain	Res	Type	Atoms
3	F	2	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	E	2	NAG	C1-C2-N2-C7

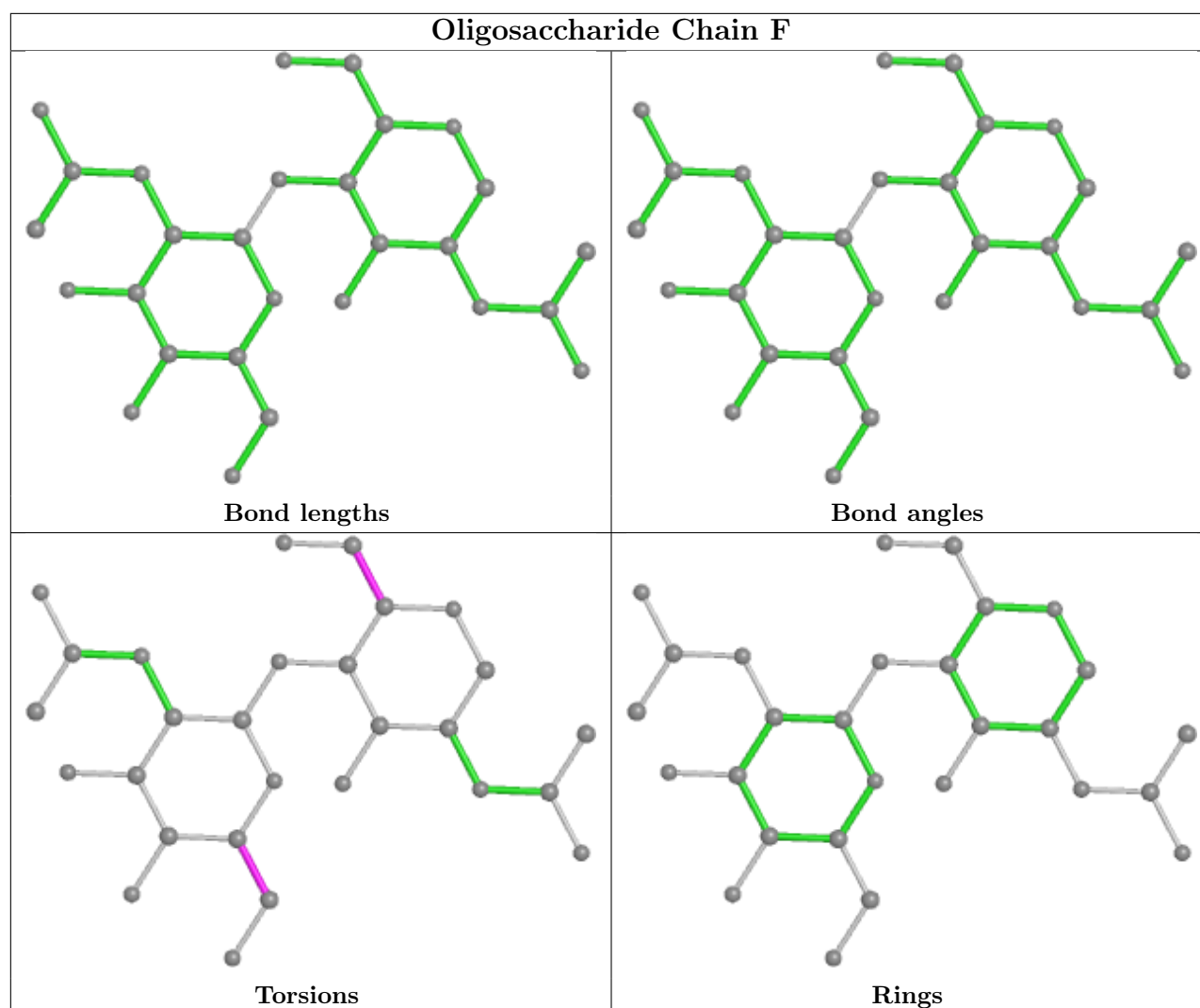
There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	NAG	1	0
3	F	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](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

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	B	801	1	14,14,15	0.31	0	17,19,21	0.57	0
5	AKG	A	802	6	9,9,9	2.15	3 (33%)	11,11,11	4.13	5 (45%)
4	NAG	A	801	1	14,14,15	0.20	0	17,19,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GDU	V	701	8	35,38,38	0.49	0	53,58,58	1.03	4 (7%)
5	AKG	B	803	6	9,9,9	2.02	2 (22%)	11,11,11	4.30	5 (45%)
7	GDU	U	701	8	35,38,38	0.52	0	53,58,58	0.77	1 (1%)
4	NAG	B	802	1	14,14,15	0.20	0	17,19,21	0.39	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	B	801	1	-	2/6/23/26	0/1/1/1
5	AKG	A	802	6	-	4/9/9/9	-
4	NAG	A	801	1	-	3/6/23/26	0/1/1/1
7	GDU	V	701	8	-	12/23/59/59	0/3/3/3
5	AKG	B	803	6	-	0/9/9/9	-
7	GDU	U	701	8	-	9/23/59/59	0/3/3/3
4	NAG	B	802	1	-	4/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	803	AKG	C3-C2	-4.23	1.46	1.51
5	A	802	AKG	C3-C2	-4.21	1.46	1.51
5	A	802	AKG	C2-C1	-3.56	1.48	1.53
5	B	803	AKG	C2-C1	-2.95	1.49	1.53
5	A	802	AKG	O2-C1	-2.20	1.24	1.30

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	803	AKG	O1-C1-C2	-11.75	106.04	121.72
5	A	802	AKG	O1-C1-C2	-10.95	107.10	121.72
5	A	802	AKG	O2-C1-O1	5.26	135.64	123.61
5	B	803	AKG	O2-C1-O1	4.96	134.96	123.61
5	A	802	AKG	O5-C2-C3	4.43	131.02	121.20
5	B	803	AKG	C4-C3-C2	-4.13	105.25	113.03
7	V	701	GDU	PB-O3A-PA	-3.75	119.95	132.83
5	B	803	AKG	O5-C2-C3	3.51	128.99	121.20
5	A	802	AKG	C4-C3-C2	-2.85	107.67	113.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	V	701	GDU	C3'-C4'-C5'	2.84	115.31	110.24
7	V	701	GDU	O5'-C1'-O3B	-2.64	107.91	111.36
5	A	802	AKG	C3-C2-C1	-2.50	111.34	115.97
5	B	803	AKG	C3-C2-C1	-2.44	111.44	115.97
7	U	701	GDU	C3D-C2D-C1D	-2.28	97.08	101.43
7	V	701	GDU	C4'-C3'-C2'	2.03	114.37	110.82

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	U	701	GDU	O4D-C4D-C5D-O5D
7	U	701	GDU	C5D-O5D-PA-O3A
7	U	701	GDU	C1'-O3B-PB-O2B
7	V	701	GDU	C5D-O5D-PA-O1A
7	V	701	GDU	C5D-O5D-PA-O2A
7	V	701	GDU	C5D-O5D-PA-O3A
7	U	701	GDU	C4'-C5'-C6'-O6'
7	U	701	GDU	O5'-C5'-C6'-O6'
4	B	801	NAG	O5-C5-C6-O6
4	B	802	NAG	O5-C5-C6-O6
7	V	701	GDU	O4D-C4D-C5D-O5D
4	B	801	NAG	C4-C5-C6-O6
4	A	801	NAG	C8-C7-N2-C2
4	A	801	NAG	O7-C7-N2-C2
4	B	802	NAG	C8-C7-N2-C2
4	B	802	NAG	O7-C7-N2-C2
7	V	701	GDU	O5'-C5'-C6'-O6'
7	U	701	GDU	C3D-C4D-C5D-O5D
7	V	701	GDU	C3D-C4D-C5D-O5D
4	B	802	NAG	C4-C5-C6-O6
4	A	801	NAG	O5-C5-C6-O6
7	U	701	GDU	C1'-O3B-PB-O3A
7	V	701	GDU	PB-O3A-PA-O2A
7	U	701	GDU	C5D-O5D-PA-O1A
7	U	701	GDU	C5D-O5D-PA-O2A
7	V	701	GDU	C1'-O3B-PB-O3A
7	V	701	GDU	O5'-C1'-O3B-PB
7	V	701	GDU	C4'-C5'-C6'-O6'
5	A	802	AKG	C2-C3-C4-C5
5	A	802	AKG	C3-C4-C5-O3
5	A	802	AKG	C3-C4-C5-O4

