



## Full wwPDB EM Validation Report ⓘ

Oct 10, 2022 – 11:12 AM EDT

PDB ID : 7TCC  
EMDB ID : EMD-25808  
Title : Cryo-EM structure of SARS-CoV-2 Omicron spike in complex with antibodies A19-46.1 and B1-182.1  
Authors : Zhou, T.; Kwong, P.D.  
Deposited on : 2021-12-23  
Resolution : 3.86 Å (reported)  
Based on initial model : 7MM0

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:

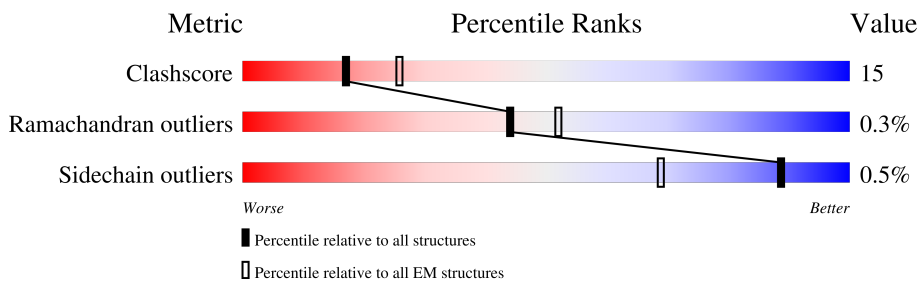
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.86 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	1272	
1	B	1272	
1	C	1272	
2	D	126	
2	H	126	
2	M	126	
3	E	110	
3	L	110	

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Mol	Chain	Length	Quality of chain
3	N	110	
4	F	123	
4	J	123	
4	O	123	
5	G	108	
5	K	108	
5	P	108	
6	I	2	
6	Q	2	
6	R	2	
6	S	2	
6	T	2	
6	U	2	
6	V	2	
6	W	2	
6	X	2	
6	Y	2	
6	Z	2	
6	a	2	
6	b	2	

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 37493 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
			Total	C	N	O	S		
1	A	1118	8755	5595	1464	1656	40	0	0
1	B	1116	8735	5584	1459	1652	40	0	0
1	C	1118	8755	5595	1464	1656	40	0	0

There are 384 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	conflict	UNP P0DTC2
A	?	-	GLY	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	142	ASP	TYR	conflict	UNP P0DTC2
A	212	ILE	-	insertion	UNP P0DTC2
A	213	VAL	-	insertion	UNP P0DTC2
A	214	ARG	ASN	conflict	UNP P0DTC2
A	214A	GLU	LEU	conflict	UNP P0DTC2
A	214B	PRO	VAL	conflict	UNP P0DTC2
A	214C	GLU	ARG	conflict	UNP P0DTC2
A	339	ASP	GLY	conflict	UNP P0DTC2
A	371	LEU	SER	conflict	UNP P0DTC2
A	373	PRO	SER	conflict	UNP P0DTC2
A	375	PHE	SER	conflict	UNP P0DTC2
A	417	ASN	LYS	conflict	UNP P0DTC2
A	440	LYS	ASN	conflict	UNP P0DTC2
A	446	SER	GLY	conflict	UNP P0DTC2
A	477	ASN	SER	conflict	UNP P0DTC2
A	478	LYS	THR	conflict	UNP P0DTC2
A	484	ALA	GLU	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	493	ARG	GLN	conflict	UNP P0DTC2
A	496	SER	GLY	conflict	UNP P0DTC2
A	498	ARG	GLN	conflict	UNP P0DTC2
A	501	TYR	ASN	conflict	UNP P0DTC2
A	505	HIS	TYR	conflict	UNP P0DTC2
A	547	LYS	THR	conflict	UNP P0DTC2
A	614	GLY	ASP	conflict	UNP P0DTC2
A	655	TYR	HIS	conflict	UNP P0DTC2
A	679	LYS	ASN	conflict	UNP P0DTC2
A	681	HIS	PRO	conflict	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	764	LYS	ASN	conflict	UNP P0DTC2
A	796	TYR	ASP	conflict	UNP P0DTC2
A	856	LYS	ASN	conflict	UNP P0DTC2
A	954	HIS	GLN	conflict	UNP P0DTC2
A	969	LYS	ASN	conflict	UNP P0DTC2
A	981	PHE	LEU	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1206	TYR	-	expression tag	UNP P0DTC2
A	1207	GLU	-	expression tag	UNP P0DTC2
A	1208	GLN	-	expression tag	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	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
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	TRP	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	PRO	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2
A	1265	PHE	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	LYS	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	UNP P0DTC2
B	67	VAL	ALA	conflict	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	conflict	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	142	ASP	TYR	conflict	UNP P0DTC2
B	212	ILE	-	insertion	UNP P0DTC2
B	213	VAL	-	insertion	UNP P0DTC2
B	213A	ARG	ASN	conflict	UNP P0DTC2
B	213B	GLU	LEU	conflict	UNP P0DTC2
B	214B	PRO	VAL	conflict	UNP P0DTC2
B	214C	GLU	ARG	conflict	UNP P0DTC2
B	339	ASP	GLY	conflict	UNP P0DTC2
B	371	LEU	SER	conflict	UNP P0DTC2
B	373	PRO	SER	conflict	UNP P0DTC2
B	375	PHE	SER	conflict	UNP P0DTC2
B	417	ASN	LYS	conflict	UNP P0DTC2
B	440	LYS	ASN	conflict	UNP P0DTC2
B	446	SER	GLY	conflict	UNP P0DTC2
B	477	ASN	SER	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	478	LYS	THR	conflict	UNP P0DTC2
B	484	ALA	GLU	conflict	UNP P0DTC2
B	493	ARG	GLN	conflict	UNP P0DTC2
B	496	SER	GLY	conflict	UNP P0DTC2
B	498	ARG	GLN	conflict	UNP P0DTC2
B	501	TYR	ASN	conflict	UNP P0DTC2
B	505	HIS	TYR	conflict	UNP P0DTC2
B	547	LYS	THR	conflict	UNP P0DTC2
B	614	GLY	ASP	conflict	UNP P0DTC2
B	655	TYR	HIS	conflict	UNP P0DTC2
B	679	LYS	ASN	conflict	UNP P0DTC2
B	681	HIS	PRO	conflict	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	764	LYS	ASN	conflict	UNP P0DTC2
B	796	TYR	ASP	conflict	UNP P0DTC2
B	856	LYS	ASN	conflict	UNP P0DTC2
B	954	HIS	GLN	conflict	UNP P0DTC2
B	969	LYS	ASN	conflict	UNP P0DTC2
B	981	PHE	LEU	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1206	TYR	-	expression tag	UNP P0DTC2
B	1207	GLU	-	expression tag	UNP P0DTC2
B	1208	GLN	-	expression tag	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLY	-	expression tag	UNP P0DTC2
B	1239	ARG	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	GLN	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	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	SER	-	expression tag	UNP P0DTC2
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	TRP	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	PRO	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	PHE	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1267	LYS	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	ALA	-	expression tag	UNP P0DTC2
B	1281	TRP	-	expression tag	UNP P0DTC2
B	1282	SER	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	PRO	-	expression tag	UNP P0DTC2
B	1285	GLN	-	expression tag	UNP P0DTC2
B	1286	PHE	-	expression tag	UNP P0DTC2
B	1287	GLU	-	expression tag	UNP P0DTC2
B	1288	LYS	-	expression tag	UNP P0DTC2
C	67	VAL	ALA	conflict	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	conflict	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	142	ASP	TYR	conflict	UNP P0DTC2
C	212	ILE	-	insertion	UNP P0DTC2
C	213	VAL	-	insertion	UNP P0DTC2
C	214	ARG	ASN	conflict	UNP P0DTC2
C	214A	GLU	LEU	conflict	UNP P0DTC2
C	214B	PRO	VAL	conflict	UNP P0DTC2
C	214C	GLU	ARG	conflict	UNP P0DTC2
C	339	ASP	GLY	conflict	UNP P0DTC2
C	371	LEU	SER	conflict	UNP P0DTC2
C	373	PRO	SER	conflict	UNP P0DTC2
C	375	PHE	SER	conflict	UNP P0DTC2
C	417	ASN	LYS	conflict	UNP P0DTC2
C	440	LYS	ASN	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	446	SER	GLY	conflict	UNP P0DTC2
C	477	ASN	SER	conflict	UNP P0DTC2
C	478	LYS	THR	conflict	UNP P0DTC2
C	484	ALA	GLU	conflict	UNP P0DTC2
C	493	ARG	GLN	conflict	UNP P0DTC2
C	496	SER	GLY	conflict	UNP P0DTC2
C	498	ARG	GLN	conflict	UNP P0DTC2
C	501	TYR	ASN	conflict	UNP P0DTC2
C	505	HIS	TYR	conflict	UNP P0DTC2
C	547	LYS	THR	conflict	UNP P0DTC2
C	614	GLY	ASP	conflict	UNP P0DTC2
C	655	TYR	HIS	conflict	UNP P0DTC2
C	679	LYS	ASN	conflict	UNP P0DTC2
C	681	HIS	PRO	conflict	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	conflict	UNP P0DTC2
C	796	TYR	ASP	conflict	UNP P0DTC2
C	856	LYS	ASN	conflict	UNP P0DTC2
C	954	HIS	GLN	conflict	UNP P0DTC2
C	969	LYS	ASN	conflict	UNP P0DTC2
C	981	PHE	LEU	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1206	TYR	-	expression tag	UNP P0DTC2
C	1207	GLU	-	expression tag	UNP P0DTC2
C	1208	GLN	-	expression tag	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	GLY	-	expression tag	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	GLN	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	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	SER	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	TRP	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	PRO	-	expression tag	UNP P0DTC2
C	1264	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1265	PHE	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	LYS	-	expression tag	UNP P0DTC2
C	1268	GLY	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	GLY	-	expression tag	UNP P0DTC2
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	ALA	-	expression tag	UNP P0DTC2
C	1281	TRP	-	expression tag	UNP P0DTC2
C	1282	SER	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	PRO	-	expression tag	UNP P0DTC2
C	1285	GLN	-	expression tag	UNP P0DTC2
C	1286	PHE	-	expression tag	UNP P0DTC2
C	1287	GLU	-	expression tag	UNP P0DTC2
C	1288	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Heavy chain of antibody A19-46.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	126	990	629	168	188	5	0	0
2	H	126	990	629	168	188	5	0	0
2	M	126	990	629	168	188	5	0	0

- Molecule 3 is a protein called Light chain of antibody A19-46.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	110	806	507	133	163	3	0	0
3	L	110	806	507	133	163	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	N	110	806	507	133	163	3	0	0

- Molecule 4 is a protein called heavy chain of antibody B1-182.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	J	122	932	584	159	181	8	1	0
4	O	122	932	584	159	181	8	1	0
4	F	122	932	584	159	181	8	1	0

- Molecule 5 is a protein called Light chain of antibody B1-182.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	K	108	830	522	142	164	2	1	0
5	P	108	830	522	142	164	2	1	0
5	G	108	830	522	142	164	2	1	0

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



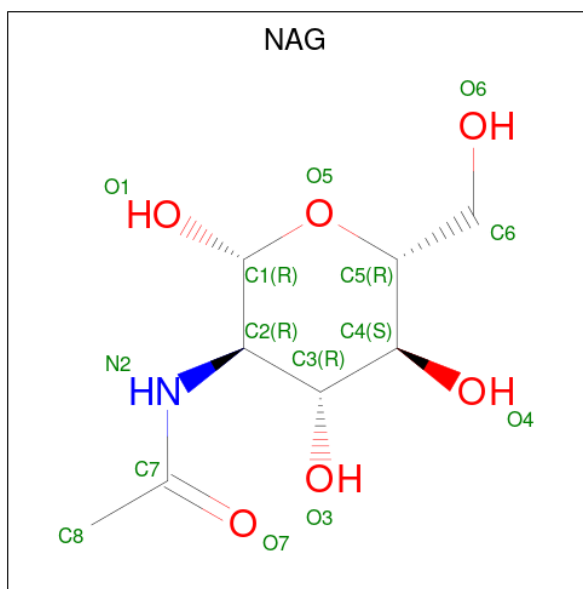
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	I	2	28	16	2	10	0	0
6	Q	2	28	16	2	10	0	0
6	R	2	28	16	2	10	0	0
6	S	2	28	16	2	10	0	0
6	T	2	28	16	2	10	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	U	2	Total 28	C 16	N 2	O 10	0	0
6	V	2	Total 28	C 16	N 2	O 10	0	0
6	W	2	Total 28	C 16	N 2	O 10	0	0
6	X	2	Total 28	C 16	N 2	O 10	0	0
6	Y	2	Total 28	C 16	N 2	O 10	0	0
6	Z	2	Total 28	C 16	N 2	O 10	0	0
6	a	2	Total 28	C 16	N 2	O 10	0	0
6	b	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	A	1	Total 84	C 48	N 6	O 30	0
7	A	1	Total 84	C 48	N 6	O 30	0
7	A	1	Total 84	C 48	N 6	O 30	0

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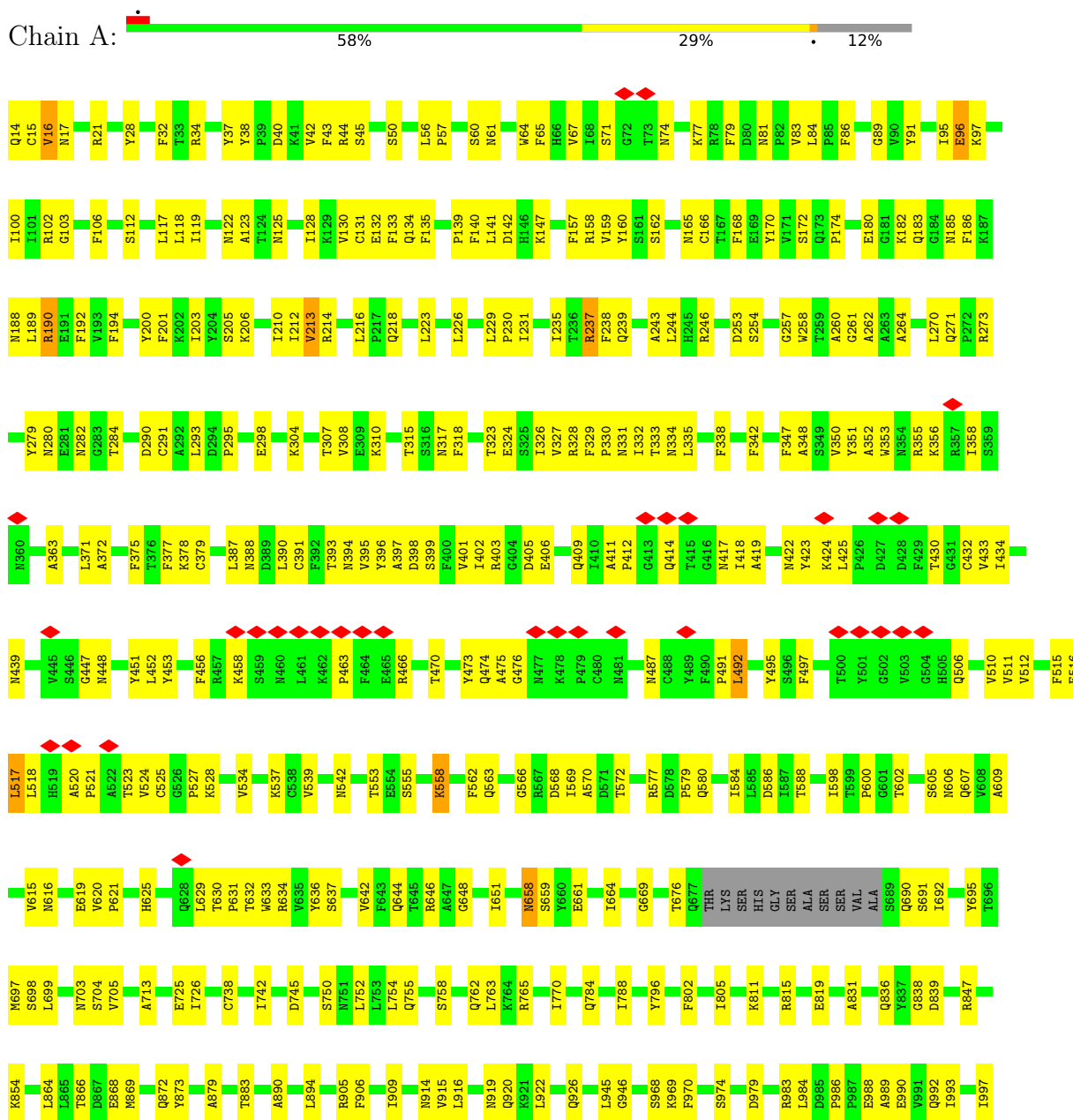
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	A	1	Total 84	C 48	N 6	O 30	0
7	A	1	Total 84	C 48	N 6	O 30	0
7	A	1	Total 84	C 48	N 6	O 30	0
7	B	1	Total 70	C 40	N 5	O 25	0
7	B	1	Total 70	C 40	N 5	O 25	0
7	B	1	Total 70	C 40	N 5	O 25	0
7	B	1	Total 70	C 40	N 5	O 25	0
7	B	1	Total 70	C 40	N 5	O 25	0
7	C	1	Total 56	C 32	N 4	O 20	0
7	C	1	Total 56	C 32	N 4	O 20	0
7	C	1	Total 56	C 32	N 4	O 20	0
7	C	1	Total 56	C 32	N 4	O 20	0



### 3 Residue-property plots

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

#### • Molecule 1: Spike glycoprotein





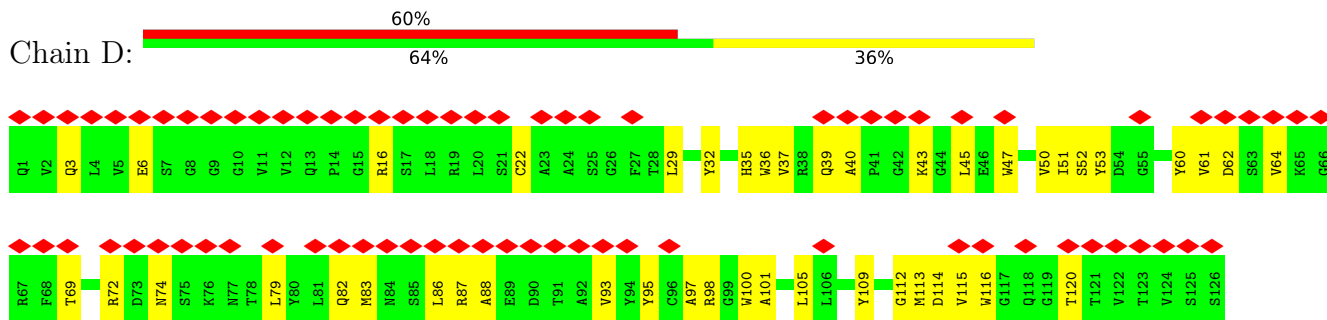
GLY LYS TYR GLY GLN GLY SER GLY TYR TYR ILE GLY PRO GLY GLU SER ALA PRO ARG ASP GLY GLN GLY ALA TRP GLN SER TRP TYR VAL GLN ARG LYS ASP GLY GLU GLY	GLN PHE GLU LYS GLY GLY SER GLY TYR GLY ILE GLY PRO GLY GLU SER ALA PRO ARG ASP SER SER GLY TRP ALA TRP VAL GLN PHE GLY GLU LYS
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● Molecule 1: Spike glycoprotein

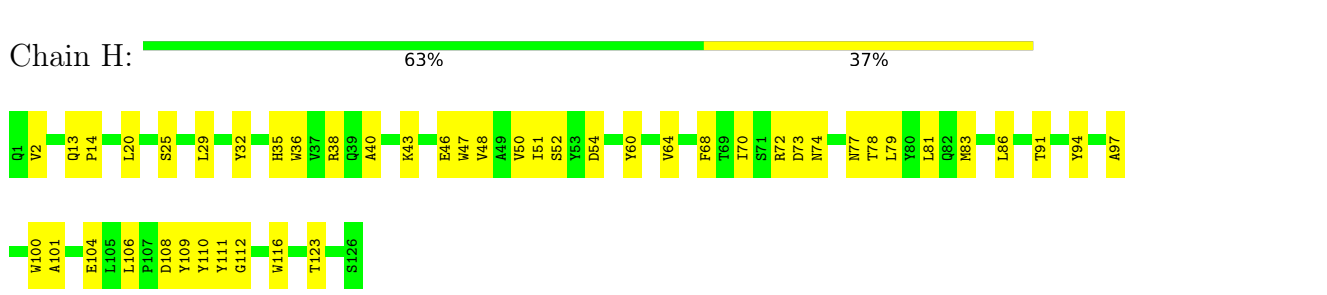


Q14 C15 V16 N17 R21 L24 P25 P26 A27 Y28 F32 T33 R34 Y37 D40 K41 V42 F43 S46 L54 N61 V62 T63 W64 V67 M65 I68 S71 G72 T73 N74 K77 R78 F79 F86 N87 D88 F92 E96 K97 S98 N99 I100 I101 T108 S112	K113 T114 S115 S116 L117 L118 N125 K129 E122 V130 A27 C131 L226 E132 F133 Q134 F135 F140 L141 D142 H146 K147 M148 E154 S155 E156 F157 Y159 Y160 M164 M165 C166 P174 M177 D178 L179 E180 G181 K182 Q183 F186 K187 M188 L189 R190 F194 I203 Y204 K206 K207 T208	P209 I210 R214 Q218 G219 L223 E224 P225 L226 W227 I231 G232 G233 R237 F238 L241 L242 A243 R246 S247 Y248 P251 G252 D253 S254 S255 S256 W258 V267 Y279 L293 L296 K300 V308 K309 K310 N317 F318 R319 I326 K327 R328 P330	N331 C336 D339 Y341 F342 N343 R346 F347 A348 S349 V350 Y351 A352 K356 N437 R357 I358 V362 Y365 L371 A372 F375 F377 K378 C379 S383 K386 L387 C391 F392 T393 A397 D398 S399 F400 I402 R403 E406 F407 R408 Q409 I410 A411 Q414	I418 A419 D420 N422 Y423 K424 L425 P426 D427 D428 F429 T430 G431 C432 V433 W436 N437 S438 N439 K440 L441 D442 V445 S446 G447 Y451 L452 K458 A459 M460 L461 K462 R466 T470 S471 I472 Y473 C480 M481 F490 P491 L492 R493 S494 F497 R498 P499 V503	G504 H505 Q506 P507 Y508 R509 V512 L513 S514 F515 E516 L517 L518 H519 A520 P521 A522 T523 W524 C525 G526 P527 K528 L533 V534 K535 M536 K537 L546 S555 M556 K557 K558 F559 L560 Q563 G566 R567 D568 D578 P579 Q580 I584 L585 D586 G594 T602 M605 M606	Q607 V615 T618 E619 W620 P621 V612 H625 T628 E629 T630 P631 R634 S637 T638 V642 F643 R646 L650 I651 Y660 D663 I664 P665 V674 Q675 T676 Q677 THR LYS SER GLY GLY SER ALA SER SER SER VAL ALA G689 Q690 V695 L699 E702 N703 S704	A713 N717 S721 T724 T732 C738 I742 C743 S746 C749 S750 L754 F759 K776 M777 T778 V781 Q787 P792 I805 R806 P807 R815 S816 D820 L821 K825 W826 T827 L828 Q832 F833 R834 K835 Q836 Y837 L841 Q842 D843	Y873 L878 A879 T882 T883 Q895 R905 V915 E918 N919 I931 T934 L938 S939 K947 H954 N955 A956 Q957 V963 L966 K969 F970 G971 A972 S974 L977 I980 Q992 R995 L996 I997 R1000 L1001 N1134 M1135 T1136 L1145 ASP	R1014 R1019 M1029 C1032 R1039 V1040 D1041 K1045 G1046 L1049 M1050 S1051 F1062 T1066 Q1071 T1077 A1078 I1081 C1082 A1087 H1088 E1092 V1104 R1107 E1111 P1112 Q1113 I1114 I1115 V1122 S1123 V1129 I1130 G1131 I1132 V1133 N1134 M1135 T1136 L1145 ASP	SER PHE LYS GLU GLU LEU ASP LYS TYR PHE LYS ASN HIS THR SER PRO ALA TYR SER VAL VAL ASP GLY ASP GLY ILE GLU TRP SER GLY VAL ILE ASN GLN SER LEU LEU VAL ILE ASP ARG GLN GLY SER GLU GLY VAL VAL ILE LEU LEU SER THR PHE VAL LEU GLY ASN ILE GLN LEU GLU GLY VAL ILE ASN GLY PRO GLY VAL ALA HIS GLY SER HIS HIS HIS HIS HIS HIS SER ILE ASP TRP LEU GLN GLY LEU TYR	GLU GLN GLY SER GLY TYR ILE PRO GLY GLU SER ALA PRO GLY GLY ASN ASP GLY GLN SER ALA TYR SER VAL VAL ASP GLY ASP GLY ILE GLU TRP SER GLY VAL ILE LEU LEU SER THR PHE VAL LEU GLY ASN ILE GLN SER LEU GLU GLY VAL VAL ILE LEU LEU SER THR PHE VAL LEU GLY ASN ILE GLN LEU GLU GLY VAL ALA HIS GLY SER HIS HIS HIS SER ILE ASP TRP LEU GLN GLY LEU TYR	LYS GLY GLY SER GLY GLY TYR ILE PRO GLY GLU SER ALA TRP SER SER HIS PRO GLN PHE LYS
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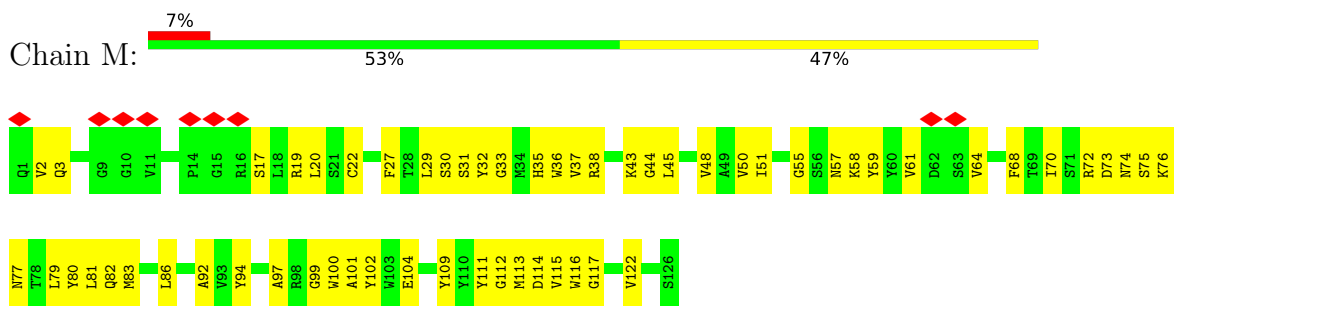
• Molecule 2: Heavy chain of antibody A19-46.1



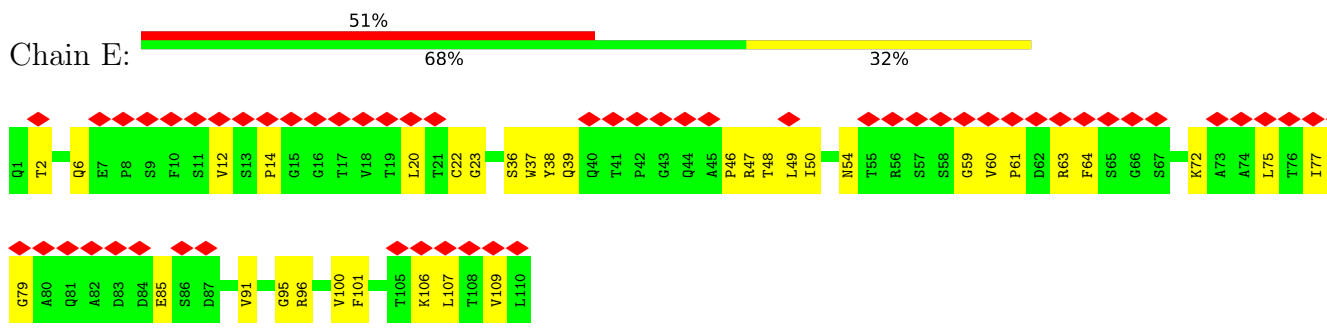
• Molecule 2: Heavy chain of antibody A19-46.1



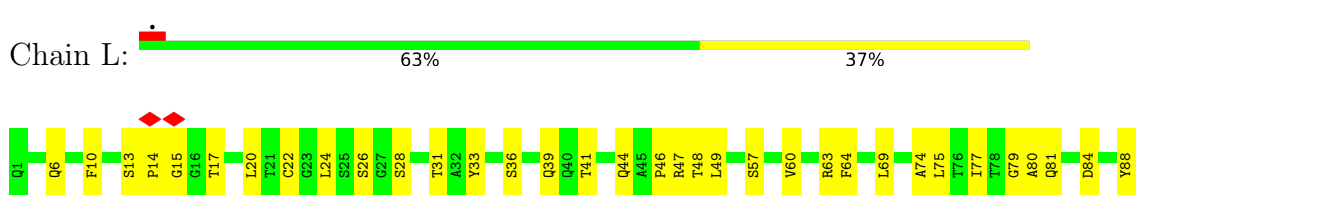
• Molecule 2: Heavy chain of antibody A19-46.1

