



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 02:54 PM UTC

PDB ID : 8YZ6 / pdb_00008yz6
EMDB ID : EMD-39686
Title : SARS-CoV-2 Spike (BA.1) in complex with Fab of JH-8B
Authors : Chen, X.; Wu, Y.-M.
Deposited on : 2024-04-06
Resolution : 4.55 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
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

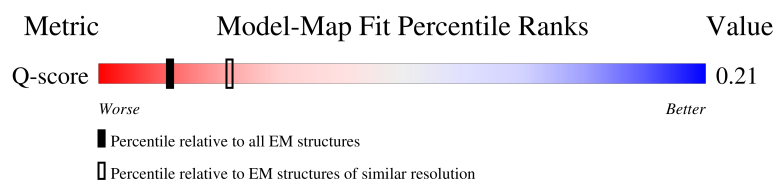
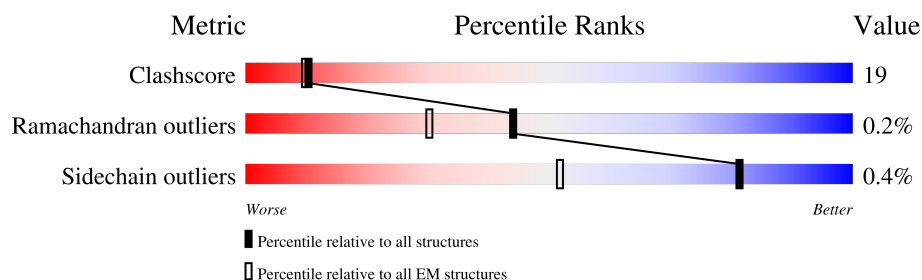
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.55 Å.

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



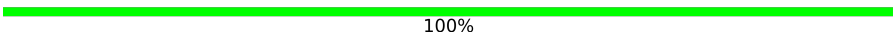
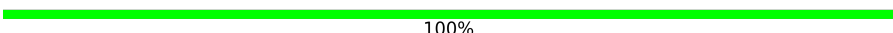
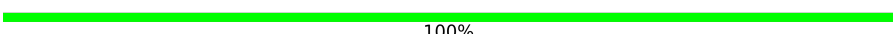
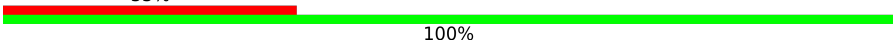
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2458 (4.05 - 5.04)

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	1261	15% 47% 29% 24%
1	B	1261	15% 49% 28% 22%
1	C	1261	17% 53% 25% 21%
2	D	119	51% 55% 43% ..

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Mol	Chain	Length	Quality of chain
3	E	110	
4	F	2	
4	L	2	
4	N	2	
4	U	2	
5	T	3	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24972 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	959	Total	C	N	O	S	0	0
			7521	4826	1255	1408	32		
1	B	984	Total	C	N	O	S	0	0
			7704	4944	1281	1446	33		
1	C	990	Total	C	N	O	S	0	0
			7773	4982	1296	1461	34		

There are 333 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP P0DTC2
A	-4	LYS	-	expression tag	UNP P0DTC2
A	-3	VAL	-	expression tag	UNP P0DTC2
A	-2	LYS	-	expression tag	UNP P0DTC2
A	-1	LEU	-	expression tag	UNP P0DTC2
A	0	LEU	-	expression tag	UNP P0DTC2
A	1	VAL	-	expression tag	UNP P0DTC2
A	2	LEU	-	expression tag	UNP P0DTC2
A	3	LEU	-	expression tag	UNP P0DTC2
A	4	CYS	-	expression tag	UNP P0DTC2
A	5	THR	-	expression tag	UNP P0DTC2
A	6	PHE	-	expression tag	UNP P0DTC2
A	7	THR	-	expression tag	UNP P0DTC2
A	8	ALA	-	expression tag	UNP P0DTC2
A	9	THR	-	expression tag	UNP P0DTC2
A	10	TYR	-	expression tag	UNP P0DTC2
A	11	ALA	-	expression tag	UNP P0DTC2
A	12	GLY	-	expression tag	UNP P0DTC2
A	13	THR	-	expression tag	UNP P0DTC2
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	variant	UNP P0DTC2
A	145	ASP	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	210A	ILE	LEU	variant	UNP P0DTC2
A	210D	GLU	-	insertion	UNP P0DTC2
A	210E	PRO	-	insertion	UNP P0DTC2
A	210F	GLU	-	insertion	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2
A	496	SER	GLY	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	547	LYS	THR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	variant	UNP P0DTC2
A	683	SER	ARG	variant	UNP P0DTC2
A	685	SER	ARG	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	856	LYS	ASN	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	981	PHE	LEU	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1211	LYS	-	expression tag	UNP P0DTC2
A	1212	ASP	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1214	ARG	-	expression tag	UNP P0DTC2
A	1215	SER	-	expression tag	UNP P0DTC2
A	1216	LEU	-	expression tag	UNP P0DTC2
A	1217	VAL	-	expression tag	UNP P0DTC2
A	1218	PRO	-	expression tag	UNP P0DTC2
A	1219	ARG	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	SER	-	expression tag	UNP P0DTC2
A	1222	PRO	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	SER	-	expression tag	UNP P0DTC2
A	1225	GLY	-	expression tag	UNP P0DTC2
A	1226	TYR	-	expression tag	UNP P0DTC2
A	1227	ILE	-	expression tag	UNP P0DTC2
A	1228	PRO	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	ALA	-	expression tag	UNP P0DTC2
A	1231	PRO	-	expression tag	UNP P0DTC2
A	1232	ARG	-	expression tag	UNP P0DTC2
A	1233	ASP	-	expression tag	UNP P0DTC2
A	1234	GLY	-	expression tag	UNP P0DTC2
A	1235	GLN	-	expression tag	UNP P0DTC2
A	1236	ALA	-	expression tag	UNP P0DTC2
A	1237	TYR	-	expression tag	UNP P0DTC2
A	1238	VAL	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	LYS	-	expression tag	UNP P0DTC2
A	1241	ASP	-	expression tag	UNP P0DTC2
A	1242	GLY	-	expression tag	UNP P0DTC2
A	1243	GLU	-	expression tag	UNP P0DTC2
A	1244	TRP	-	expression tag	UNP P0DTC2
A	1245	VAL	-	expression tag	UNP P0DTC2
A	1246	LEU	-	expression tag	UNP P0DTC2
A	1247	LEU	-	expression tag	UNP P0DTC2
A	1248	SER	-	expression tag	UNP P0DTC2
A	1249	THR	-	expression tag	UNP P0DTC2
A	1250	PHE	-	expression tag	UNP P0DTC2
A	1251	LEU	-	expression tag	UNP P0DTC2
A	1252	GLY	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2
B	-5	MET	-	initiating methionine	UNP P0DTC2
B	-4	LYS	-	expression tag	UNP P0DTC2
B	-3	VAL	-	expression tag	UNP P0DTC2
B	-2	LYS	-	expression tag	UNP P0DTC2
B	-1	LEU	-	expression tag	UNP P0DTC2
B	0	LEU	-	expression tag	UNP P0DTC2
B	1	VAL	-	expression tag	UNP P0DTC2
B	2	LEU	-	expression tag	UNP P0DTC2
B	3	LEU	-	expression tag	UNP P0DTC2
B	4	CYS	-	expression tag	UNP P0DTC2
B	5	THR	-	expression tag	UNP P0DTC2
B	6	PHE	-	expression tag	UNP P0DTC2
B	7	THR	-	expression tag	UNP P0DTC2
B	8	ALA	-	expression tag	UNP P0DTC2
B	9	THR	-	expression tag	UNP P0DTC2
B	10	TYR	-	expression tag	UNP P0DTC2
B	11	ALA	-	expression tag	UNP P0DTC2
B	12	GLY	-	expression tag	UNP P0DTC2
B	13	THR	-	expression tag	UNP P0DTC2
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	variant	UNP P0DTC2
B	145	ASP	GLY	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	210A	ILE	LEU	variant	UNP P0DTC2
B	210D	GLU	-	insertion	UNP P0DTC2
B	210E	PRO	-	insertion	UNP P0DTC2
B	210F	GLU	-	insertion	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	496	SER	GLY	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	547	LYS	THR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	variant	UNP P0DTC2
B	683	SER	ARG	variant	UNP P0DTC2
B	685	SER	ARG	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	856	LYS	ASN	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	981	PHE	LEU	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1211	LYS	-	expression tag	UNP P0DTC2
B	1212	ASP	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	ARG	-	expression tag	UNP P0DTC2
B	1215	SER	-	expression tag	UNP P0DTC2
B	1216	LEU	-	expression tag	UNP P0DTC2
B	1217	VAL	-	expression tag	UNP P0DTC2
B	1218	PRO	-	expression tag	UNP P0DTC2
B	1219	ARG	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	SER	-	expression tag	UNP P0DTC2
B	1222	PRO	-	expression tag	UNP P0DTC2
B	1223	GLY	-	expression tag	UNP P0DTC2
B	1224	SER	-	expression tag	UNP P0DTC2
B	1225	GLY	-	expression tag	UNP P0DTC2
B	1226	TYR	-	expression tag	UNP P0DTC2
B	1227	ILE	-	expression tag	UNP P0DTC2
B	1228	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	ALA	-	expression tag	UNP P0DTC2
B	1231	PRO	-	expression tag	UNP P0DTC2
B	1232	ARG	-	expression tag	UNP P0DTC2
B	1233	ASP	-	expression tag	UNP P0DTC2
B	1234	GLY	-	expression tag	UNP P0DTC2
B	1235	GLN	-	expression tag	UNP P0DTC2
B	1236	ALA	-	expression tag	UNP P0DTC2
B	1237	TYR	-	expression tag	UNP P0DTC2
B	1238	VAL	-	expression tag	UNP P0DTC2
B	1239	ARG	-	expression tag	UNP P0DTC2
B	1240	LYS	-	expression tag	UNP P0DTC2
B	1241	ASP	-	expression tag	UNP P0DTC2
B	1242	GLY	-	expression tag	UNP P0DTC2
B	1243	GLU	-	expression tag	UNP P0DTC2
B	1244	TRP	-	expression tag	UNP P0DTC2
B	1245	VAL	-	expression tag	UNP P0DTC2
B	1246	LEU	-	expression tag	UNP P0DTC2
B	1247	LEU	-	expression tag	UNP P0DTC2
B	1248	SER	-	expression tag	UNP P0DTC2
B	1249	THR	-	expression tag	UNP P0DTC2
B	1250	PHE	-	expression tag	UNP P0DTC2
B	1251	LEU	-	expression tag	UNP P0DTC2
B	1252	GLY	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	HIS	-	expression tag	UNP P0DTC2
C	-5	MET	-	initiating methionine	UNP P0DTC2
C	-4	LYS	-	expression tag	UNP P0DTC2
C	-3	VAL	-	expression tag	UNP P0DTC2
C	-2	LYS	-	expression tag	UNP P0DTC2
C	-1	LEU	-	expression tag	UNP P0DTC2
C	0	LEU	-	expression tag	UNP P0DTC2
C	1	VAL	-	expression tag	UNP P0DTC2
C	2	LEU	-	expression tag	UNP P0DTC2
C	3	LEU	-	expression tag	UNP P0DTC2
C	4	CYS	-	expression tag	UNP P0DTC2
C	5	THR	-	expression tag	UNP P0DTC2
C	6	PHE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	7	THR	-	expression tag	UNP P0DTC2
C	8	ALA	-	expression tag	UNP P0DTC2
C	9	THR	-	expression tag	UNP P0DTC2
C	10	TYR	-	expression tag	UNP P0DTC2
C	11	ALA	-	expression tag	UNP P0DTC2
C	12	GLY	-	expression tag	UNP P0DTC2
C	13	THR	-	expression tag	UNP P0DTC2
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	210A	ILE	LEU	variant	UNP P0DTC2
C	210D	GLU	-	insertion	UNP P0DTC2
C	210E	PRO	-	insertion	UNP P0DTC2
C	210F	GLU	-	insertion	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	LEU	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	496	SER	GLY	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	547	LYS	THR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	variant	UNP P0DTC2
C	683	SER	ARG	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	685	SER	ARG	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	856	LYS	ASN	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	981	PHE	LEU	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1211	LYS	-	expression tag	UNP P0DTC2
C	1212	ASP	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	ARG	-	expression tag	UNP P0DTC2
C	1215	SER	-	expression tag	UNP P0DTC2
C	1216	LEU	-	expression tag	UNP P0DTC2
C	1217	VAL	-	expression tag	UNP P0DTC2
C	1218	PRO	-	expression tag	UNP P0DTC2
C	1219	ARG	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	SER	-	expression tag	UNP P0DTC2
C	1222	PRO	-	expression tag	UNP P0DTC2
C	1223	GLY	-	expression tag	UNP P0DTC2
C	1224	SER	-	expression tag	UNP P0DTC2
C	1225	GLY	-	expression tag	UNP P0DTC2
C	1226	TYR	-	expression tag	UNP P0DTC2
C	1227	ILE	-	expression tag	UNP P0DTC2
C	1228	PRO	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	ALA	-	expression tag	UNP P0DTC2
C	1231	PRO	-	expression tag	UNP P0DTC2
C	1232	ARG	-	expression tag	UNP P0DTC2
C	1233	ASP	-	expression tag	UNP P0DTC2
C	1234	GLY	-	expression tag	UNP P0DTC2
C	1235	GLN	-	expression tag	UNP P0DTC2
C	1236	ALA	-	expression tag	UNP P0DTC2
C	1237	TYR	-	expression tag	UNP P0DTC2
C	1238	VAL	-	expression tag	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP P0DTC2
C	1240	LYS	-	expression tag	UNP P0DTC2
C	1241	ASP	-	expression tag	UNP P0DTC2
C	1242	GLY	-	expression tag	UNP P0DTC2
C	1243	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1244	TRP	-	expression tag	UNP P0DTC2
C	1245	VAL	-	expression tag	UNP P0DTC2
C	1246	LEU	-	expression tag	UNP P0DTC2
C	1247	LEU	-	expression tag	UNP P0DTC2
C	1248	SER	-	expression tag	UNP P0DTC2
C	1249	THR	-	expression tag	UNP P0DTC2
C	1250	PHE	-	expression tag	UNP P0DTC2
C	1251	LEU	-	expression tag	UNP P0DTC2
C	1252	GLY	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Fab heavy chain of JH-8B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	118	Total	C	N	O	S	0	0
			888	554	151	178	5		

- Molecule 3 is a protein called Fab light chain of JH-8B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	110	Total	C	N	O	S	0	0
			837	529	139	167	2		

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



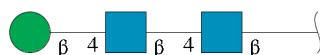
Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	2	Total	C	N	O		0	0
			28	16	2	10			
4	L	2	Total	C	N	O		0	0
			28	16	2	10			
4	N	2	Total	C	N	O		0	0
			28	16	2	10			

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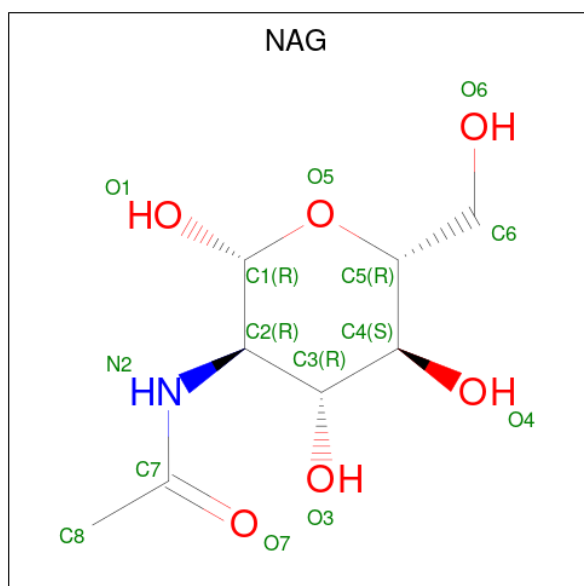
Mol	Chain	Residues	Atoms				AltConf	Trace
4	U	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 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
5	T	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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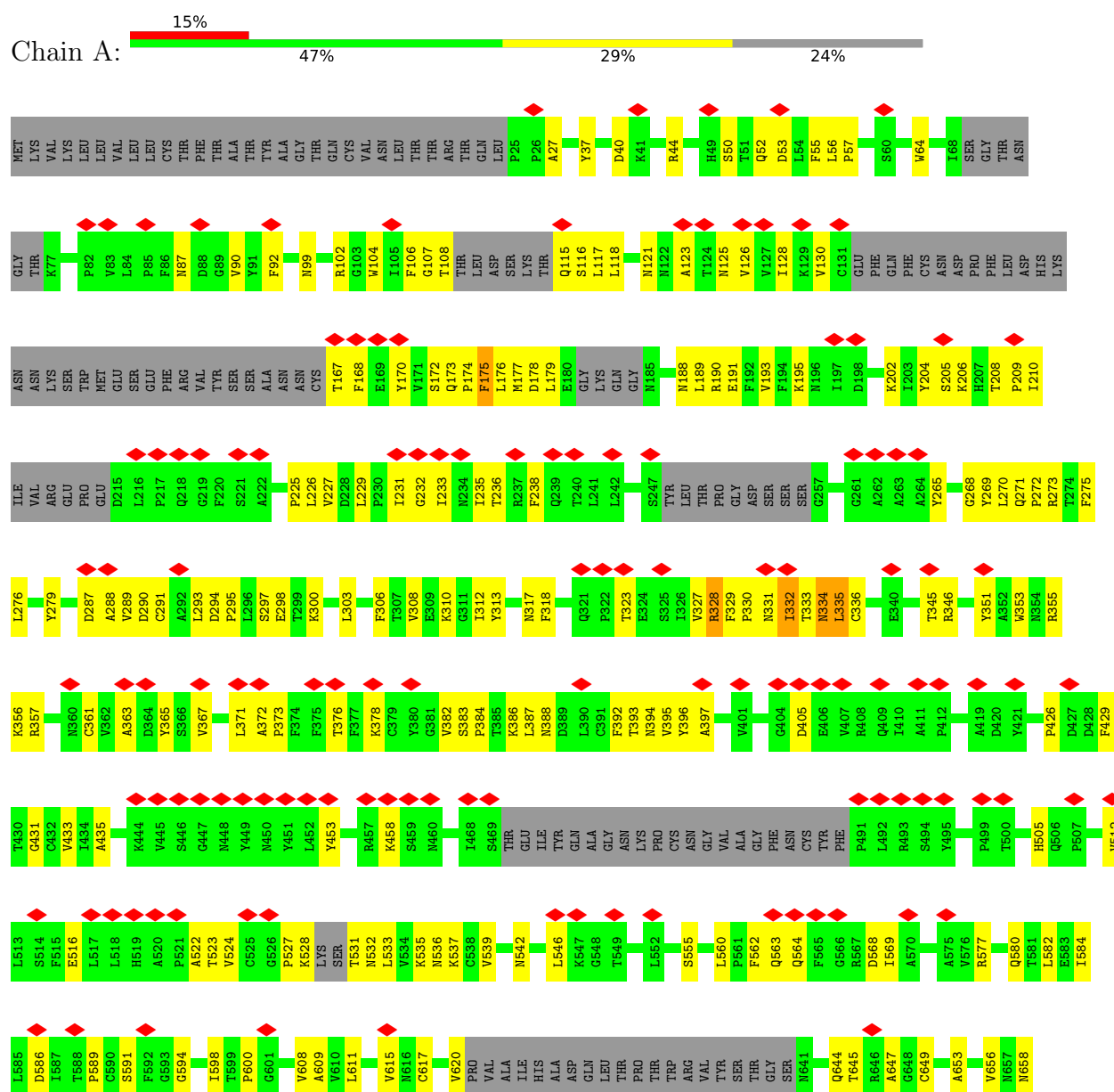
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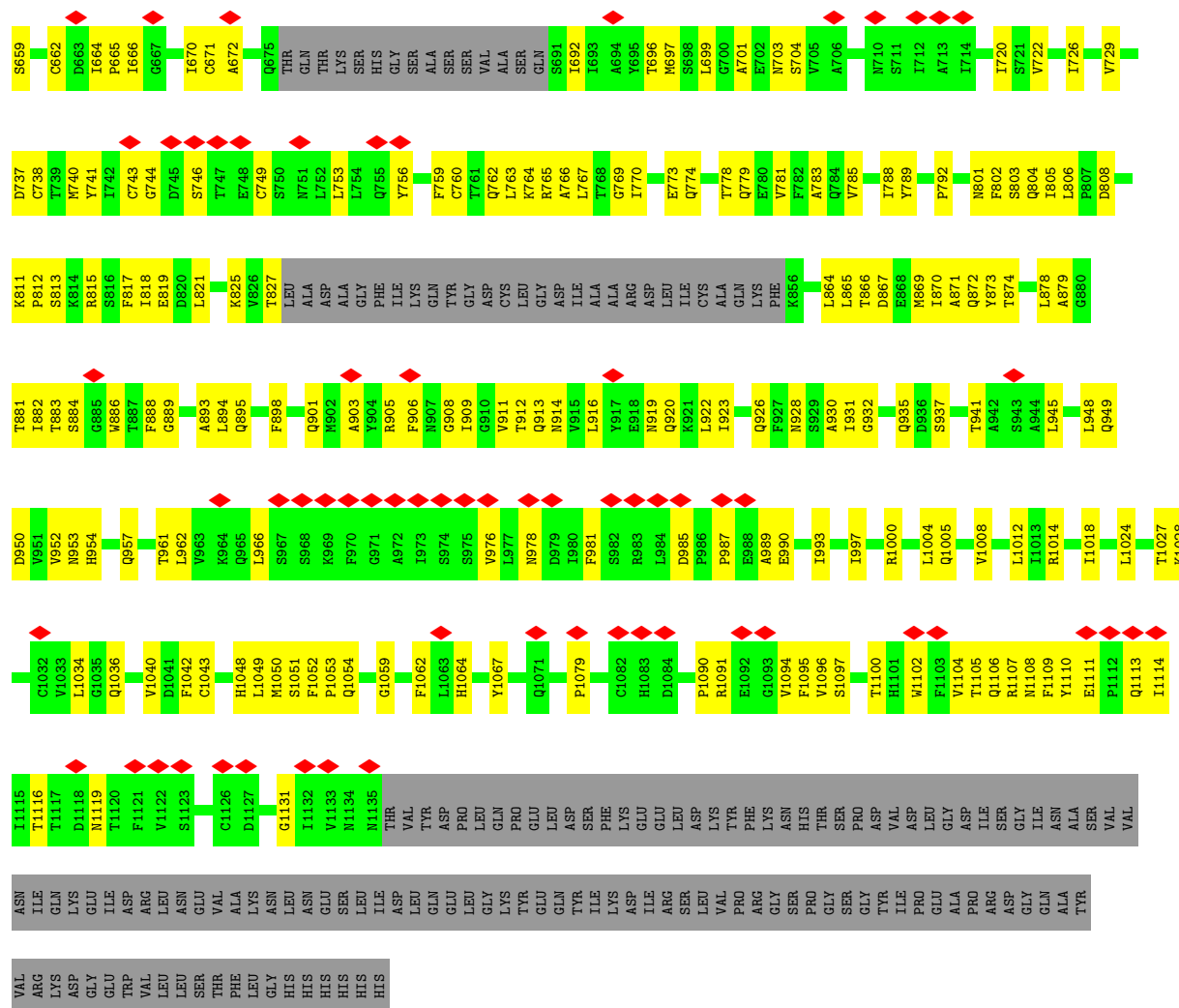
Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots