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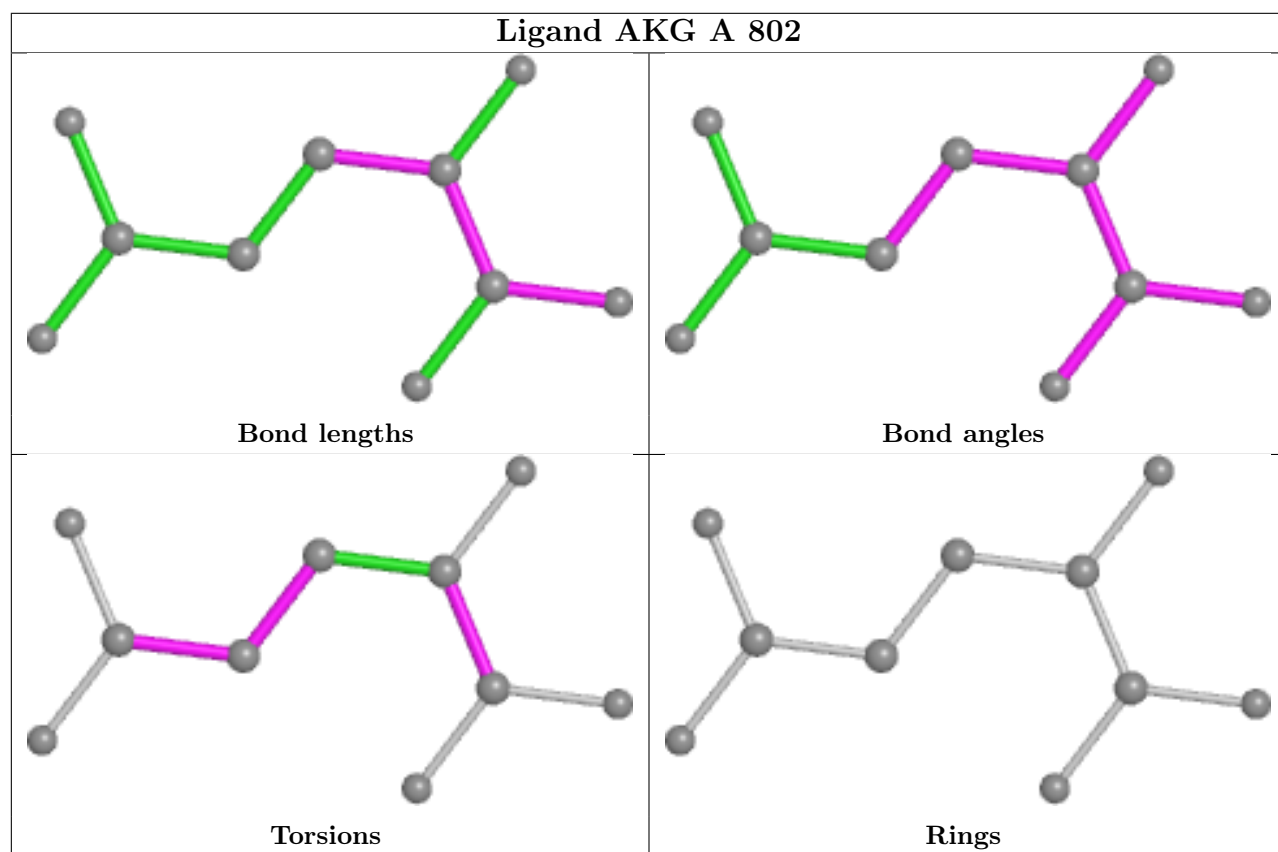
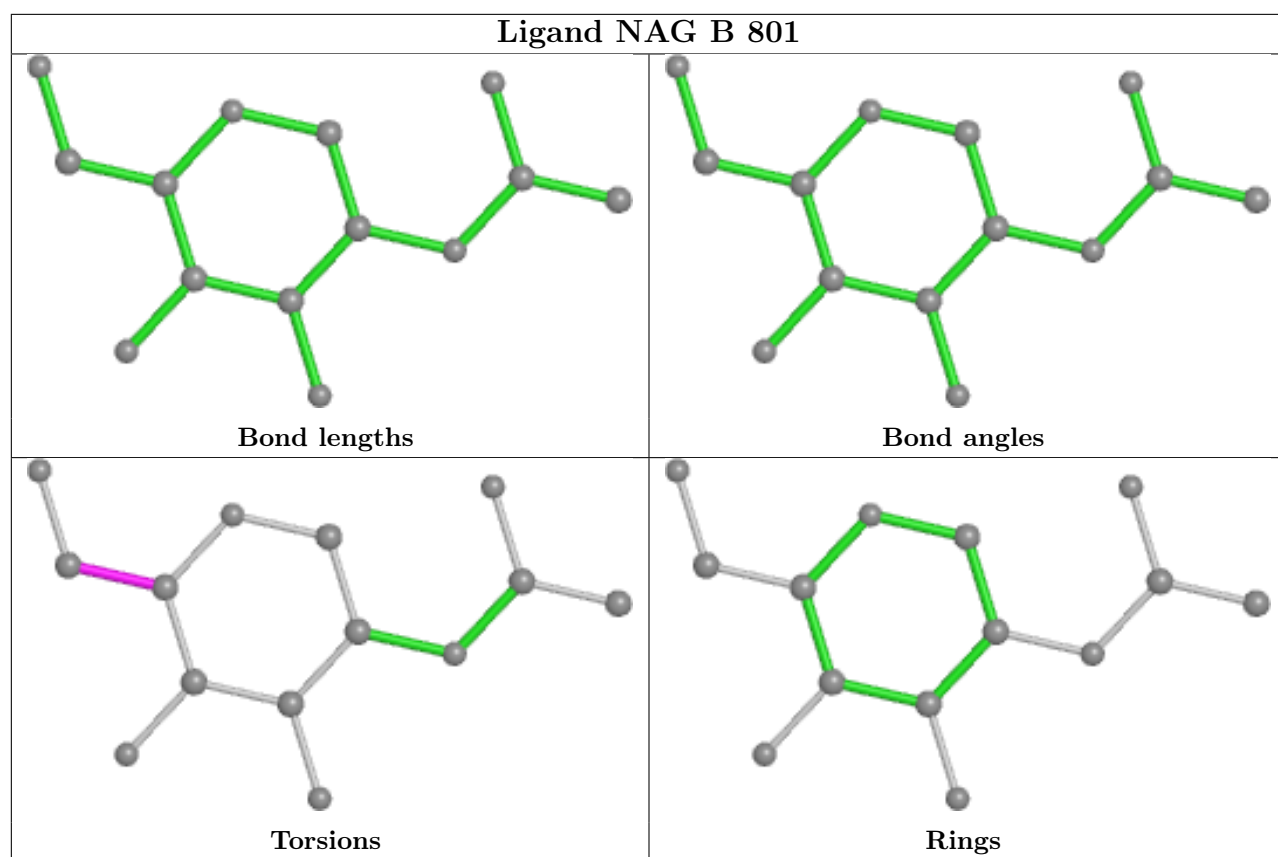
Mol	Chain	Res	Type	Atoms
5	A	802	AKG	O2-C1-C2-C3
7	V	701	GDU	C4D-C5D-O5D-PA
7	V	701	GDU	PB-O3A-PA-O1A