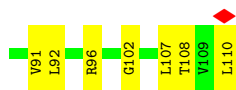


• Molecule 3: Light chain of antibody A19-46.1

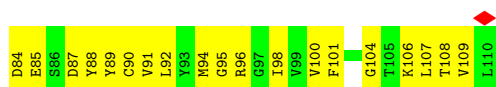
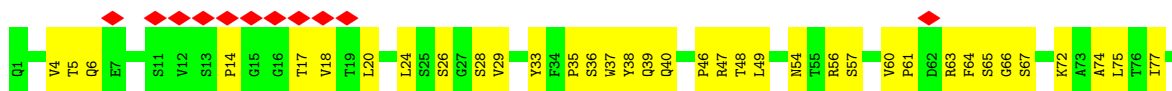


• Molecule 3: Light chain of antibody A19-46.1

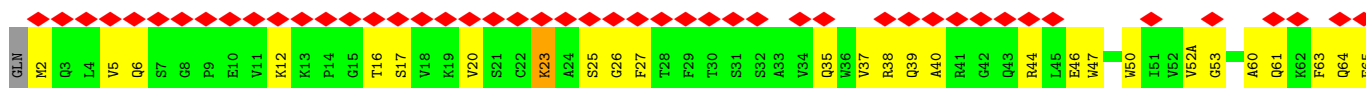




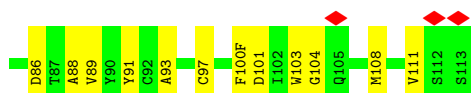
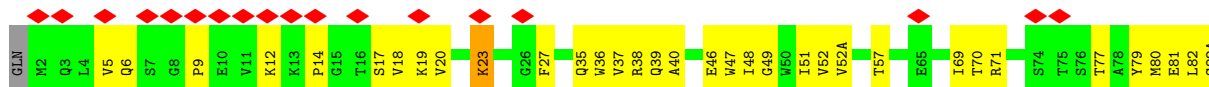
- Molecule 3: Light chain of antibody A19-46.1



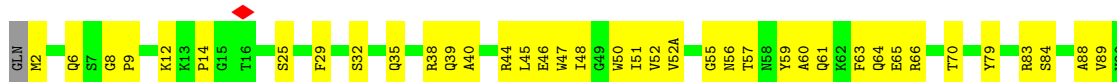
- Molecule 4: heavy chain of antibody B1-182.1



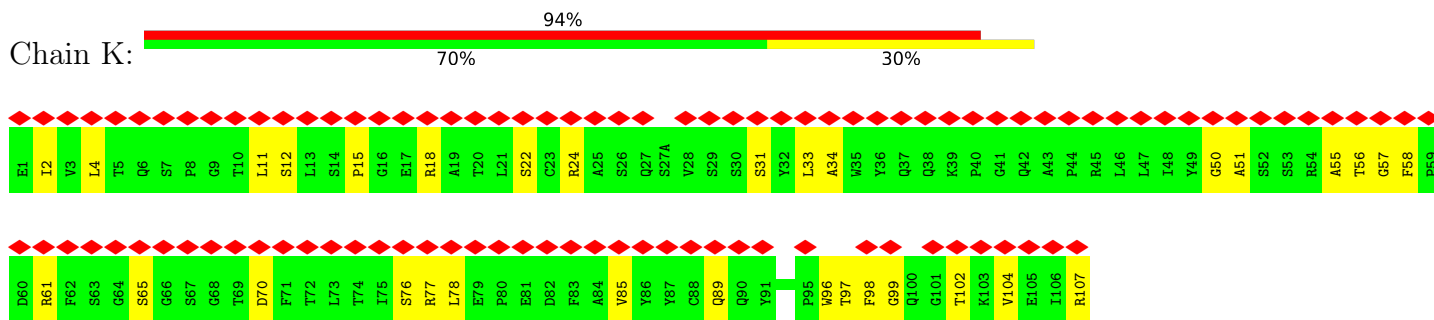
- Molecule 4: heavy chain of antibody B1-182.1



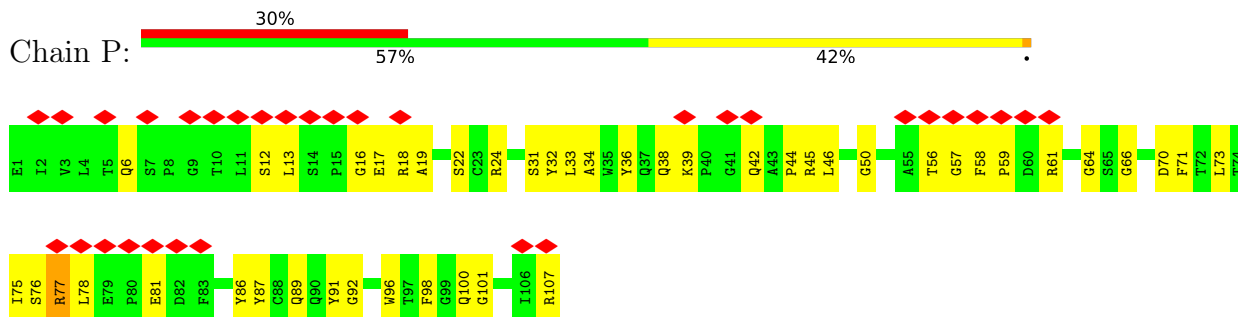
- Molecule 4: heavy chain of antibody B1-182.1



- Molecule 5: Light chain of antibody B1-182.1



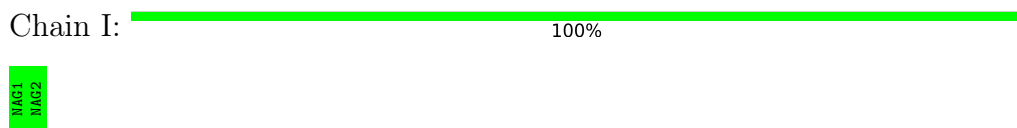
• Molecule 5: Light chain of antibody B1-182.1



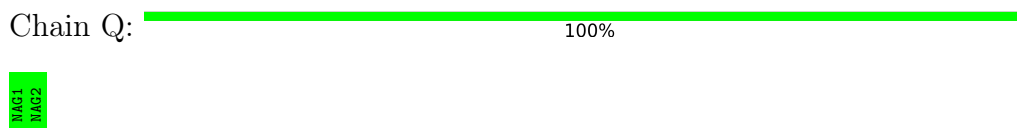
• Molecule 5: Light chain of antibody B1-182.1



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  100%

MAG1  
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  100%

MAG1  
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  100%

MAG1  
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  50% 50%

MAG1  
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  100%

MAG1  
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  100%

MAG1  
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  50% 50%

MAG1  
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  100%

MAG1  
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  50% 50%

MAG1  
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  100%

MAG1  
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  100%

MAG1  
MAG2



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46244	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	OTHER	Depositor
Maximum map value	0.797	Depositor
Minimum map value	-0.191	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.116	Depositor
Map size (Å)	513.0, 513.0, 513.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.855, 0.855, 0.855	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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.27	0/8965	0.51	1/12202 (0.0%)
1	B	0.27	0/8944	0.51	0/12172
1	C	0.27	0/8965	0.52	2/12202 (0.0%)
2	D	0.25	0/1016	0.53	0/1381
2	H	0.26	0/1016	0.54	0/1381
2	M	0.26	0/1016	0.54	0/1381
3	E	0.26	0/823	0.51	0/1123
3	L	0.26	0/823	0.53	0/1123
3	N	0.26	0/823	0.52	0/1123
4	F	0.26	0/952	0.54	0/1289
4	J	0.24	0/952	0.54	0/1289
4	O	0.25	0/952	0.59	0/1289
5	G	0.52	1/851 (0.1%)	0.82	3/1156 (0.3%)
5	K	0.25	0/851	0.57	0/1156
5	P	0.26	0/851	0.56	0/1156
All	All	0.27	1/37800 (0.0%)	0.53	6/51423 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	8	PRO	CG-CD	-12.64	1.08	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	8	PRO	N-CD-CG	-15.40	80.11	103.20
5	G	8	PRO	CA-CB-CG	-8.38	88.08	104.00
5	G	8	PRO	CA-N-CD	-7.11	101.55	111.50
1	A	517	LEU	CA-CB-CG	5.04	126.89	115.30
1	C	452	LEU	CA-CB-CG	5.04	126.89	115.30
1	C	526	GLY	C-N-CD	-5.01	109.57	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	183	GLN	Peptide

## 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	8755	0	8562	279	0
1	B	8735	0	8544	248	0
1	C	8755	0	8563	258	0
2	D	990	0	947	36	0
2	H	990	0	947	31	0
2	M	990	0	947	51	0
3	E	806	0	787	30	0
3	L	806	0	787	32	0
3	N	806	0	787	42	0
4	F	932	0	893	43	0
4	J	932	0	893	31	0
4	O	932	0	893	37	0
5	G	830	0	797	34	0
5	K	830	0	797	24	0
5	P	830	0	797	37	0
6	I	28	0	25	0	0
6	Q	28	0	25	0	0
6	R	28	0	25	0	0
6	S	28	0	25	0	0
6	T	28	0	25	0	0
6	U	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	V	28	0	25	0	0
6	W	28	0	25	0	0
6	X	28	0	25	0	0
6	Y	28	0	25	0	0
6	Z	28	0	25	1	0
6	a	28	0	25	0	0
6	b	28	0	25	0	0
7	A	84	0	78	1	0
7	B	70	0	65	0	0
7	C	56	0	52	1	0
All	All	37493	0	36461	1140	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 15.

