



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 01:54 PM UTC

PDB ID : 9D2M / pdb_00009d2m
EMDB ID : EMD-46500
Title : Map of hemagglutinin A/Sing/INFIMH/16 expressed in 293F cells
Authors : Torrents de la Pena, A.; Ward, A.B.; de Paiva Froes Rocha, R.
Deposited on : 2024-08-08
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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) : 2.49

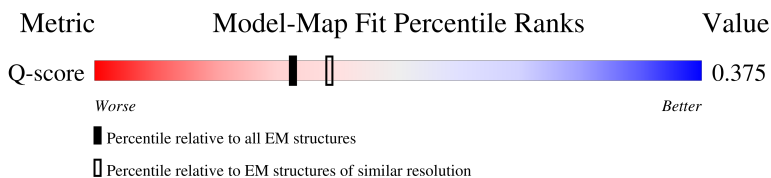
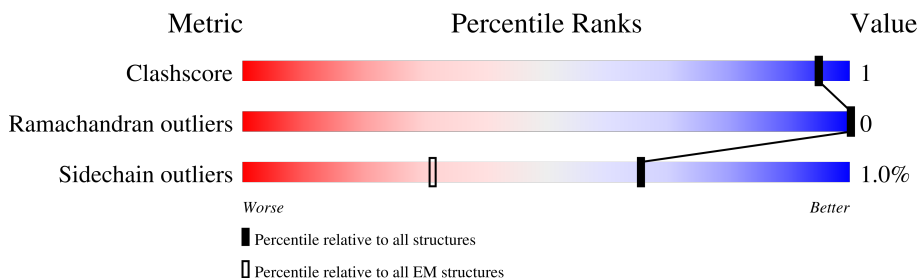
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	826	
1	B	826	
1	C	826	
2	D	2	

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Mol	Chain	Length	Quality of chain
2	F	2	<div><div></div><div>50%</div><div></div><div>50%</div></div>
2	H	2	<div><div></div><div>50%</div><div></div><div>50%</div></div>
2	J	2	<div><div></div><div>50%</div><div></div><div>50%</div></div>
2	L	2	<div><div></div><div>50%</div><div></div><div>50%</div></div>
2	N	2	<div><div></div><div>50%</div><div></div><div>50%</div></div>
3	E	3	<div><div></div><div>67%</div><div></div><div>33%</div></div>
3	G	3	<div><div></div><div>67%</div><div></div><div>33%</div></div>
3	I	3	<div><div></div><div>67%</div><div></div><div>33%</div></div>
3	K	3	<div><div></div><div>67%</div><div></div><div>33%</div></div>
3	M	3	<div><div></div><div>67%</div><div></div><div>33%</div></div>
3	O	3	<div><div></div><div>67%</div><div></div><div>33%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12090 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	478	Total	C	N	O	S	0	0
			3798	2375	672	733	18		
1	B	478	Total	C	N	O	S	0	0
			3798	2375	672	733	18		
1	C	478	Total	C	N	O	S	0	0
			3798	2375	672	733	18		

