



## Full wwPDB EM Validation Report ⓘ

Dec 5, 2022 – 12:14 PM JST

PDB ID : 7DKJ  
EMDB ID : EMD-30707  
Title : Hemagglutinin Influenza A virus (A/Okuda/1957(H2N2) bound with a neutralizing antibody  
Authors : Shirouzu, M.  
Deposited on : 2020-11-24  
Resolution : 3.70 Å(reported)  
Based on initial models : 5XCX, 4HLZ

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

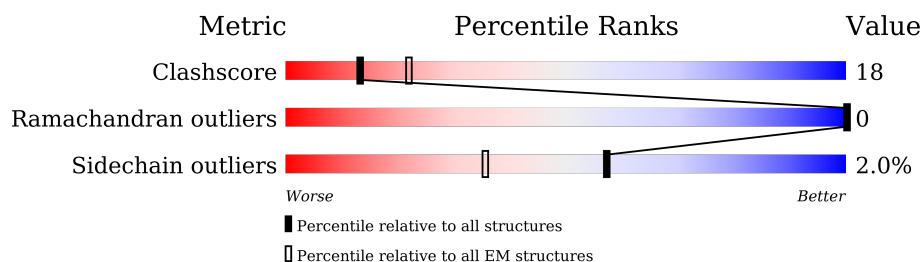
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.70 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	599	<div> <div>12%</div> <div>56%</div> <div>26%</div> <div>•</div> <div>17%</div> </div>
1	E	599	<div> <div>13%</div> <div>56%</div> <div>27%</div> <div>•</div> <div>17%</div> </div>
1	I	599	<div> <div>13%</div> <div>55%</div> <div>27%</div> <div>•</div> <div>17%</div> </div>
2	C	203	<div> <div>48%</div> <div>47%</div> <div>37%</div> <div>15%</div> </div>
2	G	203	<div> <div>49%</div> <div>45%</div> <div>39%</div> <div>15%</div> </div>
2	K	203	<div> <div>49%</div> <div>47%</div> <div>38%</div> <div>15%</div> </div>
3	D	189	<div> <div>58%</div> <div>47%</div> <div>36%</div> <div>•</div> <div>16%</div> </div>
3	H	189	<div> <div>58%</div> <div>47%</div> <div>35%</div> <div>•</div> <div>16%</div> </div>

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Mol	Chain	Length	Quality of chain
3	L	189	<div><div></div><div>58%</div><div>45%</div><div>38%</div><div>16%</div></div>
4	B	3	<div><div></div><div>67%</div><div>100%</div></div>
4	F	3	<div><div></div><div>67%</div><div>33%</div><div>67%</div></div>
4	J	3	<div><div></div><div>67%</div><div>100%</div></div>
4	M	3	<div><div></div><div>67%</div><div>33%</div><div>67%</div></div>
4	N	3	<div><div></div><div>67%</div><div>100%</div></div>
4	O	3	<div><div></div><div>67%</div><div>33%</div><div>67%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20112 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	498	Total	C	N	O	S	0	0
			3947	2477	680	766	24		
1	E	498	Total	C	N	O	S	0	0
			3947	2477	680	766	24		
1	I	498	Total	C	N	O	S	0	0
			3947	2477	680	766	24		

There are 306 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	initiating methionine	UNP A0A0A7E4R0
A	-34	LEU	-	expression tag	UNP A0A0A7E4R0
A	-33	LEU	-	expression tag	UNP A0A0A7E4R0
A	-32	VAL	-	expression tag	UNP A0A0A7E4R0
A	-31	ASN	-	expression tag	UNP A0A0A7E4R0
A	-30	GLN	-	expression tag	UNP A0A0A7E4R0
A	-29	SER	-	expression tag	UNP A0A0A7E4R0
A	-28	HIS	-	expression tag	UNP A0A0A7E4R0
A	-27	GLN	-	expression tag	UNP A0A0A7E4R0
A	-26	GLY	-	expression tag	UNP A0A0A7E4R0
A	-25	PHE	-	expression tag	UNP A0A0A7E4R0
A	-24	ASN	-	expression tag	UNP A0A0A7E4R0
A	-23	LYS	-	expression tag	UNP A0A0A7E4R0
A	-22	GLU	-	expression tag	UNP A0A0A7E4R0
A	-21	HIS	-	expression tag	UNP A0A0A7E4R0
A	-20	THR	-	expression tag	UNP A0A0A7E4R0
A	-19	SER	-	expression tag	UNP A0A0A7E4R0
A	-18	LYS	-	expression tag	UNP A0A0A7E4R0
A	-17	MET	-	expression tag	UNP A0A0A7E4R0
A	-16	VAL	-	expression tag	UNP A0A0A7E4R0
A	-15	SER	-	expression tag	UNP A0A0A7E4R0
A	-14	ALA	-	expression tag	UNP A0A0A7E4R0
A	-13	ILE	-	expression tag	UNP A0A0A7E4R0
A	-12	VAL	-	expression tag	UNP A0A0A7E4R0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	LEU	-	expression tag	UNP A0A0A7E4R0
A	-10	TYR	-	expression tag	UNP A0A0A7E4R0
A	-9	VAL	-	expression tag	UNP A0A0A7E4R0
A	-8	LEU	-	expression tag	UNP A0A0A7E4R0
A	-7	LEU	-	expression tag	UNP A0A0A7E4R0
A	-6	ALA	-	expression tag	UNP A0A0A7E4R0
A	-5	ALA	-	expression tag	UNP A0A0A7E4R0
A	-4	ALA	-	expression tag	UNP A0A0A7E4R0
A	-3	ALA	-	expression tag	UNP A0A0A7E4R0
A	-2	HIS	-	expression tag	UNP A0A0A7E4R0
A	-1	SER	-	expression tag	UNP A0A0A7E4R0
A	0	ALA	-	expression tag	UNP A0A0A7E4R0
A	1	PHE	-	expression tag	UNP A0A0A7E4R0
A	2	ALA	-	expression tag	UNP A0A0A7E4R0
A	22	CYS	LEU	engineered mutation	UNP A0A0A7E4R0
A	93	PHE	TYR	engineered mutation	UNP A0A0A7E4R0
A	98	SER	ASN	engineered mutation	UNP A0A0A7E4R0
A	374	CYS	GLY	engineered mutation	UNP A0A0A7E4R0
A	504	LEU	-	expression tag	UNP A0A0A7E4R0
A	505	VAL	-	expression tag	UNP A0A0A7E4R0
A	506	PRO	-	expression tag	UNP A0A0A7E4R0
A	507	ARG	-	expression tag	UNP A0A0A7E4R0
A	508	GLY	-	expression tag	UNP A0A0A7E4R0
A	509	SER	-	expression tag	UNP A0A0A7E4R0
A	510	PRO	-	expression tag	UNP A0A0A7E4R0
A	511	GLY	-	expression tag	UNP A0A0A7E4R0
A	512	SER	-	expression tag	UNP A0A0A7E4R0
A	513	GLY	-	expression tag	UNP A0A0A7E4R0
A	514	TYR	-	expression tag	UNP A0A0A7E4R0
A	515	ILE	-	expression tag	UNP A0A0A7E4R0
A	516	PRO	-	expression tag	UNP A0A0A7E4R0
A	517	GLU	-	expression tag	UNP A0A0A7E4R0
A	518	ALA	-	expression tag	UNP A0A0A7E4R0
A	519	PRO	-	expression tag	UNP A0A0A7E4R0
A	520	ARG	-	expression tag	UNP A0A0A7E4R0
A	521	ASP	-	expression tag	UNP A0A0A7E4R0
A	522	GLY	-	expression tag	UNP A0A0A7E4R0
A	523	GLN	-	expression tag	UNP A0A0A7E4R0
A	524	ALA	-	expression tag	UNP A0A0A7E4R0
A	525	TYR	-	expression tag	UNP A0A0A7E4R0
A	526	VAL	-	expression tag	UNP A0A0A7E4R0
A	527	ARG	-	expression tag	UNP A0A0A7E4R0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	528	LYS	-	expression tag	UNP A0A0A7E4R0
A	529	ASP	-	expression tag	UNP A0A0A7E4R0
A	530	GLY	-	expression tag	UNP A0A0A7E4R0
A	531	GLU	-	expression tag	UNP A0A0A7E4R0
A	532	TRP	-	expression tag	UNP A0A0A7E4R0
A	533	VAL	-	expression tag	UNP A0A0A7E4R0
A	534	LEU	-	expression tag	UNP A0A0A7E4R0
A	535	LEU	-	expression tag	UNP A0A0A7E4R0
A	536	SER	-	expression tag	UNP A0A0A7E4R0
A	537	THR	-	expression tag	UNP A0A0A7E4R0
A	538	PHE	-	expression tag	UNP A0A0A7E4R0
A	539	LEU	-	expression tag	UNP A0A0A7E4R0
A	540	GLY	-	expression tag	UNP A0A0A7E4R0
A	541	SER	-	expression tag	UNP A0A0A7E4R0
A	542	GLY	-	expression tag	UNP A0A0A7E4R0
A	543	LEU	-	expression tag	UNP A0A0A7E4R0
A	544	ASN	-	expression tag	UNP A0A0A7E4R0
A	545	ASP	-	expression tag	UNP A0A0A7E4R0
A	546	ILE	-	expression tag	UNP A0A0A7E4R0
A	547	PHE	-	expression tag	UNP A0A0A7E4R0
A	548	GLU	-	expression tag	UNP A0A0A7E4R0
A	549	ALA	-	expression tag	UNP A0A0A7E4R0
A	550	GLN	-	expression tag	UNP A0A0A7E4R0
A	551	LYS	-	expression tag	UNP A0A0A7E4R0
A	552	ILE	-	expression tag	UNP A0A0A7E4R0
A	553	GLU	-	expression tag	UNP A0A0A7E4R0
A	554	TRP	-	expression tag	UNP A0A0A7E4R0
A	555	HIS	-	expression tag	UNP A0A0A7E4R0
A	556	GLU	-	expression tag	UNP A0A0A7E4R0
A	557	GLY	-	expression tag	UNP A0A0A7E4R0
A	558	HIS	-	expression tag	UNP A0A0A7E4R0
A	559	HIS	-	expression tag	UNP A0A0A7E4R0
A	560	HIS	-	expression tag	UNP A0A0A7E4R0
A	561	HIS	-	expression tag	UNP A0A0A7E4R0
A	562	HIS	-	expression tag	UNP A0A0A7E4R0
A	563	HIS	-	expression tag	UNP A0A0A7E4R0
E	-35	MET	-	initiating methionine	UNP A0A0A7E4R0
E	-34	LEU	-	expression tag	UNP A0A0A7E4R0
E	-33	LEU	-	expression tag	UNP A0A0A7E4R0
E	-32	VAL	-	expression tag	UNP A0A0A7E4R0
E	-31	ASN	-	expression tag	UNP A0A0A7E4R0
E	-30	GLN	-	expression tag	UNP A0A0A7E4R0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-29	SER	-	expression tag	UNP A0A0A7E4R0
E	-28	HIS	-	expression tag	UNP A0A0A7E4R0
E	-27	GLN	-	expression tag	UNP A0A0A7E4R0
E	-26	GLY	-	expression tag	UNP A0A0A7E4R0
E	-25	PHE	-	expression tag	UNP A0A0A7E4R0
E	-24	ASN	-	expression tag	UNP A0A0A7E4R0
E	-23	LYS	-	expression tag	UNP A0A0A7E4R0
E	-22	GLU	-	expression tag	UNP A0A0A7E4R0
E	-21	HIS	-	expression tag	UNP A0A0A7E4R0
E	-20	THR	-	expression tag	UNP A0A0A7E4R0
E	-19	SER	-	expression tag	UNP A0A0A7E4R0
E	-18	LYS	-	expression tag	UNP A0A0A7E4R0
E	-17	MET	-	expression tag	UNP A0A0A7E4R0
E	-16	VAL	-	expression tag	UNP A0A0A7E4R0
E	-15	SER	-	expression tag	UNP A0A0A7E4R0
E	-14	ALA	-	expression tag	UNP A0A0A7E4R0
E	-13	ILE	-	expression tag	UNP A0A0A7E4R0
E	-12	VAL	-	expression tag	UNP A0A0A7E4R0
E	-11	LEU	-	expression tag	UNP A0A0A7E4R0
E	-10	TYR	-	expression tag	UNP A0A0A7E4R0
E	-9	VAL	-	expression tag	UNP A0A0A7E4R0
E	-8	LEU	-	expression tag	UNP A0A0A7E4R0
E	-7	LEU	-	expression tag	UNP A0A0A7E4R0
E	-6	ALA	-	expression tag	UNP A0A0A7E4R0
E	-5	ALA	-	expression tag	UNP A0A0A7E4R0
E	-4	ALA	-	expression tag	UNP A0A0A7E4R0
E	-3	ALA	-	expression tag	UNP A0A0A7E4R0
E	-2	HIS	-	expression tag	UNP A0A0A7E4R0
E	-1	SER	-	expression tag	UNP A0A0A7E4R0
E	0	ALA	-	expression tag	UNP A0A0A7E4R0
E	1	PHE	-	expression tag	UNP A0A0A7E4R0
E	2	ALA	-	expression tag	UNP A0A0A7E4R0
E	22	CYS	LEU	engineered mutation	UNP A0A0A7E4R0
E	93	PHE	TYR	engineered mutation	UNP A0A0A7E4R0
E	98	SER	ASN	engineered mutation	UNP A0A0A7E4R0
E	374	CYS	GLY	engineered mutation	UNP A0A0A7E4R0
E	504	LEU	-	expression tag	UNP A0A0A7E4R0
E	505	VAL	-	expression tag	UNP A0A0A7E4R0
E	506	PRO	-	expression tag	UNP A0A0A7E4R0
E	507	ARG	-	expression tag	UNP A0A0A7E4R0
E	508	GLY	-	expression tag	UNP A0A0A7E4R0
E	509	SER	-	expression tag	UNP A0A0A7E4R0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	510	PRO	-	expression tag	UNP A0A0A7E4R0
E	511	GLY	-	expression tag	UNP A0A0A7E4R0
E	512	SER	-	expression tag	UNP A0A0A7E4R0
E	513	GLY	-	expression tag	UNP A0A0A7E4R0
E	514	TYR	-	expression tag	UNP A0A0A7E4R0
E	515	ILE	-	expression tag	UNP A0A0A7E4R0
E	516	PRO	-	expression tag	UNP A0A0A7E4R0
E	517	GLU	-	expression tag	UNP A0A0A7E4R0
E	518	ALA	-	expression tag	UNP A0A0A7E4R0
E	519	PRO	-	expression tag	UNP A0A0A7E4R0
E	520	ARG	-	expression tag	UNP A0A0A7E4R0
E	521	ASP	-	expression tag	UNP A0A0A7E4R0
E	522	GLY	-	expression tag	UNP A0A0A7E4R0
E	523	GLN	-	expression tag	UNP A0A0A7E4R0
E	524	ALA	-	expression tag	UNP A0A0A7E4R0
E	525	TYR	-	expression tag	UNP A0A0A7E4R0
E	526	VAL	-	expression tag	UNP A0A0A7E4R0
E	527	ARG	-	expression tag	UNP A0A0A7E4R0
E	528	LYS	-	expression tag	UNP A0A0A7E4R0
E	529	ASP	-	expression tag	UNP A0A0A7E4R0
E	530	GLY	-	expression tag	UNP A0A0A7E4R0
E	531	GLU	-	expression tag	UNP A0A0A7E4R0
E	532	TRP	-	expression tag	UNP A0A0A7E4R0
E	533	VAL	-	expression tag	UNP A0A0A7E4R0
E	534	LEU	-	expression tag	UNP A0A0A7E4R0
E	535	LEU	-	expression tag	UNP A0A0A7E4R0
E	536	SER	-	expression tag	UNP A0A0A7E4R0
E	537	THR	-	expression tag	UNP A0A0A7E4R0
E	538	PHE	-	expression tag	UNP A0A0A7E4R0
E	539	LEU	-	expression tag	UNP A0A0A7E4R0
E	540	GLY	-	expression tag	UNP A0A0A7E4R0
E	541	SER	-	expression tag	UNP A0A0A7E4R0
E	542	GLY	-	expression tag	UNP A0A0A7E4R0
E	543	LEU	-	expression tag	UNP A0A0A7E4R0
E	544	ASN	-	expression tag	UNP A0A0A7E4R0
E	545	ASP	-	expression tag	UNP A0A0A7E4R0
E	546	ILE	-	expression tag	UNP A0A0A7E4R0
E	547	PHE	-	expression tag	UNP A0A0A7E4R0
E	548	GLU	-	expression tag	UNP A0A0A7E4R0
E	549	ALA	-	expression tag	UNP A0A0A7E4R0
E	550	GLN	-	expression tag	UNP A0A0A7E4R0
E	551	LYS	-	expression tag	UNP A0A0A7E4R0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	552	ILE	-	expression tag	UNP A0A0A7E4R0
E	553	GLU	-	expression tag	UNP A0A0A7E4R0
E	554	TRP	-	expression tag	UNP A0A0A7E4R0
E	555	HIS	-	expression tag	UNP A0A0A7E4R0
E	556	GLU	-	expression tag	UNP A0A0A7E4R0
E	557	GLY	-	expression tag	UNP A0A0A7E4R0
E	558	HIS	-	expression tag	UNP A0A0A7E4R0
E	559	HIS	-	expression tag	UNP A0A0A7E4R0
E	560	HIS	-	expression tag	UNP A0A0A7E4R0
E	561	HIS	-	expression tag	UNP A0A0A7E4R0
E	562	HIS	-	expression tag	UNP A0A0A7E4R0
E	563	HIS	-	expression tag	UNP A0A0A7E4R0
I	-35	MET	-	initiating methionine	UNP A0A0A7E4R0
I	-34	LEU	-	expression tag	UNP A0A0A7E4R0
I	-33	LEU	-	expression tag	UNP A0A0A7E4R0
I	-32	VAL	-	expression tag	UNP A0A0A7E4R0
I	-31	ASN	-	expression tag	UNP A0A0A7E4R0
I	-30	GLN	-	expression tag	UNP A0A0A7E4R0
I	-29	SER	-	expression tag	UNP A0A0A7E4R0
I	-28	HIS	-	expression tag	UNP A0A0A7E4R0
I	-27	GLN	-	expression tag	UNP A0A0A7E4R0
I	-26	GLY	-	expression tag	UNP A0A0A7E4R0
I	-25	PHE	-	expression tag	UNP A0A0A7E4R0
I	-24	ASN	-	expression tag	UNP A0A0A7E4R0
I	-23	LYS	-	expression tag	UNP A0A0A7E4R0
I	-22	GLU	-	expression tag	UNP A0A0A7E4R0
I	-21	HIS	-	expression tag	UNP A0A0A7E4R0
I	-20	THR	-	expression tag	UNP A0A0A7E4R0
I	-19	SER	-	expression tag	UNP A0A0A7E4R0
I	-18	LYS	-	expression tag	UNP A0A0A7E4R0
I	-17	MET	-	expression tag	UNP A0A0A7E4R0
I	-16	VAL	-	expression tag	UNP A0A0A7E4R0
I	-15	SER	-	expression tag	UNP A0A0A7E4R0
I	-14	ALA	-	expression tag	UNP A0A0A7E4R0
I	-13	ILE	-	expression tag	UNP A0A0A7E4R0
I	-12	VAL	-	expression tag	UNP A0A0A7E4R0
I	-11	LEU	-	expression tag	UNP A0A0A7E4R0
I	-10	TYR	-	expression tag	UNP A0A0A7E4R0
I	-9	VAL	-	expression tag	UNP A0A0A7E4R0
I	-8	LEU	-	expression tag	UNP A0A0A7E4R0
I	-7	LEU	-	expression tag	UNP A0A0A7E4R0
I	-6	ALA	-	expression tag	UNP A0A0A7E4R0