All (1140) 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)
3:N:85:GLU:HA	3:N:107:LEU:O	1.59	1.00
3:N:17:THR:HA	3:N:77:ILE:O	1.69	0.93
1:A:97:LYS:O	1:A:188:ASN:ND2	2.03	0.90
3:E:36:SER:HB2	3:E:91:VAL:HB	1.59	0.84
1:C:391:CYS:HA	1:C:525:CYS:HA	1.60	0.82
1:A:71:SER:HB3	1:A:261:GLY:H	1.47	0.80
1:C:206:LYS:NZ	1:C:208:THR:OG1	2.13	0.80
3:N:63:ARG:HG3	3:N:64:PHE:HD1	1.47	0.80
4:O:38:ARG:HB3	4:O:46:GLU:HB3	1.64	0.80
5:K:22:SER:HB2	5:K:24:ARG:HH22	1.47	0.79
1:C:1129:VAL:HB	1:C:1132:ILE:HD11	1.64	0.79
1:C:246:ARG:NH1	1:C:254:SER:O	2.16	0.79
1:C:403:ARG:HG3	1:C:505:HIS:HA	1.65	0.79
5:G:22:SER:HB2	5:G:24:ARG:HH22	1.46	0.79
4:F:35:GLN:HB3	4:F:93:ALA:HB3	1.65	0.78
1:A:102:ARG:HG2	1:A:243:ALA:HB2	1.63	0.78
1:C:555:SER:HB3	1:C:586:ASP:HB2	1.65	0.78
1:A:81:ASN:OD1	1:A:239:GLN:NE2	2.17	0.77
1:B:231:ILE:HG13	1:B:232:GLY:H	1.50	0.77
1:A:95:ILE:HD11	1:A:186:PHE:HB3	1.67	0.77
1:C:675:GLN:O	1:C:690:GLN:HA	1.84	0.76
1:A:333:THR:HG22	1:A:334:ASN:H	1.50	0.76
1:C:452:LEU:HD12	1:C:492:LEU:HB3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:PRO:HA	1:A:637:SER:HB2	1.67	0.76
4:F:6:GLN:H	4:F:105:GLN:HE22	1.33	0.76
1:B:656:VAL:HB	1:B:693:ILE:HD11	1.67	0.76
2:M:22:CYS:HB3	2:M:79:LEU:HB3	1.67	0.75
4:O:35:GLN:HB3	4:O:93:ALA:HB3	1.68	0.75
1:A:452:LEU:HD12	1:A:492:LEU:HB3	1.66	0.75
1:B:705:VAL:HG21	1:C:883:THR:HG21	1.67	0.75
1:B:246:ARG:NH1	1:B:257:GLY:O	2.19	0.75
1:B:346:ARG:NH1	1:B:347:PHE:O	2.18	0.75
1:C:131:CYS:HA	1:C:166:CYS:HB3	1.69	0.75
4:F:14:PRO:HG3	4:F:111:VAL:HB	1.68	0.75
1:A:474:GLN:HG2	1:A:476:GLY:H	1.49	0.75
1:B:433:VAL:HG12	1:B:512:VAL:HG12	1.69	0.75
1:C:525:CYS:SG	1:C:526:GLY:N	2.57	0.74
1:C:96:GLU:O	1:C:188:ASN:HB3	1.87	0.74
1:B:815:ARG:HG2	1:B:819:GLU:HG3	1.68	0.74
1:B:15:CYS:O	1:B:17:ASN:N	2.20	0.74
1:C:742:ILE:O	1:C:1000:ARG:NH1	2.21	0.73
1:A:555:SER:HB3	1:A:586:ASP:HB2	1.69	0.73
1:B:566:GLY:HA2	1:C:43:PHE:HB3	1.69	0.73
5:P:39:LYS:NZ	5:P:81:GLU:O	2.19	0.72
3:L:24:LEU:HG	3:L:26:SER:H	1.54	0.72
5:P:66:GLY:HA3	5:P:71:PHE:HA	1.70	0.72
4:F:61:GLN:HA	4:F:64:GLN:HE22	1.53	0.72
1:A:330:PRO:HA	1:A:579:PRO:HB2	1.71	0.72
1:B:474:GLN:HG2	1:B:476:GLY:H	1.53	0.72
1:C:433:VAL:HG12	1:C:512:VAL:HG12	1.70	0.72
5:G:24:ARG:NH2	5:G:70:ASP:OD1	2.22	0.72
4:O:6:GLN:HE22	4:O:91:TYR:HA	1.55	0.72
1:A:15:CYS:O	1:A:17:ASN:N	2.23	0.71
4:O:6:GLN:HE21	4:O:104:GLY:HA3	1.55	0.71
5:P:22:SER:HB2	5:P:24:ARG:HH22	1.56	0.71
1:A:752:LEU:O	1:A:755:GLN:NE2	2.22	0.71
1:A:433:VAL:HG12	1:A:512:VAL:HG12	1.73	0.71
1:C:68:ILE:H	1:C:78:ARG:HG2	1.56	0.71
2:M:51:ILE:HD11	2:M:55:GLY:HA2	1.71	0.71
1:A:271:GLN:HE21	1:A:273:ARG:HG3	1.56	0.70
1:B:746:SER:OG	1:B:749:CYS:SG	2.50	0.70
1:B:858:LEU:HD11	1:B:962:LEU:HD22	1.73	0.70
2:D:97:ALA:HA	2:D:116:TRP:HB3	1.72	0.70
5:K:24:ARG:NH2	5:K:70:ASP:OD1	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:2:ILE:HB	5:K:97:THR:HG21	1.73	0.70
3:E:85:GLU:HB3	3:E:109:VAL:HG23	1.73	0.70
5:G:54:ARG:NH2	5:G:62:PHE:O	2.25	0.70
1:C:746:SER:OG	1:C:749:CYS:SG	2.50	0.69
1:B:140:PHE:HE1	1:B:244:LEU:HD22	1.58	0.69
1:A:212:ILE:O	1:A:214:ARG:N	2.25	0.69
1:C:1092:GLU:O	1:C:1107:ARG:NH1	2.25	0.69
5:P:34:ALA:HB3	5:P:89:GLN:HB2	1.75	0.69
2:M:48:VAL:HG13	2:M:64:VAL:HG11	1.75	0.69
1:A:258:TRP:HZ3	1:A:260:ALA:HB2	1.59	0.68
1:A:866:THR:HG23	1:A:868:GLU:H	1.59	0.68
1:C:724:THR:HG22	1:C:934:ILE:HD11	1.74	0.68
1:C:1081:ILE:O	1:C:1088:HIS:HB2	1.93	0.68
1:B:400:PHE:HE2	1:B:402:ILE:HD11	1.59	0.68
1:C:732:THR:OG1	1:C:955:ASN:ND2	2.27	0.68
1:A:122:ASN:OD1	1:A:123:ALA:N	2.27	0.67
1:B:644:GLN:NE2	1:B:645:THR:O	2.27	0.67
1:C:1111:GLU:OE1	1:C:1113:GLN:NE2	2.28	0.67
1:A:237:ARG:NH1	1:A:238:PHE:O	2.28	0.67
1:C:310:LYS:HB2	1:C:664:ILE:HD11	1.77	0.67
1:A:118:LEU:HD21	1:A:135:PHE:HZ	1.58	0.67
1:C:605:SER:OG	1:C:607:GLN:OE1	2.13	0.67
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.77	0.67
3:L:6:GLN:NE2	3:L:22:CYS:SG	2.68	0.67
1:A:403:ARG:HD2	1:A:405:ASP:H	1.59	0.67
1:C:115:GLN:NE2	1:C:130:VAL:O	2.28	0.67
1:C:409:GLN:O	1:C:414:GLN:NE2	2.28	0.67
1:A:293:LEU:O	1:A:632:THR:OG1	2.12	0.66
1:C:490:PHE:O	1:C:493:ARG:NH1	2.28	0.66
1:C:125:ASN:HA	1:C:174:PRO:HD3	1.78	0.66
1:A:363:ALA:O	1:A:528:LYS:NZ	2.22	0.66
2:M:97:ALA:HB1	2:M:113:MET:HA	1.78	0.66
1:A:74:ASN:HB3	1:A:77:LYS:HB2	1.78	0.66
5:G:88:CYS:H	5:G:99:GLY:HA3	1.61	0.65
1:C:970:PHE:O	1:C:995:ARG:NH1	2.30	0.65
1:C:905:ARG:NH1	1:C:1049:LEU:O	2.28	0.65
3:N:39:GLN:HE21	3:N:47:ARG:HB3	1.61	0.65
1:A:836:GLN:NE2	1:A:839:ASP:OD2	2.30	0.65
1:A:56:LEU:HD12	1:A:57:PRO:HD2	1.78	0.65
1:C:188:ASN:OD1	1:C:207:HIS:NE2	2.30	0.65
1:C:743:CYS:SG	1:C:746:SER:OG	2.55	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:PHE:O	1:B:580:GLN:NE2	2.29	0.65
1:B:524:VAL:HG13	1:B:525:CYS:H	1.61	0.65
3:L:28:SER:HB2	4:F:56:ASN:HD22	1.62	0.65
2:D:22:CYS:HB3	2:D:79:LEU:HB3	1.77	0.65
1:A:1087:ALA:O	1:A:1088:HIS:ND1	2.30	0.65
1:B:139:PRO:HB2	1:B:159:VAL:HA	1.78	0.65
2:M:35:HIS:HA	2:M:50:VAL:HG12	1.79	0.65
1:A:327:VAL:HG23	1:A:542:ASN:HB3	1.79	0.64
1:B:477:ASN:ND2	4:F:100(B):CYS:O	2.24	0.64
3:E:39:GLN:HE21	3:E:47:ARG:HB3	1.62	0.64
1:A:915:VAL:O	1:A:919:ASN:ND2	2.30	0.64
1:B:621:PRO:O	1:B:625:HIS:ND1	2.31	0.64
4:J:5:VAL:HB	4:J:23:LYS:HE3	1.78	0.64
1:A:566:GLY:HA2	1:B:43:PHE:HB3	1.78	0.64
4:J:6:GLN:HE21	4:J:104:GLY:HA3	1.61	0.64
3:L:28:SER:CB	4:F:56:ASN:HD22	2.11	0.64
4:O:39:GLN:O	4:O:89:VAL:N	2.27	0.64
4:O:93:ALA:HB1	4:O:100(F):PHE:HB3	1.78	0.64
1:B:147:LYS:HA	1:B:246:ARG:HG3	1.78	0.64
5:P:12:SER:OG	5:P:107:ARG:NH1	2.30	0.64
1:A:642:VAL:HG22	1:A:651:ILE:HG12	1.80	0.64
4:J:6:GLN:HE22	4:J:91:TYR:HA	1.61	0.64
5:K:12:SER:OG	5:K:107:ARG:NH1	2.30	0.64
2:H:2:VAL:HA	2:H:25:SER:O	1.98	0.64
1:A:95:ILE:HG23	1:A:96:GLU:OE1	1.98	0.64
1:A:147:LYS:HG2	1:A:246:ARG:HE	1.63	0.64
1:B:725:GLU:OE2	1:B:1064:HIS:NE2	2.29	0.64
3:L:63:ARG:NH2	3:L:84:ASP:OD2	2.28	0.63
1:C:329:PHE:O	1:C:580:GLN:NE2	2.32	0.63
2:H:20:LEU:HB2	2:H:81:LEU:HB3	1.80	0.63
1:B:314:GLN:OE1	1:B:596:SER:OG	2.17	0.63
1:C:15:CYS:O	1:C:17:ASN:N	2.31	0.63
4:O:35:GLN:NE2	4:O:36:TRP:O	2.32	0.63
1:C:447:GLY:O	3:N:54:ASN:ND2	2.28	0.63
1:C:621:PRO:O	1:C:625:HIS:ND1	2.31	0.63
3:N:5:THR:OG1	3:N:72:LYS:NZ	2.29	0.63
4:F:93:ALA:HB1	4:F:100(F):PHE:HB3	1.79	0.63
2:D:100:TRP:H	2:D:112:GLY:HA2	1.63	0.63
1:A:705:VAL:HG21	1:B:883:THR:HG21	1.80	0.62
1:A:577:ARG:HB2	1:A:584:ILE:HG13	1.80	0.62
1:B:426:PRO:HG2	1:B:429:PHE:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:915:VAL:O	1:B:919:ASN:ND2	2.32	0.62
1:A:186:PHE:HB2	1:A:210:ILE:HG22	1.80	0.62
1:C:535:LYS:O	1:C:537:LYS:NZ	2.32	0.62
1:A:562:PHE:HD2	1:B:41:LYS:HE2	1.65	0.62
1:C:141:LEU:O	1:C:243:ALA:HA	1.99	0.62
5:P:33:LEU:HB3	5:P:50:GLY:HA2	1.82	0.62
3:N:47:ARG:HH21	3:N:60:VAL:HG22	1.64	0.62
1:B:645:THR:OG1	1:B:648:GLY:O	2.17	0.61
1:B:809:PRO:O	1:B:814:LYS:NZ	2.32	0.61
1:A:388:ASN:HB3	1:A:528:LYS:HD2	1.80	0.61
1:B:357:ARG:HB2	1:B:396:TYR:HE1	1.65	0.61
3:E:63:ARG:NH2	3:E:79:GLY:O	2.33	0.61
1:A:103:GLY:HA3	1:A:119:ILE:O	2.00	0.61
3:L:69:LEU:HD13	3:L:74:ALA:HB3	1.82	0.61
3:N:94:MET:HB2	3:N:98:ILE:HB	1.81	0.61
1:A:34:ARG:HH22	1:A:216:LEU:HB3	1.65	0.61
1:B:375:PHE:HE1	1:B:434:ILE:HG23	1.63	0.61
1:A:356:LYS:HB3	1:A:397:ALA:HB3	1.82	0.61
1:C:115:GLN:HA	1:C:132:GLU:HG2	1.83	0.61
1:B:409:GLN:O	1:B:414:GLN:NE2	2.34	0.61
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.33	0.61
1:C:642:VAL:HG22	1:C:651:ILE:HG12	1.81	0.61
4:F:84:SER:HA	4:F:111:VAL:HG21	1.83	0.61
2:D:47:TRP:HB2	3:E:101:PHE:HE2	1.66	0.60
1:A:1115:ILE:HG22	1:A:1137:VAL:HG23	1.83	0.60
1:B:328:ARG:NH1	1:B:533:LEU:HB2	2.16	0.60
1:C:491:PRO:O	1:C:492:LEU:HB2	2.01	0.60
1:B:675:GLN:O	1:B:690:GLN:HA	2.00	0.60
1:C:328:ARG:HH12	1:C:533:LEU:HD12	1.65	0.60
5:P:19:ALA:HB3	5:P:75:ILE:HB	1.82	0.60
1:C:214:ARG:HH12	1:C:218:GLN:H	1.48	0.60
5:G:88:CYS:O	5:G:99:GLY:N	2.33	0.60
1:B:245:HIS:NE2	1:B:259:THR:O	2.34	0.60
1:B:277:LEU:HD12	1:B:288:ALA:HB2	1.83	0.60
2:H:52:SER:OG	2:H:54:ASP:OD1	2.18	0.60
1:B:324:GLU:HG2	1:B:539:VAL:HG13	1.84	0.60
2:H:48:VAL:HG13	2:H:64:VAL:HG11	1.82	0.60
2:M:50:VAL:HG23	2:M:59:TYR:HB2	1.82	0.60
1:A:21:ARG:HH12	1:A:81:ASN:H	1.50	0.60
1:B:327:VAL:O	1:B:531:THR:OG1	2.19	0.60
2:M:109:TYR:HB3	3:N:95:GLY:HA2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:36:TYR:HB2	5:P:87:TYR:HB2	1.84	0.60
3:E:91:VAL:HG22	3:E:101:PHE:HE1	1.67	0.60
1:C:164:ASN:OD1	1:C:165:ASN:N	2.34	0.60
1:A:470:THR:HB	3:E:95:GLY:HA3	1.83	0.59
1:B:472:ILE:HD11	1:B:482:GLY:HA2	1.84	0.59
2:D:116:TRP:HE1	3:E:46:PRO:HD2	1.67	0.59
1:A:57:PRO:HG2	1:A:60:SER:HB2	1.84	0.59
4:J:60:ALA:O	4:J:64:GLN:NE2	2.35	0.59
3:L:10:PHE:O	3:L:108:THR:OG1	2.20	0.59
1:A:86:PHE:HB2	1:A:238:PHE:HD1	1.67	0.59
1:C:118:LEU:HD11	1:C:135:PHE:HZ	1.66	0.59
1:C:1032:CYS:O	1:C:1051:SER:OG	2.20	0.59
1:B:472:ILE:HG22	1:B:490:PHE:HD1	1.66	0.59
1:B:90:VAL:HG12	1:B:92:PHE:H	1.67	0.59
1:B:142:ASP:HA	1:B:244:LEU:HB3	1.85	0.59
5:K:51:ALA:HB1	5:K:65:SER:HA	1.84	0.59
5:G:33:LEU:HB3	5:G:50:GLY:HA2	1.85	0.59
1:A:229:LEU:HB3	1:A:231:ILE:HG12	1.85	0.59
3:N:67:SER:N	3:N:74:ALA:O	2.35	0.59
1:C:807:PRO:HA	1:C:816:SER:HB3	1.84	0.58
3:N:39:GLN:HB3	3:N:49:LEU:HD11	1.84	0.58
1:A:253:ASP:O	1:A:257:GLY:N	2.34	0.58
1:B:425:LEU:HD12	1:B:426:PRO:HD2	1.86	0.58
1:B:616:ASN:OD1	1:B:618:THR:N	2.29	0.58
1:A:290:ASP:OD1	1:A:291:CYS:N	2.36	0.58
4:F:2:MET:N	4:F:25:SER:O	2.37	0.58
4:J:12:LYS:NZ	4:J:16:THR:OG1	2.37	0.58
3:N:36:SER:HB2	3:N:91:VAL:HB	1.86	0.58
1:A:112:SER:OG	1:A:134:GLN:NE2	2.37	0.58
1:A:894:LEU:HB3	1:C:713:ALA:HB3	1.86	0.58
1:B:92:PHE:HA	1:B:266:TYR:O	2.03	0.58
3:E:61:PRO:HB2	3:E:63:ARG:HG2	1.85	0.58
4:O:18:VAL:O	4:O:81:GLU:HA	2.03	0.58
1:B:368:LEU:HD11	1:B:434:ILE:HD13	1.86	0.58
1:A:763:LEU:HD12	1:A:1008:VAL:HG21	1.86	0.58
3:L:49:LEU:HA	3:L:60:VAL:HG21	1.85	0.58
1:A:905:ARG:NH1	1:A:1049:LEU:O	2.33	0.58
1:A:1116:THR:OG1	1:A:1118:ASP:OD1	2.21	0.57
4:J:44:ARG:NE	5:K:99:GLY:O	2.36	0.57
2:M:29:LEU:HG	2:M:72:ARG:HH21	1.69	0.57
1:C:439:ASN:HA	1:C:507:PRO:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:GLN:HB3	2:D:95:TYR:HE1	1.68	0.57
3:E:37:TRP:HB2	3:E:50:ILE:HB	1.85	0.57
1:B:328:ARG:HH12	1:B:533:LEU:HB2	1.69	0.57
1:C:357:ARG:HH12	1:C:523:THR:HG21	1.68	0.57
5:P:6:GLN:NE2	5:P:101:GLY:O	2.37	0.57
1:C:180:GLU:OE2	1:C:182:LYS:NZ	2.34	0.57
3:L:64:PHE:HB3	3:L:75:LEU:HD11	1.85	0.57
1:C:429:PHE:HE1	1:C:514:SER:HB3	1.69	0.57
1:C:743:CYS:HB2	1:C:977:LEU:HG	1.86	0.57
1:C:246:ARG:HG3	1:C:258:TRP:HB3	1.86	0.57
2:M:100:TRP:CD1	2:M:111:TYR:HB2	2.40	0.57
1:A:568:ASP:OD1	1:A:569:ILE:N	2.33	0.57
1:B:646:ARG:HH21	1:C:835:LYS:HA	1.69	0.57
2:D:113:MET:O	3:E:38:TYR:OH	2.21	0.57
5:P:24:ARG:NH2	5:P:70:ASP:OD1	2.38	0.57
5:G:33:LEU:O	5:G:50:GLY:N	2.38	0.57
1:B:775:ASP:HA	1:B:778:THR:HG22	1.87	0.57
1:C:974:SER:HB3	1:C:980:ILE:HG13	1.87	0.57
3:E:106:LYS:NZ	3:E:107:LEU:O	2.36	0.57
1:A:491:PRO:O	1:A:492:LEU:HB2	2.05	0.57
1:C:352:ALA:HA	1:C:466:ARG:NH2	2.19	0.57
1:A:524:VAL:HG13	1:A:525:CYS:H	1.69	0.56
1:B:452:LEU:HG	1:B:492:LEU:HD12	1.86	0.56
1:A:67:VAL:HG12	1:A:79:PHE:HA	1.86	0.56
1:A:141:LEU:HD11	1:A:157:PHE:HD1	1.70	0.56
1:A:430:THR:OG1	1:A:515:PHE:O	2.19	0.56
1:A:555:SER:OG	1:A:584:ILE:O	2.21	0.56
1:B:642:VAL:HG22	1:B:651:ILE:HD12	1.86	0.56
1:C:37:TYR:OH	1:C:54:LEU:O	2.15	0.56
1:C:375:PHE:HE1	1:C:377:PHE:HB2	1.70	0.56
1:A:323:THR:OG1	1:A:537:LYS:NZ	2.38	0.56
1:A:629:LEU:HD13	1:A:633:TRP:CD2	2.41	0.56
1:A:920:GLN:N	1:A:920:GLN:OE1	2.38	0.56
1:B:99:ASN:ND2	1:B:177:MET:HG2	2.20	0.56
1:A:106:PHE:HB2	1:A:117:LEU:HB2	1.87	0.56
1:C:1041:ASP:OD2	1:C:1045:LYS:NZ	2.35	0.56
3:L:48:THR:HG22	3:L:57:SER:HB2	1.87	0.56
3:L:41:THR:OG1	3:L:44:GLN:NE2	2.39	0.56
1:C:825:LYS:NZ	1:C:938:LEU:O	2.33	0.56
1:B:68:ILE:HG22	1:B:78:ARG:HG2	1.87	0.56
1:C:34:ARG:HH12	1:C:219:GLY:H	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:37:TRP:CD1	3:E:75:LEU:HB2	2.41	0.56
1:B:141:LEU:HD22	1:B:157:PHE:HA	1.86	0.56
1:C:407:VAL:HG11	1:C:508:TYR:HD2	1.71	0.56
4:J:39:GLN:NE2	4:J:40:ALA:O	2.39	0.56
2:M:70:ILE:HD11	2:M:79:LEU:HG	1.88	0.56
5:P:31:SER:HA	5:P:50:GLY:HA3	1.87	0.56
1:A:375:PHE:HE1	1:A:377:PHE:HB2	1.71	0.55
1:B:106:PHE:HD1	1:B:238:PHE:HB2	1.71	0.55
1:B:491:PRO:O	1:B:492:LEU:HB2	2.06	0.55
1:A:738:CYS:O	1:A:742:ILE:HG22	2.06	0.55
1:B:67:VAL:O	1:B:262:ALA:HA	2.06	0.55
1:B:993:ILE:O	1:B:997:ILE:HG12	2.06	0.55
1:C:557:LYS:HZ2	1:C:559:PHE:HD1	1.54	0.55
1:C:560:LEU:H	1:C:563:GLN:HG3	1.70	0.55
1:C:1135:ASN:OD1	1:C:1136:THR:N	2.36	0.55
3:L:84:ASP:O	3:L:88:TYR:OH	2.21	0.55
1:A:412:PRO:HG3	1:A:425:LEU:HD23	1.88	0.55
1:A:439:ASN:ND2	1:A:506:GLN:OE1	2.40	0.55
1:A:563:GLN:O	1:A:577:ARG:NH1	2.38	0.55
1:B:449:TYR:HB3	3:L:31:THR:HG21	1.87	0.55
2:M:83:MET:HB3	2:M:86:LEU:HD21	1.88	0.55
1:A:212:ILE:O	1:A:214:ARG:HG2	2.05	0.55
1:A:520:ALA:HB3	1:A:521:PRO:HD3	1.88	0.55
1:B:185:ASN:HB2	1:B:213:VAL:HA	1.87	0.55
1:B:394:ASN:HA	1:B:523:THR:HG21	1.88	0.55
1:B:562:PHE:HD2	1:C:41:LYS:HZ2	1.53	0.55
1:C:402:ILE:HG22	1:C:403:ARG:O	2.07	0.55
5:G:51:ALA:HB1	5:G:65:SER:HA	1.87	0.55
1:A:605:SER:OG	1:A:607:GLN:OE1	2.24	0.55
5:K:33:LEU:HD12	5:K:89:GLN:O	2.07	0.55
2:M:116:TRP:NE1	3:N:46:PRO:O	2.39	0.55
1:A:802:PHE:HD2	1:A:805:ILE:HD11	1.72	0.55
1:C:621:PRO:HB3	1:C:638:THR:HB	1.88	0.55
2:H:60:TYR:HB3	2:H:64:VAL:HG23	1.89	0.55
1:B:228:ASP:OD1	1:B:229:LEU:N	2.40	0.55
4:O:52:VAL:HG22	4:O:52(A):VAL:H	1.72	0.55
1:A:83:VAL:HA	1:A:237:ARG:HH22	1.71	0.55
1:C:832:GLY:H	1:C:835:LYS:HZ3	1.55	0.55
1:B:409:GLN:NE2	1:B:417:ASN:OD1	2.31	0.55
1:B:1009:THR:O	1:B:1013:ILE:HG12	2.06	0.55
1:C:357:ARG:NH1	1:C:358:ILE:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:30:SER:HA	2:M:72:ARG:HH22	1.70	0.55
1:A:395:VAL:HB	1:A:515:PHE:HB3	1.88	0.54
1:A:588:THR:HG21	1:B:841:LEU:HD13	1.89	0.54
1:B:106:PHE:CD1	1:B:238:PHE:HB2	2.41	0.54
1:A:815:ARG:HG2	1:A:819:GLU:HG3	1.87	0.54
1:B:97:LYS:HB2	1:B:186:PHE:HA	1.90	0.54
2:D:37:VAL:HG11	2:D:45:LEU:HD12	1.89	0.54
2:D:69:THR:HB	2:D:82:GLN:HB3	1.89	0.54
2:H:36:TRP:HZ3	2:H:94:TYR:HB3	1.72	0.54
1:A:298:GLU:OE2	1:A:315:THR:OG1	2.23	0.54
1:A:338:PHE:HE1	1:A:358:ILE:HG13	1.71	0.54
1:B:661:GLU:O	1:B:695:TYR:OH	2.24	0.54
5:K:12:SER:O	5:K:107:ARG:NH1	2.39	0.54
3:E:12:VAL:HG23	3:E:107:LEU:HD11	1.88	0.54
4:J:60:ALA:HB3	4:J:63:PHE:HD2	1.72	0.54
4:O:5:VAL:HB	4:O:23:LYS:HE3	1.90	0.54
5:G:4:LEU:HD13	5:G:88:CYS:HB2	1.89	0.54
1:B:99:ASN:HD21	1:B:177:MET:HG2	1.73	0.54
1:B:200:TYR:HA	1:B:230:PRO:HA	1.90	0.54
2:H:47:TRP:HE1	2:H:50:VAL:HG13	1.71	0.54
5:P:33:LEU:O	5:P:50:GLY:N	2.40	0.54
1:A:71:SER:HB3	1:A:261:GLY:N	2.21	0.54
1:A:350:VAL:HB	1:A:452:LEU:O	2.08	0.54
1:A:906:PHE:HD2	1:A:916:LEU:HB2	1.72	0.54
1:B:280:ASN:OD1	1:B:284:THR:N	2.38	0.54
1:B:520:ALA:HB3	1:B:521:PRO:HD3	1.88	0.54
2:D:60:TYR:HB3	2:D:64:VAL:HG23	1.89	0.54
2:H:91:THR:HG23	2:H:123:THR:HA	1.88	0.54
1:B:527:PRO:O	1:B:529:LYS:NZ	2.34	0.54
1:A:37:TYR:HA	1:A:223:LEU:HB2	1.89	0.54
1:A:329:PHE:O	1:A:580:GLN:NE2	2.40	0.54
1:B:316:SER:HB2	1:B:595:VAL:HB	1.89	0.54
1:C:356:LYS:HG3	1:C:397:ALA:HB3	1.90	0.54
3:E:49:LEU:HA	3:E:60:VAL:HG21	1.88	0.54
2:H:29:LEU:HD21	2:H:74:ASN:HA	1.90	0.54
1:A:517:LEU:HD23	1:A:518:LEU:N	2.23	0.54
1:C:406:GLU:HB2	1:C:409:GLN:HB3	1.89	0.54
1:C:805:ILE:HD12	1:C:878:LEU:HD11	1.90	0.54
5:K:61:ARG:NH1	5:K:77:ARG:O	2.41	0.54
1:C:520:ALA:HB3	1:C:521:PRO:HD3	1.90	0.53
3:E:2:THR:HG23	3:E:100:VAL:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:17:THR:HA	3:L:77:ILE:O	2.08	0.53
1:A:1077:THR:OG1	1:A:1078:ALA:N	2.40	0.53
1:B:559:PHE:HB3	1:B:563:GLN:HB2	1.90	0.53
2:D:35:HIS:HD2	2:D:50:VAL:HG12	1.71	0.53
5:G:66:GLY:HA3	5:G:71:PHE:HA	1.90	0.53
1:B:379:CYS:HA	1:B:432:CYS:HB3	1.90	0.53
1:C:470:THR:HB	3:N:95:GLY:HA3	1.90	0.53
2:D:29:LEU:HD11	2:D:74:ASN:HA	1.90	0.53
5:K:33:LEU:HB3	5:K:50:GLY:HA2	1.90	0.53
5:P:36:TYR:HE1	5:P:46:LEU:HD12	1.72	0.53
1:A:661:GLU:O	1:A:695:TYR:OH	2.20	0.53
1:B:102:ARG:HD3	1:B:243:ALA:HB3	1.91	0.53
1:B:835:LYS:HD2	1:B:835:LYS:O	2.08	0.53
2:H:38:ARG:HA	2:H:94:TYR:HA	1.89	0.53
5:G:4:LEU:HD12	5:G:99:GLY:HA2	1.89	0.53
1:A:43:PHE:CZ	1:C:557:LYS:HE3	2.44	0.53
1:A:659:SER:HB3	1:A:698:SER:HB3	1.90	0.53
1:C:14:GLN:HG3	1:C:16:VAL:H	1.72	0.53
2:D:35:HIS:CD2	2:D:50:VAL:HG12	2.43	0.53
4:J:6:GLN:H	4:J:105:GLN:HE22	1.56	0.53
1:B:66:HIS:O	1:B:78:ARG:NH1	2.41	0.53
1:C:1134:ASN:OD1	6:Z:1:NAG:N2	2.40	0.53
4:J:81:GLU:OE2	4:J:82(A):SER:OG	2.18	0.53
1:B:321:GLN:NE2	1:B:626:ALA:O	2.42	0.53
1:B:475:ALA:HB3	1:B:487:ASN:HB3	1.91	0.53
1:A:1104:VAL:HG23	1:A:1115:ILE:HG13	1.90	0.53
1:C:96:GLU:OE1	1:C:100:ILE:N	2.39	0.53
1:C:915:VAL:O	1:C:919:ASN:ND2	2.41	0.53
1:A:210:ILE:HG13	1:A:214:ARG:HG3	1.91	0.53
2:H:108:ASP:OD1	2:H:109:TYR:N	2.36	0.53
5:G:47:LEU:HB3	5:G:54:ARG:HH11	1.74	0.53
1:A:879:ALA:O	1:A:883:THR:HG22	2.09	0.52
1:B:378:LYS:NZ	1:B:380:TYR:OH	2.25	0.52
1:C:963:VAL:O	1:C:966:LEU:HB3	2.08	0.52
2:D:114:ASP:OD1	2:D:115:VAL:N	2.41	0.52
1:A:447:GLY:O	3:E:54:ASN:ND2	2.43	0.52
1:A:563:GLN:NE2	1:B:42:VAL:O	2.42	0.52
1:B:298:GLU:OE2	1:B:316:SER:OG	2.27	0.52
1:C:362:VAL:HG21	1:C:528:LYS:HE3	1.92	0.52
1:C:815:ARG:HD3	1:C:820:ASP:HA	1.90	0.52
3:E:20:LEU:HD23	3:E:77:ILE:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:35:GLN:HB3	4:J:93:ALA:HB3	1.90	0.52
5:G:6:GLN:NE2	5:G:101:GLY:O	2.42	0.52
1:A:989:ALA:O	1:A:993:ILE:HG12	2.10	0.52
5:P:12:SER:O	5:P:107:ARG:NH1	2.42	0.52
1:B:231:ILE:HG13	1:B:232:GLY:N	2.21	0.52
1:C:146:HIS:HB3	1:C:154:GLU:HA	1.91	0.52
1:B:452:LEU:HD12	1:B:492:LEU:HB3	1.92	0.52
3:L:20:LEU:O	3:L:74:ALA:HA	2.08	0.52
1:A:134:GLN:OE1	1:A:162:SER:OG	2.27	0.52
1:A:517:LEU:HD23	1:A:518:LEU:H	1.74	0.52
1:B:142:ASP:OD2	1:B:254:SER:OG	2.26	0.52
1:C:365:TYR:CE1	1:C:387:LEU:HB2	2.45	0.52
5:K:61:ARG:HH12	5:K:78:LEU:HA	1.75	0.52
3:N:40:GLN:N	3:N:87:ASP:O	2.30	0.52
4:O:27:PHE:HB2	4:O:97:CYS:H	1.75	0.52
1:A:558:LYS:HE3	1:B:282:ASN:HB2	1.91	0.52
1:A:307:THR:HA	1:A:602:THR:HG21	1.92	0.52
4:J:2:MET:N	4:J:25:SER:O	2.43	0.52
4:J:17:SER:OG	4:J:81:GLU:OE1	2.24	0.52
1:C:430:THR:OG1	1:C:515:PHE:O	2.18	0.52
1:C:451:TYR:HB2	1:C:497:PHE:CE2	2.45	0.52
1:C:517:LEU:HG	1:C:518:LEU:H	1.74	0.52
4:F:6:GLN:H	4:F:105:GLN:NE2	2.05	0.52
1:B:328:ARG:HE	1:B:580:GLN:HG3	1.75	0.51
1:C:1009:THR:O	1:C:1013:ILE:HG12	2.09	0.51
3:E:6:GLN:HG2	3:E:22:CYS:HB2	1.92	0.51
4:F:60:ALA:O	4:F:64:GLN:NE2	2.43	0.51
3:N:48:THR:HG22	3:N:57:SER:HB2	1.92	0.51
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.76	0.51
1:C:410:ILE:HD11	1:C:423:TYR:HD2	1.75	0.51
4:F:51:ILE:HD11	4:F:57:THR:HB	1.91	0.51
1:B:544:ASN:H	1:B:546:LEU:HD23	1.75	0.51
4:F:89:VAL:HG13	4:F:107:THR:H	1.76	0.51
2:D:29:LEU:O	2:D:72:ARG:NH2	2.44	0.51
2:D:82:GLN:NE2	2:D:83:MET:O	2.44	0.51
1:A:644:GLN:NE2	1:A:648:GLY:O	2.43	0.51
1:B:136:CYS:HB2	1:B:139:PRO:HB3	1.92	0.51
1:C:350:VAL:HG23	1:C:451:TYR:HD2	1.76	0.51
4:O:23:LYS:HA	4:O:77:THR:HA	1.92	0.51
4:O:101:ASP:O	5:P:45:ARG:NH2	2.44	0.51
1:C:204:TYR:CD1	1:C:225:PRO:HA	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:29:VAL:HG13	3:N:33:TYR:HD2	1.75	0.51
1:B:122:ASN:OD1	1:B:123:ALA:N	2.43	0.51
1:A:409:GLN:O	1:A:414:GLN:NE2	2.44	0.51
1:C:156:GLU:HB3	1:C:158:ARG:HG2	1.93	0.51
1:C:296:LEU:HG	1:C:300:LYS:HE3	1.92	0.51
3:N:88:TYR:O	3:N:104:GLY:HA2	2.11	0.51
5:G:89:GLN:HG3	5:G:98:PHE:CE1	2.46	0.51
1:B:1116:THR:OG1	1:B:1118:ASP:OD1	2.28	0.51
1:C:1132:ILE:HD12	1:C:1132:ILE:H	1.75	0.51
3:L:14:PRO:HA	3:L:80:ALA:HB3	1.93	0.51
1:A:185:ASN:OD1	1:A:212:ILE:HG23	2.11	0.50
1:B:141:LEU:HB3	1:B:154:GLU:HB3	1.93	0.50
1:A:89:GLY:HA3	1:A:270:LEU:HD12	1.94	0.50
1:A:406:GLU:HG3	1:A:418:ILE:HD13	1.92	0.50
1:B:293:LEU:HA	1:B:630:THR:HG21	1.93	0.50
1:C:317:ASN:HA	1:C:594:GLY:HA2	1.94	0.50
1:C:339:ASP:O	1:C:343:ASN:N	2.29	0.50
2:H:70:ILE:HD11	2:H:79:LEU:HG	1.93	0.50
3:N:18:VAL:HG12	3:N:77:ILE:HB	1.93	0.50
5:P:38:GLN:HB2	5:P:44:PRO:HG3	1.93	0.50
1:A:393:THR:OG1	1:A:516:GLU:HG2	2.11	0.50
1:A:399:SER:OG	1:A:510:VAL:O	2.24	0.50
1:B:244:LEU:HD11	1:B:258:TRP:CE2	2.46	0.50
1:C:115:GLN:HE21	1:C:130:VAL:HG12	1.77	0.50
1:A:387:LEU:HG	1:A:390:LEU:HD12	1.94	0.50
1:B:793:PRO:O	1:B:795:LYS:NZ	2.44	0.50
1:C:972:ALA:HB2	1:C:995:ARG:HH12	1.76	0.50
2:D:35:HIS:CE1	2:D:112:GLY:HA3	2.47	0.50
1:A:106:PHE:HB3	1:A:235:ILE:HD13	1.93	0.50
3:N:66:GLY:HA2	3:N:75:LEU:HA	1.92	0.50
5:P:24:ARG:HH21	5:P:70:ASP:HA	1.77	0.50
4:F:97:CYS:HA	4:F:100(B):CYS:CB	2.42	0.50
5:G:43:ALA:HB3	5:G:45:ARG:HH22	1.77	0.50
1:A:395:VAL:HA	1:A:515:PHE:HA	1.93	0.50
1:B:21:ARG:HH11	1:B:79:PHE:HE2	1.60	0.50
1:B:357:ARG:NH1	1:B:359:SER:HB3	2.26	0.50
1:C:605:SER:OG	1:C:606:ASN:N	2.45	0.50
4:F:9:PRO:HB3	4:F:108:MET:HB2	1.94	0.50
5:G:64:GLY:HA3	5:G:73:LEU:HA	1.93	0.50
1:B:409:GLN:NE2	1:B:418:ILE:HG12	2.27	0.50
1:C:253:ASP:OD2	1:C:256:SER:OG	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:438:SER:HB2	1:C:441:LEU:HB2	1.94	0.50
2:M:61:VAL:HG12	2:M:64:VAL:HG22	1.93	0.50
1:A:399:SER:HB2	1:A:511:VAL:HG23	1.94	0.50
1:A:658:ASN:HD22	1:A:658:ASN:C	2.15	0.50
1:B:256:SER:HA	1:B:258:TRP:HE1	1.76	0.50
1:B:477:ASN:HB3	1:B:478:LYS:HD2	1.94	0.50
1:B:1102:TRP:HB2	1:B:1135:ASN:ND2	2.26	0.50
1:C:178:ASP:N	1:C:207:HIS:HE1	2.10	0.50
2:H:35:HIS:HB2	2:H:97:ALA:HB3	1.94	0.50
3:L:13:SER:HA	3:L:110:LEU:HB2	1.94	0.50
2:M:51:ILE:HD13	2:M:58:LYS:HZ2	1.77	0.50
3:N:56:ARG:NH2	3:N:65:SER:HB3	2.26	0.50
4:F:38:ARG:HB3	4:F:46:GLU:HG2	1.94	0.50
1:B:473:TYR:N	1:B:489:TYR:O	2.45	0.49
4:J:61:GLN:HA	4:J:64:GLN:HE22	1.76	0.49
1:B:115:GLN:HA	1:B:132:GLU:HG2	1.94	0.49
1:B:309:GLU:O	1:B:313:TYR:OH	2.22	0.49
1:B:954:HIS:HB3	1:B:1014:ARG:NH1	2.27	0.49
1:C:74:ASN:HB2	1:C:77:LYS:HB2	1.93	0.49
4:J:50:TRP:CD1	5:K:96:TRP:HZ3	2.30	0.49
4:F:103:TRP:HB2	5:G:45:ARG:HH21	1.77	0.49
1:C:293:LEU:HA	1:C:630:THR:HG21	1.93	0.49
2:D:36:TRP:HE1	2:D:79:LEU:HD21	1.77	0.49
4:J:52(A):VAL:O	4:J:71:ARG:NH2	2.42	0.49
1:A:280:ASN:ND2	1:A:282:ASN:OD1	2.43	0.49
1:A:350:VAL:HG12	1:A:422:ASN:ND2	2.27	0.49
1:A:796:TYR:HE2	7:C:1301:NAG:H2	1.78	0.49
1:B:91:TYR:HB3	1:B:268:GLY:HA3	1.93	0.49
1:B:625:HIS:HA	1:B:634:ARG:HH22	1.77	0.49
1:B:954:HIS:HB3	1:B:1014:ARG:CZ	2.43	0.49
1:C:738:CYS:O	1:C:742:ILE:HG12	2.13	0.49
2:H:51:ILE:HD11	2:H:72:ARG:HD2	1.94	0.49
2:M:100:TRP:HD1	2:M:111:TYR:HB2	1.77	0.49
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.95	0.49
1:C:159:VAL:HG13	1:C:160:TYR:CD2	2.47	0.49
1:C:328:ARG:HH21	1:C:580:GLN:HB2	1.77	0.49
3:N:36:SER:O	3:N:90:CYS:HA	2.13	0.49
1:A:112:SER:HA	1:A:132:GLU:HB3	1.94	0.49
1:A:631:PRO:HA	1:A:634:ARG:HB2	1.94	0.49
1:A:703:ASN:OD1	1:A:704:SER:N	2.46	0.49
1:A:770:ILE:HD11	1:A:1012:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ASP:O	1:B:216:LEU:HD22	2.13	0.49
1:B:391:CYS:O	1:B:519:HIS:NE2	2.45	0.49
1:B:469:SER:HA	3:L:96:ARG:HH12	1.78	0.49
1:C:132:GLU:HB2	1:C:164:ASN:HD21	1.77	0.49
1:C:165:ASN:OD1	1:C:166:CYS:N	2.45	0.49
1:C:375:PHE:CE1	1:C:377:PHE:HB2	2.48	0.49
5:G:88:CYS:HB3	5:G:90:GLN:HE22	1.76	0.49
1:A:253:ASP:N	1:A:253:ASP:OD1	2.45	0.49
1:B:91:TYR:OH	1:B:191:GLU:OE1	2.27	0.49
5:K:31:SER:HA	5:K:50:GLY:HA3	1.94	0.49
4:F:65:GLU:O	4:F:66:ARG:HG2	2.13	0.49
1:B:190:ARG:HB3	1:B:192:PHE:HE1	1.77	0.49
1:B:836:GLN:NE2	1:B:839:ASP:OD1	2.45	0.49
2:M:31:SER:HA	2:M:102:TYR:HE2	1.76	0.49
5:G:36:TYR:HE1	5:G:46:LEU:HD12	1.76	0.49
1:A:324:GLU:HG2	1:A:539:VAL:HG23	1.94	0.49
1:B:399:SER:HB2	1:B:511:VAL:HG23	1.94	0.49
1:C:27:ALA:HB3	1:C:64:TRP:HB3	1.94	0.49
1:C:203:ILE:HB	1:C:227:VAL:HG23	1.94	0.49
1:C:660:TYR:H	1:C:695:TYR:HE2	1.61	0.49
2:D:116:TRP:HZ2	3:E:46:PRO:HB2	1.78	0.49
1:A:139:PRO:HB2	1:A:159:VAL:HG23	1.95	0.49
1:B:80:ASP:O	1:B:265:TYR:OH	2.30	0.49
4:O:69:ILE:O	4:O:71:ARG:NH1	2.45	0.49
1:A:403:ARG:NE	1:A:406:GLU:OE1	2.46	0.48
1:A:411:ALA:N	1:A:414:GLN:HE22	2.11	0.48
1:C:759:PHE:CD2	1:C:1001:LEU:HD12	2.48	0.48
2:H:32:TYR:CD2	2:H:101:ALA:HB2	2.47	0.48
4:O:18:VAL:HB	4:O:82(A):SER:HB3	1.94	0.48
1:C:99:ASN:HA	1:C:190:ARG:HH22	1.78	0.48
1:C:918:GLU:N	1:C:918:GLU:OE1	2.47	0.48
1:A:43:PHE:CZ	1:A:45:SER:HB2	2.48	0.48
1:A:742:ILE:HD11	1:A:997:ILE:HA	1.94	0.48
1:C:703:ASN:OD1	1:C:704:SER:N	2.47	0.48
1:A:168:PHE:CZ	1:A:170:TYR:HB2	2.49	0.48
1:A:205:SER:HB3	1:A:226:LEU:HD21	1.96	0.48
1:B:314:GLN:HE22	1:B:613:GLN:HE22	1.60	0.48
1:B:327:VAL:HG12	1:B:542:ASN:HB2	1.96	0.48
1:B:707:TYR:HB3	1:C:792:PRO:HG3	1.96	0.48
1:C:834:ILE:HA	1:C:837:TYR:CD2	2.48	0.48
1:C:1082:CYS:SG	1:C:1132:ILE:HG21	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:33:GLY:O	2:M:99:GLY:N	2.33	0.48
4:O:47:TRP:HD1	5:P:98:PHE:CZ	2.31	0.48
1:A:159:VAL:HG13	1:A:160:TYR:CD2	2.47	0.48
1:A:371:LEU:HG	1:A:372:ALA:H	1.79	0.48
1:A:906:PHE:CD2	1:A:916:LEU:HB2	2.48	0.48
1:B:244:LEU:HD11	1:B:258:TRP:CZ2	2.49	0.48
1:C:555:SER:OG	1:C:584:ILE:O	2.31	0.48
1:C:674:TYR:CZ	1:C:690:GLN:HB3	2.48	0.48
3:E:38:TYR:HE1	3:E:48:THR:HG23	1.78	0.48
2:H:35:HIS:CD2	2:H:110:TYR:HH	2.31	0.48
2:M:51:ILE:HG12	2:M:72:ARG:HD2	1.93	0.48
1:A:185:ASN:HA	1:A:213:VAL:H	1.78	0.48
1:A:409:GLN:NE2	1:A:417:ASN:OD1	2.46	0.48
1:A:909:ILE:O	1:A:909:ILE:HG13	2.13	0.48
4:O:70:THR:OG1	4:O:79:TYR:HB2	2.14	0.48
5:P:16:GLY:HA2	5:P:77:ARG:HG3	1.94	0.48
1:A:57:PRO:HD3	1:A:271:GLN:OE1	2.13	0.48
1:A:165:ASN:OD1	1:A:166:CYS:N	2.47	0.48
1:A:335:LEU:HD23	1:A:335:LEU:H	1.79	0.48
1:A:873:TYR:CE1	1:C:699:LEU:HD22	2.49	0.48
1:C:403:ARG:HB3	1:C:406:GLU:OE2	2.13	0.48
1:C:631:PRO:HA	1:C:634:ARG:HB2	1.96	0.48
