



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:33 PM UTC

PDB ID : 7E5R / pdb_00007e5r
EMDB ID : EMD-30993
Title : SARS-CoV-2 S trimer with three-antibody cocktail complex
Authors : Sun, Y.; Wang, L.; Wang, N.; Feng, R.; Wang, X.
Deposited on : 2021-02-20
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

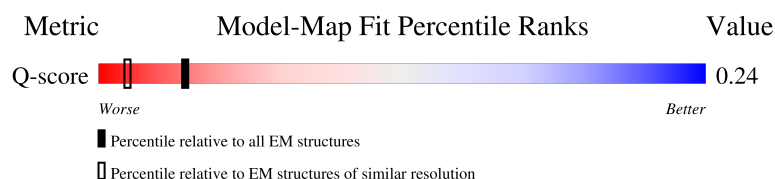
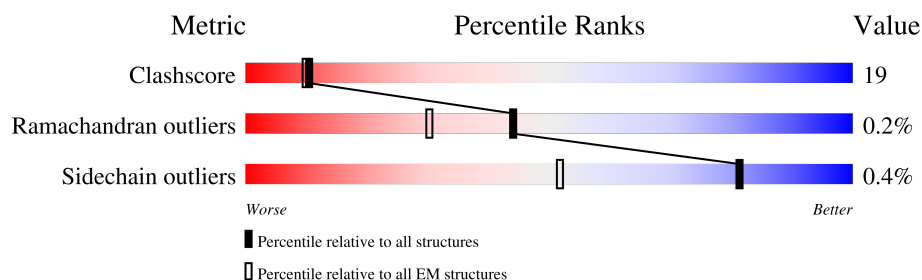
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 Å.

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



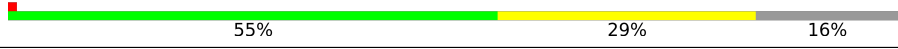
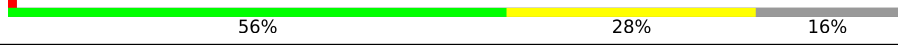
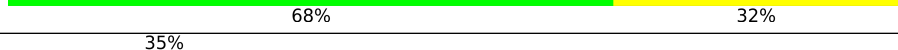
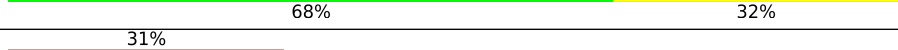
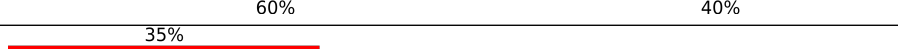
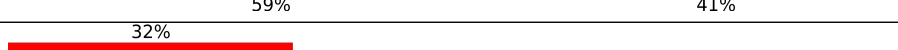
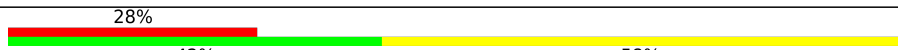
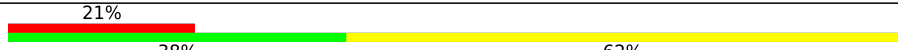
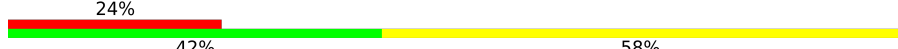
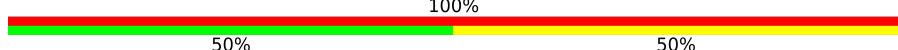
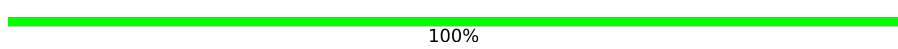
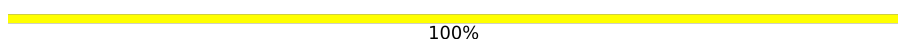
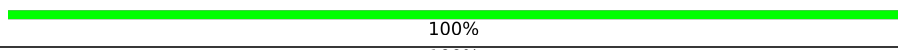
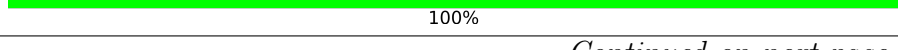
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	D	210	
1	E	210	
1	H	210	
2	L	223	

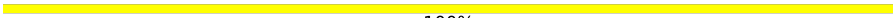
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Mol	Chain	Length	Quality of chain
2	N	223	
2	O	223	
3	A	1281	
3	B	1281	
3	C	1281	
4	I	120	
4	M	120	
4	T	120	
5	K	108	
5	U	108	
5	V	108	
6	Q	109	
6	R	109	
6	S	109	
7	P	120	
7	W	120	
7	X	120	
8	F	2	
8	G	2	
8	J	2	
8	Y	2	
8	Z	2	
8	a	2	
8	b	2	
8	c	2	

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Mol	Chain	Length	Quality of chain
8	d	2	 100%
8	e	2	 100%
8	f	2	 50%  50%
8	g	2	 50%  50%
8	h	2	 100%
8	i	2	 100%
8	j	2	 100%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 40683 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 H014 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	105	Total	C	N	O	S	0	0
			704	447	116	140	1		
1	D	105	Total	C	N	O	S	0	0
			704	447	116	140	1		
1	E	105	Total	C	N	O	S	0	0
			704	447	116	140	1		

- Molecule 2 is a protein called H014 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	120	Total	C	N	O	S	0	0
			903	575	144	182	2		
2	N	120	Total	C	N	O	S	0	0
			903	575	144	182	2		
2	O	120	Total	C	N	O	S	0	0
			903	575	144	182	2		

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1072	Total	C	N	O	S	0	0
			8360	5337	1400	1585	38		
3	B	1072	Total	C	N	O	S	0	0
			8360	5337	1400	1585	38		
3	C	1072	Total	C	N	O	S	0	0
			8360	5337	1400	1585	38		