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-5	ALA	-	expression tag	UNP A0A0A7E4R0
I	-4	ALA	-	expression tag	UNP A0A0A7E4R0
I	-3	ALA	-	expression tag	UNP A0A0A7E4R0
I	-2	HIS	-	expression tag	UNP A0A0A7E4R0
I	-1	SER	-	expression tag	UNP A0A0A7E4R0
I	0	ALA	-	expression tag	UNP A0A0A7E4R0
I	1	PHE	-	expression tag	UNP A0A0A7E4R0
I	2	ALA	-	expression tag	UNP A0A0A7E4R0
I	22	CYS	LEU	engineered mutation	UNP A0A0A7E4R0
I	93	PHE	TYR	engineered mutation	UNP A0A0A7E4R0
I	98	SER	ASN	engineered mutation	UNP A0A0A7E4R0
I	374	CYS	GLY	engineered mutation	UNP A0A0A7E4R0
I	504	LEU	-	expression tag	UNP A0A0A7E4R0
I	505	VAL	-	expression tag	UNP A0A0A7E4R0
I	506	PRO	-	expression tag	UNP A0A0A7E4R0
I	507	ARG	-	expression tag	UNP A0A0A7E4R0
I	508	GLY	-	expression tag	UNP A0A0A7E4R0
I	509	SER	-	expression tag	UNP A0A0A7E4R0
I	510	PRO	-	expression tag	UNP A0A0A7E4R0
I	511	GLY	-	expression tag	UNP A0A0A7E4R0
I	512	SER	-	expression tag	UNP A0A0A7E4R0
I	513	GLY	-	expression tag	UNP A0A0A7E4R0
I	514	TYR	-	expression tag	UNP A0A0A7E4R0
I	515	ILE	-	expression tag	UNP A0A0A7E4R0
I	516	PRO	-	expression tag	UNP A0A0A7E4R0
I	517	GLU	-	expression tag	UNP A0A0A7E4R0
I	518	ALA	-	expression tag	UNP A0A0A7E4R0
I	519	PRO	-	expression tag	UNP A0A0A7E4R0
I	520	ARG	-	expression tag	UNP A0A0A7E4R0
I	521	ASP	-	expression tag	UNP A0A0A7E4R0
I	522	GLY	-	expression tag	UNP A0A0A7E4R0
I	523	GLN	-	expression tag	UNP A0A0A7E4R0
I	524	ALA	-	expression tag	UNP A0A0A7E4R0
I	525	TYR	-	expression tag	UNP A0A0A7E4R0
I	526	VAL	-	expression tag	UNP A0A0A7E4R0
I	527	ARG	-	expression tag	UNP A0A0A7E4R0
I	528	LYS	-	expression tag	UNP A0A0A7E4R0
I	529	ASP	-	expression tag	UNP A0A0A7E4R0
I	530	GLY	-	expression tag	UNP A0A0A7E4R0
I	531	GLU	-	expression tag	UNP A0A0A7E4R0
I	532	TRP	-	expression tag	UNP A0A0A7E4R0
I	533	VAL	-	expression tag	UNP A0A0A7E4R0

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Chain	Residue	Modelled	Actual	Comment	Reference
I	534	LEU	-	expression tag	UNP A0A0A7E4R0
I	535	LEU	-	expression tag	UNP A0A0A7E4R0
I	536	SER	-	expression tag	UNP A0A0A7E4R0
I	537	THR	-	expression tag	UNP A0A0A7E4R0
I	538	PHE	-	expression tag	UNP A0A0A7E4R0
I	539	LEU	-	expression tag	UNP A0A0A7E4R0
I	540	GLY	-	expression tag	UNP A0A0A7E4R0
I	541	SER	-	expression tag	UNP A0A0A7E4R0
I	542	GLY	-	expression tag	UNP A0A0A7E4R0
I	543	LEU	-	expression tag	UNP A0A0A7E4R0
I	544	ASN	-	expression tag	UNP A0A0A7E4R0
I	545	ASP	-	expression tag	UNP A0A0A7E4R0
I	546	ILE	-	expression tag	UNP A0A0A7E4R0
I	547	PHE	-	expression tag	UNP A0A0A7E4R0
I	548	GLU	-	expression tag	UNP A0A0A7E4R0
I	549	ALA	-	expression tag	UNP A0A0A7E4R0
I	550	GLN	-	expression tag	UNP A0A0A7E4R0
I	551	LYS	-	expression tag	UNP A0A0A7E4R0
I	552	ILE	-	expression tag	UNP A0A0A7E4R0
I	553	GLU	-	expression tag	UNP A0A0A7E4R0
I	554	TRP	-	expression tag	UNP A0A0A7E4R0
I	555	HIS	-	expression tag	UNP A0A0A7E4R0
I	556	GLU	-	expression tag	UNP A0A0A7E4R0
I	557	GLY	-	expression tag	UNP A0A0A7E4R0
I	558	HIS	-	expression tag	UNP A0A0A7E4R0
I	559	HIS	-	expression tag	UNP A0A0A7E4R0
I	560	HIS	-	expression tag	UNP A0A0A7E4R0
I	561	HIS	-	expression tag	UNP A0A0A7E4R0
I	562	HIS	-	expression tag	UNP A0A0A7E4R0
I	563	HIS	-	expression tag	UNP A0A0A7E4R0

- Molecule 2 is a protein called Fv-clasp heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	173	Total	C	N	O	S	0	0
			1381	873	232	268	8		
2	G	173	Total	C	N	O	S	0	0
			1381	873	232	268	8		
2	K	173	Total	C	N	O	S	0	0
			1381	873	232	268	8		

- Molecule 3 is a protein called Fv-clasp light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	159	Total	C	N	O	S	0	0
			1256	793	208	249	6		
3	H	159	Total	C	N	O	S	0	0
			1256	793	208	249	6		
3	L	159	Total	C	N	O	S	0	0
			1256	793	208	249	6		

- Molecule 4 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
4	B	3	Total	C	N	O	0	0
			39	22	2	15		
4	F	3	Total	C	N	O	0	0
			39	22	2	15		
4	J	3	Total	C	N	O	0	0
			39	22	2	15		
4	M	3	Total	C	N	O	0	0
			39	22	2	15		
4	N	3	Total	C	N	O	0	0
			39	22	2	15		
4	O	3	Total	C	N	O	0	0
			39	22	2	15		

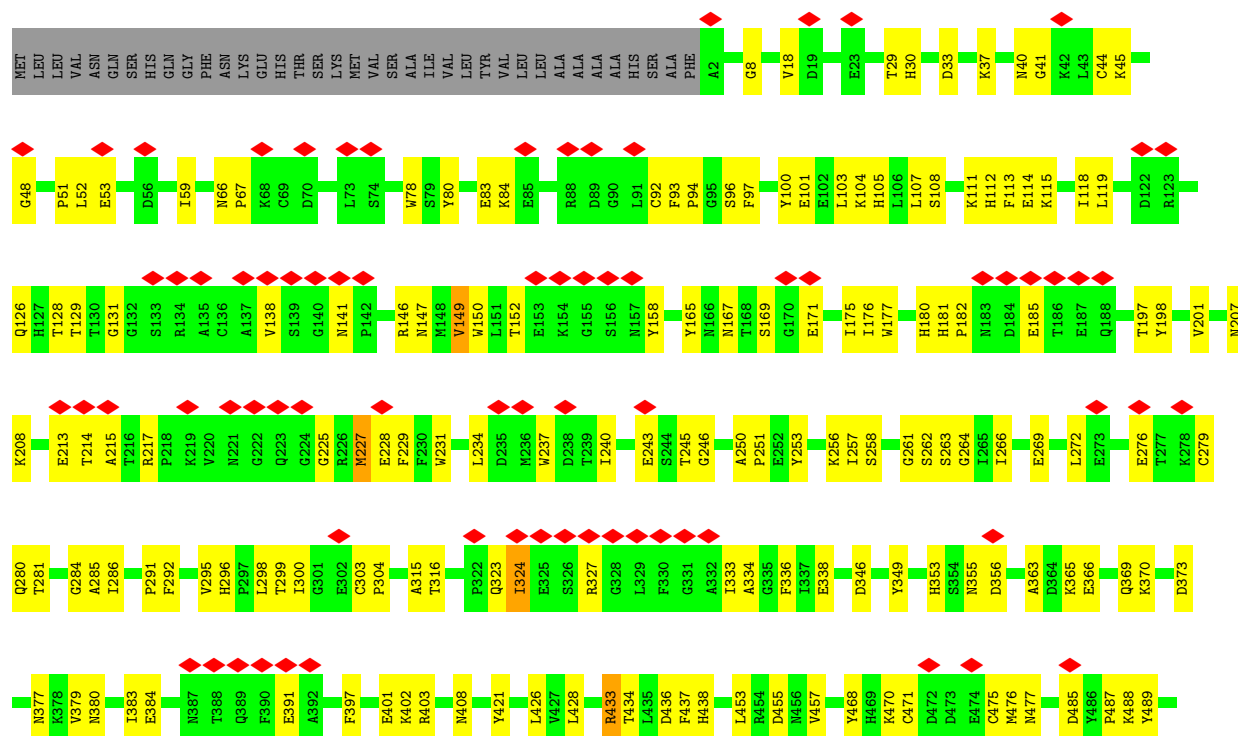
- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

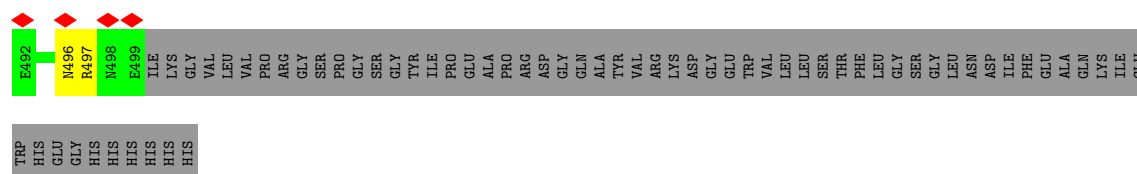


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			42	24	3	15	
5	A	1	Total	C	N	O	0
			42	24	3	15	
5	A	1	Total	C	N	O	0
			42	24	3	15	
5	E	1	Total	C	N	O	0
			42	24	3	15	
5	E	1	Total	C	N	O	0
			42	24	3	15	
5	E	1	Total	C	N	O	0
			42	24	3	15	
5	I	1	Total	C	N	O	0
			42	24	3	15	
5	I	1	Total	C	N	O	0
			42	24	3	15	
5	I	1	Total	C	N	O	0
			42	24	3	15	



- Molecule 1: Hemagglutinin

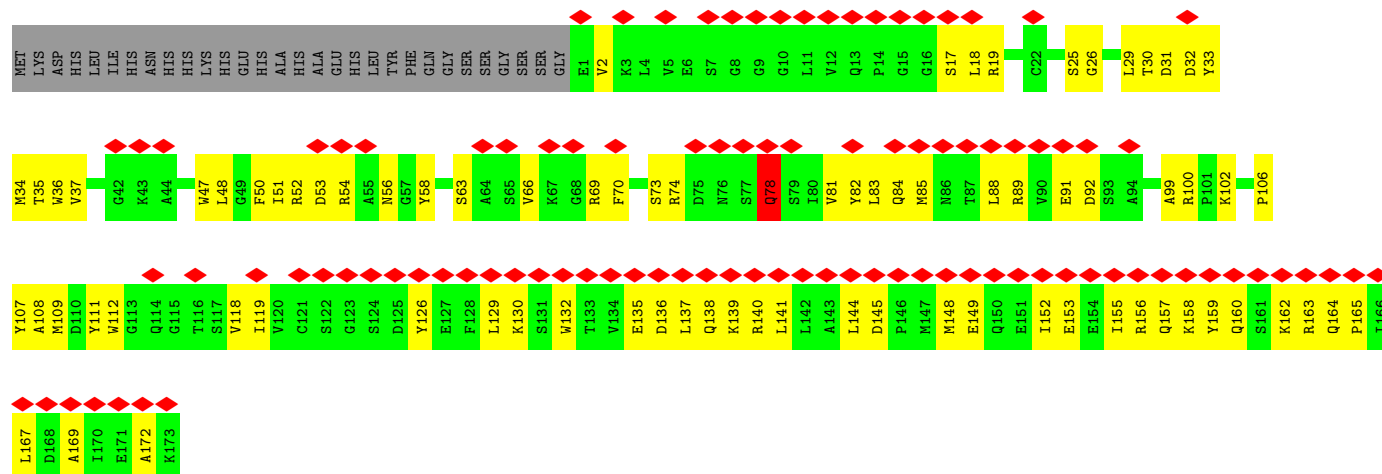




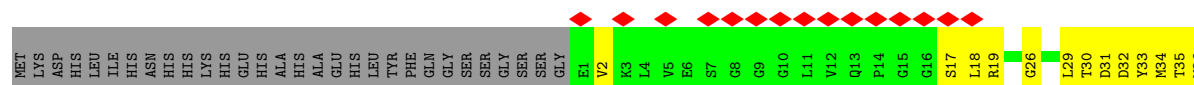
• Molecule 2: Fv-clasp heavy chain



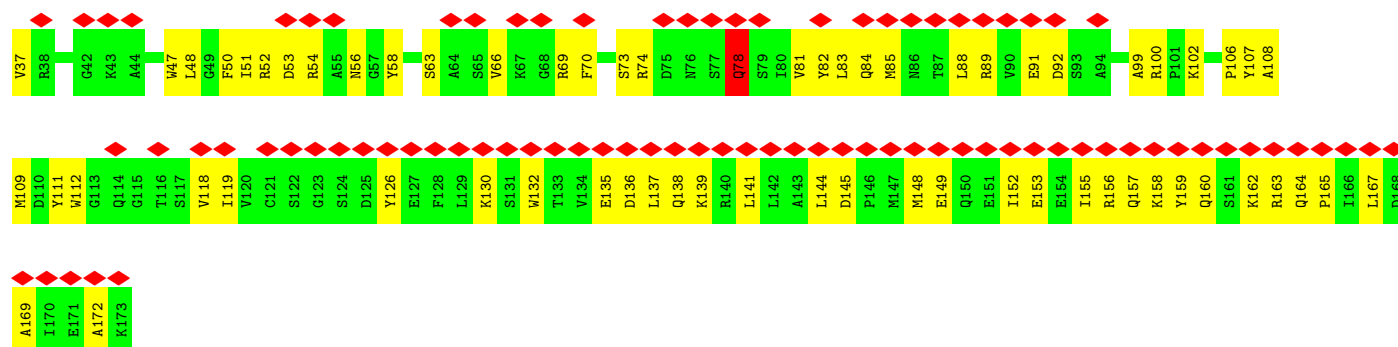
• Molecule 2: Fv-clasp heavy chain



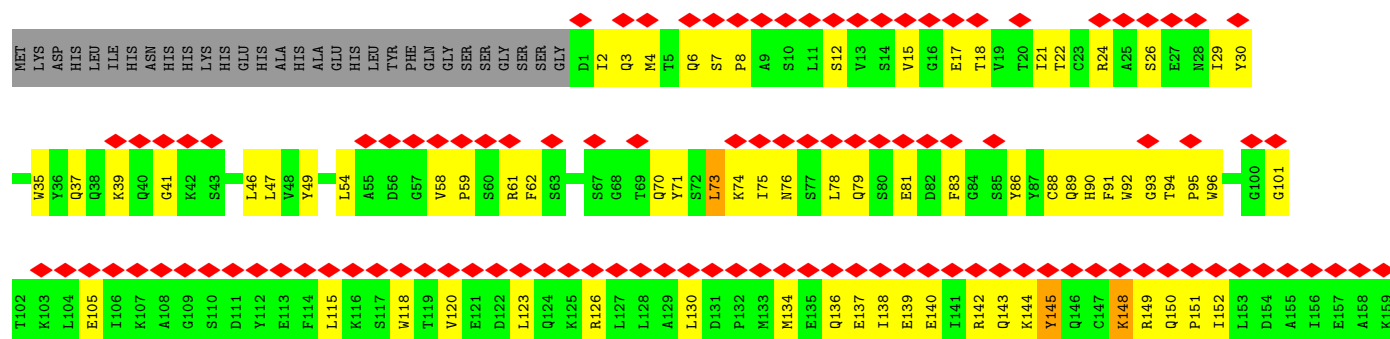
• Molecule 2: Fv-clasp heavy chain



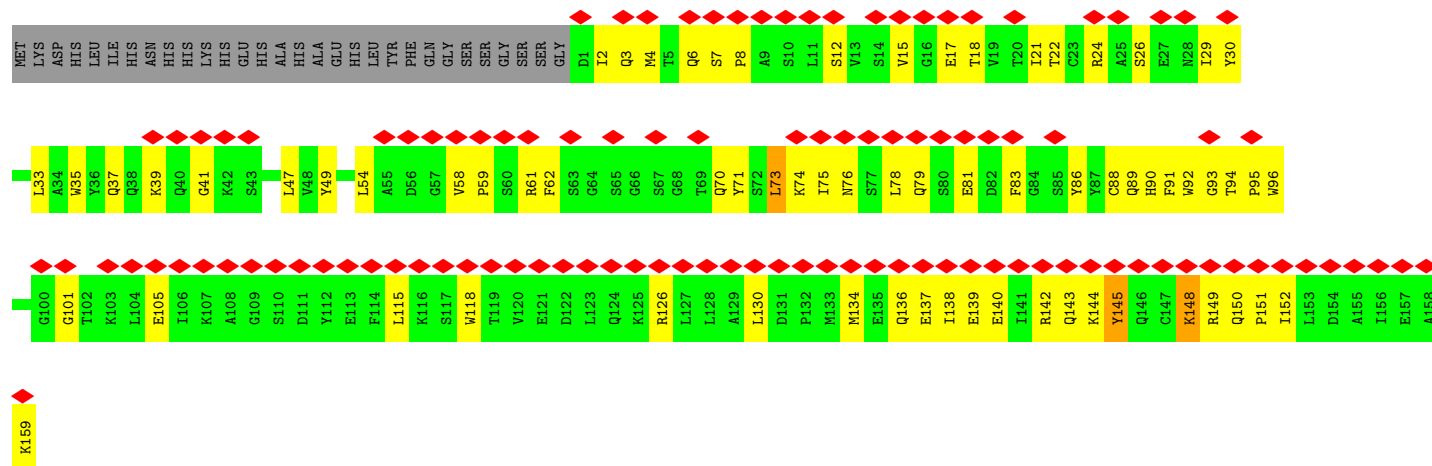




• Molecule 3: Fv-clasp light chain

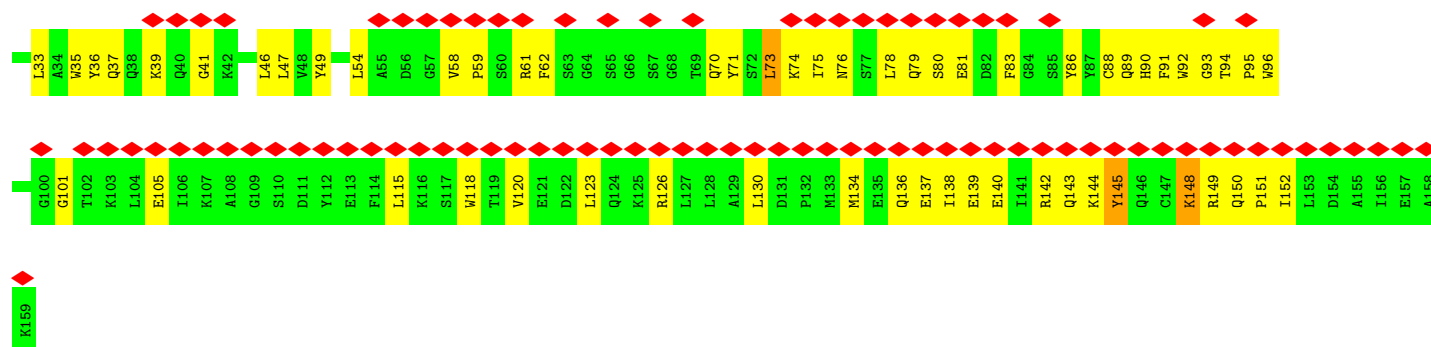


• Molecule 3: Fv-clasp light chain



• Molecule 3: Fv-clasp light chain





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



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



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



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



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





- Molecule 4: beta-D-mannopyranose-(1-4)-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, C3	Depositor
Number of particles used	52314	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.388	Depositor
Minimum map value	-0.231	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	220.5, 220.5, 220.5	wwPDB
Map dimensions	150, 150, 150	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.47, 1.47, 1.47	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.43	0/4036	0.52	0/5458
1	E	0.43	0/4036	0.52	0/5458
1	I	0.43	0/4036	0.52	0/5458
2	C	0.40	0/1411	0.59	1/1906 (0.1%)
2	G	0.39	0/1411	0.59	1/1906 (0.1%)
2	K	0.39	0/1411	0.59	1/1906 (0.1%)
3	D	0.34	0/1283	0.54	0/1734
3	H	0.34	0/1283	0.54	0/1734
3	L	0.34	0/1283	0.54	0/1734
All	All	0.41	0/20190	0.54	3/27294 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	78	GLN	CA-CB-CG	5.06	124.54	113.40
2	C	78	GLN	CA-CB-CG	5.06	124.53	113.40
2	G	78	GLN	CA-CB-CG	5.05	124.52	113.40

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	3947	0	3803	120	0
1	E	3947	0	3803	125	0
1	I	3947	0	3803	122	0
2	C	1381	0	1347	83	0
2	G	1381	0	1347	77	0
2	K	1381	0	1347	73	0
3	D	1256	0	1220	71	0
3	H	1256	0	1220	65	0
3	L	1256	0	1220	64	0
4	B	39	0	34	0	0
4	F	39	0	34	0	0
4	J	39	0	34	0	0
4	M	39	0	34	0	0
4	N	39	0	34	0	0
4	O	39	0	34	0	0
5	A	42	0	39	0	0
5	E	42	0	39	0	0
5	I	42	0	39	0	0
All	All	20112	0	19431	719	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 18.