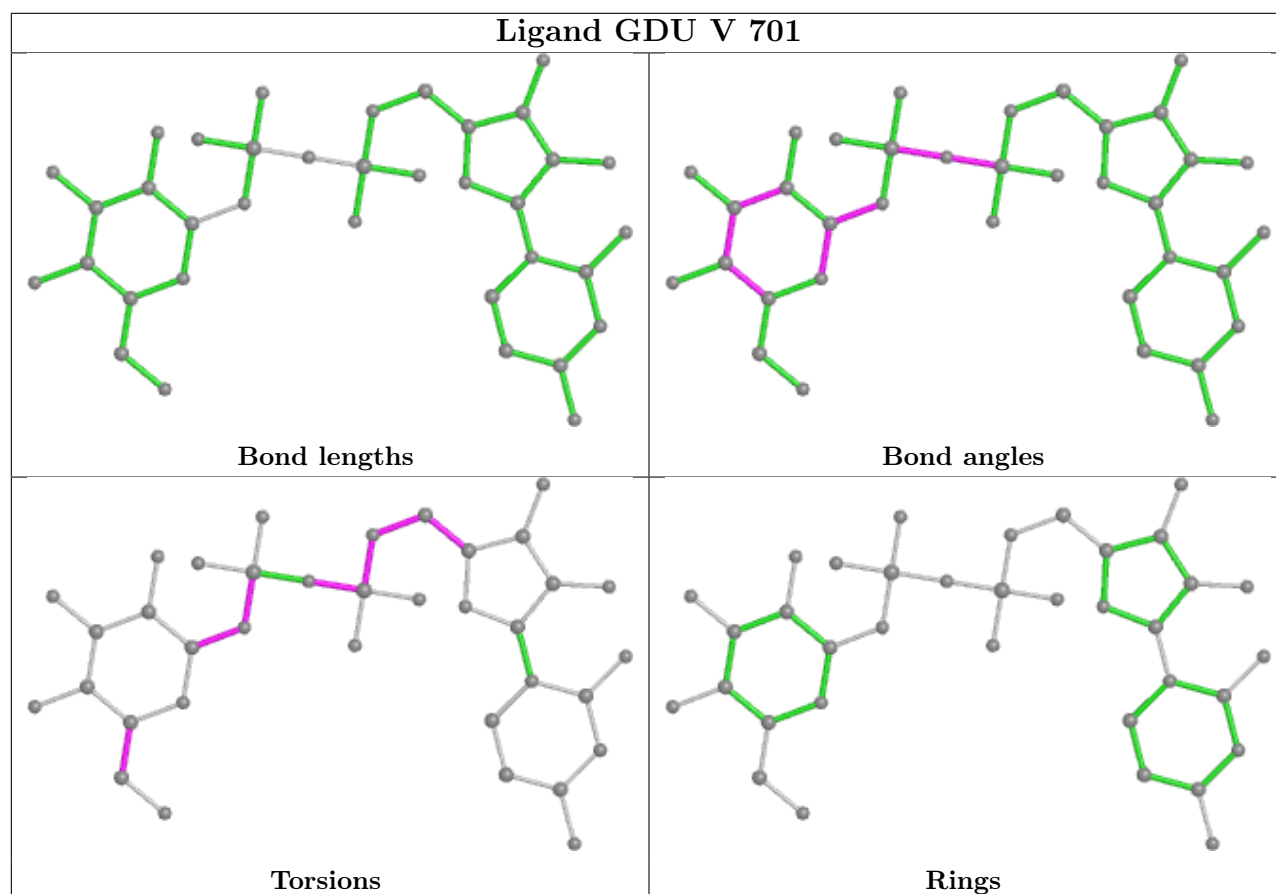
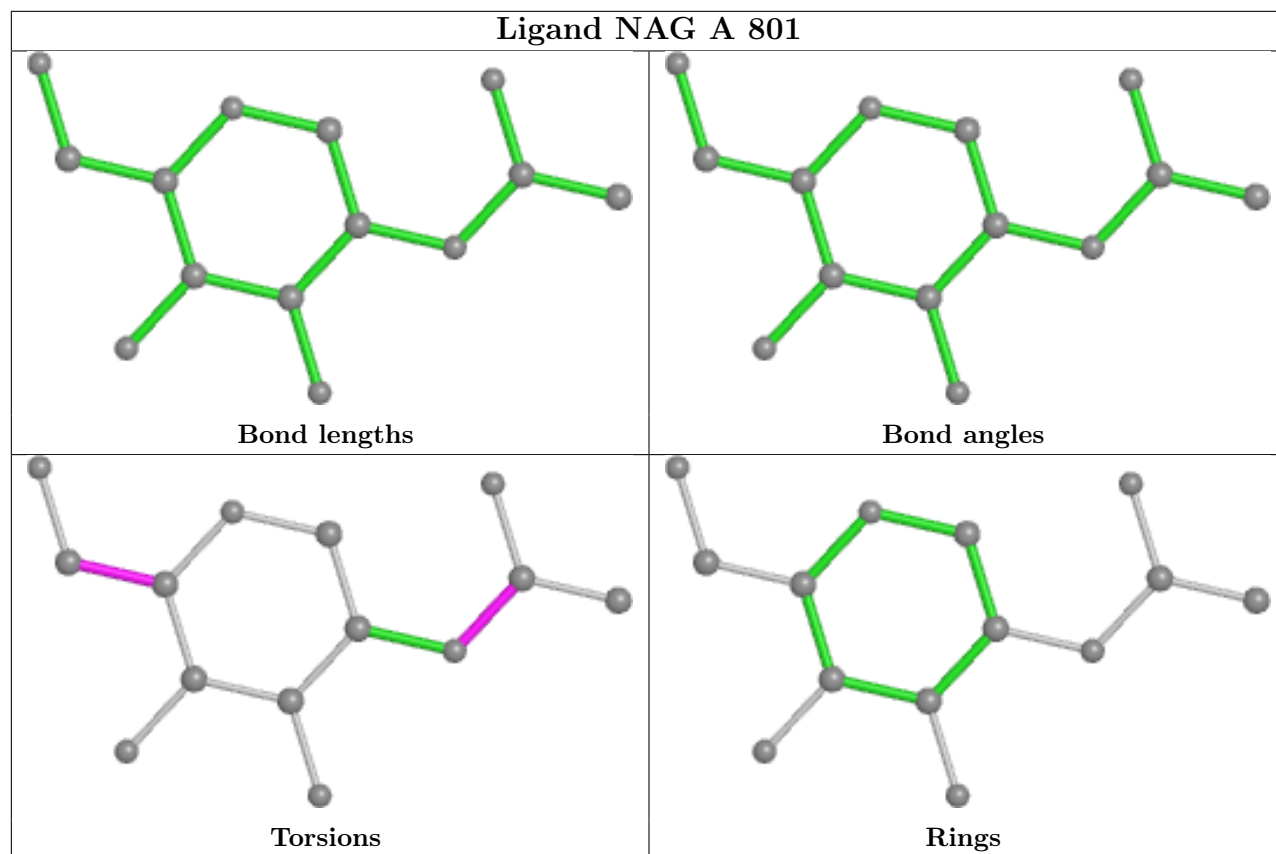
There are no ring outliers.

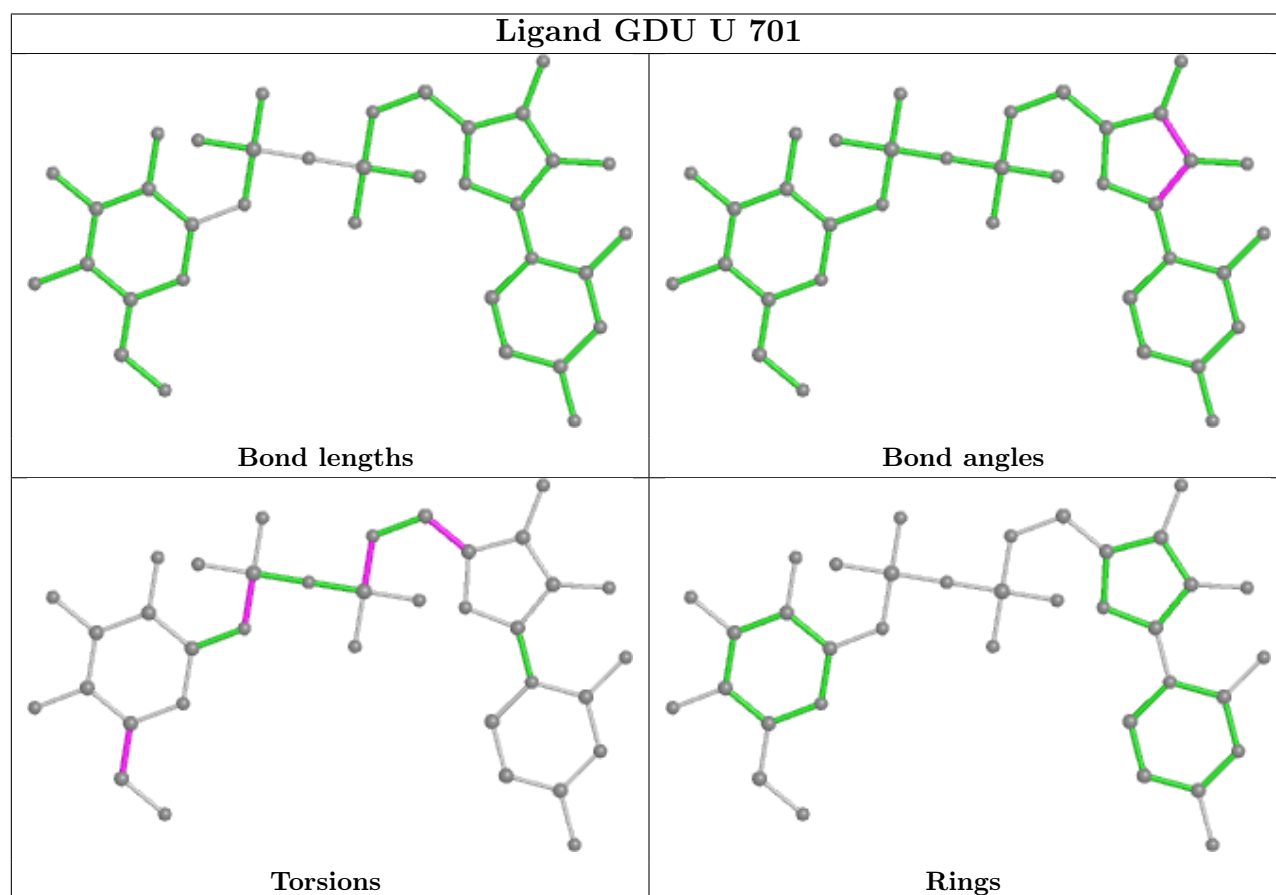
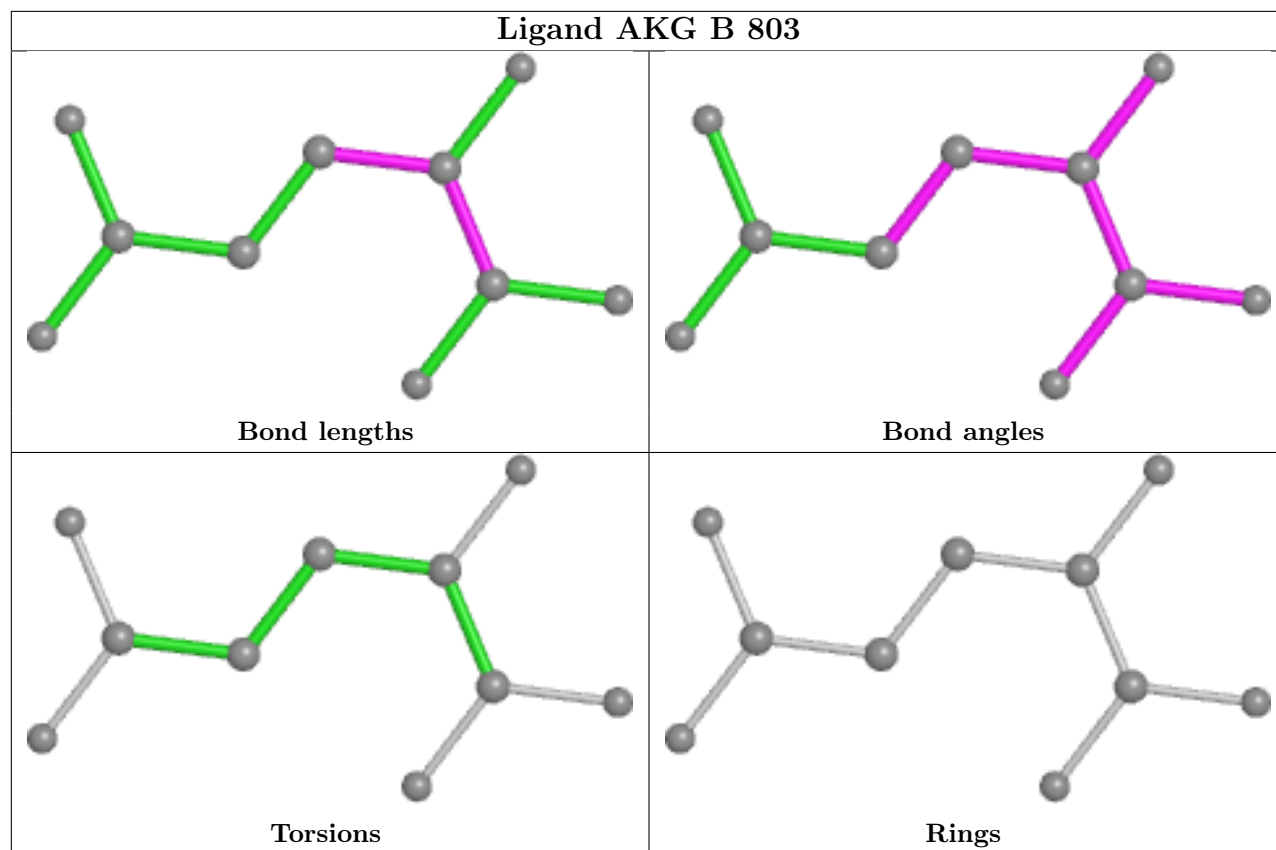
1 monomer is involved in 1 short contact:

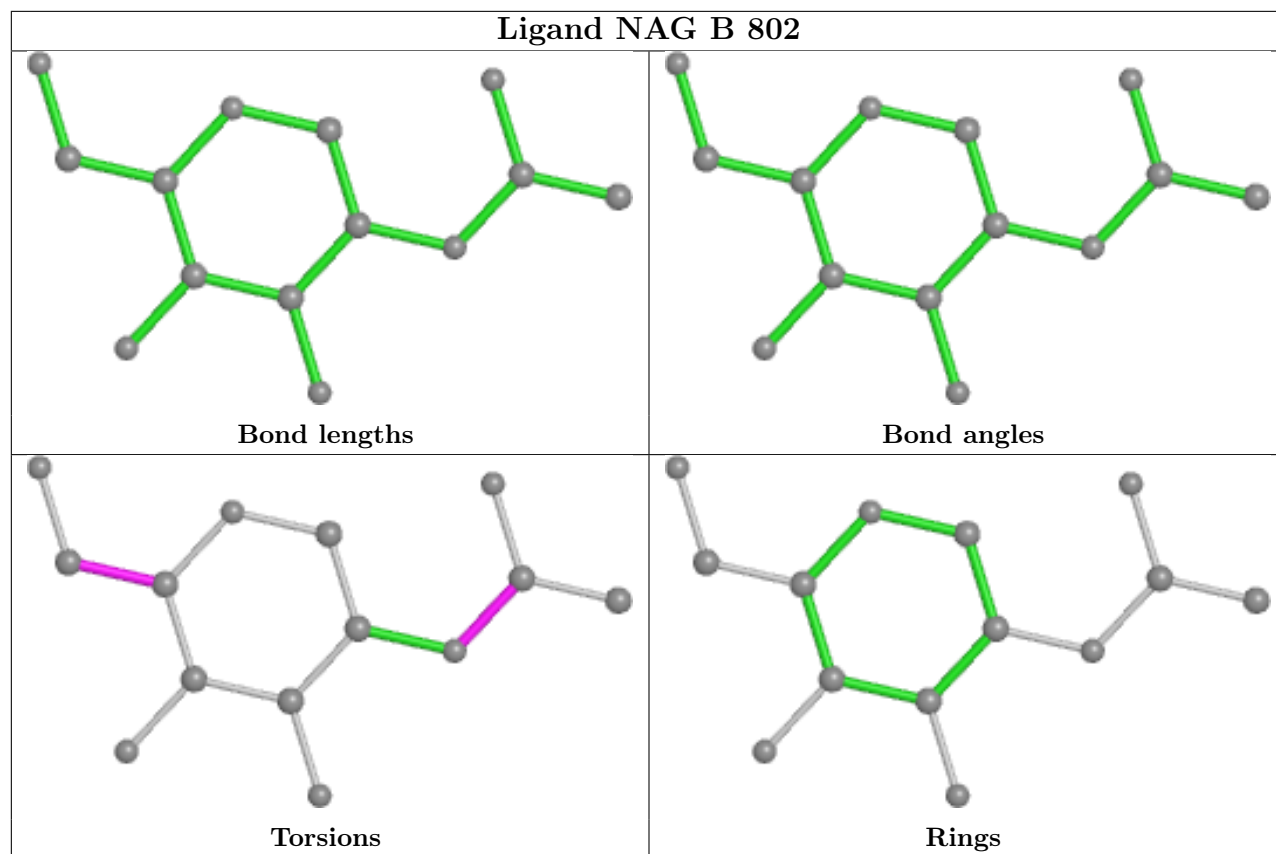
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	803	AKG	1	0

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.

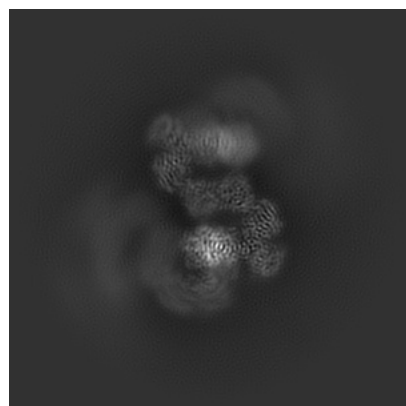
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60079. These allow visual inspection of the internal detail of the map and identification of artifacts.

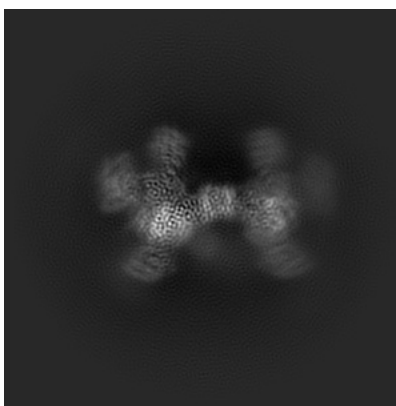
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

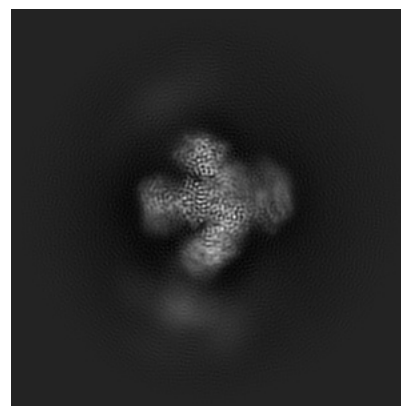
6.1.1 Primary map



X

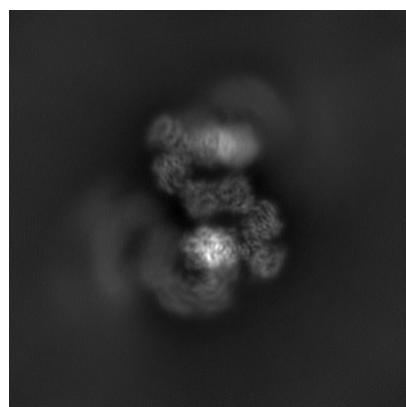


Y

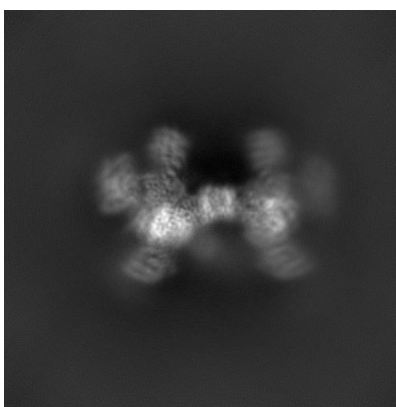


Z

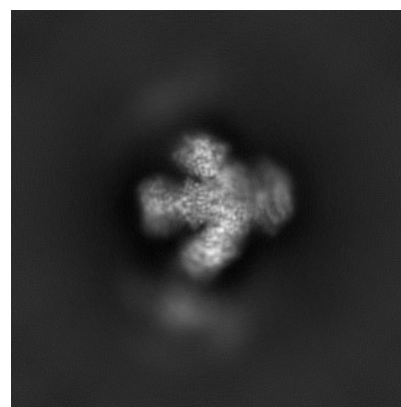
6.1.2 Raw map



X



Y

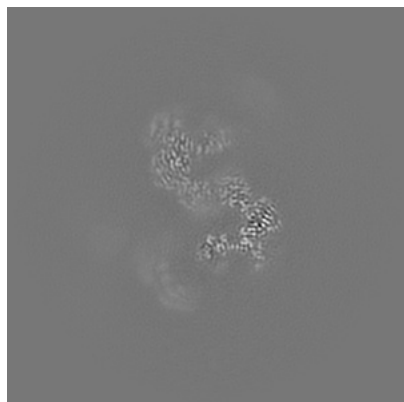


Z

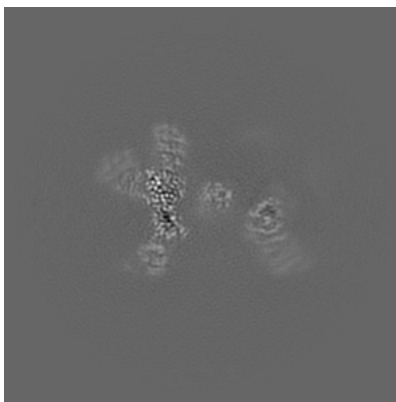
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