1:A:391:CYS:HA	1:A:525:CYS:HA	1.95	0.48
1:A:598:ILE:HB	1:A:609:ALA:HB3	1.96	0.48
1:B:206:LYS:HD3	1:B:222:ALA:O	2.13	0.48
1:B:578:ASP:OD1	1:B:583:GLU:N	2.28	0.48
1:C:750:SER:O	1:C:754:LEU:HG	2.13	0.48
2:M:37:VAL:O	2:M:94:TYR:HA	2.14	0.48
1:C:40:ASP:N	1:C:40:ASP:OD1	2.44	0.48
1:C:180:GLU:HG2	1:C:187:LYS:HD2	1.95	0.48
3:N:85:GLU:HB3	3:N:109:VAL:H	1.77	0.48
4:F:70:THR:OG1	4:F:79:TYR:HB2	2.14	0.48
1:A:40:ASP:HB3	1:A:42:VAL:HG22	1.95	0.48
1:A:379:CYS:HA	1:A:432:CYS:HB3	1.96	0.48
1:C:248:TYR:HB2	1:C:251:PRO:HB3	1.94	0.48
1:C:401:VAL:HG12	1:C:451:TYR:CE2	2.49	0.48
2:M:73:ASP:OD1	2:M:75:SER:OG	2.27	0.48
3:N:56:ARG:NH1	3:N:61:PRO:O	2.47	0.48
4:F:32:SER:H	4:F:52(A):VAL:HB	1.79	0.48
1:A:83:VAL:HA	1:A:237:ARG:NH2	2.29	0.47
1:A:691:SER:OG	1:A:692:ILE:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:CYS:N	1:C:362:VAL:O	2.45	0.47
3:L:88:TYR:HE1	3:L:107:LEU:HB3	1.79	0.47
4:F:32:SER:O	4:F:52(A):VAL:N	2.39	0.47
5:G:86:TYR:HB2	5:G:102:THR:HB	1.95	0.47
1:A:453:TYR:CE1	1:A:495:TYR:HE1	2.32	0.47
1:A:620:VAL:N	1:A:621:PRO:HD2	2.29	0.47
1:B:399:SER:OG	1:B:510:VAL:O	2.18	0.47
1:B:1029:MET:HB2	1:B:1062:PHE:HZ	1.79	0.47
1:C:148:ASN:HB3	1:C:247:SER:HA	1.96	0.47
1:C:931:ILE:O	1:C:934:ILE:HG22	2.14	0.47
5:K:2:ILE:HD12	5:K:4:LEU:HG	1.95	0.47
1:B:762:GLN:HA	1:B:765:ARG:HG2	1.96	0.47
1:B:1010:GLN:HE22	1:B:1014:ARG:CZ	2.27	0.47
1:C:37:TYR:HB3	1:C:223:LEU:HB2	1.96	0.47
1:C:177:MET:SD	1:C:179:LEU:N	2.85	0.47
1:C:643:PHE:HD2	1:C:650:LEU:HD21	1.79	0.47
5:G:2:ILE:HD12	5:G:4:LEU:HG	1.95	0.47
1:A:866:THR:HG22	1:A:869:MET:CE	2.44	0.47
1:B:451:TYR:HB2	1:B:497:PHE:CE2	2.49	0.47
1:C:371:LEU:HG	1:C:372:ALA:H	1.80	0.47
1:C:1115:ILE:HD12	1:C:1115:ILE:H	1.80	0.47
2:H:68:PHE:CD1	2:H:83:MET:HA	2.49	0.47
1:A:350:VAL:HG23	1:A:451:TYR:HB3	1.96	0.47
1:A:456:PHE:HZ	4:J:53:GLY:HA3	1.79	0.47
1:A:869:MET:CG	1:C:699:LEU:HD21	2.45	0.47
1:B:389:ASP:OD1	1:B:389:ASP:N	2.47	0.47
1:B:1111:GLU:O	1:B:1113:GLN:NE2	2.48	0.47
1:C:96:GLU:O	1:C:188:ASN:CB	2.60	0.47
2:H:38:ARG:HG2	2:H:46:GLU:HB3	1.96	0.47
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.97	0.47
1:B:111:ASP:HB3	1:B:113:LYS:HE3	1.96	0.47
1:B:919:ASN:O	1:B:923:ILE:HG12	2.14	0.47
4:J:65:GLU:O	4:J:66:ARG:HG2	2.15	0.47
2:M:19:ARG:HH11	2:M:80:TYR:HD1	1.63	0.47
2:M:37:VAL:HG11	2:M:45:LEU:HD12	1.97	0.47
4:F:38:ARG:HB2	4:F:48:ILE:HD11	1.97	0.47
4:F:103:TRP:CZ3	5:G:44:PRO:HD2	2.50	0.47
1:A:331:ASN:OD1	1:A:332:ILE:N	2.46	0.47
1:A:398:ASP:N	1:A:398:ASP:OD1	2.47	0.47
1:B:147:LYS:HB2	1:B:149:ASN:OD1	2.15	0.47
1:B:1135:ASN:OD1	1:B:1136:THR:N	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ILE:HG13	1:C:232:GLY:N	2.29	0.47
1:C:721:SER:OG	1:C:1066:THR:OG1	2.31	0.47
2:H:13:GLN:OE1	2:H:14:PRO:HD2	2.15	0.47
1:A:125:ASN:HB2	1:A:172:SER:O	2.15	0.47
1:A:348:ALA:HB3	1:A:399:SER:O	2.15	0.47
1:B:159:VAL:HG13	1:B:160:TYR:CD2	2.50	0.47
1:B:190:ARG:HB3	1:B:192:PHE:CE1	2.50	0.47
1:B:524:VAL:HG13	1:B:525:CYS:N	2.29	0.47
1:B:532:ASN:OD1	1:B:533:LEU:N	2.41	0.47
1:C:92:PHE:HZ	1:C:101:ILE:HD13	1.80	0.47
2:M:27:PHE:O	2:M:77:ASN:ND2	2.48	0.47
1:A:201:PHE:HB3	1:A:229:LEU:HB2	1.96	0.47
1:B:307:THR:HA	1:B:602:THR:HG21	1.97	0.47
1:B:346:ARG:NH1	1:B:451:TYR:OH	2.48	0.47
1:B:785:VAL:HG12	1:B:787:GLN:H	1.80	0.47
4:O:37:VAL:HG11	4:O:103:TRP:HH2	1.79	0.47
1:A:1089:PHE:O	1:A:1120:THR:OG1	2.27	0.46
3:L:63:ARG:NH2	3:L:79:GLY:O	2.48	0.46
4:F:44:ARG:HH12	5:G:2:ILE:HD11	1.79	0.46
1:C:777:ASN:HD21	1:C:1019:ARG:HD3	1.79	0.46
1:B:834:ILE:HA	1:B:837:TYR:CG	2.49	0.46
1:C:503:VAL:HA	1:C:506:GLN:HB2	1.97	0.46
3:E:47:ARG:NH2	3:E:59:GLY:O	2.48	0.46
4:J:2:MET:HG3	4:J:26:GLY:HA3	1.96	0.46
5:P:18:ARG:HH12	5:P:77:ARG:NH1	2.14	0.46
1:A:100:ILE:C	1:A:243:ALA:HB3	2.36	0.46
1:A:329:PHE:CG	1:A:527:PRO:HB2	2.50	0.46
1:A:524:VAL:HG13	1:A:525:CYS:N	2.30	0.46
1:B:71:SER:HB3	1:B:261:GLY:H	1.80	0.46
1:C:406:GLU:HG3	1:C:418:ILE:HD13	1.97	0.46
5:K:34:ALA:HB3	5:K:89:GLN:HB2	1.96	0.46
2:M:64:VAL:HB	2:M:68:PHE:HD2	1.81	0.46
2:M:114:ASP:OD1	2:M:115:VAL:N	2.48	0.46
1:A:246:ARG:HH12	1:A:254:SER:HA	1.80	0.46
1:A:353:TRP:H	1:A:466:ARG:HH22	1.63	0.46
1:B:244:LEU:HD21	1:B:258:TRP:CD1	2.50	0.46
1:C:208:THR:HG22	1:C:210:ILE:HG23	1.97	0.46
1:C:535:LYS:H	1:C:537:LYS:HZ1	1.64	0.46
4:J:35:GLN:OE1	4:J:47:TRP:NE1	2.48	0.46
2:H:29:LEU:HD22	2:H:77:ASN:OD1	2.15	0.46
4:F:6:GLN:HE22	4:F:91:TYR:HA	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ARG:HH12	1:A:81:ASN:N	2.14	0.46
1:B:620:VAL:N	1:B:621:PRO:HD2	2.30	0.46
1:C:436:TRP:CZ2	1:C:509:ARG:HG2	2.51	0.46
4:J:37:VAL:HG12	5:K:98:PHE:HE2	1.80	0.46
4:O:38:ARG:HH22	4:O:86:ASP:HB3	1.81	0.46
1:A:14:GLN:N	1:A:158:ARG:HD3	2.31	0.46
1:A:95:ILE:HD13	1:A:189:LEU:HB2	1.97	0.46
1:A:758:SER:O	1:A:762:GLN:NE2	2.49	0.46
1:B:403:ARG:HD3	1:B:505:HIS:CD2	2.50	0.46
1:B:480:CYS:O	1:B:483:VAL:HG23	2.15	0.46
1:C:879:ALA:HA	1:C:882:ILE:HG22	1.98	0.46
1:A:402:ILE:HG23	1:A:406:GLU:HG2	1.97	0.46
1:A:456:PHE:CZ	4:J:53:GLY:HA3	2.51	0.46
1:A:577:ARG:HA	1:A:584:ILE:HA	1.98	0.46
1:B:729:VAL:HG22	1:B:1059:GLY:HA2	1.97	0.46
1:C:108:THR:O	1:C:237:ARG:NH2	2.49	0.46
1:C:992:GLN:HG3	1:C:995:ARG:HH21	1.81	0.46
2:D:40:ALA:HB3	2:D:43:LYS:HB2	1.98	0.46
4:F:47:TRP:HZ2	4:F:50:TRP:HB3	1.81	0.46
4:F:48:ILE:HG12	4:F:63:PHE:HE2	1.80	0.46
1:A:192:PHE:HB3	1:A:194:PHE:HE1	1.81	0.46
1:A:458:LYS:HB2	1:A:473:TYR:HE1	1.81	0.46
1:A:784:GLN:N	1:A:784:GLN:OE1	2.49	0.46
1:C:142:ASP:OD2	1:C:246:ARG:NH2	2.49	0.46
1:C:451:TYR:HB2	1:C:497:PHE:HE2	1.79	0.46
4:J:27:PHE:HB2	4:J:97:CYS:O	2.16	0.46
2:M:43:LYS:O	3:N:89:TYR:OH	2.32	0.46
3:N:4:VAL:HG22	3:N:92:LEU:HD12	1.97	0.46
1:A:96:GLU:HG2	1:A:262:ALA:O	2.15	0.46
1:A:324:GLU:OE1	1:A:537:LYS:NZ	2.47	0.46
1:A:351:TYR:HE1	1:A:452:LEU:HG	1.81	0.46
1:B:20:THR:HB	1:B:77:LYS:HG2	1.98	0.46
1:B:112:SER:HA	1:B:132:GLU:HB3	1.98	0.46
1:C:350:VAL:HG23	1:C:451:TYR:CD2	2.51	0.46
1:C:350:VAL:O	1:C:422:ASN:ND2	2.47	0.46
3:N:20:LEU:HB3	3:N:37:TRP:CZ3	2.50	0.46
1:C:341:VAL:HG13	1:C:356:LYS:HE3	1.97	0.45
2:H:104:GLU:O	2:H:106:LEU:HG	2.16	0.45
2:M:32:TYR:CE1	2:M:101:ALA:HB2	2.51	0.45
1:A:131:CYS:HB2	1:A:133:PHE:CZ	2.51	0.45
1:A:890:ALA:HB1	1:C:1046:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:914:ASN:OD1	1:A:915:VAL:N	2.49	0.45
2:D:52:SER:OG	2:D:53:TYR:N	2.49	0.45
3:L:64:PHE:HD2	3:L:75:LEU:HD21	1.81	0.45
4:F:8:GLY:O	4:F:107:THR:OG1	2.34	0.45
1:A:201:PHE:CE2	1:A:203:ILE:HD11	2.52	0.45
1:A:355:ARG:HD2	1:A:396:TYR:HB3	1.99	0.45
1:A:424:LYS:HB3	1:A:463:PRO:HG3	1.98	0.45
1:A:1081:ILE:O	1:A:1088:HIS:N	2.49	0.45
1:C:398:ASP:OD1	1:C:512:VAL:HG23	2.17	0.45
5:P:36:TYR:CD2	5:P:89:GLN:HG3	2.51	0.45
4:F:48:ILE:HG12	4:F:63:PHE:CE2	2.51	0.45
1:A:125:ASN:HA	1:A:174:PRO:HD3	1.98	0.45
1:B:770:ILE:HD11	1:B:1012:LEU:HD12	1.98	0.45
1:C:401:VAL:HG21	1:C:442:ASP:OD2	2.17	0.45
2:M:113:MET:O	3:N:38:TYR:OH	2.20	0.45
4:O:47:TRP:CH2	4:O:49:GLY:HA2	2.51	0.45
5:G:1:GLU:HB3	5:G:93:ASN:HD22	1.81	0.45
1:A:375:PHE:CE1	1:A:377:PHE:HB2	2.51	0.45
1:A:713:ALA:HB3	1:B:894:LEU:HB3	1.97	0.45
1:C:133:PHE:HB2	1:C:135:PHE:CZ	2.52	0.45
5:K:56:THR:OG1	5:K:57:GLY:N	2.50	0.45
2:M:38:ARG:HG3	2:M:48:VAL:HG21	1.98	0.45
4:O:51:ILE:HG22	4:O:52:VAL:N	2.31	0.45
1:A:130:VAL:HG12	1:A:130:VAL:O	2.15	0.45
1:B:133:PHE:HB3	1:B:160:TYR:CG	2.52	0.45
1:B:458:LYS:HB2	1:B:473:TYR:HE1	1.82	0.45
1:C:895:GLN:OE1	1:C:895:GLN:N	2.42	0.45
2:D:114:ASP:O	3:E:48:THR:OG1	2.29	0.45
5:G:34:ALA:HA	5:G:49:TYR:HA	1.99	0.45
1:A:969:LYS:HZ3	1:A:974:SER:HA	1.81	0.45
1:B:398:ASP:OD1	1:B:512:VAL:HG23	2.16	0.45
1:B:639:GLY:HA2	1:B:642:VAL:HG23	1.98	0.45
3:L:81:GLN:N	3:L:84:ASP:OD2	2.43	0.45
2:M:2:VAL:HG13	2:M:27:PHE:CD1	2.52	0.45
4:O:52:VAL:HG22	4:O:52(A):VAL:N	2.32	0.45
1:A:351:TYR:HD1	1:A:452:LEU:O	2.00	0.45
1:A:394:ASN:HB3	1:A:523:THR:HG21	1.98	0.45
1:A:750:SER:O	1:A:754:LEU:HD23	2.17	0.45
1:A:866:THR:H	1:A:869:MET:HE2	1.82	0.45
1:A:986:PRO:O	1:A:990:GLU:HG2	2.17	0.45
1:B:131:CYS:HB2	1:B:133:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:616:ASN:OD1	1:B:617:CYS:N	2.49	0.45
1:B:906:PHE:CD2	1:B:916:LEU:HB2	2.52	0.45
1:C:117:LEU:HA	1:C:129:LYS:O	2.17	0.45
1:C:140:PHE:HA	1:C:241:LEU:HD12	1.99	0.45
1:C:826:VAL:O	1:C:828:LEU:HG	2.16	0.45
4:O:19:LYS:HZ3	4:O:81:GLU:HG2	1.82	0.45
5:P:92:GLY:N	5:P:96:TRP:HE1	2.14	0.45
4:F:59:TYR:CD2	4:F:64:GLN:HA	2.52	0.45
5:G:58:PHE:HD1	5:G:59:PRO:HD2	1.81	0.45
1:C:87:ASN:OD1	1:C:88:ASP:N	2.45	0.45
1:C:115:GLN:NE2	1:C:130:VAL:HG12	2.31	0.45
2:M:58:LYS:NZ	2:M:70:ILE:HG23	2.32	0.45
1:A:338:PHE:HB3	1:A:342:PHE:CE2	2.52	0.45
1:A:419:ALA:HA	1:A:423:TYR:O	2.17	0.45
1:B:204:TYR:CE2	1:B:225:PRO:HG3	2.52	0.45
1:B:903:ALA:HB1	1:B:913:GLN:HG2	1.99	0.45
1:C:21:ARG:HA	1:C:79:PHE:HE1	1.81	0.45
1:C:931:ILE:HA	1:C:934:ILE:HG22	1.99	0.45
1:C:1077:THR:OG1	1:C:1078:ALA:N	2.50	0.45
3:L:15:GLY:HA2	3:L:79:GLY:HA2	1.98	0.45
1:A:417:ASN:OD1	1:A:418:ILE:N	2.49	0.44
1:C:663:ASP:OD1	1:C:664:ILE:N	2.50	0.44
2:D:47:TRP:CZ2	2:D:50:VAL:HG13	2.51	0.44
4:J:70:THR:OG1	4:J:79:TYR:HB2	2.17	0.44
3:N:6:GLN:NE2	3:N:90:CYS:HB2	2.32	0.44
4:O:20:VAL:CG1	4:O:80:MET:HB3	2.47	0.44
4:F:39:GLN:HB2	4:F:45:LEU:HD23	1.98	0.44
1:A:355:ARG:NH1	1:A:398:ASP:OD2	2.50	0.44
1:B:66:HIS:ND1	1:B:264:ALA:HB2	2.32	0.44
1:B:229:LEU:HG	1:B:231:ILE:HG23	1.99	0.44
1:B:398:ASP:OD1	1:B:398:ASP:N	2.50	0.44
1:B:815:ARG:HD2	1:B:820:ASP:OD1	2.17	0.44
2:D:6:GLU:O	2:D:120:THR:OG1	2.32	0.44
3:N:84:ASP:HB2	3:N:109:VAL:HG21	1.99	0.44
4:O:17:SER:HB2	4:O:82:LEU:HA	2.00	0.44
4:O:52:VAL:O	4:O:71:ARG:HD2	2.16	0.44
1:B:493:ARG:NH1	4:F:55:GLY:H	2.16	0.44
1:C:420:ASP:HB2	1:C:460:ASN:HA	1.99	0.44
1:C:445:VAL:HA	1:C:499:PRO:HB3	1.99	0.44
4:O:38:ARG:HE	4:O:88:ALA:HB3	1.82	0.44
1:A:600:PRO:HB3	1:A:692:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:PHE:CE2	1:B:170:TYR:HB2	2.53	0.44
1:B:347:PHE:HB3	1:B:509:ARG:NH1	2.33	0.44
1:B:443:SER:HB2	1:B:499:PRO:HA	2.00	0.44
1:C:14:GLN:O	1:C:158:ARG:HD3	2.17	0.44
1:C:546:LEU:H	1:C:546:LEU:HD23	1.82	0.44
3:N:90:CYS:O	3:N:101:PHE:HA	2.17	0.44
1:A:147:LYS:HA	1:A:246:ARG:HB3	1.99	0.44
1:A:310:LYS:HG2	1:A:664:ILE:HD11	2.00	0.44
1:A:387:LEU:HA	1:A:390:LEU:HG	1.99	0.44
1:B:559:PHE:CD2	1:B:584:ILE:HG12	2.52	0.44
1:A:621:PRO:O	1:A:625:HIS:ND1	2.51	0.44
2:H:73:ASP:OD1	2:H:78:THR:HB	2.17	0.44
2:H:109:TYR:HB2	3:L:96:ARG:H	1.83	0.44
1:B:249:LEU:HD12	1:B:259:THR:HG21	1.98	0.44
1:C:147:LYS:NZ	1:C:246:ARG:HD2	2.33	0.44
2:D:116:TRP:CZ2	3:E:46:PRO:HB2	2.53	0.44
4:J:44:ARG:HH22	5:K:2:ILE:HD11	1.82	0.44
5:P:61:ARG:HH12	5:P:78:LEU:HA	1.82	0.44
4:F:65:GLU:N	4:F:65:GLU:OE2	2.51	0.44
1:A:34:ARG:NH2	1:A:216:LEU:HB3	2.33	0.44
1:C:14:GLN:OE1	1:C:16:VAL:N	2.51	0.44
1:C:16:VAL:HG13	1:C:17:ASN:N	2.33	0.44
1:C:326:ILE:HG13	1:C:534:VAL:HG22	2.00	0.44
1:C:702:GLU:OE1	1:C:702:GLU:N	2.51	0.44
5:P:13:LEU:HD22	5:P:17:GLU:HG3	2.00	0.44
1:A:605:SER:OG	1:A:606:ASN:N	2.51	0.44
1:B:357:ARG:HB2	1:B:396:TYR:CE1	2.50	0.44
1:C:26:PRO:HG2	1:C:28:TYR:HE1	1.82	0.44
1:C:62:VAL:HB	1:C:267:VAL:O	2.18	0.44
1:C:253:ASP:N	1:C:253:ASP:OD1	2.48	0.44
2:M:109:TYR:HB3	3:N:96:ARG:H	1.83	0.44
3:N:35:PRO:HA	3:N:91:VAL:O	2.18	0.44
1:A:128:ILE:HB	1:A:170:TYR:HB3	2.00	0.43
1:A:838:GLY:N	1:A:854:LYS:HZ2	2.16	0.43
1:C:533:LEU:HD21	1:C:535:LYS:HG3	2.00	0.43
1:C:620:VAL:N	1:C:621:PRO:HD2	2.33	0.43
1:C:1087:ALA:O	1:C:1122:VAL:HG23	2.18	0.43
2:M:3:GLN:HE22	2:M:117:GLY:HA3	1.83	0.43
4:O:12:LYS:NZ	4:O:17:SER:H	2.16	0.43
4:O:47:TRP:NE1	5:P:96:TRP:HB2	2.33	0.43
5:G:56:THR:OG1	5:G:57:GLY:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:619:GLU:OE1	1:A:619:GLU:N	2.51	0.43
1:B:620:VAL:O	1:B:624:ILE:HG12	2.19	0.43
3:E:23:GLY:HA3	3:E:72:LYS:HG3	2.01	0.43
5:G:83:PHE:HD1	5:G:104:VAL:HG23	1.83	0.43
1:A:984:LEU:HD12	1:A:984:LEU:HA	1.84	0.43
1:A:1009:THR:O	1:A:1013:ILE:HG12	2.18	0.43
1:B:1093:GLY:HA3	1:B:1105:THR:O	2.17	0.43
1:C:426:PRO:O	1:C:429:PHE:HB2	2.18	0.43
1:B:405:ASP:HB2	1:B:504:GLY:O	2.18	0.43
1:B:553:THR:HG21	1:C:842:GLY:HA2	2.00	0.43
1:B:737:ASP:OD1	1:B:738:CYS:N	2.51	0.43
1:B:1047:TYR:HD2	1:B:1067:TYR:HD2	1.66	0.43
1:C:717:ASN:HB2	1:C:1071:GLN:HG3	2.00	0.43
3:L:36:SER:O	3:L:91:VAL:N	2.51	0.43
1:A:745:ASP:OD1	1:C:319:ARG:NH1	2.52	0.43
1:B:18:LEU:HB2	1:B:256:SER:HB3	2.00	0.43
1:B:290:ASP:OD1	1:B:291:CYS:N	2.51	0.43
1:C:411:ALA:HB3	1:C:414:GLN:NE2	2.34	0.43
1:A:293:LEU:O	1:A:630:THR:OG1	2.35	0.43
1:B:1082:CYS:HB2	1:B:1126:CYS:HB2	1.85	0.43
2:M:17:SER:HB3	2:M:82:GLN:HE22	1.84	0.43
1:A:86:PHE:HB2	1:A:238:PHE:CD1	2.49	0.43
1:A:102:ARG:HG2	1:A:243:ALA:CB	2.43	0.43
1:A:475:ALA:HB3	1:A:487:ASN:HB3	2.01	0.43
1:A:922:LEU:HD11	1:A:926:GLN:HE21	1.84	0.43
1:B:1117:THR:N	1:B:1138:TYR:O	2.47	0.43
1:C:112:SER:O	1:C:164:ASN:ND2	2.52	0.43
1:C:618:THR:OG1	1:C:619:GLU:OE1	2.30	0.43
1:C:1104:VAL:HG23	1:C:1115:ILE:HG13	2.01	0.43
2:M:29:LEU:HB2	2:M:77:ASN:OD1	2.19	0.43
2:M:72:ARG:NH2	2:M:74:ASN:OD1	2.51	0.43
2:M:92:ALA:HB3	2:M:94:TYR:HE1	1.84	0.43
3:N:20:LEU:HB3	3:N:37:TRP:HZ3	1.83	0.43
1:A:553:THR:HG23	1:A:586:ASP:HB3	2.00	0.43
1:A:920:GLN:HE21	1:C:1130:ILE:HG12	1.83	0.43
1:B:156:GLU:HB3	1:B:158:ARG:HG2	1.99	0.43
1:B:1101:HIS:CE1	6:U:1:NAG:H3	2.53	0.43
3:E:91:VAL:HG22	3:E:101:PHE:CE1	2.49	0.43
4:J:66:ARG:HD2	4:J:82(B):SER:HB2	2.01	0.43
1:A:347:PHE:O	2:D:105:LEU:HD22	2.19	0.43
1:C:24:LEU:HD23	1:C:78:ARG:HH22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:LYS:HD2	1:C:186:PHE:HA	2.00	0.43
4:J:67:VAL:HG22	4:J:82:LEU:HD13	2.01	0.43
5:P:64:GLY:HA3	5:P:73:LEU:HA	2.00	0.43
4:F:40:ALA:HB2	4:F:88:ALA:HB2	2.01	0.43
1:A:811:LYS:HB2	1:A:811:LYS:HE3	1.88	0.43
1:A:1039:ARG:NE	1:B:1031:GLU:OE2	2.51	0.43
1:C:331:ASN:N	1:C:331:ASN:OD1	2.51	0.43
1:C:383:SER:OG	1:C:386:LYS:HG2	2.19	0.43
1:C:821:LEU:HD21	1:C:939:SER:HB2	2.01	0.43
2:M:36:TRP:CE3	2:M:81:LEU:HD22	2.53	0.43
4:F:29:PHE:O	4:F:52(A):VAL:HG11	2.18	0.43
4:F:97:CYS:HA	4:F:100(B):CYS:HB3	2.00	0.43
1:A:765:ARG:NH2	1:C:957:GLN:OE1	2.52	0.42
1:A:802:PHE:CD2	1:A:805:ILE:HD11	2.54	0.42
1:B:37:TYR:HB3	1:B:223:LEU:HB2	2.01	0.42
1:B:735:SER:OG	1:B:736:VAL:N	2.52	0.42
3:E:39:GLN:HB3	3:E:49:LEU:HD11	2.00	0.42
2:M:83:MET:HE2	2:M:122:VAL:HG11	2.01	0.42
5:P:32:TYR:O	5:P:91:TYR:N	2.47	0.42
5:P:76:SER:HB2	5:P:77:ARG:NH1	2.34	0.42
1:A:32:PHE:HB3	1:A:218:GLN:HE22	1.84	0.42
1:A:38:TYR:HH	1:A:284:THR:HG1	1.63	0.42
1:A:326:ILE:HD13	1:A:534:VAL:HG22	2.00	0.42
1:A:451:TYR:HB2	1:A:497:PHE:CZ	2.54	0.42
1:B:89:GLY:C	1:B:270:LEU:HD23	2.40	0.42
1:B:146:HIS:CE1	1:B:245:HIS:HA	2.54	0.42
1:B:328:ARG:HH21	1:B:580:GLN:HB2	1.84	0.42
1:B:834:ILE:HD11	1:B:862:PRO:HD3	2.01	0.42
1:C:67:VAL:HG12	1:C:79:PHE:HA	2.00	0.42
4:O:39:GLN:NE2	4:O:40:ALA:O	2.46	0.42
5:P:6:GLN:HE22	5:P:100:GLN:HB2	1.83	0.42
1:A:16:VAL:HG11	1:A:140:PHE:HE1	1.84	0.42
1:A:1031:GLU:OE2	1:C:1039:ARG:NE	2.42	0.42
1:B:501:TYR:CD2	1:B:505:HIS:HB2	2.54	0.42
1:B:879:ALA:HA	1:B:882:ILE:HG22	2.01	0.42
1:C:214:ARG:NH1	1:C:218:GLN:H	2.14	0.42
1:C:628:GLN:OE1	1:C:634:ARG:NH2	2.52	0.42
2:D:93:VAL:HG23	2:D:95:TYR:CE1	2.54	0.42
4:J:38:ARG:HB3	4:J:46:GLU:HB2	2.02	0.42
2:M:99:GLY:HA2	2:M:112:GLY:HA2	2.00	0.42
4:O:14:PRO:HG3	4:O:111:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ARG:HD2	1:A:91:TYR:OH	2.20	0.42
1:A:180:GLU:OE1	1:A:182:LYS:HB2	2.19	0.42
1:A:188:ASN:O	1:A:190:ARG:N	2.52	0.42
1:B:104:TRP:HB3	1:B:106:PHE:CE1	2.55	0.42
1:B:960:ASN:HA	1:B:963:VAL:HG12	2.01	0.42
2:D:32:TYR:CD2	2:D:101:ALA:HB2	2.54	0.42
3:N:33:TYR:HB3	3:N:92:LEU:HD22	2.00	0.42
3:N:106:LYS:HG3	3:N:108:THR:HG23	2.00	0.42
1:A:847:ARG:HD3	1:C:568:ASP:OD2	2.20	0.42
1:A:979:ASP:HB2	1:A:983:ARG:HE	1.83	0.42
1:B:244:LEU:HD21	1:B:258:TRP:NE1	2.34	0.42
1:C:318:PHE:HZ	1:C:615:VAL:HG21	1.85	0.42
1:C:348:ALA:HB3	1:C:399:SER:O	2.18	0.42
1:C:351:TYR:HA	1:C:422:ASN:OD1	2.19	0.42
1:C:997:ILE:O	1:C:1001:LEU:HD23	2.20	0.42
2:D:61:VAL:HG22	2:D:62:ASP:H	1.84	0.42
2:D:87:ARG:HG2	2:D:88:ALA:H	1.83	0.42
4:O:9:PRO:HB3	4:O:108:MET:HB2	2.01	0.42
5:P:33:LEU:HD22	5:P:71:PHE:CG	2.55	0.42
1:A:44:ARG:NH1	1:A:279:TYR:OH	2.52	0.42
1:A:205:SER:OG	1:A:206:LYS:N	2.52	0.42
7:A:1304:NAG:H5	1:B:836:GLN:NE2	2.34	0.42
1:B:1139:ASP:OD2	1:B:1142:GLN:HG2	2.20	0.42
1:C:954:HIS:HB3	1:C:1014:ARG:NH2	2.34	0.42
3:L:28:SER:HB2	4:F:56:ASN:ND2	2.32	0.42
5:P:56:THR:OG1	5:P:57:GLY:N	2.52	0.42
1:A:200:TYR:HD1	1:A:230:PRO:HA	1.84	0.42
1:A:328:ARG:HH21	1:A:580:GLN:HG3	1.84	0.42
1:A:864:LEU:HD11	1:C:665:PRO:HB2	2.01	0.42
1:C:379:CYS:HA	1:C:432:CYS:HB3	2.01	0.42
1:C:462:LYS:HE2	1:C:462:LYS:HB2	1.89	0.42
1:C:505:HIS:O	1:C:505:HIS:ND1	2.53	0.42
1:A:448:ASN:O	1:A:497:PHE:HB2	2.19	0.42
1:B:121:ASN:HA	1:B:126:VAL:HG23	2.01	0.42
1:B:310:LYS:HG3	1:B:664:ILE:HD11	2.01	0.42
1:B:407:VAL:HG11	1:B:508:TYR:HD2	1.84	0.42
1:C:452:LEU:HG	1:C:492:LEU:HD12	2.02	0.42
2:D:32:TYR:CD2	2:D:98:ARG:HD3	2.55	0.42
2:M:30:SER:HA	2:M:72:ARG:NH2	2.34	0.42
1:A:351:TYR:CE1	1:A:452:LEU:HG	2.55	0.42
1:A:586:ASP:OD2	1:B:843:ASP:N	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:LEU:HB3	1:B:873:TYR:CE1	2.55	0.42
1:A:1135:ASN:OD1	1:A:1136:THR:N	2.39	0.42
1:B:106:PHE:HB3	1:B:235:ILE:HD11	2.01	0.42
1:B:188:ASN:OD1	1:B:207:HIS:ND1	2.52	0.42
1:B:386:LYS:HD3	1:B:386:LYS:HA	1.80	0.42
1:B:451:TYR:HB2	1:B:497:PHE:HE2	1.85	0.42
1:B:755:GLN:OE1	1:B:755:GLN:N	2.40	0.42
1:B:940:SER:OG	1:B:941:THR:N	2.53	0.42
1:B:992:GLN:OE1	1:B:995:ARG:NH2	2.47	0.42
5:K:22:SER:HB2	5:K:24:ARG:NH2	2.26	0.42
3:N:14:PRO:HG3	3:N:109:VAL:HG12	2.02	0.42
5:P:91:TYR:HA	5:P:96:TRP:CD1	2.53	0.42
1:B:438:SER:HB2	1:B:441:LEU:HB2	2.01	0.42
1:C:425:LEU:HD12	1:C:426:PRO:HD2	2.01	0.42
2:M:20:LEU:N	2:M:81:LEU:O	2.49	0.42
1:A:21:ARG:HH22	1:A:81:ASN:H	1.66	0.41
1:A:570:ALA:O	1:A:572:THR:HG23	2.19	0.41
1:A:968:SER:HB3	1:A:970:PHE:CE1	2.55	0.41
1:B:203:ILE:O	1:B:225:PRO:HA	2.20	0.41
1:C:32:PHE:HB3	1:C:218:GLN:OE1	2.20	0.41
1:C:194:PHE:HD1	1:C:203:ILE:HG12	1.85	0.41
1:C:452:LEU:CB	1:C:494:SER:HA	2.49	0.41
3:E:64:PHE:HB3	3:E:75:LEU:HD11	2.02	0.41
3:L:6:GLN:NE2	3:L:102:GLY:HA3	2.35	0.41
2:M:31:SER:HA	2:M:102:TYR:CE2	2.55	0.41
2:M:44:GLY:HA2	3:N:89:TYR:CZ	2.55	0.41
3:N:24:LEU:HD11	3:N:26:SER:HB3	2.02	0.41
1:A:43:PHE:HB3	1:C:566:GLY:HA2	2.01	0.41
1:A:50:SER:HB3	1:A:304:LYS:NZ	2.35	0.41
1:A:295:PRO:HG3	1:A:633:TRP:CZ3	2.55	0.41
1:A:377:PHE:HD1	1:A:434:ILE:HG12	1.84	0.41
1:A:945:LEU:HD23	1:A:946:GLY:H	1.85	0.41
1:C:118:LEU:HD11	1:C:135:PHE:CZ	2.52	0.41
1:C:1123:SER:O	1:C:1123:SER:OG	2.28	0.41
2:H:100:TRP:CD1	2:H:111:TYR:HB2	2.55	0.41
1:C:97:LYS:HZ1	1:C:187:LYS:HE3	1.84	0.41
1:C:458:LYS:HB2	1:C:473:TYR:HE1	1.84	0.41
1:C:776:LYS:HB3	1:C:776:LYS:HE3	1.86	0.41
4:J:87:THR:HG23	4:J:110:THR:HA	2.03	0.41
2:H:48:VAL:HG21	2:H:94:TYR:CE2	2.55	0.41
2:H:52:SER:O	2:H:72:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:51:ILE:HD13	2:M:58:LYS:NZ	2.34	0.41
2:M:76:LYS:HD2	2:M:76:LYS:HA	1.93	0.41
4:O:38:ARG:N	4:O:46:GLU:O	2.40	0.41
1:A:77:LYS:HB2	1:A:77:LYS:HE3	1.75	0.41
1:B:947:LYS:HE2	1:B:947:LYS:HB2	1.92	0.41
4:J:65:GLU:O	4:J:67:VAL:HG23	2.20	0.41
5:G:33:LEU:HD11	5:G:90:GLN:HE21	1.85	0.41
1:A:333:THR:HG22	1:A:334:ASN:N	2.25	0.41
1:A:403:ARG:HB2	1:A:495:TYR:HE2	1.85	0.41
1:A:1086:LYS:HE3	1:A:1086:LYS:HB2	1.86	0.41
1:B:173:GLN:HG2	1:B:174:PRO:HD2	2.01	0.41
1:B:328:ARG:HD2	1:B:328:ARG:HA	1.89	0.41
1:B:699:LEU:HB3	1:C:873:TYR:HE1	1.84	0.41
1:B:708:SER:OG	1:B:709:ASN:N	2.53	0.41
1:B:821:LEU:O	1:B:825:LYS:HG2	2.20	0.41
1:C:393:THR:HG21	1:C:521:PRO:HD2	2.01	0.41
1:C:1039:ARG:H	1:C:1039:ARG:HG3	1.66	0.41
2:M:57:ASN:OD1	2:M:58:LYS:N	2.50	0.41
5:P:38:GLN:HG3	5:P:42:GLN:O	2.19	0.41
4:F:35:GLN:HB2	4:F:100(F):PHE:CZ	2.55	0.41
5:G:22:SER:CB	5:G:24:ARG:HH22	2.26	0.41
5:G:31:SER:HA	5:G:50:GLY:HA3	2.02	0.41
1:A:725:GLU:OE1	1:A:1028:LYS:HE2	2.21	0.41
1:B:516:GLU:C	1:B:517:LEU:HD12	2.41	0.41
1:B:731:MET:HE3	1:B:1018:ILE:HG13	2.02	0.41
1:C:86:PHE:HB2	1:C:238:PHE:CD1	2.56	0.41
1:C:346:ARG:HB2	2:M:104:GLU:OE2	2.20	0.41
1:C:947:LYS:HD3	1:C:947:LYS:H	1.85	0.41
2:D:112:GLY:C	2:D:113:MET:HG2	2.41	0.41
2:H:35:HIS:HE1	2:H:112:GLY:HA3	1.86	0.41
3:N:38:TYR:CE1	3:N:48:THR:HG23	2.56	0.41
4:O:36:TRP:O	4:O:48:ILE:HB	2.19	0.41
5:G:35:TRP:HE3	5:G:48:ILE:HG23	1.84	0.41
1:B:867:ASP:OD1	1:B:868:GLU:N	2.53	0.41
1:C:411:ALA:HB3	1:C:414:GLN:HE22	1.85	0.41
2:M:20:LEU:HD22	2:M:36:TRP:CH2	2.55	0.41
1:B:81:ASN:N	1:B:82:PRO:HD3	2.36	0.41
1:B:83:VAL:HA	1:B:239:GLN:HB3	2.02	0.41
1:B:675:GLN:OE1	1:B:677:GLN:HB3	2.21	0.41
1:C:46:SER:HA	1:C:279:TYR:O	2.21	0.41
1:C:527:PRO:O	1:C:528:LYS:HE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:578:ASP:N	1:C:578:ASP:OD1	2.54	0.41
1:C:969:LYS:HD2	1:C:972:ALA:O	2.21	0.41
2:D:16:ARG:O	2:D:86:LEU:HD23	2.21	0.41
5:K:18:ARG:HH12	5:K:76:SER:HB3	1.84	0.41
5:K:55:ALA:HB3	5:K:58:PHE:CD2	2.56	0.41
2:H:116:TRP:HH2	3:L:48:THR:HG1	1.64	0.41
5:P:58:PHE:HD1	5:P:59:PRO:HD2	1.84	0.41
1:A:106:PHE:HD1	1:A:238:PHE:HB2	1.86	0.41
1:A:317:ASN:OD1	1:A:318:PHE:N	2.54	0.41
1:A:646:ARG:HD2	1:B:835:LYS:HA	2.03	0.41
1:A:1072:GLU:OE1	1:A:1072:GLU:N	2.49	0.41
1:B:208:THR:HG22	1:B:210:ILE:HG23	2.02	0.41
1:B:403:ARG:HB3	1:B:406:GLU:OE1	2.21	0.41
1:B:449:TYR:CD1	1:B:496:SER:HA	2.56	0.41
1:B:984:LEU:HD22	1:B:988:GLU:HG3	2.02	0.41
1:C:113:LYS:HD2	1:C:113:LYS:HA	1.80	0.41
1:C:466:ARG:HA	1:C:466:ARG:NE	2.36	0.41
1:C:646:ARG:HA	1:C:646:ARG:HD3	1.85	0.41
2:D:51:ILE:HG21	2:D:72:ARG:HD2	2.03	0.41
4:O:38:ARG:NH2	4:O:86:ASP:HB3	2.36	0.41
5:P:92:GLY:H	5:P:96:TRP:HE1	1.67	0.41
1:A:84:LEU:H	1:A:237:ARG:NH1	2.18	0.41
1:A:142:ASP:HA	1:A:244:LEU:HB3	2.02	0.41
1:B:425:LEU:HD11	1:B:429:PHE:CD2	2.56	0.41
1:B:489:TYR:OH	4:F:52:VAL:HG11	2.20	0.41
1:C:480:CYS:SG	1:C:481:ASN:N	2.94	0.41
1:C:778:THR:HA	1:C:781:VAL:HG12	2.03	0.41
2:D:109:TYR:HB3	3:E:96:ARG:H	1.86	0.41
2:H:47:TRP:NE1	2:H:50:VAL:HG13	2.34	0.41
4:F:94:ALA:HA	4:F:95:PRO:HD3	1.96	0.41
1:A:106:PHE:CD1	1:A:238:PHE:HB2	2.56	0.40
1:A:350:VAL:HG12	1:A:422:ASN:HD21	1.86	0.40
1:A:676:THR:HA	1:A:690:GLN:HA	2.03	0.40
1:B:971:GLY:O	1:B:995:ARG:NH1	2.43	0.40
1:B:986:PRO:N	1:B:987:PRO:HD2	2.36	0.40
1:B:1140:PRO:O	1:B:1143:PRO:HD2	2.21	0.40
1:C:61:ASN:OD1	1:C:61:ASN:N	2.55	0.40
1:C:472:ILE:HG22	1:C:490:PHE:CD1	2.56	0.40
4:J:20:VAL:HG21	4:J:90:TYR:HD2	1.86	0.40
1:A:28:TYR:HD2	1:A:61:ASN:ND2	2.19	0.40
1:A:210:ILE:HD12	1:A:210:ILE:HA	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:988:GLU:O	1:A:992:GLN:HG2	2.21	0.40
1:B:673:SER:OG	1:B:674:TYR:N	2.54	0.40
3:L:39:GLN:HE21	3:L:47:ARG:HB2	1.86	0.40
3:L:39:GLN:N	3:L:47:ARG:O	2.49	0.40
2:M:51:ILE:HD13	2:M:58:LYS:HD2	2.03	0.40
1:A:64:TRP:HD1	1:A:65:PHE:N	2.19	0.40
1:A:308:VAL:HG12	1:A:602:THR:HB	2.02	0.40
1:A:401:VAL:HG11	1:A:451:TYR:CD2	2.56	0.40
1:A:636:TYR:O	1:A:651:ILE:HG21	2.21	0.40
1:B:474:GLN:HA	1:B:488:CYS:HA	2.02	0.40
1:B:835:LYS:HG3	1:B:837:TYR:HE1	1.87	0.40
1:B:941:THR:HG22	1:B:943:SER:H	1.86	0.40
1:C:74:ASN:ND2	1:C:78:ARG:HB2	2.36	0.40
1:C:129:LYS:HG3	1:C:131:CYS:H	1.86	0.40
1:C:204:TYR:HD1	1:C:225:PRO:HA	1.84	0.40
1:C:356:LYS:HZ1	1:C:398:ASP:HA	1.86	0.40
1:C:634:ARG:HA	1:C:637:SER:HB3	2.02	0.40
1:C:787:GLN:OE1	1:C:787:GLN:N	2.54	0.40
2:H:83:MET:HB3	2:H:86:LEU:HD21	2.03	0.40
3:L:33:TYR:HB3	3:L:92:LEU:HD12	2.03	0.40
5:G:17:GLU:O	5:G:18:ARG:HD3	2.21	0.40
1:A:452:LEU:HD11	2:D:109:TYR:OH	2.22	0.40
1:A:615:VAL:HG22	1:A:616:ASN:O	2.22	0.40
1:A:669:GLY:HA2	1:A:697:MET:HE2	2.02	0.40
1:A:788:ILE:HG21	1:A:872:GLN:HE21	1.86	0.40
1:B:743:CYS:HB2	1:B:977:LEU:HD22	2.04	0.40
1:B:900:MET:HG2	1:B:917:TYR:OH	2.22	0.40
1:C:308:VAL:H	1:C:602:THR:HG22	1.85	0.40
1:C:425:LEU:HD11	1:C:429:PHE:CZ	2.57	0.40
1:C:676:THR:HG22	1:C:690:GLN:HG3	2.03	0.40
5:K:11:LEU:O	5:K:104:VAL:HA	2.22	0.40
5:K:85:VAL:HA	5:K:102:THR:O	2.22	0.40
3:L:46:PRO:O	3:L:47:ARG:HD2	2.21	0.40
3:N:28:SER:OG	4:O:57:THR:N	2.54	0.40
3:N:91:VAL:HA	3:N:100:VAL:O	2.21	0.40
5:P:86:TYR:O	5:P:101:GLY:HA2	2.21	0.40
4:F:6:GLN:NE2	4:F:92:CYS:SG	2.94	0.40
1:A:213:VAL:HG13	1:A:214:ARG:N	2.37	0.40
1:A:676:THR:HA	1:A:690:GLN:HG3	2.03	0.40
1:B:197:ILE:O	1:B:200:TYR:HD1	2.05	0.40
1:B:331:ASN:H	1:B:580:GLN:NE2	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:822:LEU:HD21	1:B:1061:VAL:HG21	2.04	0.40
1:C:205:SER:H	1:C:226:LEU:HD23	1.87	0.40
1:C:1029:MET:HB2	1:C:1062:PHE:HZ	1.87	0.40
1:C:1092:GLU:OE1	1:C:1092:GLU:N	2.55	0.40
3:E:14:PRO:HG3	3:E:109:VAL:HG12	2.04	0.40
5:K:15:PRO:HA	5:K:78:LEU:HD23	2.03	0.40
4:F:39:GLN:NE2	4:F:40:ALA:O	2.54	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	1114/1272 (88%)	1011 (91%)	97 (9%)	6 (0%)	29	66
1	B	1110/1272 (87%)	1005 (90%)	100 (9%)	5 (0%)	29	66
1	C	1114/1272 (88%)	1010 (91%)	99 (9%)	5 (0%)	34	70
2	D	124/126 (98%)	117 (94%)	7 (6%)	0	100	100
2	H	124/126 (98%)	113 (91%)	11 (9%)	0	100	100
2	M	124/126 (98%)	116 (94%)	8 (6%)	0	100	100
3	E	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
3	L	108/110 (98%)	99 (92%)	9 (8%)	0	100	100
3	N	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
4	F	120/123 (98%)	109 (91%)	11 (9%)	0	100	100
4	J	120/123 (98%)	108 (90%)	12 (10%)	0	100	100
4	O	120/123 (98%)	105 (88%)	15 (12%)	0	100	100
5	G	106/108 (98%)	97 (92%)	9 (8%)	0	100	100
5	K	106/108 (98%)	95 (90%)	11 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	P	106/108 (98%)	98 (92%)	8 (8%)	0	100	100
All	All	4712/5217 (90%)	4289 (91%)	407 (9%)	16 (0%)	44	74