There are 1002 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A2R4U2X2
A	2	PRO	-	expression tag	UNP A0A2R4U2X2
A	3	MET	-	expression tag	UNP A0A2R4U2X2
A	4	GLY	-	expression tag	UNP A0A2R4U2X2
A	5	SER	-	expression tag	UNP A0A2R4U2X2
A	6	LEU	-	expression tag	UNP A0A2R4U2X2
A	7	GLN	-	expression tag	UNP A0A2R4U2X2
A	8	PRO	-	expression tag	UNP A0A2R4U2X2
A	9	LEU	-	expression tag	UNP A0A2R4U2X2
A	10	ALA	-	expression tag	UNP A0A2R4U2X2
A	11	THR	-	expression tag	UNP A0A2R4U2X2
A	12	LEU	-	expression tag	UNP A0A2R4U2X2
A	13	TYR	-	expression tag	UNP A0A2R4U2X2
A	14	LEU	-	expression tag	UNP A0A2R4U2X2
A	15	LEU	-	expression tag	UNP A0A2R4U2X2
A	16	GLY	-	expression tag	UNP A0A2R4U2X2
A	17	MET	-	expression tag	UNP A0A2R4U2X2
A	18	LEU	-	expression tag	UNP A0A2R4U2X2
A	19	VAL	-	expression tag	UNP A0A2R4U2X2
A	20	ALA	-	expression tag	UNP A0A2R4U2X2
A	21	SER	-	expression tag	UNP A0A2R4U2X2
A	22	VAL	-	expression tag	UNP A0A2R4U2X2
A	23	LEU	-	expression tag	UNP A0A2R4U2X2
A	24	ALA	-	expression tag	UNP A0A2R4U2X2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	493	GLU	GLY	conflict	UNP A0A2R4U2X2
A	518	ARG	-	expression tag	UNP A0A2R4U2X2
A	519	MET	-	expression tag	UNP A0A2R4U2X2
A	520	LYS	-	expression tag	UNP A0A2R4U2X2
A	521	GLN	-	expression tag	UNP A0A2R4U2X2
A	522	ILE	-	expression tag	UNP A0A2R4U2X2
A	523	GLU	-	expression tag	UNP A0A2R4U2X2
A	524	ASP	-	expression tag	UNP A0A2R4U2X2
A	525	LYS	-	expression tag	UNP A0A2R4U2X2
A	526	ILE	-	expression tag	UNP A0A2R4U2X2
A	527	GLU	-	expression tag	UNP A0A2R4U2X2
A	528	GLU	-	expression tag	UNP A0A2R4U2X2
A	529	ILE	-	expression tag	UNP A0A2R4U2X2
A	530	GLU	-	expression tag	UNP A0A2R4U2X2
A	531	SER	-	expression tag	UNP A0A2R4U2X2
A	532	LYS	-	expression tag	UNP A0A2R4U2X2
A	533	GLN	-	expression tag	UNP A0A2R4U2X2
A	534	LYS	-	expression tag	UNP A0A2R4U2X2
A	535	LYS	-	expression tag	UNP A0A2R4U2X2
A	536	ILE	-	expression tag	UNP A0A2R4U2X2
A	537	GLU	-	expression tag	UNP A0A2R4U2X2
A	538	ASN	-	expression tag	UNP A0A2R4U2X2
A	539	GLU	-	expression tag	UNP A0A2R4U2X2
A	540	ILE	-	expression tag	UNP A0A2R4U2X2
A	541	ALA	-	expression tag	UNP A0A2R4U2X2
A	542	ARG	-	expression tag	UNP A0A2R4U2X2
A	543	ILE	-	expression tag	UNP A0A2R4U2X2
A	544	LYS	-	expression tag	UNP A0A2R4U2X2
A	545	LYS	-	expression tag	UNP A0A2R4U2X2
A	546	ILE	-	expression tag	UNP A0A2R4U2X2
A	547	LYS	-	expression tag	UNP A0A2R4U2X2
A	548	LEU	-	expression tag	UNP A0A2R4U2X2
A	549	VAL	-	expression tag	UNP A0A2R4U2X2
A	550	PRO	-	expression tag	UNP A0A2R4U2X2
A	551	ARG	-	expression tag	UNP A0A2R4U2X2
A	552	GLY	-	expression tag	UNP A0A2R4U2X2
A	553	SER	-	expression tag	UNP A0A2R4U2X2
A	554	VAL	-	expression tag	UNP A0A2R4U2X2
A	555	ASP	-	expression tag	UNP A0A2R4U2X2
A	556	GLU	-	expression tag	UNP A0A2R4U2X2
A	557	ASN	-	expression tag	UNP A0A2R4U2X2
A	558	LEU	-	expression tag	UNP A0A2R4U2X2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	559	TYR	-	expression tag	UNP A0A2R4U2X2
A	560	PHE	-	expression tag	UNP A0A2R4U2X2
A	561	GLN	-	expression tag	UNP A0A2R4U2X2
A	562	ALA	-	expression tag	UNP A0A2R4U2X2
A	563	MET	-	expression tag	UNP A0A2R4U2X2
A	564	SER	-	expression tag	UNP A0A2R4U2X2
A	565	LYS	-	expression tag	UNP A0A2R4U2X2
A	566	GLY	-	expression tag	UNP A0A2R4U2X2
A	567	GLU	-	expression tag	UNP A0A2R4U2X2
A	568	GLU	-	expression tag	UNP A0A2R4U2X2
A	569	LEU	-	expression tag	UNP A0A2R4U2X2
A	570	PHE	-	expression tag	UNP A0A2R4U2X2
A	571	THR	-	expression tag	UNP A0A2R4U2X2
A	572	GLY	-	expression tag	UNP A0A2R4U2X2
A	573	VAL	-	expression tag	UNP A0A2R4U2X2
A	574	VAL	-	expression tag	UNP A0A2R4U2X2
A	575	PRO	-	expression tag	UNP A0A2R4U2X2
A	576	ILE	-	expression tag	UNP A0A2R4U2X2
A	577	LEU	-	expression tag	UNP A0A2R4U2X2
A	578	VAL	-	expression tag	UNP A0A2R4U2X2
A	579	GLU	-	expression tag	UNP A0A2R4U2X2
A	580	LEU	-	expression tag	UNP A0A2R4U2X2
A	581	ASP	-	expression tag	UNP A0A2R4U2X2
A	582	GLY	-	expression tag	UNP A0A2R4U2X2
A	583	ASP	-	expression tag	UNP A0A2R4U2X2
A	584	VAL	-	expression tag	UNP A0A2R4U2X2
A	585	ASN	-	expression tag	UNP A0A2R4U2X2
A	586	GLY	-	expression tag	UNP A0A2R4U2X2
A	587	HIS	-	expression tag	UNP A0A2R4U2X2
A	588	LYS	-	expression tag	UNP A0A2R4U2X2
A	589	PHE	-	expression tag	UNP A0A2R4U2X2
A	590	SER	-	expression tag	UNP A0A2R4U2X2
A	591	VAL	-	expression tag	UNP A0A2R4U2X2
A	592	ARG	-	expression tag	UNP A0A2R4U2X2
A	593	GLY	-	expression tag	UNP A0A2R4U2X2
A	594	GLU	-	expression tag	UNP A0A2R4U2X2
A	595	GLY	-	expression tag	UNP A0A2R4U2X2
A	596	GLU	-	expression tag	UNP A0A2R4U2X2
A	597	GLY	-	expression tag	UNP A0A2R4U2X2
A	598	ASP	-	expression tag	UNP A0A2R4U2X2
A	599	ALA	-	expression tag	UNP A0A2R4U2X2
A	600	THR	-	expression tag	UNP A0A2R4U2X2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	601	ASN	-	expression tag	UNP A0A2R4U2X2
A	602	GLY	-	expression tag	UNP A0A2R4U2X2
A	603	LYS	-	expression tag	UNP A0A2R4U2X2
A	604	LEU	-	expression tag	UNP A0A2R4U2X2
A	605	THR	-	expression tag	UNP A0A2R4U2X2
A	606	LEU	-	expression tag	UNP A0A2R4U2X2
A	607	LYS	-	expression tag	UNP A0A2R4U2X2
A	608	PHE	-	expression tag	UNP A0A2R4U2X2
A	609	ILE	-	expression tag	UNP A0A2R4U2X2
A	610	CYS	-	expression tag	UNP A0A2R4U2X2
A	611	THR	-	expression tag	UNP A0A2R4U2X2
A	612	THR	-	expression tag	UNP A0A2R4U2X2
A	613	GLY	-	expression tag	UNP A0A2R4U2X2
A	614	LYS	-	expression tag	UNP A0A2R4U2X2
A	615	LEU	-	expression tag	UNP A0A2R4U2X2
A	616	PRO	-	expression tag	UNP A0A2R4U2X2
A	617	VAL	-	expression tag	UNP A0A2R4U2X2
A	618	PRO	-	expression tag	UNP A0A2R4U2X2
A	619	TRP	-	expression tag	UNP A0A2R4U2X2
A	620	PRO	-	expression tag	UNP A0A2R4U2X2
A	621	THR	-	expression tag	UNP A0A2R4U2X2
A	622	LEU	-	expression tag	UNP A0A2R4U2X2
A	623	VAL	-	expression tag	UNP A0A2R4U2X2
A	624	THR	-	expression tag	UNP A0A2R4U2X2
A	625	THR	-	expression tag	UNP A0A2R4U2X2
A	626	LEU	-	expression tag	UNP A0A2R4U2X2
A	627	THR	-	expression tag	UNP A0A2R4U2X2
A	628	TYR	-	expression tag	UNP A0A2R4U2X2
A	629	GLY	-	expression tag	UNP A0A2R4U2X2
A	630	VAL	-	expression tag	UNP A0A2R4U2X2
A	631	GLN	-	expression tag	UNP A0A2R4U2X2
A	632	CYS	-	expression tag	UNP A0A2R4U2X2
A	633	PHE	-	expression tag	UNP A0A2R4U2X2
A	634	SER	-	expression tag	UNP A0A2R4U2X2
A	635	ARG	-	expression tag	UNP A0A2R4U2X2
A	636	TYR	-	expression tag	UNP A0A2R4U2X2
A	637	PRO	-	expression tag	UNP A0A2R4U2X2
A	638	ASP	-	expression tag	UNP A0A2R4U2X2
A	639	HIS	-	expression tag	UNP A0A2R4U2X2
A	640	MET	-	expression tag	UNP A0A2R4U2X2
A	641	LYS	-	expression tag	UNP A0A2R4U2X2
A	642	ARG	-	expression tag	UNP A0A2R4U2X2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	643	HIS	-	expression tag	UNP A0A2R4U2X2
A	644	ASP	-	expression tag	UNP A0A2R4U2X2
A	645	PHE	-	expression tag	UNP A0A2R4U2X2
A	646	PHE	-	expression tag	UNP A0A2R4U2X2
A	647	LYS	-	expression tag	UNP A0A2R4U2X2
A	648	SER	-	expression tag	UNP A0A2R4U2X2
A	649	ALA	-	expression tag	UNP A0A2R4U2X2
A	650	MET	-	expression tag	UNP A0A2R4U2X2
A	651	PRO	-	expression tag	UNP A0A2R4U2X2
A	652	GLU	-	expression tag	UNP A0A2R4U2X2
A	653	GLY	-	expression tag	UNP A0A2R4U2X2
A	654	TYR	-	expression tag	UNP A0A2R4U2X2
A	655	VAL	-	expression tag	UNP A0A2R4U2X2
A	656	GLN	-	expression tag	UNP A0A2R4U2X2
A	657	GLU	-	expression tag	UNP A0A2R4U2X2
A	658	ARG	-	expression tag	UNP A0A2R4U2X2
A	659	THR	-	expression tag	UNP A0A2R4U2X2
A	660	ILE	-	expression tag	UNP A0A2R4U2X2
A	661	SER	-	expression tag	UNP A0A2R4U2X2
A	662	PHE	-	expression tag	UNP A0A2R4U2X2
A	663	LYS	-	expression tag	UNP A0A2R4U2X2
A	664	ASP	-	expression tag	UNP A0A2R4U2X2
A	665	ASP	-	expression tag	UNP A0A2R4U2X2
A	666	GLY	-	expression tag	UNP A0A2R4U2X2
A	667	THR	-	expression tag	UNP A0A2R4U2X2
A	668	TYR	-	expression tag	UNP A0A2R4U2X2
A	669	LYS	-	expression tag	UNP A0A2R4U2X2
A	670	THR	-	expression tag	UNP A0A2R4U2X2
A	671	ARG	-	expression tag	UNP A0A2R4U2X2
A	672	ALA	-	expression tag	UNP A0A2R4U2X2
A	673	GLU	-	expression tag	UNP A0A2R4U2X2
A	674	VAL	-	expression tag	UNP A0A2R4U2X2
A	675	LYS	-	expression tag	UNP A0A2R4U2X2
A	676	PHE	-	expression tag	UNP A0A2R4U2X2
A	677	GLU	-	expression tag	UNP A0A2R4U2X2
A	678	GLY	-	expression tag	UNP A0A2R4U2X2
A	679	ASP	-	expression tag	UNP A0A2R4U2X2
A	680	THR	-	expression tag	UNP A0A2R4U2X2
A	681	LEU	-	expression tag	UNP A0A2R4U2X2
A	682	VAL	-	expression tag	UNP A0A2R4U2X2
A	683	ASN	-	expression tag	UNP A0A2R4U2X2
A	684	ARG	-	expression tag	UNP A0A2R4U2X2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	685	ILE	-	expression tag	UNP A0A2R4U2X2
A	686	GLU	-	expression tag	UNP A0A2R4U2X2
A	687	LEU	-	expression tag	UNP A0A2R4U2X2
A	688	LYS	-	expression tag	UNP A0A2R4U2X2
A	689	GLY	-	expression tag	UNP A0A2R4U2X2
A	690	ILE	-	expression tag	UNP A0A2R4U2X2
A	691	ASP	-	expression tag	UNP A0A2R4U2X2
A	692	PHE	-	expression tag	UNP A0A2R4U2X2
A	693	LYS	-	expression tag	UNP A0A2R4U2X2
A	694	GLU	-	expression tag	UNP A0A2R4U2X2
A	695	ASP	-	expression tag	UNP A0A2R4U2X2
A	696	GLY	-	expression tag	UNP A0A2R4U2X2
A	697	ASN	-	expression tag	UNP A0A2R4U2X2
A	698	ILE	-	expression tag	UNP A0A2R4U2X2
A	699	LEU	-	expression tag	UNP A0A2R4U2X2
A	700	GLY	-	expression tag	UNP A0A2R4U2X2
A	701	HIS	-	expression tag	UNP A0A2R4U2X2
A	702	LYS	-	expression tag	UNP A0A2R4U2X2
A	703	LEU	-	expression tag	UNP A0A2R4U2X2
A	704	GLU	-	expression tag	UNP A0A2R4U2X2
A	705	TYR	-	expression tag	UNP A0A2R4U2X2
A	706	ASN	-	expression tag	UNP A0A2R4U2X2
A	707	PHE	-	expression tag	UNP A0A2R4U2X2
A	708	ASN	-	expression tag	UNP A0A2R4U2X2
A	709	SER	-	expression tag	UNP A0A2R4U2X2
A	710	HIS	-	expression tag	UNP A0A2R4U2X2
A	711	ASN	-	expression tag	UNP A0A2R4U2X2
A	712	VAL	-	expression tag	UNP A0A2R4U2X2
A	713	TYR	-	expression tag	UNP A0A2R4U2X2
A	714	ILE	-	expression tag	UNP A0A2R4U2X2
A	715	THR	-	expression tag	UNP A0A2R4U2X2
A	716	ALA	-	expression tag	UNP A0A2R4U2X2
A	717	ASP	-	expression tag	UNP A0A2R4U2X2
A	718	LYS	-	expression tag	UNP A0A2R4U2X2
A	719	GLN	-	expression tag	UNP A0A2R4U2X2
A	720	LYS	-	expression tag	UNP A0A2R4U2X2
A	721	ASN	-	expression tag	UNP A0A2R4U2X2
A	722	GLY	-	expression tag	UNP A0A2R4U2X2
A	723	ILE	-	expression tag	UNP A0A2R4U2X2
A	724	LYS	-	expression tag	UNP A0A2R4U2X2
A	725	ALA	-	expression tag	UNP A0A2R4U2X2
A	726	ASN	-	expression tag	UNP A0A2R4U2X2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	727	PHE	-	expression tag	UNP A0A2R4U2X2
A	728	LYS	-	expression tag	UNP A0A2R4U2X2
A	729	ILE	-	expression tag	UNP A0A2R4U2X2
A	730	ARG	-	expression tag	UNP A0A2R4U2X2
A	731	HIS	-	expression tag	UNP A0A2R4U2X2
A	732	ASN	-	expression tag	UNP A0A2R4U2X2
A	733	VAL	-	expression tag	UNP A0A2R4U2X2
A	734	GLU	-	expression tag	UNP A0A2R4U2X2
A	735	ASP	-	expression tag	UNP A0A2R4U2X2
A	736	GLY	-	expression tag	UNP A0A2R4U2X2
A	737	SER	-	expression tag	UNP A0A2R4U2X2
A	738	VAL	-	expression tag	UNP A0A2R4U2X2
A	739	GLN	-	expression tag	UNP A0A2R4U2X2
A	740	LEU	-	expression tag	UNP A0A2R4U2X2
A	741	ALA	-	expression tag	UNP A0A2R4U2X2
A	742	ASP	-	expression tag	UNP A0A2R4U2X2
A	743	HIS	-	expression tag	UNP A0A2R4U2X2
A	744	TYR	-	expression tag	UNP A0A2R4U2X2
A	745	GLN	-	expression tag	UNP A0A2R4U2X2
A	746	GLN	-	expression tag	UNP A0A2R4U2X2
A	747	ASN	-	expression tag	UNP A0A2R4U2X2
A	748	THR	-	expression tag	UNP A0A2R4U2X2
A	749	PRO	-	expression tag	UNP A0A2R4U2X2
A	750	ILE	-	expression tag	UNP A0A2R4U2X2
A	751	GLY	-	expression tag	UNP A0A2R4U2X2
A	752	ASP	-	expression tag	UNP A0A2R4U2X2
A	753	GLY	-	expression tag	UNP A0A2R4U2X2
A	754	PRO	-	expression tag	UNP A0A2R4U2X2
A	755	VAL	-	expression tag	UNP A0A2R4U2X2
A	756	LEU	-	expression tag	UNP A0A2R4U2X2
A	757	LEU	-	expression tag	UNP A0A2R4U2X2
A	758	PRO	-	expression tag	UNP A0A2R4U2X2
A	759	ASP	-	expression tag	UNP A0A2R4U2X2
A	760	ASN	-	expression tag	UNP A0A2R4U2X2
A	761	HIS	-	expression tag	UNP A0A2R4U2X2
A	762	TYR	-	expression tag	UNP A0A2R4U2X2
A	763	LEU	-	expression tag	UNP A0A2R4U2X2
A	764	SER	-	expression tag	UNP A0A2R4U2X2
A	765	THR	-	expression tag	UNP A0A2R4U2X2
A	766	GLN	-	expression tag	UNP A0A2R4U2X2
A	767	SER	-	expression tag	UNP A0A2R4U2X2
A	768	VAL	-	expression tag	UNP A0A2R4U2X2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	769	LEU	-	expression tag	UNP A0A2R4U2X2
A	770	SER	-	expression tag	UNP A0A2R4U2X2
A	771	LYS	-	expression tag	UNP A0A2R4U2X2
A	772	ASP	-	expression tag	UNP A0A2R4U2X2
A	773	PRO	-	expression tag	UNP A0A2R4U2X2
A	774	ASN	-	expression tag	UNP A0A2R4U2X2
A	775	GLU	-	expression tag	UNP A0A2R4U2X2
A	776	LYS	-	expression tag	UNP A0A2R4U2X2
A	777	ARG	-	expression tag	UNP A0A2R4U2X2
A	778	ASP	-	expression tag	UNP A0A2R4U2X2
A	779	HIS	-	expression tag	UNP A0A2R4U2X2
A	780	MET	-	expression tag	UNP A0A2R4U2X2
A	781	VAL	-	expression tag	UNP A0A2R4U2X2
A	782	LEU	-	expression tag	UNP A0A2R4U2X2
A	783	LEU	-	expression tag	UNP A0A2R4U2X2
A	784	GLU	-	expression tag	UNP A0A2R4U2X2
A	785	PHE	-	expression tag	UNP A0A2R4U2X2
A	786	VAL	-	expression tag	UNP A0A2R4U2X2
A	787	THR	-	expression tag	UNP A0A2R4U2X2
A	788	ALA	-	expression tag	UNP A0A2R4U2X2
A	789	ALA	-	expression tag	UNP A0A2R4U2X2
A	790	GLY	-	expression tag	UNP A0A2R4U2X2
A	791	ILE	-	expression tag	UNP A0A2R4U2X2
A	792	THR	-	expression tag	UNP A0A2R4U2X2
A	793	HIS	-	expression tag	UNP A0A2R4U2X2
A	794	GLY	-	expression tag	UNP A0A2R4U2X2
A	795	MET	-	expression tag	UNP A0A2R4U2X2
A	796	SER	-	expression tag	UNP A0A2R4U2X2
A	797	SER	-	expression tag	UNP A0A2R4U2X2
A	798	ALA	-	expression tag	UNP A0A2R4U2X2
A	799	TRP	-	expression tag	UNP A0A2R4U2X2
A	800	SER	-	expression tag	UNP A0A2R4U2X2
A	801	HIS	-	expression tag	UNP A0A2R4U2X2
A	802	PRO	-	expression tag	UNP A0A2R4U2X2
A	803	GLN	-	expression tag	UNP A0A2R4U2X2
A	804	PHE	-	expression tag	UNP A0A2R4U2X2
A	805	GLU	-	expression tag	UNP A0A2R4U2X2
A	806	LYS	-	expression tag	UNP A0A2R4U2X2
A	807	GLY	-	expression tag	UNP A0A2R4U2X2
A	808	GLY	-	expression tag	UNP A0A2R4U2X2
A	809	GLY	-	expression tag	UNP A0A2R4U2X2
A	810	SER	-	expression tag	UNP A0A2R4U2X2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	811	GLY	-	expression tag	UNP A0A2R4U2X2
A	812	GLY	-	expression tag	UNP A0A2R4U2X2
A	813	GLY	-	expression tag	UNP A0A2R4U2X2
A	814	SER	-	expression tag	UNP A0A2R4U2X2
A	815	GLY	-	expression tag	UNP A0A2R4U2X2
A	816	GLY	-	expression tag	UNP A0A2R4U2X2
A	817	SER	-	expression tag	UNP A0A2R4U2X2
A	818	ALA	-	expression tag	UNP A0A2R4U2X2
A	819	TRP	-	expression tag	UNP A0A2R4U2X2
A	820	SER	-	expression tag	UNP A0A2R4U2X2
A	821	HIS	-	expression tag	UNP A0A2R4U2X2
A	822	PRO	-	expression tag	UNP A0A2R4U2X2
A	823	GLN	-	expression tag	UNP A0A2R4U2X2
A	824	PHE	-	expression tag	UNP A0A2R4U2X2
A	825	GLU	-	expression tag	UNP A0A2R4U2X2
A	826	LYS	-	expression tag	UNP A0A2R4U2X2
B	1	MET	-	initiating methionine	UNP A0A2R4U2X2
B	2	PRO	-	expression tag	UNP A0A2R4U2X2
B	3	MET	-	expression tag	UNP A0A2R4U2X2
B	4	GLY	-	expression tag	UNP A0A2R4U2X2
B	5	SER	-	expression tag	UNP A0A2R4U2X2
B	6	LEU	-	expression tag	UNP A0A2R4U2X2
B	7	GLN	-	expression tag	UNP A0A2R4U2X2
B	8	PRO	-	expression tag	UNP A0A2R4U2X2
B	9	LEU	-	expression tag	UNP A0A2R4U2X2
B	10	ALA	-	expression tag	UNP A0A2R4U2X2
B	11	THR	-	expression tag	UNP A0A2R4U2X2
B	12	LEU	-	expression tag	UNP A0A2R4U2X2
B	13	TYR	-	expression tag	UNP A0A2R4U2X2
B	14	LEU	-	expression tag	UNP A0A2R4U2X2
B	15	LEU	-	expression tag	UNP A0A2R4U2X2
B	16	GLY	-	expression tag	UNP A0A2R4U2X2
B	17	MET	-	expression tag	UNP A0A2R4U2X2
B	18	LEU	-	expression tag	UNP A0A2R4U2X2
B	19	VAL	-	expression tag	UNP A0A2R4U2X2
B	20	ALA	-	expression tag	UNP A0A2R4U2X2
B	21	SER	-	expression tag	UNP A0A2R4U2X2
B	22	VAL	-	expression tag	UNP A0A2R4U2X2
B	23	LEU	-	expression tag	UNP A0A2R4U2X2
B	24	ALA	-	expression tag	UNP A0A2R4U2X2
B	493	GLU	GLY	conflict	UNP A0A2R4U2X2
B	518	ARG	-	expression tag	UNP A0A2R4U2X2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	519	MET	-	expression tag	UNP A0A2R4U2X2
B	520	LYS	-	expression tag	UNP A0A2R4U2X2
B	521	GLN	-	expression tag	UNP A0A2R4U2X2
B	522	ILE	-	expression tag	UNP A0A2R4U2X2
B	523	GLU	-	expression tag	UNP A0A2R4U2X2
B	524	ASP	-	expression tag	UNP A0A2R4U2X2
B	525	LYS	-	expression tag	UNP A0A2R4U2X2
B	526	ILE	-	expression tag	UNP A0A2R4U2X2
B	527	GLU	-	expression tag	UNP A0A2R4U2X2
B	528	GLU	-	expression tag	UNP A0A2R4U2X2
B	529	ILE	-	expression tag	UNP A0A2R4U2X2
B	530	GLU	-	expression tag	UNP A0A2R4U2X2
B	531	SER	-	expression tag	UNP A0A2R4U2X2
B	532	LYS	-	expression tag	UNP A0A2R4U2X2
B	533	GLN	-	expression tag	UNP A0A2R4U2X2
B	534	LYS	-	expression tag	UNP A0A2R4U2X2
B	535	LYS	-	expression tag	UNP A0A2R4U2X2
B	536	ILE	-	expression tag	UNP A0A2R4U2X2
B	537	GLU	-	expression tag	UNP A0A2R4U2X2
B	538	ASN	-	expression tag	UNP A0A2R4U2X2
B	539	GLU	-	expression tag	UNP A0A2R4U2X2
B	540	ILE	-	expression tag	UNP A0A2R4U2X2
B	541	ALA	-	expression tag	UNP A0A2R4U2X2
B	542	ARG	-	expression tag	UNP A0A2R4U2X2
B	543	ILE	-	expression tag	UNP A0A2R4U2X2
B	544	LYS	-	expression tag	UNP A0A2R4U2X2
B	545	LYS	-	expression tag	UNP A0A2R4U2X2
B	546	ILE	-	expression tag	UNP A0A2R4U2X2
B	547	LYS	-	expression tag	UNP A0A2R4U2X2
B	548	LEU	-	expression tag	UNP A0A2R4U2X2
B	549	VAL	-	expression tag	UNP A0A2R4U2X2
B	550	PRO	-	expression tag	UNP A0A2R4U2X2
B	551	ARG	-	expression tag	UNP A0A2R4U2X2
B	552	GLY	-	expression tag	UNP A0A2R4U2X2
B	553	SER	-	expression tag	UNP A0A2R4U2X2
B	554	VAL	-	expression tag	UNP A0A2R4U2X2
B	555	ASP	-	expression tag	UNP A0A2R4U2X2
B	556	GLU	-	expression tag	UNP A0A2R4U2X2
B	557	ASN	-	expression tag	UNP A0A2R4U2X2
B	558	LEU	-	expression tag	UNP A0A2R4U2X2
B	559	TYR	-	expression tag	UNP A0A2R4U2X2
B	560	PHE	-	expression tag	UNP A0A2R4U2X2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	561	GLN	-	expression tag	UNP A0A2R4U2X2
B	562	ALA	-	expression tag	UNP A0A2R4U2X2
B	563	MET	-	expression tag	UNP A0A2R4U2X2
B	564	SER	-	expression tag	UNP A0A2R4U2X2
B	565	LYS	-	expression tag	UNP A0A2R4U2X2
B	566	GLY	-	expression tag	UNP A0A2R4U2X2
B	567	GLU	-	expression tag	UNP A0A2R4U2X2
B	568	GLU	-	expression tag	UNP A0A2R4U2X2
B	569	LEU	-	expression tag	UNP A0A2R4U2X2
B	570	PHE	-	expression tag	UNP A0A2R4U2X2
B	571	THR	-	expression tag	UNP A0A2R4U2X2
B	572	GLY	-	expression tag	UNP A0A2R4U2X2
B	573	VAL	-	expression tag	UNP A0A2R4U2X2
B	574	VAL	-	expression tag	UNP A0A2R4U2X2
B	575	PRO	-	expression tag	UNP A0A2R4U2X2
B	576	ILE	-	expression tag	UNP A0A2R4U2X2
B	577	LEU	-	expression tag	UNP A0A2R4U2X2
B	578	VAL	-	expression tag	UNP A0A2R4U2X2
B	579	GLU	-	expression tag	UNP A0A2R4U2X2
B	580	LEU	-	expression tag	UNP A0A2R4U2X2
B	581	ASP	-	expression tag	UNP A0A2R4U2X2
B	582	GLY	-	expression tag	UNP A0A2R4U2X2
B	583	ASP	-	expression tag	UNP A0A2R4U2X2
B	584	VAL	-	expression tag	UNP A0A2R4U2X2
B	585	ASN	-	expression tag	UNP A0A2R4U2X2
B	586	GLY	-	expression tag	UNP A0A2R4U2X2
B	587	HIS	-	expression tag	UNP A0A2R4U2X2
B	588	LYS	-	expression tag	UNP A0A2R4U2X2
B	589	PHE	-	expression tag	UNP A0A2R4U2X2
B	590	SER	-	expression tag	UNP A0A2R4U2X2
B	591	VAL	-	expression tag	UNP A0A2R4U2X2
B	592	ARG	-	expression tag	UNP A0A2R4U2X2
B	593	GLY	-	expression tag	UNP A0A2R4U2X2
B	594	GLU	-	expression tag	UNP A0A2R4U2X2
B	595	GLY	-	expression tag	UNP A0A2R4U2X2
B	596	GLU	-	expression tag	UNP A0A2R4U2X2
B	597	GLY	-	expression tag	UNP A0A2R4U2X2
B	598	ASP	-	expression tag	UNP A0A2R4U2X2
B	599	ALA	-	expression tag	UNP A0A2R4U2X2
B	600	THR	-	expression tag	UNP A0A2R4U2X2
B	601	ASN	-	expression tag	UNP A0A2R4U2X2
B	602	GLY	-	expression tag	UNP A0A2R4U2X2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	603	LYS	-	expression tag	UNP A0A2R4U2X2
B	604	LEU	-	expression tag	UNP A0A2R4U2X2
B	605	THR	-	expression tag	UNP A0A2R4U2X2
B	606	LEU	-	expression tag	UNP A0A2R4U2X2
B	607	LYS	-	expression tag	UNP A0A2R4U2X2
B	608	PHE	-	expression tag	UNP A0A2R4U2X2
B	609	ILE	-	expression tag	UNP A0A2R4U2X2
B	610	CYS	-	expression tag	UNP A0A2R4U2X2
B	611	THR	-	expression tag	UNP A0A2R4U2X2
B	612	THR	-	expression tag	UNP A0A2R4U2X2
B	613	GLY	-	expression tag	UNP A0A2R4U2X2
B	614	LYS	-	expression tag	UNP A0A2R4U2X2
B	615	LEU	-	expression tag	UNP A0A2R4U2X2
B	616	PRO	-	expression tag	UNP A0A2R4U2X2
B	617	VAL	-	expression tag	UNP A0A2R4U2X2
B	618	PRO	-	expression tag	UNP A0A2R4U2X2
B	619	TRP	-	expression tag	UNP A0A2R4U2X2
B	620	PRO	-	expression tag	UNP A0A2R4U2X2
B	621	THR	-	expression tag	UNP A0A2R4U2X2
B	622	LEU	-	expression tag	UNP A0A2R4U2X2
B	623	VAL	-	expression tag	UNP A0A2R4U2X2
B	624	THR	-	expression tag	UNP A0A2R4U2X2
B	625	THR	-	expression tag	UNP A0A2R4U2X2
B	626	LEU	-	expression tag	UNP A0A2R4U2X2
B	627	THR	-	expression tag	UNP A0A2R4U2X2
B	628	TYR	-	expression tag	UNP A0A2R4U2X2
B	629	GLY	-	expression tag	UNP A0A2R4U2X2
B	630	VAL	-	expression tag	UNP A0A2R4U2X2
B	631	GLN	-	expression tag	UNP A0A2R4U2X2
B	632	CYS	-	expression tag	UNP A0A2R4U2X2
B	633	PHE	-	expression tag	UNP A0A2R4U2X2
B	634	SER	-	expression tag	UNP A0A2R4U2X2
B	635	ARG	-	expression tag	UNP A0A2R4U2X2
B	636	TYR	-	expression tag	UNP A0A2R4U2X2
B	637	PRO	-	expression tag	UNP A0A2R4U2X2
B	638	ASP	-	expression tag	UNP A0A2R4U2X2
B	639	HIS	-	expression tag	UNP A0A2R4U2X2
B	640	MET	-	expression tag	UNP A0A2R4U2X2
B	641	LYS	-	expression tag	UNP A0A2R4U2X2
B	642	ARG	-	expression tag	UNP A0A2R4U2X2
B	643	HIS	-	expression tag	UNP A0A2R4U2X2
B	644	ASP	-	expression tag	UNP A0A2R4U2X2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	645	PHE	-	expression tag	UNP A0A2R4U2X2
B	646	PHE	-	expression tag	UNP A0A2R4U2X2
B	647	LYS	-	expression tag	UNP A0A2R4U2X2
B	648	SER	-	expression tag	UNP A0A2R4U2X2
B	649	ALA	-	expression tag	UNP A0A2R4U2X2
B	650	MET	-	expression tag	UNP A0A2R4U2X2
B	651	PRO	-	expression tag	UNP A0A2R4U2X2
B	652	GLU	-	expression tag	UNP A0A2R4U2X2