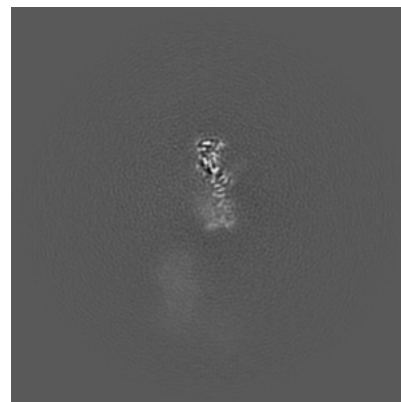
6.2.1 Primary map



X Index: 192

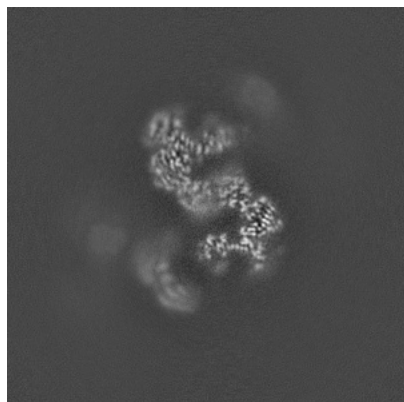


Y Index: 192

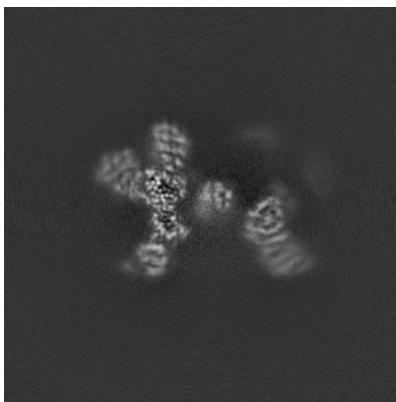


Z Index: 192

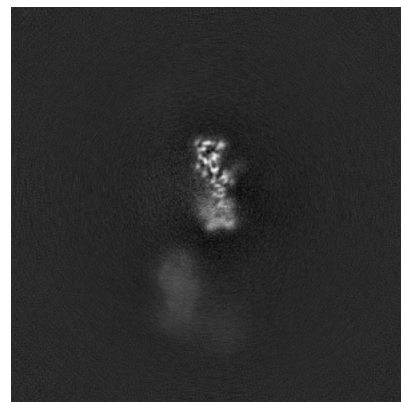
6.2.2 Raw map



X Index: 192



Y Index: 192

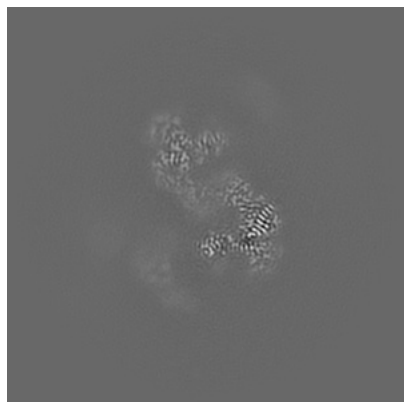


Z Index: 192

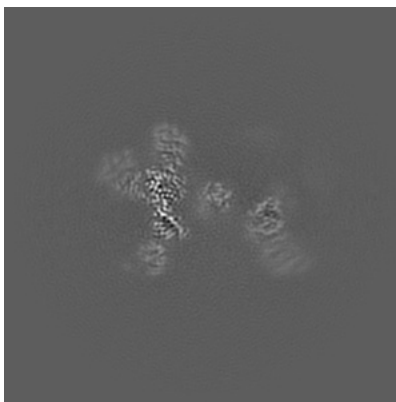
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

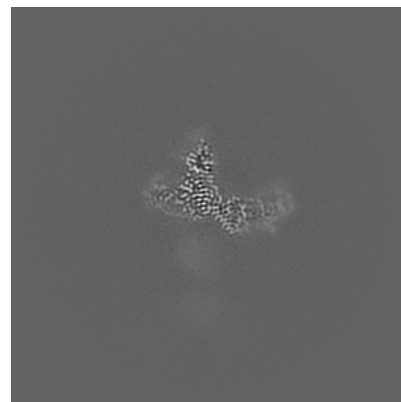
6.3.1 Primary map



X Index: 189

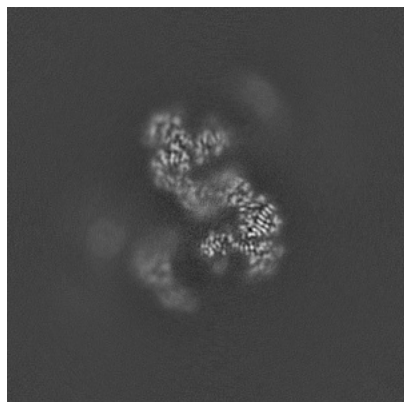


Y Index: 191

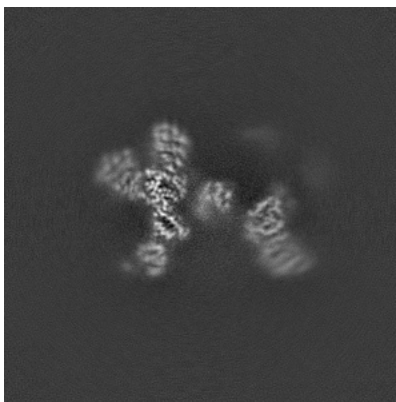


Z Index: 154

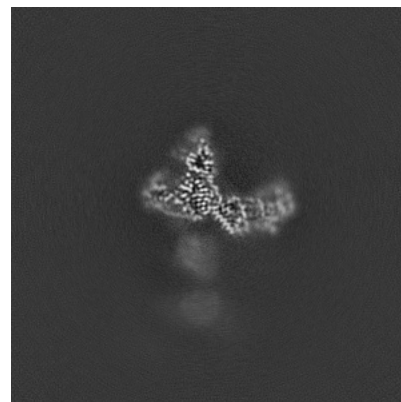
6.3.2 Raw map



X Index: 189



Y Index: 191

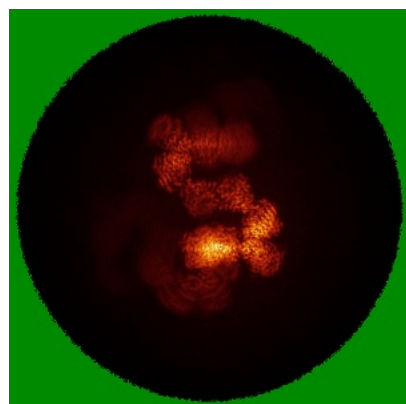


Z Index: 154

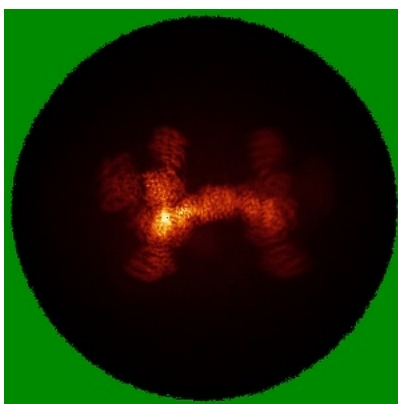
The images above show the largest variance slices of the map in three orthogonal directions.

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

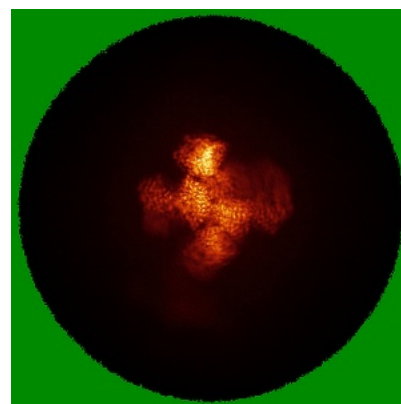
6.4.1 Primary map



X

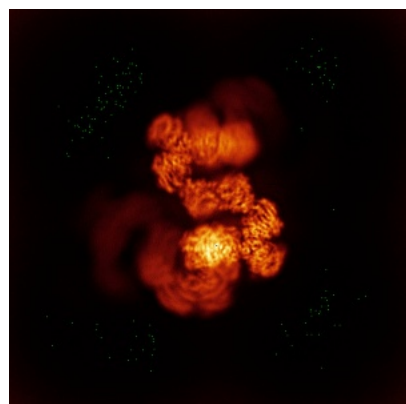


Y



Z

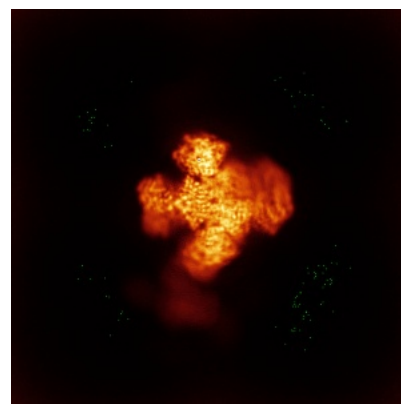
6.4.2 Raw map



X



Y

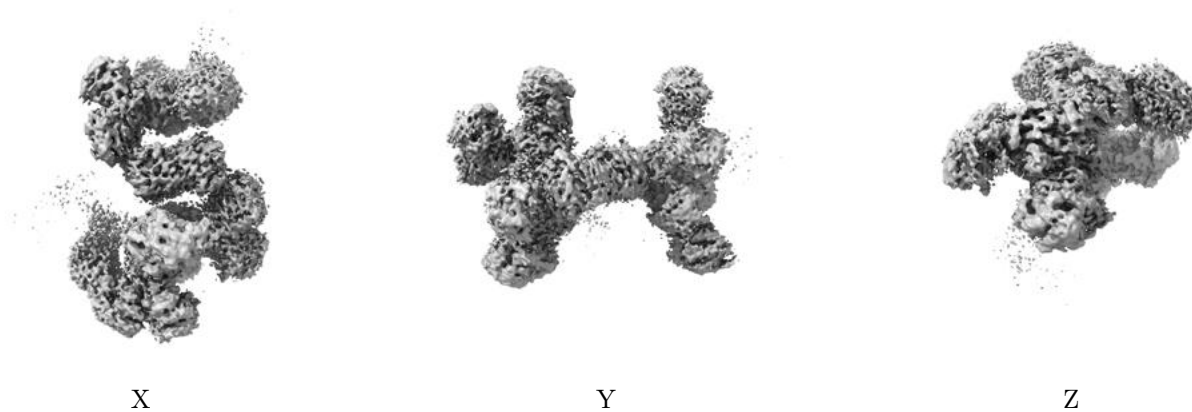


Z

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.