All (719) 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:K:70:PHE:HB3	2:K:83:LEU:HD11	1.53	0.91
2:G:70:PHE:HB3	2:G:83:LEU:HD11	1.53	0.90
3:L:18:THR:HA	3:L:75:ILE:O	1.72	0.89
3:H:18:THR:HA	3:H:75:ILE:O	1.72	0.89
2:C:70:PHE:HB3	2:C:83:LEU:HD11	1.53	0.89
3:D:18:THR:HA	3:D:75:ILE:O	1.72	0.88
1:E:349:TYR:HH	1:E:438:HIS:HD1	1.14	0.88
1:I:349:TYR:HH	1:I:438:HIS:HD1	1.14	0.88
2:C:85:MET:HB3	2:C:88:LEU:HD11	1.56	0.87
2:G:85:MET:HB3	2:G:88:LEU:HD11	1.56	0.87
2:K:85:MET:HB3	2:K:88:LEU:HD11	1.56	0.87
3:L:39:LYS:NZ	3:L:81:GLU:O	2.09	0.85
2:C:137:LEU:HB3	3:D:152:ILE:HG23	1.57	0.84
3:H:39:LYS:NZ	3:H:81:GLU:O	2.09	0.84
3:D:39:LYS:NZ	3:D:81:GLU:O	2.09	0.84
1:A:349:TYR:HH	1:A:438:HIS:HD1	1.25	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:109:MET:O	2:K:112:TRP:NE1	2.12	0.82
2:G:137:LEU:HB3	3:H:152:ILE:HG23	1.60	0.81
2:G:109:MET:O	2:G:112:TRP:NE1	2.12	0.81
2:C:109:MET:O	2:C:112:TRP:NE1	2.12	0.80
1:A:349:TYR:OH	1:A:438:HIS:ND1	2.14	0.79
1:I:355:ASN:OD1	1:I:356:ASP:N	2.18	0.77
2:C:148:MET:HG3	3:D:145:TYR:CD2	2.21	0.76
2:K:78:GLN:N	2:K:78:GLN:OE1	2.20	0.75
3:H:6:GLN:NE2	3:H:88:CYS:SG	2.57	0.75
1:A:355:ASN:OD1	1:A:356:ASP:N	2.19	0.75
2:C:78:GLN:OE1	2:C:78:GLN:N	2.20	0.75
2:C:141:LEU:HD13	3:D:149:ARG:HD2	1.69	0.74
1:A:379:VAL:O	1:A:383:ILE:HG12	1.88	0.74
1:E:379:VAL:O	1:E:383:ILE:HG12	1.87	0.74
1:I:379:VAL:O	1:I:383:ILE:HG12	1.87	0.74
2:C:17:SER:HA	2:C:85:MET:O	1.88	0.74
1:A:128:THR:OG1	1:A:152:THR:OG1	2.06	0.74
3:H:18:THR:HG22	3:H:76:ASN:HA	1.69	0.74
2:G:78:GLN:N	2:G:78:GLN:OE1	2.20	0.73
2:K:17:SER:HA	2:K:85:MET:O	1.88	0.73
3:L:18:THR:HG22	3:L:76:ASN:HA	1.69	0.73
2:G:17:SER:HA	2:G:85:MET:O	1.88	0.73
1:I:128:THR:OG1	1:I:152:THR:OG1	2.06	0.73
1:E:128:THR:OG1	1:E:152:THR:OG1	2.06	0.73
3:D:18:THR:HG22	3:D:76:ASN:HA	1.69	0.73
1:I:433:ARG:NE	1:I:433:ARG:HA	2.04	0.73
3:D:7:SER:OG	3:D:24:ARG:NH2	2.22	0.72
3:H:7:SER:OG	3:H:24:ARG:NH2	2.22	0.72
3:L:7:SER:OG	3:L:24:ARG:NH2	2.22	0.72
1:E:355:ASN:OD1	1:E:356:ASP:N	2.19	0.72
1:E:433:ARG:HA	1:E:433:ARG:NE	2.04	0.72
1:I:349:TYR:OH	1:I:438:HIS:ND1	2.14	0.72
1:A:433:ARG:HA	1:A:433:ARG:NE	2.04	0.72
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.72	0.72
1:I:111:LYS:HD2	1:I:261:GLY:HA3	1.72	0.71
3:H:37:GLN:HB2	3:H:47:LEU:HD11	1.72	0.71
1:E:111:LYS:HD2	1:E:261:GLY:HA3	1.72	0.71
1:A:111:LYS:HD2	1:A:261:GLY:HA3	1.72	0.70
3:D:6:GLN:NE2	3:D:88:CYS:SG	2.57	0.70
3:D:37:GLN:HB2	3:D:47:LEU:HD11	1.72	0.70
2:K:51:ILE:HG23	2:K:74:ARG:HH21	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:153:GLU:O	2:C:157:GLN:NE2	2.26	0.69
2:K:153:GLU:O	2:K:157:GLN:NE2	2.26	0.69
2:C:51:ILE:HG23	2:C:74:ARG:HH21	1.57	0.69
3:L:6:GLN:NE2	3:L:88:CYS:SG	2.57	0.69
2:G:51:ILE:HG23	2:G:74:ARG:HH21	1.57	0.69
2:C:69:ARG:NH1	2:C:92:ASP:OD2	2.21	0.69
2:K:148:MET:HG3	3:L:145:TYR:CD2	2.27	0.69
2:C:144:LEU:HD22	3:D:149:ARG:HH21	1.56	0.68
2:G:153:GLU:O	2:G:157:GLN:NE2	2.26	0.68
1:A:401:GLU:OE1	1:I:403:ARG:NH1	2.26	0.68
3:H:78:LEU:HD21	3:H:83:PHE:HE1	1.59	0.68
1:E:217:ARG:HE	1:I:207:ASN:HD21	1.42	0.68
3:L:17:GLU:HG3	3:L:18:THR:H	1.58	0.68
3:D:17:GLU:HG3	3:D:18:THR:H	1.58	0.67
3:D:78:LEU:HD21	3:D:83:PHE:HE1	1.59	0.67
1:E:349:TYR:OH	1:E:438:HIS:ND1	2.14	0.67
2:K:69:ARG:NH1	2:K:92:ASP:OD2	2.21	0.67
3:L:78:LEU:HD21	3:L:83:PHE:HE1	1.59	0.67
1:E:215:ALA:O	1:E:217:ARG:NH1	2.27	0.67
1:A:197:THR:HG23	1:A:245:THR:HG23	1.76	0.67
1:E:197:THR:HG23	1:E:245:THR:HG23	1.76	0.67
3:H:17:GLU:HG3	3:H:18:THR:H	1.58	0.67
2:G:152:ILE:HD11	3:H:138:ILE:HG23	1.76	0.67
1:I:112:HIS:HB3	1:I:258:SER:HB3	1.77	0.67
1:A:215:ALA:O	1:A:217:ARG:NH1	2.27	0.67
1:A:217:ARG:HE	1:E:207:ASN:HD21	1.42	0.67
2:K:153:GLU:HB3	2:K:157:GLN:HE22	1.60	0.67
1:A:113:PHE:HE1	1:A:257:ILE:HG22	1.60	0.66
2:C:153:GLU:HB3	2:C:157:GLN:HE22	1.60	0.66
1:E:112:HIS:HB3	1:E:258:SER:HB3	1.77	0.66
1:I:215:ALA:O	1:I:217:ARG:NH1	2.28	0.66
1:A:112:HIS:HB3	1:A:258:SER:HB3	1.77	0.66
1:A:403:ARG:NH1	1:E:401:GLU:OE1	2.28	0.66
2:G:160:GLN:OE1	2:G:163:ARG:NH2	2.28	0.66
2:G:145:ASP:O	2:G:148:MET:HB3	1.96	0.66
1:A:207:ASN:HD21	1:I:217:ARG:HE	1.41	0.66
1:A:274:ASN:O	1:A:274:ASN:ND2	2.29	0.66
2:C:126:TYR:HB2	2:C:130:LYS:HG2	1.78	0.66
2:G:69:ARG:NH1	2:G:92:ASP:OD2	2.21	0.66
2:G:153:GLU:HB3	2:G:157:GLN:HE22	1.60	0.66
1:I:197:THR:HG23	1:I:245:THR:HG23	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:145:ASP:O	2:C:148:MET:HB3	1.96	0.66
1:I:213:GLU:O	1:I:217:ARG:NH2	2.30	0.66
2:K:152:ILE:HG23	2:K:156:ARG:HH21	1.61	0.66
1:E:403:ARG:NH1	1:I:401:GLU:OE1	2.28	0.65
1:A:40:ASN:HD21	1:A:285:ALA:HB3	1.62	0.65
2:C:160:GLN:OE1	2:C:163:ARG:NH2	2.28	0.65
1:I:113:PHE:HE1	1:I:257:ILE:HG22	1.60	0.65
2:K:160:GLN:OE1	2:K:163:ARG:NH2	2.28	0.65
2:K:145:ASP:O	2:K:148:MET:HB3	1.96	0.65
2:K:126:TYR:HB2	2:K:130:LYS:HG2	1.78	0.65
2:K:164:GLN:HA	2:K:167:LEU:HD13	1.79	0.65
2:C:152:ILE:HG23	2:C:156:ARG:HH21	1.61	0.65
2:C:164:GLN:HA	2:C:167:LEU:HD13	1.79	0.65
2:G:126:TYR:HB2	2:G:130:LYS:HG2	1.78	0.65
1:E:213:GLU:O	1:E:217:ARG:NH2	2.30	0.65
2:G:152:ILE:HG23	2:G:156:ARG:HH21	1.61	0.65
1:A:213:GLU:O	1:A:217:ARG:NH2	2.30	0.64
2:C:148:MET:HG3	3:D:145:TYR:HD2	1.61	0.64
2:G:164:GLN:HA	2:G:167:LEU:HD13	1.79	0.64
1:I:40:ASN:HD21	1:I:285:ALA:HB3	1.62	0.64
3:D:29:ILE:O	3:D:71:TYR:OH	2.16	0.64
1:E:40:ASN:HD21	1:E:285:ALA:HB3	1.62	0.64
1:E:113:PHE:HE1	1:E:257:ILE:HG22	1.60	0.64
3:D:140:GLU:OE1	3:D:143:GLN:NE2	2.31	0.64
2:C:58:TYR:CE2	2:C:74:ARG:HD2	2.33	0.63
2:G:58:TYR:CE2	2:G:74:ARG:HD2	2.33	0.63
3:L:140:GLU:OE1	3:L:143:GLN:NE2	2.31	0.63
3:H:140:GLU:OE1	3:H:143:GLN:NE2	2.31	0.63
2:K:58:TYR:CE2	2:K:74:ARG:HD2	2.33	0.63
1:E:323:GLN:HE22	1:E:334:ALA:HB3	1.64	0.63
1:E:18:VAL:HG21	1:E:315:ALA:HB2	1.80	0.63
3:H:22:THR:HB	3:H:24:ARG:HH12	1.64	0.63
1:E:291:PRO:HB3	1:E:383:ILE:HD12	1.81	0.63
3:H:29:ILE:O	3:H:71:TYR:OH	2.16	0.62
1:I:18:VAL:HG21	1:I:315:ALA:HB2	1.80	0.62
1:I:291:PRO:HB3	1:I:383:ILE:HD12	1.81	0.62
3:L:22:THR:HB	3:L:24:ARG:HH12	1.64	0.62
1:A:291:PRO:HB3	1:A:383:ILE:HD12	1.81	0.62
1:E:286:ILE:HD11	1:E:295:VAL:HG21	1.81	0.62
2:K:119:ILE:HD13	3:L:143:GLN:OE1	1.98	0.62
3:D:22:THR:HB	3:D:24:ARG:HH12	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:29:ILE:O	3:L:71:TYR:OH	2.16	0.62
2:C:152:ILE:HD11	3:D:138:ILE:HG23	1.81	0.62
1:I:323:GLN:HE22	1:I:334:ALA:HB3	1.64	0.62
1:A:323:GLN:HE22	1:A:334:ALA:HB3	1.64	0.62
1:A:18:VAL:HG21	1:A:315:ALA:HB2	1.80	0.62
1:A:286:ILE:HD11	1:A:295:VAL:HG21	1.81	0.62
1:E:167:ASN:HB3	1:E:237:TRP:HA	1.81	0.62
2:K:106:PRO:HB3	3:L:96:TRP:CH2	2.34	0.62
3:L:29:ILE:HG22	3:L:92:TRP:HB3	1.82	0.62
1:E:215:ALA:H	1:E:217:ARG:HH12	1.48	0.61
2:G:148:MET:HG3	3:H:145:TYR:CD2	2.35	0.61
2:C:37:VAL:HG23	2:C:47:TRP:HA	1.83	0.61
2:C:50:PHE:HZ	3:D:96:TRP:CZ2	2.17	0.61
3:D:29:ILE:HG22	3:D:92:TRP:HB3	1.82	0.61
2:K:37:VAL:HG23	2:K:47:TRP:HA	1.83	0.61
1:I:215:ALA:H	1:I:217:ARG:HH12	1.48	0.61
1:I:286:ILE:HD11	1:I:295:VAL:HG21	1.81	0.61
1:A:167:ASN:HB3	1:A:237:TRP:HA	1.81	0.61
1:A:215:ALA:H	1:A:217:ARG:HH12	1.48	0.61
1:I:167:ASN:HB3	1:I:237:TRP:HA	1.81	0.61
1:A:158:TYR:CZ	1:A:246:GLY:HA2	2.36	0.60
1:A:115:LYS:NZ	1:A:147:ASN:HD21	1.99	0.60
2:G:37:VAL:HG23	2:G:47:TRP:HA	1.83	0.60
1:I:158:TYR:CZ	1:I:246:GLY:HA2	2.36	0.60
3:H:94:THR:OG1	3:H:95:PRO:HD3	2.01	0.60
1:I:115:LYS:NZ	1:I:147:ASN:HD21	1.99	0.60
3:L:94:THR:OG1	3:L:95:PRO:HD3	2.01	0.60
1:E:48:GLY:N	1:E:276:GLU:OE2	2.30	0.60
1:A:434:THR:O	1:A:437:PHE:HB3	2.02	0.60
1:E:115:LYS:NZ	1:E:147:ASN:HD21	1.99	0.60
2:K:31:ASP:HA	2:K:100:ARG:HE	1.66	0.60
3:H:29:ILE:HG22	3:H:92:TRP:HB3	1.82	0.60
1:I:434:THR:O	1:I:437:PHE:HB3	2.02	0.60
1:E:263:SER:OG	1:E:264:GLY:N	2.34	0.60
1:E:158:TYR:CZ	1:E:246:GLY:HA2	2.36	0.60
3:D:89:GLN:HE21	3:D:96:TRP:HB3	1.67	0.59
2:C:144:LEU:HB3	3:D:149:ARG:NH2	2.17	0.59
3:H:4:MET:SD	3:H:90:HIS:ND1	2.75	0.59
3:L:89:GLN:HE21	3:L:96:TRP:HB3	1.67	0.59
3:L:35:TRP:CH2	3:L:88:CYS:HB3	2.38	0.59
2:C:31:ASP:HA	2:C:100:ARG:HE	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4:MET:SD	3:D:90:HIS:ND1	2.75	0.59
3:H:35:TRP:CH2	3:H:88:CYS:HB3	2.38	0.59
1:I:263:SER:OG	1:I:264:GLY:N	2.34	0.59
3:L:4:MET:SD	3:L:90:HIS:ND1	2.75	0.59
3:H:24:ARG:NH1	3:H:70:GLN:OE1	2.34	0.59
1:I:373:ASP:O	1:I:377:ASN:ND2	2.32	0.59
2:K:137:LEU:HB3	3:L:152:ILE:HG23	1.84	0.59
3:H:89:GLN:HE21	3:H:96:TRP:HB3	1.67	0.59
3:D:35:TRP:CH2	3:D:88:CYS:HB3	2.38	0.59
2:G:31:ASP:HA	2:G:100:ARG:HE	1.66	0.59
3:D:24:ARG:NH1	3:D:70:GLN:OE1	2.35	0.59
1:E:434:THR:O	1:E:437:PHE:HB3	2.02	0.58
2:C:152:ILE:HD13	3:D:142:ARG:NH1	2.18	0.58
2:G:163:ARG:HG2	3:H:130:LEU:HD11	1.84	0.58
3:D:94:THR:OG1	3:D:95:PRO:HD3	2.01	0.58
1:A:468:TYR:O	1:A:496:ASN:ND2	2.37	0.58
1:A:263:SER:OG	1:A:264:GLY:N	2.34	0.58
1:I:48:GLY:N	1:I:276:GLU:OE2	2.30	0.58
2:C:132:TRP:HB3	2:C:136:ASP:HB3	1.86	0.57
2:K:51:ILE:HG21	2:K:81:VAL:HG21	1.86	0.57
1:A:266:ILE:HD11	1:A:300:ILE:HD12	1.87	0.57
1:I:468:TYR:O	1:I:496:ASN:ND2	2.37	0.57
1:E:436:ASP:OD1	1:E:437:PHE:N	2.38	0.57
2:K:132:TRP:HB3	2:K:136:ASP:HB3	1.86	0.57
1:A:397:PHE:HE2	1:A:408:ASN:HD22	1.52	0.57
2:C:51:ILE:HG21	2:C:81:VAL:HG21	1.86	0.57
1:I:266:ILE:HD11	1:I:300:ILE:HD12	1.87	0.57
1:I:436:ASP:OD1	1:I:437:PHE:N	2.38	0.57
2:C:32:ASP:O	2:C:52:ARG:HA	2.05	0.56
3:L:139:GLU:HA	3:L:142:ARG:HB2	1.87	0.56
1:A:436:ASP:OD1	1:A:437:PHE:N	2.38	0.56
2:G:51:ILE:HG21	2:G:81:VAL:HG21	1.86	0.56
3:L:29:ILE:O	3:L:29:ILE:HG13	2.04	0.56
2:C:50:PHE:HZ	3:D:96:TRP:CE2	2.23	0.56
3:D:29:ILE:O	3:D:29:ILE:HG13	2.04	0.56
2:G:32:ASP:O	2:G:52:ARG:HA	2.05	0.56
2:G:132:TRP:HB3	2:G:136:ASP:HB3	1.86	0.56
2:K:53:ASP:OD2	2:K:54:ARG:N	2.34	0.56
3:L:24:ARG:NH1	3:L:70:GLN:OE1	2.35	0.56
1:E:397:PHE:HE2	1:E:408:ASN:HD22	1.52	0.56
1:I:397:PHE:HE2	1:I:408:ASN:HD22	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:468:TYR:O	1:E:496:ASN:ND2	2.37	0.56
3:H:29:ILE:O	3:H:29:ILE:HG13	2.04	0.56
2:C:53:ASP:OD2	2:C:54:ARG:N	2.34	0.56
3:H:126:ARG:O	3:H:130:LEU:HB2	2.06	0.56
3:H:139:GLU:HA	3:H:142:ARG:HB2	1.87	0.56
2:K:32:ASP:O	2:K:52:ARG:HA	2.05	0.56
1:E:266:ILE:HD11	1:E:300:ILE:HD12	1.87	0.56
1:A:323:GLN:CD	1:A:327:ARG:HH22	2.10	0.56
3:D:126:ARG:O	3:D:130:LEU:HB2	2.06	0.56
3:L:126:ARG:O	3:L:130:LEU:HB2	2.06	0.56
2:G:106:PRO:HB3	3:H:96:TRP:CH2	2.41	0.55
1:A:113:PHE:CE1	1:A:257:ILE:HG22	2.41	0.55
1:E:323:GLN:HG2	1:E:324:ILE:H	1.72	0.55
2:G:163:ARG:HD2	3:H:130:LEU:HD21	1.89	0.55
1:E:373:ASP:O	1:E:377:ASN:ND2	2.32	0.55
1:E:323:GLN:CD	1:E:327:ARG:HH22	2.10	0.55
1:A:33:ASP:OD2	1:A:37:LYS:NZ	2.39	0.55
1:I:33:ASP:OD2	1:I:37:LYS:NZ	2.39	0.55
1:A:262:SER:HB3	1:A:391:GLU:HG2	1.89	0.55
1:I:113:PHE:CE1	1:I:257:ILE:HG22	2.41	0.55
1:A:213:GLU:N	1:A:213:GLU:OE2	2.40	0.55
2:C:70:PHE:CE1	2:C:85:MET:HG2	2.42	0.55
3:D:139:GLU:HA	3:D:142:ARG:HB2	1.87	0.55
1:E:33:ASP:OD2	1:E:37:LYS:NZ	2.39	0.55
2:G:70:PHE:CE1	2:G:85:MET:HG2	2.42	0.55
2:K:70:PHE:CE1	2:K:85:MET:HG2	2.42	0.55
2:G:144:LEU:HD22	3:H:149:ARG:HH21	1.72	0.54
1:I:213:GLU:N	1:I:213:GLU:OE2	2.40	0.54
1:I:215:ALA:H	1:I:217:ARG:NH1	2.05	0.54
1:A:48:GLY:N	1:A:276:GLU:OE2	2.30	0.54
1:A:176:ILE:O	1:A:251:PRO:HB3	2.08	0.54
1:E:147:ASN:HA	1:E:253:TYR:HD1	1.72	0.54
1:I:105:HIS:O	1:I:108:SER:OG	2.22	0.54
1:I:296:HIS:CE1	1:I:298:LEU:HD12	2.42	0.54
1:E:215:ALA:H	1:E:217:ARG:NH1	2.05	0.54
1:I:176:ILE:O	1:I:251:PRO:HB3	2.08	0.54
1:I:323:GLN:HG2	1:I:324:ILE:H	1.72	0.54
1:I:323:GLN:CD	1:I:327:ARG:HH22	2.10	0.54
2:C:108:ALA:HB2	3:D:49:TYR:HB3	1.90	0.54
1:E:176:ILE:O	1:E:251:PRO:HB3	2.08	0.54
1:A:323:GLN:HG2	1:A:324:ILE:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ASP:O	1:A:377:ASN:ND2	2.32	0.54
2:C:66:VAL:HG12	2:C:66:VAL:O	2.08	0.54
1:E:262:SER:HB3	1:E:391:GLU:HG2	1.89	0.54
1:E:296:HIS:CE1	1:E:298:LEU:HD12	2.43	0.54
1:I:147:ASN:HA	1:I:253:TYR:HD1	1.73	0.54
2:K:144:LEU:HD22	3:L:149:ARG:HH21	1.71	0.54
1:I:97:PHE:CZ	1:I:176:ILE:HD11	2.43	0.54
2:G:53:ASP:OD2	2:G:54:ARG:N	2.34	0.54
1:I:262:SER:HB3	1:I:391:GLU:HG2	1.89	0.54
1:E:213:GLU:OE2	1:E:213:GLU:N	2.40	0.53
1:I:44:CYS:H	1:I:280:GLN:NE2	2.06	0.53
2:K:66:VAL:HG12	2:K:66:VAL:O	2.08	0.53
1:A:296:HIS:CE1	1:A:298:LEU:HD12	2.43	0.53
1:E:44:CYS:H	1:E:280:GLN:NE2	2.07	0.53
1:E:323:GLN:NE2	1:E:334:ALA:HB3	2.23	0.53
1:A:281:THR:OG1	1:A:284:GLY:O	2.22	0.53
1:I:323:GLN:NE2	1:I:334:ALA:HB3	2.23	0.53
1:A:44:CYS:H	1:A:280:GLN:NE2	2.07	0.53
1:A:147:ASN:HA	1:A:253:TYR:HD1	1.72	0.53
1:A:215:ALA:H	1:A:217:ARG:NH1	2.05	0.53
2:C:141:LEU:HA	3:D:149:ARG:NH1	2.23	0.53
1:E:234:LEU:HD21	1:E:240:ILE:HB	1.91	0.53
1:I:234:LEU:HD21	1:I:240:ILE:HB	1.91	0.53
2:C:163:ARG:HG2	3:D:130:LEU:HD11	1.90	0.53
1:E:113:PHE:CE1	1:E:257:ILE:HG22	2.41	0.53
2:K:50:PHE:HZ	3:L:96:TRP:CE2	2.26	0.53
1:A:97:PHE:CZ	1:A:176:ILE:HD11	2.43	0.53
1:E:97:PHE:CZ	1:E:176:ILE:HD11	2.43	0.53
2:G:66:VAL:HG12	2:G:66:VAL:O	2.08	0.53
1:I:52:LEU:HD12	1:I:78:TRP:CE3	2.44	0.53
1:I:369:GLN:HG3	3:L:49:TYR:CE1	2.43	0.53
1:A:52:LEU:HD12	1:A:78:TRP:CE3	2.44	0.53
1:A:66:ASN:HD21	1:A:92:CYS:H	1.57	0.53
1:E:51:PRO:HB3	1:E:80:TYR:CE1	2.44	0.53
1:E:66:ASN:HD21	1:E:92:CYS:H	1.57	0.53
2:G:140:ARG:NH2	3:H:152:ILE:HG13	2.24	0.53
1:I:51:PRO:HB3	1:I:80:TYR:CE1	2.44	0.53
1:A:323:GLN:NE2	1:A:334:ALA:HB3	2.23	0.53
1:E:353:HIS:HB2	1:E:476:MET:HE2	1.91	0.53
1:E:8:GLY:HA2	1:E:336:PHE:HB3	1.91	0.53
1:A:8:GLY:HA2	1:A:336:PHE:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:PRO:HG3	1:A:146:ARG:HH12	1.74	0.52
1:A:138:VAL:HG23	1:A:141:ASN:HB2	1.91	0.52
1:A:234:LEU:HD21	1:A:240:ILE:HB	1.91	0.52
1:E:52:LEU:HD12	1:E:78:TRP:CE3	2.44	0.52
1:E:353:HIS:HB2	1:E:476:MET:CE	2.39	0.52
1:I:181:HIS:O	1:I:225:GLY:CA	2.57	0.52
1:A:51:PRO:HB3	1:A:80:TYR:CE1	2.44	0.52
3:D:59:PRO:HG2	3:D:62:PHE:CD2	2.45	0.52
2:C:163:ARG:HD2	3:D:130:LEU:HD21	1.90	0.52
1:E:181:HIS:O	1:E:225:GLY:CA	2.57	0.52
1:A:181:HIS:O	1:A:225:GLY:CA	2.57	0.52
1:I:67:PRO:HG3	1:I:146:ARG:HH12	1.74	0.52
1:I:353:HIS:HB2	1:I:476:MET:CE	2.39	0.52
1:A:353:HIS:HB2	1:A:476:MET:CE	2.39	0.52
1:E:138:VAL:HG23	1:E:141:ASN:HB2	1.91	0.52
3:H:59:PRO:HG2	3:H:62:PHE:CD2	2.45	0.52
1:E:67:PRO:HG3	1:E:146:ARG:HH12	1.74	0.52
3:D:86:TYR:O	3:D:101:GLY:HA2	2.10	0.52
1:E:97:PHE:HB3	1:E:100:TYR:HD2	1.75	0.52
1:E:100:TYR:CE1	1:E:104:LYS:HD2	2.45	0.52
1:I:66:ASN:HD21	1:I:92:CYS:H	1.57	0.52
1:I:281:THR:OG1	1:I:284:GLY:O	2.22	0.52
1:A:353:HIS:HB2	1:A:476:MET:HE2	1.92	0.51
2:C:70:PHE:CD1	2:C:85:MET:HA	2.45	0.51
1:E:97:PHE:HZ	1:E:176:ILE:HD11	1.75	0.51
1:I:100:TYR:CE1	1:I:104:LYS:HD2	2.45	0.51
1:A:97:PHE:HZ	1:A:176:ILE:HD11	1.75	0.51
2:G:148:MET:HG3	3:H:145:TYR:HD2	1.74	0.51
1:I:8:GLY:HA2	1:I:336:PHE:HB3	1.91	0.51
2:K:70:PHE:CD1	2:K:85:MET:HA	2.45	0.51
3:H:41:GLY:HA2	3:H:136:GLN:OE1	2.10	0.51
3:H:86:TYR:O	3:H:101:GLY:HA2	2.10	0.51
1:A:100:TYR:CE1	1:A:104:LYS:HD2	2.45	0.51
1:I:138:VAL:HG23	1:I:141:ASN:HB2	1.91	0.51
1:A:380:ASN:O	1:A:384:GLU:HG2	2.11	0.51
2:G:152:ILE:O	2:G:155:ILE:HG22	2.11	0.51
1:I:29:THR:O	1:I:30:HIS:ND1	2.44	0.51
1:A:29:THR:O	1:A:30:HIS:ND1	2.44	0.51
1:E:453:LEU:HD13	1:E:457:VAL:HG11	1.93	0.51
1:I:97:PHE:HZ	1:I:176:ILE:HD11	1.75	0.51
1:A:346:ASP:O	2:C:107:TYR:OH	2.16	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:86:TYR:O	3:L:101:GLY:HA2	2.10	0.51
2:G:70:PHE:CD1	2:G:85:MET:HA	2.45	0.51
2:C:152:ILE:O	2:C:155:ILE:HG22	2.11	0.50
3:D:41:GLY:HA2	3:D:136:GLN:OE1	2.10	0.50
3:D:90:HIS:C	3:D:91:PHE:HD1	2.15	0.50
1:I:97:PHE:HB3	1:I:100:TYR:HD2	1.75	0.50
3:L:41:GLY:HA2	3:L:136:GLN:OE1	2.10	0.50
3:L:59:PRO:HG2	3:L:62:PHE:CD2	2.45	0.50
1:E:29:THR:O	1:E:30:HIS:ND1	2.44	0.50
1:E:380:ASN:O	1:E:384:GLU:HG2	2.11	0.50
2:K:152:ILE:O	2:K:155:ILE:HG22	2.11	0.50
1:A:97:PHE:HB3	1:A:100:TYR:HD2	1.75	0.50
1:I:380:ASN:O	1:I:384:GLU:HG2	2.11	0.50
1:E:185:GLU:OE2	1:E:214:THR:OG1	2.29	0.50
1:E:227:MET:HB3	1:E:229:PHE:CE1	2.47	0.50
1:I:227:MET:HB3	1:I:229:PHE:CE1	2.47	0.50
3:L:35:TRP:CZ3	3:L:88:CYS:HB3	2.47	0.50
1:A:66:ASN:ND2	1:A:92:CYS:SG	2.85	0.50
1:I:66:ASN:ND2	1:I:92:CYS:SG	2.85	0.50
1:A:453:LEU:HD13	1:A:457:VAL:HG11	1.93	0.50
3:D:35:TRP:CZ3	3:D:88:CYS:HB3	2.47	0.50
1:I:185:GLU:OE2	1:I:214:THR:OG1	2.29	0.50
3:H:35:TRP:CZ3	3:H:88:CYS:HB3	2.47	0.49
1:A:227:MET:HB3	1:A:229:PHE:CE1	2.47	0.49
1:E:66:ASN:ND2	1:E:92:CYS:SG	2.85	0.49
3:H:90:HIS:C	3:H:91:PHE:HD1	2.15	0.49