There are 234 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	GLY	-	expression tag	UNP P0DTC2
A	1211	ARG	-	expression tag	UNP P0DTC2
A	1212	GLY	-	expression tag	UNP P0DTC2
A	1213	SER	-	expression tag	UNP P0DTC2
A	1214	GLY	-	expression tag	UNP P0DTC2
A	1215	TYR	-	expression tag	UNP P0DTC2
A	1216	ILE	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	GLU	-	expression tag	UNP P0DTC2
A	1219	ALA	-	expression tag	UNP P0DTC2
A	1220	PRO	-	expression tag	UNP P0DTC2
A	1221	ARG	-	expression tag	UNP P0DTC2
A	1222	ASP	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	GLN	-	expression tag	UNP P0DTC2
A	1225	ALA	-	expression tag	UNP P0DTC2
A	1226	TYR	-	expression tag	UNP P0DTC2
A	1227	VAL	-	expression tag	UNP P0DTC2
A	1228	ARG	-	expression tag	UNP P0DTC2
A	1229	LYS	-	expression tag	UNP P0DTC2
A	1230	ASP	-	expression tag	UNP P0DTC2
A	1231	GLY	-	expression tag	UNP P0DTC2
A	1232	GLU	-	expression tag	UNP P0DTC2
A	1233	TRP	-	expression tag	UNP P0DTC2
A	1234	VAL	-	expression tag	UNP P0DTC2
A	1235	LEU	-	expression tag	UNP P0DTC2
A	1236	LEU	-	expression tag	UNP P0DTC2
A	1237	SER	-	expression tag	UNP P0DTC2
A	1238	THR	-	expression tag	UNP P0DTC2
A	1239	PHE	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	GLY	-	expression tag	UNP P0DTC2
A	1242	ARG	-	expression tag	UNP P0DTC2
A	1243	SER	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	GLU	-	expression tag	UNP P0DTC2
A	1246	VAL	-	expression tag	UNP P0DTC2
A	1247	LEU	-	expression tag	UNP P0DTC2
A	1248	PHE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1249	GLN	-	expression tag	UNP P0DTC2
A	1250	GLY	-	expression tag	UNP P0DTC2
A	1251	PRO	-	expression tag	UNP P0DTC2
A	1252	GLY	-	expression tag	UNP P0DTC2
A	1253	TRP	-	expression tag	UNP P0DTC2
A	1254	SER	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	PRO	-	expression tag	UNP P0DTC2
A	1257	GLN	-	expression tag	UNP P0DTC2
A	1258	PHE	-	expression tag	UNP P0DTC2
A	1259	GLU	-	expression tag	UNP P0DTC2
A	1260	LYS	-	expression tag	UNP P0DTC2
A	1261	GLY	-	expression tag	UNP P0DTC2
A	1262	GLY	-	expression tag	UNP P0DTC2
A	1263	GLY	-	expression tag	UNP P0DTC2
A	1264	SER	-	expression tag	UNP P0DTC2
A	1265	GLY	-	expression tag	UNP P0DTC2
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	SER	-	expression tag	UNP P0DTC2
A	1273	ALA	-	expression tag	UNP P0DTC2
A	1274	TRP	-	expression tag	UNP P0DTC2
A	1275	SER	-	expression tag	UNP P0DTC2
A	1276	HIS	-	expression tag	UNP P0DTC2
A	1277	PRO	-	expression tag	UNP P0DTC2
A	1278	GLN	-	expression tag	UNP P0DTC2
A	1279	PHE	-	expression tag	UNP P0DTC2
A	1280	GLU	-	expression tag	UNP P0DTC2
A	1281	LYS	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	GLY	-	expression tag	UNP P0DTC2
B	1211	ARG	-	expression tag	UNP P0DTC2
B	1212	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1213	SER	-	expression tag	UNP P0DTC2
B	1214	GLY	-	expression tag	UNP P0DTC2
B	1215	TYR	-	expression tag	UNP P0DTC2
B	1216	ILE	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	GLU	-	expression tag	UNP P0DTC2
B	1219	ALA	-	expression tag	UNP P0DTC2
B	1220	PRO	-	expression tag	UNP P0DTC2
B	1221	ARG	-	expression tag	UNP P0DTC2
B	1222	ASP	-	expression tag	UNP P0DTC2
B	1223	GLY	-	expression tag	UNP P0DTC2
B	1224	GLN	-	expression tag	UNP P0DTC2
B	1225	ALA	-	expression tag	UNP P0DTC2
B	1226	TYR	-	expression tag	UNP P0DTC2
B	1227	VAL	-	expression tag	UNP P0DTC2
B	1228	ARG	-	expression tag	UNP P0DTC2
B	1229	LYS	-	expression tag	UNP P0DTC2
B	1230	ASP	-	expression tag	UNP P0DTC2
B	1231	GLY	-	expression tag	UNP P0DTC2
B	1232	GLU	-	expression tag	UNP P0DTC2
B	1233	TRP	-	expression tag	UNP P0DTC2
B	1234	VAL	-	expression tag	UNP P0DTC2
B	1235	LEU	-	expression tag	UNP P0DTC2
B	1236	LEU	-	expression tag	UNP P0DTC2
B	1237	SER	-	expression tag	UNP P0DTC2
B	1238	THR	-	expression tag	UNP P0DTC2
B	1239	PHE	-	expression tag	UNP P0DTC2
B	1240	LEU	-	expression tag	UNP P0DTC2
B	1241	GLY	-	expression tag	UNP P0DTC2
B	1242	ARG	-	expression tag	UNP P0DTC2
B	1243	SER	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	GLU	-	expression tag	UNP P0DTC2
B	1246	VAL	-	expression tag	UNP P0DTC2
B	1247	LEU	-	expression tag	UNP P0DTC2
B	1248	PHE	-	expression tag	UNP P0DTC2
B	1249	GLN	-	expression tag	UNP P0DTC2
B	1250	GLY	-	expression tag	UNP P0DTC2
B	1251	PRO	-	expression tag	UNP P0DTC2
B	1252	GLY	-	expression tag	UNP P0DTC2
B	1253	TRP	-	expression tag	UNP P0DTC2
B	1254	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	PRO	-	expression tag	UNP P0DTC2
B	1257	GLN	-	expression tag	UNP P0DTC2
B	1258	PHE	-	expression tag	UNP P0DTC2
B	1259	GLU	-	expression tag	UNP P0DTC2
B	1260	LYS	-	expression tag	UNP P0DTC2
B	1261	GLY	-	expression tag	UNP P0DTC2
B	1262	GLY	-	expression tag	UNP P0DTC2
B	1263	GLY	-	expression tag	UNP P0DTC2
B	1264	SER	-	expression tag	UNP P0DTC2
B	1265	GLY	-	expression tag	UNP P0DTC2
B	1266	GLY	-	expression tag	UNP P0DTC2
B	1267	GLY	-	expression tag	UNP P0DTC2
B	1268	SER	-	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	SER	-	expression tag	UNP P0DTC2
B	1273	ALA	-	expression tag	UNP P0DTC2
B	1274	TRP	-	expression tag	UNP P0DTC2
B	1275	SER	-	expression tag	UNP P0DTC2
B	1276	HIS	-	expression tag	UNP P0DTC2
B	1277	PRO	-	expression tag	UNP P0DTC2
B	1278	GLN	-	expression tag	UNP P0DTC2
B	1279	PHE	-	expression tag	UNP P0DTC2
B	1280	GLU	-	expression tag	UNP P0DTC2
B	1281	LYS	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	GLY	-	expression tag	UNP P0DTC2
C	1211	ARG	-	expression tag	UNP P0DTC2
C	1212	GLY	-	expression tag	UNP P0DTC2
C	1213	SER	-	expression tag	UNP P0DTC2
C	1214	GLY	-	expression tag	UNP P0DTC2
C	1215	TYR	-	expression tag	UNP P0DTC2
C	1216	ILE	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1219	ALA	-	expression tag	UNP P0DTC2
C	1220	PRO	-	expression tag	UNP P0DTC2
C	1221	ARG	-	expression tag	UNP P0DTC2
C	1222	ASP	-	expression tag	UNP P0DTC2
C	1223	GLY	-	expression tag	UNP P0DTC2
C	1224	GLN	-	expression tag	UNP P0DTC2
C	1225	ALA	-	expression tag	UNP P0DTC2
C	1226	TYR	-	expression tag	UNP P0DTC2
C	1227	VAL	-	expression tag	UNP P0DTC2
C	1228	ARG	-	expression tag	UNP P0DTC2
C	1229	LYS	-	expression tag	UNP P0DTC2
C	1230	ASP	-	expression tag	UNP P0DTC2
C	1231	GLY	-	expression tag	UNP P0DTC2
C	1232	GLU	-	expression tag	UNP P0DTC2
C	1233	TRP	-	expression tag	UNP P0DTC2
C	1234	VAL	-	expression tag	UNP P0DTC2
C	1235	LEU	-	expression tag	UNP P0DTC2
C	1236	LEU	-	expression tag	UNP P0DTC2
C	1237	SER	-	expression tag	UNP P0DTC2
C	1238	THR	-	expression tag	UNP P0DTC2
C	1239	PHE	-	expression tag	UNP P0DTC2
C	1240	LEU	-	expression tag	UNP P0DTC2
C	1241	GLY	-	expression tag	UNP P0DTC2
C	1242	ARG	-	expression tag	UNP P0DTC2
C	1243	SER	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	GLU	-	expression tag	UNP P0DTC2
C	1246	VAL	-	expression tag	UNP P0DTC2
C	1247	LEU	-	expression tag	UNP P0DTC2
C	1248	PHE	-	expression tag	UNP P0DTC2
C	1249	GLN	-	expression tag	UNP P0DTC2
C	1250	GLY	-	expression tag	UNP P0DTC2
C	1251	PRO	-	expression tag	UNP P0DTC2
C	1252	GLY	-	expression tag	UNP P0DTC2
C	1253	TRP	-	expression tag	UNP P0DTC2
C	1254	SER	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	PRO	-	expression tag	UNP P0DTC2
C	1257	GLN	-	expression tag	UNP P0DTC2
C	1258	PHE	-	expression tag	UNP P0DTC2
C	1259	GLU	-	expression tag	UNP P0DTC2
C	1260	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1261	GLY	-	expression tag	UNP P0DTC2
C	1262	GLY	-	expression tag	UNP P0DTC2
C	1263	GLY	-	expression tag	UNP P0DTC2
C	1264	SER	-	expression tag	UNP P0DTC2
C	1265	GLY	-	expression tag	UNP P0DTC2
C	1266	GLY	-	expression tag	UNP P0DTC2
C	1267	GLY	-	expression tag	UNP P0DTC2
C	1268	SER	-	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	SER	-	expression tag	UNP P0DTC2
C	1273	ALA	-	expression tag	UNP P0DTC2
C	1274	TRP	-	expression tag	UNP P0DTC2
C	1275	SER	-	expression tag	UNP P0DTC2
C	1276	HIS	-	expression tag	UNP P0DTC2
C	1277	PRO	-	expression tag	UNP P0DTC2
C	1278	GLN	-	expression tag	UNP P0DTC2
C	1279	PHE	-	expression tag	UNP P0DTC2
C	1280	GLU	-	expression tag	UNP P0DTC2
C	1281	LYS	-	expression tag	UNP P0DTC2