B	653	GLY	-	expression tag	UNP A0A2R4U2X2
B	654	TYR	-	expression tag	UNP A0A2R4U2X2
B	655	VAL	-	expression tag	UNP A0A2R4U2X2
B	656	GLN	-	expression tag	UNP A0A2R4U2X2
B	657	GLU	-	expression tag	UNP A0A2R4U2X2
B	658	ARG	-	expression tag	UNP A0A2R4U2X2
B	659	THR	-	expression tag	UNP A0A2R4U2X2
B	660	ILE	-	expression tag	UNP A0A2R4U2X2
B	661	SER	-	expression tag	UNP A0A2R4U2X2
B	662	PHE	-	expression tag	UNP A0A2R4U2X2
B	663	LYS	-	expression tag	UNP A0A2R4U2X2
B	664	ASP	-	expression tag	UNP A0A2R4U2X2
B	665	ASP	-	expression tag	UNP A0A2R4U2X2
B	666	GLY	-	expression tag	UNP A0A2R4U2X2
B	667	THR	-	expression tag	UNP A0A2R4U2X2
B	668	TYR	-	expression tag	UNP A0A2R4U2X2
B	669	LYS	-	expression tag	UNP A0A2R4U2X2
B	670	THR	-	expression tag	UNP A0A2R4U2X2
B	671	ARG	-	expression tag	UNP A0A2R4U2X2
B	672	ALA	-	expression tag	UNP A0A2R4U2X2
B	673	GLU	-	expression tag	UNP A0A2R4U2X2
B	674	VAL	-	expression tag	UNP A0A2R4U2X2
B	675	LYS	-	expression tag	UNP A0A2R4U2X2
B	676	PHE	-	expression tag	UNP A0A2R4U2X2
B	677	GLU	-	expression tag	UNP A0A2R4U2X2
B	678	GLY	-	expression tag	UNP A0A2R4U2X2
B	679	ASP	-	expression tag	UNP A0A2R4U2X2
B	680	THR	-	expression tag	UNP A0A2R4U2X2
B	681	LEU	-	expression tag	UNP A0A2R4U2X2
B	682	VAL	-	expression tag	UNP A0A2R4U2X2
B	683	ASN	-	expression tag	UNP A0A2R4U2X2
B	684	ARG	-	expression tag	UNP A0A2R4U2X2
B	685	ILE	-	expression tag	UNP A0A2R4U2X2
B	686	GLU	-	expression tag	UNP A0A2R4U2X2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	687	LEU	-	expression tag	UNP A0A2R4U2X2
B	688	LYS	-	expression tag	UNP A0A2R4U2X2
B	689	GLY	-	expression tag	UNP A0A2R4U2X2
B	690	ILE	-	expression tag	UNP A0A2R4U2X2
B	691	ASP	-	expression tag	UNP A0A2R4U2X2
B	692	PHE	-	expression tag	UNP A0A2R4U2X2
B	693	LYS	-	expression tag	UNP A0A2R4U2X2
B	694	GLU	-	expression tag	UNP A0A2R4U2X2
B	695	ASP	-	expression tag	UNP A0A2R4U2X2
B	696	GLY	-	expression tag	UNP A0A2R4U2X2
B	697	ASN	-	expression tag	UNP A0A2R4U2X2
B	698	ILE	-	expression tag	UNP A0A2R4U2X2
B	699	LEU	-	expression tag	UNP A0A2R4U2X2
B	700	GLY	-	expression tag	UNP A0A2R4U2X2
B	701	HIS	-	expression tag	UNP A0A2R4U2X2
B	702	LYS	-	expression tag	UNP A0A2R4U2X2
B	703	LEU	-	expression tag	UNP A0A2R4U2X2
B	704	GLU	-	expression tag	UNP A0A2R4U2X2
B	705	TYR	-	expression tag	UNP A0A2R4U2X2
B	706	ASN	-	expression tag	UNP A0A2R4U2X2
B	707	PHE	-	expression tag	UNP A0A2R4U2X2
B	708	ASN	-	expression tag	UNP A0A2R4U2X2
B	709	SER	-	expression tag	UNP A0A2R4U2X2
B	710	HIS	-	expression tag	UNP A0A2R4U2X2
B	711	ASN	-	expression tag	UNP A0A2R4U2X2
B	712	VAL	-	expression tag	UNP A0A2R4U2X2
B	713	TYR	-	expression tag	UNP A0A2R4U2X2
B	714	ILE	-	expression tag	UNP A0A2R4U2X2
B	715	THR	-	expression tag	UNP A0A2R4U2X2
B	716	ALA	-	expression tag	UNP A0A2R4U2X2
B	717	ASP	-	expression tag	UNP A0A2R4U2X2
B	718	LYS	-	expression tag	UNP A0A2R4U2X2
B	719	GLN	-	expression tag	UNP A0A2R4U2X2
B	720	LYS	-	expression tag	UNP A0A2R4U2X2
B	721	ASN	-	expression tag	UNP A0A2R4U2X2
B	722	GLY	-	expression tag	UNP A0A2R4U2X2
B	723	ILE	-	expression tag	UNP A0A2R4U2X2
B	724	LYS	-	expression tag	UNP A0A2R4U2X2
B	725	ALA	-	expression tag	UNP A0A2R4U2X2
B	726	ASN	-	expression tag	UNP A0A2R4U2X2
B	727	PHE	-	expression tag	UNP A0A2R4U2X2
B	728	LYS	-	expression tag	UNP A0A2R4U2X2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	729	ILE	-	expression tag	UNP A0A2R4U2X2
B	730	ARG	-	expression tag	UNP A0A2R4U2X2
B	731	HIS	-	expression tag	UNP A0A2R4U2X2
B	732	ASN	-	expression tag	UNP A0A2R4U2X2
B	733	VAL	-	expression tag	UNP A0A2R4U2X2
B	734	GLU	-	expression tag	UNP A0A2R4U2X2
B	735	ASP	-	expression tag	UNP A0A2R4U2X2
B	736	GLY	-	expression tag	UNP A0A2R4U2X2
B	737	SER	-	expression tag	UNP A0A2R4U2X2
B	738	VAL	-	expression tag	UNP A0A2R4U2X2
B	739	GLN	-	expression tag	UNP A0A2R4U2X2
B	740	LEU	-	expression tag	UNP A0A2R4U2X2
B	741	ALA	-	expression tag	UNP A0A2R4U2X2
B	742	ASP	-	expression tag	UNP A0A2R4U2X2
B	743	HIS	-	expression tag	UNP A0A2R4U2X2
B	744	TYR	-	expression tag	UNP A0A2R4U2X2
B	745	GLN	-	expression tag	UNP A0A2R4U2X2
B	746	GLN	-	expression tag	UNP A0A2R4U2X2
B	747	ASN	-	expression tag	UNP A0A2R4U2X2
B	748	THR	-	expression tag	UNP A0A2R4U2X2
B	749	PRO	-	expression tag	UNP A0A2R4U2X2
B	750	ILE	-	expression tag	UNP A0A2R4U2X2
B	751	GLY	-	expression tag	UNP A0A2R4U2X2
B	752	ASP	-	expression tag	UNP A0A2R4U2X2
B	753	GLY	-	expression tag	UNP A0A2R4U2X2
B	754	PRO	-	expression tag	UNP A0A2R4U2X2
B	755	VAL	-	expression tag	UNP A0A2R4U2X2
B	756	LEU	-	expression tag	UNP A0A2R4U2X2
B	757	LEU	-	expression tag	UNP A0A2R4U2X2
B	758	PRO	-	expression tag	UNP A0A2R4U2X2
B	759	ASP	-	expression tag	UNP A0A2R4U2X2
B	760	ASN	-	expression tag	UNP A0A2R4U2X2
B	761	HIS	-	expression tag	UNP A0A2R4U2X2
B	762	TYR	-	expression tag	UNP A0A2R4U2X2
B	763	LEU	-	expression tag	UNP A0A2R4U2X2
B	764	SER	-	expression tag	UNP A0A2R4U2X2
B	765	THR	-	expression tag	UNP A0A2R4U2X2
B	766	GLN	-	expression tag	UNP A0A2R4U2X2
B	767	SER	-	expression tag	UNP A0A2R4U2X2
B	768	VAL	-	expression tag	UNP A0A2R4U2X2
B	769	LEU	-	expression tag	UNP A0A2R4U2X2
B	770	SER	-	expression tag	UNP A0A2R4U2X2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	771	LYS	-	expression tag	UNP A0A2R4U2X2
B	772	ASP	-	expression tag	UNP A0A2R4U2X2
B	773	PRO	-	expression tag	UNP A0A2R4U2X2
B	774	ASN	-	expression tag	UNP A0A2R4U2X2
B	775	GLU	-	expression tag	UNP A0A2R4U2X2
B	776	LYS	-	expression tag	UNP A0A2R4U2X2
B	777	ARG	-	expression tag	UNP A0A2R4U2X2
B	778	ASP	-	expression tag	UNP A0A2R4U2X2
B	779	HIS	-	expression tag	UNP A0A2R4U2X2
B	780	MET	-	expression tag	UNP A0A2R4U2X2
B	781	VAL	-	expression tag	UNP A0A2R4U2X2
B	782	LEU	-	expression tag	UNP A0A2R4U2X2
B	783	LEU	-	expression tag	UNP A0A2R4U2X2
B	784	GLU	-	expression tag	UNP A0A2R4U2X2
B	785	PHE	-	expression tag	UNP A0A2R4U2X2
B	786	VAL	-	expression tag	UNP A0A2R4U2X2
B	787	THR	-	expression tag	UNP A0A2R4U2X2
B	788	ALA	-	expression tag	UNP A0A2R4U2X2
B	789	ALA	-	expression tag	UNP A0A2R4U2X2
B	790	GLY	-	expression tag	UNP A0A2R4U2X2
B	791	ILE	-	expression tag	UNP A0A2R4U2X2
B	792	THR	-	expression tag	UNP A0A2R4U2X2
B	793	HIS	-	expression tag	UNP A0A2R4U2X2
B	794	GLY	-	expression tag	UNP A0A2R4U2X2
B	795	MET	-	expression tag	UNP A0A2R4U2X2
B	796	SER	-	expression tag	UNP A0A2R4U2X2
B	797	SER	-	expression tag	UNP A0A2R4U2X2
B	798	ALA	-	expression tag	UNP A0A2R4U2X2
B	799	TRP	-	expression tag	UNP A0A2R4U2X2
B	800	SER	-	expression tag	UNP A0A2R4U2X2
B	801	HIS	-	expression tag	UNP A0A2R4U2X2
B	802	PRO	-	expression tag	UNP A0A2R4U2X2
B	803	GLN	-	expression tag	UNP A0A2R4U2X2
B	804	PHE	-	expression tag	UNP A0A2R4U2X2
B	805	GLU	-	expression tag	UNP A0A2R4U2X2
B	806	LYS	-	expression tag	UNP A0A2R4U2X2
B	807	GLY	-	expression tag	UNP A0A2R4U2X2
B	808	GLY	-	expression tag	UNP A0A2R4U2X2
B	809	GLY	-	expression tag	UNP A0A2R4U2X2
B	810	SER	-	expression tag	UNP A0A2R4U2X2
B	811	GLY	-	expression tag	UNP A0A2R4U2X2
B	812	GLY	-	expression tag	UNP A0A2R4U2X2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	813	GLY	-	expression tag	UNP A0A2R4U2X2
B	814	SER	-	expression tag	UNP A0A2R4U2X2
B	815	GLY	-	expression tag	UNP A0A2R4U2X2
B	816	GLY	-	expression tag	UNP A0A2R4U2X2
B	817	SER	-	expression tag	UNP A0A2R4U2X2
B	818	ALA	-	expression tag	UNP A0A2R4U2X2
B	819	TRP	-	expression tag	UNP A0A2R4U2X2
B	820	SER	-	expression tag	UNP A0A2R4U2X2
B	821	HIS	-	expression tag	UNP A0A2R4U2X2
B	822	PRO	-	expression tag	UNP A0A2R4U2X2
B	823	GLN	-	expression tag	UNP A0A2R4U2X2
B	824	PHE	-	expression tag	UNP A0A2R4U2X2
B	825	GLU	-	expression tag	UNP A0A2R4U2X2
B	826	LYS	-	expression tag	UNP A0A2R4U2X2
C	1	MET	-	initiating methionine	UNP A0A2R4U2X2
C	2	PRO	-	expression tag	UNP A0A2R4U2X2
C	3	MET	-	expression tag	UNP A0A2R4U2X2
C	4	GLY	-	expression tag	UNP A0A2R4U2X2
C	5	SER	-	expression tag	UNP A0A2R4U2X2
C	6	LEU	-	expression tag	UNP A0A2R4U2X2
C	7	GLN	-	expression tag	UNP A0A2R4U2X2
C	8	PRO	-	expression tag	UNP A0A2R4U2X2
C	9	LEU	-	expression tag	UNP A0A2R4U2X2
C	10	ALA	-	expression tag	UNP A0A2R4U2X2
C	11	THR	-	expression tag	UNP A0A2R4U2X2
C	12	LEU	-	expression tag	UNP A0A2R4U2X2
C	13	TYR	-	expression tag	UNP A0A2R4U2X2
C	14	LEU	-	expression tag	UNP A0A2R4U2X2
C	15	LEU	-	expression tag	UNP A0A2R4U2X2
C	16	GLY	-	expression tag	UNP A0A2R4U2X2
C	17	MET	-	expression tag	UNP A0A2R4U2X2
C	18	LEU	-	expression tag	UNP A0A2R4U2X2
C	19	VAL	-	expression tag	UNP A0A2R4U2X2
C	20	ALA	-	expression tag	UNP A0A2R4U2X2
C	21	SER	-	expression tag	UNP A0A2R4U2X2
C	22	VAL	-	expression tag	UNP A0A2R4U2X2
C	23	LEU	-	expression tag	UNP A0A2R4U2X2
C	24	ALA	-	expression tag	UNP A0A2R4U2X2
C	493	GLU	GLY	conflict	UNP A0A2R4U2X2
C	518	ARG	-	expression tag	UNP A0A2R4U2X2
C	519	MET	-	expression tag	UNP A0A2R4U2X2
C	520	LYS	-	expression tag	UNP A0A2R4U2X2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	521	GLN	-	expression tag	UNP A0A2R4U2X2
C	522	ILE	-	expression tag	UNP A0A2R4U2X2
C	523	GLU	-	expression tag	UNP A0A2R4U2X2
C	524	ASP	-	expression tag	UNP A0A2R4U2X2
C	525	LYS	-	expression tag	UNP A0A2R4U2X2
C	526	ILE	-	expression tag	UNP A0A2R4U2X2
C	527	GLU	-	expression tag	UNP A0A2R4U2X2
C	528	GLU	-	expression tag	UNP A0A2R4U2X2
C	529	ILE	-	expression tag	UNP A0A2R4U2X2
C	530	GLU	-	expression tag	UNP A0A2R4U2X2
C	531	SER	-	expression tag	UNP A0A2R4U2X2
C	532	LYS	-	expression tag	UNP A0A2R4U2X2
C	533	GLN	-	expression tag	UNP A0A2R4U2X2
C	534	LYS	-	expression tag	UNP A0A2R4U2X2
C	535	LYS	-	expression tag	UNP A0A2R4U2X2
C	536	ILE	-	expression tag	UNP A0A2R4U2X2
C	537	GLU	-	expression tag	UNP A0A2R4U2X2
C	538	ASN	-	expression tag	UNP A0A2R4U2X2
C	539	GLU	-	expression tag	UNP A0A2R4U2X2
C	540	ILE	-	expression tag	UNP A0A2R4U2X2
C	541	ALA	-	expression tag	UNP A0A2R4U2X2
C	542	ARG	-	expression tag	UNP A0A2R4U2X2
C	543	ILE	-	expression tag	UNP A0A2R4U2X2
C	544	LYS	-	expression tag	UNP A0A2R4U2X2
C	545	LYS	-	expression tag	UNP A0A2R4U2X2
C	546	ILE	-	expression tag	UNP A0A2R4U2X2
C	547	LYS	-	expression tag	UNP A0A2R4U2X2
C	548	LEU	-	expression tag	UNP A0A2R4U2X2
C	549	VAL	-	expression tag	UNP A0A2R4U2X2
C	550	PRO	-	expression tag	UNP A0A2R4U2X2
C	551	ARG	-	expression tag	UNP A0A2R4U2X2
C	552	GLY	-	expression tag	UNP A0A2R4U2X2
C	553	SER	-	expression tag	UNP A0A2R4U2X2
C	554	VAL	-	expression tag	UNP A0A2R4U2X2
C	555	ASP	-	expression tag	UNP A0A2R4U2X2
C	556	GLU	-	expression tag	UNP A0A2R4U2X2
C	557	ASN	-	expression tag	UNP A0A2R4U2X2
C	558	LEU	-	expression tag	UNP A0A2R4U2X2
C	559	TYR	-	expression tag	UNP A0A2R4U2X2
C	560	PHE	-	expression tag	UNP A0A2R4U2X2
C	561	GLN	-	expression tag	UNP A0A2R4U2X2
C	562	ALA	-	expression tag	UNP A0A2R4U2X2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	563	MET	-	expression tag	UNP A0A2R4U2X2
C	564	SER	-	expression tag	UNP A0A2R4U2X2
C	565	LYS	-	expression tag	UNP A0A2R4U2X2
C	566	GLY	-	expression tag	UNP A0A2R4U2X2
C	567	GLU	-	expression tag	UNP A0A2R4U2X2
C	568	GLU	-	expression tag	UNP A0A2R4U2X2
C	569	LEU	-	expression tag	UNP A0A2R4U2X2
C	570	PHE	-	expression tag	UNP A0A2R4U2X2
C	571	THR	-	expression tag	UNP A0A2R4U2X2
C	572	GLY	-	expression tag	UNP A0A2R4U2X2
C	573	VAL	-	expression tag	UNP A0A2R4U2X2
C	574	VAL	-	expression tag	UNP A0A2R4U2X2
C	575	PRO	-	expression tag	UNP A0A2R4U2X2
C	576	ILE	-	expression tag	UNP A0A2R4U2X2
C	577	LEU	-	expression tag	UNP A0A2R4U2X2
C	578	VAL	-	expression tag	UNP A0A2R4U2X2
C	579	GLU	-	expression tag	UNP A0A2R4U2X2
C	580	LEU	-	expression tag	UNP A0A2R4U2X2
C	581	ASP	-	expression tag	UNP A0A2R4U2X2
C	582	GLY	-	expression tag	UNP A0A2R4U2X2
C	583	ASP	-	expression tag	UNP A0A2R4U2X2
C	584	VAL	-	expression tag	UNP A0A2R4U2X2
C	585	ASN	-	expression tag	UNP A0A2R4U2X2
C	586	GLY	-	expression tag	UNP A0A2R4U2X2
C	587	HIS	-	expression tag	UNP A0A2R4U2X2
C	588	LYS	-	expression tag	UNP A0A2R4U2X2
C	589	PHE	-	expression tag	UNP A0A2R4U2X2
C	590	SER	-	expression tag	UNP A0A2R4U2X2
C	591	VAL	-	expression tag	UNP A0A2R4U2X2
C	592	ARG	-	expression tag	UNP A0A2R4U2X2
C	593	GLY	-	expression tag	UNP A0A2R4U2X2
C	594	GLU	-	expression tag	UNP A0A2R4U2X2
C	595	GLY	-	expression tag	UNP A0A2R4U2X2
C	596	GLU	-	expression tag	UNP A0A2R4U2X2
C	597	GLY	-	expression tag	UNP A0A2R4U2X2
C	598	ASP	-	expression tag	UNP A0A2R4U2X2
C	599	ALA	-	expression tag	UNP A0A2R4U2X2
C	600	THR	-	expression tag	UNP A0A2R4U2X2
C	601	ASN	-	expression tag	UNP A0A2R4U2X2
C	602	GLY	-	expression tag	UNP A0A2R4U2X2
C	603	LYS	-	expression tag	UNP A0A2R4U2X2
C	604	LEU	-	expression tag	UNP A0A2R4U2X2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	605	THR	-	expression tag	UNP A0A2R4U2X2
C	606	LEU	-	expression tag	UNP A0A2R4U2X2
C	607	LYS	-	expression tag	UNP A0A2R4U2X2
C	608	PHE	-	expression tag	UNP A0A2R4U2X2
C	609	ILE	-	expression tag	UNP A0A2R4U2X2
C	610	CYS	-	expression tag	UNP A0A2R4U2X2
C	611	THR	-	expression tag	UNP A0A2R4U2X2
C	612	THR	-	expression tag	UNP A0A2R4U2X2
C	613	GLY	-	expression tag	UNP A0A2R4U2X2
C	614	LYS	-	expression tag	UNP A0A2R4U2X2
C	615	LEU	-	expression tag	UNP A0A2R4U2X2
C	616	PRO	-	expression tag	UNP A0A2R4U2X2
C	617	VAL	-	expression tag	UNP A0A2R4U2X2
C	618	PRO	-	expression tag	UNP A0A2R4U2X2
C	619	TRP	-	expression tag	UNP A0A2R4U2X2
C	620	PRO	-	expression tag	UNP A0A2R4U2X2
C	621	THR	-	expression tag	UNP A0A2R4U2X2
C	622	LEU	-	expression tag	UNP A0A2R4U2X2
C	623	VAL	-	expression tag	UNP A0A2R4U2X2
C	624	THR	-	expression tag	UNP A0A2R4U2X2
C	625	THR	-	expression tag	UNP A0A2R4U2X2
C	626	LEU	-	expression tag	UNP A0A2R4U2X2
C	627	THR	-	expression tag	UNP A0A2R4U2X2
C	628	TYR	-	expression tag	UNP A0A2R4U2X2
C	629	GLY	-	expression tag	UNP A0A2R4U2X2
C	630	VAL	-	expression tag	UNP A0A2R4U2X2
C	631	GLN	-	expression tag	UNP A0A2R4U2X2
C	632	CYS	-	expression tag	UNP A0A2R4U2X2
C	633	PHE	-	expression tag	UNP A0A2R4U2X2
C	634	SER	-	expression tag	UNP A0A2R4U2X2
C	635	ARG	-	expression tag	UNP A0A2R4U2X2
C	636	TYR	-	expression tag	UNP A0A2R4U2X2
C	637	PRO	-	expression tag	UNP A0A2R4U2X2
C	638	ASP	-	expression tag	UNP A0A2R4U2X2
C	639	HIS	-	expression tag	UNP A0A2R4U2X2
C	640	MET	-	expression tag	UNP A0A2R4U2X2
C	641	LYS	-	expression tag	UNP A0A2R4U2X2
C	642	ARG	-	expression tag	UNP A0A2R4U2X2
C	643	HIS	-	expression tag	UNP A0A2R4U2X2
C	644	ASP	-	expression tag	UNP A0A2R4U2X2
C	645	PHE	-	expression tag	UNP A0A2R4U2X2
C	646	PHE	-	expression tag	UNP A0A2R4U2X2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	647	LYS	-	expression tag	UNP A0A2R4U2X2
C	648	SER	-	expression tag	UNP A0A2R4U2X2
C	649	ALA	-	expression tag	UNP A0A2R4U2X2
C	650	MET	-	expression tag	UNP A0A2R4U2X2
C	651	PRO	-	expression tag	UNP A0A2R4U2X2
C	652	GLU	-	expression tag	UNP A0A2R4U2X2
C	653	GLY	-	expression tag	UNP A0A2R4U2X2
C	654	TYR	-	expression tag	UNP A0A2R4U2X2
C	655	VAL	-	expression tag	UNP A0A2R4U2X2
C	656	GLN	-	expression tag	UNP A0A2R4U2X2
C	657	GLU	-	expression tag	UNP A0A2R4U2X2
C	658	ARG	-	expression tag	UNP A0A2R4U2X2
C	659	THR	-	expression tag	UNP A0A2R4U2X2
C	660	ILE	-	expression tag	UNP A0A2R4U2X2
C	661	SER	-	expression tag	UNP A0A2R4U2X2
C	662	PHE	-	expression tag	UNP A0A2R4U2X2
C	663	LYS	-	expression tag	UNP A0A2R4U2X2
C	664	ASP	-	expression tag	UNP A0A2R4U2X2
C	665	ASP	-	expression tag	UNP A0A2R4U2X2
C	666	GLY	-	expression tag	UNP A0A2R4U2X2
C	667	THR	-	expression tag	UNP A0A2R4U2X2
C	668	TYR	-	expression tag	UNP A0A2R4U2X2
C	669	LYS	-	expression tag	UNP A0A2R4U2X2
C	670	THR	-	expression tag	UNP A0A2R4U2X2
C	671	ARG	-	expression tag	UNP A0A2R4U2X2
C	672	ALA	-	expression tag	UNP A0A2R4U2X2
C	673	GLU	-	expression tag	UNP A0A2R4U2X2
C	674	VAL	-	expression tag	UNP A0A2R4U2X2
C	675	LYS	-	expression tag	UNP A0A2R4U2X2
C	676	PHE	-	expression tag	UNP A0A2R4U2X2
C	677	GLU	-	expression tag	UNP A0A2R4U2X2
C	678	GLY	-	expression tag	UNP A0A2R4U2X2
C	679	ASP	-	expression tag	UNP A0A2R4U2X2
C	680	THR	-	expression tag	UNP A0A2R4U2X2
C	681	LEU	-	expression tag	UNP A0A2R4U2X2
C	682	VAL	-	expression tag	UNP A0A2R4U2X2
C	683	ASN	-	expression tag	UNP A0A2R4U2X2
C	684	ARG	-	expression tag	UNP A0A2R4U2X2
C	685	ILE	-	expression tag	UNP A0A2R4U2X2
C	686	GLU	-	expression tag	UNP A0A2R4U2X2
C	687	LEU	-	expression tag	UNP A0A2R4U2X2
C	688	LYS	-	expression tag	UNP A0A2R4U2X2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	689	GLY	-	expression tag	UNP A0A2R4U2X2
C	690	ILE	-	expression tag	UNP A0A2R4U2X2
C	691	ASP	-	expression tag	UNP A0A2R4U2X2
C	692	PHE	-	expression tag	UNP A0A2R4U2X2
C	693	LYS	-	expression tag	UNP A0A2R4U2X2
C	694	GLU	-	expression tag	UNP A0A2R4U2X2
C	695	ASP	-	expression tag	UNP A0A2R4U2X2
C	696	GLY	-	expression tag	UNP A0A2R4U2X2
C	697	ASN	-	expression tag	UNP A0A2R4U2X2
C	698	ILE	-	expression tag	UNP A0A2R4U2X2
C	699	LEU	-	expression tag	UNP A0A2R4U2X2
C	700	GLY	-	expression tag	UNP A0A2R4U2X2
C	701	HIS	-	expression tag	UNP A0A2R4U2X2
C	702	LYS	-	expression tag	UNP A0A2R4U2X2
C	703	LEU	-	expression tag	UNP A0A2R4U2X2
C	704	GLU	-	expression tag	UNP A0A2R4U2X2
C	705	TYR	-	expression tag	UNP A0A2R4U2X2
C	706	ASN	-	expression tag	UNP A0A2R4U2X2
C	707	PHE	-	expression tag	UNP A0A2R4U2X2
C	708	ASN	-	expression tag	UNP A0A2R4U2X2
C	709	SER	-	expression tag	UNP A0A2R4U2X2
C	710	HIS	-	expression tag	UNP A0A2R4U2X2
C	711	ASN	-	expression tag	UNP A0A2R4U2X2
C	712	VAL	-	expression tag	UNP A0A2R4U2X2
C	713	TYR	-	expression tag	UNP A0A2R4U2X2
C	714	ILE	-	expression tag	UNP A0A2R4U2X2
C	715	THR	-	expression tag	UNP A0A2R4U2X2
C	716	ALA	-	expression tag	UNP A0A2R4U2X2
C	717	ASP	-	expression tag	UNP A0A2R4U2X2
C	718	LYS	-	expression tag	UNP A0A2R4U2X2
C	719	GLN	-	expression tag	UNP A0A2R4U2X2
C	720	LYS	-	expression tag	UNP A0A2R4U2X2
C	721	ASN	-	expression tag	UNP A0A2R4U2X2
C	722	GLY	-	expression tag	UNP A0A2R4U2X2
C	723	ILE	-	expression tag	UNP A0A2R4U2X2
C	724	LYS	-	expression tag	UNP A0A2R4U2X2
C	725	ALA	-	expression tag	UNP A0A2R4U2X2
C	726	ASN	-	expression tag	UNP A0A2R4U2X2
C	727	PHE	-	expression tag	UNP A0A2R4U2X2
C	728	LYS	-	expression tag	UNP A0A2R4U2X2
C	729	ILE	-	expression tag	UNP A0A2R4U2X2
C	730	ARG	-	expression tag	UNP A0A2R4U2X2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	731	HIS	-	expression tag	UNP A0A2R4U2X2
C	732	ASN	-	expression tag	UNP A0A2R4U2X2
C	733	VAL	-	expression tag	UNP A0A2R4U2X2
C	734	GLU	-	expression tag	UNP A0A2R4U2X2
C	735	ASP	-	expression tag	UNP A0A2R4U2X2
C	736	GLY	-	expression tag	UNP A0A2R4U2X2
C	737	SER	-	expression tag	UNP A0A2R4U2X2
C	738	VAL	-	expression tag	UNP A0A2R4U2X2
C	739	GLN	-	expression tag	UNP A0A2R4U2X2
C	740	LEU	-	expression tag	UNP A0A2R4U2X2
C	741	ALA	-	expression tag	UNP A0A2R4U2X2
C	742	ASP	-	expression tag	UNP A0A2R4U2X2
C	743	HIS	-	expression tag	UNP A0A2R4U2X2
C	744	TYR	-	expression tag	UNP A0A2R4U2X2
C	745	GLN	-	expression tag	UNP A0A2R4U2X2
C	746	GLN	-	expression tag	UNP A0A2R4U2X2
C	747	ASN	-	expression tag	UNP A0A2R4U2X2
C	748	THR	-	expression tag	UNP A0A2R4U2X2
C	749	PRO	-	expression tag	UNP A0A2R4U2X2
C	750	ILE	-	expression tag	UNP A0A2R4U2X2
C	751	GLY	-	expression tag	UNP A0A2R4U2X2
C	752	ASP	-	expression tag	UNP A0A2R4U2X2
C	753	GLY	-	expression tag	UNP A0A2R4U2X2
C	754	PRO	-	expression tag	UNP A0A2R4U2X2
C	755	VAL	-	expression tag	UNP A0A2R4U2X2
C	756	LEU	-	expression tag	UNP A0A2R4U2X2
C	757	LEU	-	expression tag	UNP A0A2R4U2X2
C	758	PRO	-	expression tag	UNP A0A2R4U2X2
C	759	ASP	-	expression tag	UNP A0A2R4U2X2
C	760	ASN	-	expression tag	UNP A0A2R4U2X2
C	761	HIS	-	expression tag	UNP A0A2R4U2X2
C	762	TYR	-	expression tag	UNP A0A2R4U2X2
C	763	LEU	-	expression tag	UNP A0A2R4U2X2
C	764	SER	-	expression tag	UNP A0A2R4U2X2
C	765	THR	-	expression tag	UNP A0A2R4U2X2
C	766	GLN	-	expression tag	UNP A0A2R4U2X2
C	767	SER	-	expression tag	UNP A0A2R4U2X2
C	768	VAL	-	expression tag	UNP A0A2R4U2X2
C	769	LEU	-	expression tag	UNP A0A2R4U2X2
C	770	SER	-	expression tag	UNP A0A2R4U2X2
C	771	LYS	-	expression tag	UNP A0A2R4U2X2
C	772	ASP	-	expression tag	UNP A0A2R4U2X2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	773	PRO	-	expression tag	UNP A0A2R4U2X2
C	774	ASN	-	expression tag	UNP A0A2R4U2X2
C	775	GLU	-	expression tag	UNP A0A2R4U2X2
C	776	LYS	-	expression tag	UNP A0A2R4U2X2
C	777	ARG	-	expression tag	UNP A0A2R4U2X2
C	778	ASP	-	expression tag	UNP A0A2R4U2X2
C	779	HIS	-	expression tag	UNP A0A2R4U2X2
C	780	MET	-	expression tag	UNP A0A2R4U2X2
C	781	VAL	-	expression tag	UNP A0A2R4U2X2
C	782	LEU	-	expression tag	UNP A0A2R4U2X2
C	783	LEU	-	expression tag	UNP A0A2R4U2X2
C	784	GLU	-	expression tag	UNP A0A2R4U2X2
C	785	PHE	-	expression tag	UNP A0A2R4U2X2
C	786	VAL	-	expression tag	UNP A0A2R4U2X2
C	787	THR	-	expression tag	UNP A0A2R4U2X2
C	788	ALA	-	expression tag	UNP A0A2R4U2X2
C	789	ALA	-	expression tag	UNP A0A2R4U2X2
C	790	GLY	-	expression tag	UNP A0A2R4U2X2
C	791	ILE	-	expression tag	UNP A0A2R4U2X2
C	792	THR	-	expression tag	UNP A0A2R4U2X2
C	793	HIS	-	expression tag	UNP A0A2R4U2X2
C	794	GLY	-	expression tag	UNP A0A2R4U2X2
C	795	MET	-	expression tag	UNP A0A2R4U2X2
C	796	SER	-	expression tag	UNP A0A2R4U2X2
C	797	SER	-	expression tag	UNP A0A2R4U2X2
C	798	ALA	-	expression tag	UNP A0A2R4U2X2
C	799	TRP	-	expression tag	UNP A0A2R4U2X2
C	800	SER	-	expression tag	UNP A0A2R4U2X2
C	801	HIS	-	expression tag	UNP A0A2R4U2X2
C	802	PRO	-	expression tag	UNP A0A2R4U2X2
C	803	GLN	-	expression tag	UNP A0A2R4U2X2
C	804	PHE	-	expression tag	UNP A0A2R4U2X2
C	805	GLU	-	expression tag	UNP A0A2R4U2X2
C	806	LYS	-	expression tag	UNP A0A2R4U2X2
C	807	GLY	-	expression tag	UNP A0A2R4U2X2
C	808	GLY	-	expression tag	UNP A0A2R4U2X2
C	809	GLY	-	expression tag	UNP A0A2R4U2X2
C	810	SER	-	expression tag	UNP A0A2R4U2X2
C	811	GLY	-	expression tag	UNP A0A2R4U2X2
C	812	GLY	-	expression tag	UNP A0A2R4U2X2
C	813	GLY	-	expression tag	UNP A0A2R4U2X2
C	814	SER	-	expression tag	UNP A0A2R4U2X2