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	96	GLU
1	A	213	VAL
1	A	492	LEU
1	B	16	VAL
1	B	210	ILE
1	B	492	LEU
1	C	16	VAL
1	C	210	ILE
1	C	492	LEU
1	C	527	PRO
1	A	831	ALA
1	B	813	SER
1	A	352	ALA
1	B	834	ILE
1	C	834	ILE

### 5.3.2 Protein sidechains [i](#)

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	974/1100 (88%)	969 (100%)	5 (0%)	88	93
1	B	972/1100 (88%)	967 (100%)	5 (0%)	88	93
1	C	974/1100 (88%)	969 (100%)	5 (0%)	88	93
2	D	104/104 (100%)	103 (99%)	1 (1%)	76	85
2	H	104/104 (100%)	104 (100%)	0	100	100
2	M	104/104 (100%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	89/89 (100%)	89 (100%)	0	100	100
3	L	89/89 (100%)	89 (100%)	0	100	100
3	N	89/89 (100%)	89 (100%)	0	100	100
4	F	101/103 (98%)	99 (98%)	2 (2%)	55	74
4	J	101/103 (98%)	100 (99%)	1 (1%)	76	85
4	O	101/103 (98%)	100 (99%)	1 (1%)	76	85
5	G	90/90 (100%)	90 (100%)	0	100	100
5	K	90/90 (100%)	90 (100%)	0	100	100
5	P	90/90 (100%)	89 (99%)	1 (1%)	73	84
All	All	4072/4458 (91%)	4051 (100%)	21 (0%)	89	93

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	ARG
1	A	237	ARG
1	A	378	LYS
1	A	558	LYS
1	A	658	ASN
1	B	346	ARG
1	B	378	LYS
1	B	835	LYS
1	B	955	ASN
1	B	983	ARG
1	C	357	ARG
1	C	378	LYS
1	C	498	ARG
1	C	836	GLN
1	C	1010	GLN
2	D	3	GLN
4	J	23	LYS
4	O	23	LYS
5	P	77	ARG
4	F	12	LYS
4	F	83	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	409	GLN
1	A	439	ASN
1	A	506	GLN
1	A	658	ASN
1	A	919	ASN
1	A	949	GLN
1	A	955	ASN
1	B	99	ASN
1	B	506	GLN
1	B	580	GLN
1	B	613	GLN
1	B	1010	GLN
1	B	1011	GLN
1	B	1113	GLN
1	C	115	GLN
1	C	955	ASN
2	D	35	HIS
3	E	39	GLN
3	E	40	GLN
4	J	6	GLN
4	J	64	GLN
3	L	6	GLN
3	L	44	GLN
2	M	3	GLN
2	M	82	GLN
2	M	84	ASN
4	O	6	GLN
4	F	56	ASN
4	F	64	GLN
5	G	90	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

26 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	$\# Z  > 2$
6	NAG	I	1	6,1	14,14,15	0.19	0	17,19,21	0.43	0
6	NAG	I	2	6	14,14,15	0.20	0	17,19,21	0.41	0
6	NAG	Q	1	6,1	14,14,15	0.22	0	17,19,21	0.41	0
6	NAG	Q	2	6	14,14,15	0.22	0	17,19,21	0.40	0
6	NAG	R	1	6,1	14,14,15	0.22	0	17,19,21	0.43	0
6	NAG	R	2	6	14,14,15	0.22	0	17,19,21	0.43	0
6	NAG	S	1	6,1	14,14,15	0.23	0	17,19,21	0.39	0
6	NAG	S	2	6	14,14,15	0.26	0	17,19,21	0.45	0
6	NAG	T	1	6,1	14,14,15	0.31	0	17,19,21	0.46	0
6	NAG	T	2	6	14,14,15	0.19	0	17,19,21	0.37	0
6	NAG	U	1	6,1	14,14,15	0.33	0	17,19,21	0.42	0
6	NAG	U	2	6	14,14,15	0.22	0	17,19,21	0.39	0
6	NAG	V	1	6,1	14,14,15	0.23	0	17,19,21	0.44	0
6	NAG	V	2	6	14,14,15	0.23	0	17,19,21	0.46	0
6	NAG	W	1	6,1	14,14,15	0.20	0	17,19,21	0.43	0
6	NAG	W	2	6	14,14,15	0.25	0	17,19,21	0.43	0
6	NAG	X	1	6,1	14,14,15	0.40	0	17,19,21	0.75	1 (5%)
6	NAG	X	2	6	14,14,15	0.26	0	17,19,21	0.43	0
6	NAG	Y	1	6,1	14,14,15	0.16	0	17,19,21	0.45	0
6	NAG	Y	2	6	14,14,15	0.25	0	17,19,21	0.42	0
6	NAG	Z	1	6,1	14,14,15	0.40	0	17,19,21	0.57	0
6	NAG	Z	2	6	14,14,15	0.26	0	17,19,21	0.39	0
6	NAG	a	1	6,1	14,14,15	0.31	0	17,19,21	0.58	0
6	NAG	a	2	6	14,14,15	0.23	0	17,19,21	0.43	0
6	NAG	b	1	6,1	14,14,15	0.19	0	17,19,21	0.39	0
6	NAG	b	2	6	14,14,15	0.20	0	17,19,21	0.43	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	I	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	Q	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	2/6/23/26	0/1/1/1
6	NAG	R	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	R	2	6	-	2/6/23/26	0/1/1/1
6	NAG	S	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	S	2	6	-	2/6/23/26	0/1/1/1
6	NAG	T	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	T	2	6	-	2/6/23/26	0/1/1/1
6	NAG	U	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	U	2	6	-	0/6/23/26	0/1/1/1
6	NAG	V	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	V	2	6	-	2/6/23/26	0/1/1/1
6	NAG	W	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	W	2	6	-	2/6/23/26	0/1/1/1
6	NAG	X	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	X	2	6	-	2/6/23/26	0/1/1/1
6	NAG	Y	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	Y	2	6	-	2/6/23/26	0/1/1/1
6	NAG	Z	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	2/6/23/26	0/1/1/1
6	NAG	a	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	a	2	6	-	2/6/23/26	0/1/1/1
6	NAG	b	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	b	2	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	1	NAG	C1-O5-C5	2.51	115.59	112.19

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	T	1	NAG	O5-C5-C6-O6
6	V	2	NAG	C4-C5-C6-O6
6	Z	2	NAG	C4-C5-C6-O6

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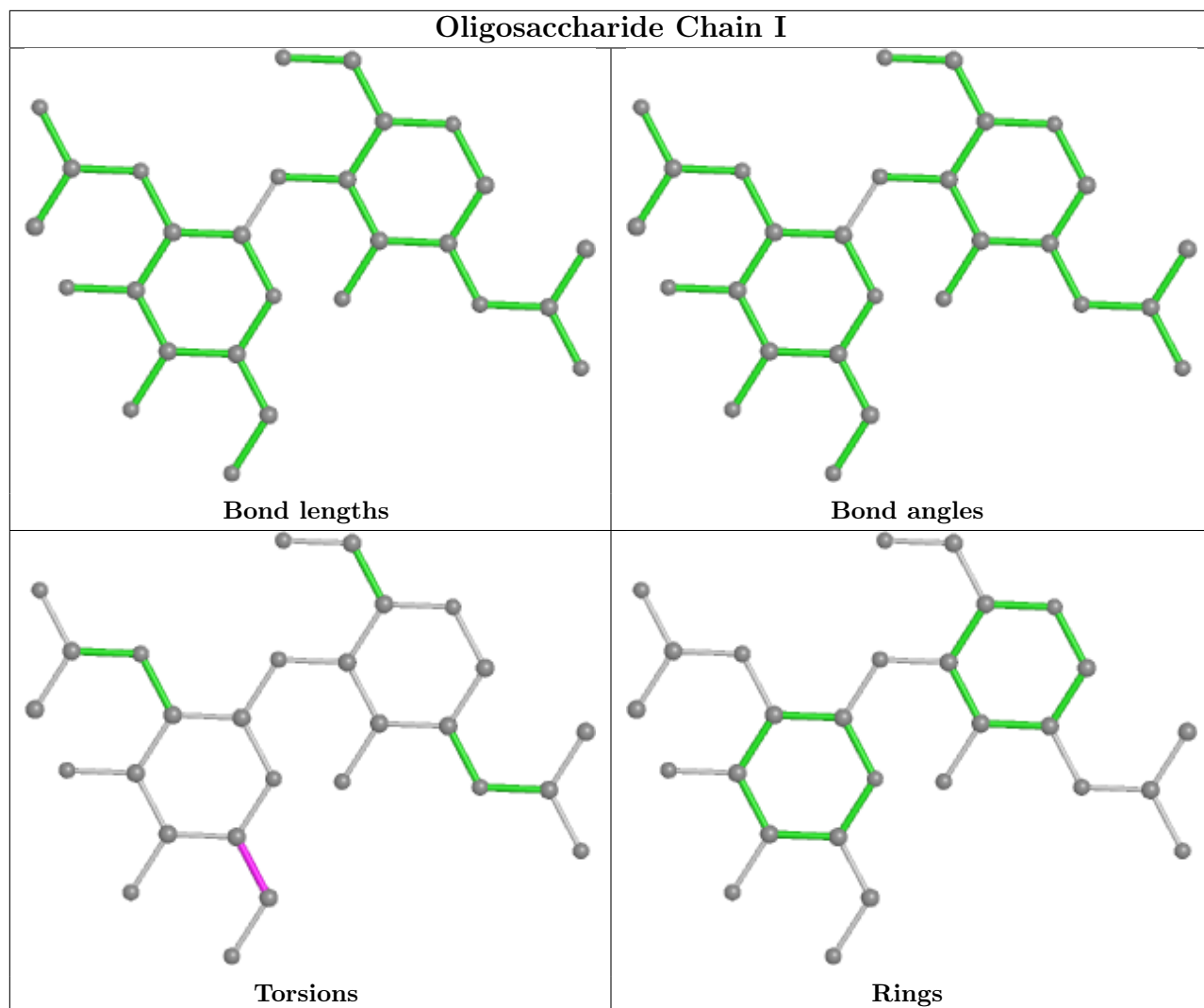
Mol	Chain	Res	Type	Atoms
6	R	2	NAG	C4-C5-C6-O6
6	T	2	NAG	C4-C5-C6-O6
6	Y	2	NAG	C4-C5-C6-O6
6	S	2	NAG	O5-C5-C6-O6
6	Q	2	NAG	O5-C5-C6-O6
6	Z	2	NAG	O5-C5-C6-O6
6	V	2	NAG	O5-C5-C6-O6
6	W	2	NAG	O5-C5-C6-O6
6	R	2	NAG	O5-C5-C6-O6
6	a	1	NAG	O5-C5-C6-O6
6	T	1	NAG	C4-C5-C6-O6
6	Y	2	NAG	O5-C5-C6-O6
6	a	1	NAG	C4-C5-C6-O6
6	S	2	NAG	C4-C5-C6-O6
6	a	2	NAG	O5-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
6	X	2	NAG	O5-C5-C6-O6
6	T	2	NAG	O5-C5-C6-O6
6	a	2	NAG	C4-C5-C6-O6
6	W	1	NAG	O5-C5-C6-O6
6	S	1	NAG	O5-C5-C6-O6
6	b	1	NAG	O5-C5-C6-O6
6	Q	2	NAG	C4-C5-C6-O6
6	W	2	NAG	C4-C5-C6-O6
6	V	1	NAG	C4-C5-C6-O6
6	R	1	NAG	C4-C5-C6-O6
6	R	1	NAG	O5-C5-C6-O6
6	V	1	NAG	O5-C5-C6-O6
6	I	2	NAG	C4-C5-C6-O6
6	X	2	NAG	C4-C5-C6-O6

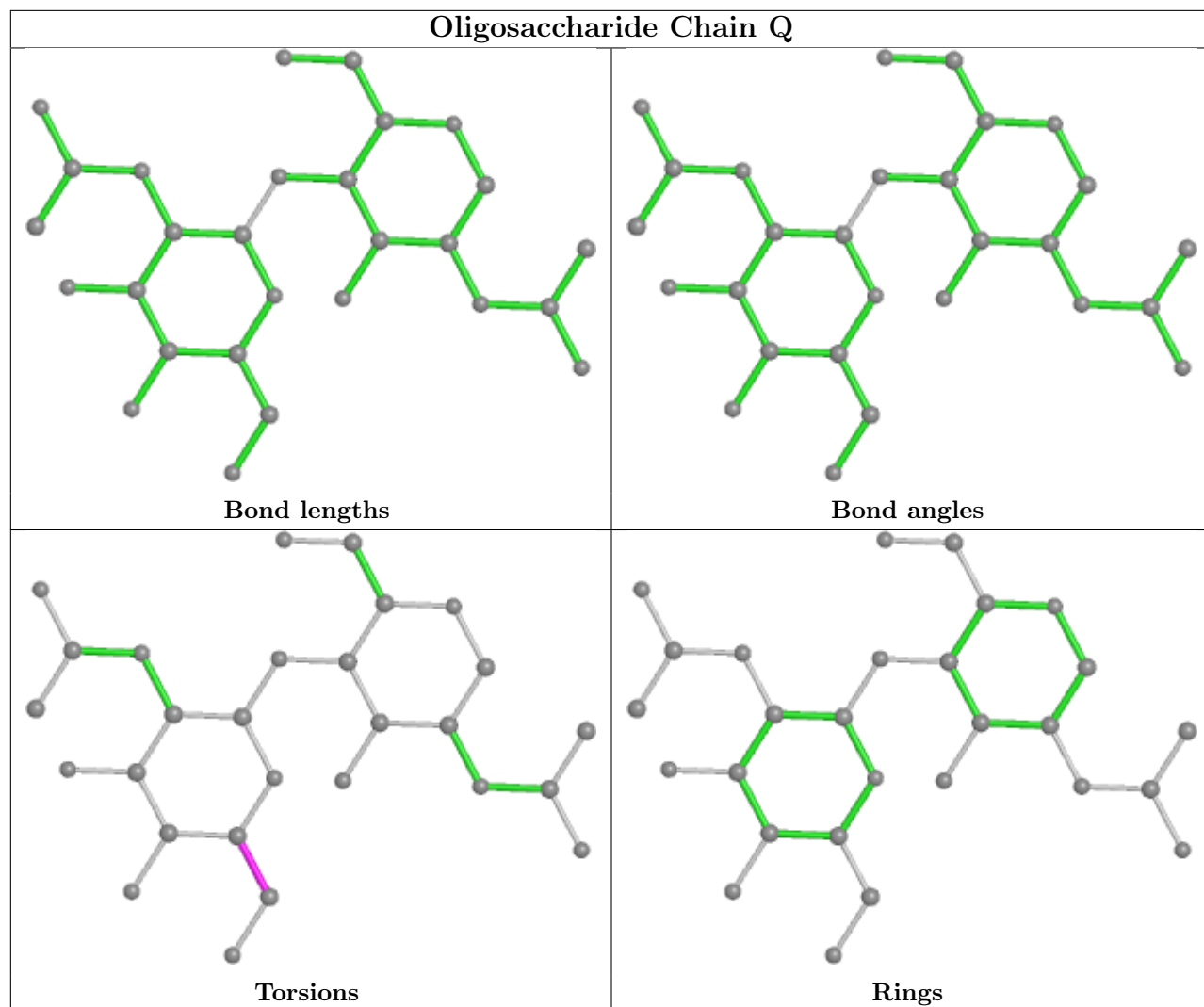
There are no ring outliers.