- Molecule 4 is a protein called P17 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	120	Total	C	N	O	S	0	0
			918	574	165	175	4		
4	T	120	Total	C	N	O	S	0	0
			918	574	165	175	4		
4	I	120	Total	C	N	O	S	0	0
			918	574	165	175	4		

- Molecule 5 is a protein called P17 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	U	108	Total	C	N	O	S	0	0
			817	511	137	167	2		
5	V	108	Total	C	N	O	S	0	0
			817	511	137	167	2		
5	K	108	Total	C	N	O	S	0	0
			817	511	137	167	2		

- Molecule 6 is a protein called FC05 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	109	Total	C	N	O	S	0	0
			788	491	132	163	2		
6	S	109	Total	C	N	O	S	0	0
			788	491	132	163	2		
6	Q	109	Total	C	N	O	S	0	0
			788	491	132	163	2		

- Molecule 7 is a protein called FC05 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	W	120	Total	C	N	O	S	0	0
			931	587	149	188	7		
7	X	120	Total	C	N	O	S	0	0
			931	587	149	188	7		
7	P	120	Total	C	N	O	S	0	0
			931	587	149	188	7		

- Molecule 8 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
8	F	2	Total	C	N	O	0	0
			28	16	2	10		
8	G	2	Total	C	N	O	0	0
			28	16	2	10		
8	J	2	Total	C	N	O	0	0
			28	16	2	10		
8	Y	2	Total	C	N	O	0	0
			28	16	2	10		
8	Z	2	Total	C	N	O	0	0
			28	16	2	10		
8	a	2	Total	C	N	O	0	0
			28	16	2	10		
8	b	2	Total	C	N	O	0	0
			28	16	2	10		
8	c	2	Total	C	N	O	0	0
			28	16	2	10		

Continued on next page...

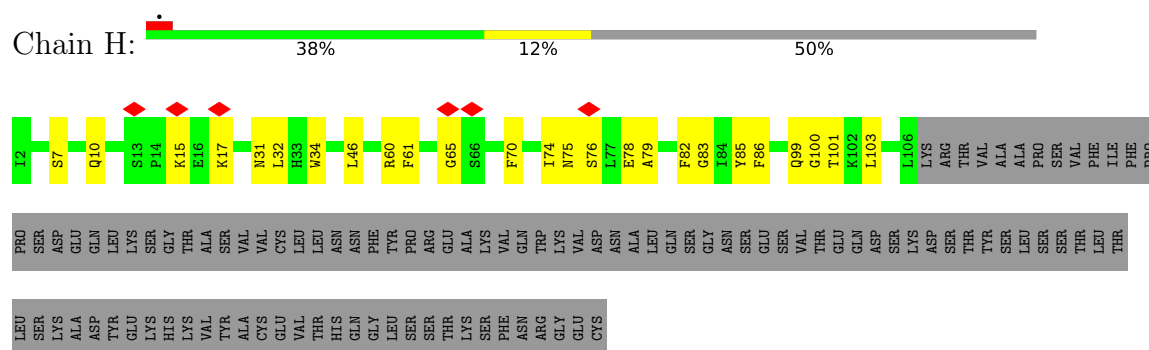
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
8	d	2	Total	C	N	O	0	0
			28	16	2	10		
8	e	2	Total	C	N	O	0	0
			28	16	2	10		
8	f	2	Total	C	N	O	0	0
			28	16	2	10		
8	g	2	Total	C	N	O	0	0
			28	16	2	10		
8	h	2	Total	C	N	O	0	0
			28	16	2	10		
8	i	2	Total	C	N	O	0	0
			28	16	2	10		
8	j	2	Total	C	N	O	0	0
			28	16	2	10		

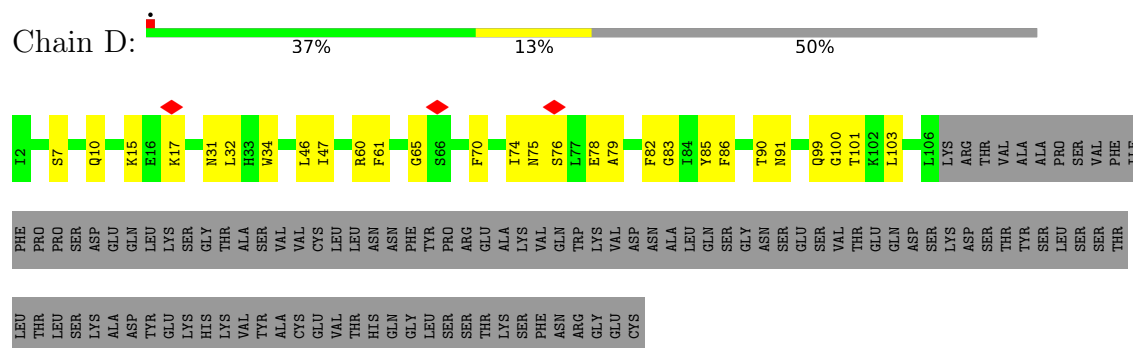
3 Residue-property plots [i](#)

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.