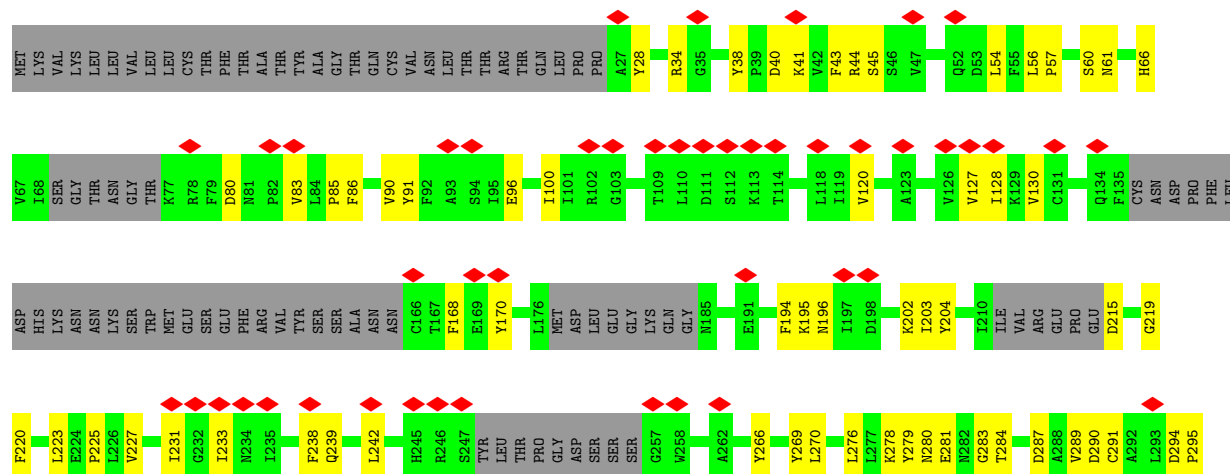
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Spike glycoprotein



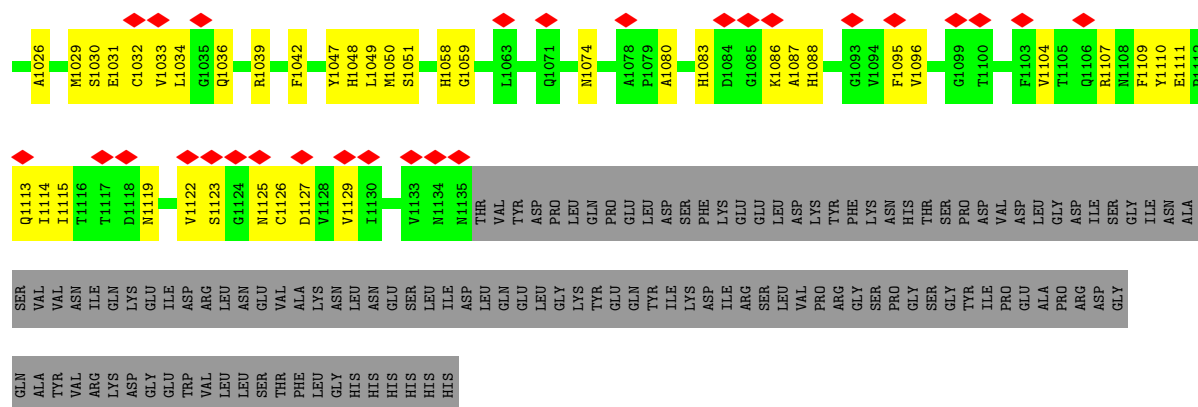


• Molecule 1: Spike glycoprotein

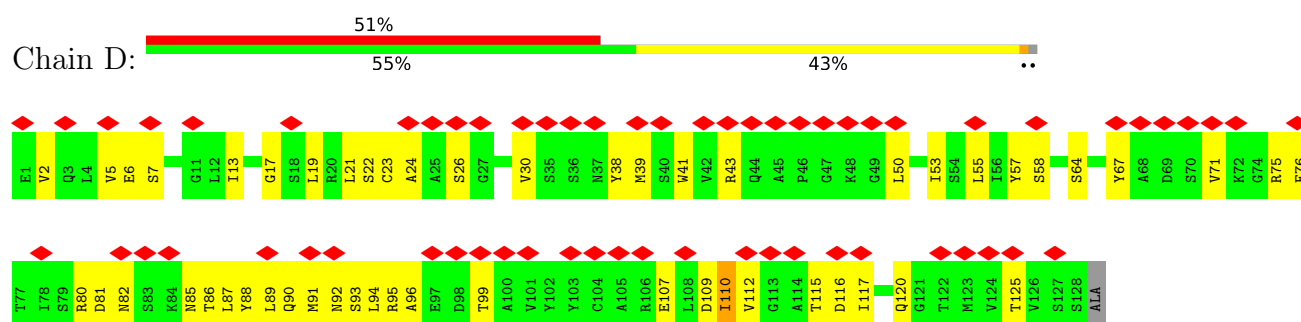




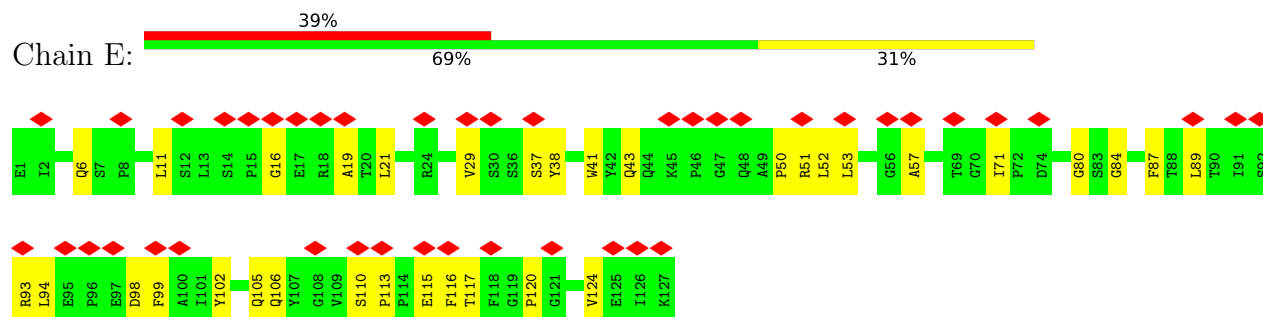




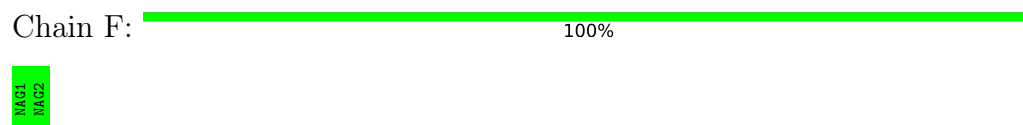
- Molecule 2: Fab heavy chain of JH-8B



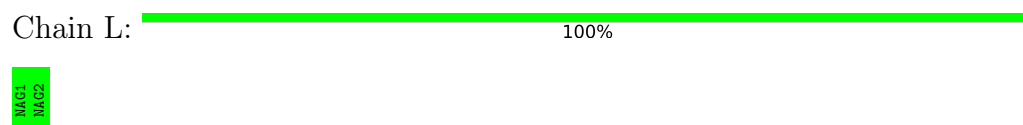
- Molecule 3: Fab light chain of JH-8B



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



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



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

Chain N:  100%

NAG1
NAG2

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

Chain U:  100%

NAG1
NAG2

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

Chain T:  33%  100%


NAG1
NAG2
BNA3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93991	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 ($e^-/\text{\AA}^2$)	1.1	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.035	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0029	Depositor
Map size (Å)	318.72, 318.72, 318.72	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA

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	0.21	0/7692	0.39	0/10453
1	B	0.20	0/7880	0.39	1/10711 (0.0%)
1	C	0.16	0/7951	0.35	0/10805
2	D	0.13	0/903	0.39	0/1224
3	E	0.13	0/858	0.35	0/1165
All	All	0.18	0/25284	0.38	1/34358 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	373	PRO	CA-N-CD	-9.01	99.38	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7521	0	7398	343	0
1	B	7704	0	7544	328	0
1	C	7773	0	7628	241	0
2	D	888	0	868	44	0
3	E	837	0	815	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	28	0	25	0	0
4	L	28	0	25	0	0
4	N	28	0	25	0	0
4	U	28	0	25	0	0
5	T	39	0	34	0	0
6	A	42	0	39	1	0
6	B	42	0	39	2	0
6	C	14	0	13	0	0
All	All	24972	0	24478	938	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 19.