2 monomers are involved in 2 short contacts:

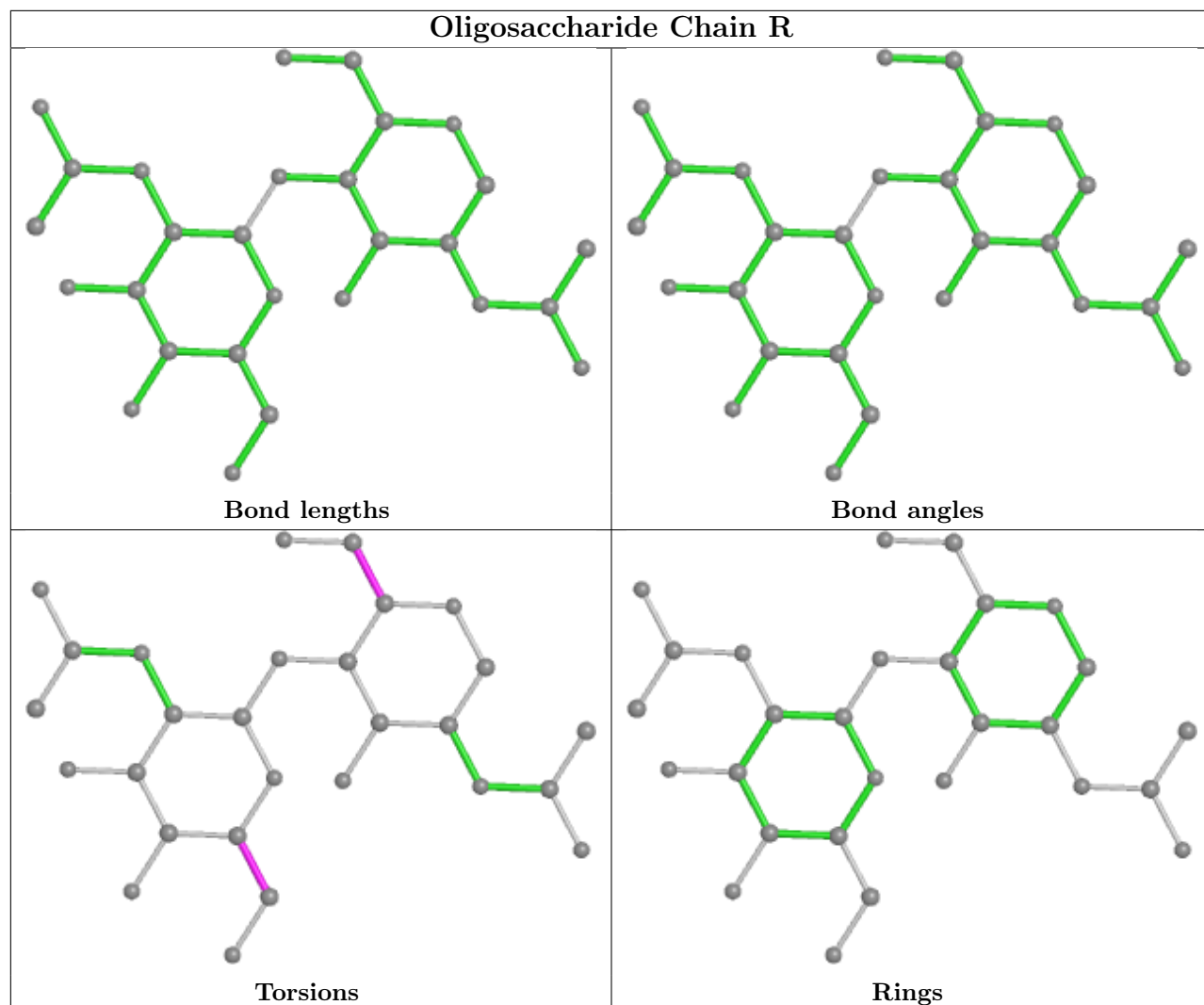
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	U	1	NAG	1	0
6	Z	1	NAG	1	0

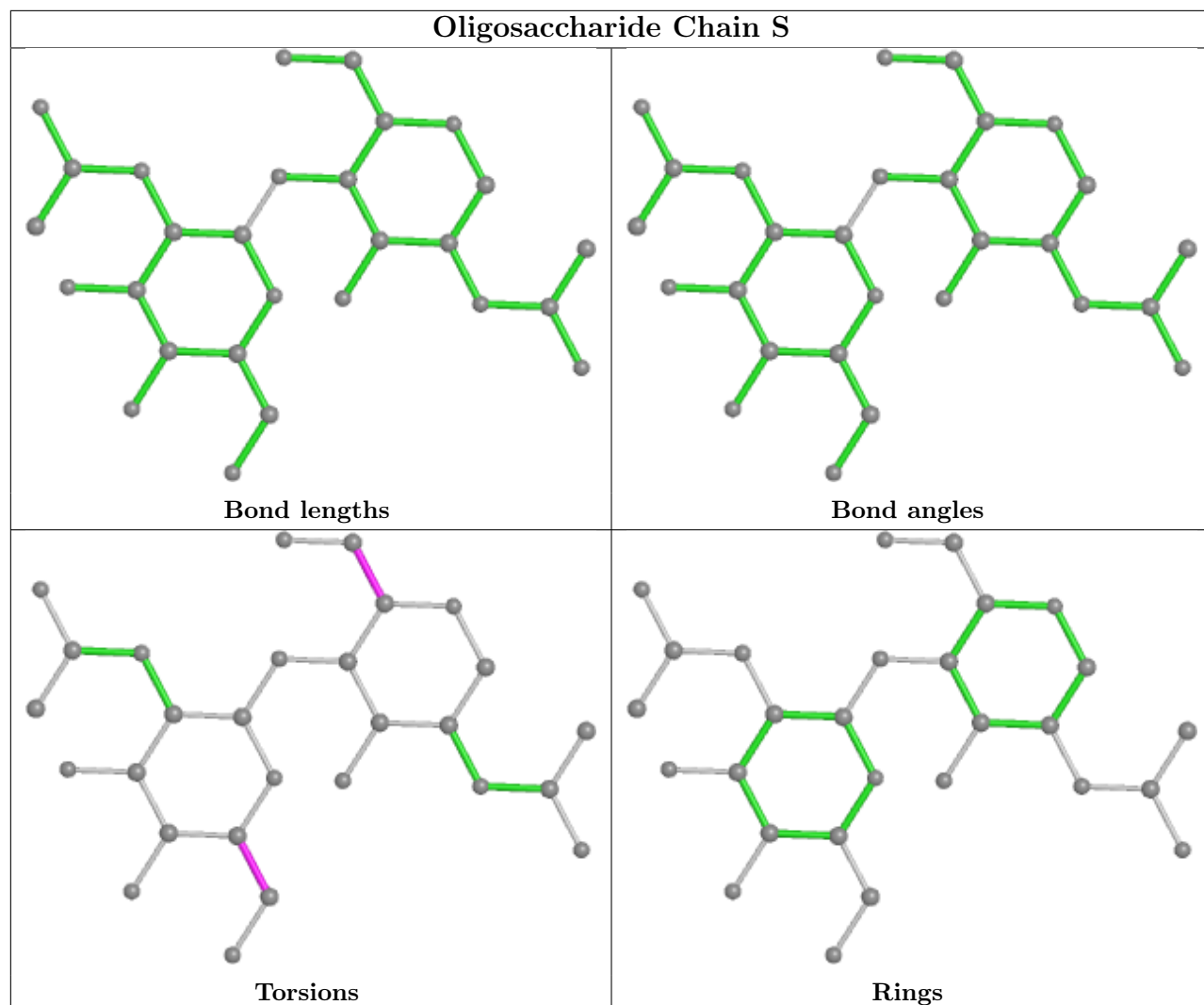
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