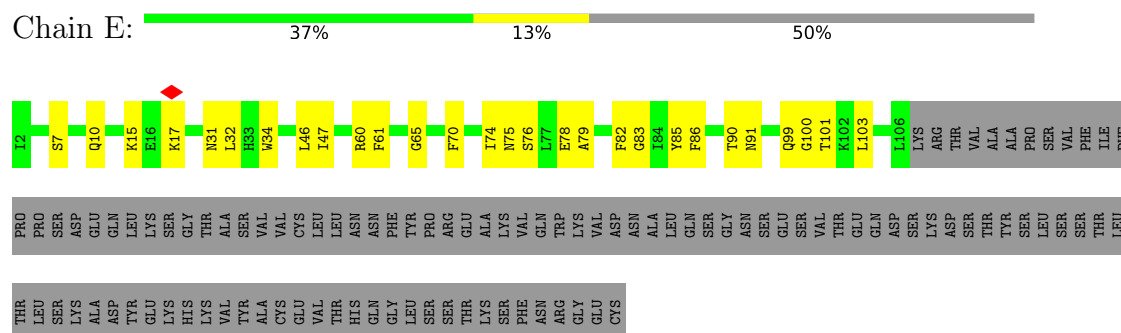
- Molecule 1: H014 light chain



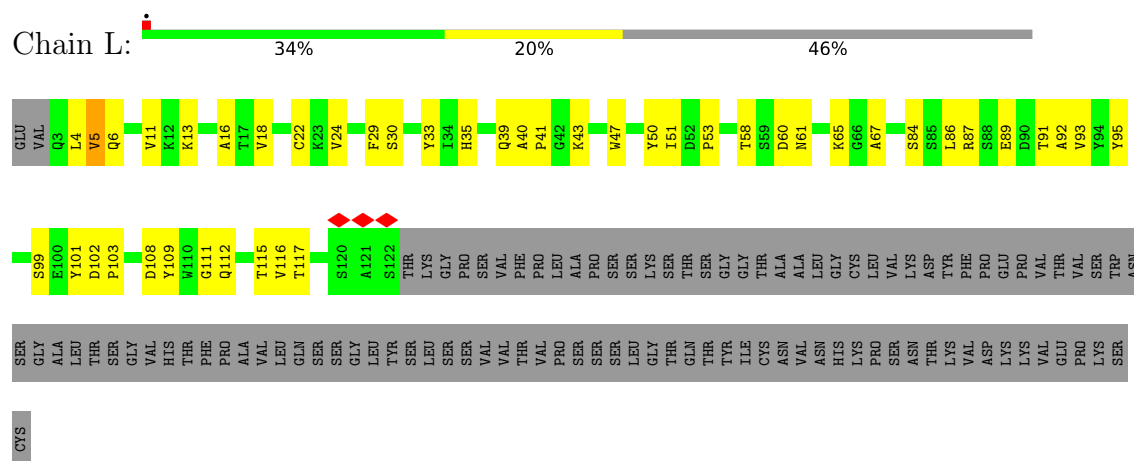
- Molecule 1: H014 light chain



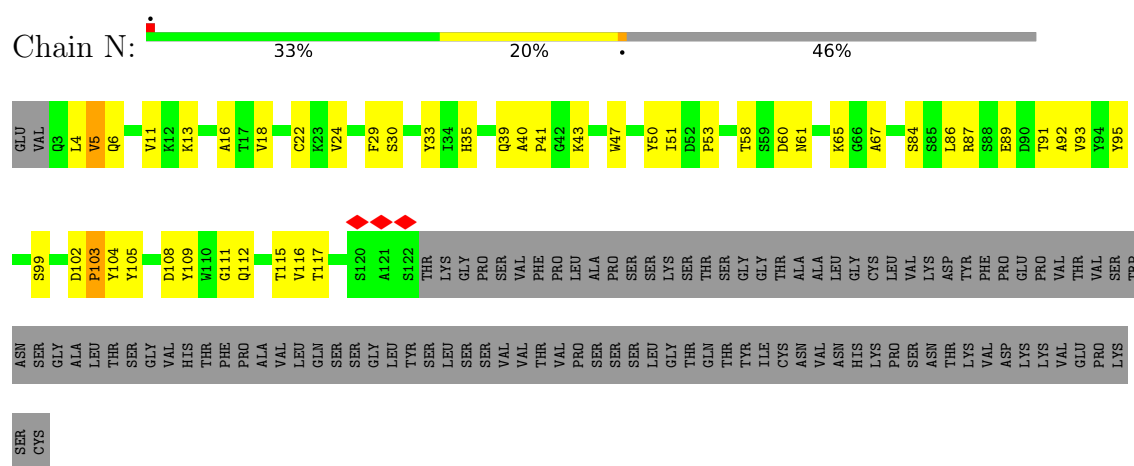
- Molecule 1: H014 light chain



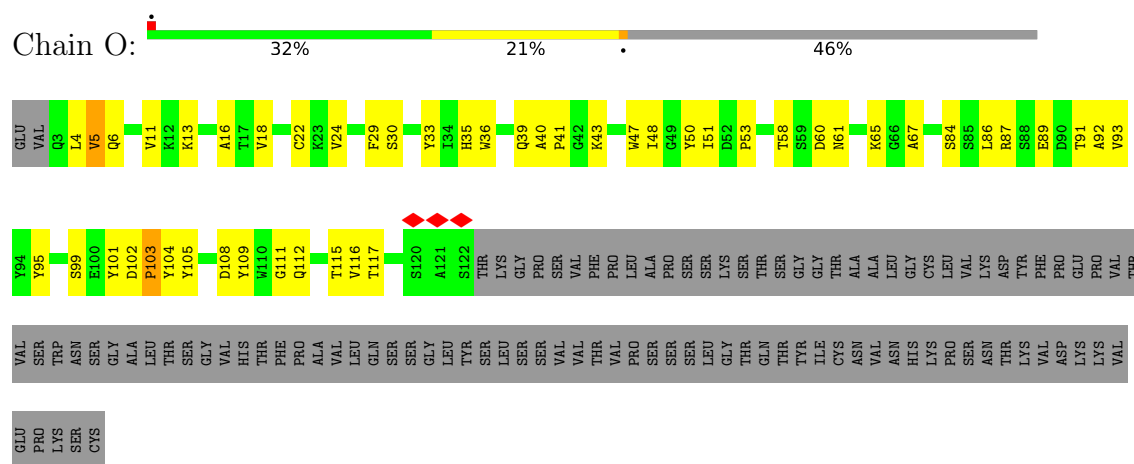
- Molecule 2: H014 heavy chain



- Molecule 2: H014 heavy chain



- Molecule 2: H014 heavy chain



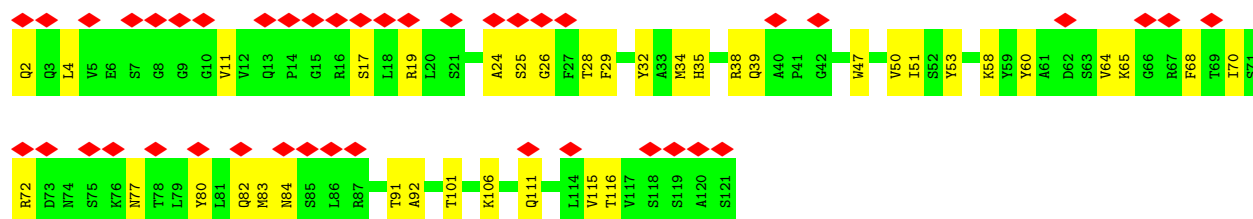
- Molecule 3: Spike glycoprotein



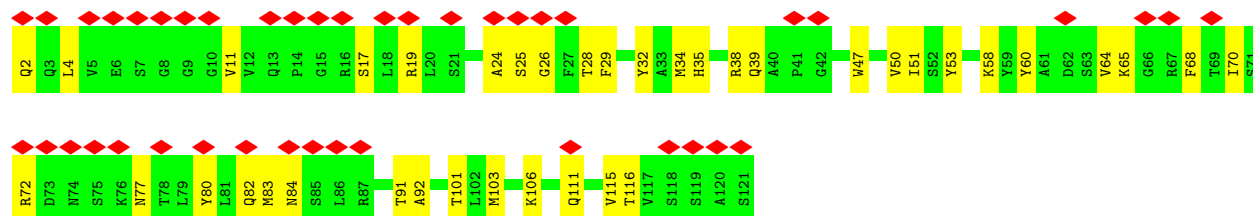




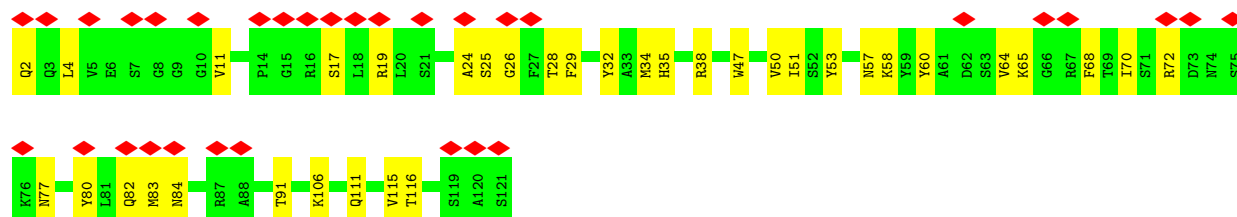




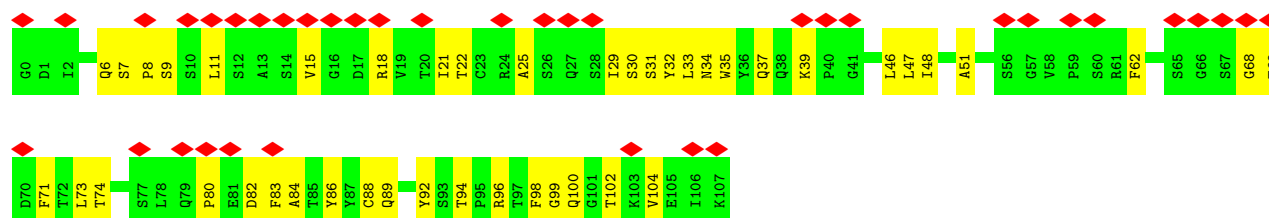
• Molecule 4: P17 heavy chain



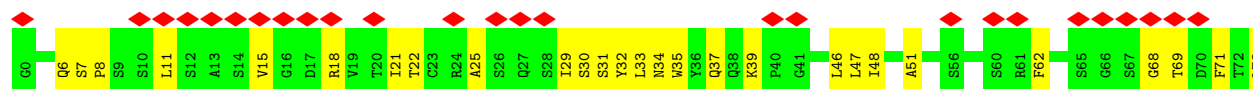
• Molecule 4: P17 heavy chain

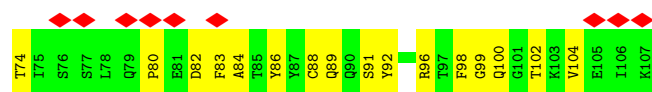


• Molecule 5: P17 light chain

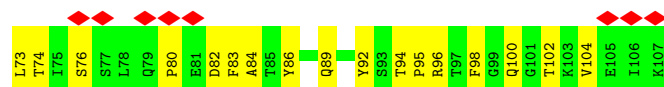


• Molecule 5: P17 light chain

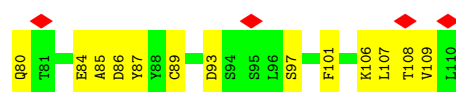
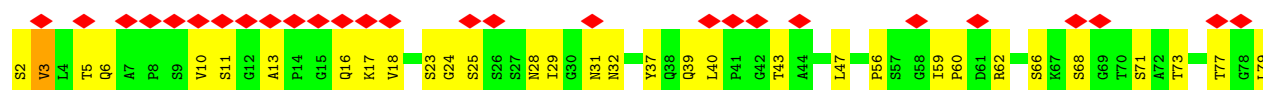




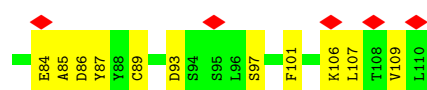
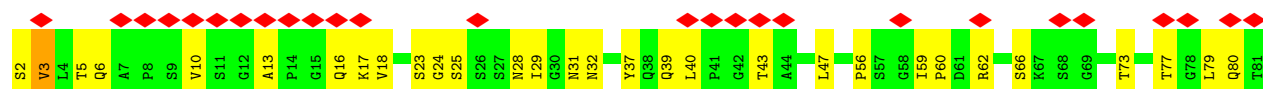
- Molecule 5: P17 light chain



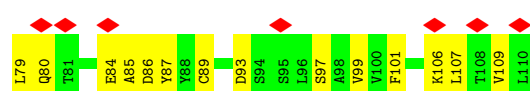
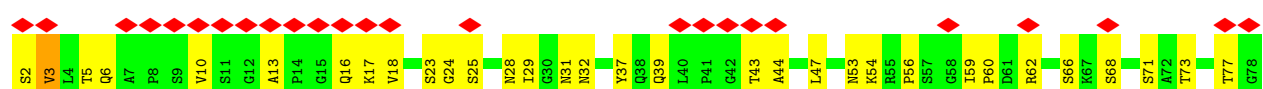
- Molecule 6: FC05 light chain



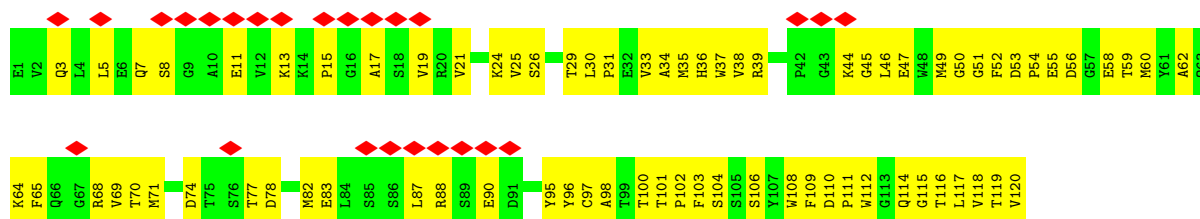
- Molecule 6: FC05 light chain



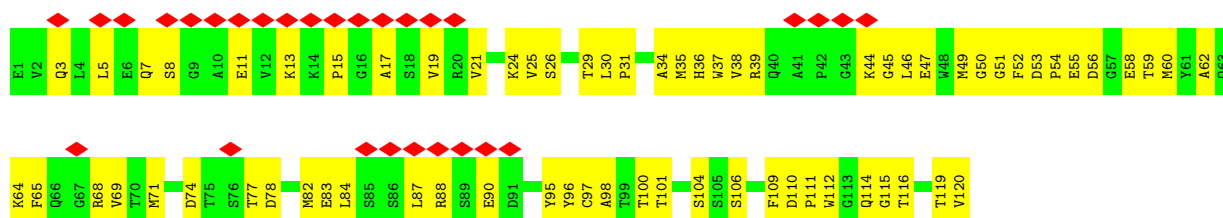
- Molecule 6: FC05 light chain



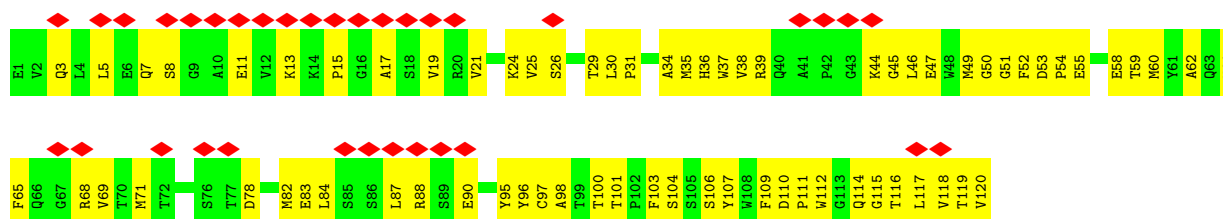
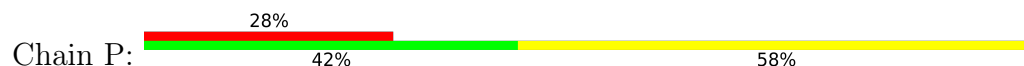
- Molecule 7: FC05 heavy chain



- Molecule 7: FC05 heavy chain



- Molecule 7: FC05 heavy chain