All (938) 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:A:106:PHE:HB2	1:A:117:LEU:O	1.23	1.29
1:A:170:TYR:OH	1:A:227:VAL:HG11	1.28	1.29
1:A:168:PHE:HZ	1:A:229:LEU:CG	1.44	1.28
1:A:106:PHE:O	1:A:116:SER:HB3	1.23	1.26
1:A:168:PHE:CE1	1:A:229:LEU:HB3	1.71	1.24
1:A:168:PHE:CZ	1:A:229:LEU:HB3	1.74	1.23
1:A:168:PHE:CZ	1:A:229:LEU:CG	2.28	1.15
1:A:168:PHE:CZ	1:A:229:LEU:HG	1.83	1.14
1:A:115:GLN:HE22	1:A:167:THR:HB	1.09	1.13
1:A:168:PHE:CZ	1:A:229:LEU:CB	2.31	1.12
1:A:170:TYR:OH	1:A:227:VAL:CG1	1.96	1.11
1:B:455:LEU:HD22	1:B:493:ARG:HD2	1.16	1.09
1:A:168:PHE:HZ	1:A:229:LEU:HG	0.92	1.05
1:B:215:ASP:N	1:B:266:TYR:HH	1.54	1.03
1:A:168:PHE:CE1	1:A:229:LEU:HD12	2.00	0.97
1:A:106:PHE:CB	1:A:117:LEU:O	2.12	0.96
1:B:455:LEU:CD2	1:B:493:ARG:HD2	1.99	0.93
1:B:371:LEU:C	1:B:373:PRO:HD3	1.93	0.92
1:A:57:PRO:HG3	1:A:271:GLN:HE22	1.35	0.92
1:B:367:VAL:O	1:B:371:LEU:HG	1.72	0.90
1:B:906:PHE:HB3	1:B:911:VAL:HB	1.55	0.88
1:B:1006:THR:HG22	1:B:1010:GLN:HE22	1.37	0.86
1:C:57:PRO:HG3	1:C:271:GLN:HE22	1.40	0.86
1:A:115:GLN:NE2	1:A:167:THR:HB	1.81	0.86
1:C:960:ASN:OD1	1:C:964:LYS:NZ	2.08	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:LEU:HD22	1:B:493:ARG:CD	2.04	0.84
1:A:168:PHE:CE1	1:A:229:LEU:CB	2.56	0.83
1:A:300:LYS:HD2	1:A:306:PHE:HA	1.61	0.82
1:A:770:ILE:HG22	1:A:774:GLN:HE22	1.43	0.82
1:A:106:PHE:O	1:A:116:SER:CB	2.19	0.82
1:B:811:LYS:NZ	1:B:813:SER:OG	2.12	0.82
1:A:170:TYR:CZ	1:A:227:VAL:HG11	2.15	0.81
1:A:170:TYR:CD1	1:A:229:LEU:HD11	2.17	0.80
1:B:1002:GLN:NE2	1:C:1002:GLN:OE1	2.14	0.80
1:B:1067:TYR:HH	1:B:1109:PHE:HZ	1.26	0.80
1:B:371:LEU:CB	1:B:373:PRO:HD3	2.12	0.80
1:C:808:ASP:H	1:C:811:LYS:HE2	1.48	0.79
1:C:950:ASP:O	1:C:954:HIS:ND1	2.15	0.78
1:B:817:PHE:CZ	1:B:821:LEU:HD11	2.17	0.78
1:A:329:PHE:HB3	1:A:527:PRO:HA	1.66	0.78
1:C:1026:ALA:HA	1:C:1029:MET:HE2	1.64	0.77
1:B:950:ASP:O	1:B:954:HIS:ND1	2.18	0.76
1:A:1106:GLN:HE21	1:A:1109:PHE:HB3	1.51	0.76
1:A:195:LYS:HD2	1:A:202:LYS:HE2	1.67	0.76
1:B:381:GLY:HA3	1:B:430:THR:HA	1.68	0.76
1:A:394:ASN:OD1	1:A:395:VAL:N	2.19	0.75
1:A:168:PHE:CZ	1:A:229:LEU:CD1	2.70	0.75
1:A:866:THR:OG1	1:A:869:MET:SD	2.44	0.75
1:B:332:ILE:CG1	1:B:580:GLN:HE21	1.98	0.75
1:B:368:LEU:HA	1:B:371:LEU:CD1	2.17	0.75
1:B:455:LEU:HD23	1:B:493:ARG:HE	1.52	0.75
1:B:335:LEU:HD22	1:B:362:VAL:HB	1.69	0.74
1:A:290:ASP:HB3	1:A:293:LEU:HD23	1.68	0.74
1:B:375:PHE:CD2	1:B:508:TYR:HE2	2.05	0.74
1:B:339:ASP:OD1	6:B:1303:NAG:H2	1.87	0.73
1:A:170:TYR:CE2	1:A:172:SER:HB2	2.23	0.73
1:B:44:ARG:NH1	1:B:279:TYR:OH	2.21	0.73
1:C:937:SER:O	1:C:941:THR:HB	1.89	0.73
1:A:922:LEU:HG	1:A:926:GLN:HE22	1.52	0.72
1:C:799:GLY:O	1:C:928:ASN:ND2	2.22	0.72
1:C:733:LYS:NZ	1:C:862:PRO:O	2.23	0.72
1:A:895:GLN:NE2	1:C:708:SER:OG	2.23	0.72
1:A:1096:VAL:HG21	1:A:1110:TYR:HE1	1.55	0.71
1:B:498:ARG:HB2	1:B:501:TYR:CD2	2.25	0.71
1:B:309:GLU:O	1:B:313:TYR:OH	2.07	0.71
1:C:34:ARG:NH1	1:C:221:SER:OG	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:ARG:NH1	3:E:38:TYR:OH	2.23	0.71
1:A:168:PHE:CZ	1:A:229:LEU:HD12	2.25	0.70
1:B:372:ALA:N	1:B:373:PRO:HD3	2.05	0.70
1:A:121:ASN:HD21	1:A:177:MET:HB2	1.56	0.70
1:B:1031:GLU:HB3	1:B:1037:SER:HB2	1.72	0.70
1:B:367:VAL:HG12	1:B:371:LEU:HD21	1.74	0.70
1:B:804:GLN:NE2	1:B:817:PHE:CD2	2.59	0.70
1:A:168:PHE:CE1	1:A:229:LEU:CD1	2.75	0.69
1:B:659:SER:OG	1:B:696:THR:O	2.10	0.69
1:B:1030:SER:HA	1:B:1034:LEU:HB2	1.73	0.69
1:A:376:THR:HB	1:A:435:ALA:HB3	1.73	0.69
1:A:564:GLN:OE1	1:A:577:ARG:NH2	2.25	0.69
1:B:498:ARG:HB2	1:B:501:TYR:HD2	1.57	0.69
3:E:98:ASP:O	3:E:102:TYR:OH	2.09	0.69
1:B:215:ASP:N	1:B:266:TYR:OH	2.24	0.69
1:B:332:ILE:HG12	1:B:580:GLN:HE21	1.57	0.69
1:B:375:PHE:CG	1:B:508:TYR:HE2	2.11	0.69
3:E:11:LEU:HB3	3:E:124:VAL:HG22	1.74	0.68
1:A:175:PHE:HD1	1:A:176:LEU:HG	1.57	0.68
1:A:433:VAL:HG23	1:A:512:VAL:HG22	1.75	0.68
1:A:170:TYR:CD1	1:A:229:LEU:HD21	2.28	0.68
1:B:371:LEU:C	1:B:373:PRO:CD	2.67	0.68
1:B:371:LEU:HD12	1:B:374:PHE:CE2	2.29	0.68
1:A:598:ILE:HD11	1:A:611:LEU:HB2	1.77	0.67
1:A:564:GLN:NE2	1:A:577:ARG:O	2.27	0.67
1:B:368:LEU:HA	1:B:371:LEU:HD12	1.75	0.67
1:B:977:LEU:HD22	1:B:993:ILE:HG12	1.76	0.66
1:A:329:PHE:CB	1:A:527:PRO:HA	2.25	0.66
1:B:1010:GLN:HB3	1:B:1014:ARG:NH1	2.10	0.66
1:C:118:LEU:HB3	1:C:129:LYS:HE3	1.77	0.66
1:B:455:LEU:CD2	1:B:493:ARG:CD	2.70	0.66
1:B:811:LYS:HZ2	1:B:815:ARG:HB2	1.59	0.66
1:B:950:ASP:HA	1:B:953:ASN:HD22	1.61	0.66
1:C:383:SER:H	1:C:386:LYS:HE2	1.61	0.66
1:B:374:PHE:HA	1:B:436:TRP:HB3	1.76	0.66
1:B:318:PHE:N	1:B:593:GLY:O	2.27	0.66
1:C:772:VAL:HG22	1:C:776:LYS:HZ1	1.61	0.66
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.24	0.66
1:B:727:LEU:HD21	1:B:1028:LYS:HZ2	1.61	0.66
1:A:168:PHE:CD2	1:A:231:ILE:HG22	2.32	0.65
1:A:825:LYS:NZ	1:A:941:THR:O	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:ARG:NH2	1:C:279:TYR:OH	2.28	0.65
1:A:740:MET:HA	1:A:744:GLY:HA2	1.77	0.65
1:A:779:GLN:NE2	1:A:783:ALA:O	2.30	0.65
1:C:666:ILE:HD11	1:C:672:ALA:HB2	1.77	0.65
1:C:717:ASN:OD1	1:C:718:PHE:N	2.27	0.65
1:A:1114:ILE:O	1:A:1119:ASN:ND2	2.30	0.65
1:B:28:TYR:HB3	1:B:61:ASN:OD1	1.96	0.65
1:A:117:LEU:HB3	1:A:235:ILE:CD1	2.27	0.65
1:A:191:GLU:HB3	1:A:206:LYS:HB3	1.79	0.65
1:B:665:PRO:HB3	1:C:864:LEU:HD11	1.79	0.65
1:A:788:ILE:HG23	1:A:872:GLN:HE22	1.62	0.64
1:C:239:GLN:NE2	1:C:240:THR:O	2.29	0.64
2:D:75:ARG:NH1	2:D:93:SER:O	2.30	0.64
1:C:906:PHE:HB3	1:C:911:VAL:HB	1.79	0.64
1:A:329:PHE:HB3	1:A:330:PRO:HD2	1.79	0.64
1:B:335:LEU:HD12	1:B:364:ASP:HB2	1.80	0.64
1:C:656:VAL:HG21	1:C:693:ILE:HD12	1.78	0.64
1:A:1014:ARG:HH22	1:A:1018:ILE:HD11	1.61	0.64
1:C:772:VAL:HG22	1:C:776:LYS:NZ	2.13	0.64
1:B:328:ARG:HG3	1:B:579:PRO:HD2	1.78	0.64
2:D:80:ARG:NH2	2:D:85:ASN:OD1	2.30	0.64
1:C:866:THR:H	1:C:869:MET:HE3	1.60	0.64
3:E:113:PRO:HB2	3:E:115:GLU:HG3	1.79	0.64
1:B:344:ALA:HB3	1:B:347:PHE:HE1	1.63	0.64
1:B:728:PRO:HB3	1:B:951:VAL:HG11	1.78	0.64
1:A:115:GLN:NE2	1:A:167:THR:CB	2.58	0.64
1:C:726:ILE:HG21	1:C:948:LEU:HG	1.79	0.64
1:C:1114:ILE:O	1:C:1119:ASN:ND2	2.30	0.63
1:B:826:VAL:HG21	1:B:1057:PRO:HG2	1.80	0.63
1:C:83:VAL:HG22	1:C:239:GLN:HG3	1.81	0.63
1:C:125:ASN:HA	1:C:174:PRO:HB3	1.80	0.63
1:A:176:LEU:O	1:A:179:LEU:HD21	1.99	0.63
1:B:770:ILE:HD11	1:B:1012:LEU:HD22	1.80	0.63
3:E:105:GLN:NE2	3:E:106:GLN:O	2.31	0.63
1:A:205:SER:H	1:A:226:LEU:HD23	1.64	0.63
1:A:763:LEU:HD11	1:A:1005:GLN:HG2	1.81	0.63
1:B:310:LYS:HG3	1:B:600:PRO:HA	1.80	0.63
1:A:99:ASN:OD1	1:A:179:LEU:HD22	1.99	0.62
1:B:916:LEU:O	1:B:920:GLN:N	2.33	0.62
1:A:170:TYR:HD1	1:A:229:LEU:HD11	1.62	0.62
1:B:953:ASN:O	1:B:956:ALA:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1010:GLN:HA	1:B:1013:ILE:HD12	1.81	0.62
1:A:170:TYR:OH	1:A:227:VAL:HG12	1.96	0.62
1:B:1067:TYR:OH	1:B:1109:PHE:HZ	1.83	0.62
1:C:759:PHE:HA	1:C:762:GLN:HE21	1.64	0.62
1:A:770:ILE:O	1:A:774:GLN:NE2	2.33	0.62
1:C:1031:GLU:OE1	1:C:1039:ARG:NH1	2.32	0.62
1:B:332:ILE:HG13	1:B:580:GLN:HE21	1.65	0.61
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.82	0.61
1:C:1006:THR:O	1:C:1010:GLN:HG2	2.00	0.61
1:A:175:PHE:CD1	1:A:176:LEU:HG	2.35	0.61
1:B:276:LEU:HD13	1:B:301:CYS:HA	1.82	0.61
1:C:204:TYR:HB3	1:C:223:LEU:HB3	1.81	0.61
1:C:817:PHE:CE2	1:C:818:ILE:HG13	2.36	0.61
1:B:371:LEU:HD12	1:B:374:PHE:HE2	1.65	0.61
1:A:27:ALA:HB3	1:A:64:TRP:HB3	1.83	0.60
1:A:722:VAL:HG22	1:A:930:ALA:HB1	1.83	0.60
1:A:881:THR:HG23	1:A:882:ILE:HD12	1.83	0.60
1:B:1049:LEU:HB2	1:B:1065:VAL:HG12	1.82	0.60
1:A:537:LYS:HG2	1:A:539:VAL:HG13	1.83	0.60
1:C:1014:ARG:O	1:C:1018:ILE:HG12	2.01	0.60
1:A:108:THR:HG22	1:A:236:THR:H	1.66	0.60
1:A:328:ARG:HH22	1:A:533:LEU:HA	1.67	0.60
1:A:106:PHE:HB3	1:A:235:ILE:HD13	1.84	0.60
1:B:928:ASN:OD1	1:B:929:SER:N	2.35	0.60
1:C:659:SER:OG	1:C:698:SER:N	2.34	0.60
1:A:788:ILE:HG23	1:A:872:GLN:NE2	2.17	0.60
1:C:48:LEU:HD22	1:C:276:LEU:HG	1.81	0.60
1:B:452:LEU:HG	1:B:494:SER:HA	1.84	0.60
1:C:773:GLU:OE1	1:C:1019:ARG:NH1	2.35	0.60
1:A:699:LEU:HB3	1:B:788:ILE:HG13	1.84	0.60
1:A:121:ASN:ND2	1:A:177:MET:HB2	2.17	0.59
1:B:376:THR:HB	1:B:435:ALA:HB3	1.83	0.59
1:A:106:PHE:HB2	1:A:117:LEU:C	2.19	0.59
1:A:276:LEU:N	1:A:289:VAL:O	2.34	0.59
1:B:371:LEU:HB3	1:B:373:PRO:HD3	1.82	0.59
1:B:749:CYS:HB2	1:B:977:LEU:HD11	1.83	0.59
1:C:905:ARG:HH12	1:C:1036:GLN:HB2	1.67	0.59
1:A:104:TRP:O	1:A:118:LEU:CD1	2.50	0.59
1:A:115:GLN:HE22	1:A:167:THR:CB	1.98	0.59
1:C:730:SER:HA	1:C:774:GLN:NE2	2.17	0.59
1:A:788:ILE:N	1:C:701:ALA:O	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:VAL:HB	1:A:168:PHE:O	2.03	0.59
1:C:317:ASN:HA	1:C:594:GLY:HA2	1.83	0.59
1:A:168:PHE:HE1	1:A:229:LEU:HD12	1.63	0.59
1:B:590:CYS:SG	1:B:591:SER:N	2.75	0.59
1:C:732:THR:OG1	1:C:1058:HIS:NE2	2.33	0.59
1:C:778:THR:HG22	1:C:865:LEU:HD12	1.85	0.59
1:A:355:ARG:HD3	1:A:357:ARG:HH22	1.68	0.58
1:A:666:ILE:HD11	1:A:672:ALA:HB2	1.85	0.58
1:B:312:ILE:HD13	1:B:598:ILE:HG13	1.84	0.58
1:B:666:ILE:HD11	1:B:672:ALA:HB2	1.85	0.58
2:D:6:GLU:HA	2:D:23:CYS:HB3	1.85	0.58
1:A:954:HIS:HA	1:A:957:GLN:HE21	1.68	0.58
1:B:330:PRO:O	1:B:580:GLN:NE2	2.36	0.58
1:C:310:LYS:HG3	1:C:600:PRO:HA	1.85	0.58
1:C:344:ALA:HB3	1:C:347:PHE:HE1	1.68	0.58
1:C:1047:TYR:OH	1:C:1107:ARG:NH1	2.27	0.58
1:A:323:THR:H	1:A:539:VAL:HG12	1.67	0.58
1:A:827:THR:OG1	1:A:949:GLN:NE2	2.37	0.58
1:B:1028:LYS:O	1:B:1032:CYS:HB2	2.04	0.58
1:C:131:CYS:SG	1:C:132:GLU:N	2.75	0.58
1:C:290:ASP:HB3	1:C:293:LEU:HB2	1.86	0.58
1:B:375:PHE:CD2	1:B:508:TYR:CE2	2.88	0.58
1:A:356:LYS:HE3	1:A:397:ALA:HB3	1.85	0.58
1:B:779:GLN:HG2	1:B:783:ALA:HB3	1.86	0.58
1:B:83:VAL:HG22	1:B:239:GLN:HG3	1.85	0.58
1:C:733:LYS:HE2	1:C:861:LEU:HB2	1.86	0.58
1:A:168:PHE:CG	1:A:231:ILE:HG22	2.39	0.57
1:B:371:LEU:HB3	1:B:373:PRO:CG	2.33	0.57
1:B:371:LEU:HB3	1:B:373:PRO:CD	2.33	0.57
1:A:535:LYS:NZ	1:A:536:ASN:OD1	2.37	0.57
1:A:873:TYR:HE1	1:C:699:LEU:HB3	1.68	0.57
1:B:437:ASN:ND2	1:B:506:GLN:OE1	2.29	0.57
1:B:457:ARG:NH1	1:B:458:LYS:HB2	2.20	0.57
1:A:990:GLU:HA	1:A:993:ILE:HD12	1.86	0.57
1:B:949:GLN:NE2	1:B:953:ASN:HD21	2.03	0.57
1:C:805:ILE:HG13	1:C:806:LEU:HD12	1.86	0.57
1:A:104:TRP:O	1:A:118:LEU:HD13	2.04	0.57
1:A:179:LEU:HA	1:A:190:ARG:HH22	1.69	0.57
1:A:275:PHE:HA	1:A:290:ASP:HA	1.86	0.57
1:A:815:ARG:HA	1:A:819:GLU:OE2	2.04	0.57
1:C:110:LEU:HG	1:C:237:ARG:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:905:ARG:NH1	1:C:1049:LEU:O	2.37	0.57
1:A:117:LEU:N	1:A:235:ILE:HD11	2.19	0.57
1:A:92:PHE:CE1	1:A:265:TYR:HB2	2.40	0.56
1:A:670:ILE:HD13	1:A:696:THR:HA	1.86	0.56
1:A:598:ILE:HB	1:A:609:ALA:HB3	1.87	0.56
1:B:322:PRO:HB3	1:B:539:VAL:HA	1.87	0.56
1:B:330:PRO:HA	1:B:580:GLN:HE22	1.69	0.56
1:B:1086:LYS:HZ1	1:B:1122:VAL:HA	1.68	0.56
1:C:1050:MET:SD	1:C:1051:SER:N	2.78	0.56
1:A:317:ASN:HA	1:A:594:GLY:HA2	1.86	0.56
1:C:273:ARG:HH12	1:C:292:ALA:HB3	1.69	0.56
3:E:41:TRP:CH2	3:E:102:TYR:HB3	2.41	0.56
1:A:756:TYR:CE1	1:C:969:LYS:HE2	2.40	0.56
1:A:901:GLN:O	1:A:905:ARG:HG2	2.06	0.56
1:C:328:ARG:HA	1:C:530:SER:HB3	1.87	0.56
1:C:614:GLY:N	1:C:647:ALA:O	2.23	0.56
1:B:880:GLY:O	1:B:885:GLY:N	2.38	0.56
1:B:926:GLN:O	1:B:926:GLN:NE2	2.38	0.56
1:A:577:ARG:HD3	1:A:582:LEU:HA	1.87	0.56
1:B:455:LEU:HD23	1:B:493:ARG:NE	2.19	0.56
2:D:13:ILE:HD11	2:D:17:GLY:HA3	1.88	0.56
1:A:294:ASP:HB3	1:A:297:SER:H	1.70	0.56
1:C:763:LEU:HD21	1:C:1005:GLN:HG3	1.88	0.56
1:A:577:ARG:HB2	1:A:584:ILE:HD13	1.88	0.56
1:A:905:ARG:HE	1:A:1036:GLN:HB2	1.70	0.56
1:C:577:ARG:HE	1:C:582:LEU:HA	1.71	0.56
2:D:43:ARG:HB3	2:D:53:ILE:HD11	1.86	0.56
1:A:168:PHE:HZ	1:A:229:LEU:CB	1.85	0.55
1:B:43:PHE:HE1	1:B:283:GLY:HA3	1.70	0.55
1:A:388:ASN:HA	1:A:528:LYS:HD2	1.87	0.55
1:A:564:GLN:HE22	1:A:577:ARG:HE	1.52	0.55
1:C:290:ASP:O	1:C:297:SER:HB2	2.06	0.55
1:C:294:ASP:OD1	1:C:297:SER:N	2.33	0.55
1:A:106:PHE:CD2	1:A:117:LEU:O	2.60	0.55
1:A:1107:ARG:HD3	1:B:886:TRP:HZ2	1.71	0.55
1:B:455:LEU:CD2	1:B:493:ARG:NE	2.69	0.55
1:A:656:VAL:HG12	1:A:658:ASN:H	1.71	0.55
1:C:722:VAL:HB	1:C:934:ILE:HG21	1.88	0.55
1:A:1040:VAL:HG13	1:B:1030:SER:HB3	1.89	0.55
1:B:960:ASN:O	1:B:964:LYS:HG3	2.06	0.55
1:C:43:PHE:CZ	1:C:45:SER:HB3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:LEU:HB3	1:A:235:ILE:HD13	1.89	0.55
1:A:895:GLN:NE2	1:C:711:SER:O	2.36	0.55
1:C:960:ASN:HA	1:C:963:VAL:HG22	1.89	0.55
1:A:310:LYS:HG3	1:A:600:PRO:HA	1.89	0.55
1:B:319:ARG:HH11	1:B:319:ARG:HA	1.72	0.55
1:B:699:LEU:HD12	1:C:788:ILE:HG12	1.88	0.55
1:B:815:ARG:NH1	1:B:868:GLU:OE2	2.39	0.55
1:A:334:ASN:HD22	1:A:361:CYS:HA	1.71	0.54
1:B:456:PHE:HE2	1:B:473:TYR:HB2	1.72	0.54
1:B:699:LEU:HB3	1:C:788:ILE:HB	1.88	0.54
1:C:424:LYS:NZ	1:C:425:LEU:O	2.40	0.54
1:B:319:ARG:HA	1:B:319:ARG:NH1	2.21	0.54
3:E:16:GLY:HA2	3:E:93:ARG:HG3	1.88	0.54
1:B:375:PHE:H	1:B:436:TRP:HA	1.73	0.54
3:E:19:ALA:HB2	3:E:94:LEU:HD11	1.89	0.54
1:A:905:ARG:NH2	1:A:1049:LEU:O	2.40	0.54
1:B:130:VAL:HB	1:B:168:PHE:HB3	1.88	0.54
1:B:731:MET:N	1:B:774:GLN:OE1	2.39	0.54
1:C:85:PRO:HA	1:C:237:ARG:HA	1.89	0.54
1:C:961:THR:O	1:C:965:GLN:HB2	2.06	0.54
1:C:577:ARG:HB2	1:C:584:ILE:HG22	1.89	0.54
1:A:329:PHE:CE2	1:A:528:LYS:HB2	2.42	0.54
1:B:607:GLN:OE1	1:B:691:SER:N	2.41	0.54
1:B:337:PRO:HG2	1:B:358:ILE:HD12	1.90	0.54
3:E:37:SER:HB3	3:E:57:ALA:HB3	1.88	0.54
1:B:333:THR:O	1:B:334:ASN:C	2.50	0.54
1:B:867:ASP:OD1	1:B:868:GLU:N	2.41	0.54
1:B:906:PHE:CE2	1:B:916:LEU:HD12	2.43	0.54
1:A:126:VAL:HG11	1:A:175:PHE:CE1	2.43	0.53
1:A:383:SER:HB3	1:A:386:LYS:HG2	1.90	0.53
1:A:937:SER:O	1:A:941:THR:OG1	2.24	0.53
1:B:38:TYR:HB2	1:B:225:PRO:HD3	1.90	0.53
1:B:785:VAL:HG11	1:B:888:PHE:HD2	1.72	0.53
1:B:1092:GLU:OE1	1:B:1092:GLU:N	2.42	0.53
1:C:365:TYR:OH	1:C:388:ASN:OD1	2.26	0.53
1:B:34:ARG:NH2	1:B:219:GLY:O	2.29	0.53
1:B:290:ASP:O	1:B:297:SER:HB2	2.07	0.53
1:A:729:VAL:H	1:A:1059:GLY:HA2	1.73	0.53
1:A:767:LEU:HA	1:A:770:ILE:HD12	1.89	0.53
1:A:906:PHE:HB3	1:A:911:VAL:HB	1.90	0.53
1:A:957:GLN:OE1	1:B:765:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:GLU:O	1:C:313:TYR:OH	2.25	0.53