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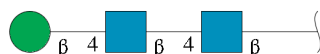
Chain	Residue	Modelled	Actual	Comment	Reference
C	815	GLY	-	expression tag	UNP A0A2R4U2X2
C	816	GLY	-	expression tag	UNP A0A2R4U2X2
C	817	SER	-	expression tag	UNP A0A2R4U2X2
C	818	ALA	-	expression tag	UNP A0A2R4U2X2
C	819	TRP	-	expression tag	UNP A0A2R4U2X2
C	820	SER	-	expression tag	UNP A0A2R4U2X2
C	821	HIS	-	expression tag	UNP A0A2R4U2X2
C	822	PRO	-	expression tag	UNP A0A2R4U2X2
C	823	GLN	-	expression tag	UNP A0A2R4U2X2
C	824	PHE	-	expression tag	UNP A0A2R4U2X2
C	825	GLU	-	expression tag	UNP A0A2R4U2X2
C	826	LYS	-	expression tag	UNP A0A2R4U2X2

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



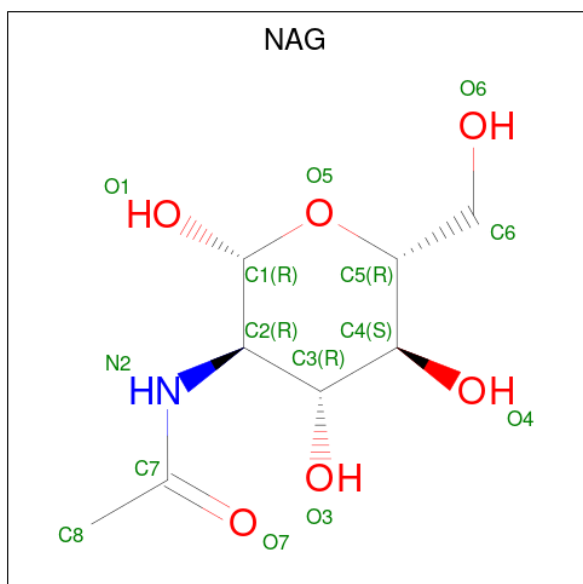
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is an oligosaccharide called 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
3	E	3	Total	C	N	O	0	0
			39	22	2	15		
3	G	3	Total	C	N	O	0	0
			39	22	2	15		
3	I	3	Total	C	N	O	0	0
			39	22	2	15		
3	K	3	Total	C	N	O	0	0
			39	22	2	15		
3	M	3	Total	C	N	O	0	0
			39	22	2	15		
3	O	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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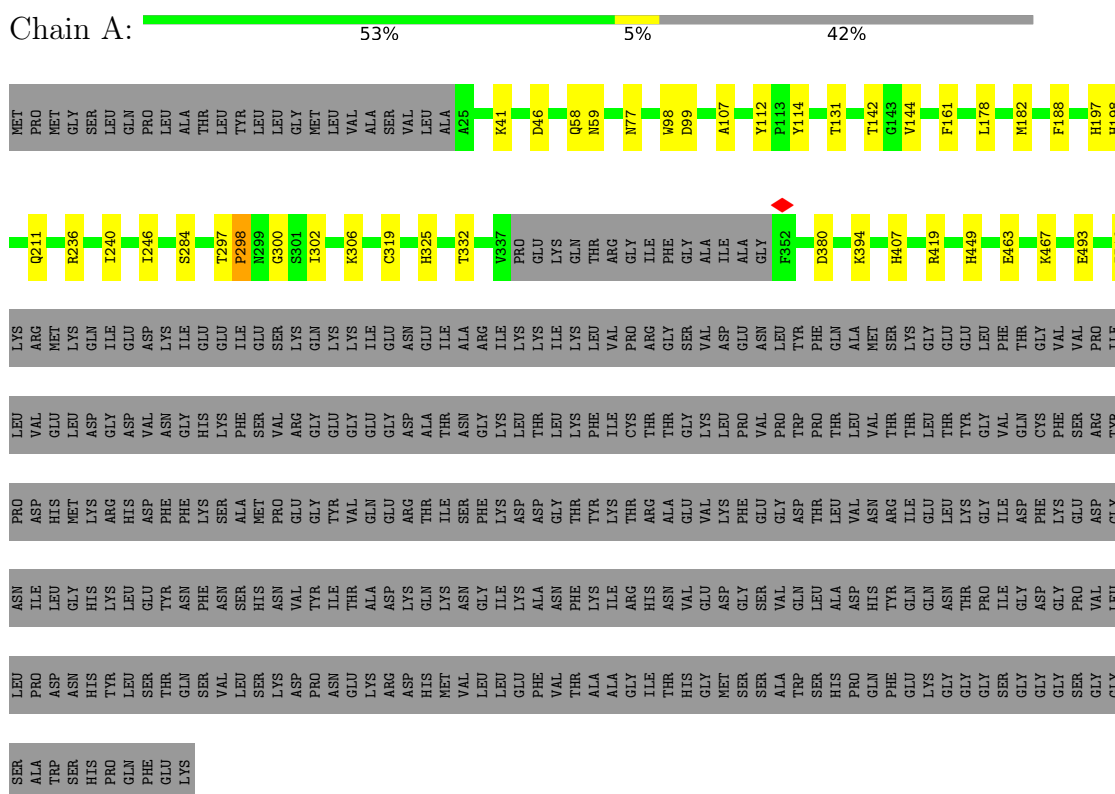
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Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total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

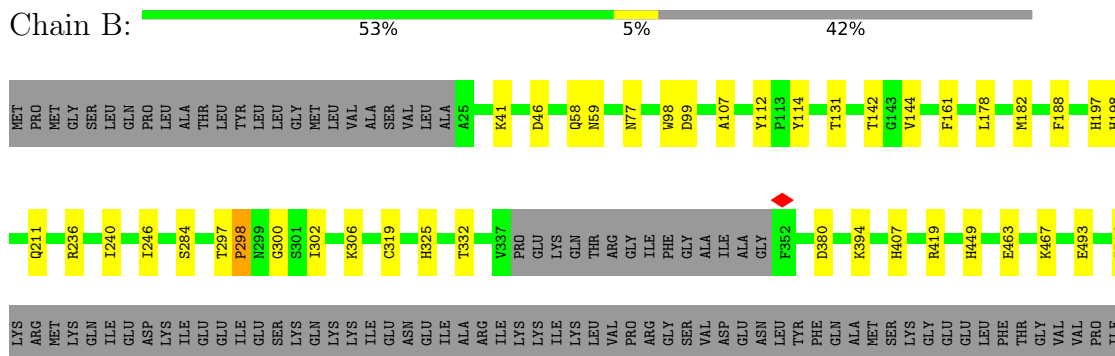
3 Residue-property plots

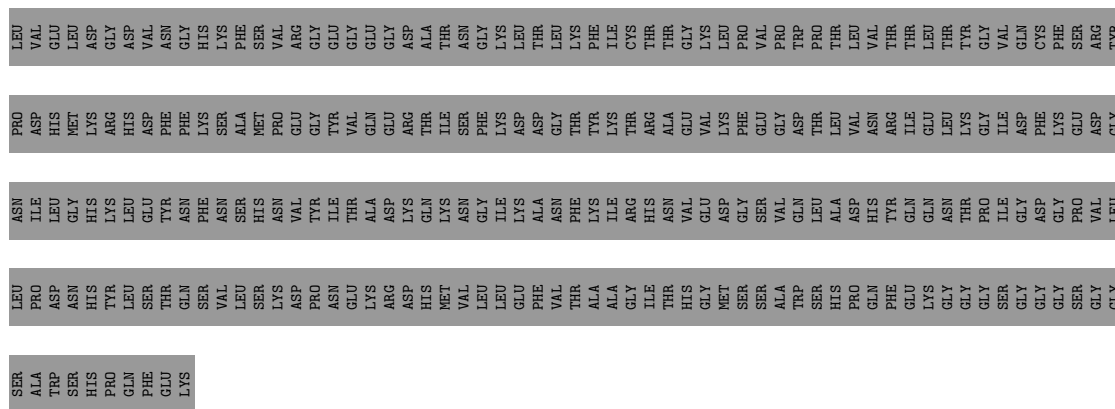
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Hemagglutinin

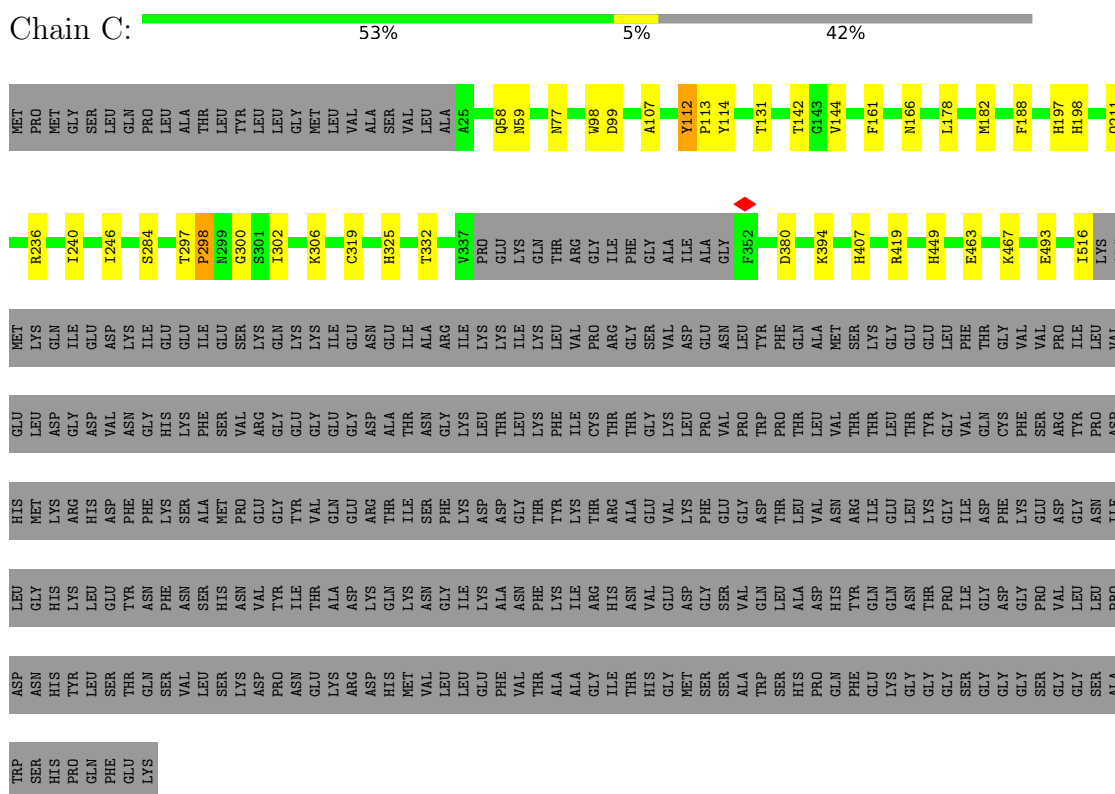


• Molecule 1: Hemagglutinin





- Molecule 1: Hemagglutinin



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



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





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

Chain H:



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

Chain J:



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

Chain L:



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

Chain N:



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

Chain E:



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

Chain G:



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

Chain I:  67% 33%



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

Chain K:  67% 33%



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

Chain M:  67% 33%



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

Chain O:  67% 33%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	76978	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.015	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.0035	Depositor
Map size (Å)	564.3, 564.3, 564.3	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	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: 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	1.21	10/3877 (0.3%)	1.24	23/5246 (0.4%)
1	B	1.21	10/3877 (0.3%)	1.24	23/5246 (0.4%)
1	C	1.21	10/3877 (0.3%)	1.24	23/5246 (0.4%)
All	All	1.21	30/11631 (0.3%)	1.24	69/15738 (0.4%)

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	114	TYR	CB-CG	-6.85	1.36	1.51
1	A	114	TYR	CB-CG	-6.85	1.36	1.51
1	B	114	TYR	CB-CG	-6.85	1.36	1.51
1	C	516	ILE	CB-CG1	6.45	1.66	1.53
1	A	516	ILE	CB-CG1	6.42	1.66	1.53

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	407	HIS	CA-CB-CG	-8.10	105.70	113.80
1	B	407	HIS	CA-CB-CG	-8.10	105.70	113.80
1	A	407	HIS	CA-CB-CG	-8.09	105.71	113.80
1	C	99	ASP	N-CA-C	-7.65	103.56	113.12
1	B	198	HIS	CA-C-N	7.65	127.36	119.56

There are no chirality outliers.

There are no planarity outliers.

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	3798	0	3680	8	0
1	B	3798	0	3680	8	0
1	C	3798	0	3680	9	0
2	D	28	0	25	0	0
2	F	28	0	25	0	0
2	H	28	0	25	0	0
2	J	28	0	25	0	0
2	L	28	0	25	0	0
2	N	28	0	25	0	0
3	E	39	0	34	0	0
3	G	39	0	34	1	0
3	I	39	0	34	0	0
3	K	39	0	34	1	0
3	M	39	0	34	0	0
3	O	39	0	34	1	0
4	A	98	0	91	1	0
4	B	98	0	91	1	0
4	C	98	0	91	1	0
All	All	12090	0	11667	25	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 1.

The worst 5 of 25 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:ASN:HA	1:C:107:ALA:HA	1.93	0.51
1:A:77:ASN:HA	1:A:107:ALA:HA	1.93	0.50
1:C:58:GLN:HG2	1:C:302:ILE:HG23	1.93	0.50
1:A:58:GLN:HG2	1:A:302:ILE:HG23	1.93	0.50
1:B:77:ASN:HA	1:B:107:ALA:HA	1.93	0.50

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	474/826 (57%)	463 (98%)	11 (2%)	0	100	100
1	B	474/826 (57%)	463 (98%)	11 (2%)	0	100	100
1	C	474/826 (57%)	463 (98%)	11 (2%)	0	100	100
All	All	1422/2478 (57%)	1389 (98%)	33 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	421/716 (59%)	417 (99%)	4 (1%)	68	74
1	B	421/716 (59%)	417 (99%)	4 (1%)	68	74
1	C	421/716 (59%)	417 (99%)	4 (1%)	68	74
All	All	1263/2148 (59%)	1251 (99%)	12 (1%)	65	74

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	394	LYS
1	C	59	ASN
1	C	394	LYS
1	C	142	THR
1	A	394	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	89	GLN
1	C	70	HIS
1	C	89	GLN
1	A	89	GLN
1	A	70	HIS

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 ⓘ

30 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	$\# Z > 2$
2	NAG	D	1	2,1	14,14,15	0.31	0	17,19,21	0.57	0
2	NAG	D	2	2	14,14,15	0.29	0	17,19,21	0.94	2 (11%)
3	NAG	E	1	3,1	14,14,15	0.39	0	17,19,21	0.81	0
3	NAG	E	2	3	14,14,15	0.27	0	17,19,21	0.95	2 (11%)
3	BMA	E	3	3	11,11,12	0.25	0	15,15,17	0.50	0
2	NAG	F	1	2,1	14,14,15	0.33	0	17,19,21	0.82	1 (5%)
2	NAG	F	2	2	14,14,15	0.28	0	17,19,21	0.57	0
3	NAG	G	1	3,1	14,14,15	0.32	0	17,19,21	0.58	0
3	NAG	G	2	3	14,14,15	0.29	0	17,19,21	0.99	1 (5%)
3	BMA	G	3	3	11,11,12	0.24	0	15,15,17	0.56	0
2	NAG	H	1	2,1	14,14,15	0.32	0	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	H	2	2	14,14,15	0.29	0	17,19,21	0.94	2 (11%)
3	NAG	I	1	3,1	14,14,15	0.39	0	17,19,21	0.81	0
3	NAG	I	2	3	14,14,15	0.28	0	17,19,21	0.95	2 (11%)
3	BMA	I	3	3	11,11,12	0.25	0	15,15,17	0.50	0
2	NAG	J	1	2,1	14,14,15	0.33	0	17,19,21	0.82	1 (5%)
2	NAG	J	2	2	14,14,15	0.28	0	17,19,21	0.57	0
3	NAG	K	1	3,1	14,14,15	0.32	0	17,19,21	0.59	0
3	NAG	K	2	3	14,14,15	0.29	0	17,19,21	0.99	1 (5%)
3	BMA	K	3	3	11,11,12	0.25	0	15,15,17	0.55	0
2	NAG	L	1	2,1	14,14,15	0.31	0	17,19,21	0.57	0
2	NAG	L	2	2	14,14,15	0.29	0	17,19,21	0.94	2 (11%)
3	NAG	M	1	3,1	14,14,15	0.39	0	17,19,21	0.81	0
3	NAG	M	2	3	14,14,15	0.28	0	17,19,21	0.95	2 (11%)
3	BMA	M	3	3	11,11,12	0.26	0	15,15,17	0.49	0
2	NAG	N	1	2,1	14,14,15	0.33	0	17,19,21	0.83	1 (5%)
2	NAG	N	2	2	14,14,15	0.29	0	17,19,21	0.57	0
3	NAG	O	1	3,1	14,14,15	0.32	0	17,19,21	0.58	0
3	NAG	O	2	3	14,14,15	0.28	0	17,19,21	0.99	1 (5%)
3	BMA	O	3	3	11,11,12	0.24	0	15,15,17	0.56	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
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	3/6/23/26	0/1/1/1
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	3/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	3/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	3/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	I	2	3	-	3/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
2	NAG	J	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	3/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1
2	NAG	L	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	3/6/23/26	0/1/1/1
3	NAG	M	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	3/6/23/26	0/1/1/1
3	BMA	M	3	3	-	0/2/19/22	0/1/1/1
2	NAG	N	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
3	NAG	O	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	O	2	3	-	3/6/23/26	0/1/1/1
3	BMA	O	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	1	NAG	C1-O5-C5	2.76	115.89	112.19
2	F	1	NAG	C1-O5-C5	2.75	115.87	112.19
2	J	1	NAG	C1-O5-C5	2.75	115.87	112.19
3	E	2	NAG	C1-O5-C5	2.63	115.71	112.19
3	I	2	NAG	C1-O5-C5	2.63	115.71	112.19