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  100%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  100%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  100%
50% 50%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  50% 50%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  100%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  100%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  100%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  50% 50%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:  50% 50%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:  100%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:  100%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92127	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.037	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

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	D	0.13	0/722	0.40	0/992
1	E	0.13	0/722	0.40	0/992
1	H	0.13	0/722	0.40	0/992
2	L	0.23	0/927	0.41	0/1266
2	N	0.26	0/927	0.37	0/1266
2	O	0.25	0/927	0.36	0/1266
3	A	0.19	0/8555	0.41	0/11646
3	B	0.19	0/8555	0.41	0/11646
3	C	0.19	0/8555	0.41	0/11646
4	I	0.11	0/937	0.35	0/1269
4	M	0.11	0/937	0.35	0/1269
4	T	0.11	0/937	0.35	0/1269
5	K	0.12	0/834	0.36	0/1131
5	U	0.16	0/834	0.37	0/1131
5	V	0.13	0/834	0.37	0/1131
6	Q	0.13	0/804	0.34	0/1095
6	R	0.13	0/804	0.35	0/1095
6	S	0.16	0/804	0.35	0/1095
7	P	0.17	0/955	0.44	0/1299
7	W	0.17	0/955	0.44	0/1299
7	X	0.17	0/955	0.44	0/1299
All	All	0.18	0/41202	0.40	0/56094