1:C:788:ILE:HG22	1:C:790:LYS:HZ1	1.72	0.53
1:A:317:ASN:ND2	1:B:737:ASP:OD2	2.41	0.53
1:A:312:ILE:HD11	1:A:664:ILE:HD12	1.91	0.53
1:A:332:ILE:HD12	1:A:580:GLN:HB3	1.90	0.53
1:B:196:ASN:ND2	1:B:233:ILE:O	2.39	0.53
2:D:81:ASP:HB2	2:D:88:TYR:CE2	2.43	0.53
1:A:1105:THR:HG21	1:A:1110:TYR:CE1	2.43	0.53
1:A:290:ASP:OD1	1:A:291:CYS:N	2.42	0.53
1:B:611:LEU:HD22	1:B:666:ILE:HG23	1.90	0.53
1:B:980:ILE:O	1:B:984:LEU:HB2	2.09	0.53
1:A:769:GLY:O	1:A:773:GLU:HG3	2.08	0.53
1:A:117:LEU:H	1:A:235:ILE:CD1	2.22	0.53
1:A:658:ASN:OD1	1:A:659:SER:N	2.35	0.53
1:A:805:ILE:HG13	1:A:806:LEU:HD22	1.91	0.53
1:B:344:ALA:HB3	1:B:347:PHE:CE1	2.44	0.53
1:C:1080:ALA:HB3	1:C:1129:VAL:HG21	1.91	0.53
2:D:91:MET:SD	2:D:94:LEU:HD21	2.48	0.53
1:A:653:ALA:HB2	1:A:692:ILE:HG22	1.91	0.53
1:C:1039:ARG:NH1	1:C:1039:ARG:HB3	2.23	0.53
1:A:56:LEU:HD11	1:A:268:GLY:HA3	1.91	0.52
1:A:920:GLN:O	1:A:923:ILE:HG22	2.10	0.52
1:B:280:ASN:OD1	1:B:283:GLY:N	2.39	0.52
2:D:109:ASP:O	2:D:110:ILE:HG22	2.09	0.52
1:A:330:PRO:HA	1:A:580:GLN:NE2	2.24	0.52
1:C:673:SER:HB2	1:C:695:TYR:HE2	1.74	0.52
1:A:966:LEU:HB2	1:A:1000:ARG:CZ	2.40	0.52
1:B:294:ASP:O	1:B:297:SER:OG	2.27	0.52
1:B:1095:PHE:HE1	1:B:1104:VAL:HB	1.74	0.52
1:C:134:GLN:NE2	1:C:161:SER:OG	2.42	0.52
1:C:312:ILE:HD13	1:C:598:ILE:HG13	1.90	0.52
1:B:353:TRP:HZ3	1:B:355:ARG:HB2	1.74	0.52
1:C:108:THR:O	1:C:237:ARG:NE	2.42	0.52
1:C:204:TYR:CD1	1:C:225:PRO:HA	2.44	0.52
1:A:106:PHE:C	1:A:116:SER:HB3	2.23	0.52
1:B:422:ASN:OD1	1:B:454:ARG:N	2.39	0.52
1:B:535:LYS:O	1:B:537:LYS:NZ	2.33	0.52
1:B:806:LEU:HD12	1:B:807:PRO:HD2	1.91	0.52
1:B:1116:THR:H	1:B:1119:ASN:HD21	1.57	0.52
1:C:1039:ARG:HH21	1:C:1042:PHE:HB3	1.75	0.52
1:A:737:ASP:HA	1:A:764:LYS:HE2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:ALA:N	1:B:373:PRO:CD	2.73	0.52
1:A:107:GLY:HA2	1:A:116:SER:OG	2.10	0.51
1:C:57:PRO:HB2	1:C:60:SER:HB3	1.92	0.51
1:C:300:LYS:HD2	1:C:306:PHE:HA	1.92	0.51
1:B:335:LEU:O	1:B:361:CYS:HB2	2.10	0.51
1:B:663:ASP:OD1	1:B:664:ILE:N	2.43	0.51
1:B:310:LYS:HG2	1:B:664:ILE:HD11	1.92	0.51
1:B:368:LEU:HD23	1:B:371:LEU:HD11	1.92	0.51
1:B:726:ILE:CG2	1:B:948:LEU:HG	2.40	0.51
1:A:90:VAL:HG11	1:A:238:PHE:CE1	2.45	0.51
1:A:932:GLY:O	1:A:935:GLN:HG3	2.10	0.51
1:C:906:PHE:HA	1:C:909:ILE:HG12	1.92	0.51
1:A:950:ASP:OD1	1:A:954:HIS:CE1	2.63	0.51
1:B:1039:ARG:NE	1:C:1031:GLU:OE2	2.44	0.51
1:C:96:GLU:OE2	1:C:100:ILE:N	2.28	0.51
2:D:19:LEU:HB2	2:D:91:MET:HB3	1.92	0.51
3:E:53:LEU:HD22	3:E:71:ILE:HG23	1.91	0.51
1:A:1105:THR:HG22	1:A:1111:GLU:C	2.35	0.51
1:B:453:TYR:CE1	1:B:493:ARG:HB2	2.45	0.51
1:B:1081:ILE:HG23	1:B:1135:ASN:HB3	1.92	0.51
1:C:134:GLN:HE22	1:C:162:SER:H	1.57	0.51
3:E:43:GLN:O	3:E:51:ARG:N	2.39	0.51
1:B:1010:GLN:HB3	1:B:1014:ARG:HH12	1.72	0.51
1:C:328:ARG:HG3	1:C:579:PRO:HD2	1.93	0.51
1:C:869:MET:HA	1:C:872:GLN:CD	2.36	0.51
1:C:1087:ALA:HB2	1:C:1126:CYS:HA	1.93	0.51
1:A:671:CYS:SG	1:A:697:MET:HG3	2.50	0.51
1:B:316:SER:O	1:B:595:VAL:N	2.32	0.51
1:C:457:ARG:NH1	1:C:459:SER:O	2.43	0.51
1:A:396:TYR:OH	1:A:516:GLU:OE2	2.27	0.51
1:A:741:TYR:CE2	1:A:1004:LEU:HB2	2.45	0.51
1:A:811:LYS:HD2	1:A:812:PRO:HD2	1.93	0.51
1:C:593:GLY:HA3	1:C:613:GLN:O	2.12	0.51
1:A:644:GLN:HA	1:A:649:CYS:HA	1.93	0.50
1:B:351:TYR:HE1	1:B:452:LEU:HB2	1.76	0.50
1:B:817:PHE:CZ	1:B:821:LEU:CD1	2.93	0.50
1:C:543:PHE:HE2	1:C:578:ASP:HB3	1.77	0.50
1:C:788:ILE:HG22	1:C:790:LYS:NZ	2.26	0.50
1:A:170:TYR:CE1	1:A:229:LEU:HD21	2.45	0.50
1:A:303:LEU:HD11	1:A:313:TYR:CE2	2.46	0.50
1:A:1100:THR:OG1	6:A:1303:NAG:N2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:773:GLU:HA	1:B:776:LYS:HG2	1.92	0.50
1:C:37:TYR:CD2	1:C:204:TYR:HE2	2.29	0.50
1:C:412:PRO:HG3	1:C:429:PHE:HB3	1.93	0.50
1:A:405:ASP:HB3	1:A:505:HIS:CD2	2.46	0.50
1:A:882:ILE:HG23	1:A:898:PHE:CD1	2.46	0.50
1:A:905:ARG:O	1:A:1036:GLN:NE2	2.45	0.50
1:B:438:SER:HB3	1:B:509:ARG:HG3	1.92	0.50
1:A:55:PHE:HB3	1:A:275:PHE:CZ	2.46	0.50
1:B:453:TYR:HE1	1:B:455:LEU:HB2	1.76	0.50
1:B:718:PHE:HE2	1:B:720:ILE:HG12	1.76	0.50
1:B:730:SER:HA	1:B:774:GLN:NE2	2.26	0.50
1:B:130:VAL:N	1:B:168:PHE:O	2.42	0.50
1:B:317:ASN:HA	1:B:594:GLY:HA2	1.93	0.50
1:C:1125:ASN:ND2	1:C:1127:ASP:OD2	2.44	0.50
1:A:976:VAL:HG12	1:A:978:ASN:H	1.77	0.50
1:B:34:ARG:HA	1:B:34:ARG:NE	2.27	0.50
1:C:45:SER:O	1:C:47:VAL:HG13	2.11	0.50
2:D:99:THR:HG23	2:D:125:THR:HA	1.93	0.50
1:B:291:CYS:O	1:B:297:SER:OG	2.28	0.50
1:B:332:ILE:O	1:B:333:THR:C	2.54	0.50
1:B:490:PHE:CE2	1:B:492:LEU:HB2	2.47	0.50
1:C:1104:VAL:O	1:C:1113:GLN:N	2.45	0.50
3:E:21:LEU:HD21	3:E:102:TYR:HD2	1.75	0.50
1:A:179:LEU:HA	1:A:190:ARG:NH2	2.26	0.50
1:A:193:VAL:HB	1:A:204:TYR:H	1.77	0.50
1:B:672:ALA:HA	1:B:694:ALA:HA	1.93	0.50
1:B:1095:PHE:CE1	1:B:1104:VAL:HB	2.47	0.50
1:C:327:VAL:O	1:C:531:THR:N	2.44	0.50
1:A:523:THR:HG23	1:A:524:VAL:HG23	1.94	0.49
1:A:864:LEU:HD11	1:C:665:PRO:HB3	1.93	0.49
1:A:125:ASN:HA	1:A:174:PRO:HB3	1.92	0.49
1:B:347:PHE:HB2	1:B:401:VAL:HG23	1.94	0.49
1:B:368:LEU:HA	1:B:371:LEU:HG	1.93	0.49
1:C:808:ASP:O	1:C:811:LYS:HG2	2.12	0.49
1:A:645:THR:HG23	1:A:647:ALA:H	1.77	0.49
1:A:1050:MET:SD	1:A:1051:SER:N	2.85	0.49
1:A:1067:TYR:OH	1:A:1108:ASN:O	2.28	0.49
1:B:204:TYR:HB3	1:B:223:LEU:HB3	1.93	0.49
1:B:276:LEU:N	1:B:289:VAL:O	2.44	0.49
1:A:130:VAL:HG21	1:A:168:PHE:HD2	1.76	0.49
1:A:173:GLN:HB2	1:A:175:PHE:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:LEU:HD22	1:B:585:LEU:HD11	1.93	0.49
1:B:666:ILE:HD12	1:B:670:ILE:HG22	1.93	0.49
1:B:937:SER:O	1:B:941:THR:OG1	2.25	0.49
2:D:55:LEU:HD22	3:E:116:PHE:HZ	1.77	0.49
1:A:532:ASN:OD1	1:A:533:LEU:N	2.46	0.49
1:A:617:CYS:O	1:A:620:VAL:HG22	2.13	0.49
1:B:730:SER:HB3	1:B:1058:HIS:HA	1.95	0.49
1:C:105:ILE:HG22	1:C:110:LEU:HD22	1.94	0.49
1:A:589:PRO:HB3	1:B:856:LYS:HE3	1.95	0.49
1:C:945:LEU:HB2	1:C:949:GLN:NE2	2.27	0.49
1:C:977:LEU:HD22	1:C:993:ILE:HG23	1.94	0.49
1:A:231:ILE:HB	1:A:233:ILE:HG12	1.94	0.49
1:A:345:THR:O	1:A:346:ARG:NE	2.40	0.49
1:B:642:VAL:HG22	1:B:651:ILE:HG12	1.94	0.49
1:A:903:ALA:HB1	1:A:913:GLN:HG2	1.93	0.49
1:A:919:ASN:OD1	1:A:922:LEU:HB3	2.13	0.49
1:A:1043:CYS:HB2	1:A:1048:HIS:CG	2.47	0.49
1:A:1090:PRO:HG3	1:A:1095:PHE:CZ	2.47	0.49
1:B:347:PHE:CE2	1:B:509:ARG:HB3	2.48	0.49
1:B:996:LEU:HB3	1:B:1000:ARG:HH12	1.78	0.49
1:B:1105:THR:OG1	1:B:1111:GLU:N	2.33	0.49
1:A:329:PHE:O	1:A:331:ASN:N	2.46	0.48
1:C:43:PHE:C	1:C:44:ARG:HD3	2.38	0.48
1:A:1051:SER:OG	1:A:1064:HIS:ND1	2.39	0.48
1:B:203:ILE:HD12	1:B:227:VAL:HB	1.95	0.48
1:B:323:THR:H	1:B:539:VAL:HG12	1.78	0.48
1:C:729:VAL:H	1:C:1059:GLY:HA2	1.77	0.48
1:A:818:ILE:O	1:A:821:LEU:HG	2.13	0.48
1:B:886:TRP:HB2	1:B:1034:LEU:O	2.13	0.48
1:B:1083:HIS:HB3	1:B:1088:HIS:CD2	2.48	0.48
1:C:190:ARG:HG2	1:C:207:HIS:CE1	2.47	0.48
2:D:41:TRP:HB3	2:D:53:ILE:HD12	1.95	0.48
1:A:740:MET:HE1	1:C:319:ARG:NH2	2.29	0.48
1:A:1014:ARG:O	1:A:1018:ILE:HG12	2.13	0.48
2:D:5:VAL:HG13	2:D:120:GLN:HE22	1.78	0.48
2:D:6:GLU:HG3	2:D:23:CYS:HB3	1.95	0.48
1:A:174:PRO:O	1:A:178:ASP:N	2.45	0.48
1:A:336:CYS:SG	1:A:363:ALA:HB2	2.53	0.48
1:A:1008:VAL:O	1:A:1012:LEU:HG	2.13	0.48
1:C:603:ASN:OD1	1:C:604:THR:N	2.46	0.48
1:A:345:THR:C	1:A:346:ARG:HE	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:ARG:NH2	1:C:405:ASP:OD2	2.35	0.48
1:C:871:ALA:O	1:C:874:THR:OG1	2.30	0.48
1:C:968:SER:HB2	1:C:970:PHE:CE2	2.48	0.48
1:C:1109:PHE:HD2	1:C:1111:GLU:HG3	1.78	0.48
2:D:80:ARG:NH2	2:D:85:ASN:HA	2.29	0.48
1:A:57:PRO:HG3	1:A:271:GLN:NE2	2.15	0.48
1:A:117:LEU:HA	1:A:130:VAL:HG22	1.96	0.48
1:B:331:ASN:CB	1:B:362:VAL:HG21	2.44	0.48
1:B:897:PRO:HB2	1:B:900:MET:HE2	1.96	0.48
1:C:781:VAL:O	1:C:1029:MET:HE1	2.14	0.48
1:C:930:ALA:HA	1:C:933:LYS:HG2	1.95	0.48
3:E:80:GLY:HA3	3:E:87:PHE:HA	1.95	0.48
1:A:945:LEU:HD23	1:A:945:LEU:H	1.78	0.48
1:C:1003:SER:O	1:C:1006:THR:OG1	2.26	0.48
1:C:1029:MET:O	1:C:1033:VAL:HB	2.13	0.48
2:D:50:LEU:HD11	3:E:50:PRO:HG2	1.96	0.48
2:D:80:ARG:NH1	2:D:81:ASP:O	2.47	0.48
1:A:208:THR:HG22	1:A:210:ILE:HG23	1.95	0.48
1:C:159:VAL:HG13	1:C:160:TYR:CD1	2.49	0.48
1:A:56:LEU:HB2	1:A:270:LEU:HD23	1.96	0.47
1:A:177:MET:C	1:A:179:LEU:HG	2.39	0.47
1:A:353:TRP:CZ3	1:A:355:ARG:HB2	2.48	0.47
1:A:873:TYR:CE1	1:C:699:LEU:HB3	2.47	0.47
1:A:873:TYR:CZ	1:C:699:LEU:HD22	2.48	0.47
1:A:889:GLY:HA3	1:A:1034:LEU:HD23	1.95	0.47
1:B:814:LYS:HD2	1:B:814:LYS:N	2.28	0.47
1:C:43:PHE:CE2	1:C:45:SER:HB3	2.49	0.47
1:A:92:PHE:HE1	1:A:265:TYR:HB2	1.79	0.47
1:A:174:PRO:HB2	1:A:177:MET:HB3	1.95	0.47
1:A:785:VAL:HG11	1:A:888:PHE:CD2	2.48	0.47
1:A:1097:SER:HB2	1:A:1102:TRP:CE2	2.49	0.47
1:B:371:LEU:HB2	1:B:373:PRO:HD3	1.93	0.47
1:B:741:TYR:HE2	1:B:962:LEU:HD21	1.79	0.47
1:C:318:PHE:N	1:C:593:GLY:O	2.35	0.47
1:A:295:PRO:HB2	1:A:608:VAL:HG21	1.96	0.47
1:A:759:PHE:O	1:A:762:GLN:HG2	2.14	0.47
1:B:811:LYS:HZ3	1:B:813:SER:HG	1.53	0.47
1:A:666:ILE:HD12	1:A:670:ILE:HG22	1.96	0.47
1:B:295:PRO:O	1:B:299:THR:HG23	2.13	0.47
1:B:368:LEU:HA	1:B:371:LEU:CG	2.43	0.47
1:B:378:LYS:O	1:B:433:VAL:N	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:785:VAL:HG11	1:B:888:PHE:CD2	2.48	0.47
1:B:1028:LYS:O	1:B:1032:CYS:CB	2.63	0.47
1:C:965:GLN:HG2	1:C:1003:SER:HB3	1.96	0.47
1:A:117:LEU:N	1:A:235:ILE:CD1	2.78	0.47
1:A:1091:ARG:HH12	1:A:1119:ASN:C	2.22	0.47
1:B:332:ILE:O	1:B:335:LEU:HD23	2.15	0.47
1:B:764:LYS:O	1:B:768:THR:HG23	2.14	0.47
1:B:781:VAL:HA	1:B:1029:MET:HE1	1.95	0.47
1:C:905:ARG:NH1	1:C:1036:GLN:HB2	2.29	0.47
2:D:23:CYS:SG	2:D:87:LEU:HB2	2.54	0.47
2:D:39:MET:CG	2:D:87:LEU:HD21	2.44	0.47
1:A:759:PHE:HZ	1:C:970:PHE:CZ	2.32	0.47
1:A:957:GLN:CD	1:B:765:ARG:HH12	2.22	0.47
1:C:516:GLU:OE1	1:C:519:HIS:N	2.46	0.47
1:C:886:TRP:HH2	1:C:904:TYR:HB3	1.79	0.47
1:A:172:SER:HB3	1:A:175:PHE:CE2	2.50	0.47
1:A:384:PRO:HA	1:A:387:LEU:HG	1.97	0.47
1:A:770:ILE:HD11	1:A:1012:LEU:HD23	1.97	0.47
1:A:870:ILE:O	1:A:874:THR:HG23	2.15	0.47
1:B:382:VAL:HG12	1:B:386:LYS:NZ	2.29	0.47
1:B:867:ASP:OD1	1:B:868:GLU:HG2	2.15	0.47
1:B:919:ASN:OD1	1:B:922:LEU:HB3	2.14	0.47
1:C:153:MET:N	1:C:153:MET:SD	2.88	0.47
1:C:886:TRP:HB2	1:C:1034:LEU:O	2.15	0.47
3:E:41:TRP:CE2	3:E:89:LEU:HD22	2.49	0.47
1:B:128:ILE:O	1:B:170:TYR:N	2.41	0.47
1:B:605:SER:OG	1:B:606:ASN:N	2.48	0.47
1:A:115:GLN:HE21	1:A:233:ILE:HG21	1.80	0.47
1:A:1116:THR:N	1:A:1119:ASN:OD1	2.38	0.47
1:B:662:CYS:HB2	1:B:697:MET:HB2	1.97	0.47
1:B:929:SER:O	1:B:933:LYS:HG2	2.14	0.47
1:B:1079:PRO:O	1:C:917:TYR:OH	2.21	0.47
1:B:730:SER:HA	1:B:774:GLN:CD	2.40	0.47
1:C:48:LEU:HD21	1:C:306:PHE:HE1	1.80	0.47
1:C:756:TYR:HE2	1:C:997:ILE:HG21	1.80	0.47
2:D:38:TYR:HB2	2:D:107:GLU:HB3	1.97	0.47
1:A:117:LEU:H	1:A:235:ILE:HD13	1.80	0.46
1:A:985:ASP:HB3	1:A:987:PRO:HD2	1.96	0.46
1:B:328:ARG:HG2	1:B:578:ASP:HB2	1.96	0.46
2:D:57:TYR:CD2	2:D:64:SER:HB2	2.49	0.46
1:A:802:PHE:HE1	1:A:1052:PHE:HE2	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ARG:O	1:B:56:LEU:HD23	2.14	0.46
1:B:645:THR:OG1	1:B:648:GLY:N	2.47	0.46
1:A:367:VAL:O	1:A:371:LEU:HD23	2.16	0.46
1:A:879:ALA:O	1:A:883:THR:OG1	2.24	0.46
1:B:85:PRO:O	1:B:269:TYR:OH	2.23	0.46
1:B:416:GLY:HA2	2:D:57:TYR:CE2	2.50	0.46
1:C:109:THR:OG1	1:C:111:ASP:OD1	2.32	0.46
1:A:591:SER:HB2	1:A:615:VAL:HG22	1.98	0.46
1:A:720:ILE:HG13	1:A:923:ILE:HD11	1.96	0.46
1:A:962:LEU:O	1:A:1000:ARG:NH1	2.36	0.46
1:B:90:VAL:HG21	1:B:238:PHE:CZ	2.50	0.46
1:B:818:ILE:O	1:B:822:LEU:HG	2.15	0.46
1:C:118:LEU:HD21	1:C:120:VAL:HG13	1.98	0.46
1:A:351:TYR:CD1	1:A:453:TYR:HA	2.50	0.46
1:B:367:VAL:HG12	1:B:371:LEU:CD2	2.45	0.46
1:B:660:TYR:HB2	1:B:695:TYR:CZ	2.50	0.46
1:C:290:ASP:OD1	1:C:291:CYS:N	2.49	0.46
1:C:316:SER:O	1:C:595:VAL:N	2.44	0.46
1:C:985:ASP:OD1	1:C:985:ASP:N	2.49	0.46
2:D:7:SER:OG	2:D:22:SER:O	2.24	0.46
1:A:763:LEU:O	1:A:767:LEU:HG	2.15	0.46
1:B:327:VAL:O	1:B:531:THR:N	2.48	0.46
1:B:795:LYS:HD3	1:B:806:LEU:HD23	1.96	0.46
1:B:817:PHE:CE2	1:B:821:LEU:HD11	2.50	0.46
1:B:403:ARG:NH1	3:E:38:TYR:HH	2.14	0.46
1:B:708:SER:HB2	1:B:711:SER:HB3	1.96	0.46
1:B:937:SER:O	1:B:941:THR:CB	2.64	0.46
1:C:598:ILE:HD11	1:C:666:ILE:HG23	1.98	0.46
1:C:865:LEU:HD13	1:C:873:TYR:CE2	2.50	0.46
3:E:110:SER:HB3	3:E:113:PRO:HD3	1.98	0.46
1:B:242:LEU:HD23	1:B:242:LEU:H	1.80	0.46
1:B:421:TYR:OH	2:D:58:SER:OG	2.24	0.46
1:B:538:CYS:HB2	1:B:590:CYS:HB2	1.77	0.46
1:C:772:VAL:HA	1:C:775:ASP:OD1	2.15	0.46
1:A:52:GLN:NE2	1:A:272:PRO:HB3	2.31	0.46
1:A:699:LEU:CB	1:B:788:ILE:HG13	2.46	0.46
1:B:789:TYR:CE2	1:B:893:ALA:HB2	2.51	0.46
1:B:811:LYS:NZ	1:B:815:ARG:HB2	2.31	0.46
3:E:106:GLN:HE21	3:E:117:THR:HB	1.80	0.46
1:B:811:LYS:HD2	1:B:815:ARG:H	1.81	0.46
1:C:95:ILE:HD13	1:C:186:PHE:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1095:PHE:HE1	1:C:1104:VAL:HB	1.81	0.46
3:E:29:VAL:N	3:E:84:GLY:O	2.46	0.46
1:A:173:GLN:C	1:A:175:PHE:H	2.23	0.45
1:A:1116:THR:H	1:A:1119:ASN:CG	2.21	0.45
1:B:120:VAL:HG23	1:B:127:VAL:HB	1.98	0.45
1:B:278:LYS:HE3	1:B:287:ASP:HB2	1.97	0.45
1:C:767:LEU:HD23	1:C:770:ILE:HD12	1.99	0.45
2:D:23:CYS:SG	2:D:87:LEU:HD22	2.56	0.45
1:A:914:ASN:HD22	1:C:1123:SER:HB2	1.80	0.45
1:B:353:TRP:CZ3	1:B:355:ARG:HB2	2.51	0.45
1:C:90:VAL:HG11	1:C:238:PHE:CZ	2.52	0.45
1:C:785:VAL:HG11	1:C:888:PHE:CD2	2.52	0.45
1:A:703:ASN:OD1	1:A:704:SER:N	2.49	0.45
1:B:408:ARG:HE	3:E:110:SER:HB2	1.80	0.45
1:B:448:ASN:HB3	1:B:497:PHE:HB2	1.96	0.45
1:C:790:LYS:HA	1:C:790:LYS:HD3	1.70	0.45
1:A:106:PHE:CG	1:A:117:LEU:O	2.68	0.45
1:A:1097:SER:HB2	1:A:1102:TRP:CD2	2.51	0.45
1:B:726:ILE:C	1:B:727:LEU:HD12	2.41	0.45
1:B:909:ILE:HG23	1:B:1036:GLN:NE2	2.32	0.45
1:B:1107:ARG:HD2	1:B:1107:ARG:O	2.16	0.45
1:A:895:GLN:HE22	1:C:711:SER:C	2.24	0.45
1:B:730:SER:N	1:B:1058:HIS:O	2.40	0.45
1:C:577:ARG:HD3	1:C:577:ARG:C	2.41	0.45
1:C:869:MET:HA	1:C:872:GLN:NE2	2.32	0.45
1:A:126:VAL:HG23	1:A:174:PRO:HA	1.99	0.45
1:A:785:VAL:HG11	1:A:888:PHE:HD2	1.81	0.45
1:A:909:ILE:HG23	1:A:1036:GLN:NE2	2.31	0.45
1:A:993:ILE:O	1:A:997:ILE:HG12	2.17	0.45
1:B:591:SER:OG	1:B:615:VAL:HA	2.17	0.45
1:C:418:ILE:O	1:C:422:ASN:ND2	2.37	0.45