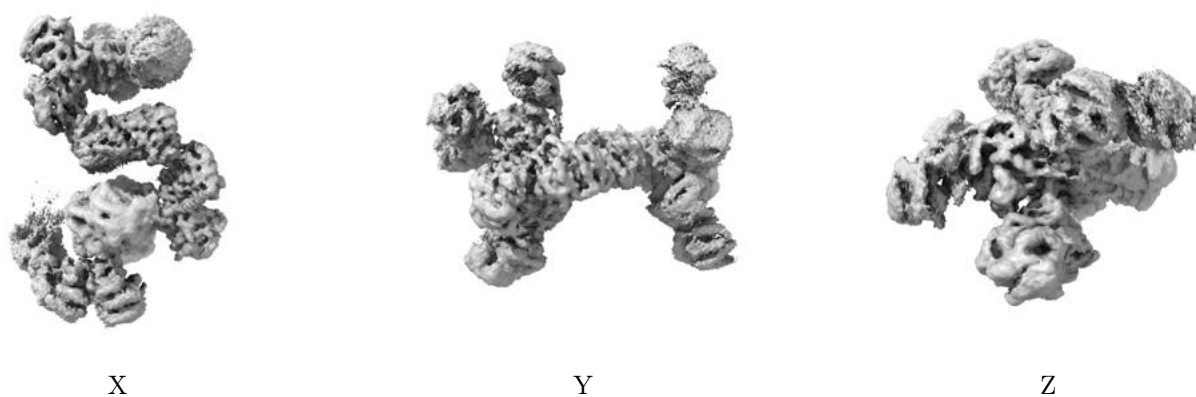
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.216. 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.

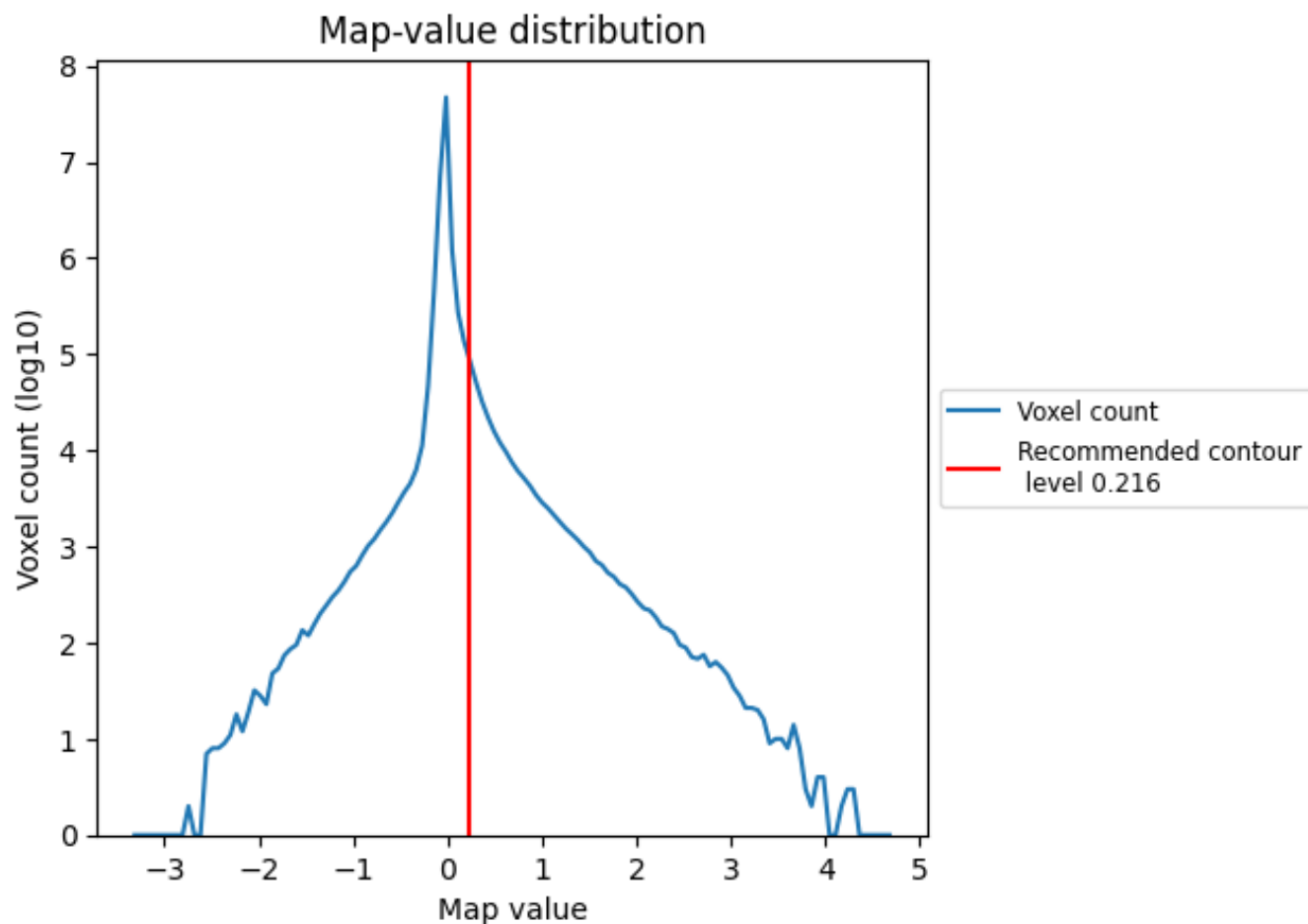
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

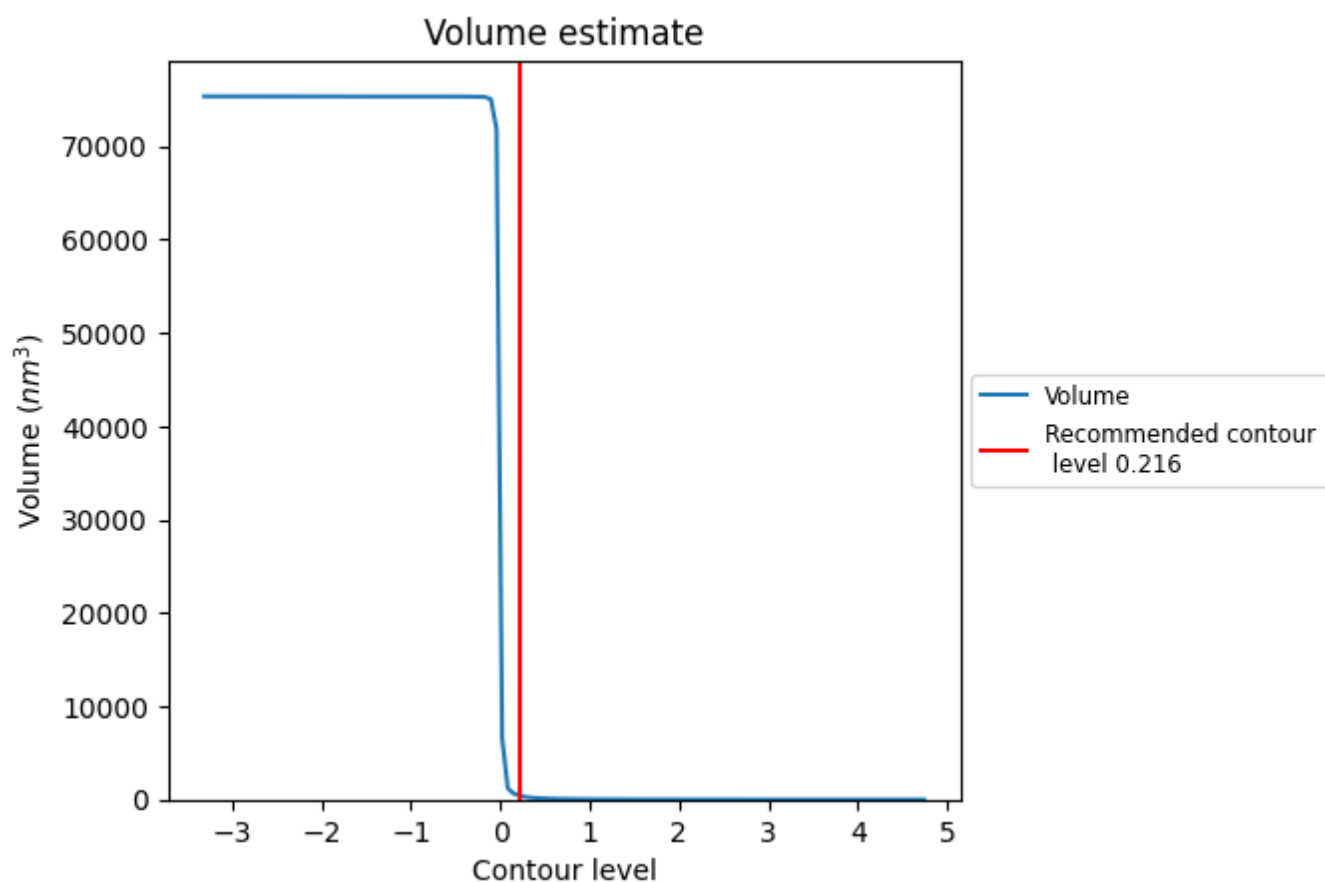
This section contains the results of statistical analysis of the map.