1:A:185:GLU:OE2	1:A:214:THR:OG1	2.29	0.49
2:C:152:ILE:HG21	3:D:142:ARG:HH22	1.78	0.49
1:E:45:LYS:NZ	1:E:276:GLU:OE1	2.38	0.49
1:I:453:LEU:HD13	1:I:457:VAL:HG11	1.93	0.49
3:L:90:HIS:C	3:L:91:PHE:HD1	2.15	0.49
2:K:109:MET:N	3:L:36:TYR:OH	2.36	0.49
1:E:281:THR:OG1	1:E:284:GLY:O	2.22	0.49
2:C:50:PHE:CZ	3:D:96:TRP:CZ2	3.01	0.49
1:E:118:ILE:HD13	1:E:175:ILE:HD12	1.95	0.48
2:G:152:ILE:HD13	3:H:142:ARG:NH1	2.28	0.48
1:A:118:ILE:HD13	1:A:175:ILE:HD12	1.95	0.48
1:A:365:LYS:HG3	2:C:107:TYR:CE1	2.49	0.48
3:H:3:GLN:H	3:H:26:SER:HB3	1.78	0.48
1:I:118:ILE:HD13	1:I:175:ILE:HD12	1.95	0.48
1:I:365:LYS:HG3	2:K:107:TYR:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:TYR:HB3	1:A:240:ILE:HG22	1.96	0.48
2:C:36:TRP:O	2:C:48:LEU:HB2	2.13	0.48
1:A:316:THR:HG21	2:C:29:LEU:HD11	1.94	0.48
1:A:333:ILE:HG13	1:A:334:ALA:H	1.79	0.48
1:I:353:HIS:HB2	1:I:476:MET:HE2	1.96	0.48
1:E:316:THR:HG21	2:G:29:LEU:HD11	1.94	0.48
1:I:333:ILE:HG13	1:I:334:ALA:H	1.79	0.48
3:L:3:GLN:H	3:L:26:SER:HB3	1.78	0.48
2:C:163:ARG:HD3	3:D:134:MET:HE1	1.95	0.48
3:D:3:GLN:H	3:D:26:SER:HB3	1.78	0.48
1:E:165:TYR:HB3	1:E:240:ILE:HG22	1.96	0.48
1:E:333:ILE:HG13	1:E:334:ALA:H	1.79	0.48
1:E:471:CYS:SG	1:E:476:MET:HG3	2.54	0.48
1:I:177:TRP:CE2	1:I:201:VAL:HG21	2.49	0.48
1:I:471:CYS:SG	1:I:476:MET:HG3	2.54	0.48
1:A:105:HIS:O	1:A:108:SER:OG	2.22	0.48
1:A:118:ILE:HG13	1:A:119:LEU:N	2.29	0.48
1:I:316:THR:HG21	2:K:29:LEU:HD11	1.95	0.48
2:K:36:TRP:O	2:K:48:LEU:HB2	2.13	0.48
1:E:118:ILE:HG13	1:E:119:LEU:N	2.29	0.48
1:I:365:LYS:HG3	2:K:107:TYR:CZ	2.49	0.48
1:A:51:PRO:HG3	1:A:272:LEU:HD13	1.96	0.47
1:E:365:LYS:HG3	2:G:107:TYR:CZ	2.49	0.47
2:G:36:TRP:O	2:G:48:LEU:HB2	2.13	0.47
1:I:167:ASN:HB3	1:I:237:TRP:CA	2.44	0.47
3:D:115:LEU:HB2	3:D:118:TRP:CG	2.50	0.47
3:D:144:LYS:O	3:D:148:LYS:HG3	2.14	0.47
1:I:118:ILE:HG13	1:I:119:LEU:N	2.29	0.47
1:E:167:ASN:HB3	1:E:237:TRP:CA	2.44	0.47
1:E:365:LYS:HG3	2:G:107:TYR:CE1	2.49	0.47
3:H:144:LYS:O	3:H:148:LYS:HG3	2.14	0.47
3:L:30:TYR:O	3:L:71:TYR:OH	2.33	0.47
1:E:346:ASP:O	2:G:107:TYR:OH	2.16	0.47
3:L:115:LEU:HB2	3:L:118:TRP:CG	2.49	0.47
1:E:51:PRO:HG3	1:E:272:LEU:HD13	1.97	0.47
2:G:50:PHE:HZ	3:H:96:TRP:CE2	2.33	0.47
3:H:115:LEU:HB2	3:H:118:TRP:CG	2.50	0.47
1:A:177:TRP:CE2	1:A:201:VAL:HG21	2.49	0.47
1:A:365:LYS:HG3	2:C:107:TYR:CZ	2.49	0.47
1:A:471:CYS:SG	1:A:476:MET:HG3	2.54	0.47
2:C:99:ALA:HA	2:C:111:TYR:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:99:ALA:HA	2:K:111:TYR:O	2.15	0.47
3:D:30:TYR:O	3:D:71:TYR:OH	2.33	0.47
1:E:177:TRP:CE2	1:E:201:VAL:HG21	2.49	0.47
2:G:159:TYR:HB3	3:H:134:MET:HE1	1.97	0.47
1:I:165:TYR:HB3	1:I:240:ILE:HG22	1.96	0.47
3:L:144:LYS:O	3:L:148:LYS:HG3	2.14	0.47
1:E:105:HIS:O	1:E:108:SER:OG	2.22	0.47
2:K:30:THR:O	2:K:100:ARG:NH2	2.36	0.47
1:E:428:LEU:HD23	1:E:428:LEU:HA	1.79	0.46
2:C:89:ARG:HH22	2:C:91:GLU:HB3	1.81	0.46
3:H:30:TYR:O	3:H:71:TYR:OH	2.33	0.46
3:H:61:ARG:HH22	3:H:79:GLN:HG3	1.80	0.46
1:I:93:PHE:CD1	1:I:94:PRO:HD2	2.51	0.46
2:C:34:MET:HB3	2:C:51:ILE:CG2	2.46	0.46
1:I:100:TYR:HE1	1:I:104:LYS:HD2	1.80	0.46
2:K:34:MET:HB3	2:K:51:ILE:CG2	2.46	0.46
1:A:100:TYR:HE1	1:A:104:LYS:HD2	1.80	0.46
2:C:110:ASP:HB3	3:D:46:LEU:HD22	1.96	0.46
3:D:61:ARG:HH22	3:D:79:GLN:HG3	1.80	0.46
1:E:96:SER:HB2	1:E:228:GLU:OE2	2.16	0.46
1:I:51:PRO:HG3	1:I:272:LEU:HD13	1.97	0.46
1:I:208:LYS:HB2	1:I:208:LYS:HE2	1.70	0.46
2:K:152:ILE:HD13	3:L:142:ARG:NH1	2.30	0.46
1:E:93:PHE:CD1	1:E:94:PRO:HD2	2.51	0.46
1:I:96:SER:HB2	1:I:228:GLU:OE2	2.16	0.46
1:A:167:ASN:HB3	1:A:237:TRP:CA	2.44	0.46
2:C:152:ILE:HG21	3:D:142:ARG:HH12	1.79	0.46
1:E:107:LEU:HD23	1:E:107:LEU:HA	1.75	0.46
1:A:334:ALA:HB1	1:A:338:GLU:OE2	2.16	0.46
2:G:99:ALA:HA	2:G:111:TYR:O	2.15	0.46
3:L:61:ARG:HH22	3:L:79:GLN:HG3	1.80	0.46
1:A:470:LYS:HA	1:A:470:LYS:HD3	1.84	0.46
1:E:131:GLY:HA2	1:E:150:TRP:CD1	2.51	0.46
1:E:334:ALA:HB1	1:E:338:GLU:OE2	2.16	0.46
2:G:155:ILE:HG13	2:G:158:LYS:HE2	1.98	0.46
2:K:35:THR:HB	2:K:109:MET:HE1	1.98	0.46
2:K:106:PRO:C	3:L:91:PHE:HD2	2.19	0.46
2:G:34:MET:HB3	2:G:51:ILE:HG23	1.98	0.46
3:L:54:LEU:HD22	3:L:58:VAL:HG13	1.98	0.46
2:G:34:MET:HB3	2:G:51:ILE:CG2	2.46	0.46
2:K:54:ARG:HB2	2:K:54:ARG:NH1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:GLY:HA2	1:A:150:TRP:CD1	2.51	0.45
2:K:18:LEU:HD12	2:K:19:ARG:H	1.81	0.45
1:E:67:PRO:HB3	1:E:138:VAL:HG12	1.98	0.45
1:E:169:SER:HB3	1:E:256:LYS:HD2	1.97	0.45
2:G:18:LEU:HD12	2:G:19:ARG:H	1.81	0.45
2:G:33:TYR:OH	2:G:52:ARG:NH2	2.49	0.45
2:G:35:THR:HB	2:G:109:MET:HE1	1.98	0.45
2:G:119:ILE:HD13	3:H:143:GLN:OE1	2.16	0.45
1:I:67:PRO:HB3	1:I:138:VAL:HG12	1.98	0.45
1:I:169:SER:HB3	1:I:256:LYS:HD2	1.97	0.45
1:I:334:ALA:HB1	1:I:338:GLU:OE2	2.16	0.45
2:K:102:LYS:HB3	2:K:111:TYR:HE1	1.80	0.45
1:A:93:PHE:CD1	1:A:94:PRO:HD2	2.51	0.45
1:A:96:SER:HB2	1:A:228:GLU:OE2	2.16	0.45
1:A:169:SER:HB3	1:A:256:LYS:HD2	1.97	0.45
2:C:18:LEU:HD12	2:C:19:ARG:H	1.81	0.45
1:E:475:CYS:HB3	1:E:489:TYR:OH	2.16	0.45
2:K:33:TYR:OH	2:K:52:ARG:NH2	2.49	0.45
2:K:89:ARG:HH22	2:K:91:GLU:HB3	1.81	0.45
2:G:54:ARG:NH1	2:G:54:ARG:HB2	2.31	0.45
2:G:102:LYS:HB3	2:G:111:TYR:HE1	1.80	0.45
1:I:475:CYS:HB3	1:I:489:TYR:OH	2.17	0.45
2:K:34:MET:HB3	2:K:51:ILE:HG23	1.98	0.45
1:A:475:CYS:HB3	1:A:489:TYR:OH	2.17	0.45
1:E:485:ASP:OD1	1:E:487:PRO:HD2	2.16	0.45
3:H:54:LEU:HD22	3:H:58:VAL:HG13	1.98	0.45
2:K:47:TRP:O	2:K:63:SER:OG	2.33	0.45
2:C:33:TYR:OH	2:C:52:ARG:NH2	2.49	0.45
2:C:34:MET:HB3	2:C:51:ILE:HG23	1.98	0.45
2:C:102:LYS:HB3	2:C:111:TYR:HE1	1.80	0.45
1:E:115:LYS:HZ3	1:E:147:ASN:HD21	1.65	0.45
2:G:141:LEU:HD13	3:H:149:ARG:HD2	1.98	0.45
3:H:140:GLU:HA	3:H:143:GLN:HG3	1.98	0.45
2:K:155:ILE:HA	2:K:158:LYS:HG2	1.99	0.45
1:A:485:ASP:OD1	1:A:487:PRO:HD2	2.17	0.45
3:D:134:MET:O	3:D:137:GLU:HG3	2.16	0.45
2:G:129:LEU:HD21	3:H:151:PRO:HB2	1.98	0.45
1:I:84:LYS:HZ2	1:I:269:GLU:HG3	1.82	0.45
1:I:131:GLY:HA2	1:I:150:TRP:CD1	2.51	0.45
1:I:485:ASP:OD1	1:I:487:PRO:HD2	2.16	0.45
2:K:102:LYS:HB3	2:K:111:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:134:MET:O	3:L:137:GLU:HG3	2.16	0.45
1:E:100:TYR:HE1	1:E:104:LYS:HD2	1.80	0.45
2:G:155:ILE:HA	2:G:158:LYS:HG2	1.99	0.45
2:G:169:ALA:HA	2:G:172:ALA:HB3	1.99	0.45
1:A:45:LYS:NZ	1:A:276:GLU:OE1	2.38	0.45
2:C:54:ARG:NH1	2:C:54:ARG:HB2	2.31	0.45
2:C:85:MET:HE1	2:C:118:VAL:HG11	1.98	0.45
1:I:324:ILE:H	1:I:324:ILE:HG13	1.61	0.45
2:K:155:ILE:HG13	2:K:158:LYS:HE2	1.98	0.45
2:C:135:GLU:O	2:C:139:LYS:HG2	2.17	0.45
2:C:155:ILE:HA	2:C:158:LYS:HG2	1.99	0.45
1:E:402:LYS:HD3	1:E:402:LYS:HA	1.83	0.45
2:G:89:ARG:HH22	2:G:91:GLU:HB3	1.81	0.45
3:H:134:MET:O	3:H:137:GLU:HG3	2.16	0.45
1:I:45:LYS:NZ	1:I:276:GLU:OE1	2.38	0.45
2:K:135:GLU:O	2:K:139:LYS:HG2	2.17	0.45
1:A:279:CYS:HB2	1:A:303:CYS:HB3	1.33	0.44
2:C:155:ILE:HG13	2:C:158:LYS:HE2	1.98	0.44
3:D:140:GLU:HA	3:D:143:GLN:HG3	1.98	0.44
1:E:171:GLU:CB	1:E:256:LYS:HZ1	2.30	0.44
1:I:107:LEU:HD23	1:I:107:LEU:HA	1.75	0.44
2:K:108:ALA:HB1	3:L:46:LEU:HD13	2.00	0.44
1:E:40:ASN:OD1	1:E:41:GLY:N	2.51	0.44
2:G:19:ARG:HD2	2:G:82:TYR:CD1	2.53	0.44
1:I:291:PRO:CB	1:I:383:ILE:HD12	2.47	0.44
3:L:150:GLN:N	3:L:151:PRO:HD2	2.33	0.44
3:D:54:LEU:HD22	3:D:58:VAL:HG13	1.98	0.44
3:L:90:HIS:CD2	3:L:93:GLY:H	2.35	0.44
2:C:141:LEU:HA	3:D:149:ARG:CZ	2.47	0.44
1:E:103:LEU:HD12	1:E:231:TRP:CG	2.52	0.44
2:K:19:ARG:HD2	2:K:82:TYR:CD1	2.53	0.44
1:A:385:LYS:HA	1:A:385:LYS:HD3	1.71	0.44
1:A:402:LYS:HA	1:A:402:LYS:HD3	1.83	0.44
2:C:19:ARG:HD2	2:C:82:TYR:CD1	2.53	0.44
2:C:47:TRP:CZ3	3:D:95:PRO:HA	2.53	0.44
1:E:470:LYS:HA	1:E:470:LYS:HD3	1.84	0.44
2:G:102:LYS:HB3	2:G:111:TYR:CE1	2.52	0.44
1:I:103:LEU:HD12	1:I:231:TRP:CG	2.52	0.44
1:I:291:PRO:HG2	1:I:292:PHE:CD2	2.53	0.44
1:A:181:HIS:O	1:A:225:GLY:HA2	2.18	0.44
3:D:90:HIS:CD2	3:D:93:GLY:H	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:GLU:CB	1:A:256:LYS:HZ1	2.31	0.44
3:H:150:GLN:N	3:H:151:PRO:HD2	2.33	0.44
2:K:148:MET:HG3	3:L:145:TYR:HD2	1.76	0.44
1:A:67:PRO:HB3	1:A:138:VAL:HG12	1.98	0.44
1:A:103:LEU:HD12	1:A:231:TRP:CG	2.52	0.44
2:C:19:ARG:NH1	2:C:84:GLN:OE1	2.51	0.44
2:G:145:ASP:O	2:G:149:GLU:OE1	2.36	0.44
3:H:90:HIS:CD2	3:H:93:GLY:H	2.35	0.44
1:E:291:PRO:HG2	1:E:292:PHE:CD2	2.53	0.43
2:G:29:LEU:HD12	2:G:29:LEU:HA	1.84	0.43
3:H:21:ILE:HD11	3:H:73:LEU:HD22	2.00	0.43
2:K:145:ASP:O	2:K:149:GLU:OE1	2.36	0.43
1:A:40:ASN:OD1	1:A:41:GLY:N	2.51	0.43
1:A:369:GLN:HG3	3:D:49:TYR:CE1	2.52	0.43
2:C:102:LYS:HB3	2:C:111:TYR:CE1	2.52	0.43
3:D:17:GLU:CG	3:D:18:THR:H	2.29	0.43
1:E:208:LYS:HB2	1:E:208:LYS:HE2	1.70	0.43
2:G:135:GLU:O	2:G:139:LYS:HG2	2.17	0.43
2:K:141:LEU:HD13	3:L:149:ARG:HD2	2.00	0.43
1:A:324:ILE:H	1:A:324:ILE:HG13	1.61	0.43
3:D:21:ILE:HD11	3:D:73:LEU:HD22	2.00	0.43
3:D:152:ILE:HD12	3:D:152:ILE:H	1.83	0.43
2:G:47:TRP:O	2:G:63:SER:OG	2.33	0.43
2:K:19:ARG:NH1	2:K:84:GLN:OE1	2.51	0.43
3:L:15:VAL:HA	3:L:78:LEU:HD22	2.00	0.43
2:C:144:LEU:HB3	3:D:149:ARG:HH22	1.81	0.43
2:C:159:TYR:HB3	3:D:134:MET:HE1	2.01	0.43
2:C:169:ALA:HA	2:C:172:ALA:HB3	1.99	0.43
3:D:150:GLN:N	3:D:151:PRO:HD2	2.33	0.43
1:E:257:ILE:HG13	1:E:257:ILE:O	2.19	0.43
1:E:385:LYS:HA	1:E:385:LYS:HD3	1.71	0.43
3:H:152:ILE:HD12	3:H:152:ILE:H	1.83	0.43
1:I:40:ASN:OD1	1:I:41:GLY:N	2.51	0.43
1:I:171:GLU:CB	1:I:256:LYS:HZ1	2.31	0.43
3:L:140:GLU:HA	3:L:143:GLN:HG3	1.99	0.43
2:C:35:THR:HB	2:C:109:MET:HE1	2.00	0.43
2:C:70:PHE:HD1	2:C:85:MET:HA	1.82	0.43
2:G:19:ARG:NH1	2:G:84:GLN:OE1	2.51	0.43
1:I:366:GLU:O	1:I:370:LYS:HG2	2.19	0.43
3:L:152:ILE:HD12	3:L:152:ILE:H	1.83	0.43
1:A:291:PRO:HG2	1:A:292:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:181:HIS:O	1:E:225:GLY:HA2	2.18	0.43
1:I:257:ILE:O	1:I:257:ILE:HG13	2.19	0.43
2:K:169:ALA:HA	2:K:172:ALA:HB3	1.99	0.43
3:L:12:SER:OG	3:L:105:GLU:HG2	2.19	0.43
1:A:126:GLN:N	1:A:126:GLN:OE1	2.52	0.43
1:A:455:ASP:O	1:A:497:ARG:NH2	2.52	0.43
3:D:15:VAL:HA	3:D:78:LEU:HD22	2.00	0.43
1:I:181:HIS:O	1:I:225:GLY:HA2	2.18	0.43
1:I:455:ASP:O	1:I:497:ARG:NH2	2.52	0.43
3:L:17:GLU:CG	3:L:18:THR:H	2.29	0.43
1:E:455:ASP:O	1:E:497:ARG:NH2	2.52	0.43
3:L:21:ILE:HD11	3:L:73:LEU:HD22	2.00	0.43
2:C:145:ASP:O	2:C:149:GLU:OE1	2.36	0.43
1:E:291:PRO:CB	1:E:383:ILE:HD12	2.47	0.43
3:H:8:PRO:HG2	3:H:21:ILE:HA	2.01	0.43
1:E:366:GLU:O	1:E:370:LYS:HG2	2.19	0.42
2:G:30:THR:O	2:G:100:ARG:NH2	2.36	0.42
2:G:70:PHE:HD1	2:G:85:MET:HA	1.82	0.42
3:H:4:MET:SD	3:H:90:HIS:HB3	2.59	0.42
1:A:257:ILE:O	1:A:257:ILE:HG13	2.19	0.42
1:E:323:GLN:HG2	1:E:324:ILE:N	2.34	0.42
1:E:126:GLN:OE1	1:E:126:GLN:N	2.52	0.42
3:H:15:VAL:HA	3:H:78:LEU:HD22	2.00	0.42
2:K:152:ILE:HD11	3:L:138:ILE:HG23	2.01	0.42
3:L:2:ILE:HD11	3:L:90:HIS:CG	2.54	0.42
1:A:198:TYR:OH	1:A:243:GLU:OE2	2.25	0.42
1:A:366:GLU:O	1:A:370:LYS:HG2	2.19	0.42
3:D:8:PRO:HG2	3:D:21:ILE:HA	2.01	0.42
2:C:159:TYR:HB3	3:D:134:MET:CE	2.50	0.42
3:D:12:SER:OG	3:D:105:GLU:HG2	2.19	0.42
1:I:126:GLN:N	1:I:126:GLN:OE1	2.52	0.42
3:L:8:PRO:HG2	3:L:21:ILE:HA	2.01	0.42
1:A:291:PRO:CB	1:A:383:ILE:HD12	2.47	0.42
1:E:198:TYR:OH	1:E:243:GLU:OE2	2.25	0.42
3:H:12:SER:OG	3:H:105:GLU:HG2	2.19	0.42
3:L:4:MET:SD	3:L:90:HIS:HB3	2.59	0.42
3:D:4:MET:SD	3:D:90:HIS:HB3	2.59	0.42
2:G:108:ALA:HB2	3:H:49:TYR:HB3	2.01	0.42
2:K:70:PHE:HD1	2:K:85:MET:HA	1.82	0.42
2:C:155:ILE:HG12	2:C:159:TYR:CE2	2.55	0.42
2:G:159:TYR:HB3	3:H:134:MET:CE	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:152:ILE:CG2	3:D:142:ARG:HH22	2.33	0.42
2:K:106:PRO:O	3:L:91:PHE:HD2	2.02	0.42
1:A:208:LYS:HB2	1:A:208:LYS:HE2	1.70	0.41
3:H:2:ILE:HD11	3:H:90:HIS:CG	2.54	0.41
3:H:17:GLU:CG	3:H:18:THR:H	2.29	0.41
2:K:164:GLN:N	2:K:165:PRO:HD2	2.35	0.41
1:E:118:ILE:HG13	1:E:119:LEU:H	1.85	0.41
1:A:323:GLN:HG2	1:A:324:ILE:N	2.34	0.41
2:G:2:VAL:HG12	2:G:26:GLY:HA3	2.02	0.41
1:I:323:GLN:HG2	1:I:324:ILE:N	2.34	0.41
1:I:470:LYS:HD3	1:I:470:LYS:HA	1.84	0.41
2:C:25:SER:OG	2:C:26:GLY:N	2.53	0.41
1:E:279:CYS:SG	1:E:280:GLN:N	2.94	0.41
2:G:155:ILE:HG12	2:G:159:TYR:CE2	2.55	0.41
2:K:2:VAL:HG12	2:K:26:GLY:HA3	2.02	0.41
2:C:30:THR:O	2:C:100:ARG:NH2	2.36	0.41
1:E:369:GLN:HG3	3:H:49:TYR:CE1	2.55	0.41
2:G:50:PHE:HZ	3:H:96:TRP:CZ2	2.38	0.41
2:G:58:TYR:CD2	2:G:74:ARG:HD2	2.56	0.41
2:G:138:GLN:OE1	2:G:141:LEU:HD23	2.21	0.41
1:I:279:CYS:SG	1:I:280:GLN:N	2.94	0.41
1:A:281:THR:HG22	1:A:299:THR:HG22	2.03	0.41
3:D:2:ILE:HD11	3:D:90:HIS:CG	2.54	0.41
1:E:29:THR:HG22	1:E:30:HIS:CE1	2.56	0.41
1:E:180:HIS:O	1:E:182:PRO:HD3	2.21	0.41
2:G:25:SER:OG	2:G:26:GLY:N	2.53	0.41
2:K:58:TYR:CD2	2:K:74:ARG:HD2	2.56	0.41
2:K:155:ILE:HG12	2:K:159:TYR:CE2	2.55	0.41
2:C:138:GLN:OE1	2:C:141:LEU:HD23	2.21	0.41
2:C:141:LEU:HD13	3:D:149:ARG:CD	2.46	0.41
1:I:118:ILE:HG13	1:I:119:LEU:H	1.85	0.41
1:A:29:THR:HG22	1:A:30:HIS:CE1	2.56	0.41
2:C:47:TRP:O	2:C:63:SER:OG	2.33	0.41
1:E:355:ASN:ND2	1:E:471:CYS:O	2.54	0.41
1:E:488:LYS:HD3	1:E:489:TYR:CZ	2.56	0.41
3:H:17:GLU:HG3	3:H:18:THR:N	2.32	0.41
1:I:29:THR:HG22	1:I:30:HIS:CE1	2.56	0.41
2:K:138:GLN:OE1	2:K:141:LEU:HD23	2.21	0.41
2:K:155:ILE:HG13	2:K:158:LYS:HZ1	1.86	0.41
1:A:44:CYS:HB3	1:A:275:CYS:HB2	1.26	0.41
1:A:118:ILE:HG13	1:A:119:LEU:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:CYS:SG	1:A:280:GLN:N	2.94	0.41
1:A:303:CYS:HB2	1:A:304:PRO:HD3	2.02	0.41
1:A:450:ARG:HB2	1:A:465:PHE:HZ	1.86	0.41
1:E:279:CYS:HB2	1:E:303:CYS:HB3	1.33	0.41
1:E:281:THR:HG22	1:E:299:THR:HG22	2.03	0.41
1:E:324:ILE:H	1:E:324:ILE:HG13	1.61	0.41
1:E:421:TYR:OH	1:I:426:LEU:HD22	2.21	0.41
2:G:85:MET:HE1	2:G:118:VAL:HG11	2.03	0.41
2:G:164:GLN:N	2:G:165:PRO:HD2	2.35	0.41
3:H:159:LYS:HA	3:H:159:LYS:HD3	1.95	0.41
1:I:428:LEU:HA	1:I:428:LEU:HD23	1.79	0.41
1:I:488:LYS:HD3	1:I:489:TYR:CZ	2.56	0.41
2:K:85:MET:HE1	2:K:118:VAL:HG11	2.03	0.41
2:K:163:ARG:HD3	3:L:134:MET:HE1	2.02	0.41
3:L:149:ARG:HA	3:L:152:ILE:HD13	2.03	0.41
2:C:2:VAL:HG12	2:C:26:GLY:HA3	2.02	0.41
2:C:164:GLN:N	2:C:165:PRO:HD2	2.35	0.41
1:E:303:CYS:HB2	1:E:304:PRO:HD3	2.02	0.41
1:I:180:HIS:O	1:I:182:PRO:HD3	2.21	0.41
1:A:58:SER:HB3	1:A:87:PRO:HB2	2.04	0.40
2:C:58:TYR:CD2	2:C:74:ARG:HD2	2.56	0.40
1:I:149:VAL:HG22	1:I:250:ALA:HB3	2.04	0.40
1:I:198:TYR:OH	1:I:243:GLU:OE2	2.25	0.40
1:A:426:LEU:HD22	1:I:421:TYR:OH	2.21	0.40
1:A:180:HIS:O	1:A:182:PRO:HD3	2.21	0.40
1:E:110:VAL:HG11	1:E:113:PHE:CE1	2.57	0.40
1:E:460:LEU:HD23	1:E:460:LEU:HA	1.96	0.40
2:G:52:ARG:NE	2:G:56:ASN:HD21	2.19	0.40
1:I:59:ILE:HG12	1:I:83:GLU:OE2	2.22	0.40
1:I:101:GLU:OE1	1:I:101:GLU:N	2.52	0.40
1:I:303:CYS:HB2	1:I:304:PRO:HD3	2.02	0.40
1:A:355:ASN:ND2	1:A:471:CYS:O	2.54	0.40
1:E:59:ILE:HG12	1:E:83:GLU:OE2	2.22	0.40
1:E:84:LYS:HZ2	1:E:269:GLU:HG3	1.86	0.40
1:E:278:LYS:HE2	1:E:278:LYS:HB2	1.96	0.40
3:H:33:LEU:HD12	3:H:90:HIS:HA	2.04	0.40
1:I:346:ASP:HB3	1:I:363:ALA:HB2	2.03	0.40
3:L:33:LEU:HD12	3:L:90:HIS:HA	2.04	0.40
3:D:120:VAL:HG23	3:D:123:LEU:HD12	2.04	0.40
1:I:114:GLU:OE1	1:I:256:LYS:HD3	2.22	0.40
1:I:281:THR:HG22	1:I:299:THR:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:402:LYS:HD3	1:I:402:LYS:HA	1.83	0.40
2:K:52:ARG:NE	2:K:56:ASN:HD21	2.19	0.40
2:K:163:ARG:HE	2:K:163:ARG:HB2	1.67	0.40
3:L:17:GLU:HG3	3:L:18:THR:N	2.31	0.40
3:L:80:SER:HA	3:L:83:PHE:CZ	2.57	0.40
3:L:120:VAL:HG23	3:L:123:LEU:HD12	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	496/599 (83%)	462 (93%)	34 (7%)	0	100	100
1	E	496/599 (83%)	462 (93%)	34 (7%)	0	100	100
1	I	496/599 (83%)	462 (93%)	34 (7%)	0	100	100
2	C	171/203 (84%)	161 (94%)	10 (6%)	0	100	100
2	G	171/203 (84%)	161 (94%)	10 (6%)	0	100	100
2	K	171/203 (84%)	161 (94%)	10 (6%)	0	100	100
3	D	157/189 (83%)	142 (90%)	15 (10%)	0	100	100
3	H	157/189 (83%)	142 (90%)	15 (10%)	0	100	100
3	L	157/189 (83%)	143 (91%)	14 (9%)	0	100	100
All	All	2472/2973 (83%)	2296 (93%)	176 (7%)	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	437/519 (84%)	429 (98%)	8 (2%)	59	77
1	E	437/519 (84%)	430 (98%)	7 (2%)	62	80
1	I	437/519 (84%)	430 (98%)	7 (2%)	62	80
2	C	149/174 (86%)	146 (98%)	3 (2%)	55	74
2	G	149/174 (86%)	146 (98%)	3 (2%)	55	74
2	K	149/174 (86%)	146 (98%)	3 (2%)	55	74
3	D	137/162 (85%)	133 (97%)	4 (3%)	42	66
3	H	137/162 (85%)	133 (97%)	4 (3%)	42	66
3	L	137/162 (85%)	133 (97%)	4 (3%)	42	66
All	All	2169/2565 (85%)	2126 (98%)	43 (2%)	57	74