1:B:1106:GLN:OE1	1:B:1109:PHE:HB2	2.17	0.45
1:C:344:ALA:HB3	1:C:347:PHE:CE1	2.49	0.45
1:C:532:ASN:OD1	1:C:533:LEU:N	2.48	0.45
1:A:175:PHE:HD1	1:A:176:LEU:H	1.64	0.45
1:A:393:THR:HA	1:A:522:ALA:HA	1.99	0.45
1:A:865:LEU:HA	1:A:869:MET:HE2	1.99	0.45
1:A:966:LEU:HD12	1:A:1000:ARG:HE	1.82	0.45
1:A:1079:PRO:HG3	1:A:1131:GLY:HA3	1.97	0.45
1:B:726:ILE:HG23	1:B:948:LEU:HG	1.98	0.45
1:C:643:PHE:CG	1:C:655:TYR:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:734:THR:HG23	1:C:859:THR:O	2.15	0.45
1:A:981:PHE:CD1	1:A:989:ALA:HB1	2.52	0.45
1:B:371:LEU:CA	1:B:373:PRO:HD3	2.47	0.45
1:B:457:ARG:HH11	1:B:458:LYS:HB2	1.81	0.45
1:C:1115:ILE:HG13	1:C:1115:ILE:O	2.15	0.45
1:A:117:LEU:CB	1:A:235:ILE:CD1	2.95	0.45
1:A:906:PHE:CE2	1:A:916:LEU:HB2	2.52	0.45
1:B:371:LEU:CD1	1:B:374:PHE:CE2	3.00	0.45
1:B:555:SER:HB3	1:B:586:ASP:HB2	1.99	0.45
3:E:6:GLN:HB2	3:E:120:PRO:HG2	1.98	0.45
1:A:766:ALA:O	1:A:770:ILE:HG13	2.16	0.44
1:B:1077:THR:HG23	1:B:1095:PHE:O	2.17	0.44
2:D:80:ARG:HD2	2:D:81:ASP:H	1.82	0.44
1:A:37:TYR:HB2	1:A:204:TYR:CD2	2.52	0.44
1:A:188:ASN:HA	1:A:209:PRO:HA	1.98	0.44
1:A:937:SER:O	1:A:941:THR:CB	2.64	0.44
1:B:318:PHE:CE1	1:B:320:VAL:HG22	2.52	0.44
1:B:977:LEU:CD2	1:B:993:ILE:HG12	2.46	0.44
1:A:563:GLN:HB3	1:B:43:PHE:HB2	1.99	0.44
1:A:1105:THR:HG21	1:A:1110:TYR:CD1	2.52	0.44
1:B:379:CYS:HA	1:B:432:CYS:HA	2.00	0.44
1:C:966:LEU:HG	1:C:1000:ARG:CZ	2.47	0.44
1:C:1086:LYS:HB3	1:C:1122:VAL:HG11	1.99	0.44
1:A:953:ASN:O	1:A:957:GLN:HG2	2.17	0.44
1:A:961:THR:HG21	1:B:762:GLN:NE2	2.33	0.44
1:B:85:PRO:HG2	1:B:269:TYR:OH	2.17	0.44
1:B:280:ASN:CG	1:B:284:THR:HG22	2.43	0.44
1:B:347:PHE:HE2	1:B:509:ARG:HB3	1.82	0.44
1:B:1073:LYS:HG2	1:B:1075:PHE:CE2	2.52	0.44
1:C:599:THR:HB	1:C:608:VAL:HG12	1.99	0.44
1:C:658:ASN:OD1	1:C:659:SER:N	2.51	0.44
1:A:912:THR:OG1	1:A:914:ASN:OD1	2.20	0.44
1:C:195:LYS:O	1:C:201:PHE:HA	2.16	0.44
1:C:758:SER:O	1:C:762:GLN:HG3	2.18	0.44
1:A:905:ARG:NE	1:A:1036:GLN:HB2	2.33	0.44
1:B:330:PRO:CA	1:B:580:GLN:HE22	2.30	0.44
1:B:969:LYS:NZ	1:B:972:ALA:HB3	2.33	0.44
2:D:90:GLN:HG3	2:D:92:ASN:OD1	2.17	0.44
1:A:40:ASP:OD1	1:A:40:ASP:N	2.48	0.44
1:A:335:LEU:HD13	1:A:335:LEU:HA	1.75	0.44
1:A:1062:PHE:HB3	1:A:1064:HIS:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:TYR:HB2	1:C:204:TYR:CD2	2.53	0.44
1:C:558:LYS:HE2	1:C:558:LYS:HB3	1.84	0.44
1:C:750:SER:O	1:C:754:LEU:HG	2.17	0.44
1:A:568:ASP:OD1	1:A:569:ILE:HD12	2.17	0.44
1:B:43:PHE:CE2	1:B:45:SER:HB2	2.53	0.44
1:B:738:CYS:HB3	1:B:760:CYS:HB3	1.80	0.44
1:C:56:LEU:HB3	1:C:270:LEU:HG	2.00	0.44
1:C:222:ALA:HB2	1:C:285:ILE:HB	2.00	0.44
3:E:99:PHE:HD1	3:E:124:VAL:HG12	1.82	0.44
1:A:99:ASN:CG	1:A:179:LEU:HD22	2.43	0.44
1:A:1091:ARG:HH22	1:A:1119:ASN:HA	1.83	0.44
1:B:901:GLN:O	1:B:905:ARG:HG2	2.17	0.44
1:C:1030:SER:O	1:C:1034:LEU:HB2	2.18	0.44
2:D:24:ALA:HA	2:D:86:THR:HA	1.98	0.44
1:C:453:TYR:CE2	1:C:455:LEU:HB2	2.53	0.43
1:C:544:ASN:HD21	1:C:579:PRO:HG3	1.83	0.43
2:D:55:LEU:HD22	3:E:116:PHE:CZ	2.53	0.43
1:A:729:VAL:HG11	1:A:781:VAL:HG11	1.99	0.43
1:A:1053:PRO:O	1:A:1054:GLN:HG2	2.18	0.43
1:C:655:TYR:HA	1:C:694:ALA:O	2.18	0.43
1:C:969:LYS:HG3	1:C:971:GLY:H	1.84	0.43
2:D:22:SER:HA	2:D:87:LEU:O	2.18	0.43
1:A:1024:LEU:O	1:A:1027:THR:OG1	2.31	0.43
1:B:403:ARG:HG2	1:B:497:PHE:HE1	1.83	0.43
1:B:457:ARG:HE	1:B:461:LEU:HD21	1.84	0.43
1:B:703:ASN:O	1:B:705:VAL:N	2.52	0.43
2:D:2:VAL:HA	2:D:26:SER:O	2.19	0.43
1:A:908:GLY:HA3	1:A:1036:GLN:OE1	2.18	0.43
1:B:330:PRO:O	1:B:331:ASN:C	2.61	0.43
1:B:332:ILE:HG22	1:B:333:THR:N	2.34	0.43
1:B:559:PHE:CD2	1:B:584:ILE:HD13	2.53	0.43
1:B:1128:VAL:HG11	1:C:918:GLU:HA	2.00	0.43
1:A:56:LEU:HD23	1:A:57:PRO:O	2.18	0.43
1:A:426:PRO:HG2	1:A:429:PHE:HB2	1.99	0.43
1:A:1094:VAL:N	1:A:1105:THR:O	2.37	0.43
1:B:563:GLN:NE2	1:C:43:PHE:HA	2.34	0.43
1:A:204:TYR:CD1	1:A:225:PRO:HA	2.53	0.43
1:A:701:ALA:HB3	1:B:787:GLN:HA	2.00	0.43
1:B:34:ARG:HA	1:B:34:ARG:HE	1.81	0.43
1:B:1081:ILE:HD11	1:B:1102:TRP:CE2	2.53	0.43
1:C:189:LEU:HD11	1:C:208:THR:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:PHE:CE2	1:C:285:ILE:HG22	2.53	0.43
2:D:21:LEU:HD13	2:D:89:LEU:HD23	2.01	0.43
1:A:801:ASN:HB2	1:A:928:ASN:ND2	2.33	0.43
1:A:867:ASP:OD1	1:A:867:ASP:N	2.52	0.43
1:B:1105:THR:OG1	1:B:1106:GLN:N	2.48	0.43
1:C:558:LYS:HA	1:C:584:ILE:HD11	2.01	0.43
1:C:800:PHE:HD1	1:C:927:PHE:HD2	1.65	0.43
1:C:919:ASN:OD1	1:C:922:LEU:HB3	2.18	0.43
1:A:803:SER:OG	1:A:804:GLN:OE1	2.17	0.43
1:A:871:ALA:O	1:A:874:THR:OG1	2.28	0.43
1:A:878:LEU:HA	1:A:881:THR:HG22	2.00	0.43
1:B:815:ARG:HD2	1:B:819:GLU:CD	2.43	0.43
1:C:104:TRP:HB2	1:C:106:PHE:CE2	2.54	0.43
1:A:189:LEU:N	1:A:208:THR:O	2.52	0.43
1:B:40:ASP:OD1	1:B:40:ASP:N	2.51	0.43
1:B:96:GLU:OE2	1:B:100:ILE:N	2.41	0.43
1:C:294:ASP:H	1:C:297:SER:HG	1.61	0.43
1:C:906:PHE:CD2	1:C:916:LEU:HD12	2.54	0.43
1:C:1083:HIS:HB2	1:C:1088:HIS:NE2	2.34	0.43
2:D:95:ARG:HH11	2:D:96:ALA:HB3	1.83	0.43
1:A:130:VAL:CG2	1:A:168:PHE:HD2	2.32	0.43
1:A:617:CYS:HB3	1:A:649:CYS:HB2	1.77	0.43
1:B:470:THR:HG22	1:B:492:LEU:HD13	2.00	0.43
1:B:863:PRO:HG2	1:B:866:THR:HA	2.01	0.43
1:B:947:LYS:HA	1:B:950:ASP:OD2	2.19	0.43
1:A:53:ASP:O	1:A:272:PRO:HA	2.19	0.42
1:A:99:ASN:HB3	1:A:102:ARG:NH2	2.33	0.42
1:A:555:SER:HA	1:A:586:ASP:OD2	2.19	0.42
1:A:808:ASP:OD1	1:A:811:LYS:HB3	2.18	0.42
1:A:886:TRP:HB2	1:A:1034:LEU:O	2.19	0.42
1:A:1004:LEU:O	1:A:1008:VAL:HG23	2.19	0.42
1:B:54:LEU:C	1:B:270:LEU:HB3	2.43	0.42
1:C:91:TYR:CZ	1:C:93:ALA:HB2	2.54	0.42
1:C:271:GLN:HE21	1:C:273:ARG:HH21	1.67	0.42
1:C:319:ARG:HG3	1:C:319:ARG:HH11	1.83	0.42
3:E:41:TRP:CD1	3:E:53:LEU:HD12	2.54	0.42
1:A:542:ASN:HA	1:A:546:LEU:O	2.20	0.42
1:C:38:TYR:CE2	1:C:285:ILE:HG13	2.53	0.42
1:C:94:SER:OG	1:C:96:GLU:HB2	2.19	0.42
1:C:974:SER:HB3	1:C:980:ILE:HG13	2.01	0.42
1:C:1095:PHE:CE1	1:C:1104:VAL:HB	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:ARG:HG3	1:A:577:ARG:HH11	1.84	0.42
1:B:399:SER:HB3	1:B:511:VAL:HG22	2.01	0.42
1:B:462:LYS:HG2	1:B:465:GLU:HB2	2.01	0.42
1:A:774:GLN:O	1:A:778:THR:HG23	2.19	0.42
1:A:789:TYR:CZ	1:A:893:ALA:HB2	2.53	0.42
1:B:326:ILE:HG13	1:B:541:PHE:HA	2.02	0.42
1:B:612:TYR:O	1:B:648:GLY:HA3	2.18	0.42
1:B:948:LEU:HA	1:B:951:VAL:HG12	2.02	0.42
1:B:949:GLN:CD	1:B:953:ASN:HD21	2.28	0.42
1:C:327:VAL:N	1:C:531:THR:OG1	2.47	0.42
1:C:966:LEU:HG	1:C:1000:ARG:NH1	2.35	0.42
1:C:1096:VAL:HG21	1:C:1110:TYR:HE1	1.83	0.42
2:D:39:MET:HG2	2:D:87:LEU:HD21	2.01	0.42
1:A:231:ILE:HG13	1:A:232:GLY:N	2.35	0.42
1:B:882:ILE:HG23	1:B:898:PHE:CE1	2.55	0.42
1:B:1005:GLN:O	1:B:1009:THR:OG1	2.24	0.42
1:C:36:VAL:HG11	1:C:220:PHE:CZ	2.55	0.42
3:E:41:TRP:O	3:E:52:LEU:HD12	2.19	0.42
3:E:99:PHE:CD1	3:E:124:VAL:HG12	2.54	0.42
1:A:126:VAL:HG11	1:A:175:PHE:HE1	1.85	0.42
1:A:318:PHE:CZ	1:A:620:VAL:HG12	2.54	0.42
1:B:318:PHE:HE2	1:B:620:VAL:HG23	1.83	0.42
1:B:415:THR:HA	1:B:419:ALA:HB3	2.00	0.42
1:B:979:ASP:OD1	1:B:983:ARG:HD3	2.19	0.42
1:B:1026:ALA:HA	1:B:1029:MET:HE3	2.02	0.42
1:C:40:ASP:N	1:C:40:ASP:OD1	2.52	0.42
1:C:102:ARG:HA	1:C:102:ARG:HD2	1.83	0.42
1:C:367:VAL:O	1:C:371:LEU:HG	2.19	0.42
2:D:115:THR:O	3:E:52:LEU:HB2	2.19	0.42
3:E:105:GLN:HE21	3:E:116:PHE:HA	1.84	0.42
1:A:90:VAL:HG11	1:A:238:PHE:HE1	1.84	0.42
1:A:948:LEU:O	1:A:952:VAL:HG23	2.20	0.42
1:B:961:THR:HG21	1:C:765:ARG:NH2	2.35	0.42
1:C:281:GLU:OE1	1:C:281:GLU:N	2.46	0.42
2:D:67:TYR:CE2	2:D:76:PHE:HB2	2.54	0.42
1:A:44:ARG:NH1	1:A:279:TYR:OH	2.53	0.42
1:A:115:GLN:HB2	1:A:233:ILE:HG21	2.02	0.42
1:A:327:VAL:O	1:A:531:THR:N	2.53	0.42
1:A:372:ALA:N	1:A:373:PRO:HD2	2.35	0.42
1:A:699:LEU:HD13	1:B:788:ILE:HG21	2.01	0.42
1:A:729:VAL:HG22	1:A:1059:GLY:HA2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:CYS:HB3	1:A:760:CYS:HB3	1.89	0.42
1:A:906:PHE:HD1	1:A:1049:LEU:HD21	1.84	0.42
1:A:928:ASN:HA	1:A:931:ILE:HG12	2.02	0.42
1:B:34:ARG:NH2	1:B:220:PHE:HA	2.34	0.42
1:C:44:ARG:HG2	1:C:49:HIS:CE1	2.55	0.42
1:C:106:PHE:HB2	1:C:117:LEU:HB3	2.02	0.42
1:C:598:ILE:HG12	1:C:666:ILE:HG12	2.01	0.42
1:C:811:LYS:NZ	1:C:816:SER:HB3	2.35	0.42
1:C:1030:SER:HA	1:C:1034:LEU:HD13	2.01	0.42
1:B:726:ILE:CG2	1:B:947:LYS:HB2	2.50	0.42
1:B:953:ASN:O	1:B:954:HIS:C	2.63	0.42
1:C:656:VAL:HB	1:C:695:TYR:HB3	2.01	0.42
1:C:1032:CYS:HA	1:C:1048:HIS:HE1	1.85	0.42
1:B:128:ILE:HB	1:B:170:TYR:HB3	2.02	0.42
1:B:995:ARG:O	1:B:998:THR:HG22	2.20	0.42
1:B:1025:ALA:HA	1:B:1028:LYS:HG2	2.02	0.42
1:B:1048:HIS:NE2	1:B:1050:MET:O	2.53	0.42
1:C:303:LEU:HD23	1:C:308:VAL:HG22	2.02	0.42
1:C:764:LYS:O	1:C:768:THR:HG23	2.20	0.42
2:D:67:TYR:HD2	2:D:71:VAL:HG23	1.85	0.42
1:A:55:PHE:O	1:A:273:ARG:NH1	2.30	0.41
1:A:87:ASN:HB2	1:A:269:TYR:CE1	2.55	0.41
1:A:746:SER:HB3	1:A:749:CYS:HB2	2.02	0.41
1:A:817:PHE:CE2	1:A:821:LEU:HD23	2.55	0.41
1:B:281:GLU:OE1	1:B:281:GLU:N	2.53	0.41
1:C:561:PRO:HG2	1:C:582:LEU:HD23	2.01	0.41
1:A:726:ILE:HG22	1:A:948:LEU:HD21	2.01	0.41
1:A:950:ASP:OD1	1:A:954:HIS:HE1	2.03	0.41
1:A:954:HIS:HA	1:A:957:GLN:NE2	2.34	0.41
2:D:30:VAL:HB	2:D:80:ARG:HE	1.85	0.41
2:D:110:ILE:HD12	2:D:110:ILE:HA	1.98	0.41
1:A:740:MET:HE1	1:C:319:ARG:HH21	1.86	0.41
1:C:916:LEU:O	1:C:920:GLN:N	2.53	0.41
2:D:94:LEU:HD23	2:D:94:LEU:HA	1.81	0.41
1:A:365:TYR:H	1:A:365:TYR:HD1	1.69	0.41
1:A:562:PHE:O	1:B:41:LYS:HB3	2.21	0.41
1:A:662:CYS:HB2	1:A:697:MET:HG3	2.03	0.41
1:B:66:HIS:NE2	1:B:80:ASP:OD2	2.53	0.41
1:B:763:LEU:O	1:B:767:LEU:HG	2.21	0.41
1:B:886:TRP:HH2	1:B:904:TYR:HD2	1.68	0.41
1:B:950:ASP:HA	1:B:953:ASN:ND2	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:950:ASP:C	1:B:954:HIS:HD1	2.25	0.41
1:C:294:ASP:N	1:C:297:SER:OG	2.45	0.41
1:C:600:PRO:HG2	1:C:605:SER:HB3	2.03	0.41
1:C:950:ASP:C	1:C:954:HIS:HD1	2.19	0.41
1:A:743:CYS:HB3	1:A:746:SER:HB3	2.02	0.41
1:A:788:ILE:HD13	1:A:788:ILE:HA	1.90	0.41
1:A:792:PRO:HG2	1:C:707:TYR:HB3	2.01	0.41
1:A:815:ARG:HG2	1:A:819:GLU:HG3	2.03	0.41
1:B:57:PRO:HB2	1:B:60:SER:OG	2.20	0.41
1:B:599:THR:HB	1:B:608:VAL:HG12	2.02	0.41
1:B:965:GLN:HG2	1:B:1003:SER:HB2	2.01	0.41
1:B:1090:PRO:HG3	1:B:1095:PHE:CE1	2.56	0.41
1:C:781:VAL:C	1:C:1029:MET:HE1	2.46	0.41
1:C:889:GLY:HA3	1:C:1034:LEU:HD23	2.02	0.41
2:D:5:VAL:O	2:D:23:CYS:HA	2.21	0.41
3:E:41:TRP:HD1	3:E:53:LEU:HB2	1.85	0.41
1:A:128:ILE:HB	1:A:170:TYR:O	2.21	0.41
1:A:741:TYR:CD2	1:A:1004:LEU:HD22	2.56	0.41
1:A:753:LEU:HA	1:A:756:TYR:HD2	1.85	0.41
1:B:559:PHE:C	1:B:577:ARG:HH22	2.28	0.41
1:A:115:GLN:NE2	1:A:233:ILE:HG21	2.36	0.41
1:B:231:ILE:HD12	1:B:233:ILE:HG12	2.02	0.41
1:B:330:PRO:C	1:B:580:GLN:HE22	2.28	0.41
1:B:430:THR:O	1:B:515:PHE:HB2	2.20	0.41
1:B:822:LEU:HD22	1:B:945:LEU:HD21	2.03	0.41
1:B:884:SER:OG	1:B:893:ALA:HB1	2.20	0.41
1:B:906:PHE:O	1:B:911:VAL:N	2.46	0.41
1:B:959:LEU:O	1:B:962:LEU:HB3	2.20	0.41
1:C:452:LEU:HD23	1:C:492:LEU:HB3	2.02	0.41
1:C:789:TYR:O	1:C:790:LYS:NZ	2.43	0.41
1:C:800:PHE:HA	1:C:928:ASN:HD21	1.85	0.41
1:C:811:LYS:HE3	1:C:814:LYS:HA	2.03	0.41
2:D:116:ASP:OD1	2:D:117:ILE:N	2.53	0.41
1:A:378:LYS:O	1:A:433:VAL:HG12	2.21	0.41
1:B:34:ARG:HB3	1:B:91:TYR:CE2	2.56	0.41
1:C:769:GLY:HA2	1:C:772:VAL:HG12	2.03	0.41
1:A:123:ALA:O	1:A:177:MET:HE2	2.21	0.41
1:A:382:VAL:HG11	1:A:392:PHE:HE2	1.85	0.41
1:A:429:PHE:CZ	1:A:431:GLY:HA3	2.56	0.41
1:A:665:PRO:HB3	1:B:864:LEU:CD1	2.51	0.41
1:A:813:SER:OG	1:A:815:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1104:VAL:HG13	1:A:1113:GLN:HB2	2.02	0.41
1:B:34:ARG:HB3	1:B:91:TYR:CZ	2.55	0.41
1:B:86:PHE:HE1	1:B:194:PHE:HB3	1.86	0.41
1:B:458:LYS:HD3	1:B:473:TYR:CE1	2.56	0.41
1:B:563:GLN:O	1:B:577:ARG:NH1	2.54	0.41
1:B:692:ILE:HG13	1:B:692:ILE:O	2.19	0.41
1:B:906:PHE:CD2	1:B:916:LEU:HD12	2.55	0.41
1:B:909:ILE:HD13	1:B:1049:LEU:HD21	2.03	0.41
1:C:762:GLN:NE2	1:C:763:LEU:HG	2.36	0.41
1:C:817:PHE:CG	1:C:818:ILE:N	2.89	0.41
1:A:287:ASP:OD1	1:A:288:ALA:N	2.54	0.41
1:A:295:PRO:HA	1:A:298:GLU:HG2	2.03	0.41
1:A:1107:ARG:HG3	1:B:904:TYR:CE2	2.56	0.41
1:B:593:GLY:HA3	1:B:613:GLN:O	2.21	0.41
1:C:86:PHE:N	1:C:236:THR:O	2.51	0.41
1:C:189:LEU:HD21	1:C:208:THR:N	2.36	0.41
1:C:729:VAL:HG13	1:C:781:VAL:HG21	2.03	0.41
1:C:868:GLU:O	1:C:872:GLN:OE1	2.39	0.41
1:C:933:LYS:HB2	1:C:933:LYS:HE2	1.84	0.41
1:C:1004:LEU:O	1:C:1008:VAL:HG23	2.21	0.41
1:A:168:PHE:CE1	1:A:229:LEU:CG	2.88	0.40
1:A:303:LEU:HD12	1:A:308:VAL:HG22	2.03	0.40
1:B:527:PRO:C	1:B:529:LYS:H	2.29	0.40
1:B:779:GLN:NE2	1:B:783:ALA:O	2.54	0.40
1:B:930:ALA:O	1:B:934:ILE:HG12	2.20	0.40
1:C:328:ARG:HD3	1:C:530:SER:HB3	2.02	0.40
1:C:713:ALA:HA	1:C:1074:ASN:HA	2.03	0.40
1:C:808:ASP:N	1:C:811:LYS:HE2	2.27	0.40
1:A:99:ASN:ND2	1:A:179:LEU:HD13	2.36	0.40
1:B:375:PHE:CG	1:B:508:TYR:CE2	3.00	0.40
1:B:403:ARG:O	1:B:407:VAL:HG23	2.21	0.40
1:B:532:ASN:OD1	1:B:533:LEU:N	2.55	0.40
1:C:742:ILE:HG22	1:C:743:CYS:SG	2.61	0.40
1:A:177:MET:O	1:A:179:LEU:HG	2.21	0.40
1:A:560:LEU:HB2	1:A:563:GLN:OE1	2.21	0.40
1:B:318:PHE:HD2	1:B:612:TYR:CE1	2.39	0.40
1:B:405:ASP:OD1	1:B:405:ASP:N	2.53	0.40
1:C:553:THR:O	1:C:586:ASP:N	2.48	0.40
1:A:50:SER:OG	1:A:275:PHE:O	2.25	0.40
1:A:458:LYS:HD3	1:A:458:LYS:HA	1.89	0.40
1:A:765:ARG:HB3	1:A:765:ARG:CZ	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:LEU:HD13	1:C:715:PRO:HG3	2.03	0.40
1:B:195:LYS:HE3	1:B:202:LYS:HE2	2.04	0.40
1:B:371:LEU:HD13	6:B:1303:NAG:H83	2.02	0.40
2:D:80:ARG:HH12	2:D:82:ASN:HA	1.86	0.40
1:A:884:SER:OG	1:A:893:ALA:HB1	2.21	0.40
1:A:923:ILE:HD12	1:A:923:ILE:HA	1.98	0.40
1:B:323:THR:N	1:B:539:VAL:HG12	2.36	0.40
1:C:44:ARG:NH2	1:C:279:TYR:CZ	2.88	0.40
1:C:728:PRO:HG3	1:C:951:VAL:HG11	2.02	0.40
1:C:743:CYS:HB3	1:C:749:CYS:HB3	1.97	0.40
2:D:80:ARG:HD2	2:D:81:ASP:N	2.37	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	935/1261 (74%)	893 (96%)	42 (4%)	0	100	100
1	B	962/1261 (76%)	915 (95%)	42 (4%)	5 (0%)	24	63
1	C	968/1261 (77%)	942 (97%)	26 (3%)	0	100	100
2	D	116/119 (98%)	112 (97%)	2 (2%)	2 (2%)	7	35
3	E	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
All	All	3089/4012 (77%)	2966 (96%)	116 (4%)	7 (0%)	44	77