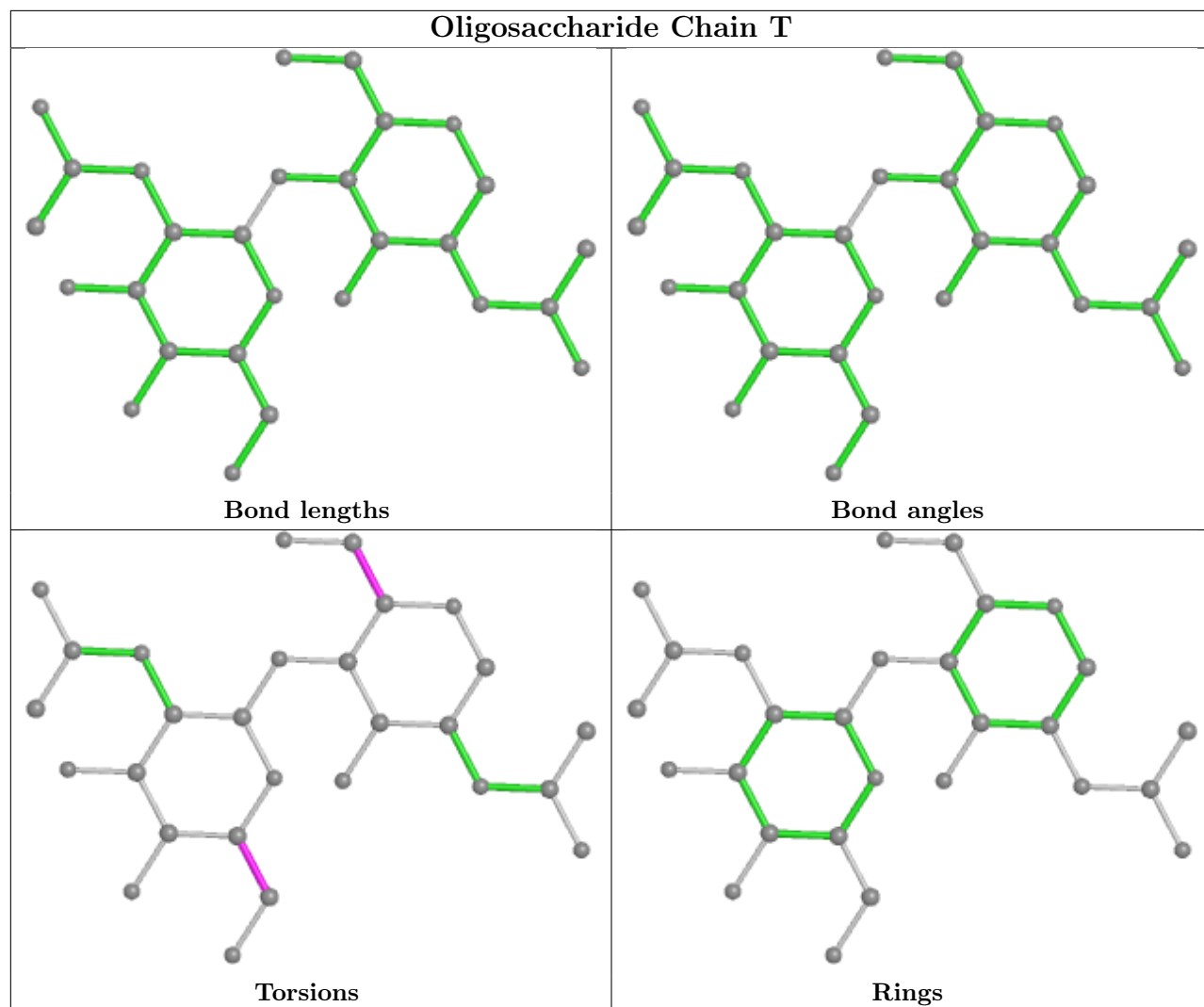


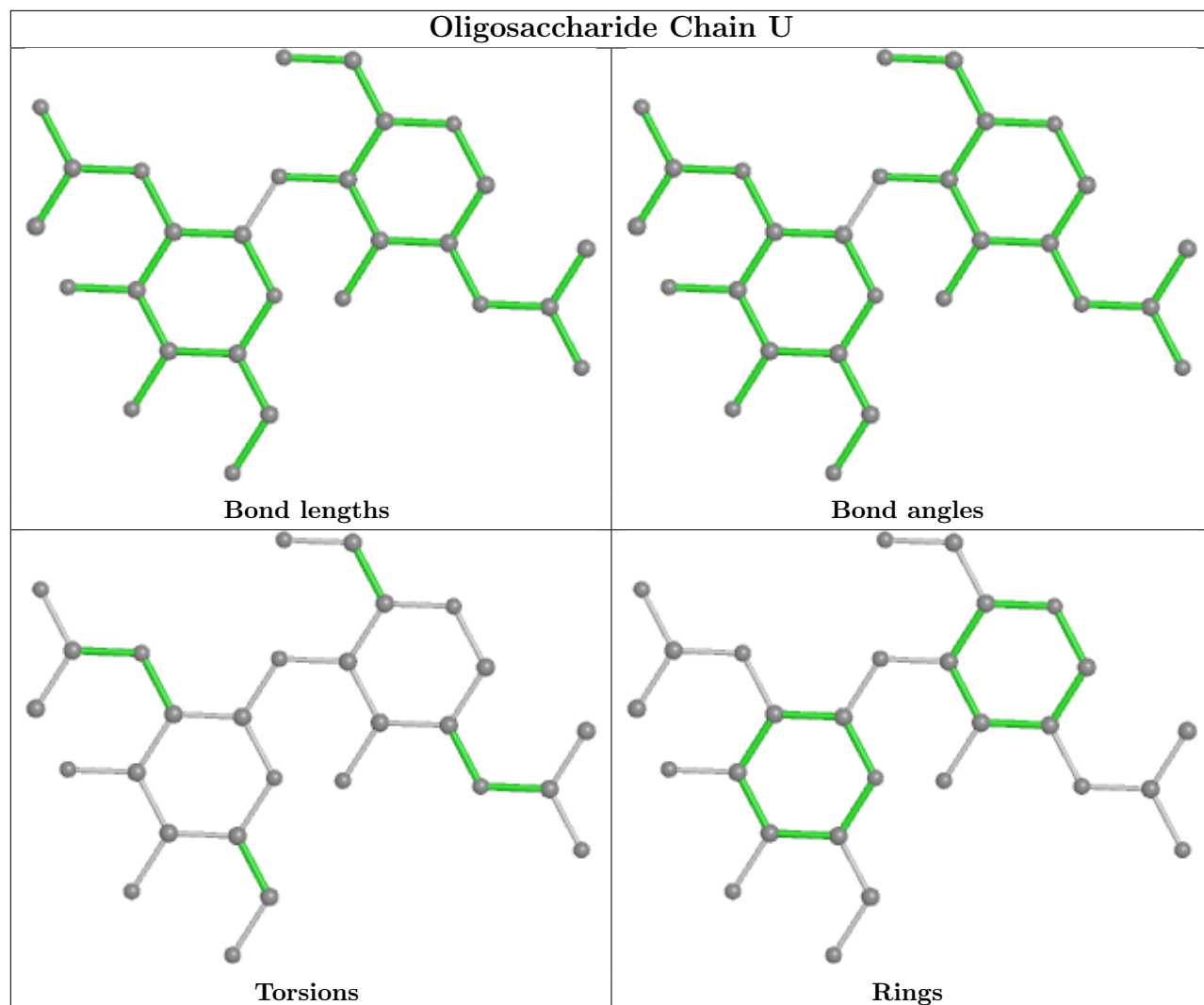


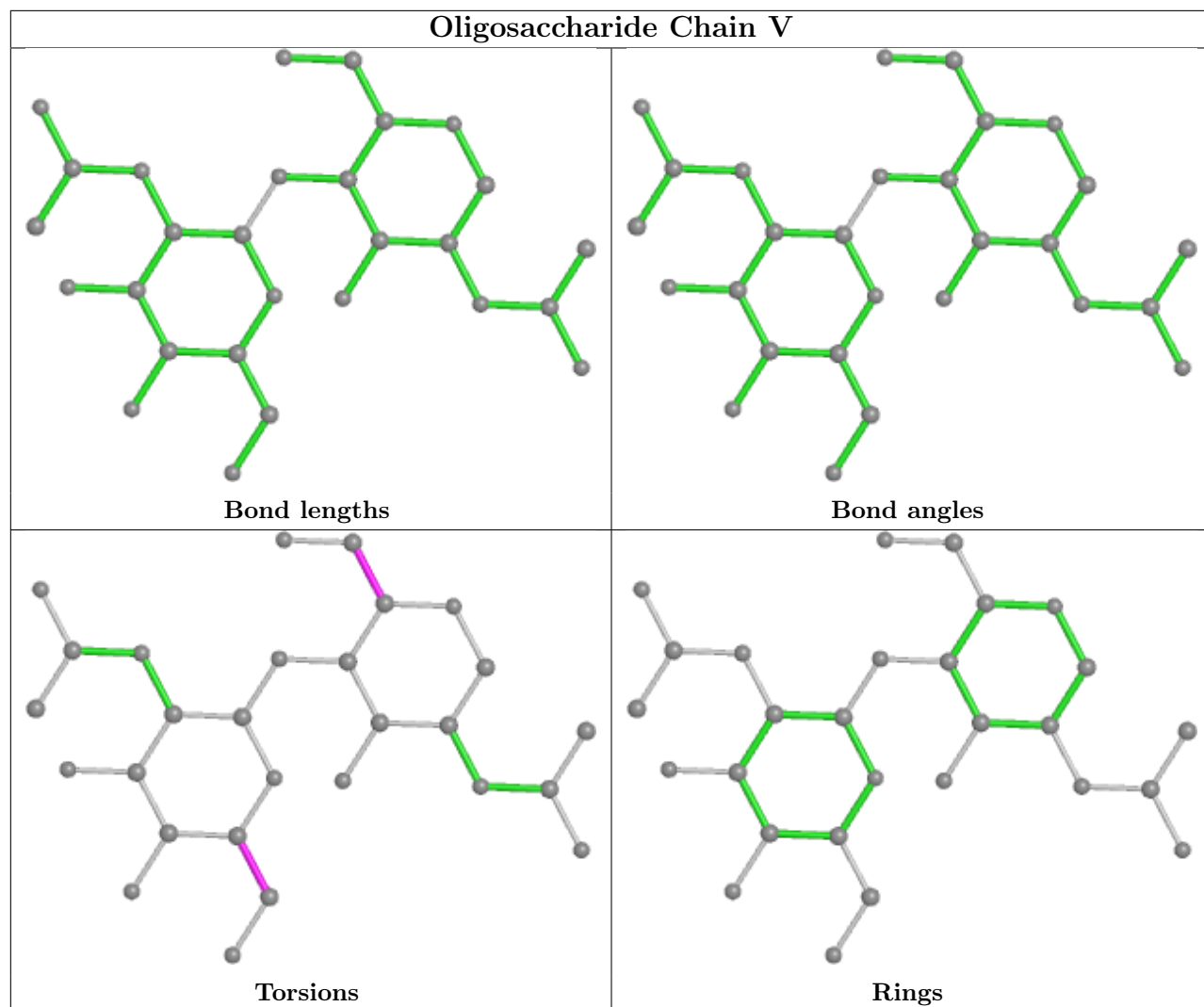


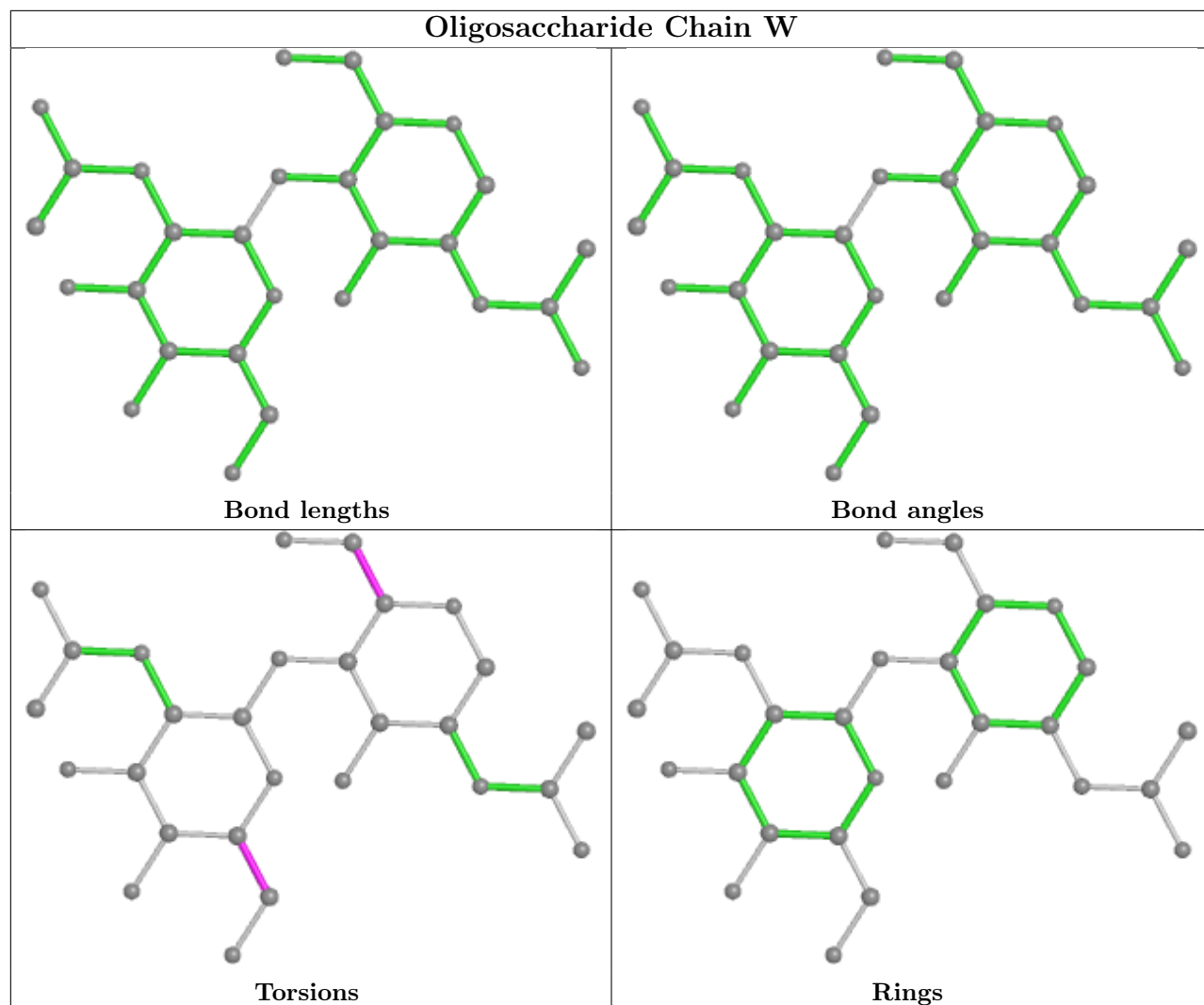


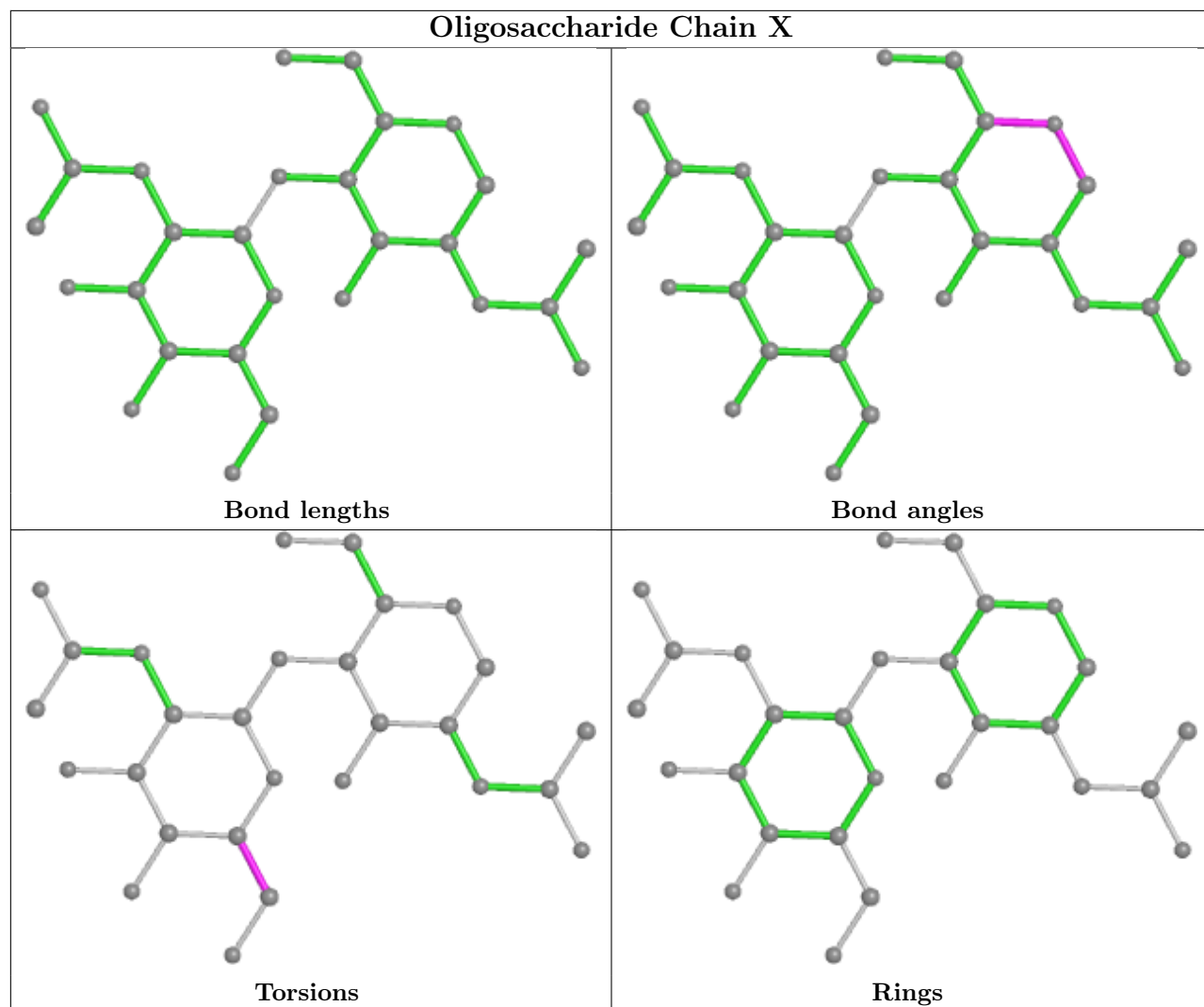


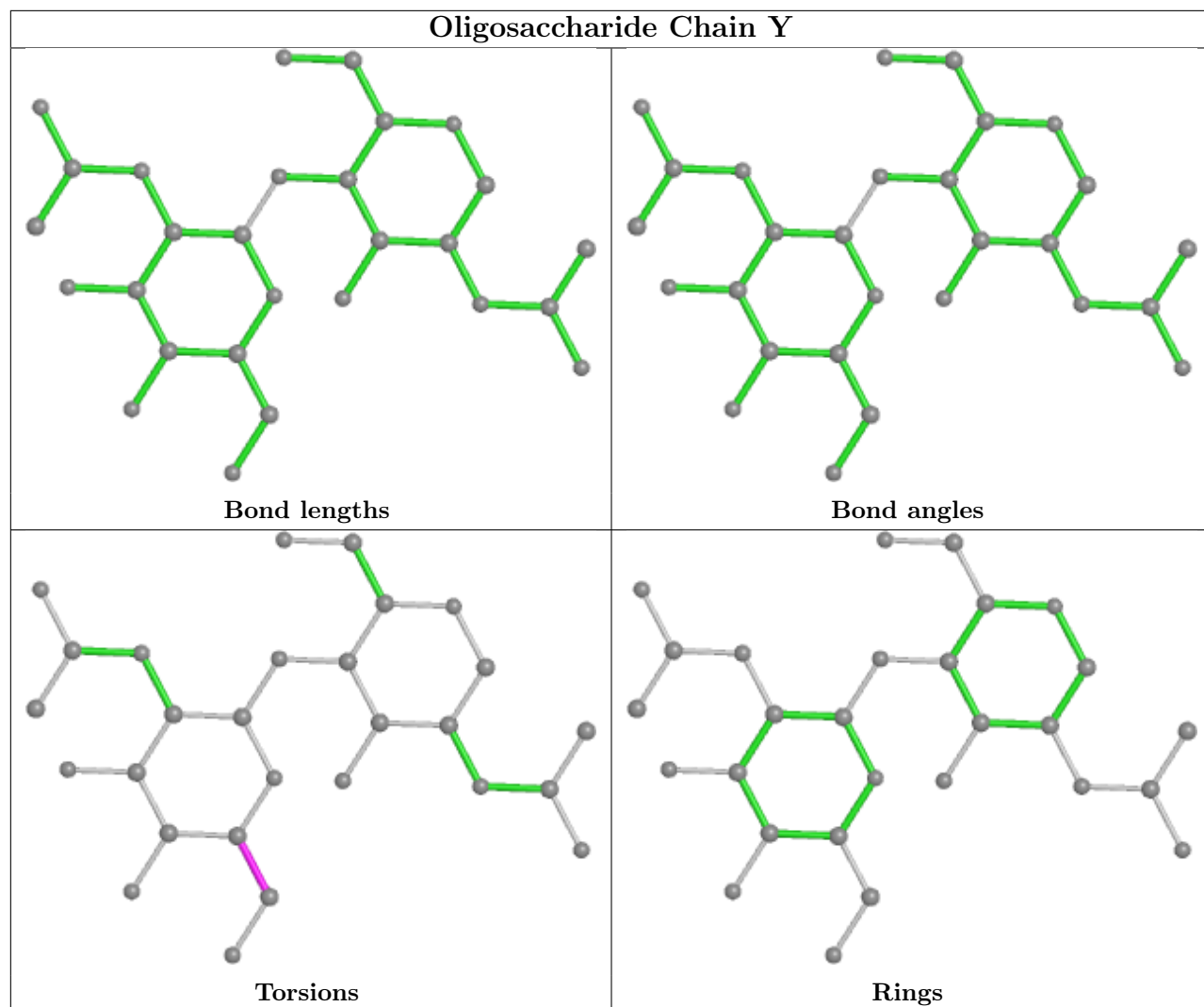




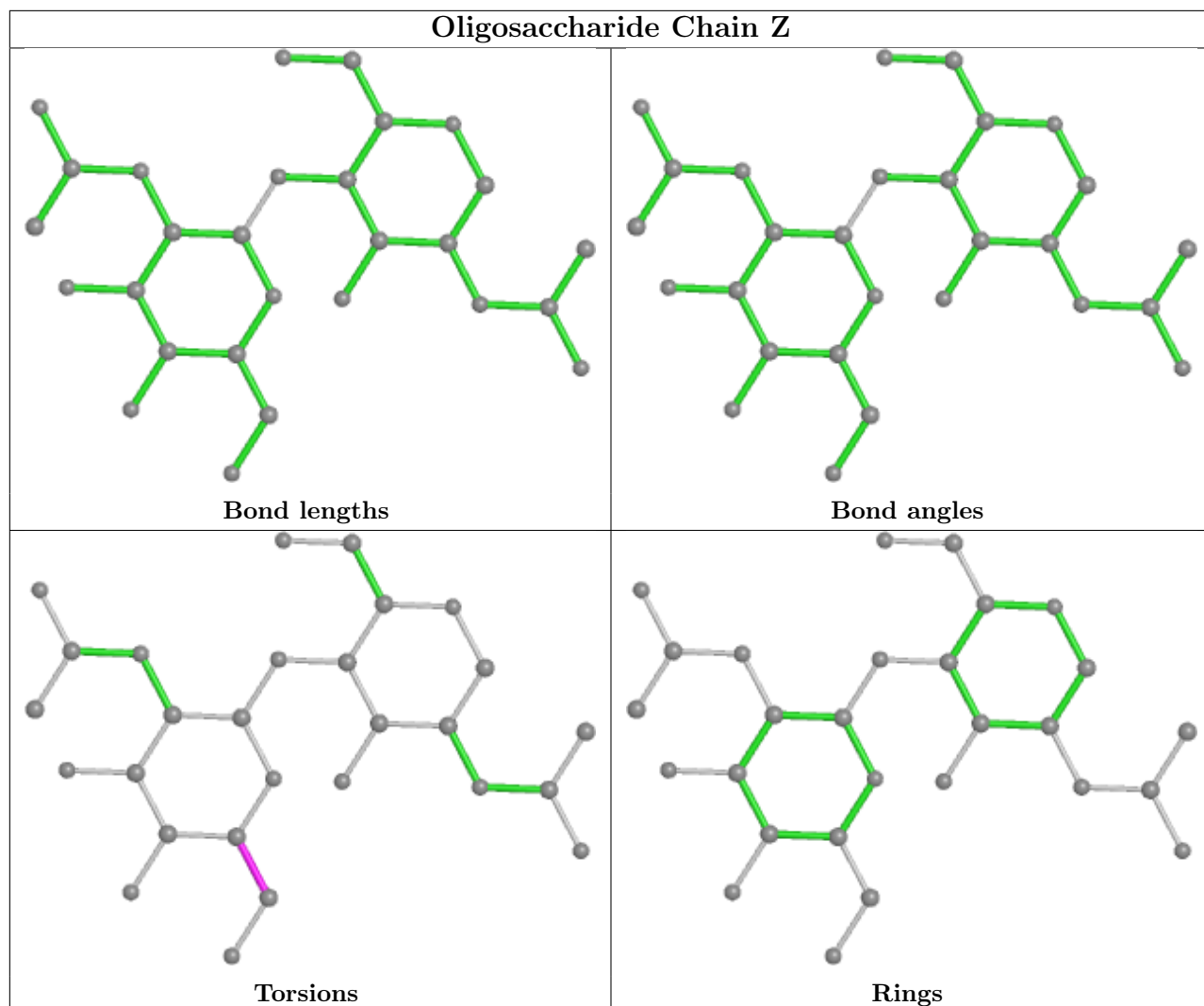


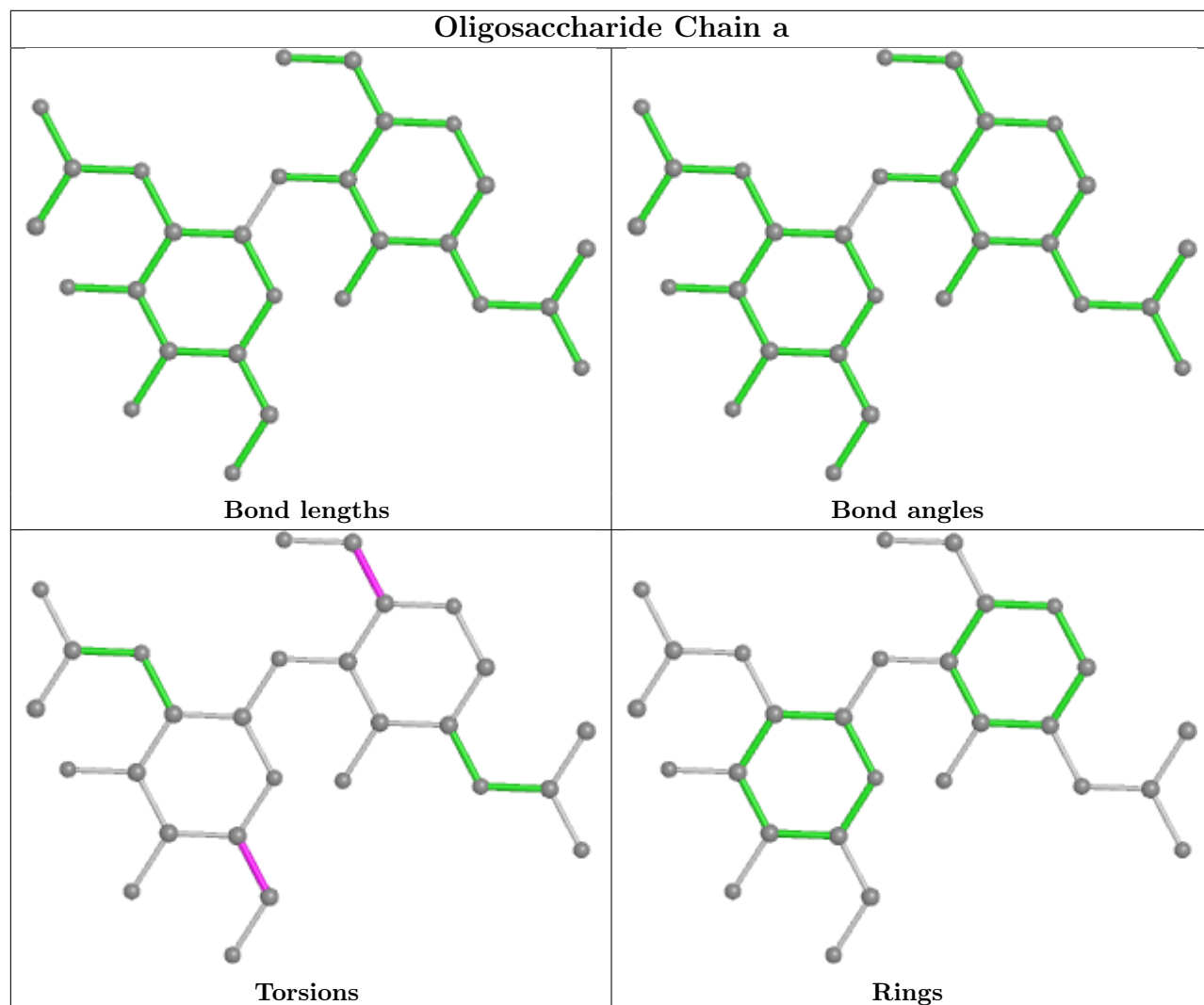


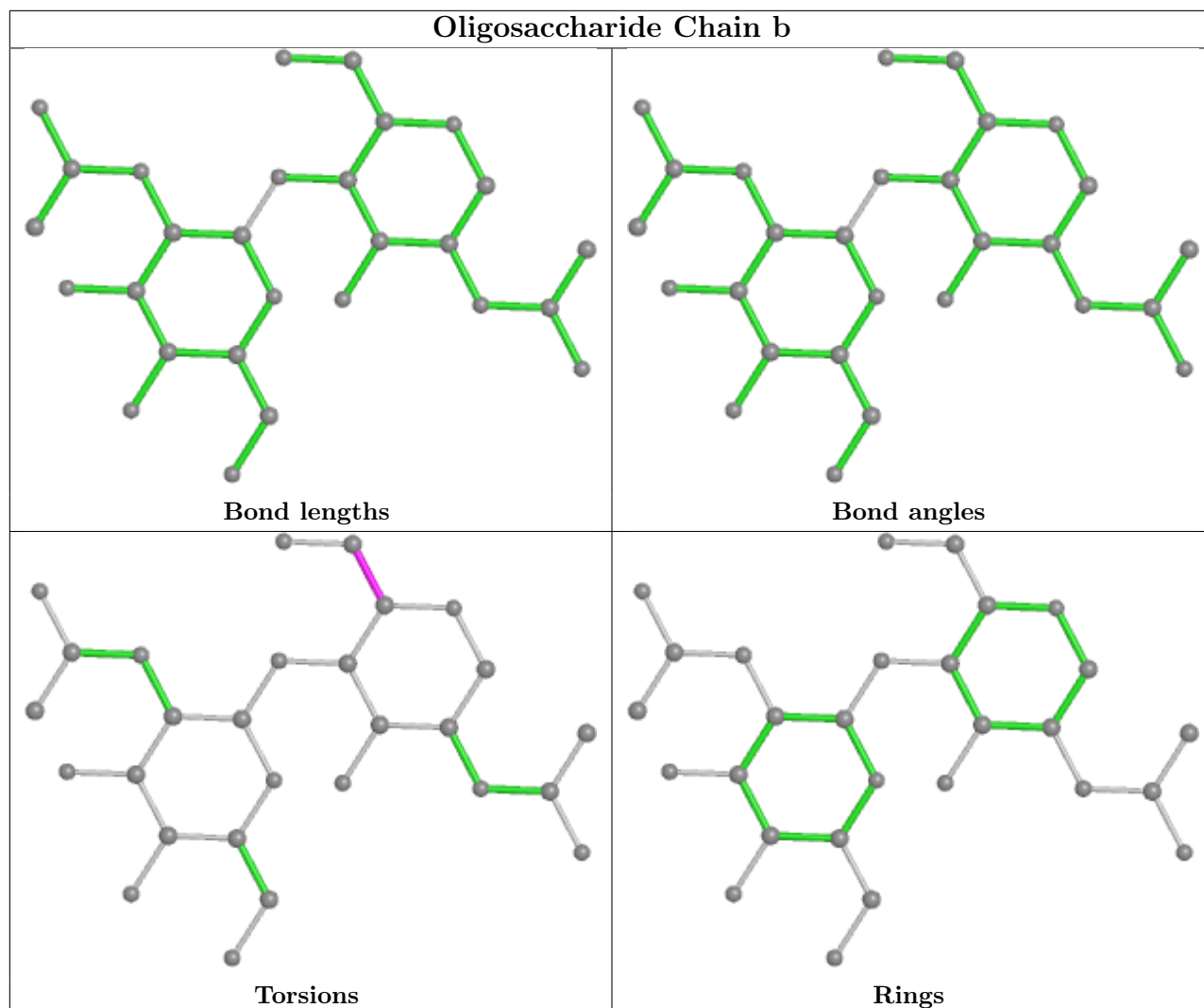












## 5.6 Ligand geometry [i](#)

15 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	$\# Z  > 2$
7	NAG	A	1306	1	14,14,15	0.21	0	17,19,21	0.42	0
7	NAG	C	1302	1	14,14,15	0.26	0	17,19,21	0.40	0
7	NAG	A	1302	1	14,14,15	0.20	0	17,19,21	0.48	0
7	NAG	B	1305	1	14,14,15	0.19	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	C	1301	1	14,14,15	0.19	0	17,19,21	0.51	0
7	NAG	A	1301	1	14,14,15	0.20	0	17,19,21	0.47	0
7	NAG	B	1302	1	14,14,15	0.23	0	17,19,21	0.52	0
7	NAG	C	1304	1	14,14,15	0.41	0	17,19,21	0.49	0
7	NAG	B	1301	1	14,14,15	0.16	0	17,19,21	0.45	0
7	NAG	C	1303	1	14,14,15	0.27	0	17,19,21	0.46	0
7	NAG	A	1305	1	14,14,15	0.23	0	17,19,21	0.42	0
7	NAG	A	1304	1	14,14,15	0.20	0	17,19,21	0.57	0
7	NAG	B	1304	1	14,14,15	0.17	0	17,19,21	0.42	0
7	NAG	B	1303	1	14,14,15	0.23	0	17,19,21	0.53	0
7	NAG	A	1303	1	14,14,15	0.23	0	17,19,21	0.41	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
7	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1305	1	-	1/6/23/26	0/1/1/1
7	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1303	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1301	NAG	C4-C5-C6-O6
7	B	1303	NAG	C4-C5-C6-O6
7	A	1301	NAG	O5-C5-C6-O6
7	A	1303	NAG	O5-C5-C6-O6
7	C	1304	NAG	C4-C5-C6-O6
7	B	1303	NAG	O5-C5-C6-O6
7	B	1304	NAG	O5-C5-C6-O6
7	C	1301	NAG	C4-C5-C6-O6
7	B	1304	NAG	C4-C5-C6-O6
7	B	1305	NAG	O5-C5-C6-O6
7	A	1303	NAG	C4-C5-C6-O6
7	C	1303	NAG	O5-C5-C6-O6
7	C	1304	NAG	O5-C5-C6-O6
7	A	1302	NAG	O5-C5-C6-O6
7	A	1302	NAG	C4-C5-C6-O6
7	C	1302	NAG	C4-C5-C6-O6
7	A	1306	NAG	O5-C5-C6-O6
7	C	1301	NAG	O5-C5-C6-O6
7	A	1306	NAG	C4-C5-C6-O6
7	A	1305	NAG	O5-C5-C6-O6
7	C	1303	NAG	C4-C5-C6-O6
7	C	1302	NAG	O5-C5-C6-O6
7	B	1302	NAG	C4-C5-C6-O6
7	B	1302	NAG	O5-C5-C6-O6
7	B	1305	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1301	NAG	1	0
7	A	1304	NAG	1	0

## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

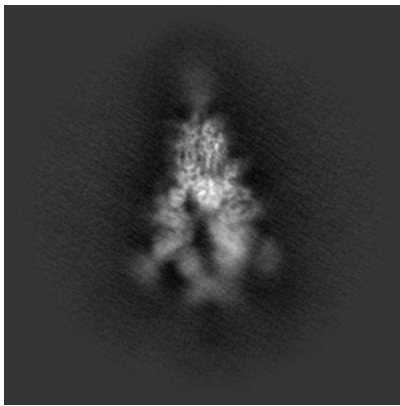
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25808. These allow visual inspection of the internal detail of the map and identification of artifacts.

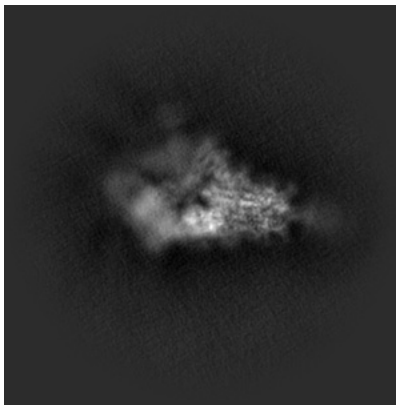
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

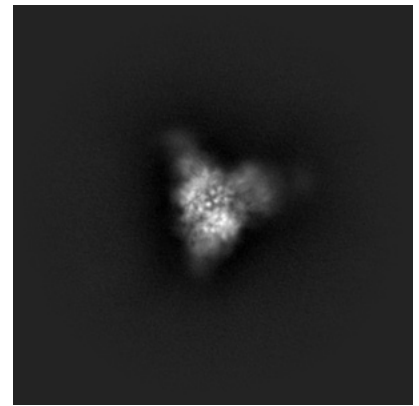
#### 6.1.1 Primary map



X

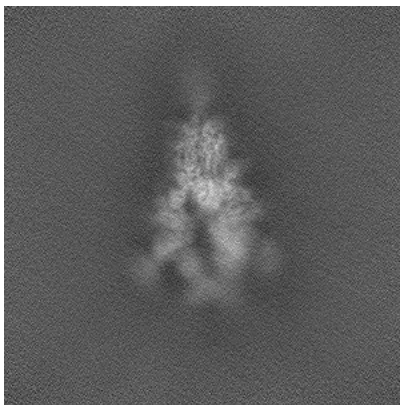


Y

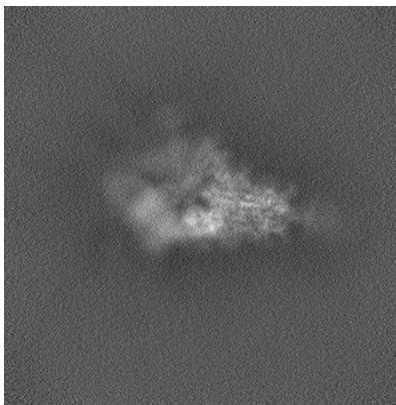


Z

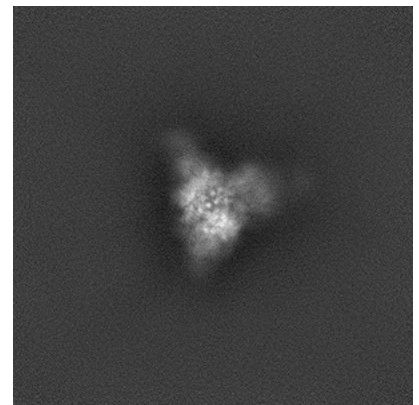
#### 6.1.2 Raw map



X



Y

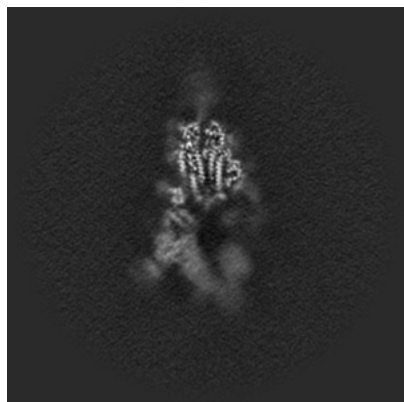


Z

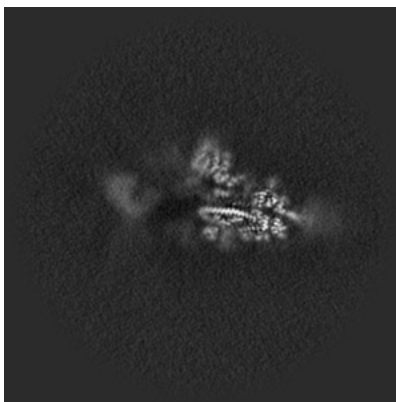
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

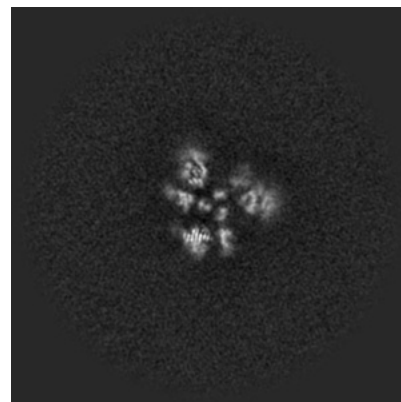
### 6.2.1 Primary map



X Index: 300

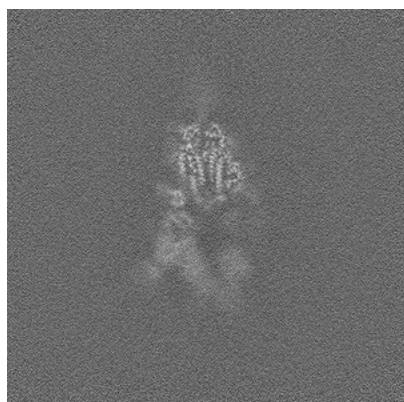


Y Index: 300



Z Index: 300

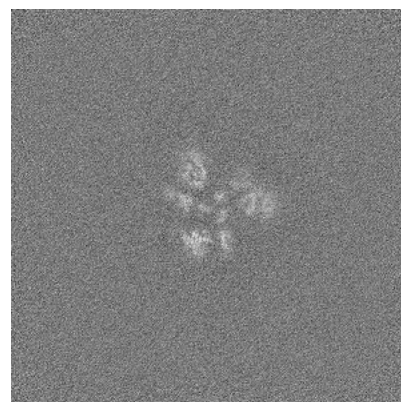
### 6.2.2 Raw map



X Index: 300



Y Index: 300



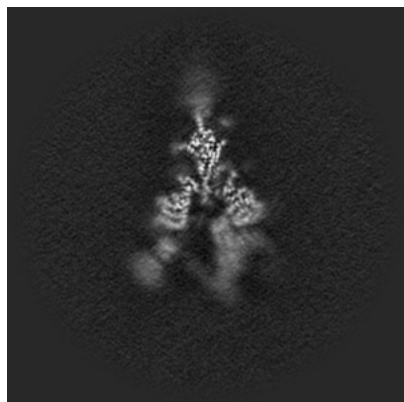
Z Index: 300

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

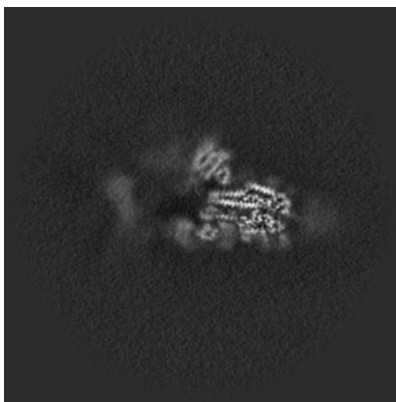


## 6.3 Largest variance slices [i](#)

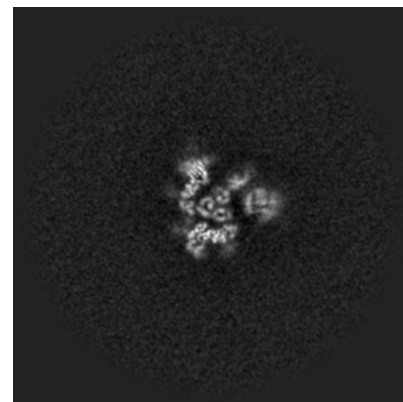
### 6.3.1 Primary map



X Index: 278

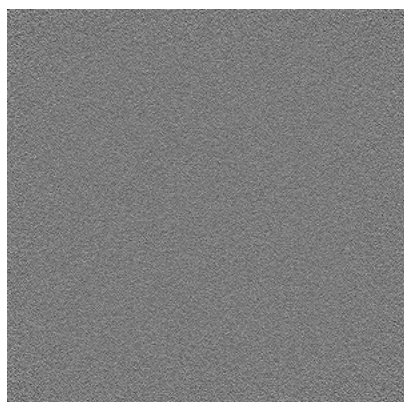


Y Index: 307

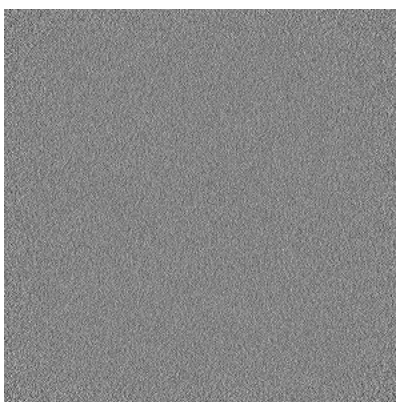


Z Index: 310

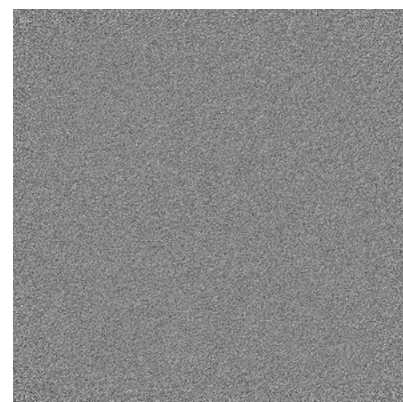
### 6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 0

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

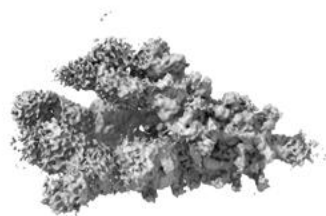


## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



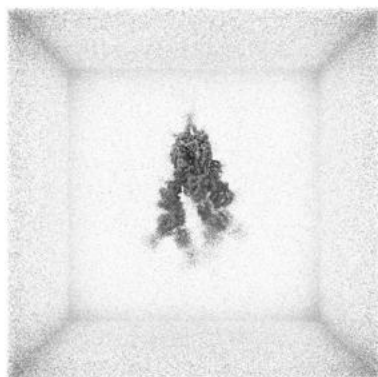
Y



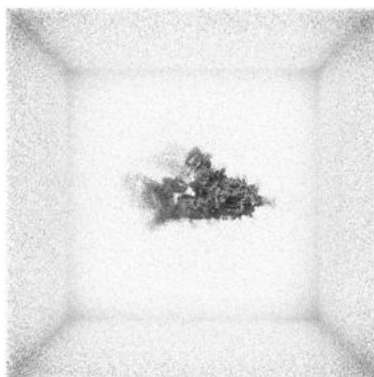
Z

The images above show the 3D surface view of the map at the recommended contour level 0.116. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

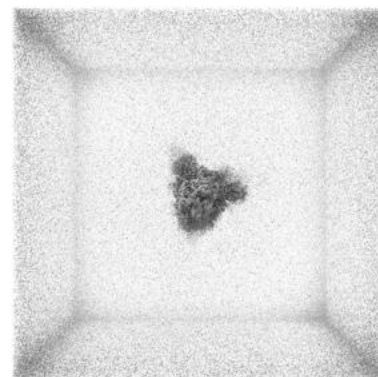
### 6.4.2 Raw map



X



Y



Z

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.