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
1	A	129	THR
1	A	149	VAL
1	A	227	MET
1	A	274	ASN
1	A	324	ILE
1	A	433	ARG
1	A	477	ASN
2	C	73	SER
2	C	78	GLN
2	C	162	LYS
3	D	73	LEU
3	D	74	LYS
3	D	145	TYR
3	D	148	LYS
1	E	53	GLU
1	E	129	THR
1	E	149	VAL

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Mol	Chain	Res	Type
1	E	227	MET
1	E	324	ILE
1	E	433	ARG
1	E	477	ASN
2	G	73	SER
2	G	78	GLN
2	G	162	LYS
3	H	73	LEU
3	H	74	LYS
3	H	145	TYR
3	H	148	LYS
1	I	53	GLU
1	I	129	THR
1	I	149	VAL
1	I	227	MET
1	I	324	ILE
1	I	433	ARG
1	I	477	ASN
2	K	73	SER
2	K	78	GLN
2	K	162	LYS
3	L	73	LEU
3	L	74	LYS
3	L	145	TYR
3	L	148	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
1	A	274	ASN
1	A	296	HIS
1	A	323	GLN
2	C	157	GLN
1	E	147	ASN
1	E	296	HIS
1	E	323	GLN
2	G	157	GLN
1	I	147	ASN
1	I	296	HIS
1	I	323	GLN
2	K	157	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