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	372	ALA
1	B	330	PRO
1	B	334	ASN

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Mol	Chain	Res	Type
1	B	529	LYS
2	D	112	VAL
1	B	373	PRO
2	D	110	ILE

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	837/1098 (76%)	831 (99%)	6 (1%)	76	79
1	B	854/1098 (78%)	850 (100%)	4 (0%)	81	81
1	C	867/1098 (79%)	867 (100%)	0	100	100
2	D	96/96 (100%)	96 (100%)	0	100	100
3	E	92/92 (100%)	92 (100%)	0	100	100
All	All	2746/3482 (79%)	2736 (100%)	10 (0%)	81	82

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	PHE
1	A	328	ARG
1	A	332	ILE
1	A	333	THR
1	A	334	ASN
1	A	335	LEU
1	B	333	THR
1	B	334	ASN
1	B	335	LEU
1	B	529	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	99	ASN
1	A	115	GLN
1	A	271	GLN
1	A	334	ASN
1	A	774	GLN
1	A	824	ASN
1	A	895	GLN
1	A	928	ASN
1	A	949	GLN
1	A	954	HIS
1	A	1010	GLN
1	A	1054	GLN
1	A	1071	GLN
1	A	1106	GLN
1	B	388	ASN
1	B	417	ASN
1	B	505	HIS
1	B	544	ASN
1	B	580	GLN
1	B	709	ASN
1	B	804	GLN
1	B	953	ASN
1	B	1002	GLN
1	B	1005	GLN
1	B	1010	GLN
1	B	1054	GLN
1	B	1071	GLN
1	B	1088	HIS
1	C	52	GLN
1	C	314	GLN
1	C	613	GLN
1	C	762	GLN
1	C	925	ASN
1	C	935	GLN
1	C	1002	GLN
1	C	1023	ASN
1	C	1083	HIS
2	D	44	GLN
3	E	43	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 ⓘ

11 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	F	1	4,1	14,14,15	0.23	0	17,19,21	0.49	0
4	NAG	F	2	4	14,14,15	0.23	0	17,19,21	0.46	0
4	NAG	L	1	4,1	14,14,15	0.29	0	17,19,21	0.45	0
4	NAG	L	2	4	14,14,15	0.28	0	17,19,21	0.43	0
4	NAG	N	1	4,1	14,14,15	0.42	0	17,19,21	0.60	0
4	NAG	N	2	4	14,14,15	0.21	0	17,19,21	0.54	0
5	NAG	T	1	5,1	14,14,15	0.38	0	17,19,21	0.53	0
5	NAG	T	2	5	14,14,15	0.25	0	17,19,21	0.40	0
5	BMA	T	3	5	11,11,12	0.51	0	15,15,17	0.67	0
4	NAG	U	1	4,1	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	U	2	4	14,14,15	0.26	0	17,19,21	0.44	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	F	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	L	1	4,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
4	NAG	N	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
5	NAG	T	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	T	2	5	-	0/6/23/26	0/1/1/1
5	BMA	T	3	5	-	0/2/19/22	0/1/1/1
4	NAG	U	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	U	2	4	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

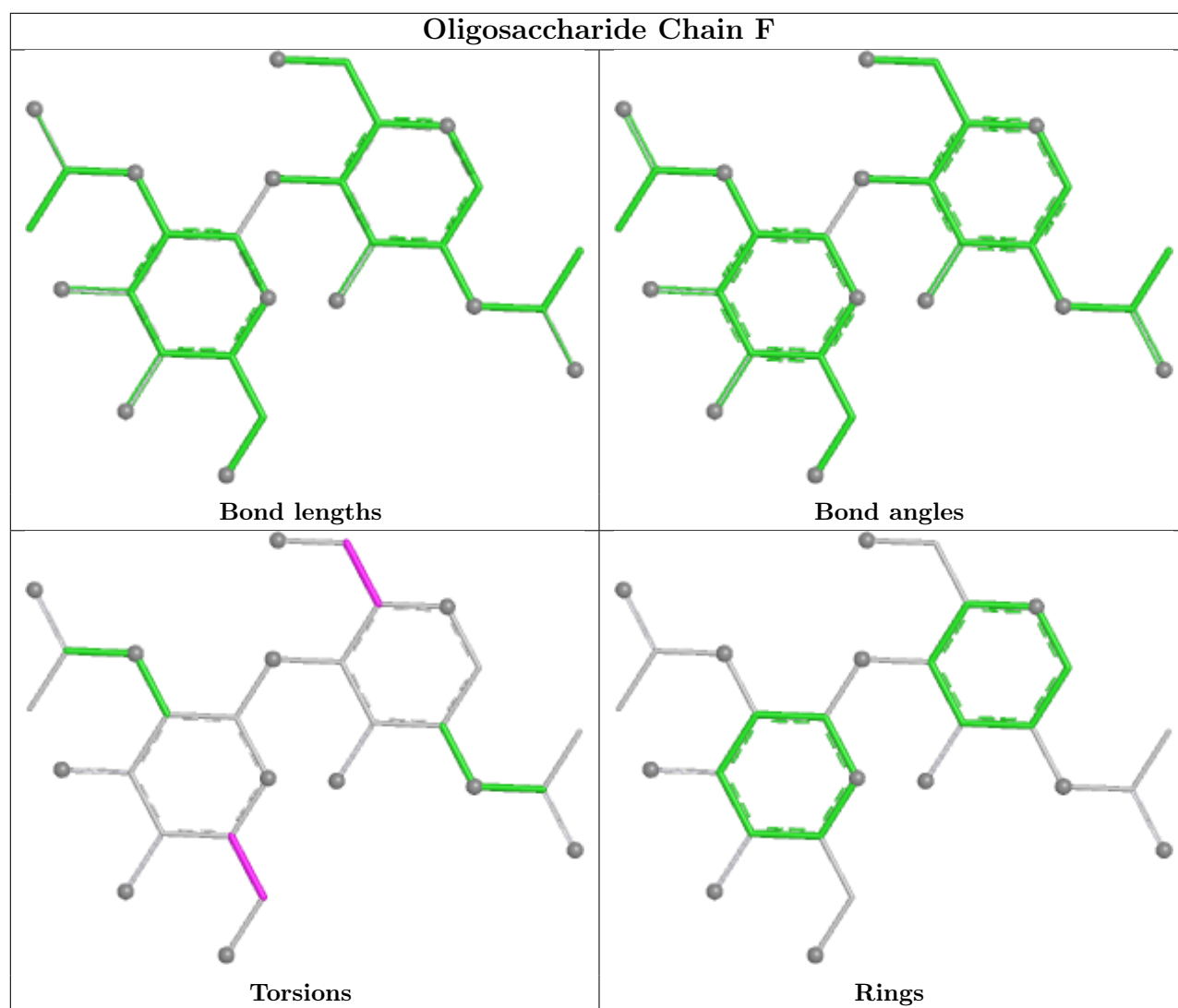
All (16) torsion outliers are listed below:

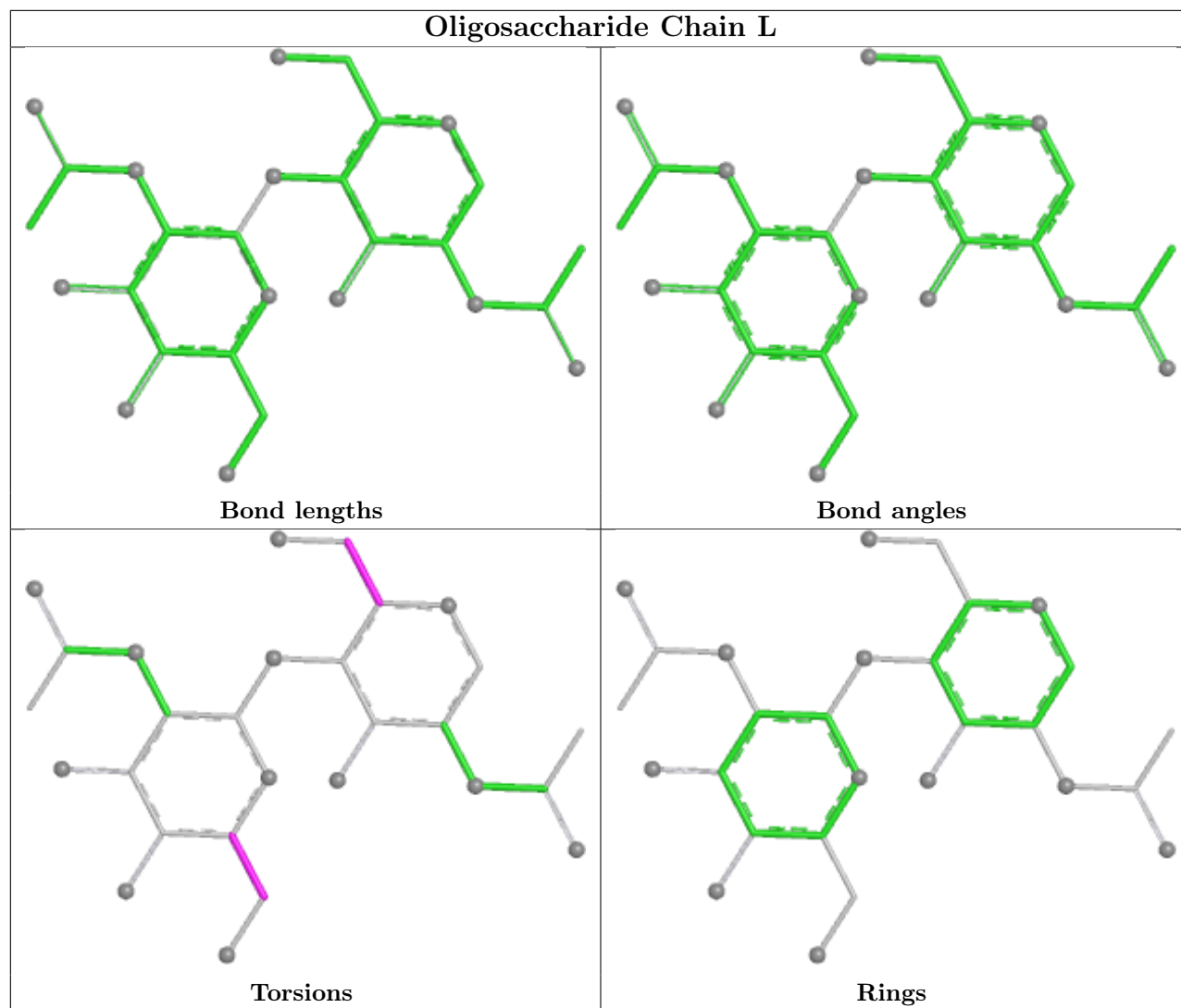
Mol	Chain	Res	Type	Atoms
4	N	2	NAG	C4-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6
5	T	1	NAG	C4-C5-C6-O6
5	T	1	NAG	O5-C5-C6-O6

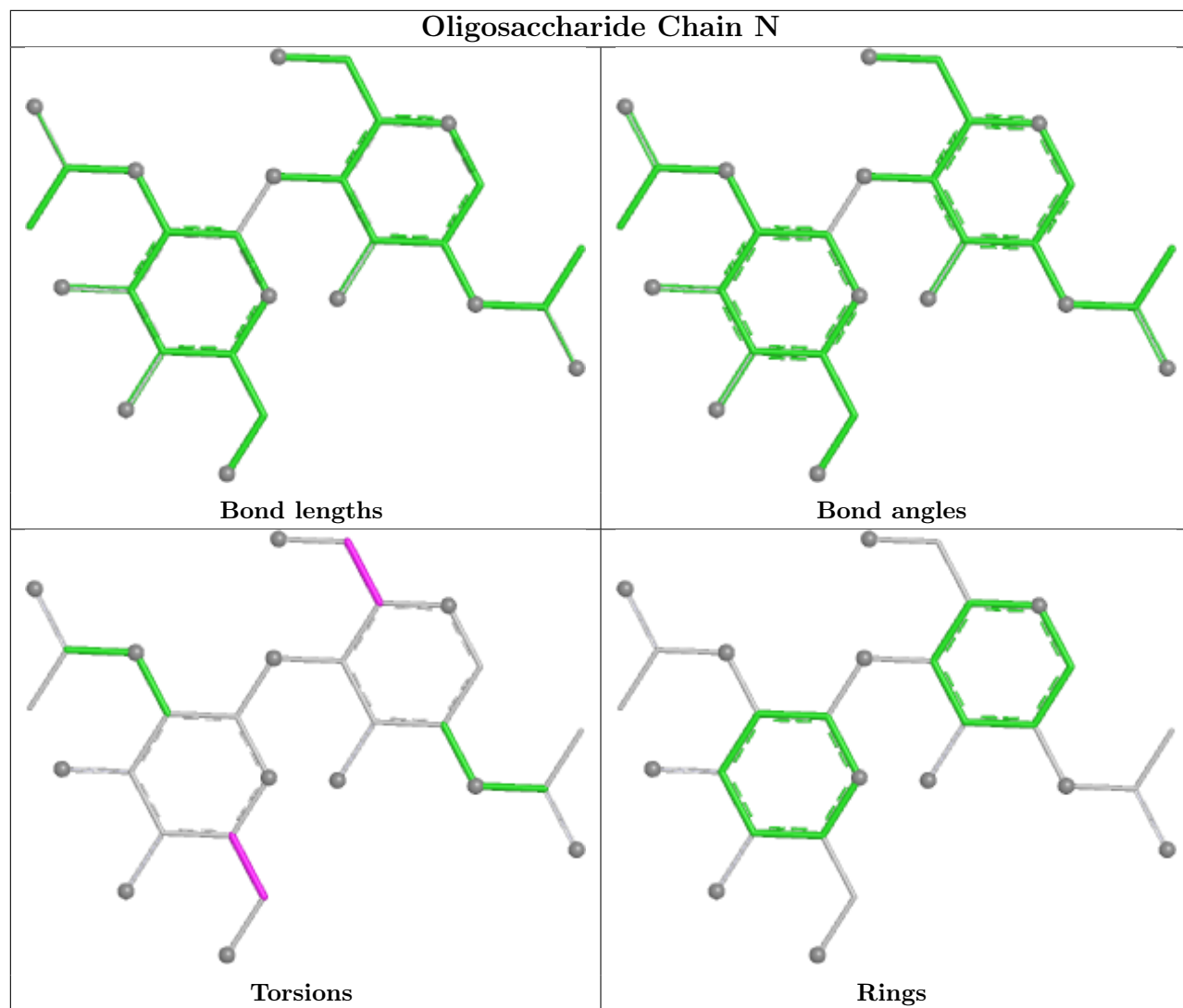
There are no ring outliers.

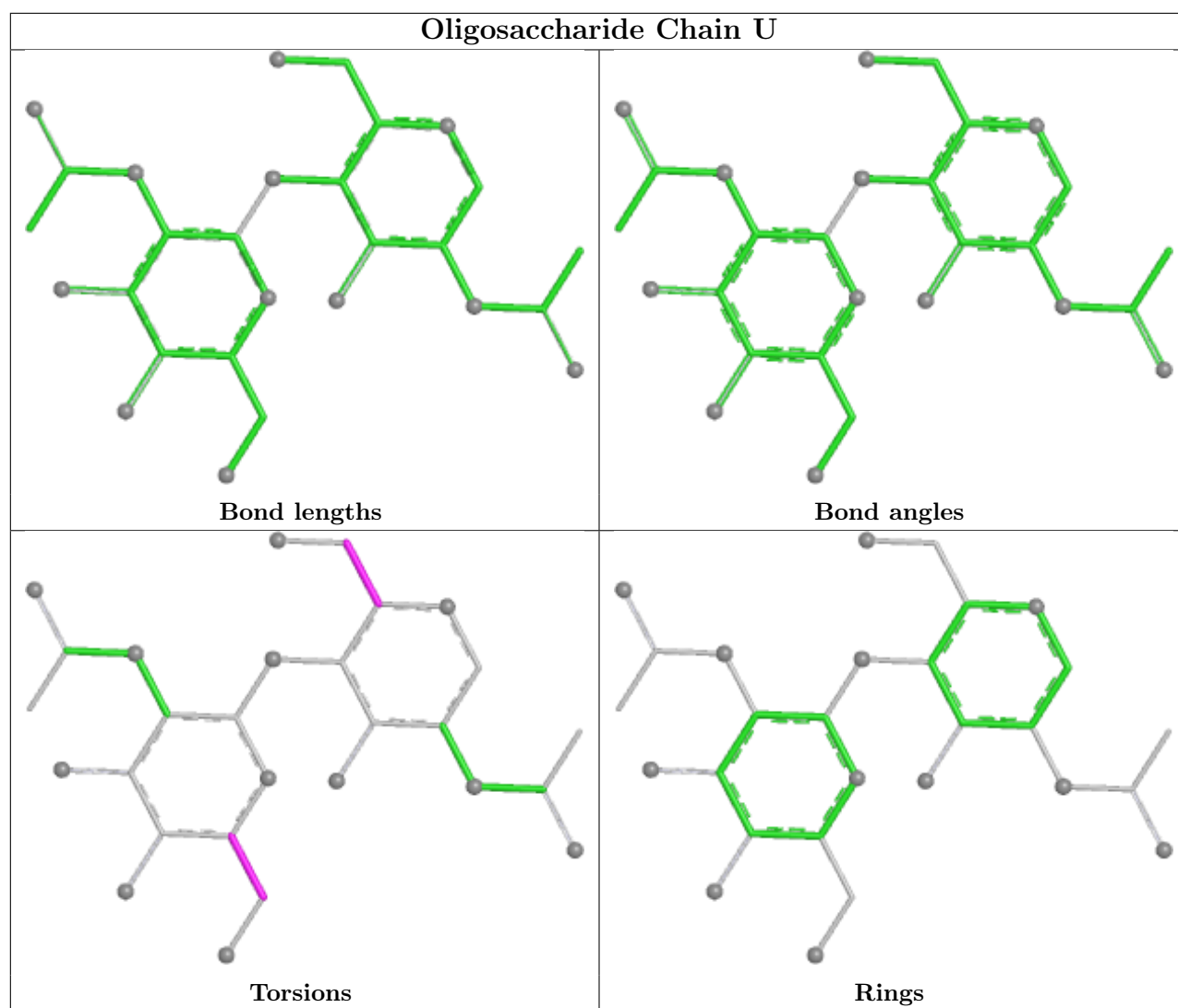
No monomer is involved in short contacts.

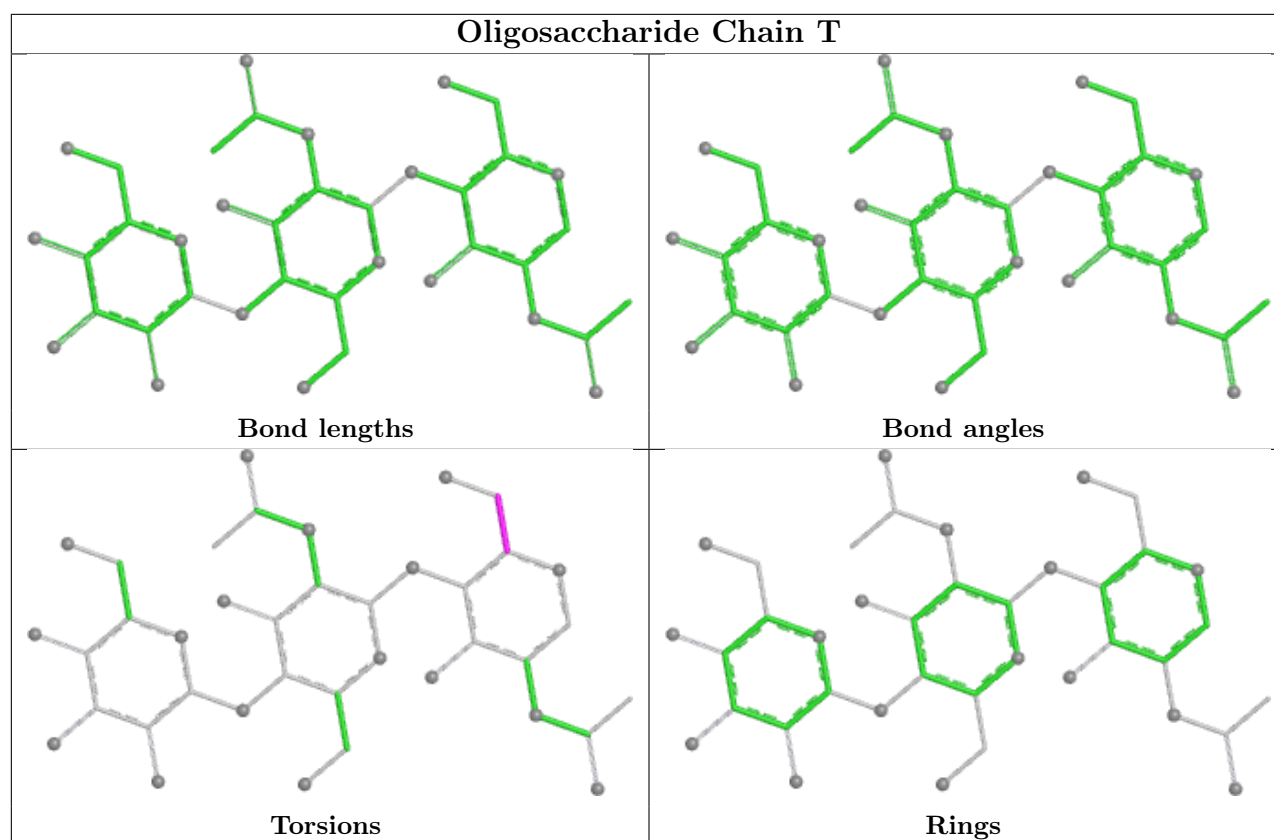
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

7 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	$\# Z > 2$
6	NAG	B	1301	1	14,14,15	0.23	0	17,19,21	0.60	0
6	NAG	A	1303	1	14,14,15	0.25	0	17,19,21	0.45	0
6	NAG	A	1301	1	14,14,15	0.17	0	17,19,21	0.56	0
6	NAG	B	1303	1	14,14,15	0.57	0	17,19,21	0.56	0
6	NAG	A	1302	1	14,14,15	0.28	0	17,19,21	0.48	0
6	NAG	B	1302	1	14,14,15	0.21	0	17,19,21	0.50	0
6	NAG	C	1301	1	14,14,15	0.19	0	17,19,21	0.54	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
6	NAG	B	1301	1	-	4/6/23/26	0/1/1/1
6	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1301	1	-	3/6/23/26	0/1/1/1
6	NAG	B	1303	1	-	3/6/23/26	0/1/1/1
6	NAG	A	1302	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1301	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1303	NAG	O5-C5-C6-O6
6	B	1303	NAG	O5-C5-C6-O6
6	B	1303	NAG	C4-C5-C6-O6
6	C	1301	NAG	O5-C5-C6-O6
6	A	1303	NAG	C4-C5-C6-O6
6	A	1301	NAG	O5-C5-C6-O6
6	B	1302	NAG	C4-C5-C6-O6
6	B	1302	NAG	O5-C5-C6-O6
6	C	1301	NAG	C4-C5-C6-O6
6	A	1302	NAG	O5-C5-C6-O6
6	B	1301	NAG	C4-C5-C6-O6
6	B	1301	NAG	O5-C5-C6-O6
6	A	1301	NAG	C1-C2-N2-C7
6	C	1301	NAG	C1-C2-N2-C7
6	A	1301	NAG	C3-C2-N2-C7
6	B	1301	NAG	C3-C2-N2-C7
6	B	1301	NAG	C1-C2-N2-C7
6	B	1303	NAG	C3-C2-N2-C7
6	C	1301	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1303	NAG	1	0
6	B	1303	NAG	2	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.