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

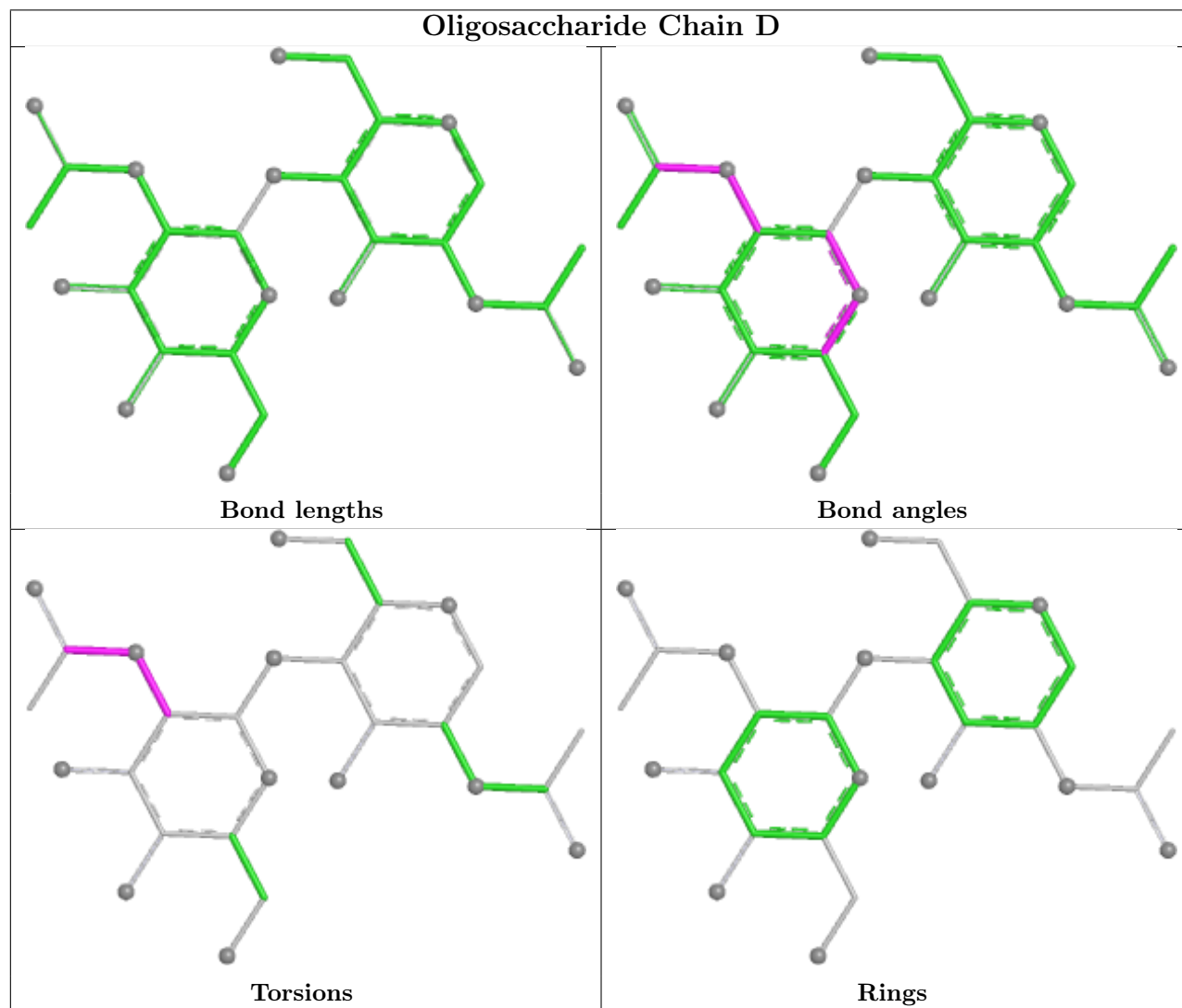
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2

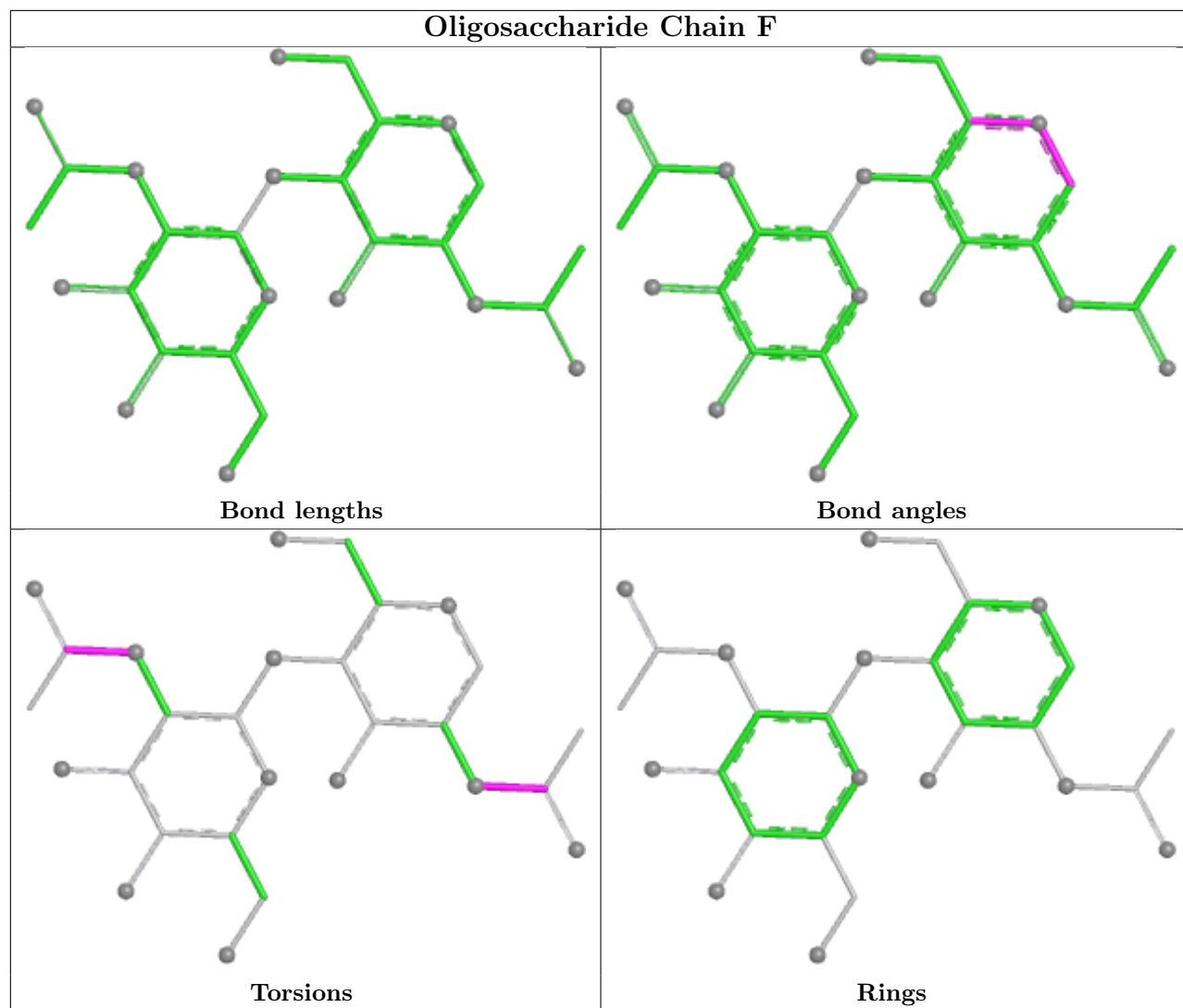
There are no ring outliers.

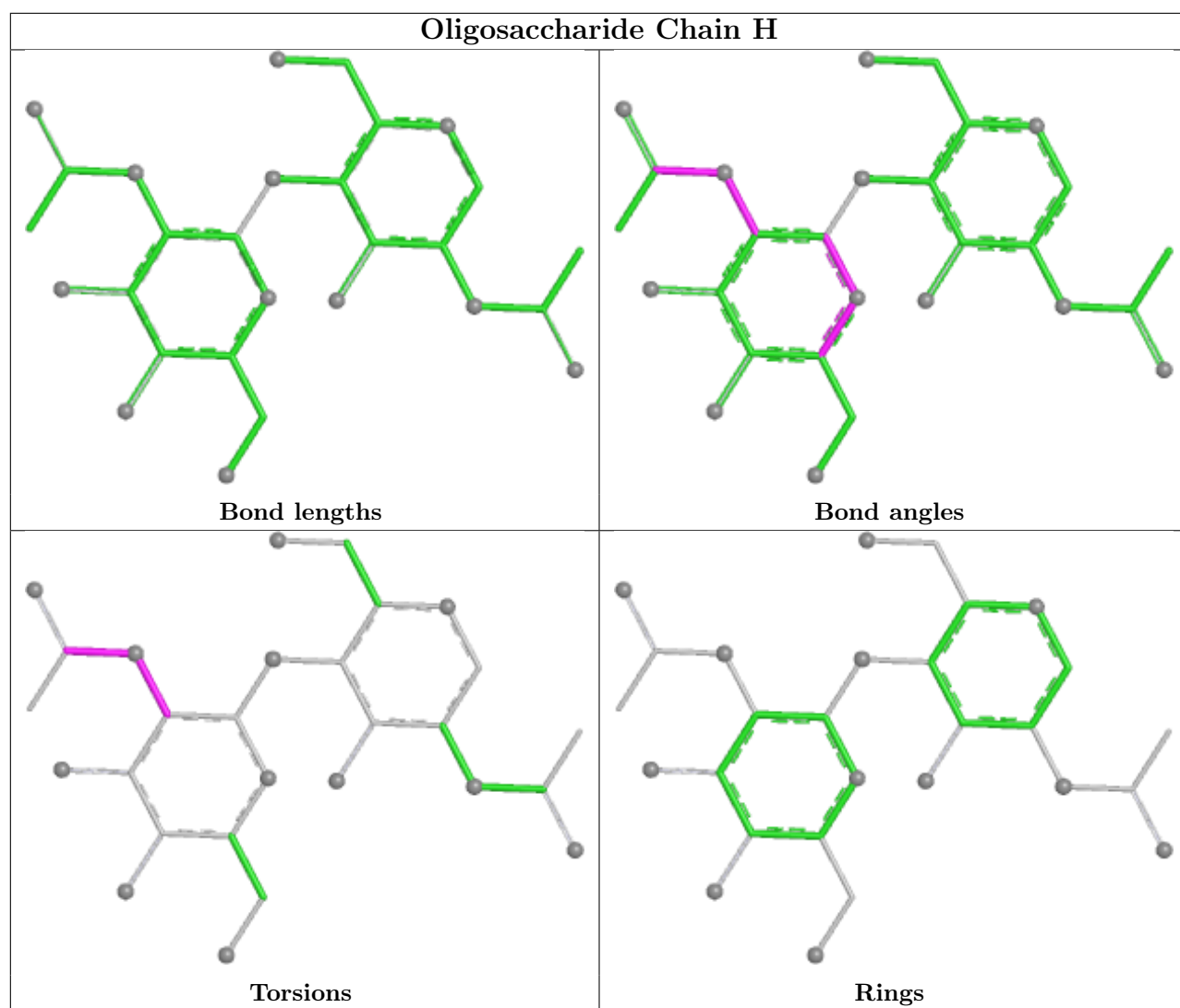
3 monomers are involved in 3 short contacts:

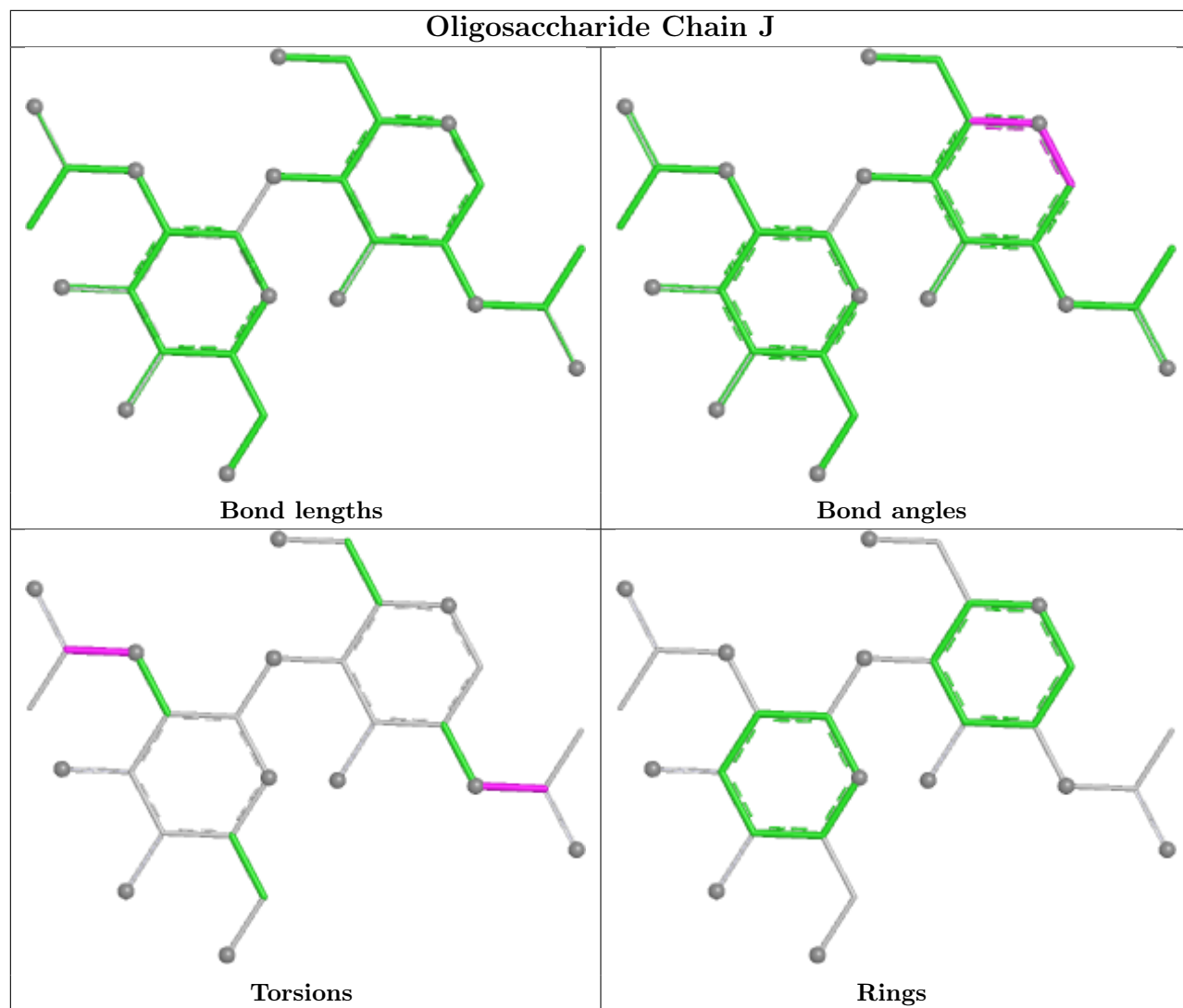
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	2	NAG	1	0
3	K	2	NAG	1	0
3	G	2	NAG	1	0

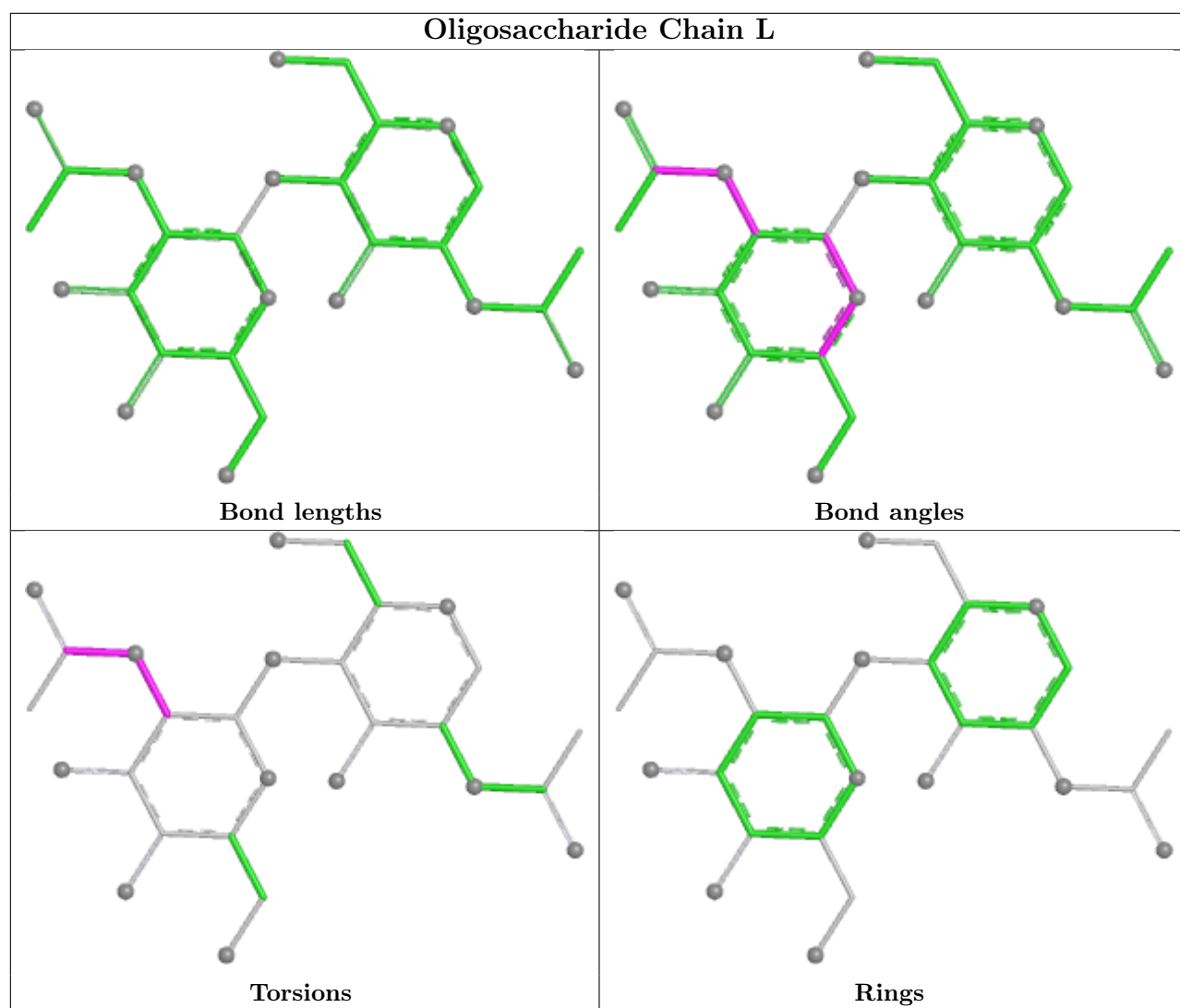
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