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.

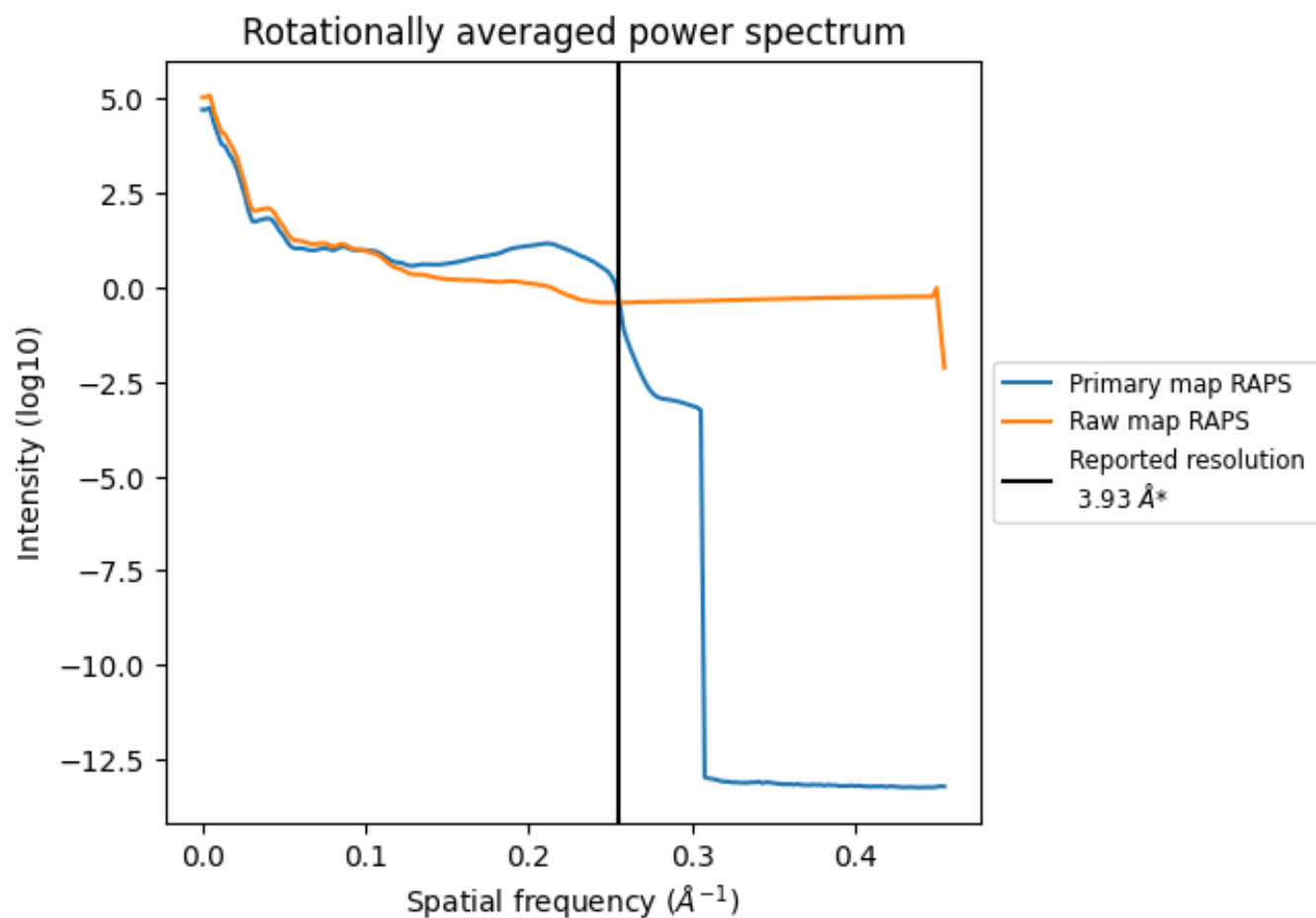
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 419 nm³; this corresponds to an approximate mass of 379 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 ⓘ

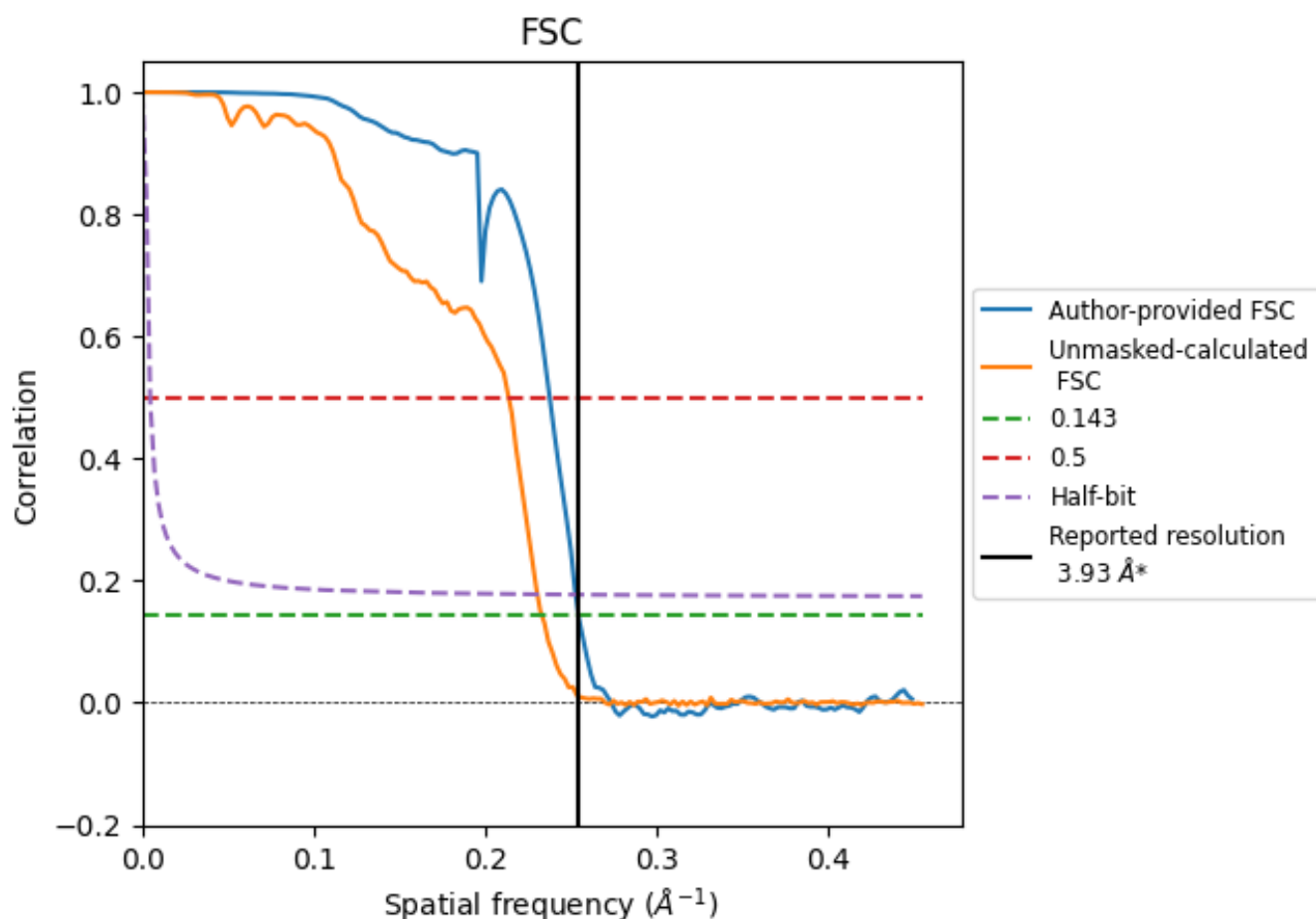


*Reported resolution corresponds to spatial frequency of 0.254 Å⁻¹

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 0.254 \AA^{-1}

8.2 Resolution estimates [i](#)

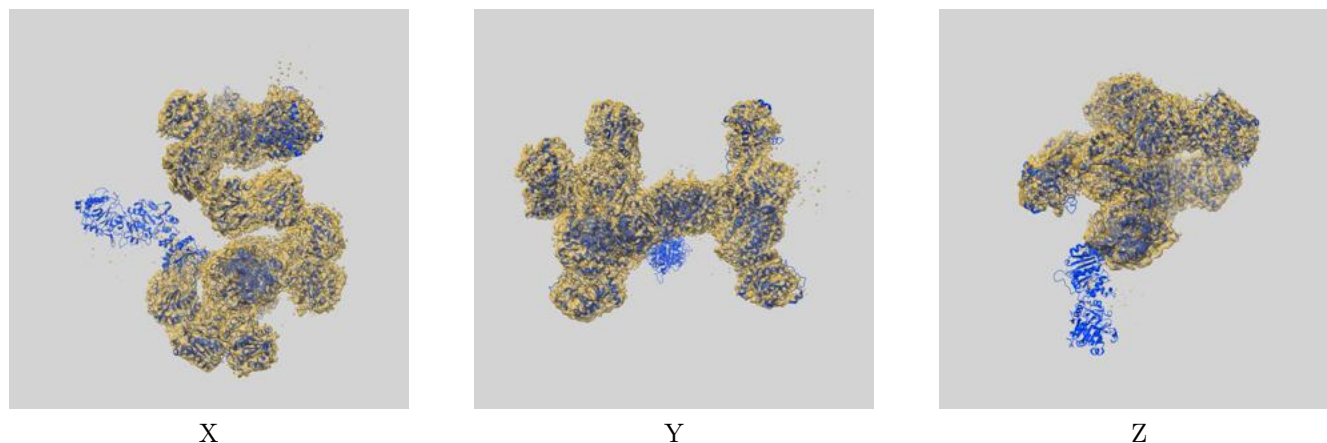
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.93	-	-
Author-provided FSC curve	3.93	4.21	3.96
Unmasked-calculated*	4.29	4.68	4.34