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	704	0	565	16	0
1	E	704	0	565	16	0
1	H	704	0	565	14	0
2	L	903	0	825	40	0
2	N	903	0	825	44	0
2	O	903	0	825	42	0
3	A	8360	0	8153	319	0
3	B	8360	0	8153	307	0
3	C	8360	0	8153	307	0
4	I	918	0	885	29	0
4	M	918	0	885	27	0
4	T	918	0	885	28	0
5	K	817	0	800	34	0
5	U	817	0	800	31	0
5	V	817	0	800	33	0
6	Q	788	0	766	34	0
6	R	788	0	766	29	0
6	S	788	0	766	26	0
7	P	931	0	878	70	0
7	W	931	0	878	67	0
7	X	931	0	878	58	0
8	F	28	0	25	2	0
8	G	28	0	25	1	0
8	J	28	0	25	0	0
8	Y	28	0	25	1	0
8	Z	28	0	25	0	0
8	a	28	0	25	2	0
8	b	28	0	25	1	0
8	c	28	0	25	0	0
8	d	28	0	25	1	0
8	e	28	0	25	0	0
8	f	28	0	25	2	0
8	g	28	0	25	1	0
8	h	28	0	25	0	0
8	i	28	0	25	1	0
8	j	28	0	25	0	0
All	All	40683	0	38991	1504	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (1504) 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)
7:P:49:MET:HE1	7:P:95:TYR:CD1	1.44	1.51
7:W:49:MET:HE1	7:W:95:TYR:CD1	1.46	1.51
7:X:49:MET:HE1	7:X:95:TYR:CD1	1.44	1.50
3:B:332:ILE:HD12	3:B:525:CYS:SG	1.56	1.44
3:A:332:ILE:HD12	3:A:525:CYS:SG	1.58	1.44
3:C:332:ILE:HD12	3:C:525:CYS:SG	1.55	1.43
3:A:391:CYS:HB3	3:A:525:CYS:CB	1.60	1.31
3:B:391:CYS:HB3	3:B:525:CYS:CB	1.60	1.30
3:B:391:CYS:CB	3:B:525:CYS:HB3	1.60	1.30
3:A:391:CYS:CB	3:A:525:CYS:HB3	1.61	1.29
3:C:391:CYS:HB3	3:C:525:CYS:CB	1.60	1.29
3:C:391:CYS:CB	3:C:525:CYS:HB3	1.60	1.29
3:B:328:ARG:NH1	3:B:533:LEU:HD22	1.49	1.28
2:N:102:ASP:OD1	2:N:103:PRO:HD2	1.25	1.27
2:O:102:ASP:OD1	2:O:103:PRO:HD2	1.25	1.26
3:C:328:ARG:NH1	3:C:533:LEU:HD22	1.48	1.25
3:A:328:ARG:NH1	3:A:533:LEU:HD22	1.49	1.24
7:P:49:MET:CE	7:P:95:TYR:HD1	1.56	1.18
7:X:49:MET:CE	7:X:95:TYR:HD1	1.56	1.17
3:C:332:ILE:CD1	3:C:525:CYS:SG	2.33	1.17
3:B:332:ILE:CD1	3:B:525:CYS:SG	2.33	1.16
2:N:102:ASP:CG	2:N:103:PRO:HD2	1.72	1.14
7:W:49:MET:CE	7:W:95:TYR:HD1	1.60	1.14
2:O:102:ASP:CG	2:O:103:PRO:HD2	1.72	1.13
3:C:328:ARG:HH11	3:C:533:LEU:HD13	1.06	1.13
2:L:102:ASP:OD1	2:L:103:PRO:CD	1.95	1.12
3:A:332:ILE:CD1	3:A:525:CYS:SG	2.36	1.12
3:B:328:ARG:HH11	3:B:533:LEU:HD13	1.07	1.12
3:A:328:ARG:HH11	3:A:533:LEU:HD13	1.07	1.10
2:L:102:ASP:OD1	2:L:103:PRO:HD2	1.48	1.09
2:N:13:LYS:HE2	2:N:16:ALA:HB2	1.33	1.09
2:L:13:LYS:HE2	2:L:16:ALA:HB2	1.33	1.08
3:A:328:ARG:HH12	3:A:533:LEU:CD2	1.66	1.07
3:C:328:ARG:HH12	3:C:533:LEU:CD2	1.65	1.07
2:L:102:ASP:CG	2:L:103:PRO:HD2	1.81	1.06
3:B:328:ARG:HH12	3:B:533:LEU:CD2	1.66	1.06
2:O:13:LYS:HE2	2:O:16:ALA:HB2	1.33	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:328:ARG:HH12	3:A:533:LEU:HD22	0.87	1.04
6:Q:43:THR:HG22	6:Q:44:ALA:H	1.19	1.02
3:B:328:ARG:NH1	3:B:533:LEU:CD2	2.22	1.02
7:W:5:LEU:HD22	7:W:24:LYS:HG2	1.42	1.02
7:X:5:LEU:HD22	7:X:24:LYS:HG2	1.42	1.00
3:C:328:ARG:HH12	3:C:533:LEU:HD22	0.86	1.00
3:B:328:ARG:HH12	3:B:533:LEU:HD22	0.87	1.00
7:P:5:LEU:HD22	7:P:24:LYS:HG2	1.42	1.00
3:A:331:ASN:ND2	3:A:362:VAL:HG23	1.78	0.99
3:A:328:ARG:NH1	3:A:533:LEU:CD2	2.22	0.99
2:N:102:ASP:OD1	2:N:103:PRO:CD	2.10	0.99
3:C:328:ARG:NH1	3:C:533:LEU:CD2	2.21	0.99
2:O:102:ASP:OD1	2:O:103:PRO:CD	2.10	0.97
3:B:328:ARG:NH1	3:B:533:LEU:HD13	1.80	0.96
2:N:13:LYS:HE2	2:N:16:ALA:CB	1.96	0.96
3:A:328:ARG:NH1	3:A:533:LEU:HD13	1.80	0.95
3:C:328:ARG:NH1	3:C:533:LEU:HD13	1.80	0.95
2:L:13:LYS:HE2	2:L:16:ALA:CB	1.96	0.95
7:X:49:MET:CE	7:X:95:TYR:CD1	2.40	0.95
2:O:13:LYS:HE2	2:O:16:ALA:CB	1.96	0.94
6:Q:93:ASP:O	6:Q:97:SER:HA	1.68	0.94
6:S:93:ASP:O	6:S:97:SER:HA	1.68	0.93
7:X:13:LYS:HD3	7:X:19:VAL:HG23	1.51	0.93
2:L:102:ASP:OD1	2:L:103:PRO:HD3	1.70	0.92
6:R:93:ASP:O	6:R:97:SER:HA	1.68	0.91
7:P:49:MET:CE	7:P:95:TYR:CD1	2.40	0.90
7:P:13:LYS:HD3	7:P:19:VAL:HG23	1.51	0.89
7:W:49:MET:CE	7:W:95:TYR:CD1	2.42	0.88
3:A:331:ASN:HD22	3:A:362:VAL:HG23	1.38	0.87
3:C:106:PHE:HB3	3:C:235:ILE:HG21	1.58	0.86
5:K:83:PHE:CD1	5:K:104:VAL:HG12	2.11	0.86
3:A:405:ASP:HA	3:A:408:ARG:NE	1.90	0.85
3:C:328:ARG:HH11	3:C:533:LEU:CD1	1.90	0.85
5:U:83:PHE:CD1	5:U:104:VAL:HG12	2.11	0.85
5:V:83:PHE:CD1	5:V:104:VAL:HG12	2.11	0.84
3:A:328:ARG:HH11	3:A:533:LEU:CD1	1.91	0.83
3:B:328:ARG:HH11	3:B:533:LEU:CD1	1.91	0.83
3:A:1102:TRP:HB2	3:A:1135:ASN:ND2	1.93	0.83
3:C:328:ARG:NH1	3:C:533:LEU:CD1	2.42	0.83
3:A:328:ARG:NH1	3:A:533:LEU:CD1	2.43	0.82
3:A:327:VAL:HA	3:A:542:ASN:HB3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:327:VAL:HA	3:B:542:ASN:HB2	1.61	0.81
3:B:328:ARG:NH1	3:B:533:LEU:CD1	2.43	0.81