18 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	B	1	1,4	14,14,15	0.31	0	17,19,21	0.53	0
4	NAG	B	2	4	14,14,15	0.52	0	17,19,21	0.39	0
4	BMA	B	3	4	11,11,12	0.61	0	15,15,17	0.75	0
4	NAG	F	1	1,4	14,14,15	0.81	1 (7%)	17,19,21	0.58	0
4	NAG	F	2	4	14,14,15	0.19	0	17,19,21	0.51	0
4	BMA	F	3	4	11,11,12	0.93	1 (9%)	15,15,17	0.79	0
4	NAG	J	1	1,4	14,14,15	0.31	0	17,19,21	0.53	0
4	NAG	J	2	4	14,14,15	0.51	0	17,19,21	0.40	0
4	BMA	J	3	4	11,11,12	0.62	0	15,15,17	0.74	0
4	NAG	M	1	1,4	14,14,15	0.80	1 (7%)	17,19,21	0.57	0
4	NAG	M	2	4	14,14,15	0.19	0	17,19,21	0.52	0
4	BMA	M	3	4	11,11,12	0.92	1 (9%)	15,15,17	0.80	0
4	NAG	N	1	1,4	14,14,15	0.31	0	17,19,21	0.54	0
4	NAG	N	2	4	14,14,15	0.49	0	17,19,21	0.39	0
4	BMA	N	3	4	11,11,12	0.63	0	15,15,17	0.74	0
4	NAG	O	1	1,4	14,14,15	0.81	1 (7%)	17,19,21	0.57	0
4	NAG	O	2	4	14,14,15	0.19	0	17,19,21	0.51	0
4	BMA	O	3	4	11,11,12	0.93	1 (9%)	15,15,17	0.80	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.  
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	B	2	4	-	2/6/23/26	0/1/1/1
4	BMA	B	3	4	-	2/2/19/22	0/1/1/1
4	NAG	F	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	BMA	F	3	4	-	2/2/19/22	0/1/1/1
4	NAG	J	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	BMA	J	3	4	-	2/2/19/22	0/1/1/1
4	NAG	M	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	BMA	M	3	4	-	2/2/19/22	0/1/1/1
4	NAG	N	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	BMA	N	3	4	-	2/2/19/22	0/1/1/1
4	NAG	O	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	BMA	O	3	4	-	2/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	1	NAG	O5-C1	-2.84	1.39	1.43
4	F	1	NAG	O5-C1	-2.81	1.39	1.43
4	M	1	NAG	O5-C1	-2.79	1.39	1.43
4	O	3	BMA	C1-C2	2.34	1.57	1.52
4	F	3	BMA	C1-C2	2.33	1.57	1.52
4	M	3	BMA	C1-C2	2.32	1.57	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	J	1	NAG	O5-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
4	B	3	BMA	O5-C5-C6-O6
4	J	3	BMA	O5-C5-C6-O6
4	N	3	BMA	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
4	M	3	BMA	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	O	3	BMA	O5-C5-C6-O6
4	F	3	BMA	C4-C5-C6-O6
4	M	3	BMA	C4-C5-C6-O6
4	O	3	BMA	C4-C5-C6-O6
4	B	1	NAG	C8-C7-N2-C2
4	B	1	NAG	O7-C7-N2-C2
4	B	2	NAG	C8-C7-N2-C2
4	B	2	NAG	O7-C7-N2-C2
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
4	J	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
4	M	1	NAG	C8-C7-N2-C2
4	M	1	NAG	O7-C7-N2-C2
4	N	1	NAG	C8-C7-N2-C2
4	N	1	NAG	O7-C7-N2-C2
4	N	2	NAG	C8-C7-N2-C2
4	N	2	NAG	O7-C7-N2-C2
4	O	1	NAG	C8-C7-N2-C2
4	O	1	NAG	O7-C7-N2-C2
4	F	2	NAG	C4-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	B	1	NAG	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6
4	B	3	BMA	C4-C5-C6-O6
4	J	3	BMA	C4-C5-C6-O6
4	N	3	BMA	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6

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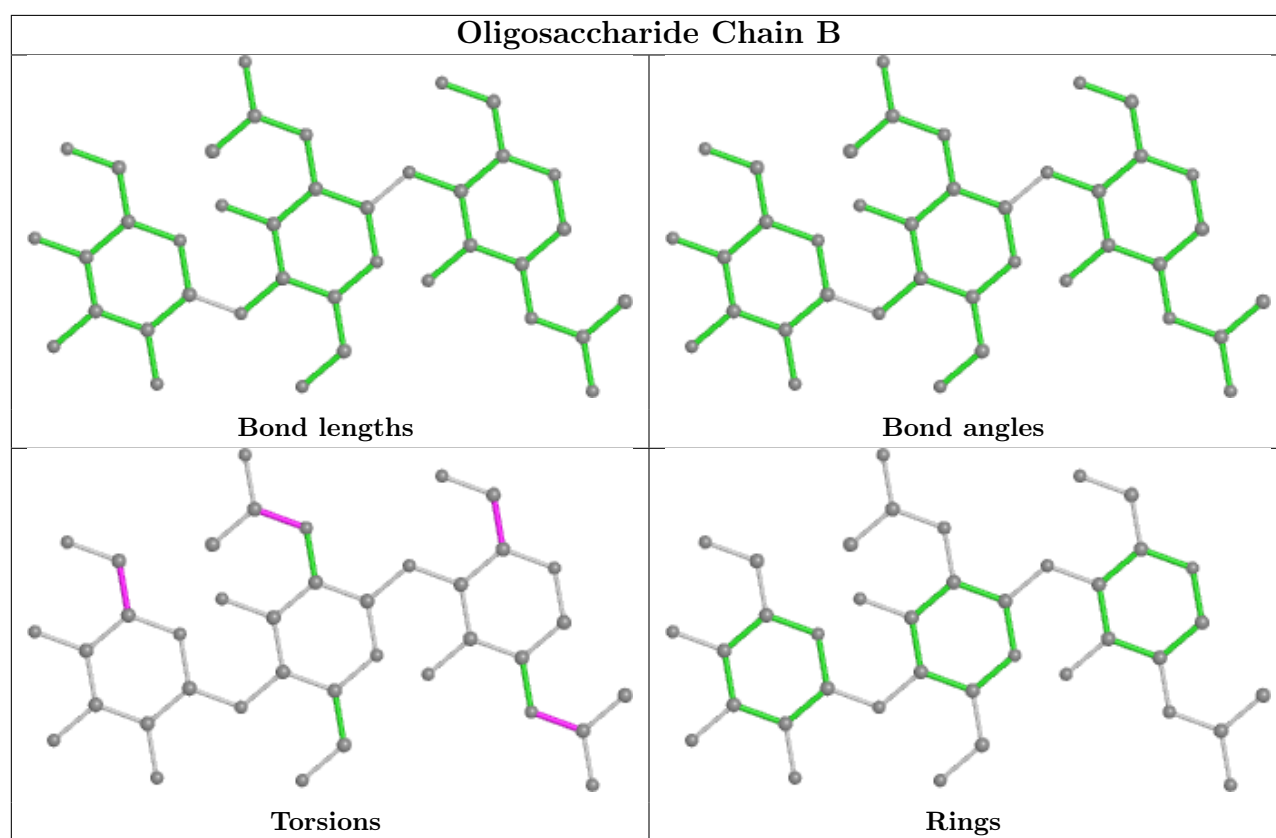
*Continued from previous page...*

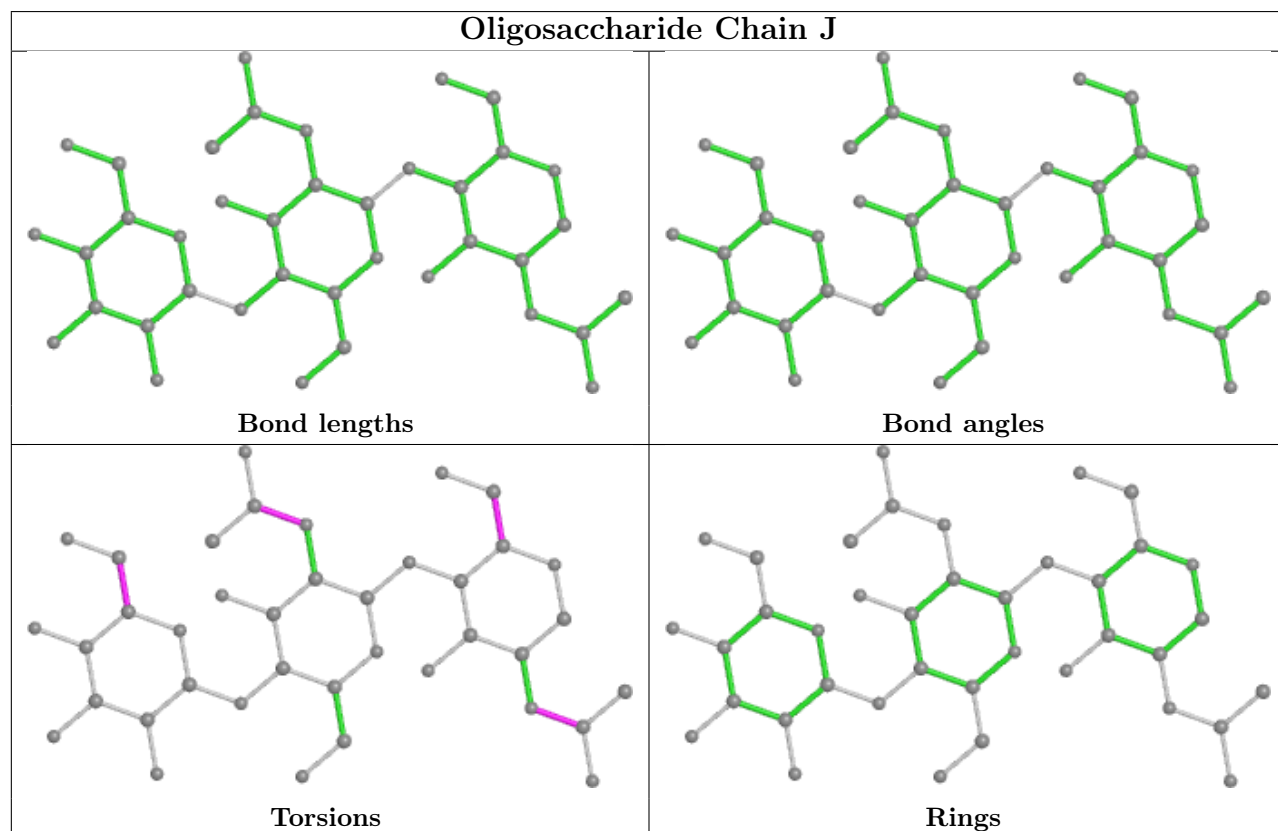
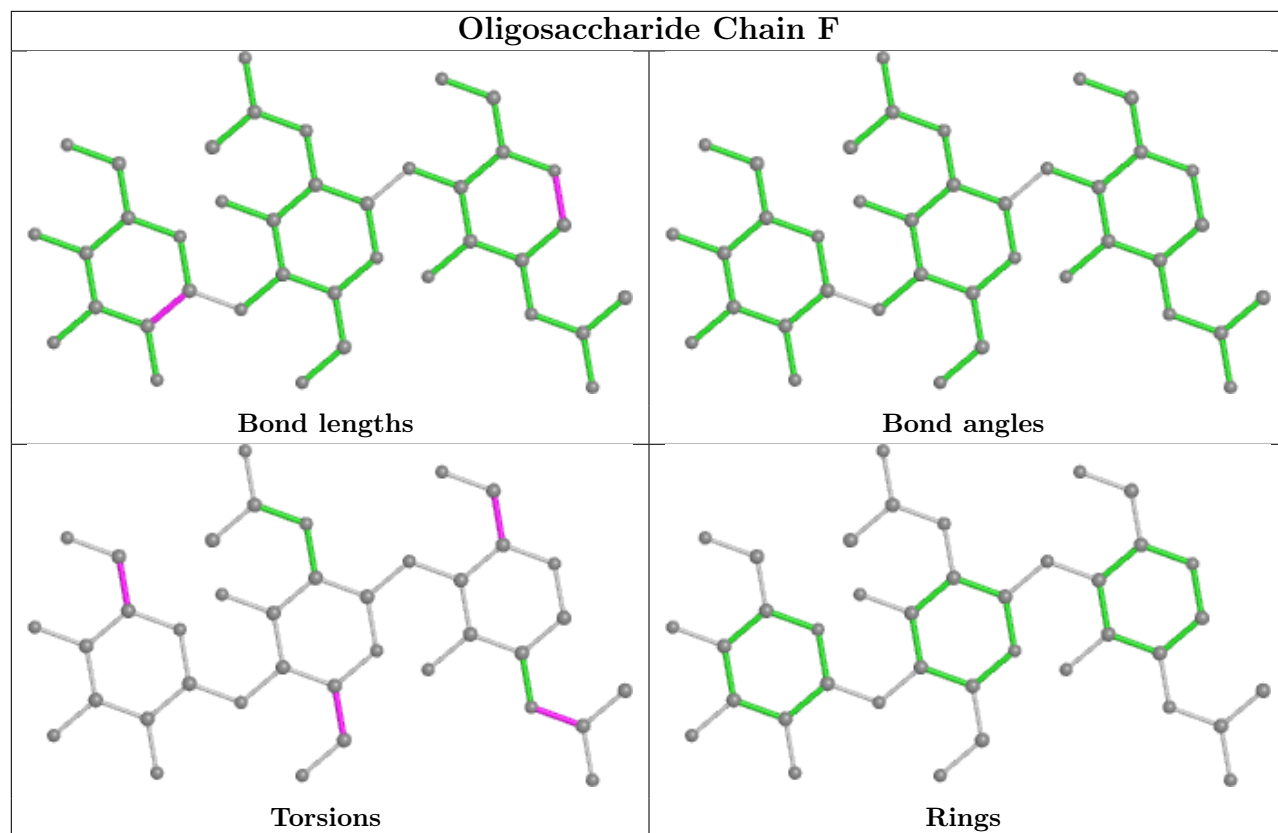
Mol	Chain	Res	Type	Atoms
4	M	1	NAG	O5-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6

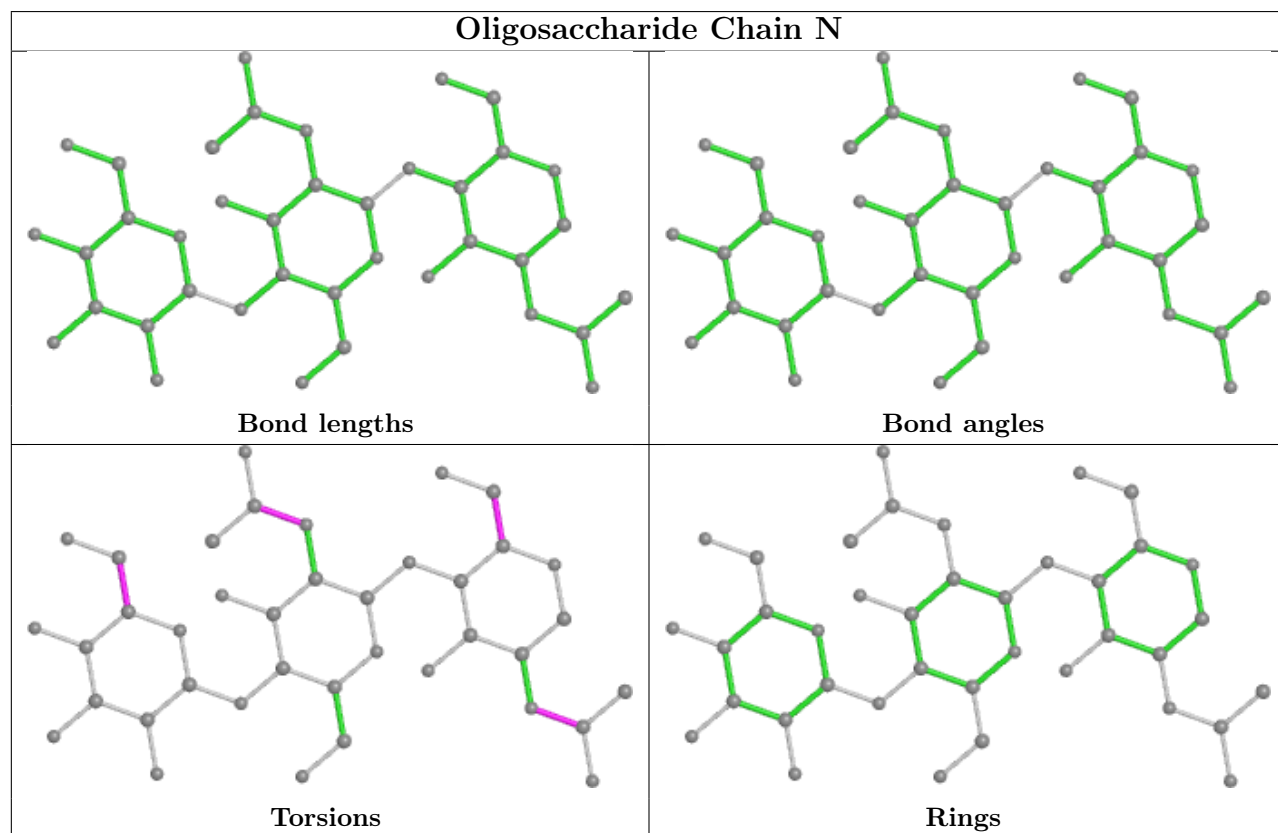
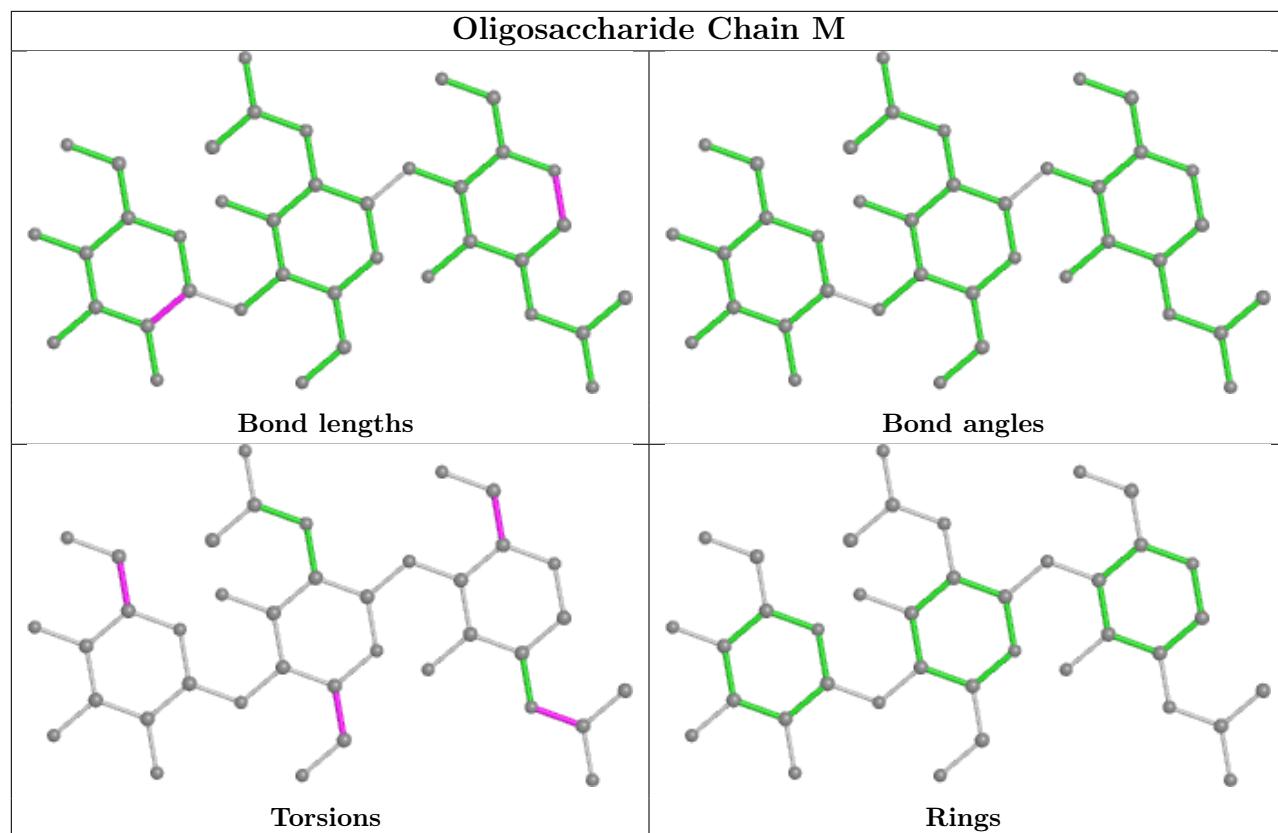
There are no ring outliers.

No monomer is involved in short contacts.