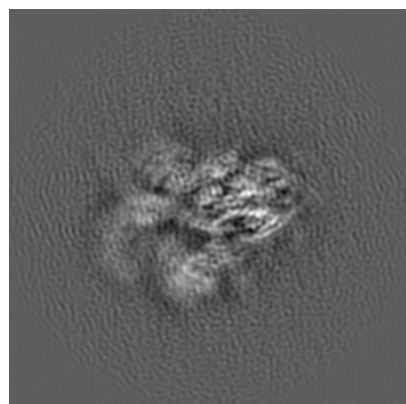
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39686. These allow visual inspection of the internal detail of the map and identification of artifacts.

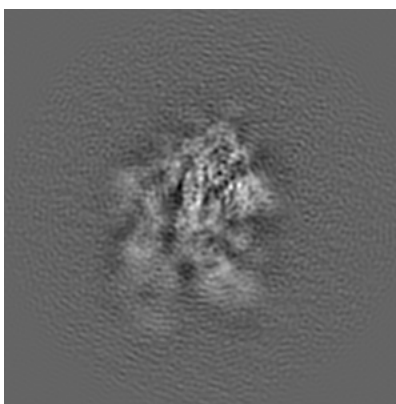
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

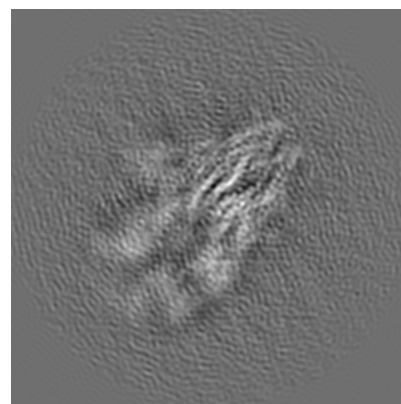
6.1.1 Primary map



X

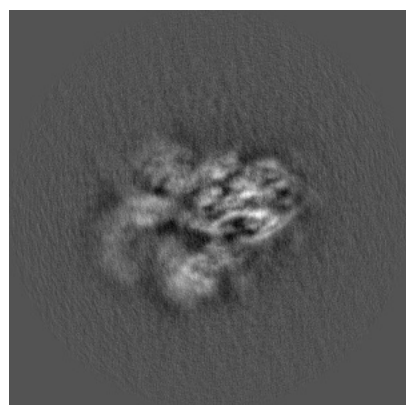


Y

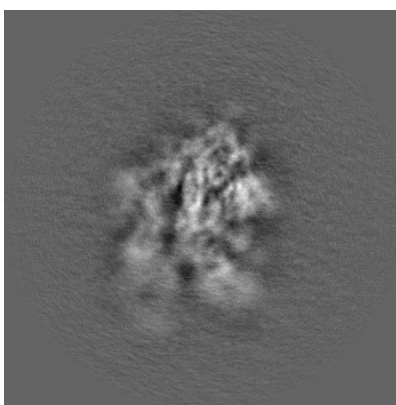


Z

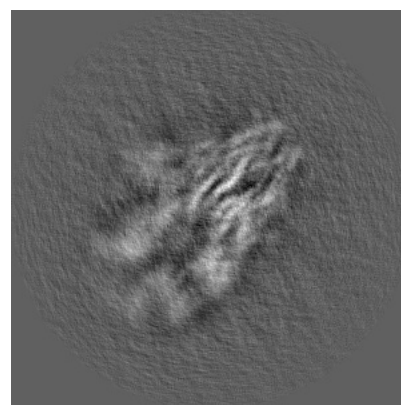
6.1.2 Raw map



X



Y

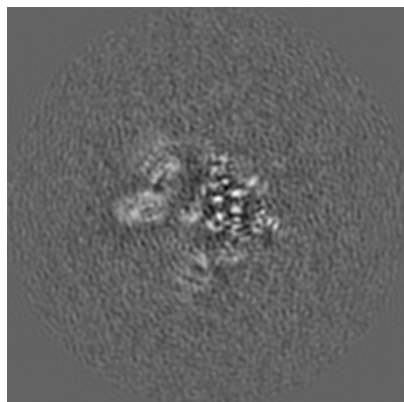


Z

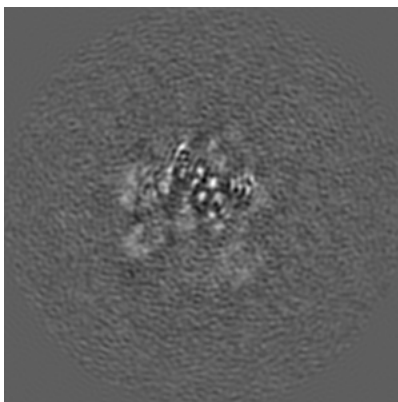
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

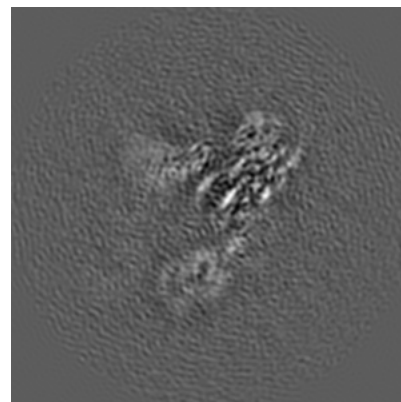
6.2.1 Primary map



X Index: 192

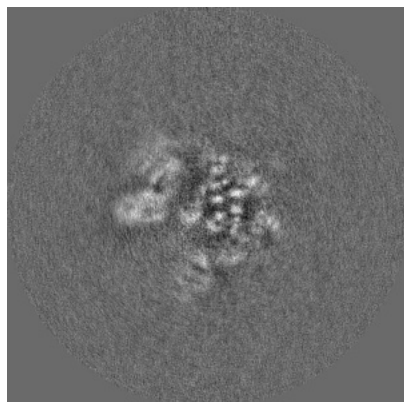


Y Index: 192

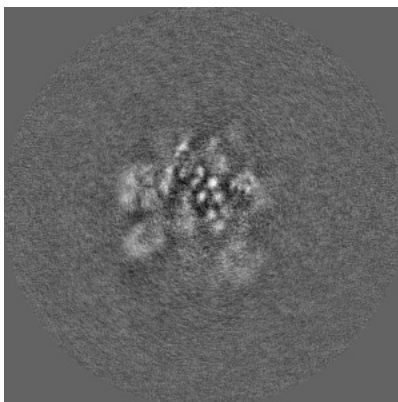


Z Index: 192

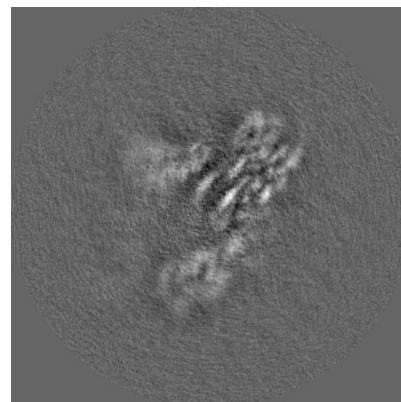
6.2.2 Raw map



X Index: 192



Y Index: 192

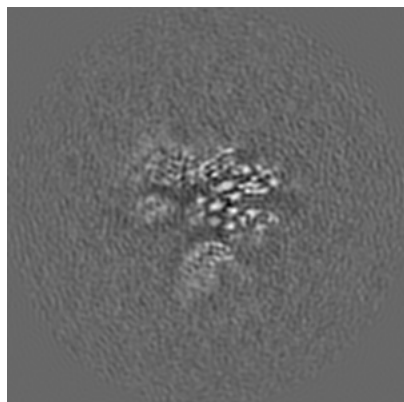


Z Index: 192

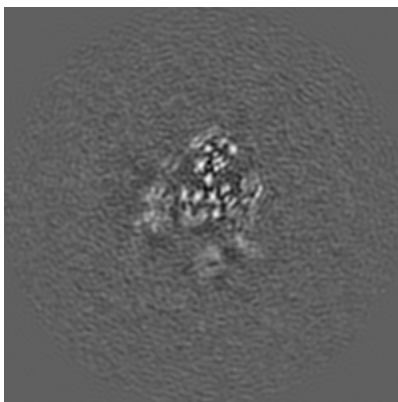
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

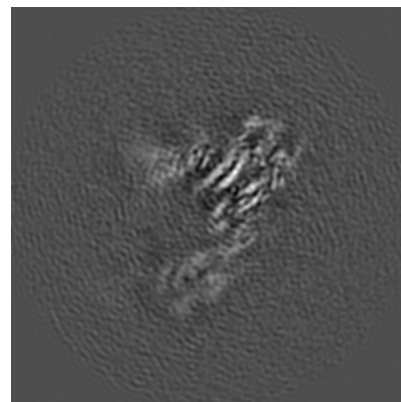
6.3.1 Primary map



X Index: 208

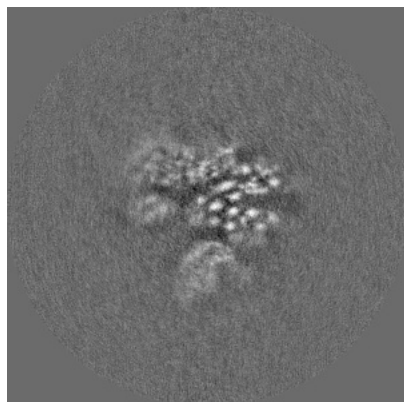


Y Index: 211

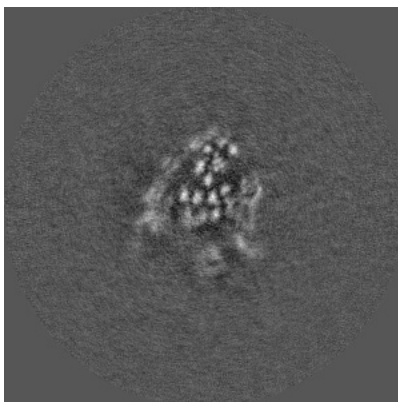


Z Index: 188

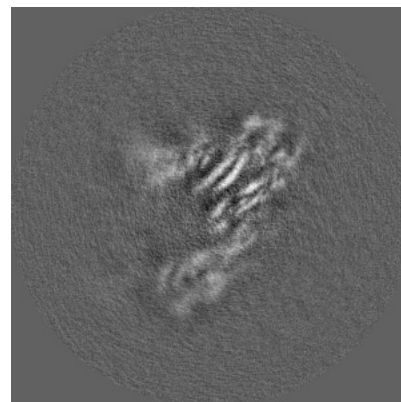
6.3.2 Raw map



X Index: 208



Y Index: 210

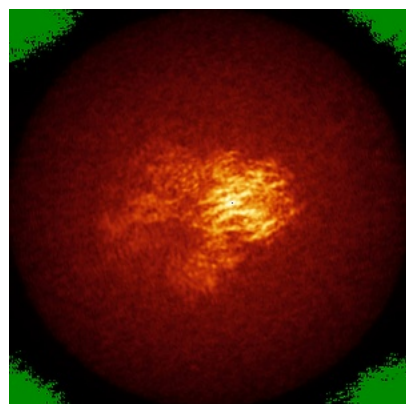


Z Index: 188

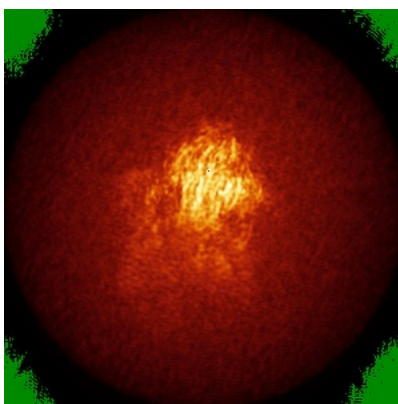
The images above show the largest variance slices of the map in three orthogonal directions.

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

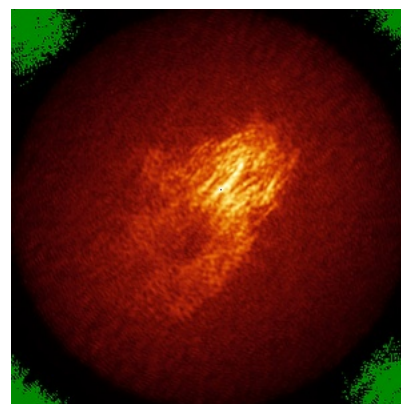
6.4.1 Primary map



X

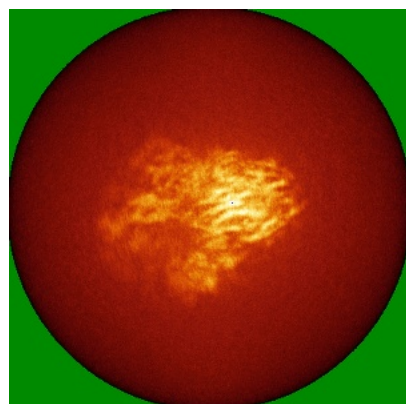


Y

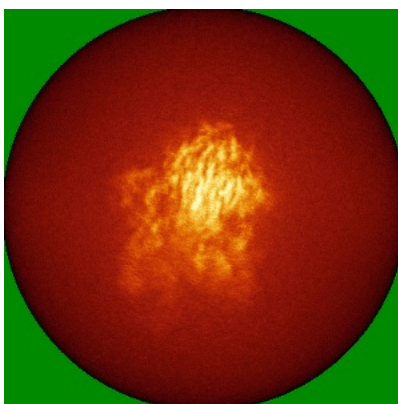


Z

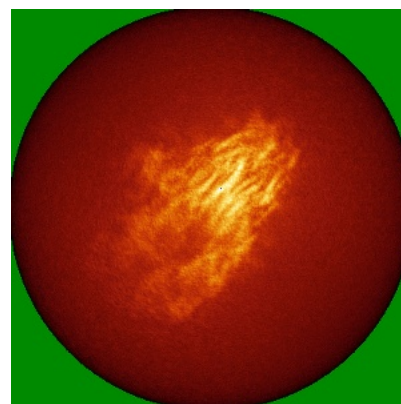
6.4.2 Raw map



X



Y

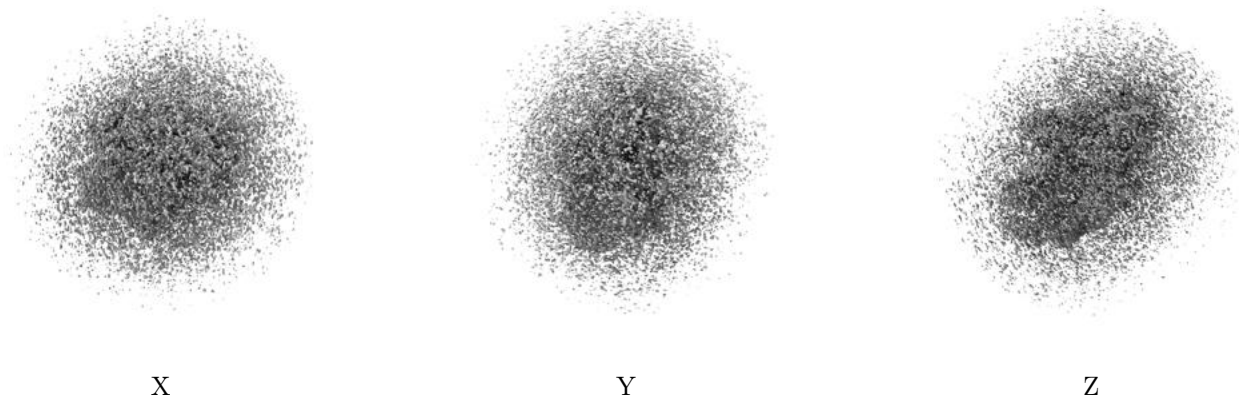


Z

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

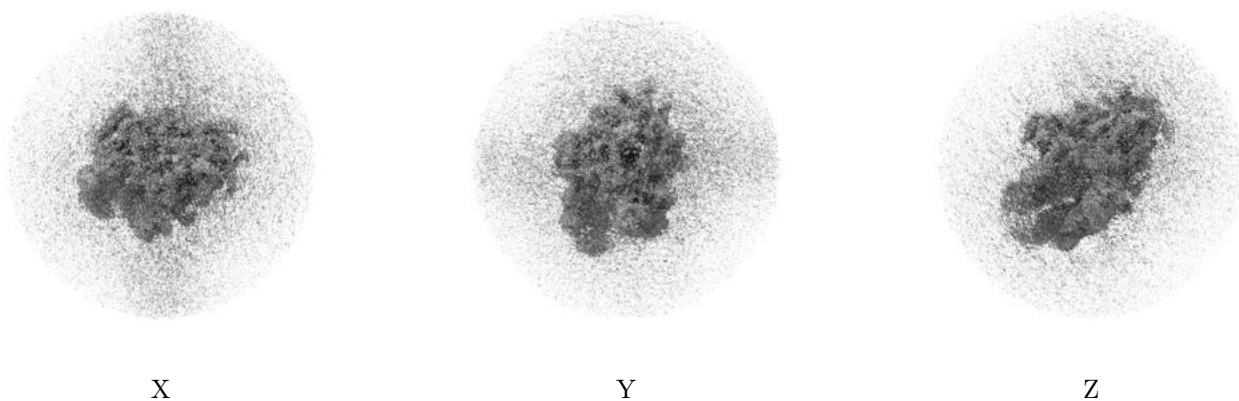
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0029. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

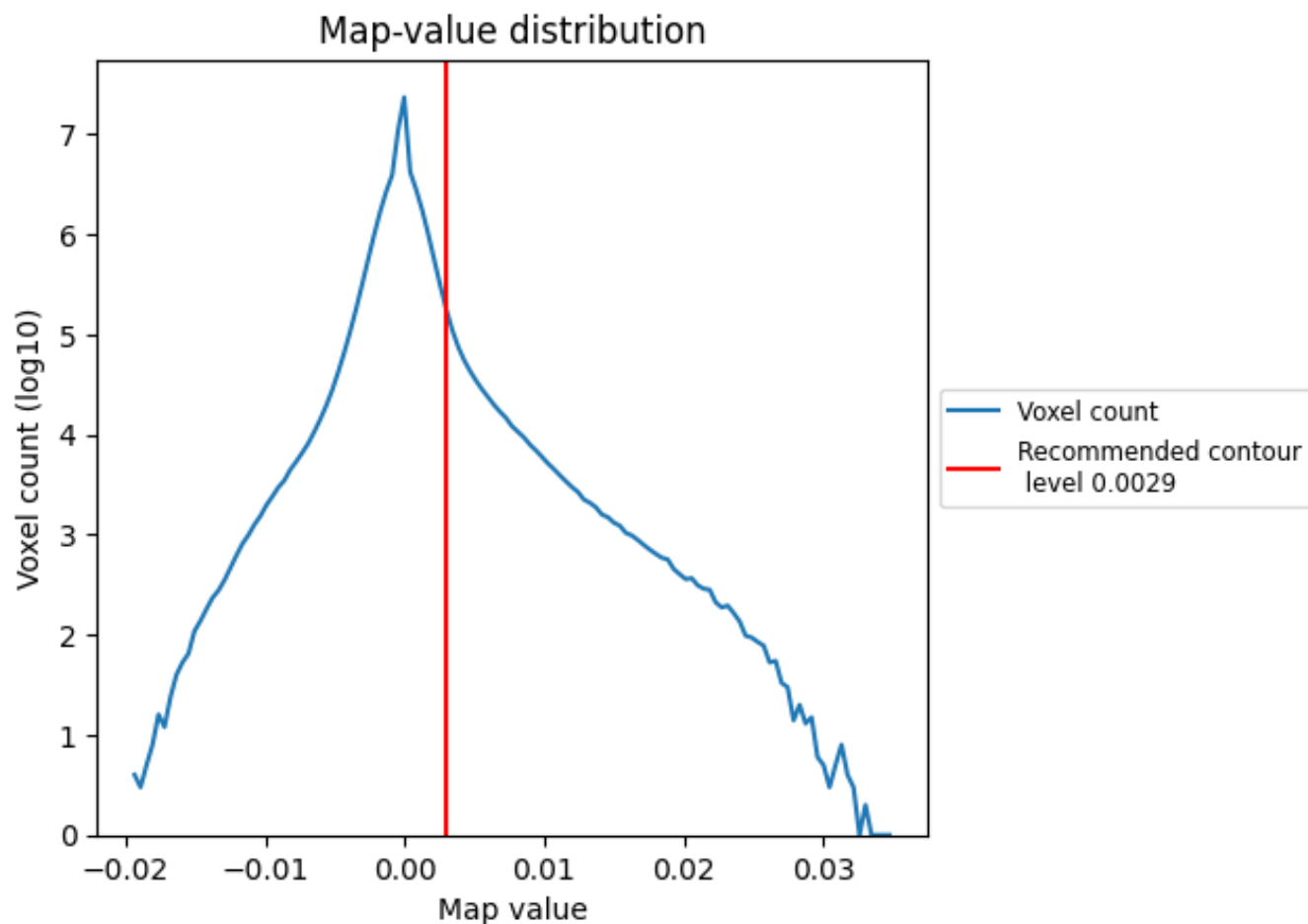
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