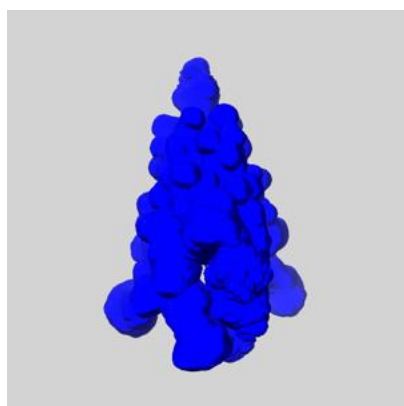
## 6.5 Mask visualisation [i](#)

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

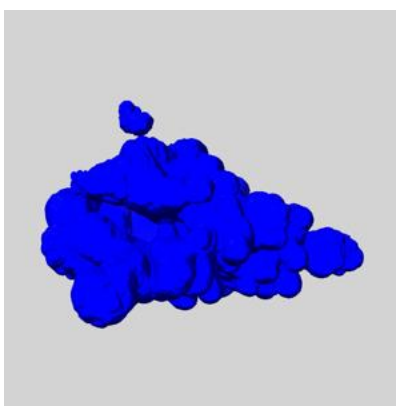
A mask typically either:

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

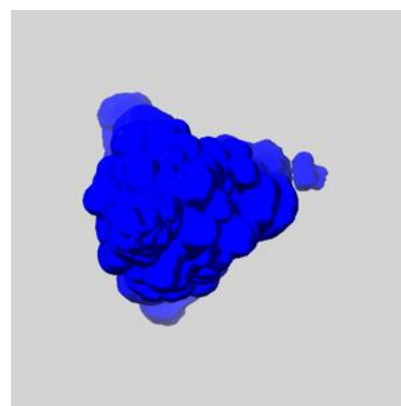
### 6.5.1 emd\_25808\_msk\_1.map [i](#)



X



Y

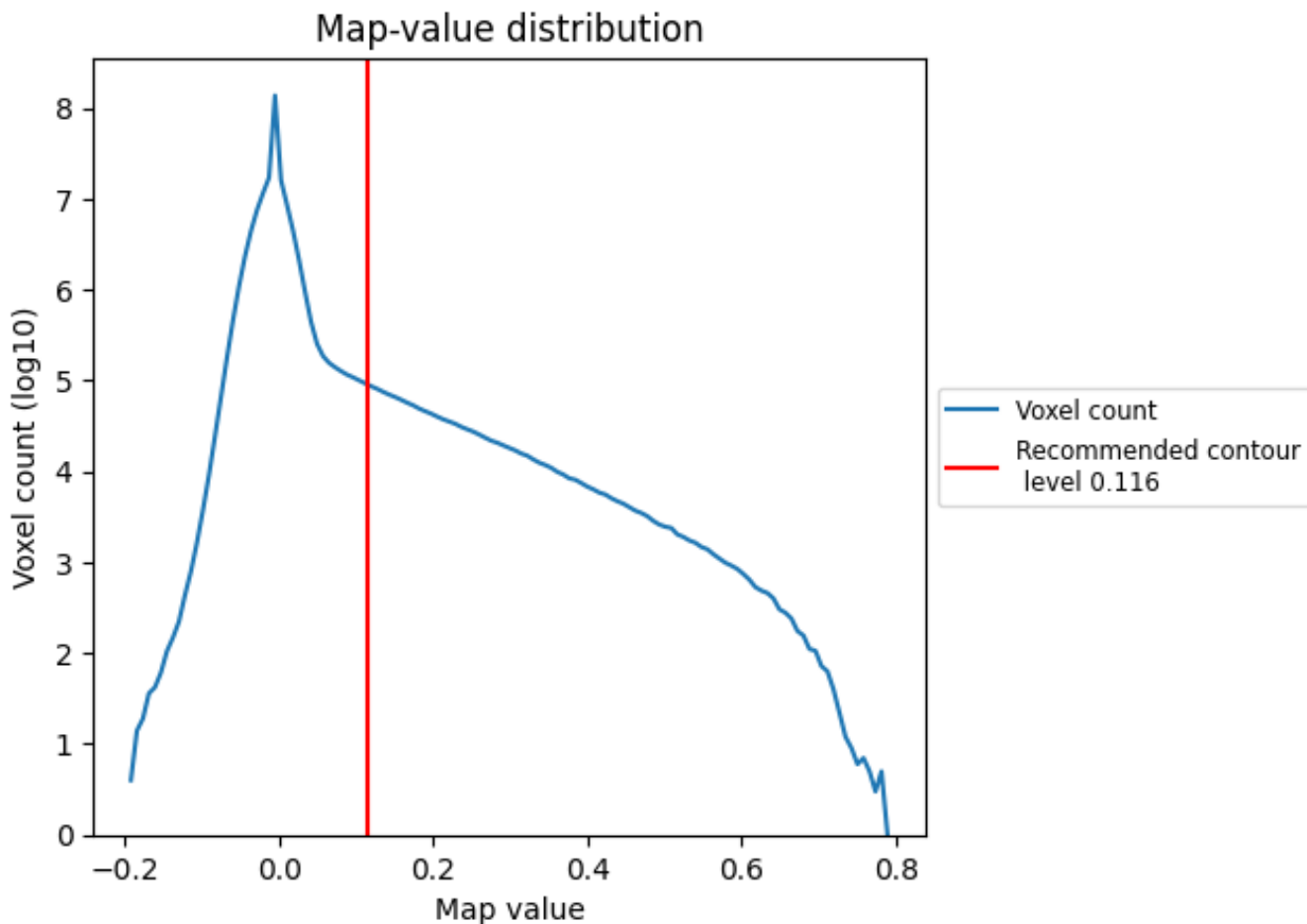


Z

## 7 Map analysis [i](#)

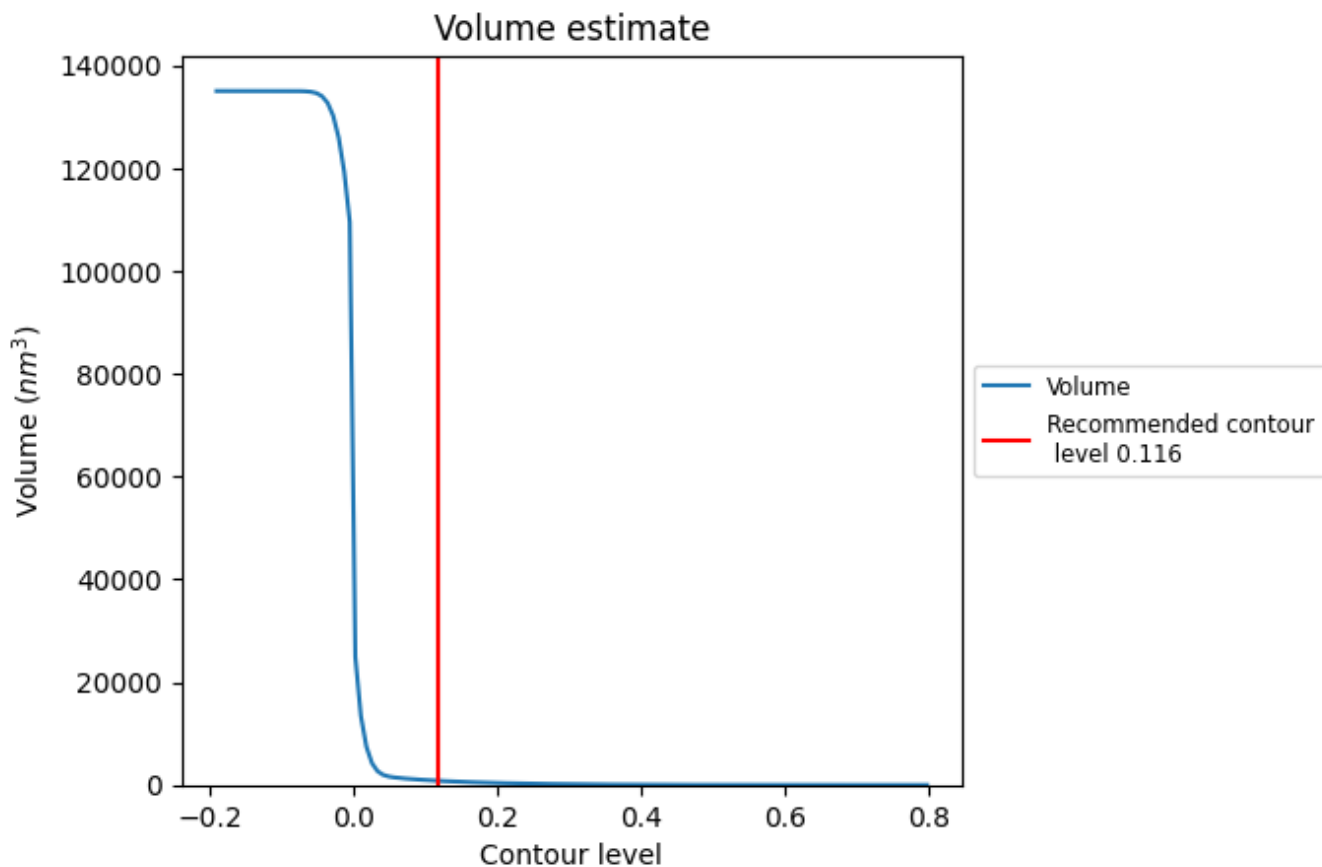
This section contains the results of statistical analysis of the map.

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



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

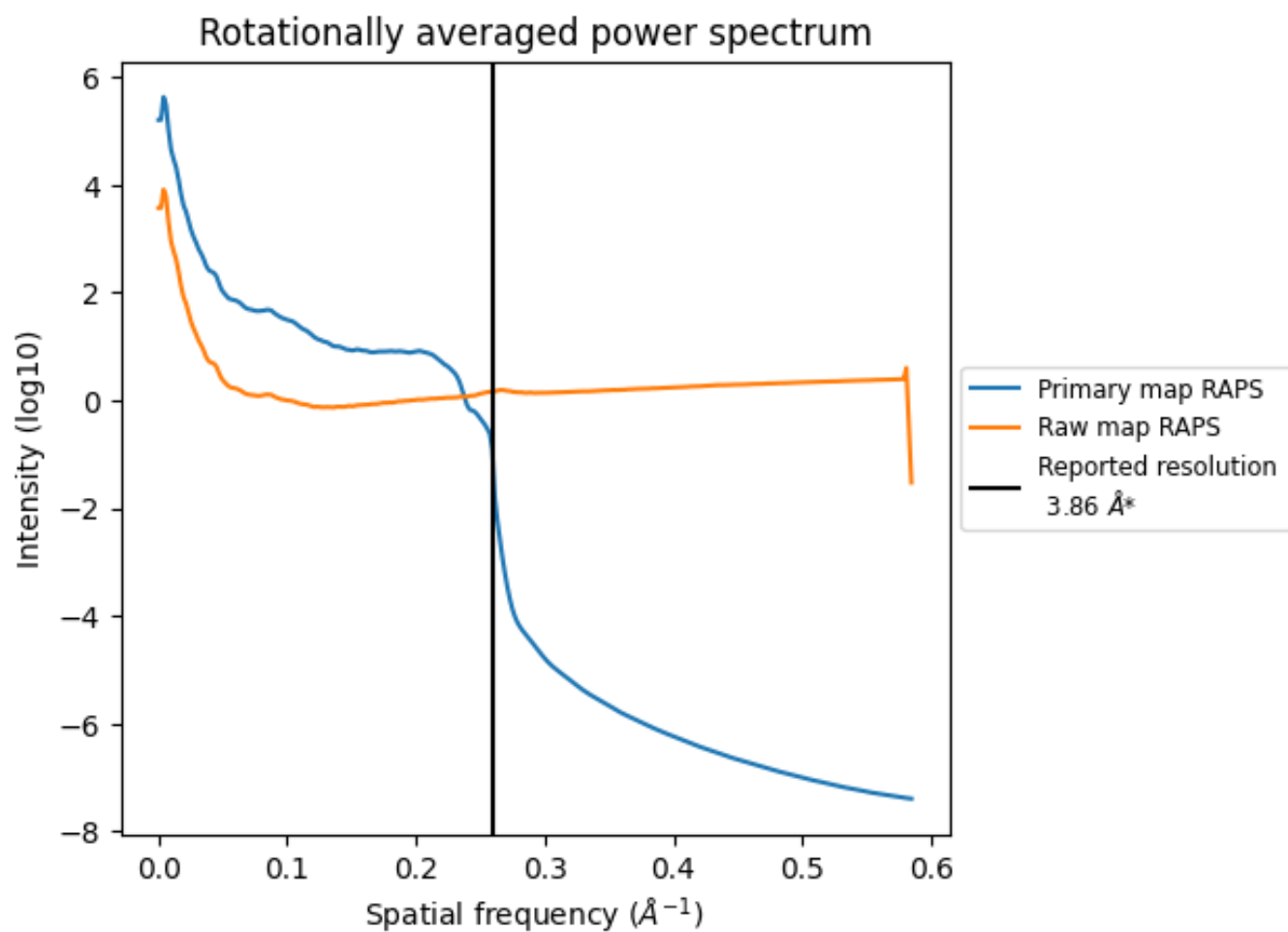
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 824 nm<sup>3</sup>; this corresponds to an approximate mass of 744 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 i

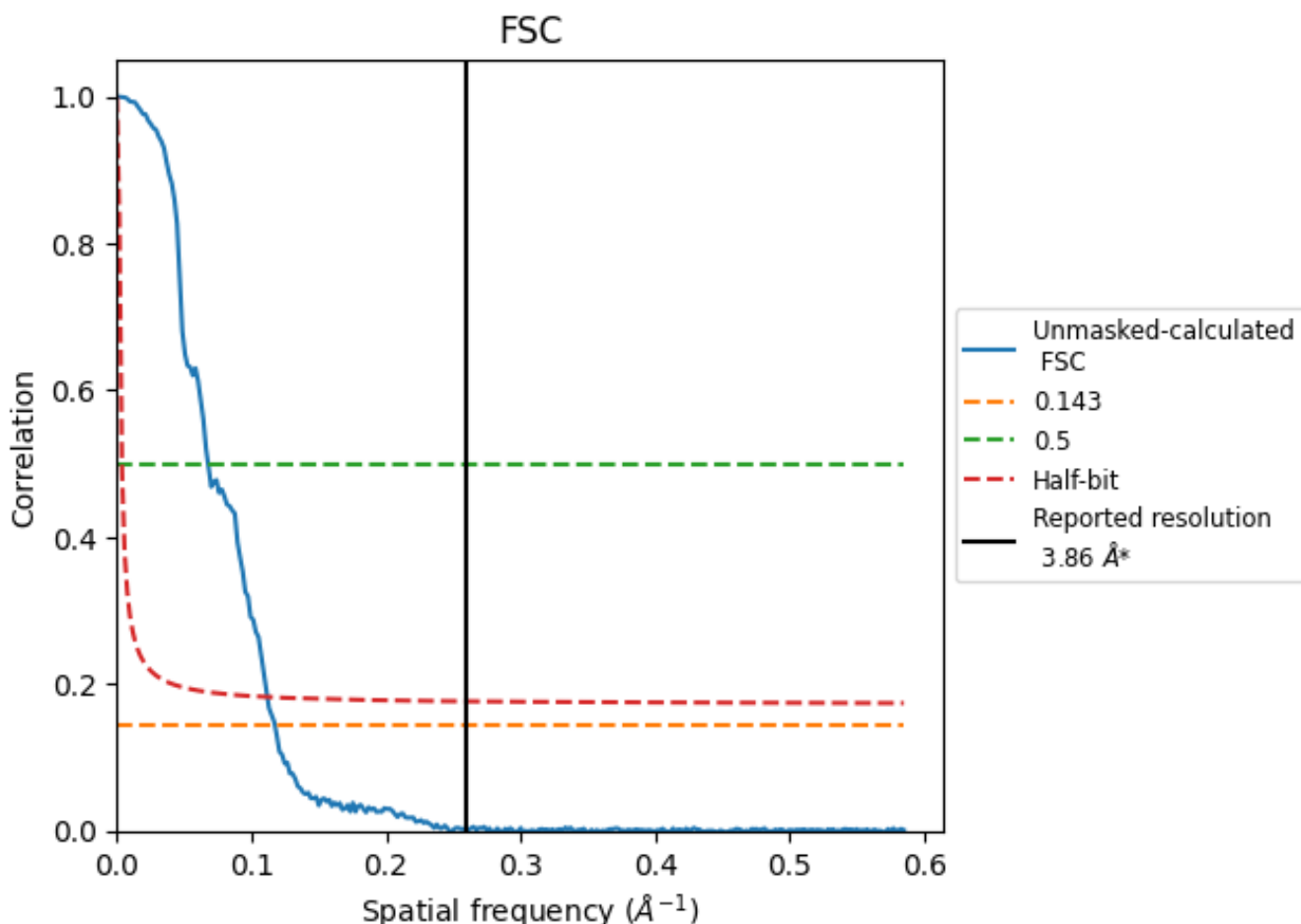


\*Reported resolution corresponds to spatial frequency of 0.259 Å<sup>-1</sup>

## 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 0.259 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

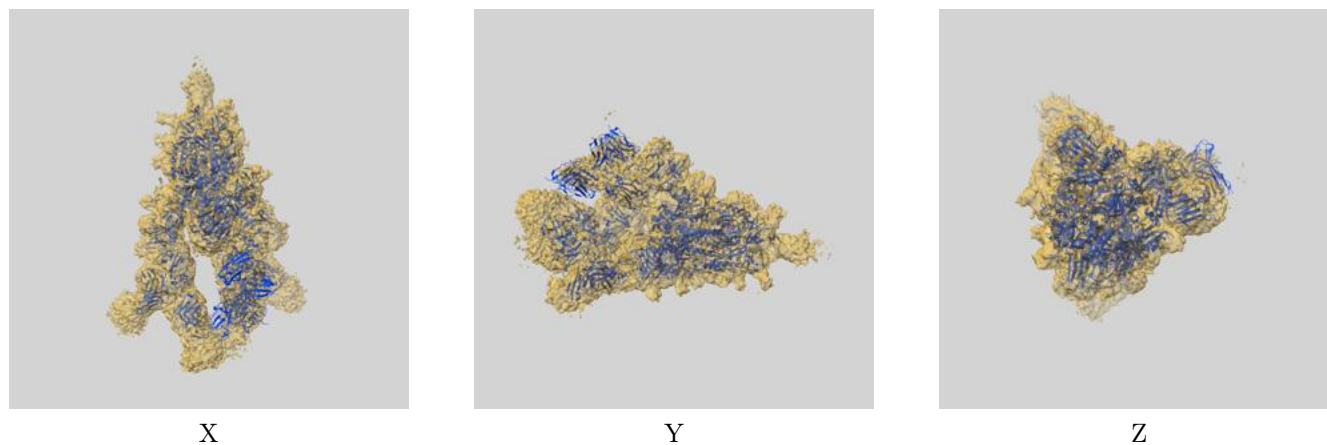
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	3.86	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.51	14.75	8.94

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.5 CUT-OFF 14.75 differs from the reported value 3.86 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-25808 and PDB model 7TCC. Per-residue inclusion information can be found in section 3 on page 17.

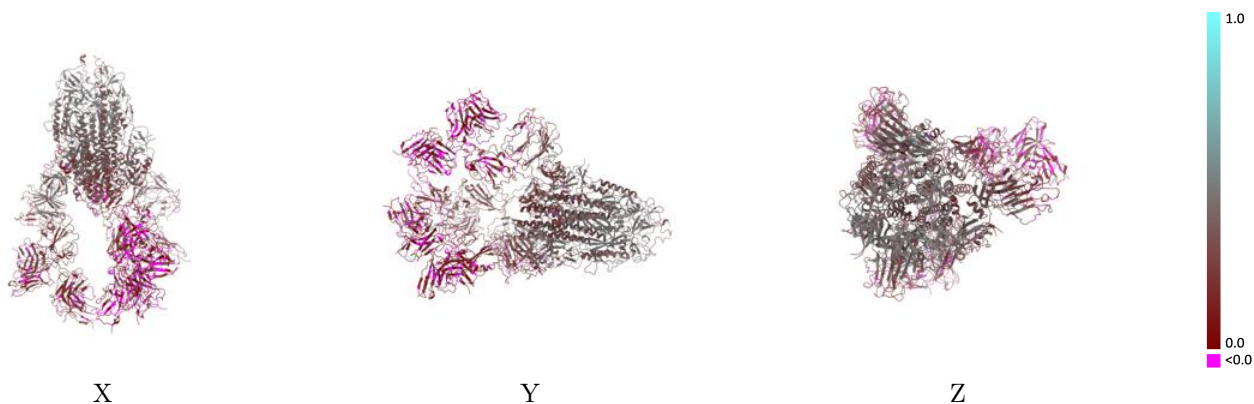
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.116 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.

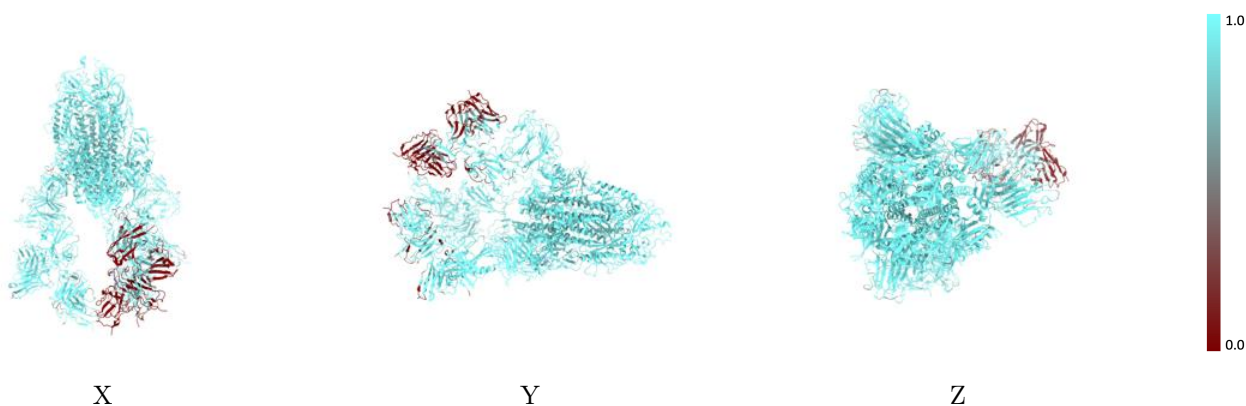


## 9.2 Q-score mapped to coordinate model [i](#)



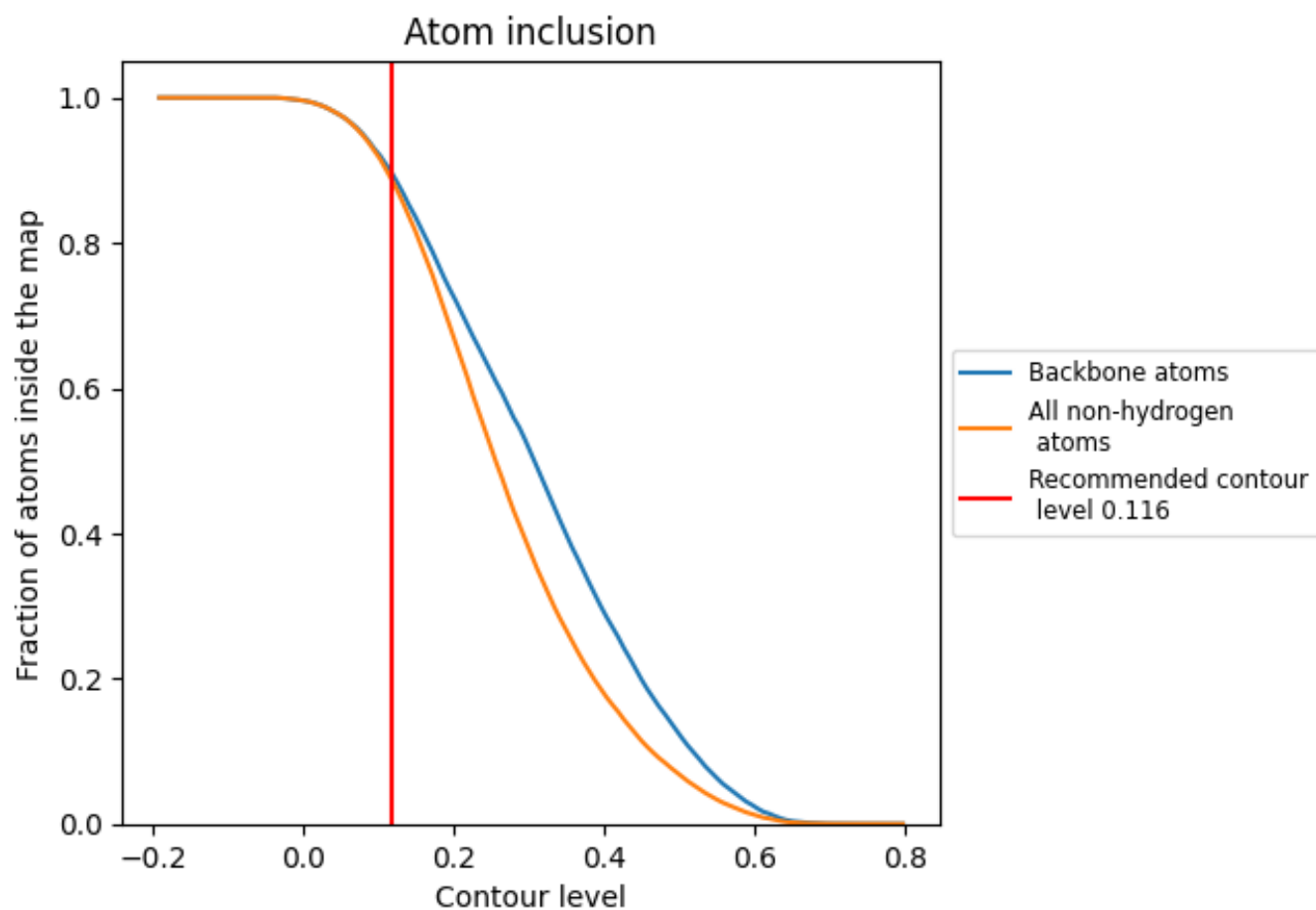
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.116).



























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 89% 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 (0.116) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8898	 0.2680
A	 0.9514	 0.3140
B	 0.9818	 0.3290
C	 0.9787	 0.3250
D	 0.3635	 0.1130
E	 0.4488	 0.1100
F	 0.9561	 0.1550
G	 0.9084	 0.1450
H	 0.9885	 0.1960
I	 1.0000	 0.4520
J	 0.1998	 0.0750
K	 0.0557	 0.0730
L	 0.9659	 0.1770
M	 0.9208	 0.1070
N	 0.8812	 0.1210
O	 0.7969	 0.1200
P	 0.6955	 0.1450
Q	 1.0000	 0.4020
R	 1.0000	 0.4470
S	 1.0000	 0.3940
T	 1.0000	 0.4510
U	 1.0000	 0.4190
V	 1.0000	 0.4110
W	 1.0000	 0.4180
X	 1.0000	 0.4550
Y	 1.0000	 0.3720
Z	 1.0000	 0.4320
a	 1.0000	 0.3220
b	 1.0000	 0.3600