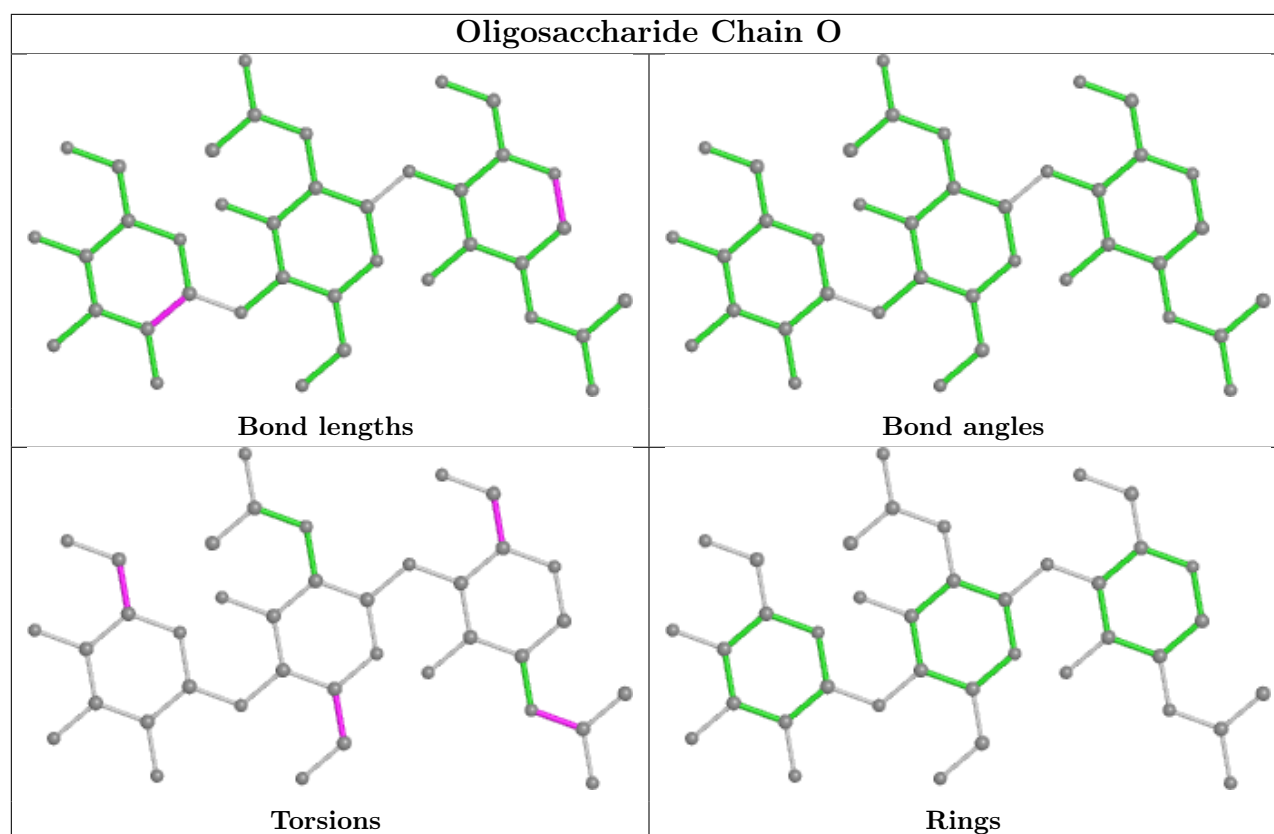
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	E	602	1	14,14,15	0.15	0	17,19,21	0.34	0
5	NAG	I	601	1	14,14,15	0.55	0	17,19,21	0.40	0
5	NAG	E	603	1	14,14,15	0.23	0	17,19,21	0.43	0
5	NAG	A	603	1	14,14,15	0.25	0	17,19,21	0.43	0
5	NAG	A	602	1	14,14,15	0.15	0	17,19,21	0.34	0
5	NAG	I	602	1	14,14,15	0.15	0	17,19,21	0.34	0
5	NAG	I	603	1	14,14,15	0.24	0	17,19,21	0.43	0
5	NAG	E	601	1	14,14,15	0.55	0	17,19,21	0.39	0
5	NAG	A	601	1	14,14,15	0.57	1 (7%)	17,19,21	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	602	1	-	4/6/23/26	0/1/1/1
5	NAG	I	601	1	-	4/6/23/26	0/1/1/1
5	NAG	E	603	1	-	2/6/23/26	0/1/1/1
5	NAG	A	603	1	-	2/6/23/26	0/1/1/1
5	NAG	A	602	1	-	4/6/23/26	0/1/1/1
5	NAG	I	602	1	-	4/6/23/26	0/1/1/1
5	NAG	I	603	1	-	2/6/23/26	0/1/1/1
5	NAG	E	601	1	-	4/6/23/26	0/1/1/1
5	NAG	A	601	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	NAG	O5-C1	-2.01	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	602	NAG	O5-C5-C6-O6
5	E	602	NAG	O5-C5-C6-O6
5	I	602	NAG	O5-C5-C6-O6
5	A	601	NAG	C8-C7-N2-C2
5	A	601	NAG	O7-C7-N2-C2
5	A	602	NAG	C8-C7-N2-C2
5	A	602	NAG	O7-C7-N2-C2
5	A	603	NAG	C8-C7-N2-C2
5	A	603	NAG	O7-C7-N2-C2
5	E	601	NAG	C8-C7-N2-C2
5	E	601	NAG	O7-C7-N2-C2
5	E	602	NAG	C8-C7-N2-C2
5	E	602	NAG	O7-C7-N2-C2
5	E	603	NAG	C8-C7-N2-C2
5	E	603	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	I	601	NAG	C8-C7-N2-C2
5	I	601	NAG	O7-C7-N2-C2
5	I	602	NAG	C8-C7-N2-C2
5	I	602	NAG	O7-C7-N2-C2
5	I	603	NAG	C8-C7-N2-C2
5	I	603	NAG	O7-C7-N2-C2
5	A	601	NAG	O5-C5-C6-O6
5	E	601	NAG	O5-C5-C6-O6
5	I	601	NAG	O5-C5-C6-O6
5	E	601	NAG	C4-C5-C6-O6
5	I	601	NAG	C4-C5-C6-O6
5	A	601	NAG	C4-C5-C6-O6
5	A	602	NAG	C4-C5-C6-O6
5	E	602	NAG	C4-C5-C6-O6
5	I	602	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

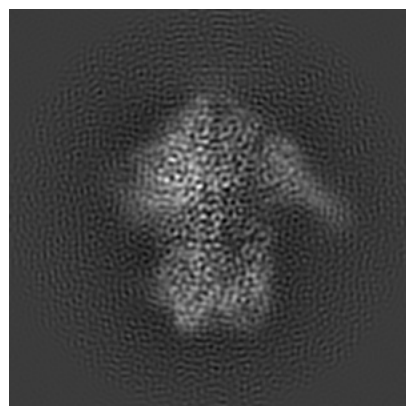
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30707. These allow visual inspection of the internal detail of the map and identification of artifacts.

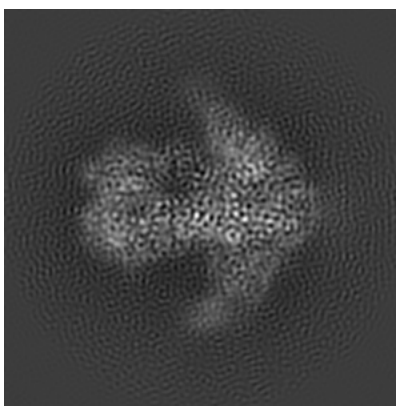
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

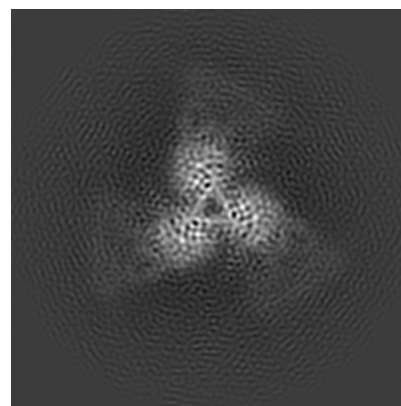
#### 6.1.1 Primary map



X

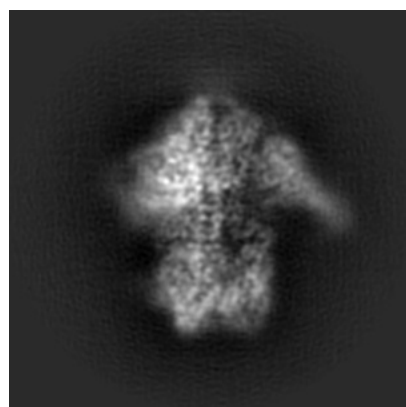


Y

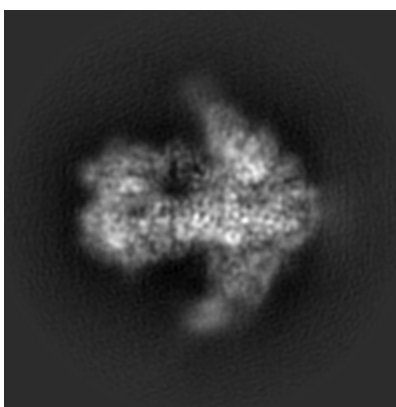


Z

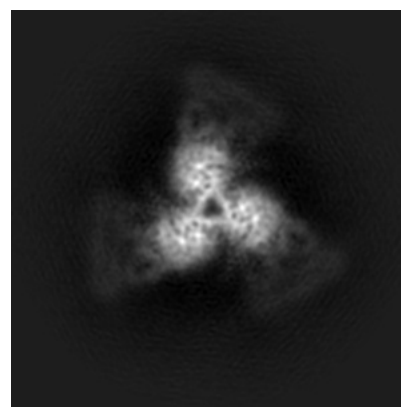
#### 6.1.2 Raw map



X



Y

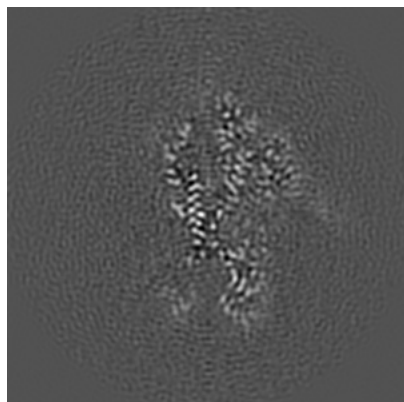


Z

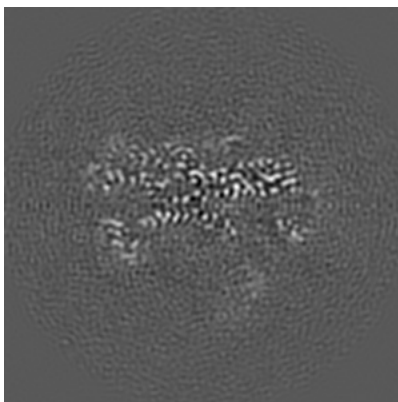
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

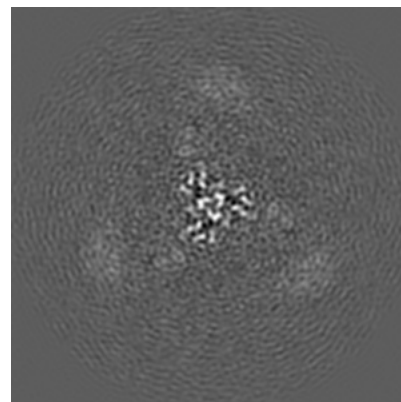
### 6.2.1 Primary map



X Index: 75

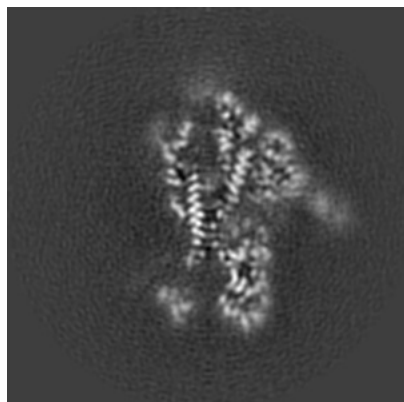


Y Index: 75

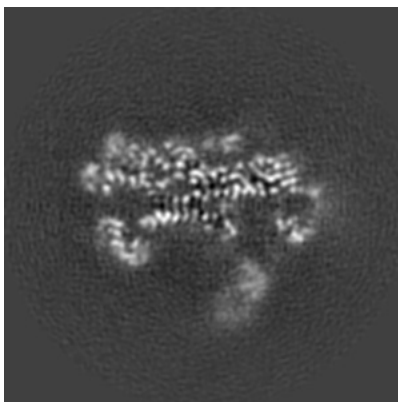


Z Index: 75

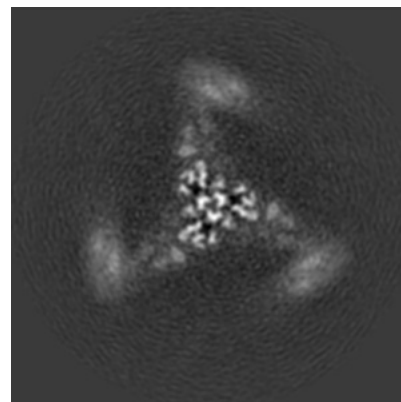
### 6.2.2 Raw map



X Index: 75



Y Index: 75

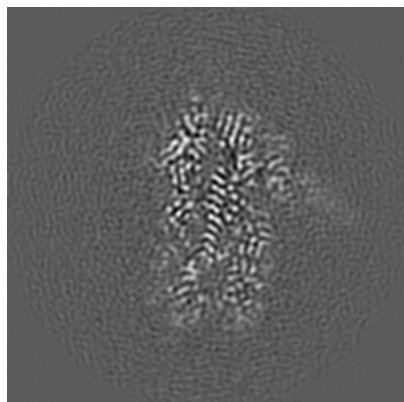


Z Index: 75

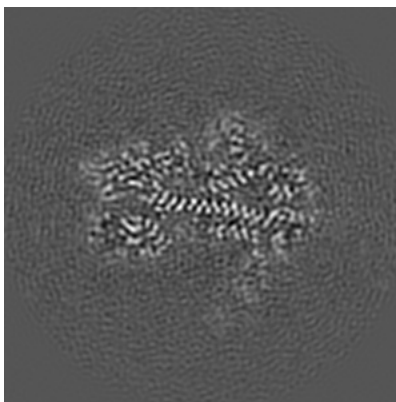
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

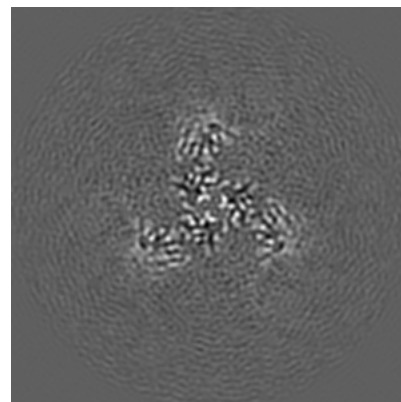
### 6.3.1 Primary map



X Index: 70

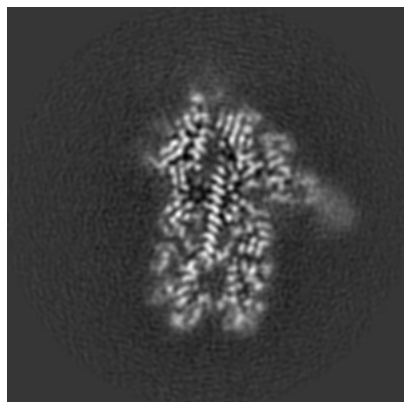


Y Index: 70

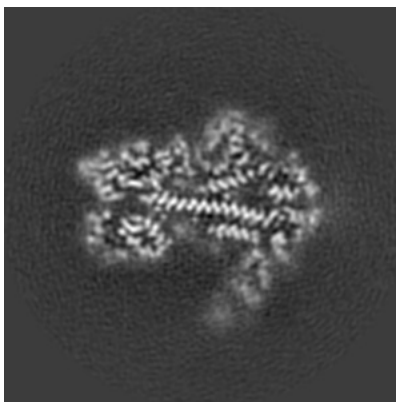


Z Index: 86

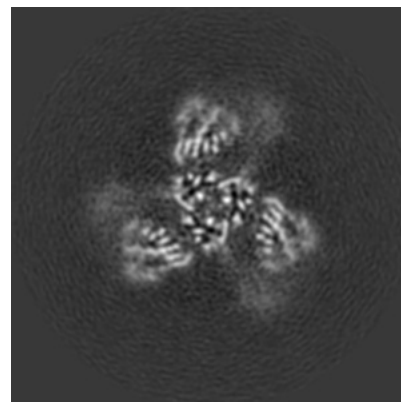
### 6.3.2 Raw map



X Index: 70



Y Index: 70

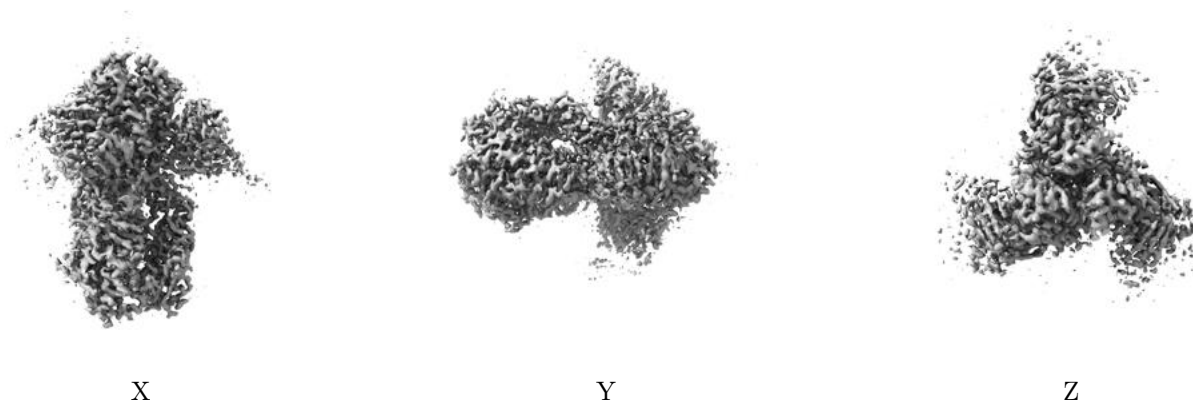


Z Index: 85

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

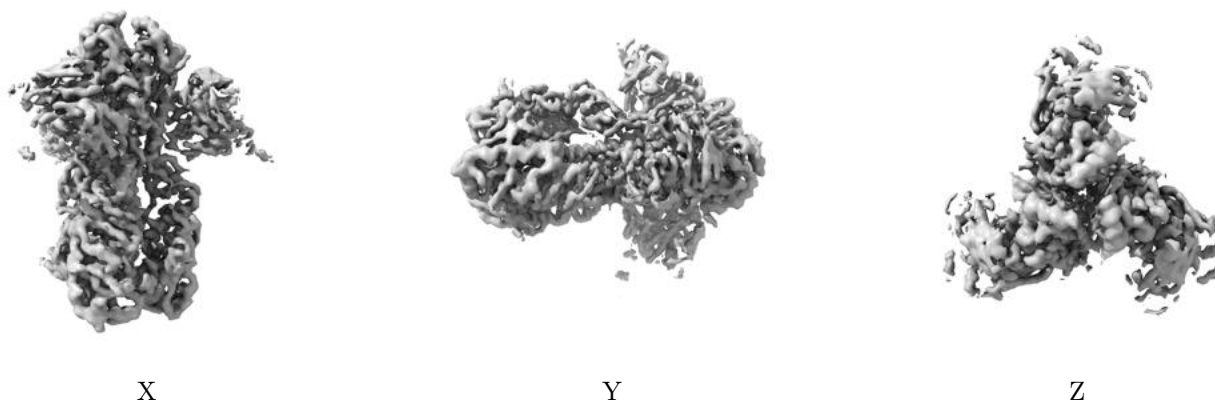
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

## 6.5 Mask visualisation [i](#)

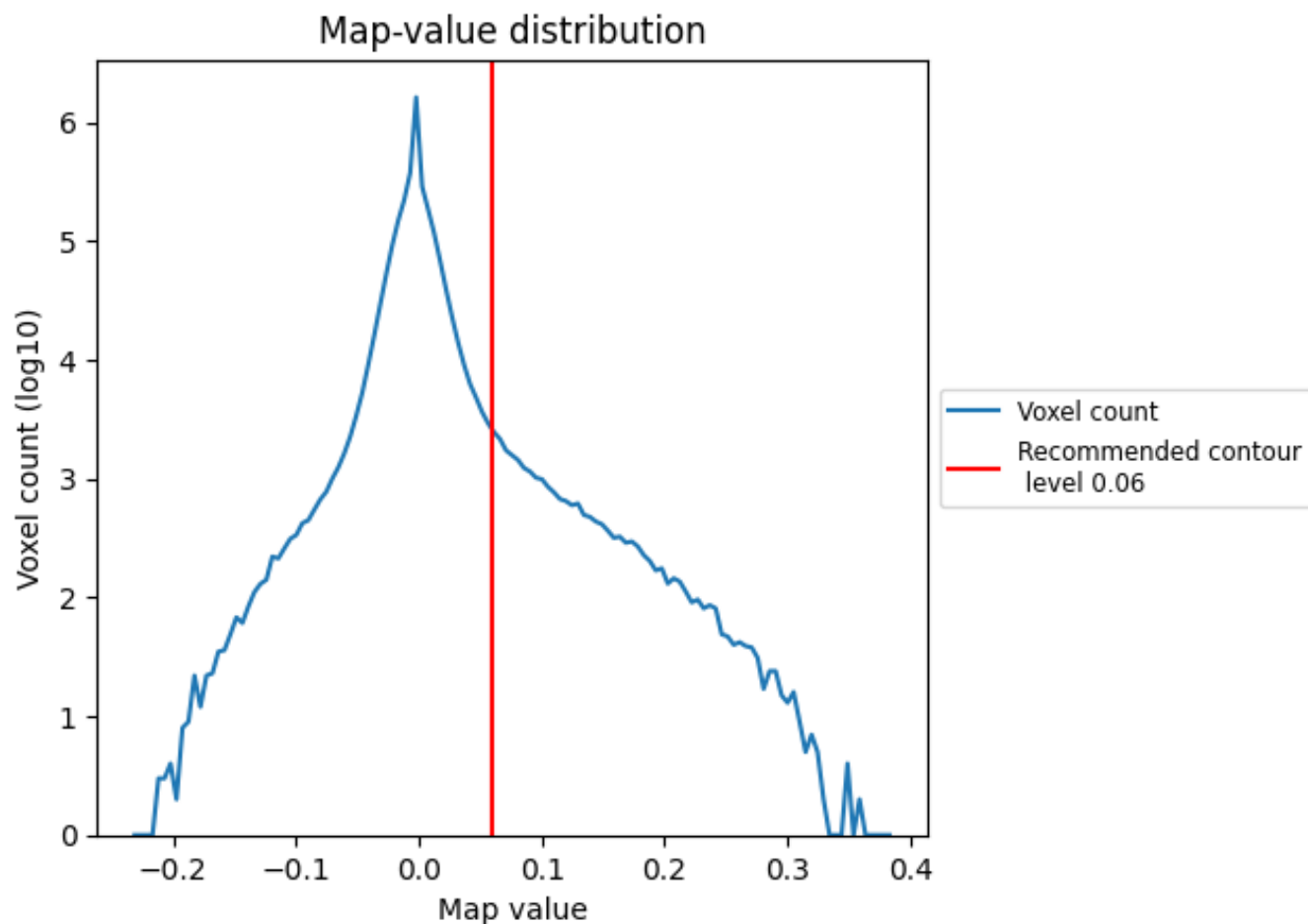
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