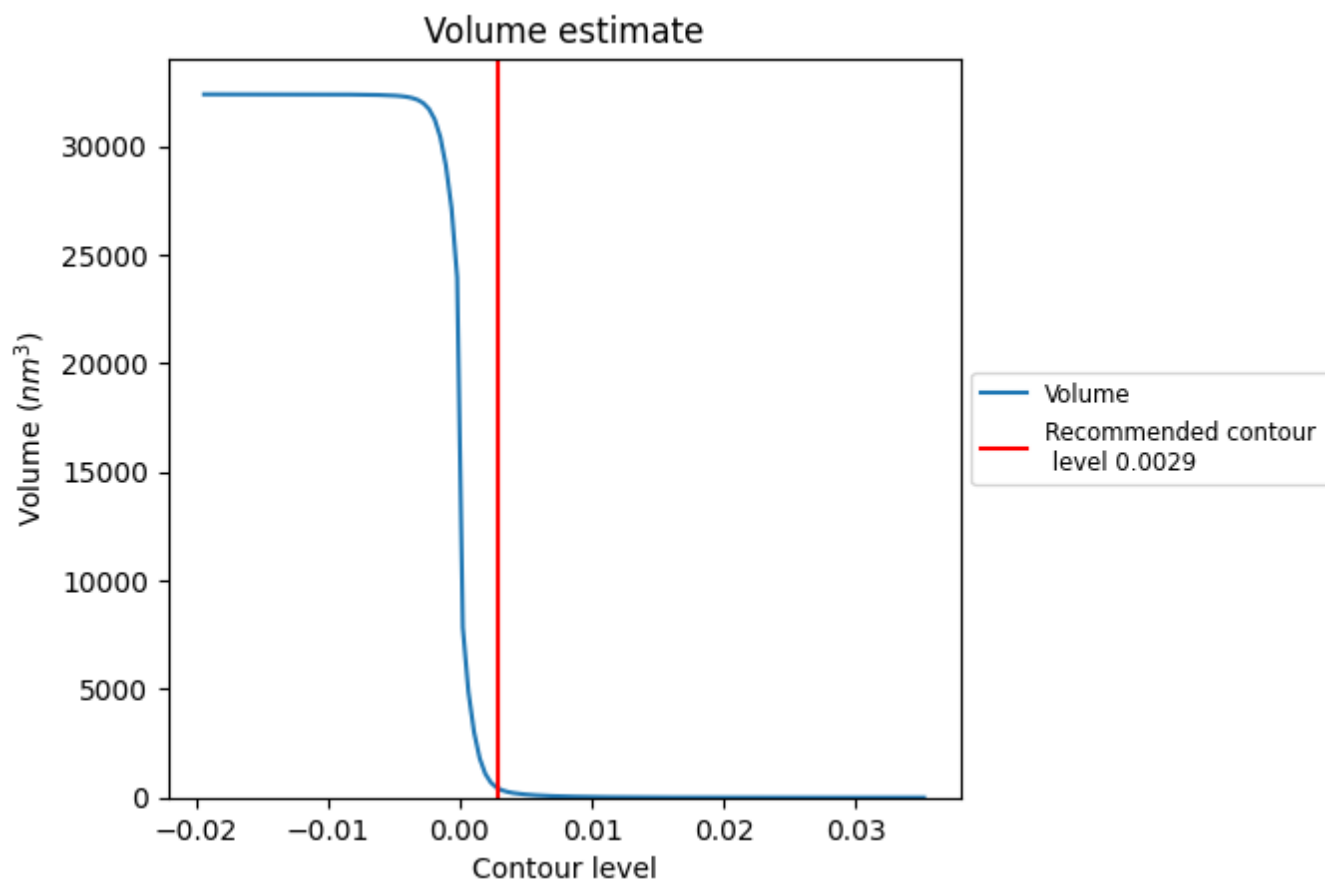
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

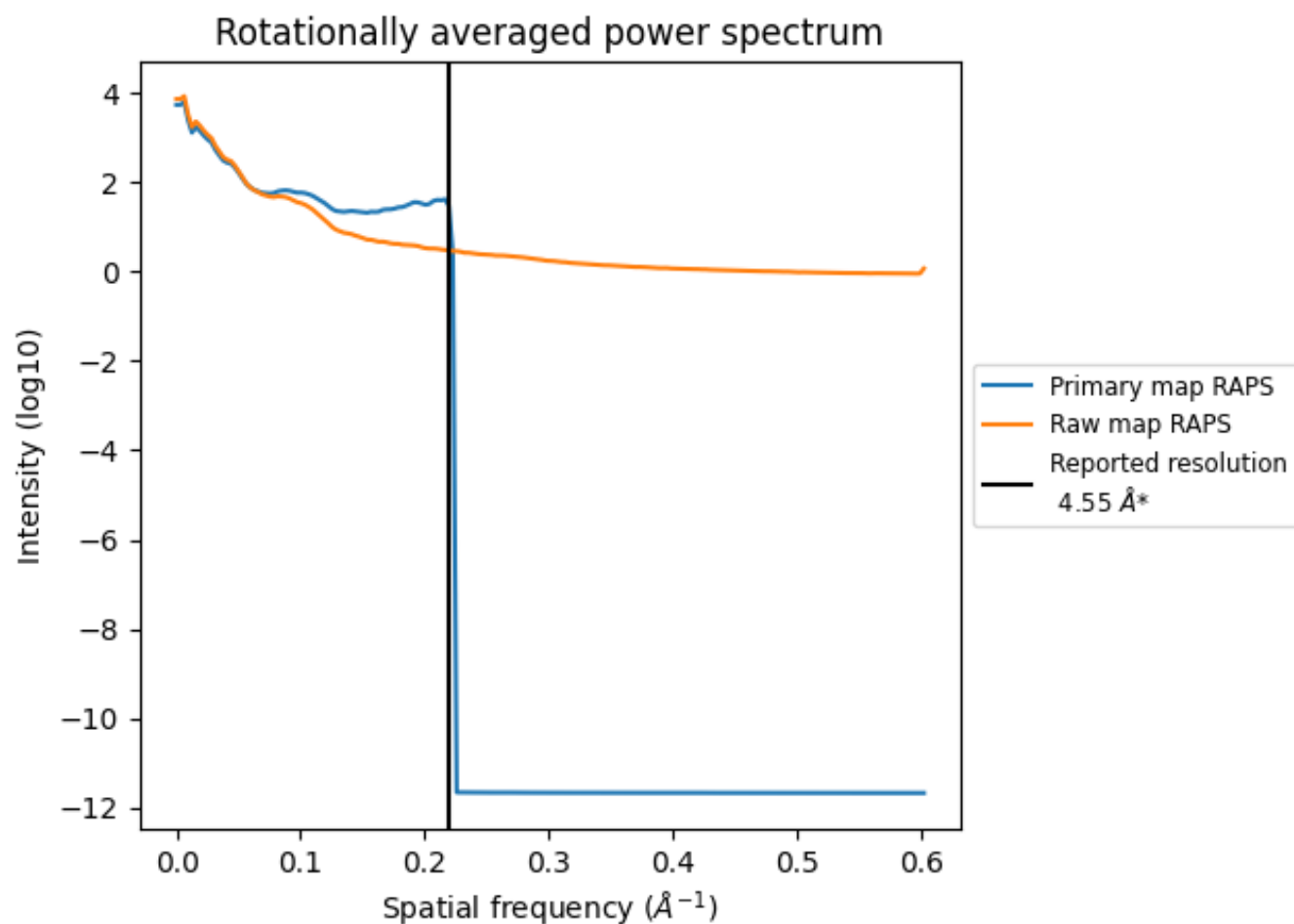
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 430 nm^3 ; this corresponds to an approximate mass of 389 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 ⓘ

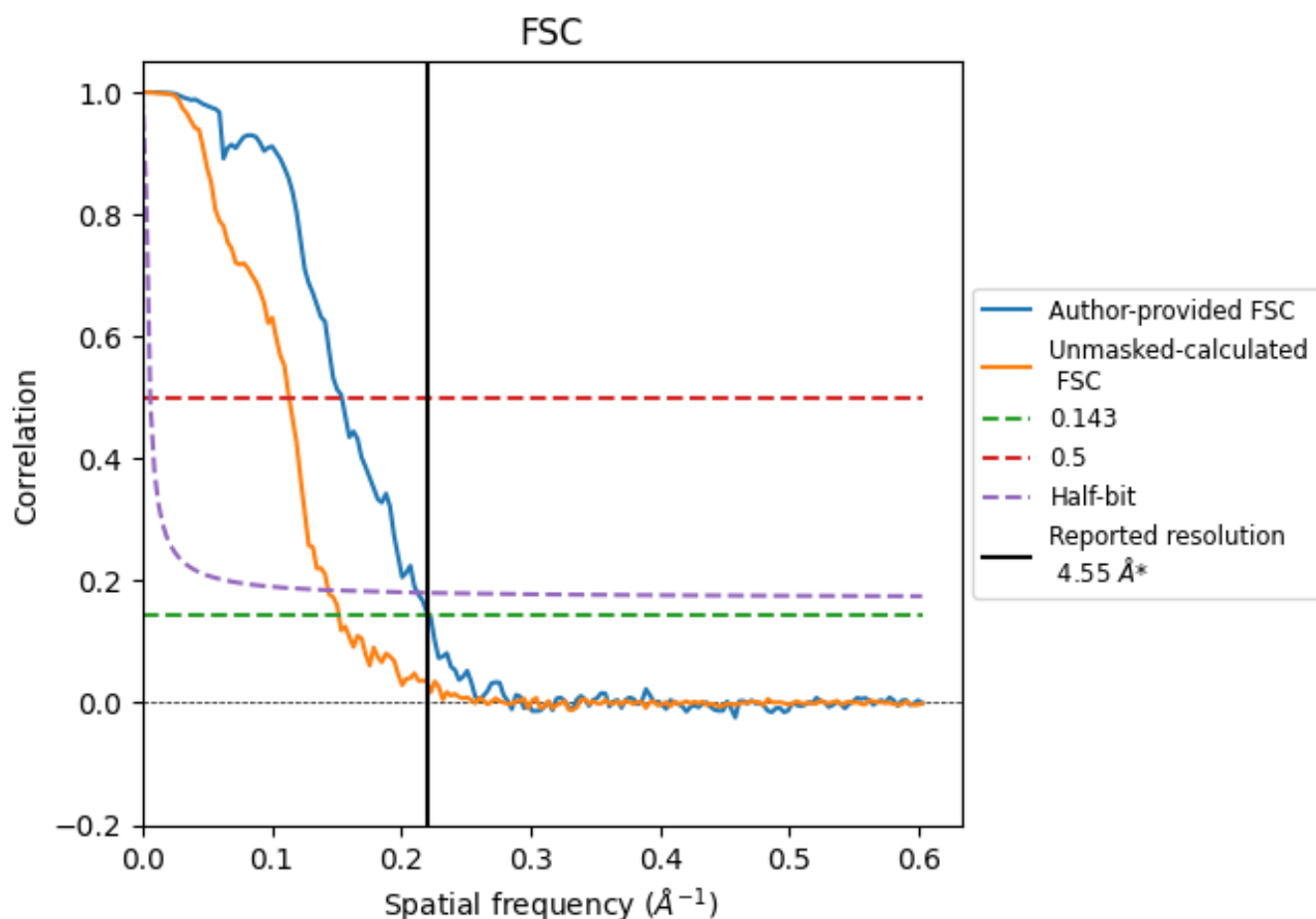


*Reported resolution corresponds to spatial frequency of 0.220 Å⁻¹

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 0.220 Å⁻¹

8.2 Resolution estimates [i](#)

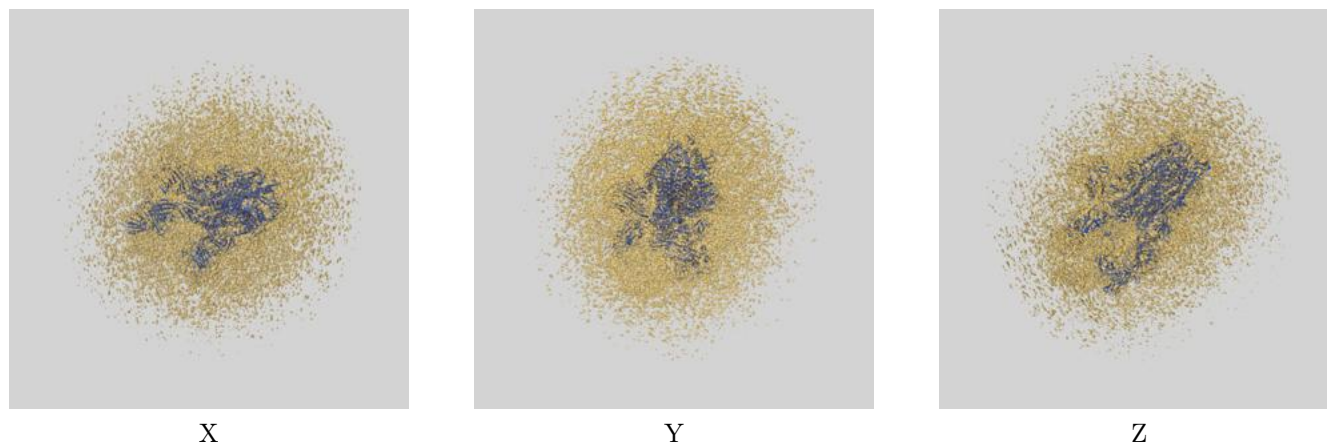
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.55	-	-
Author-provided FSC curve	4.51	6.49	4.70
Unmasked-calculated*	6.58	8.82	6.96

*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 6.58 differs from the reported value 4.55 by more than 10 %

9 Map-model fit [i](#)

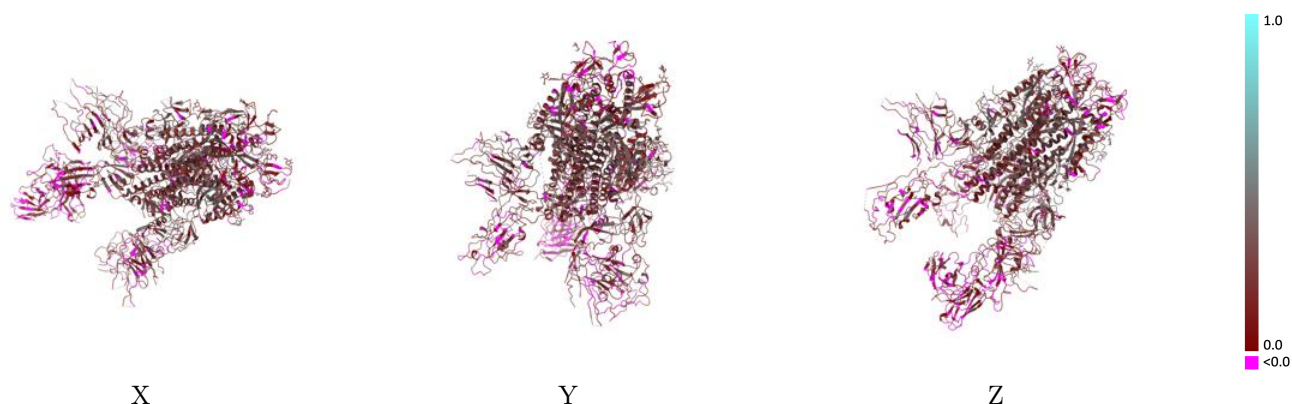
This section contains information regarding the fit between EMDB map EMD-39686 and PDB model 8YZ6. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



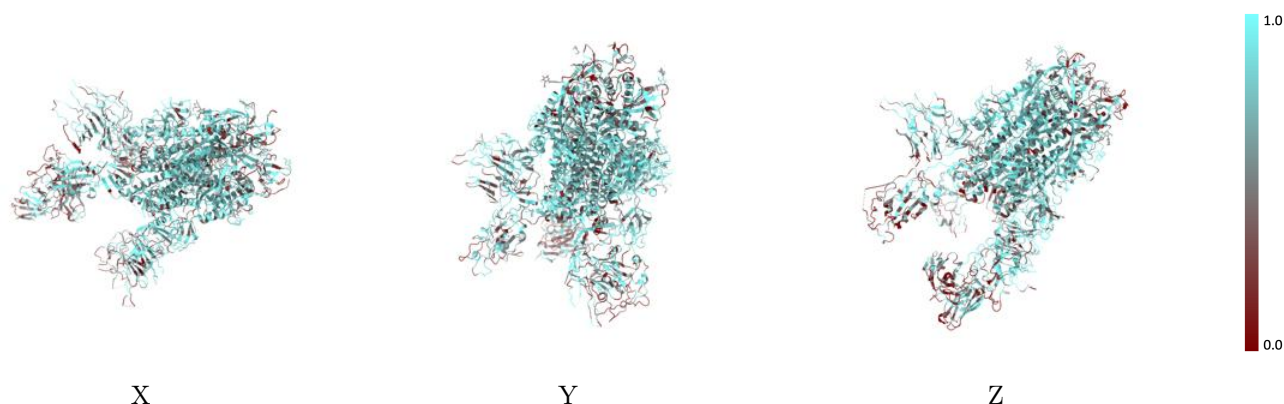
The images above show the 3D surface view of the map at the recommended contour level 0.0029 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



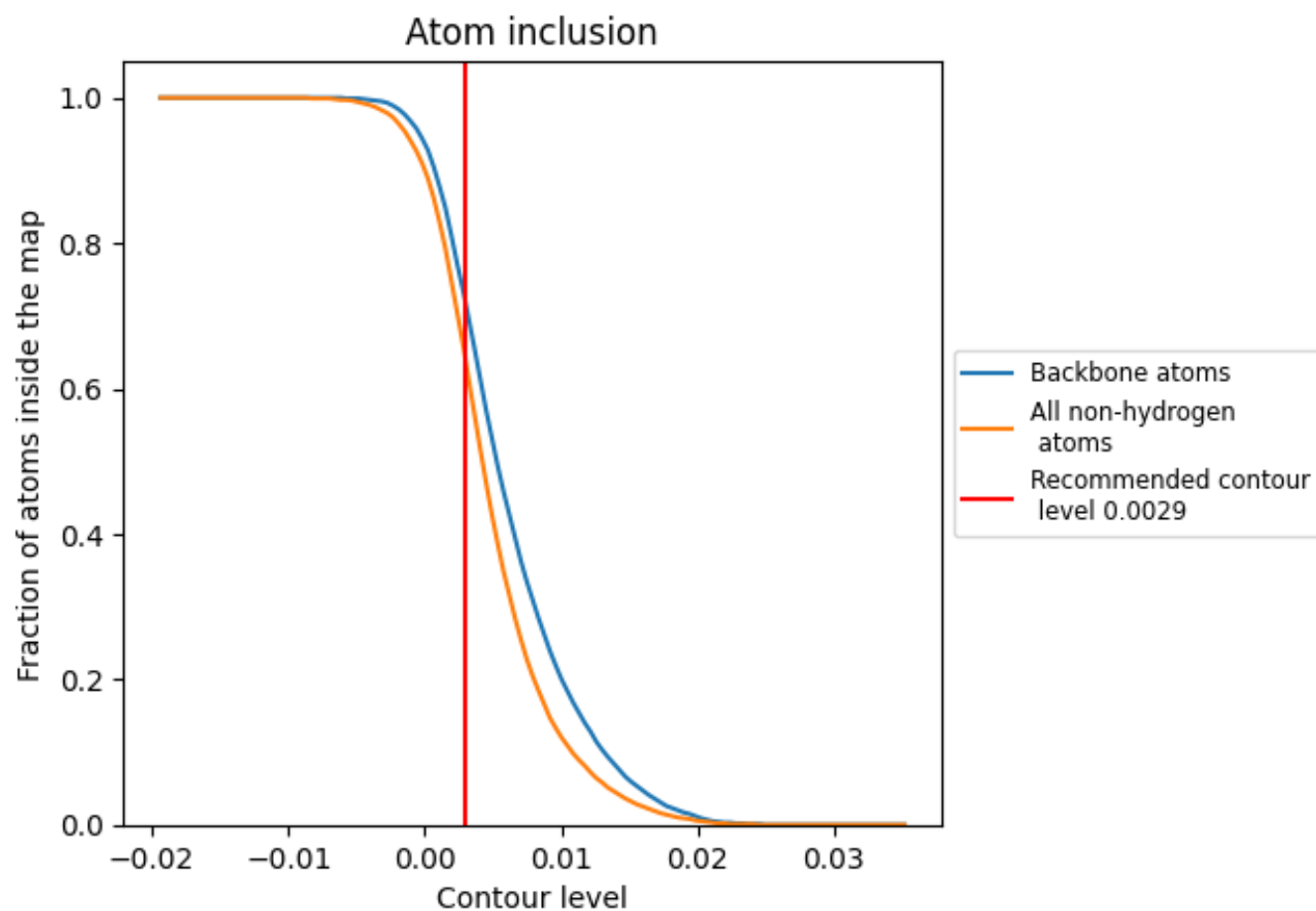
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0029).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 65% 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 (0.0029) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6500	0.2100
A	0.6670	0.2180
B	0.6750	0.2090
C	0.6520	0.2350
D	0.4060	0.0650
E	0.5110	0.0660
F	0.7140	0.3900
L	0.5000	0.2030
N	0.5360	0.3700
T	0.5640	0.2830
U	0.6430	0.2390

1.0

0.0

<0.0