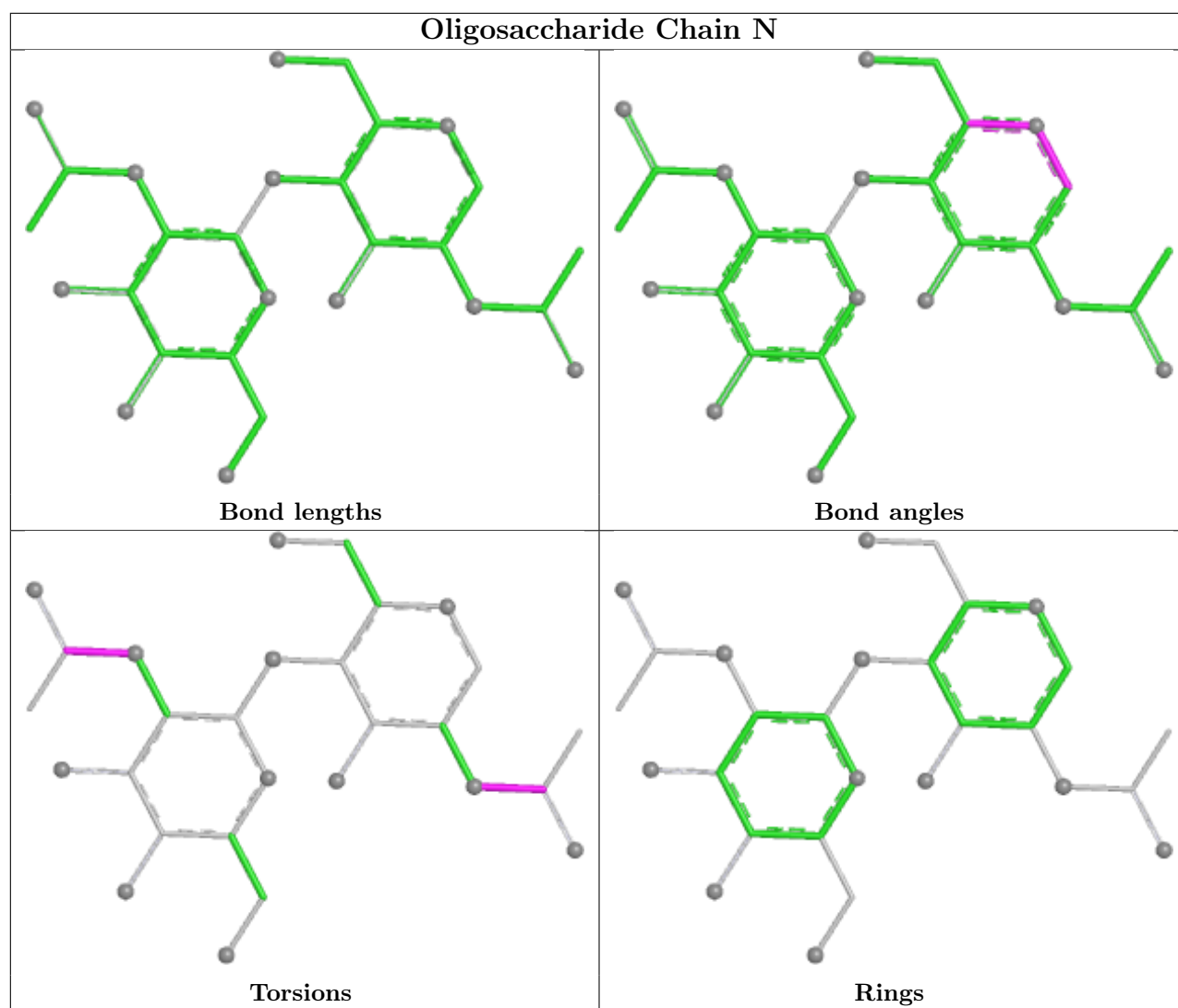


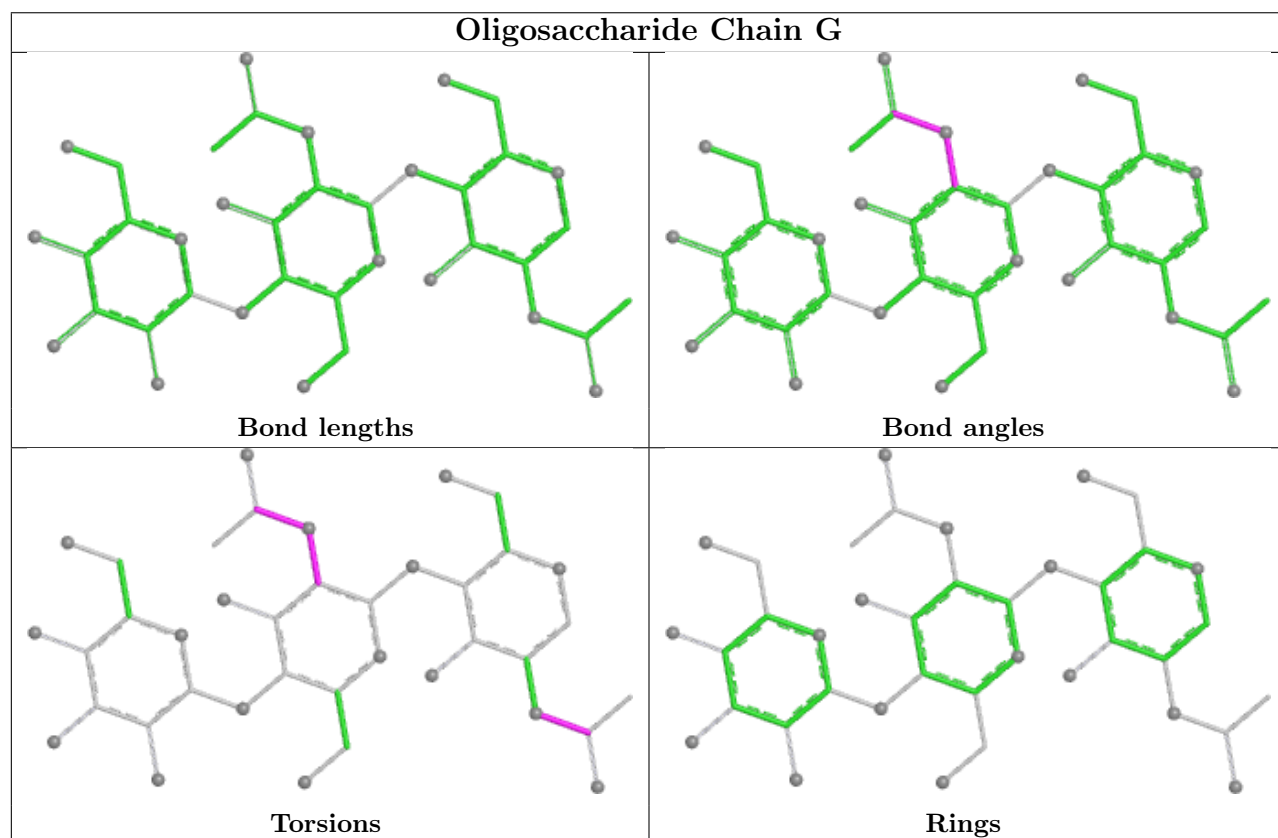
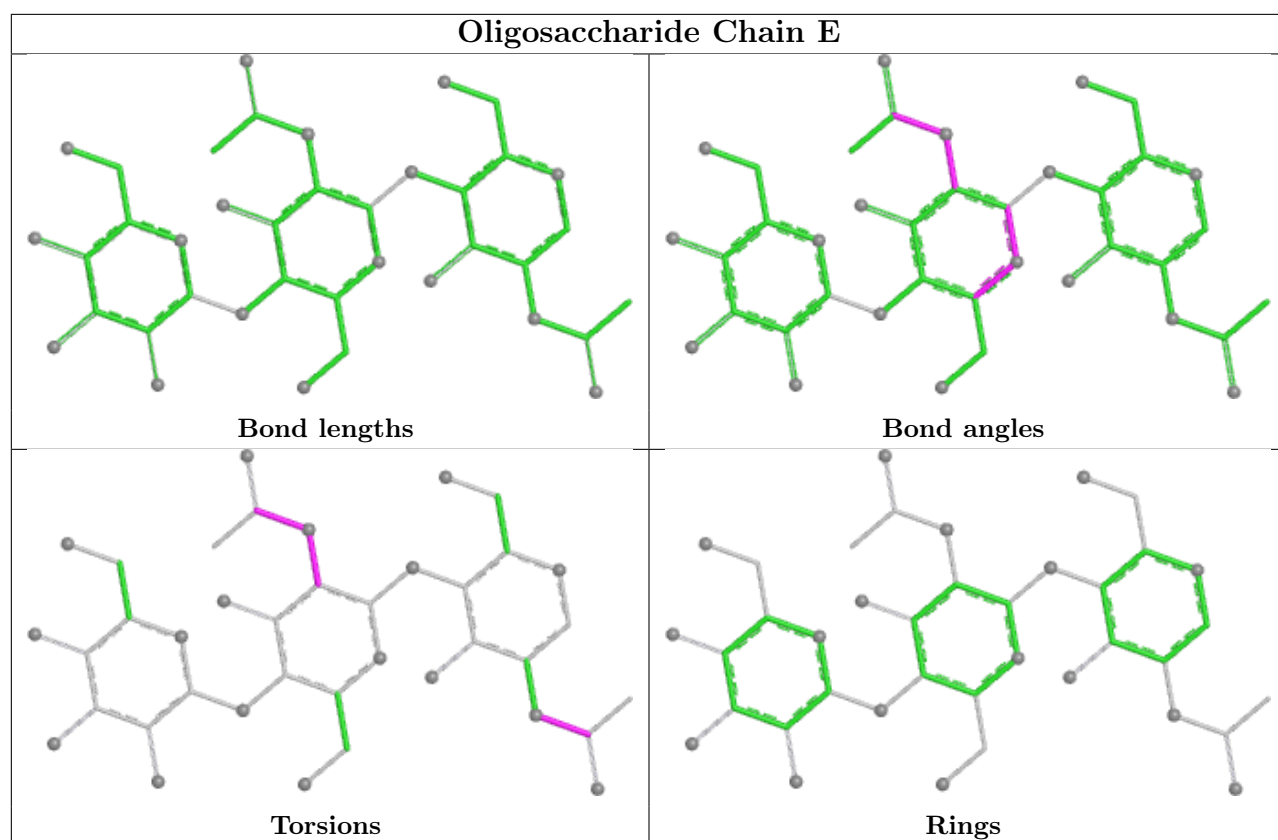


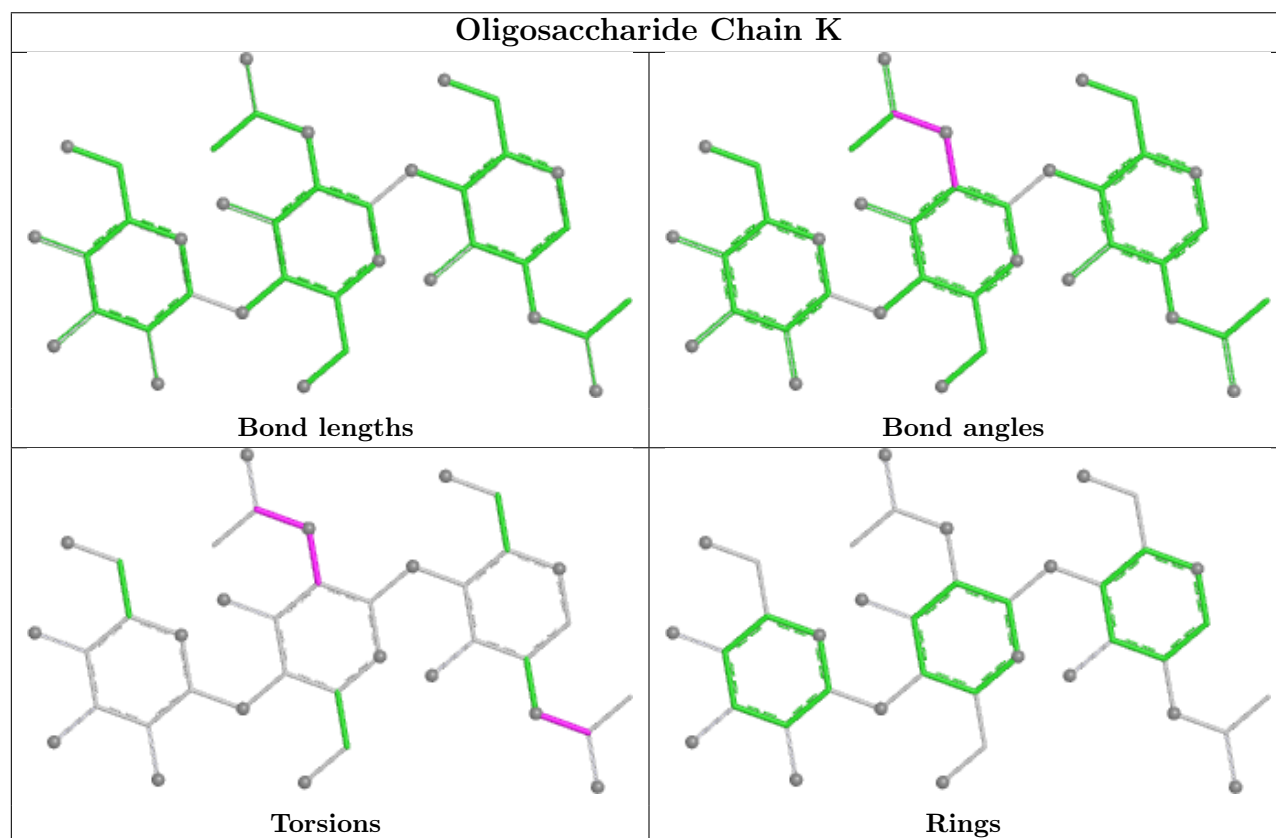
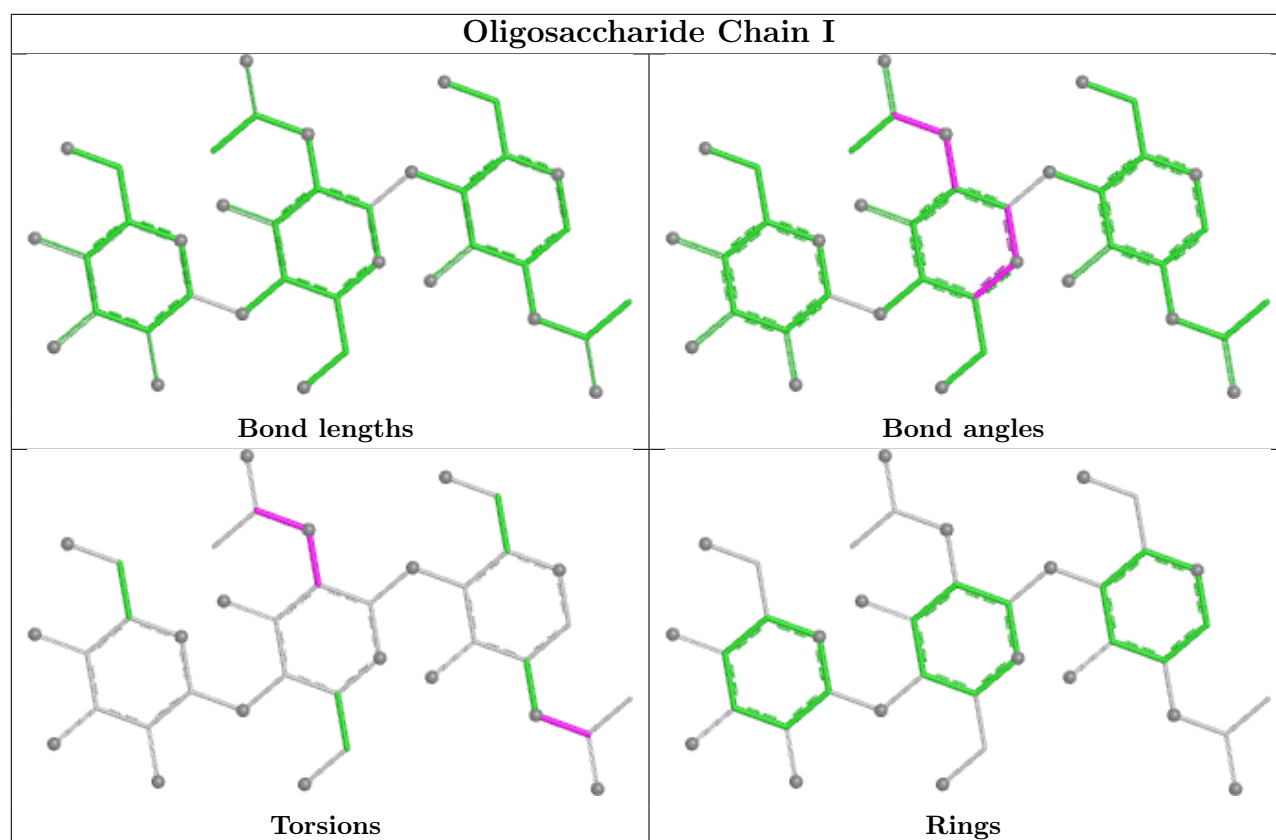


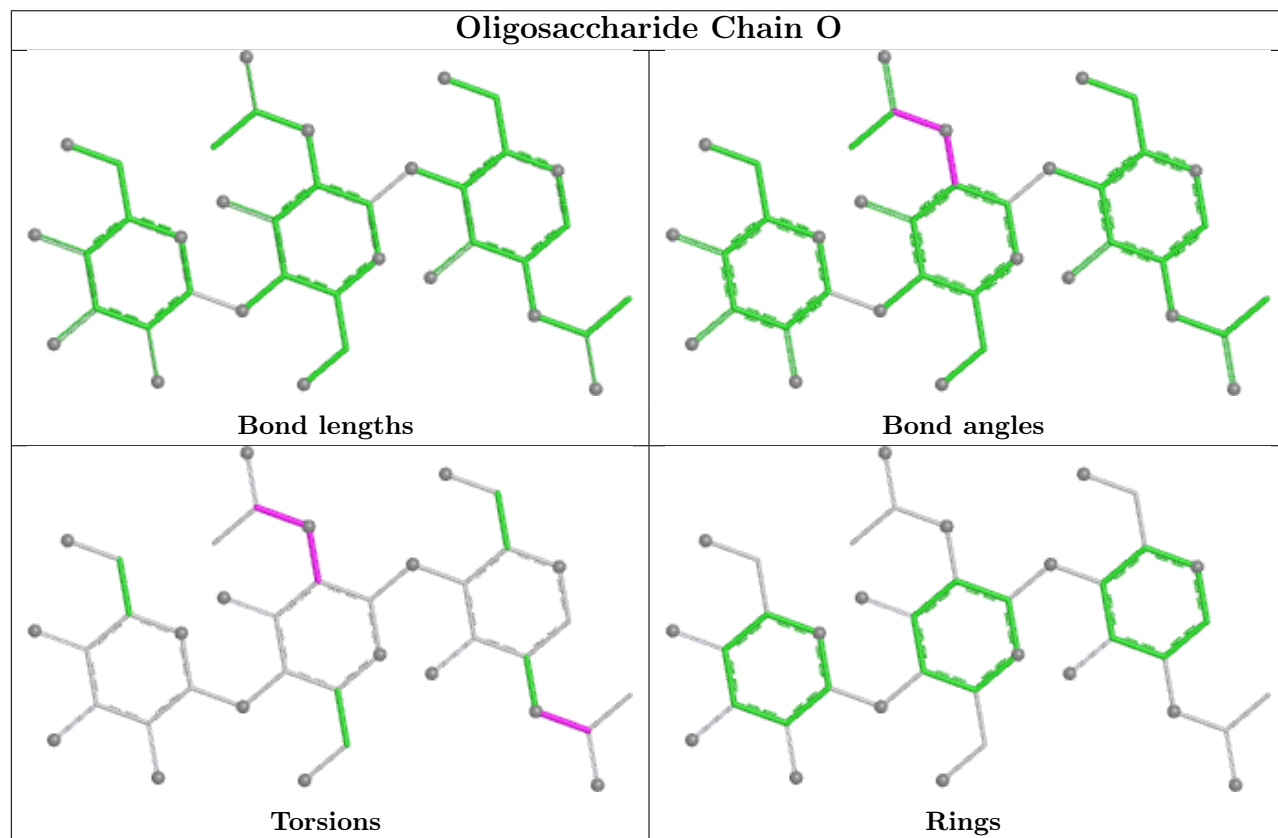
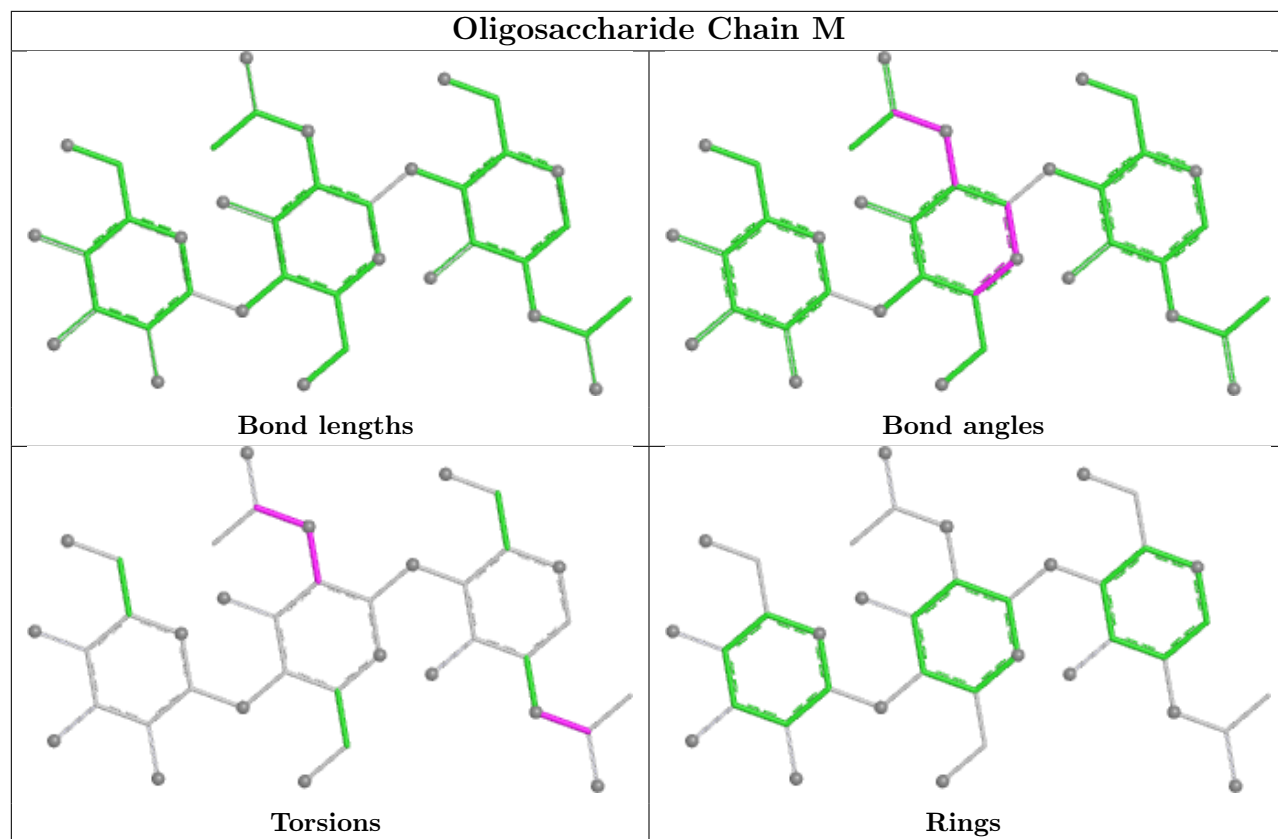