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

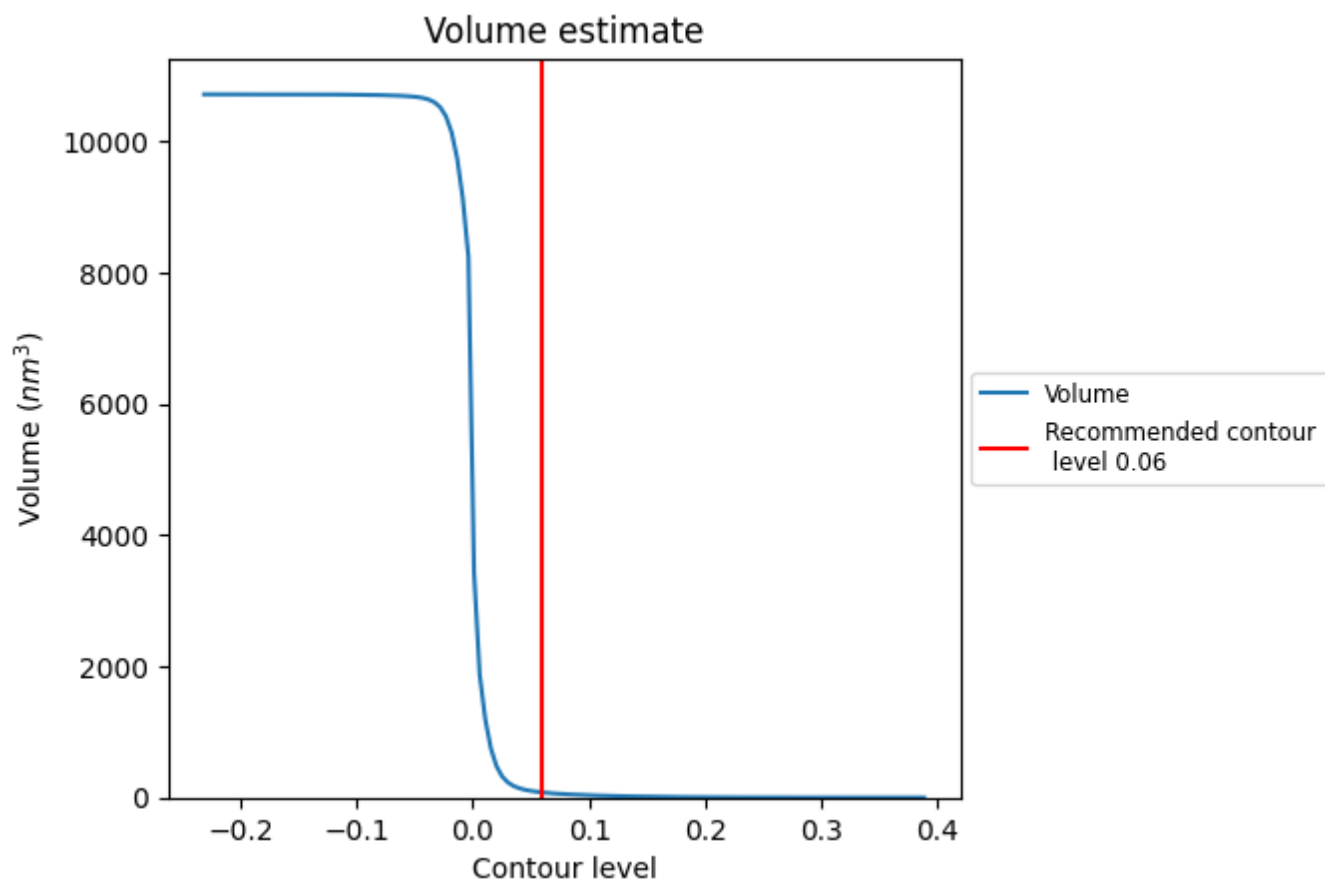
### 7.1 Map-value distribution [i](#)



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.



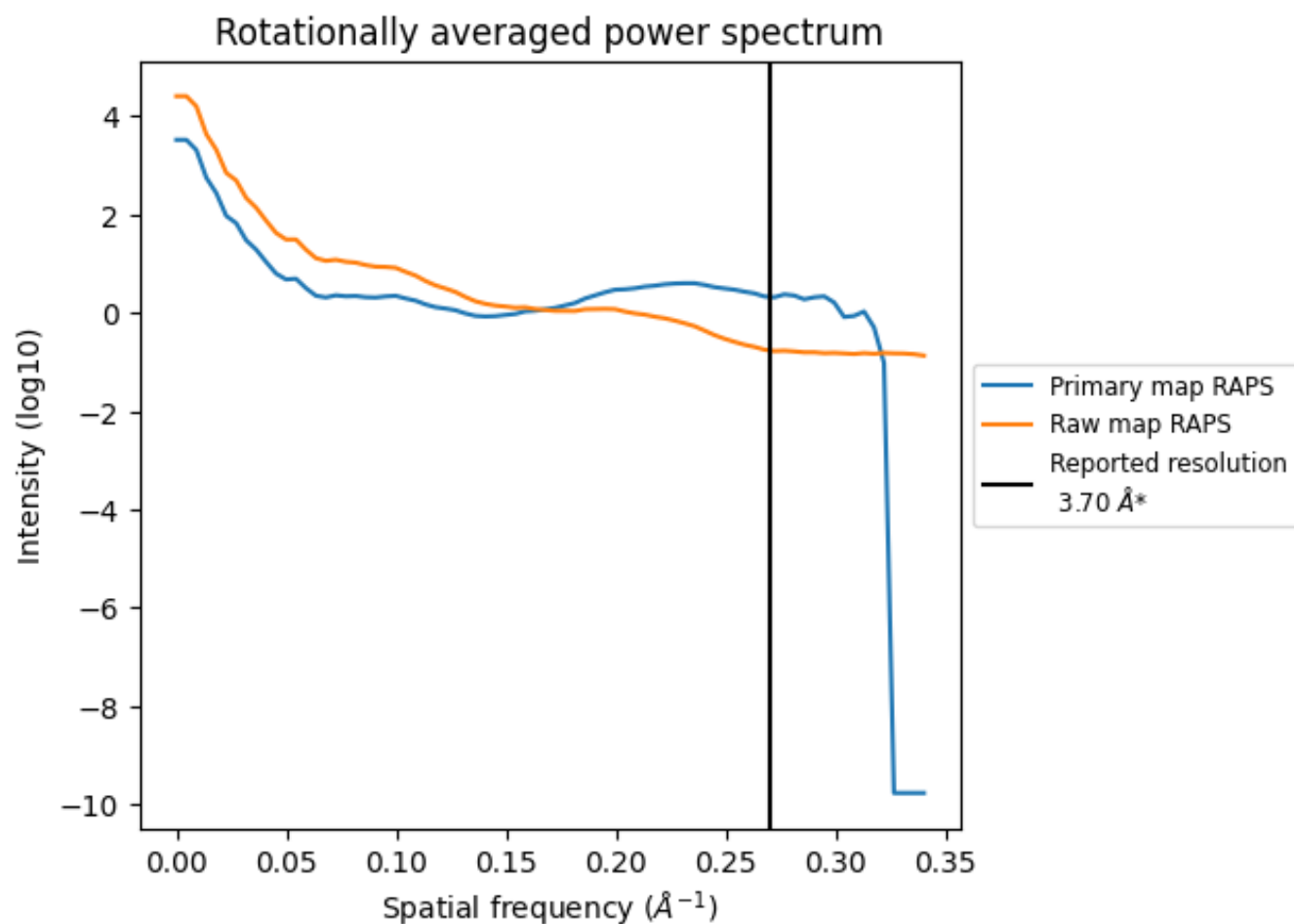
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 78 nm<sup>3</sup>; this corresponds to an approximate mass of 71 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 ⓘ

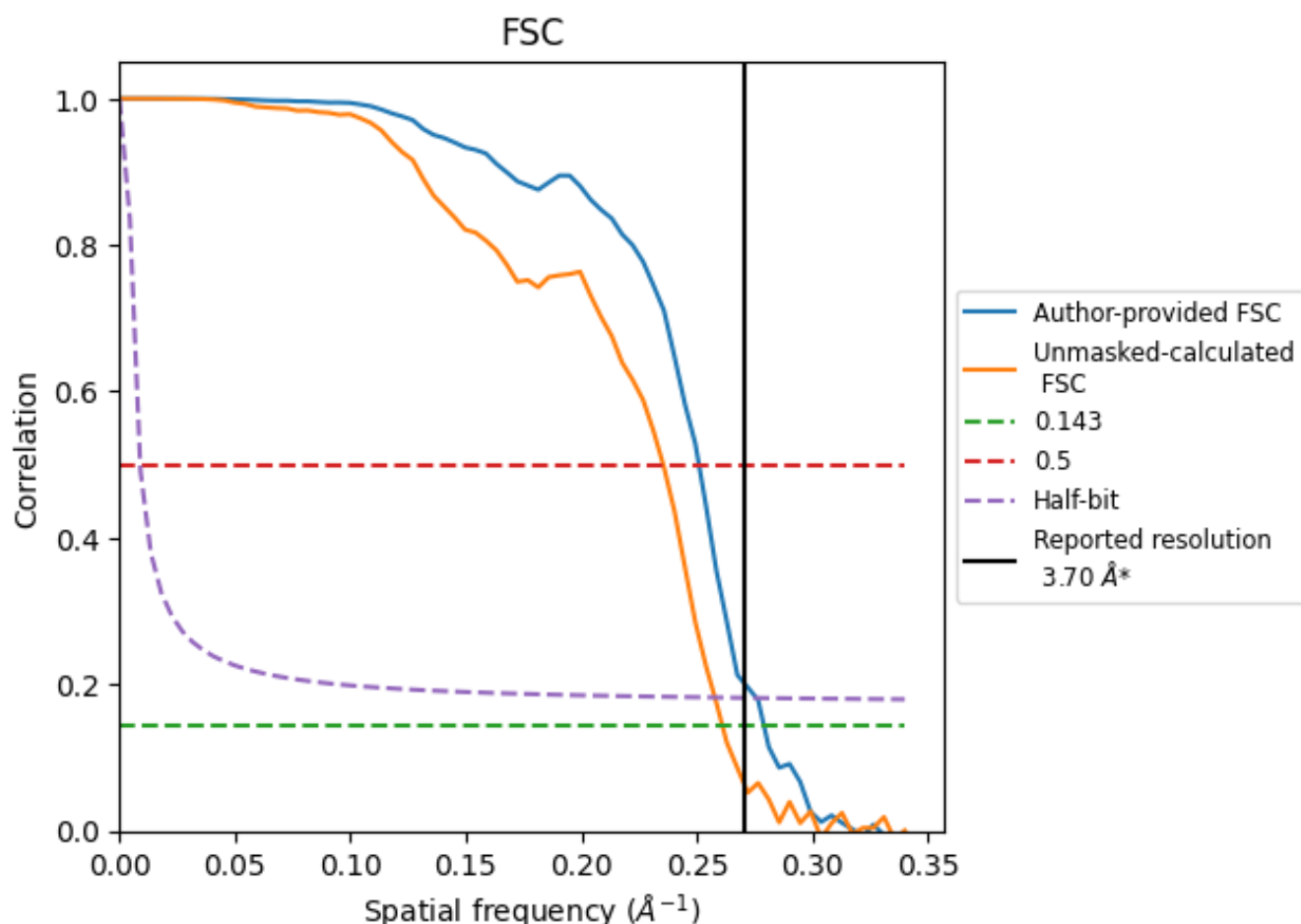


\*Reported resolution corresponds to spatial frequency of 0.270 Å<sup>-1</sup>

## 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 0.270  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

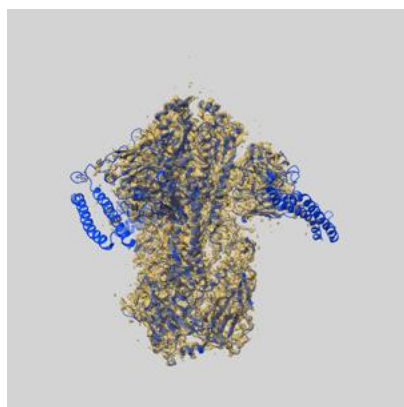
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.58	3.98	3.62
Unmasked-calculated*	3.83	4.25	3.88

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

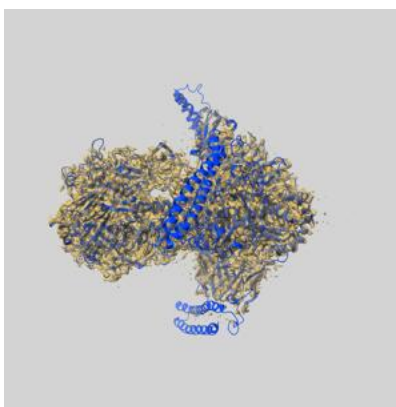
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30707 and PDB model 7DKJ. Per-residue inclusion information can be found in section 3 on page 14.

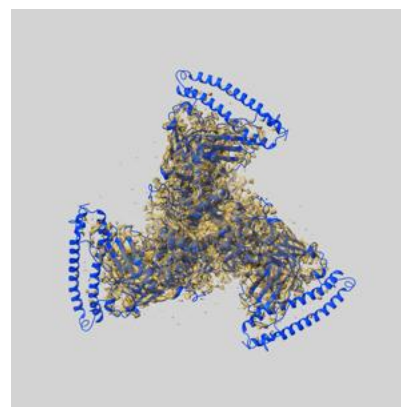
### 9.1 Map-model overlay [i](#)



X



Y



Z

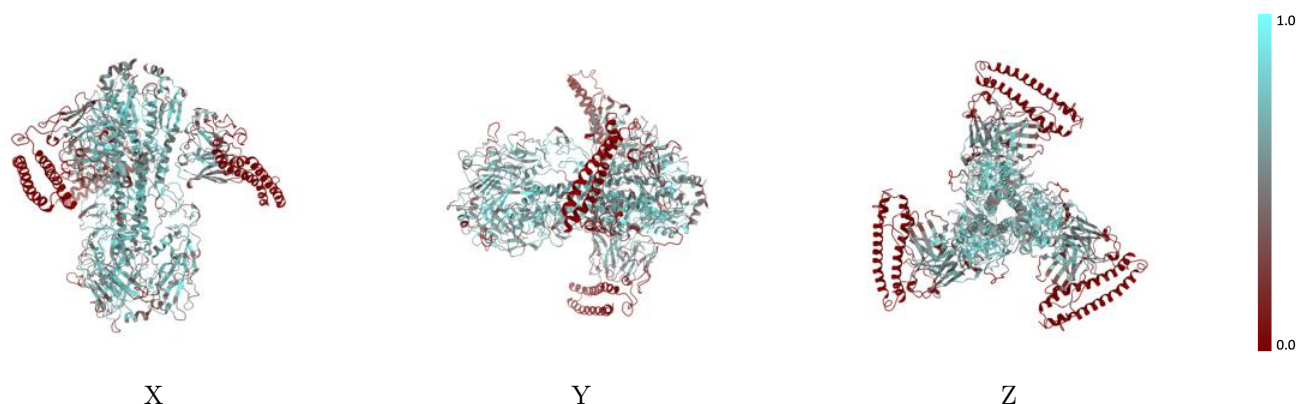
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



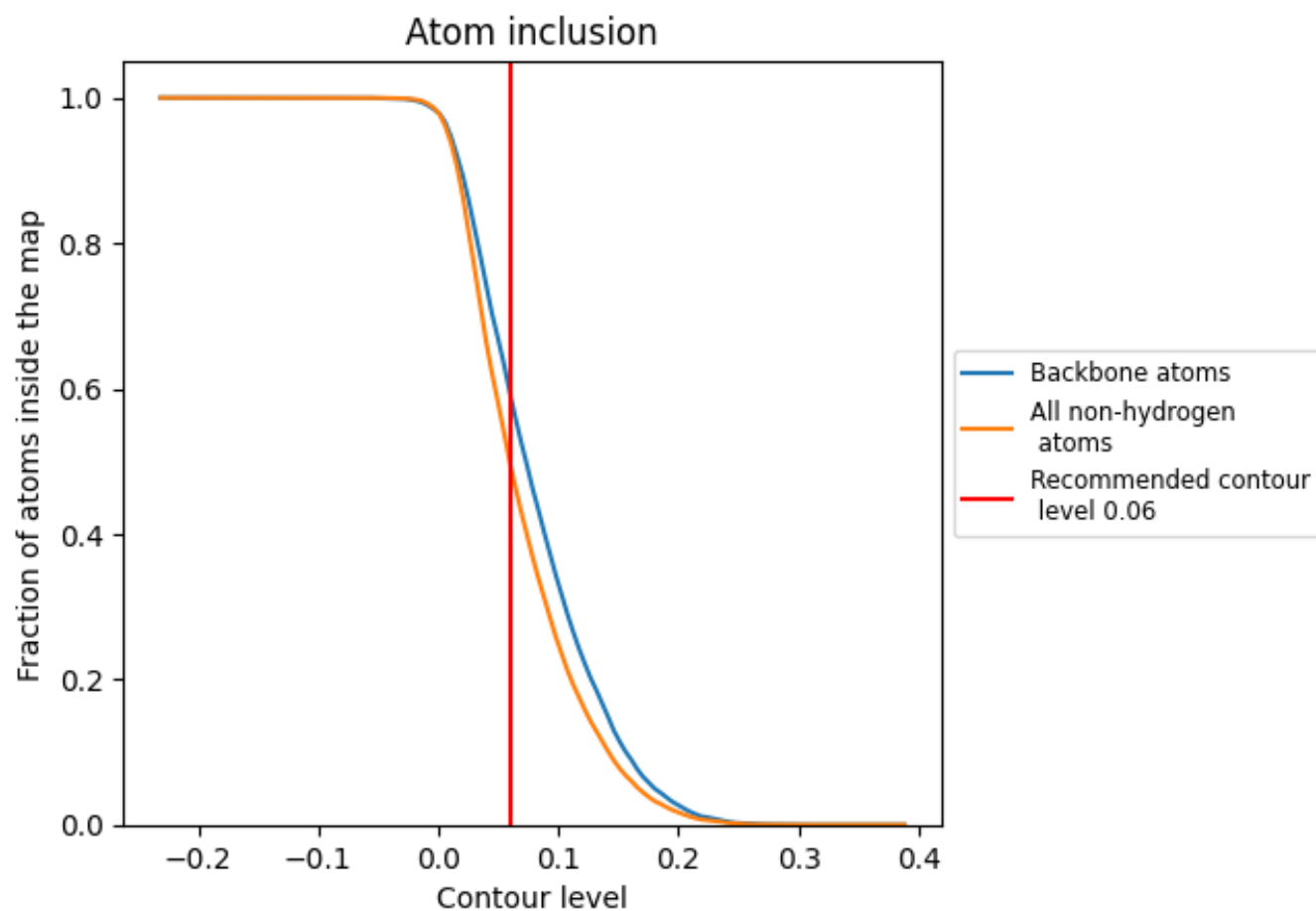
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 49% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4943	<div></div> 0.4160
A	<div></div> 0.6265	<div></div> 0.4710
B	<div></div> 0.2821	<div></div> 0.3310
C	<div></div> 0.3415	<div></div> 0.3420
D	<div></div> 0.2536	<div></div> 0.3190
E	<div></div> 0.6306	<div></div> 0.4710
F	<div></div> 0.2308	<div></div> 0.3680
G	<div></div> 0.3333	<div></div> 0.3420
H	<div></div> 0.2609	<div></div> 0.3240
I	<div></div> 0.6252	<div></div> 0.4700
J	<div></div> 0.2308	<div></div> 0.2990
K	<div></div> 0.3304	<div></div> 0.3450
L	<div></div> 0.2642	<div></div> 0.3340
M	<div></div> 0.2564	<div></div> 0.3550
N	<div></div> 0.2564	<div></div> 0.2960
O	<div></div> 0.2308	<div></div> 0.3340