3:C:332:ILE:CG1	3:C:525:CYS:SG	2.69	0.81
3:C:328:ARG:NH1	3:C:533:LEU:CG	2.44	0.81
2:N:102:ASP:CG	3:B:408:ARG:HE	1.89	0.81
3:C:1102:TRP:HB2	3:C:1135:ASN:ND2	1.94	0.81
3:B:1102:TRP:HB2	3:B:1135:ASN:ND2	1.95	0.81
7:W:117:LEU:HD23	7:W:118:VAL:O	1.81	0.81
6:Q:43:THR:HG22	6:Q:44:ALA:N	1.92	0.81
3:A:115:GLN:HB2	3:A:233:ILE:CD1	2.12	0.80
5:U:83:PHE:HD1	5:U:104:VAL:HG12	1.47	0.80
3:B:115:GLN:HB2	3:B:233:ILE:CD1	2.12	0.80
3:C:327:VAL:HA	3:C:542:ASN:HB3	1.62	0.80
3:B:332:ILE:CG1	3:B:525:CYS:SG	2.69	0.80
3:A:962:LEU:HD11	3:A:1007:TYR:HB2	1.64	0.80
3:B:962:LEU:HD11	3:B:1007:TYR:HB2	1.64	0.80
7:P:117:LEU:HD23	7:P:118:VAL:O	1.81	0.80
3:B:328:ARG:NH1	3:B:533:LEU:CG	2.45	0.80
6:R:17:LYS:HD3	6:R:77:THR:HG22	1.65	0.79
3:A:328:ARG:NH1	3:A:533:LEU:CG	2.45	0.79
6:Q:17:LYS:HD3	6:Q:77:THR:HG22	1.65	0.79
7:P:117:LEU:CD2	7:P:118:VAL:O	2.31	0.79
6:S:17:LYS:HD3	6:S:77:THR:HG22	1.65	0.79
3:C:962:LEU:HD11	3:C:1007:TYR:HB2	1.64	0.78
7:W:117:LEU:CD2	7:W:118:VAL:O	2.31	0.78
6:Q:43:THR:CG2	6:Q:44:ALA:H	1.94	0.78
3:A:332:ILE:CG1	3:A:525:CYS:SG	2.71	0.78
5:K:83:PHE:HD1	5:K:104:VAL:HG12	1.47	0.78
3:C:107:GLY:H	3:C:235:ILE:HG23	1.50	0.77
3:B:977:LEU:HD22	3:B:993:ILE:HG12	1.66	0.77
7:X:39:ARG:HB2	7:X:47:GLU:HB2	1.68	0.77
3:C:977:LEU:HD22	3:C:993:ILE:HG12	1.66	0.77
3:A:977:LEU:HD22	3:A:993:ILE:HG12	1.66	0.76
7:X:11:GLU:OE1	7:X:19:VAL:HG11	1.85	0.76
7:P:5:LEU:HD22	7:P:24:LYS:CG	2.16	0.76
7:P:11:GLU:OE1	7:P:19:VAL:HG11	1.85	0.76
7:W:5:LEU:HD22	7:W:24:LYS:CG	2.16	0.75
7:W:39:ARG:HB2	7:W:47:GLU:HB2	1.67	0.75
7:X:5:LEU:HD22	7:X:24:LYS:CG	2.16	0.75
4:M:17:SER:HA	4:M:83:MET:O	1.87	0.74
4:I:2:GLN:N	4:I:25:SER:O	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:39:ARG:HB2	7:P:47:GLU:HB2	1.68	0.74
5:V:83:PHE:HD1	5:V:104:VAL:HG12	1.47	0.74
2:O:103:PRO:HA	2:O:105:TYR:CE2	2.23	0.74
4:T:2:GLN:N	4:T:25:SER:O	2.21	0.74
5:V:11:LEU:HD11	5:V:104:VAL:HG22	1.70	0.73
4:T:17:SER:HA	4:T:83:MET:O	1.87	0.73
5:K:11:LEU:HD11	5:K:104:VAL:HG22	1.70	0.73
3:B:570:ALA:HB2	3:C:963:VAL:HG13	1.69	0.73
3:A:319:ARG:NH1	3:B:745:ASP:OD1	2.21	0.73
4:M:2:GLN:N	4:M:25:SER:O	2.21	0.73
4:I:17:SER:HA	4:I:83:MET:O	1.87	0.73
2:O:6:GLN:HE22	2:O:95:TYR:HA	1.54	0.73
7:P:25:VAL:HG12	7:P:78:ASP:HB3	1.70	0.73
5:U:11:LEU:HD11	5:U:104:VAL:HG22	1.70	0.73
3:B:115:GLN:HB2	3:B:233:ILE:HD11	1.70	0.73
2:N:6:GLN:HE22	2:N:95:TYR:HA	1.54	0.72
3:A:115:GLN:HB2	3:A:233:ILE:HD11	1.69	0.72
2:L:6:GLN:HE22	2:L:95:TYR:HA	1.54	0.72
3:C:64:TRP:HE1	3:C:264:ALA:HB1	1.55	0.72
3:C:115:GLN:HB2	3:C:233:ILE:CD1	2.19	0.72
3:A:405:ASP:CB	3:A:408:ARG:CZ	2.68	0.72
3:A:733:LYS:NZ	3:A:775:ASP:OD1	2.23	0.72
3:A:64:TRP:HE1	3:A:264:ALA:HB1	1.55	0.72
7:X:25:VAL:HG12	7:X:78:ASP:HB3	1.70	0.72
3:C:86:PHE:HD2	3:C:235:ILE:O	1.73	0.71
3:B:733:LYS:NZ	3:B:775:ASP:OD1	2.23	0.71
3:C:97:LYS:HB3	3:C:187:LYS:HG2	1.72	0.71
3:B:97:LYS:HB3	3:B:187:LYS:HG2	1.72	0.71
7:W:25:VAL:HG12	7:W:78:ASP:HB3	1.70	0.71
3:A:666:ILE:HD11	3:A:672:ALA:HB2	1.73	0.71
3:B:64:TRP:HE1	3:B:264:ALA:HB1	1.55	0.71
3:B:708:SER:HB2	3:B:711:SER:OG	1.90	0.71
3:B:328:ARG:CZ	3:B:533:LEU:HD22	2.21	0.71
7:W:37:TRP:NE1	7:W:71:MET:SD	2.63	0.71
7:X:37:TRP:NE1	7:X:71:MET:SD	2.63	0.70
7:P:37:TRP:NE1	7:P:71:MET:SD	2.63	0.70
3:B:328:ARG:CZ	3:B:533:LEU:HB2	2.21	0.70
3:C:733:LYS:NZ	3:C:775:ASP:OD1	2.23	0.70
3:C:204:TYR:HA	3:C:225:PRO:HA	1.73	0.70
3:A:204:TYR:HA	3:A:225:PRO:HA	1.74	0.70
3:B:204:TYR:HA	3:B:225:PRO:HA	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:69:VAL:HG11	7:X:82:MET:HE3	1.73	0.70
3:C:328:ARG:CZ	3:C:533:LEU:HB2	2.21	0.70
3:A:328:ARG:CZ	3:A:533:LEU:HB2	2.21	0.70
2:N:103:PRO:HA	2:N:105:TYR:CE2	2.25	0.70
7:P:69:VAL:HG11	7:P:82:MET:HE3	1.73	0.70
3:A:328:ARG:CZ	3:A:533:LEU:HD22	2.21	0.70
5:U:11:LEU:O	5:U:11:LEU:HD12	1.92	0.70
5:V:11:LEU:HD12	5:V:11:LEU:O	1.91	0.70
3:B:666:ILE:HD11	3:B:672:ALA:HB2	1.73	0.70
3:C:666:ILE:HD11	3:C:672:ALA:HB2	1.73	0.70
3:A:97:LYS:HB3	3:A:187:LYS:HG2	1.72	0.69
7:W:36:HIS:HA	7:W:51:GLY:HA2	1.74	0.69
3:C:708:SER:HB2	3:C:711:SER:OG	1.90	0.69
3:A:878:LEU:HD11	3:A:1054:GLN:HE22	1.57	0.69
3:A:563:GLN:NE2	3:B:40:ASP:O	2.26	0.69
5:K:11:LEU:O	5:K:11:LEU:HD12	1.92	0.69
3:C:328:ARG:CZ	3:C:533:LEU:HD22	2.21	0.69
3:A:562:PHE:CD1	3:B:225:PRO:HG2	2.28	0.69
3:C:878:LEU:HD11	3:C:1054:GLN:HE22	1.57	0.69
7:X:36:HIS:HA	7:X:51:GLY:HA2	1.74	0.69
3:C:106:PHE:HB3	3:C:235:ILE:HD13	1.75	0.69
3:B:391:CYS:O	3:B:522:ALA:HB1	1.94	0.68