5.6 Ligand geometry

21 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	902	1	14,14,15	0.28	0	17,19,21	0.49	0
4	NAG	C	905	1	14,14,15	0.26	0	17,19,21	0.63	0
4	NAG	A	901	1	14,14,15	0.28	0	17,19,21	0.58	0
4	NAG	B	903	1	14,14,15	0.63	0	17,19,21	2.49	5 (29%)
4	NAG	C	906	1	14,14,15	0.26	0	17,19,21	0.55	0
4	NAG	B	907	1	14,14,15	0.34	0	17,19,21	1.10	2 (11%)
4	NAG	A	903	1	14,14,15	0.62	0	17,19,21	2.49	5 (29%)
4	NAG	A	907	1	14,14,15	0.34	0	17,19,21	1.10	2 (11%)
4	NAG	B	901	1	14,14,15	0.28	0	17,19,21	0.58	0
4	NAG	C	901	1	14,14,15	0.28	0	17,19,21	0.58	0
4	NAG	B	902	1	14,14,15	0.28	0	17,19,21	0.47	0
4	NAG	A	902	1	14,14,15	0.27	0	17,19,21	0.48	0
4	NAG	B	905	1	14,14,15	0.27	0	17,19,21	0.62	0
4	NAG	A	905	1	14,14,15	0.28	0	17,19,21	0.63	1 (5%)
4	NAG	C	907	1	14,14,15	0.34	0	17,19,21	1.10	2 (11%)
4	NAG	B	904	1	14,14,15	0.32	0	17,19,21	0.62	0
4	NAG	B	906	1	14,14,15	0.25	0	17,19,21	0.55	0
4	NAG	A	906	1	14,14,15	0.25	0	17,19,21	0.55	0
4	NAG	A	904	1	14,14,15	0.32	0	17,19,21	0.62	0
4	NAG	C	903	1	14,14,15	0.63	0	17,19,21	2.49	5 (29%)
4	NAG	C	904	1	14,14,15	0.32	0	17,19,21	0.62	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	C	902	1	-	3/6/23/26	0/1/1/1
4	NAG	C	905	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	901	1	-	2/6/23/26	0/1/1/1
4	NAG	B	903	1	-	3/6/23/26	0/1/1/1
4	NAG	C	906	1	-	3/6/23/26	0/1/1/1
4	NAG	B	907	1	-	4/6/23/26	0/1/1/1
4	NAG	A	903	1	-	3/6/23/26	0/1/1/1
4	NAG	A	907	1	-	4/6/23/26	0/1/1/1
4	NAG	B	901	1	-	2/6/23/26	0/1/1/1
4	NAG	C	901	1	-	2/6/23/26	0/1/1/1
4	NAG	B	902	1	-	3/6/23/26	0/1/1/1
4	NAG	A	902	1	-	3/6/23/26	0/1/1/1
4	NAG	B	905	1	-	1/6/23/26	0/1/1/1
4	NAG	A	905	1	-	1/6/23/26	0/1/1/1
4	NAG	C	907	1	-	4/6/23/26	0/1/1/1
4	NAG	B	904	1	-	2/6/23/26	0/1/1/1
4	NAG	B	906	1	-	3/6/23/26	0/1/1/1
4	NAG	A	906	1	-	3/6/23/26	0/1/1/1
4	NAG	A	904	1	-	2/6/23/26	0/1/1/1
4	NAG	C	903	1	-	3/6/23/26	0/1/1/1
4	NAG	C	904	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	903	NAG	C1-O5-C5	6.71	121.19	112.19
4	A	903	NAG	C1-O5-C5	6.71	121.18	112.19
4	C	903	NAG	C1-O5-C5	6.69	121.15	112.19
4	C	903	NAG	C2-N2-C7	4.08	128.37	122.90
4	B	903	NAG	C2-N2-C7	4.07	128.35	122.90

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	902	NAG	C8-C7-N2-C2
4	A	902	NAG	O7-C7-N2-C2
4	A	903	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	A	903	NAG	C8-C7-N2-C2
4	A	903	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	906	NAG	1	0
4	B	906	NAG	1	0
4	A	906	NAG	1	0

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.

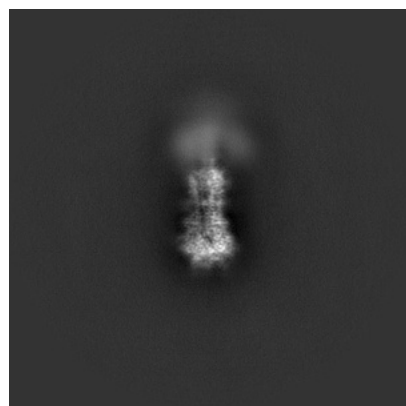
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46500. These allow visual inspection of the internal detail of the map and identification of artifacts.

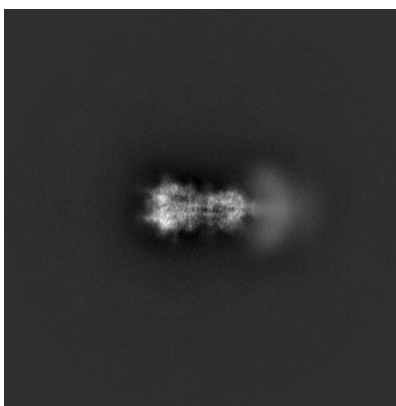
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

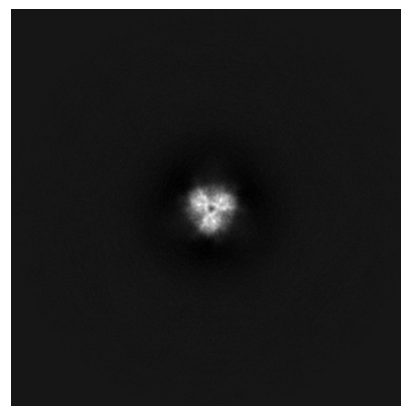
6.1.1 Primary map



X

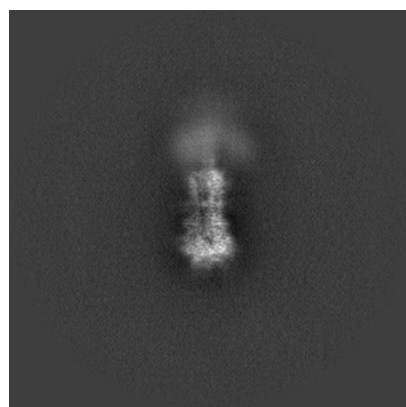


Y

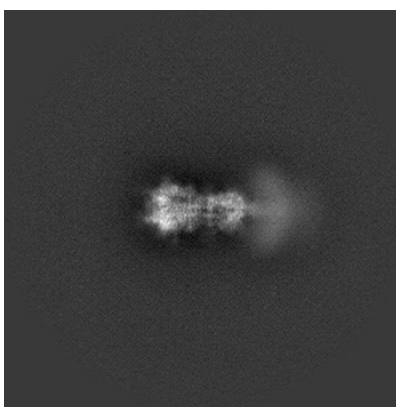


Z

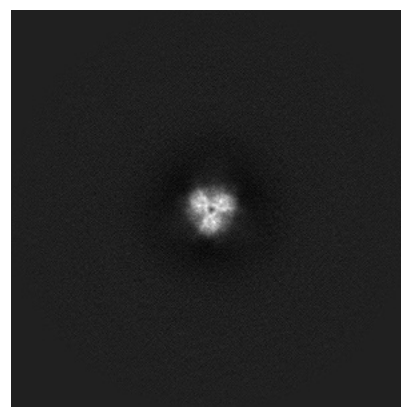
6.1.2 Raw map



X



Y

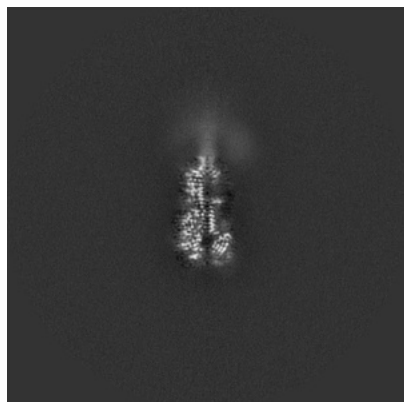


Z

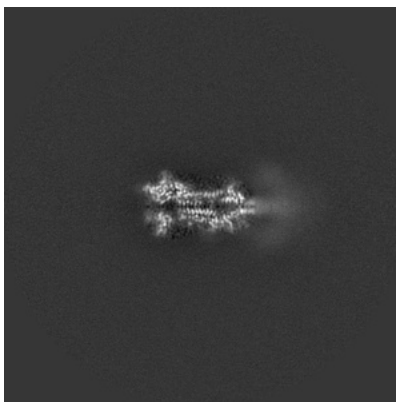
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

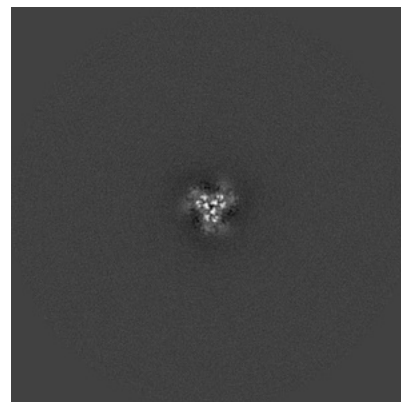
6.2.1 Primary map



X Index: 270

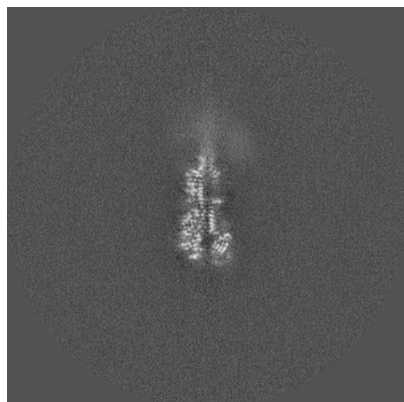


Y Index: 270

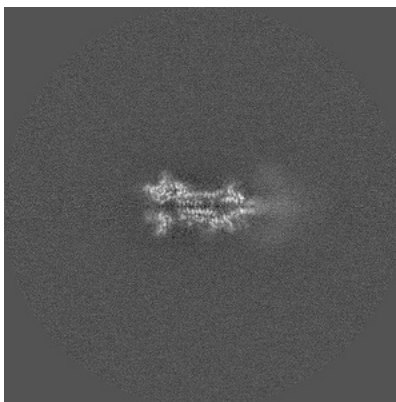


Z Index: 270

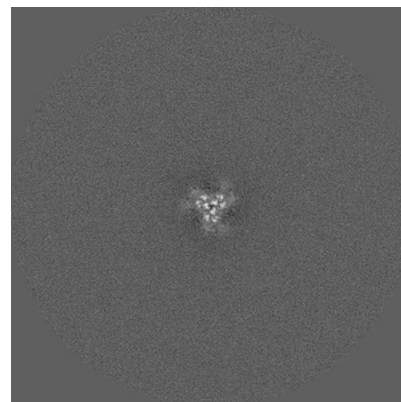
6.2.2 Raw map



X Index: 270



Y Index: 270

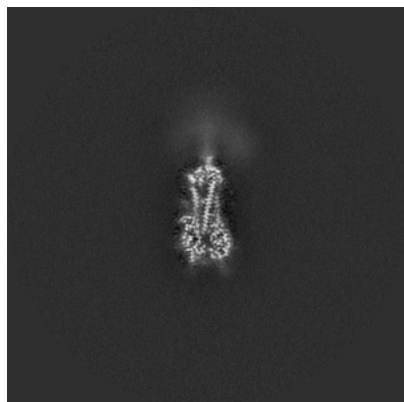


Z Index: 270

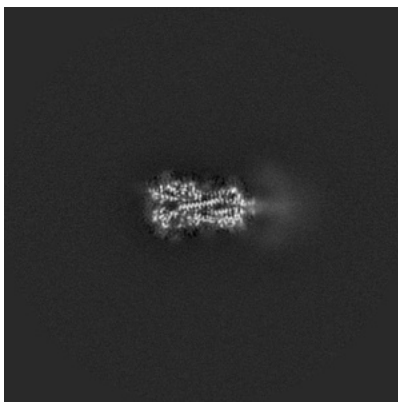
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

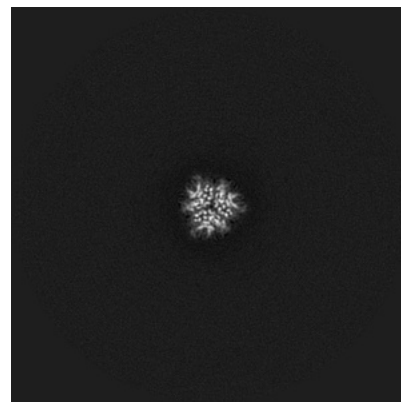
6.3.1 Primary map



X Index: 263

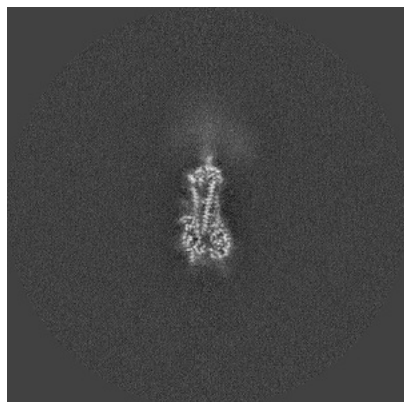


Y Index: 276

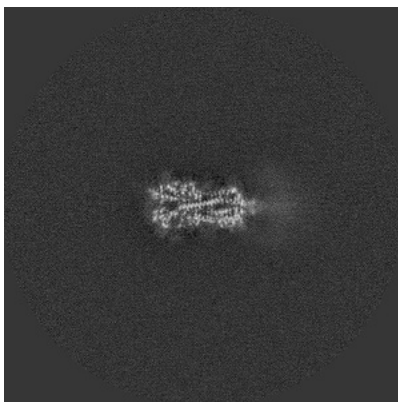


Z Index: 213

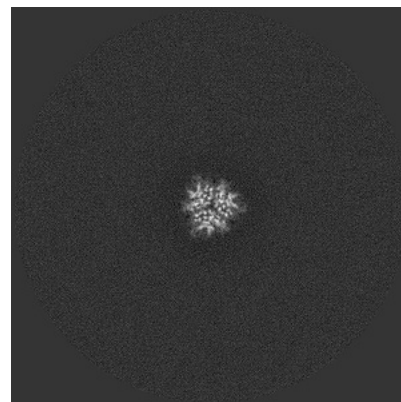
6.3.2 Raw map



X Index: 263



Y Index: 276

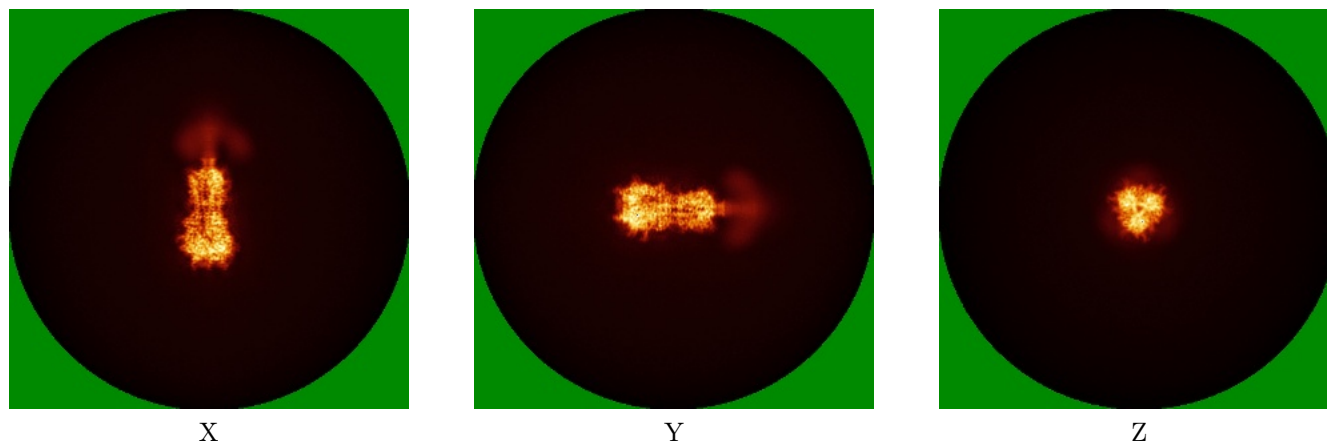


Z Index: 213

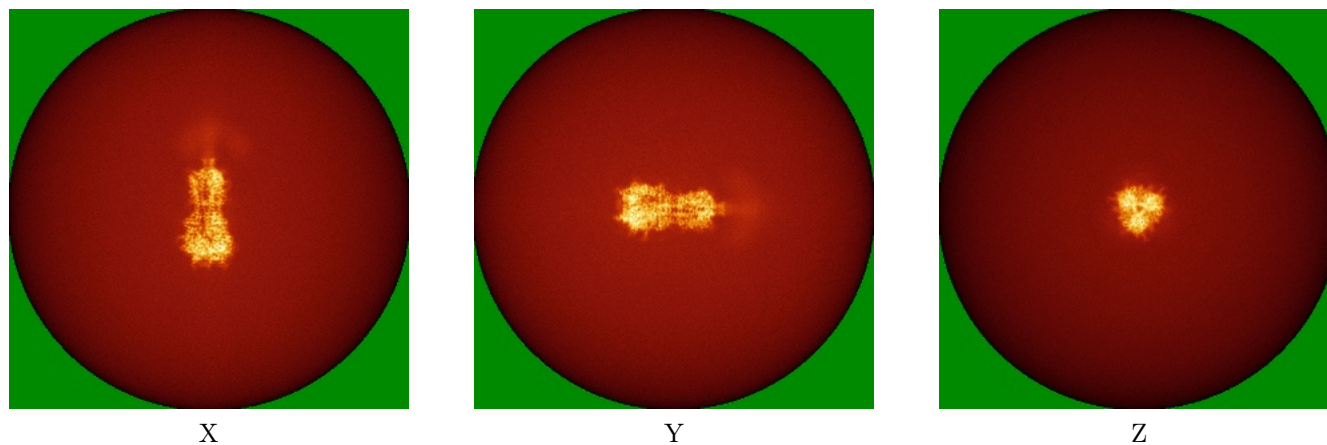
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

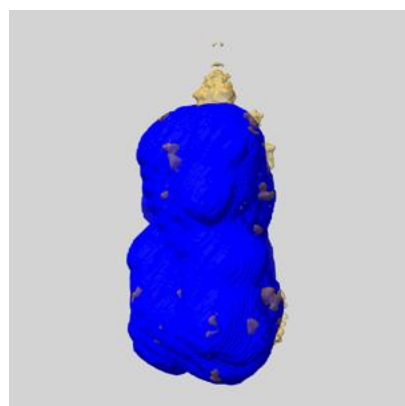
6.6 Mask visualisation [i](#)

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

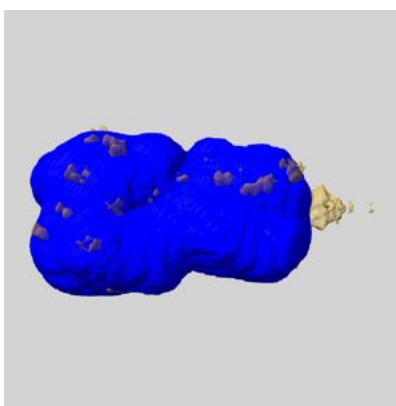
A mask typically either:

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

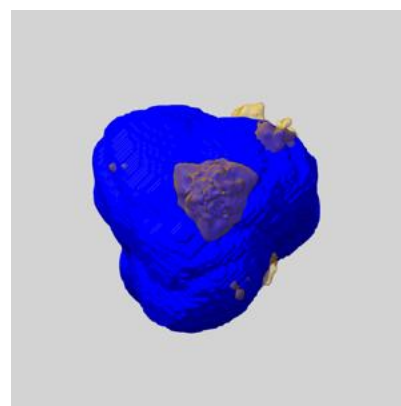
6.6.1 emd_46500_msk_1.map [i](#)