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

9 Map-model fit [i](#)

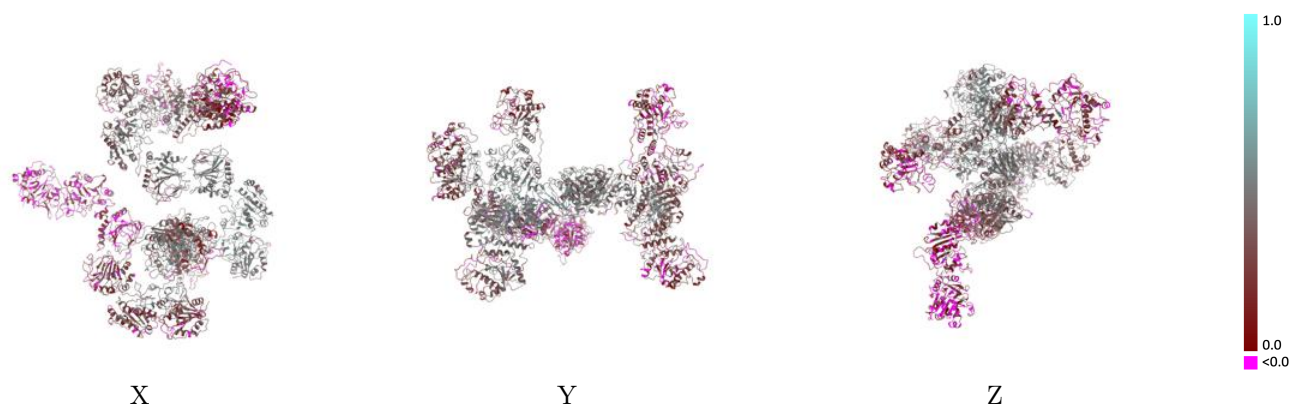
This section contains information regarding the fit between EMDB map EMD-60079 and PDB model 8ZGH. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)



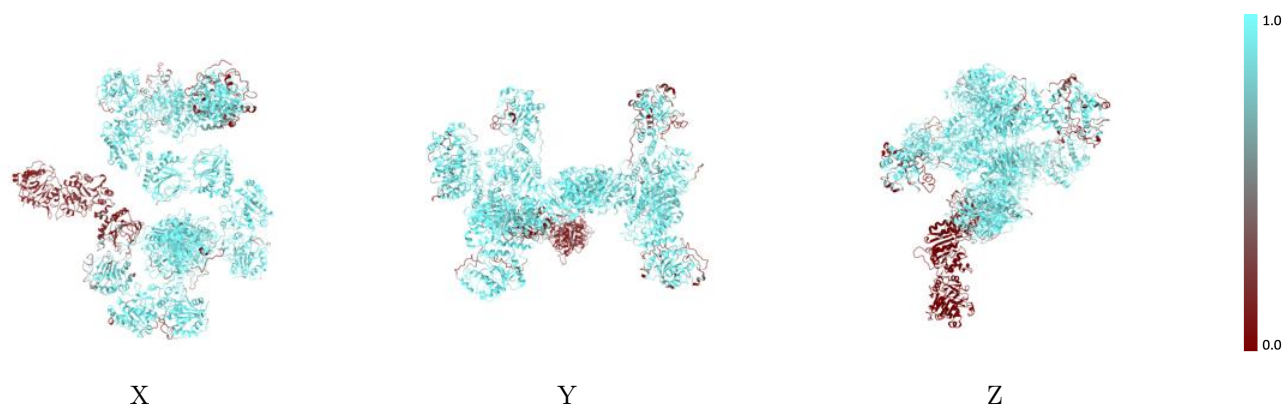
The images above show the 3D surface view of the map at the recommended contour level 0.216 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



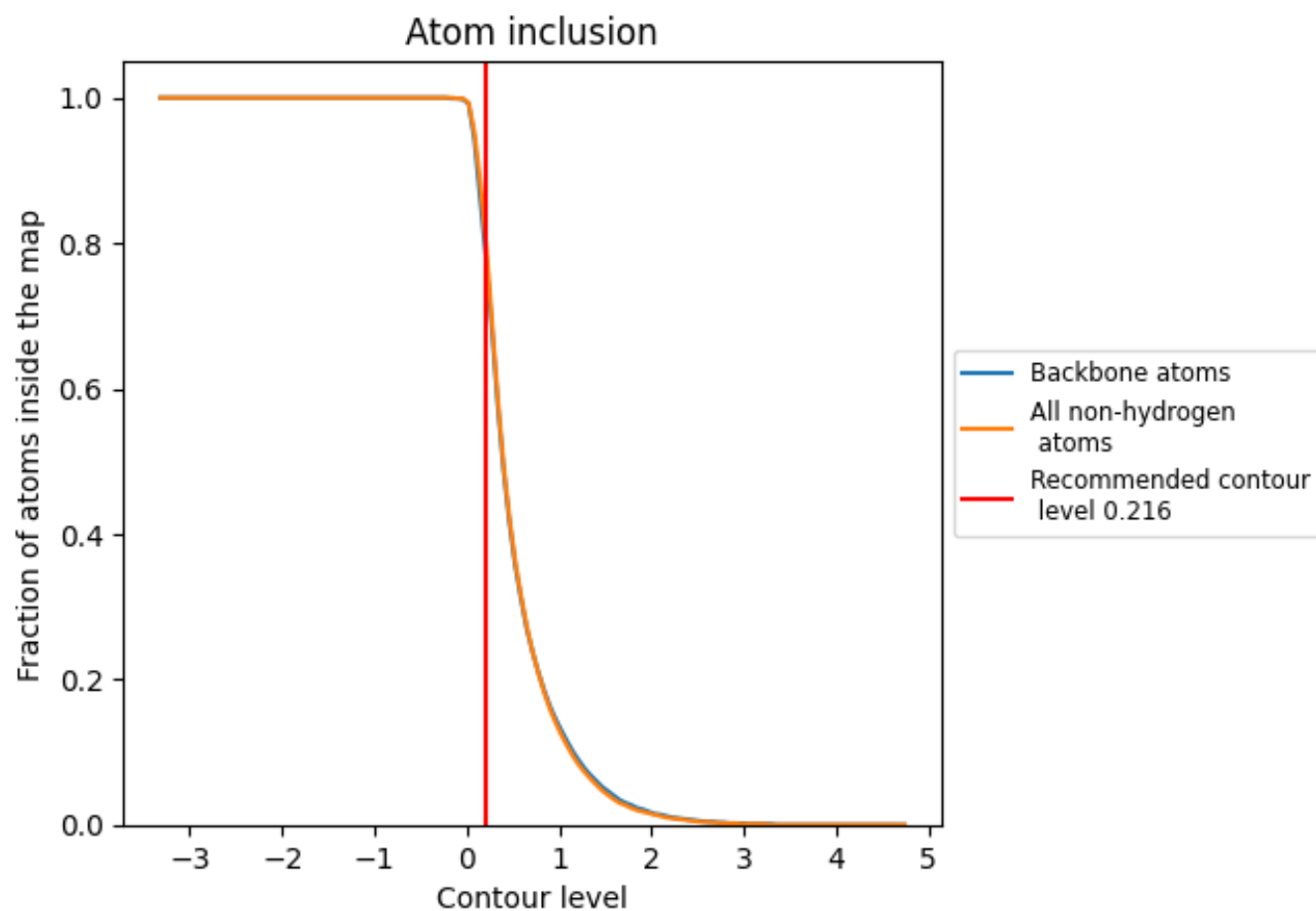
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.216).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% 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 (0.216) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7910	<div></div> 0.3400
A	<div></div> 0.9170	<div></div> 0.3900
B	<div></div> 0.9530	<div></div> 0.4720
C	<div></div> 0.0490	<div></div> 0.0730
D	<div></div> 0.8400	<div></div> 0.2780
E	<div></div> 0.8930	<div></div> 0.4390
F	<div></div> 0.9290	<div></div> 0.4990
U	<div></div> 0.8960	<div></div> 0.3940
V	<div></div> 0.8950	<div></div> 0.4110
W	<div></div> 0.7220	<div></div> 0.2170
X	<div></div> 0.7910	<div></div> 0.2830

1.0

0.0

<0.0