X



Y

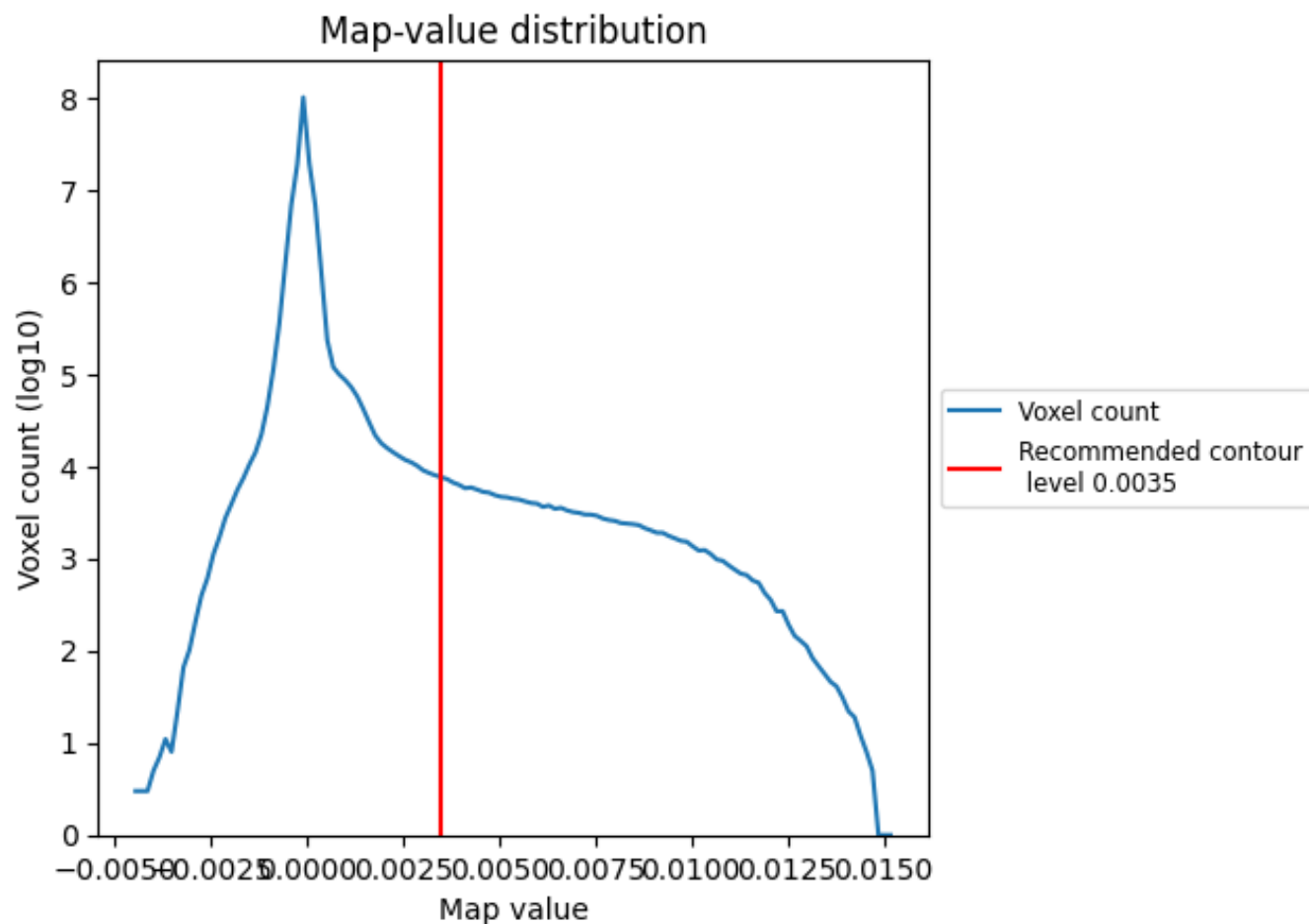


Z

7 Map analysis [i](#)

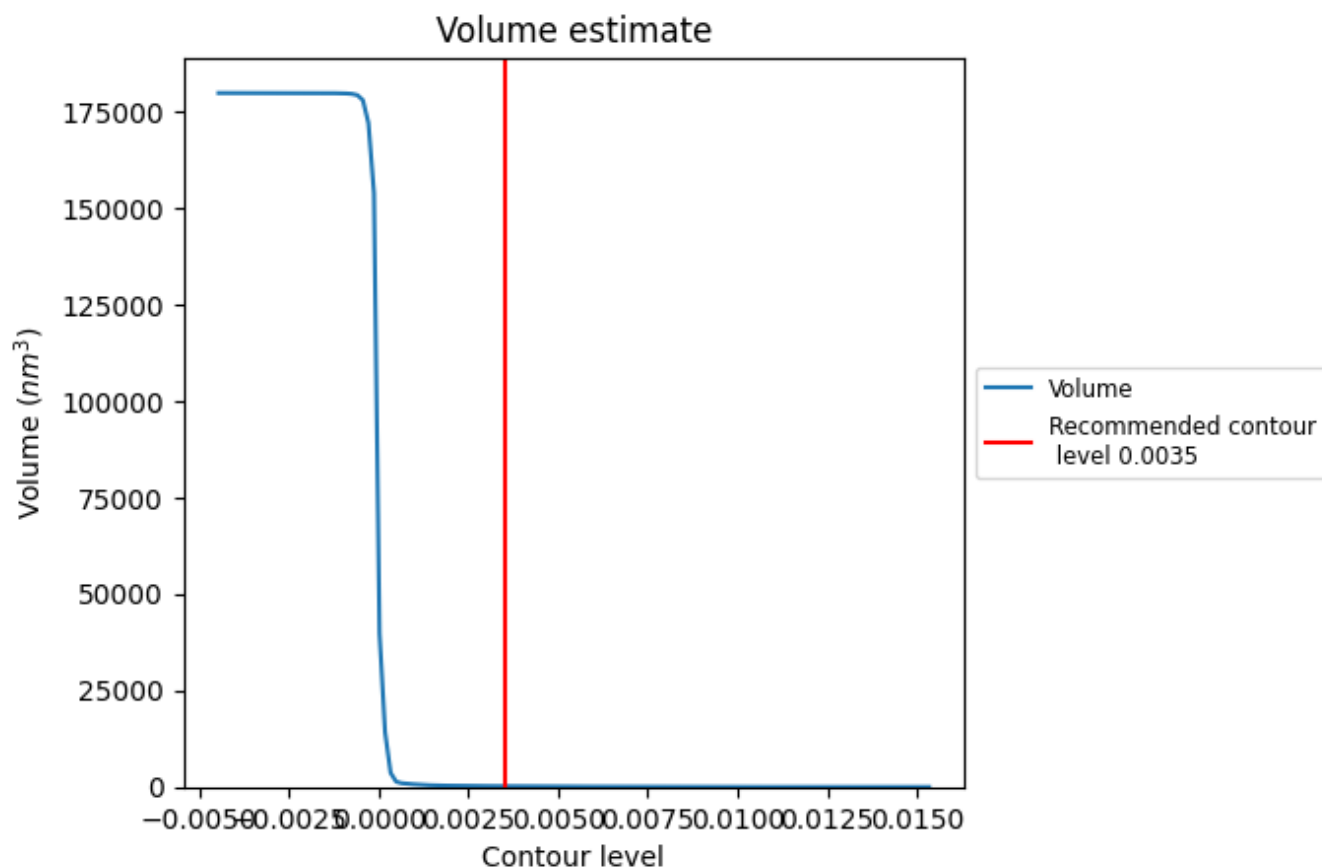
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

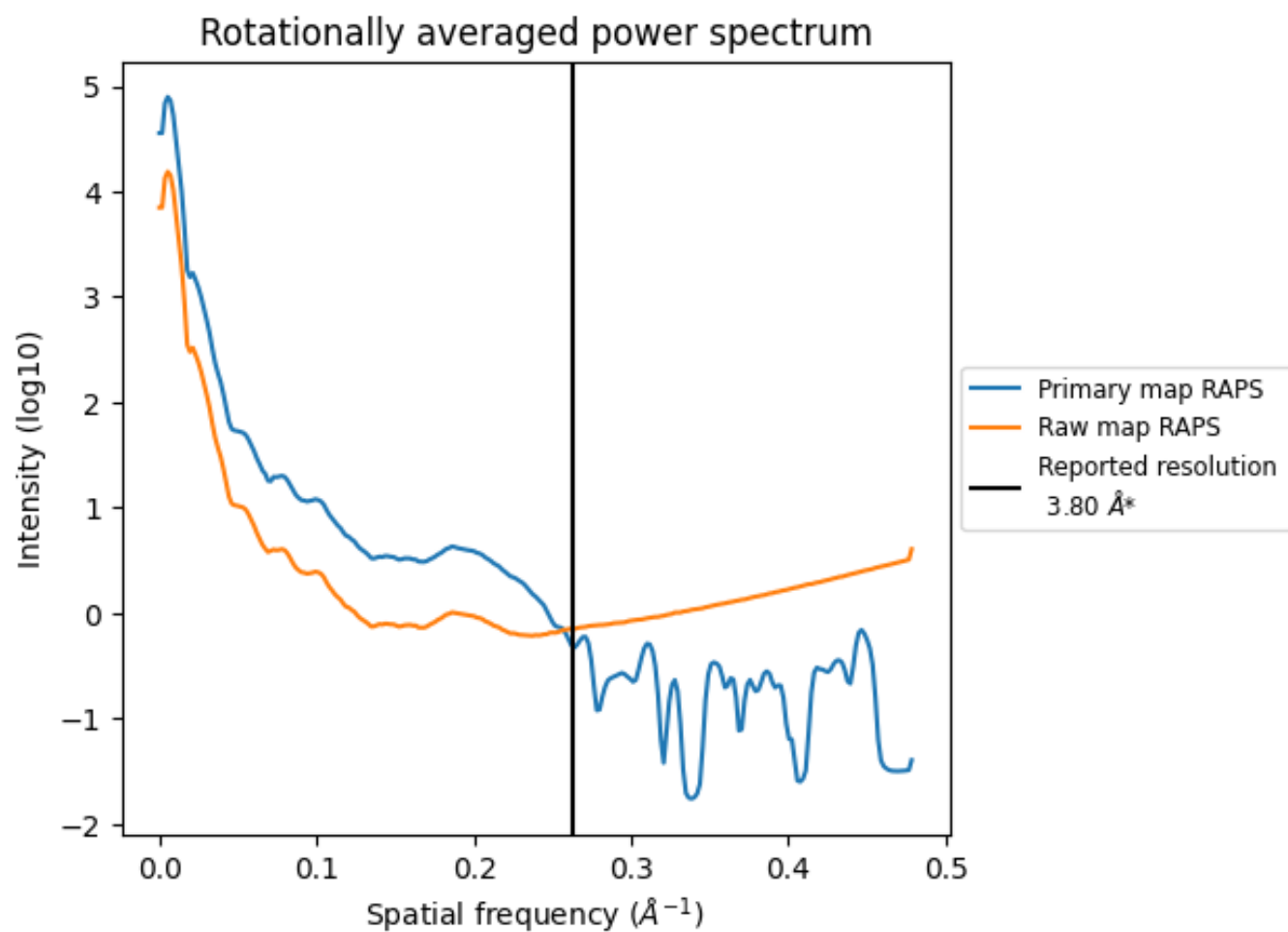
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 192 nm^3 ; this corresponds to an approximate mass of 174 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 ⓘ

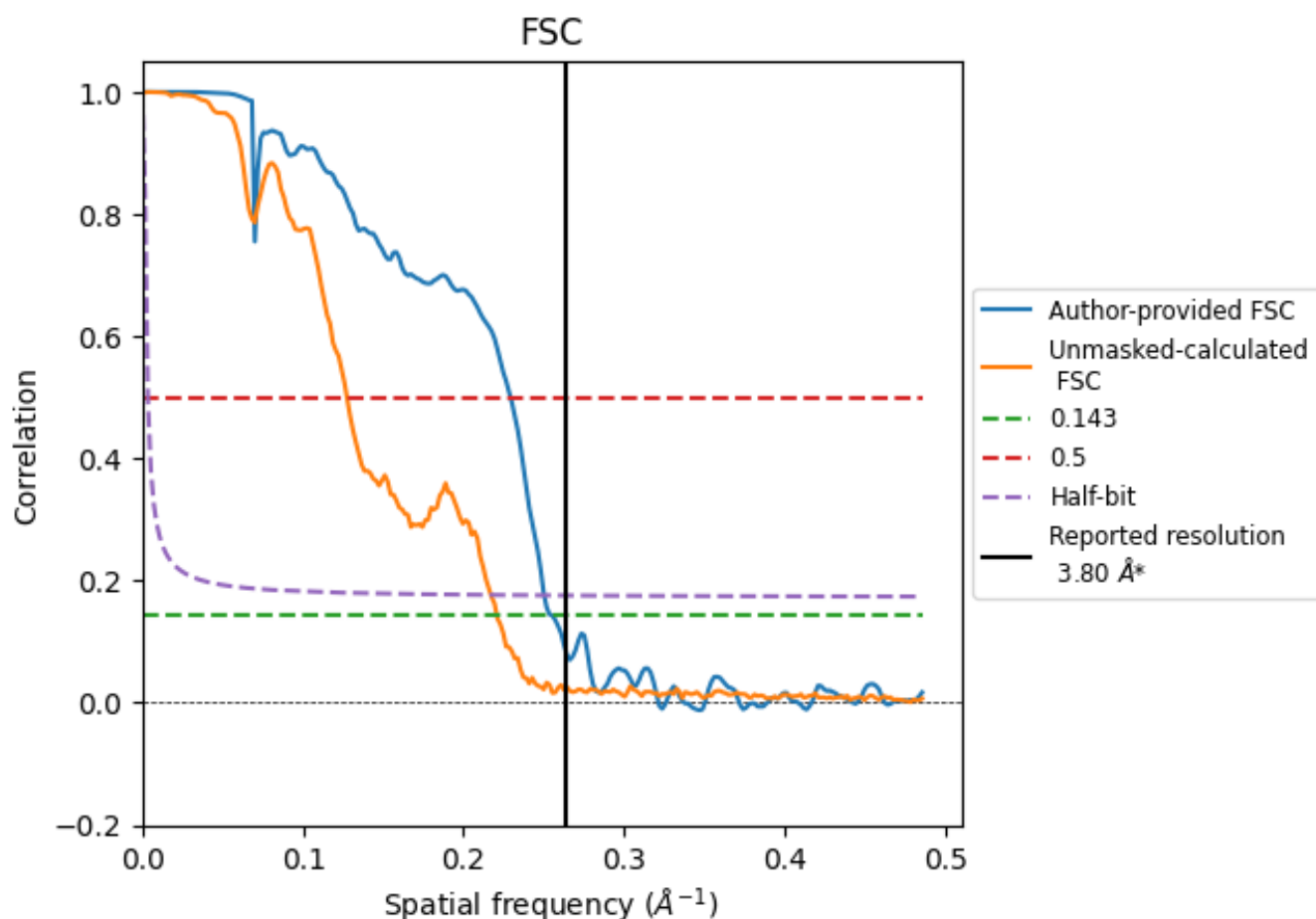


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 \AA^{-1}

8.2 Resolution estimates [i](#)

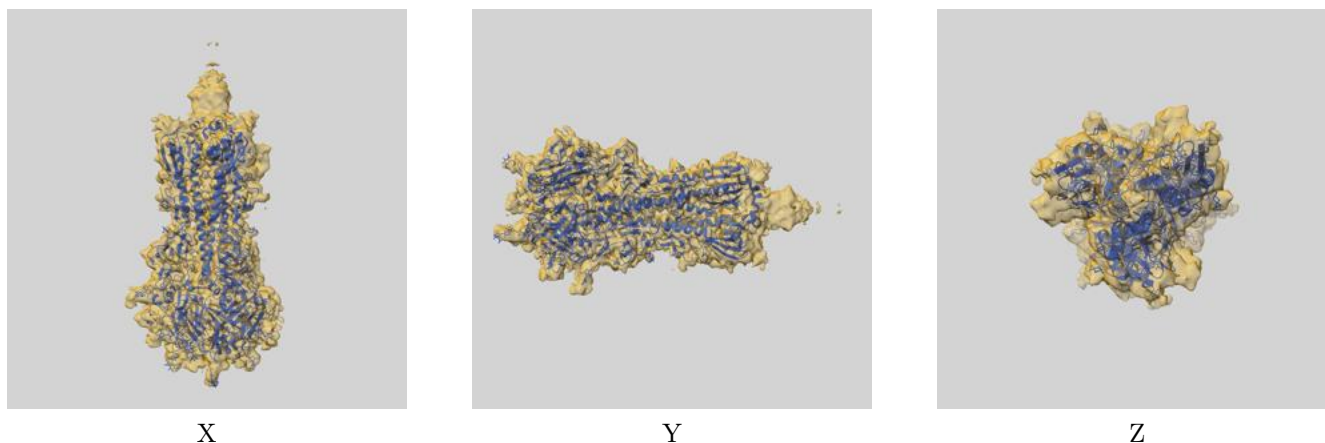
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.92	4.36	4.00
Unmasked-calculated*	4.53	7.85	4.61

*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 4.53 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

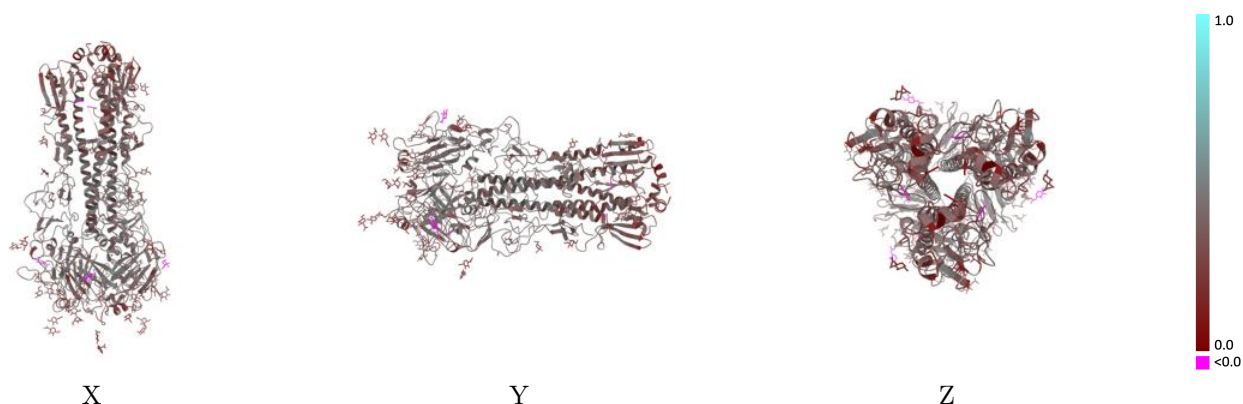
This section contains information regarding the fit between EMDB map EMD-46500 and PDB model 9D2M. Per-residue inclusion information can be found in section [3](#) on page [31](#).

9.1 Map-model overlay [i](#)



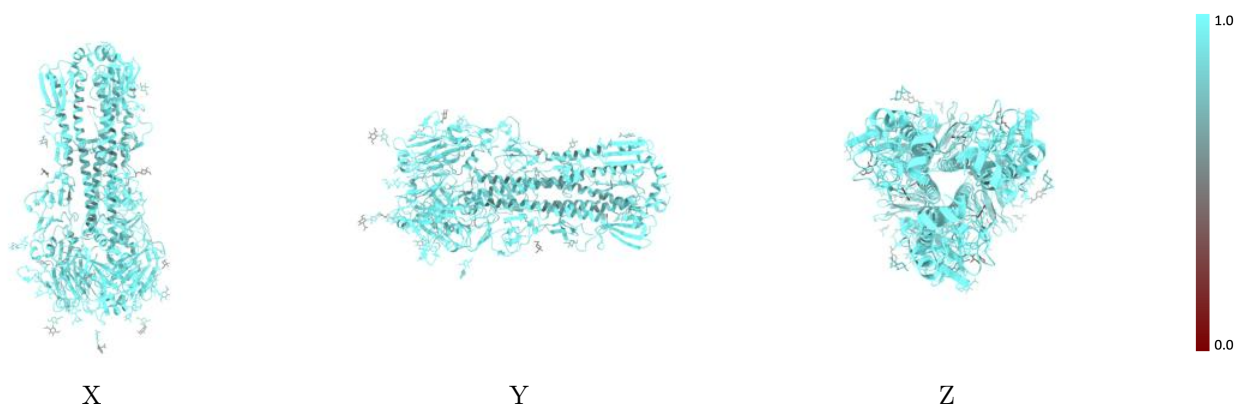
The images above show the 3D surface view of the map at the recommended contour level 0.0035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



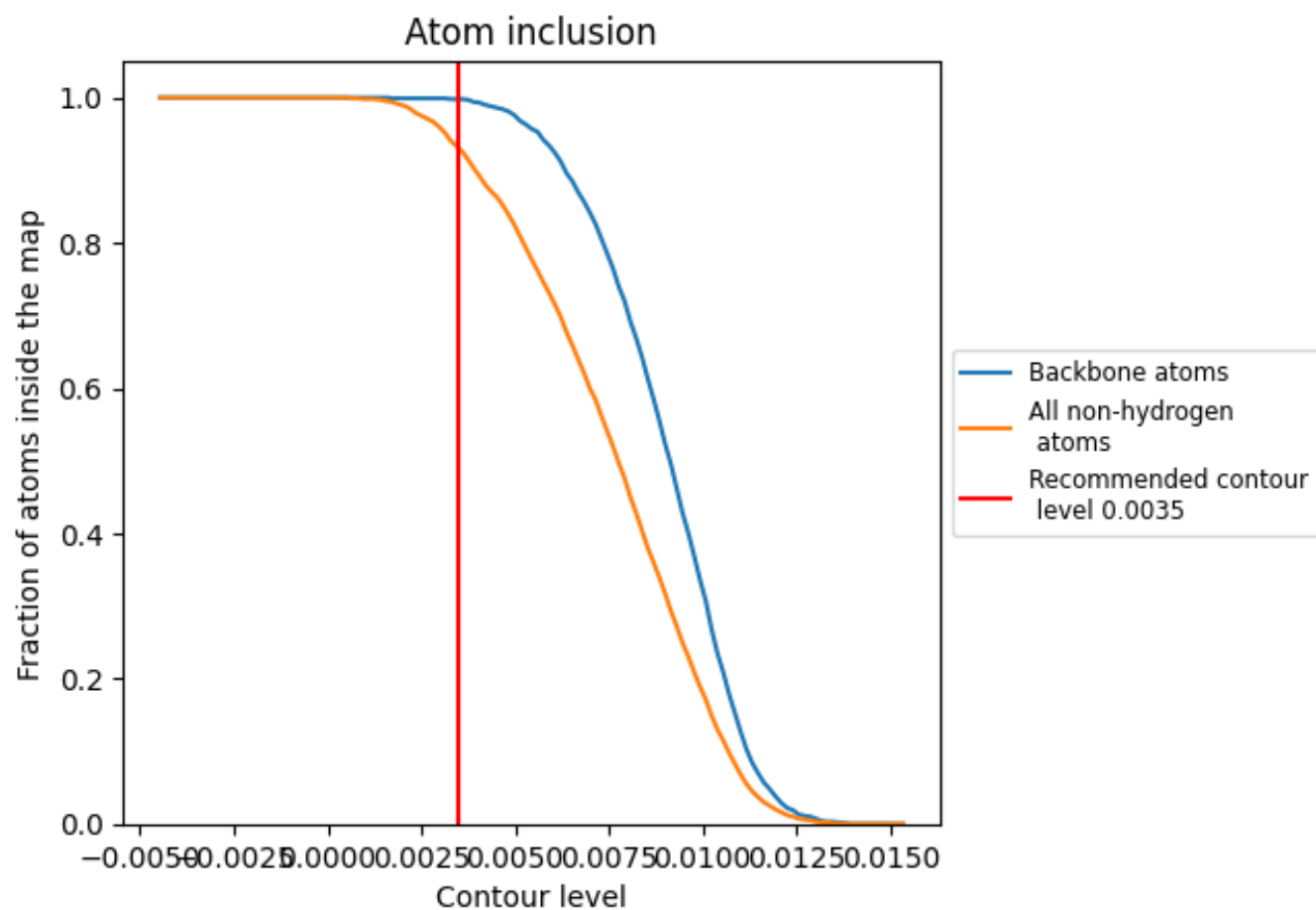
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0035).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 93% 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 (0.0035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9300	 0.3750
A	 0.9310	 0.3780
B	 0.9310	 0.3790
C	 0.9310	 0.3800
D	 0.6430	 0.2120
E	 0.9740	 0.2840
F	 0.8930	 0.2450
G	 1.0000	 0.2980
H	 0.6430	 0.2020
I	 0.9740	 0.2760
J	 0.8930	 0.2280
K	 1.0000	 0.3070
L	 0.6430	 0.2030
M	 0.9740	 0.2710
N	 0.8930	 0.2230
O	 1.0000	 0.3030