6:S:93:ASP:O	6:S:97:SER:CA	2.42	0.68
3:A:707:TYR:HB3	3:B:792:PRO:HG3	1.74	0.68
3:C:391:CYS:O	3:C:522:ALA:HB1	1.93	0.68
3:A:391:CYS:O	3:A:522:ALA:HB1	1.94	0.68
3:B:878:LEU:HD11	3:B:1054:GLN:HE22	1.57	0.68
6:R:93:ASP:O	6:R:97:SER:CA	2.42	0.68
7:P:36:HIS:HA	7:P:51:GLY:HA2	1.75	0.68
2:N:33:TYR:OH	3:B:378:LYS:NZ	2.26	0.68
6:Q:93:ASP:O	6:Q:97:SER:CA	2.42	0.67
3:A:40:ASP:O	3:C:563:GLN:NE2	2.26	0.67
3:A:1104:VAL:HG23	3:A:1115:ILE:HG12	1.76	0.67
3:B:1104:VAL:HG23	3:B:1115:ILE:HG12	1.76	0.67
7:P:98:ALA:HB1	7:P:109:PHE:HB2	1.76	0.67
3:B:1039:ARG:NE	3:C:1031:GLU:OE2	2.24	0.67
3:A:331:ASN:HD22	3:A:362:VAL:CG2	2.07	0.67
3:A:69:HIS:HB3	3:A:78:ARG:HB2	1.77	0.67
3:A:963:VAL:HG13	3:C:570:ALA:HB2	1.75	0.66
7:W:69:VAL:HG21	7:W:82:MET:CE	2.25	0.66
3:A:541:PHE:HB3	3:A:552:LEU:HD11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:69:HIS:HB3	3:C:78:ARG:HB2	1.77	0.66
3:C:722:VAL:HG22	3:C:930:ALA:HB1	1.78	0.66
3:C:424:LYS:H	3:C:461:LEU:HD22	1.61	0.66
3:A:804:GLN:OE1	3:A:935:GLN:NE2	2.29	0.66
3:B:707:TYR:HB3	3:C:792:PRO:HG3	1.78	0.66
3:B:106:PHE:HB3	3:B:235:ILE:HG21	1.77	0.66
7:W:98:ALA:HB1	7:W:109:PHE:HB2	1.76	0.66
3:B:804:GLN:OE1	3:B:935:GLN:NE2	2.29	0.66
3:C:804:GLN:OE1	3:C:935:GLN:NE2	2.29	0.66
3:C:1104:VAL:HG23	3:C:1115:ILE:HG12	1.76	0.66
3:B:87:ASN:HB3	8:a:2:NAG:H82	1.78	0.66
3:B:541:PHE:HB3	3:B:552:LEU:HD11	1.78	0.65
7:P:11:GLU:OE1	7:P:19:VAL:CG1	2.43	0.65
3:C:22:THR:HG21	3:C:78:ARG:HD2	1.78	0.65
7:X:11:GLU:OE1	7:X:19:VAL:CG1	2.43	0.65
3:C:541:PHE:HB3	3:C:552:LEU:HD11	1.78	0.65
3:B:69:HIS:HB3	3:B:78:ARG:HB2	1.77	0.65
3:B:961:THR:HG21	3:C:762:GLN:HE21	1.61	0.65
7:X:54:PRO:HB3	7:X:104:SER:HA	1.79	0.65
7:X:98:ALA:HB1	7:X:109:PHE:HB2	1.76	0.65
3:A:22:THR:HG21	3:A:78:ARG:HD2	1.78	0.65
3:C:115:GLN:HE22	3:C:167:THR:HG23	1.62	0.65
3:C:352:ALA:HA	3:C:466:ARG:HD3	1.78	0.65
3:C:376:THR:HB	3:C:435:ALA:HB3	1.79	0.65
3:A:424:LYS:H	3:A:461:LEU:HD22	1.61	0.65
3:A:115:GLN:HE22	3:A:167:THR:HG23	1.62	0.65
3:A:722:VAL:HG22	3:A:930:ALA:HB1	1.78	0.65
3:B:376:THR:HB	3:B:435:ALA:HB3	1.79	0.65
3:B:115:GLN:HE22	3:B:167:THR:HG23	1.62	0.64
7:W:54:PRO:HB3	7:W:104:SER:HA	1.79	0.64
3:C:578:ASP:OD1	3:C:581:THR:N	2.31	0.64
3:A:578:ASP:OD1	3:A:581:THR:N	2.30	0.64
3:B:352:ALA:HA	3:B:466:ARG:HD3	1.79	0.64
3:B:722:VAL:HG22	3:B:930:ALA:HB1	1.78	0.64
3:A:352:ALA:HA	3:A:466:ARG:HD3	1.78	0.64
4:T:68:PHE:HD1	4:T:83:MET:HA	1.63	0.64
3:B:578:ASP:OD1	3:B:581:THR:N	2.31	0.64
3:B:332:ILE:HD11	3:B:528:LYS:HE3	1.80	0.64
7:W:87:LEU:HD21	7:W:120:VAL:HA	1.80	0.64
7:X:87:LEU:HD21	7:X:120:VAL:HA	1.80	0.64
2:L:60:ASP:OD2	2:L:65:LYS:NZ	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:54:PRO:HB3	7:P:104:SER:HA	1.79	0.64
3:C:905:ARG:NH1	3:C:1049:LEU:O	2.31	0.64
2:L:102:ASP:CG	2:L:103:PRO:CD	2.60	0.64
3:A:332:ILE:HD11	3:A:528:LYS:HE3	1.80	0.64
3:A:350:VAL:HG13	3:A:422:ASN:HB3	1.80	0.64
3:B:424:LYS:H	3:B:461:LEU:HD22	1.60	0.64
3:B:22:THR:HG21	3:B:78:ARG:HD2	1.78	0.64
4:M:68:PHE:HD1	4:M:83:MET:HA	1.63	0.64
7:X:69:VAL:HG11	7:X:82:MET:CE	2.27	0.64
3:C:332:ILE:HD11	3:C:528:LYS:HE3	1.80	0.64
3:A:106:PHE:HB3	3:A:235:ILE:HG21	1.79	0.63
4:I:68:PHE:HD1	4:I:83:MET:HA	1.63	0.63
3:B:905:ARG:NH1	3:B:1049:LEU:O	2.31	0.63
7:P:53:ASP:HA	7:P:60:MET:HE2	1.80	0.63
3:C:350:VAL:HG13	3:C:422:ASN:HB3	1.80	0.63
3:A:376:THR:HB	3:A:435:ALA:HB3	1.79	0.63
7:P:69:VAL:HG11	7:P:82:MET:CE	2.27	0.63
7:W:49:MET:HA	7:W:62:ALA:HB2	1.81	0.63
7:P:13:LYS:HD3	7:P:19:VAL:CG2	2.26	0.63
7:P:34:ALA:HB1	7:P:52:PHE:HB3	1.81	0.63
7:P:87:LEU:HD21	7:P:120:VAL:HA	1.80	0.63
2:O:60:ASP:OD2	2:O:65:LYS:NZ	2.31	0.63
4:M:38:ARG:HH12	4:M:64:VAL:HG11	1.64	0.63
3:A:326:ILE:HD11	3:A:534:VAL:HG12	1.80	0.63
3:B:350:VAL:HG13	3:B:422:ASN:HB3	1.80	0.63
7:X:53:ASP:HA	7:X:60:MET:HE2	1.80	0.63
7:X:13:LYS:HD3	7:X:19:VAL:CG2	2.26	0.62
7:W:11:GLU:OE1	7:W:19:VAL:HG21	1.98	0.62
7:P:49:MET:HA	7:P:62:ALA:HB2	1.81	0.62
3:B:326:ILE:HD11	3:B:534:VAL:HG12	1.80	0.62
3:B:335:LEU:HA	3:B:362:VAL:HB	1.81	0.62
3:B:361:CYS:HB3	3:B:524:VAL:HG13	1.81	0.62
4:I:38:ARG:HH12	4:I:64:VAL:HG11	1.64	0.62
3:B:135:PHE:HA	3:B:160:TYR:HA	1.82	0.62
7:W:34:ALA:HB1	7:W:52:PHE:HB3	1.81	0.62
7:X:49:MET:HA	7:X:62:ALA:HB2	1.80	0.62
2:N:60:ASP:OD2	2:N:65:LYS:NZ	2.31	0.62
7:W:53:ASP:HA	7:W:60:MET:HE2	1.80	0.62
3:C:326:ILE:HD11	3:C:534:VAL:HG12	1.80	0.62
1:E:90:THR:OG1	1:E:91:ASN:N	2.33	0.62
3:B:107:GLY:H	3:B:235:ILE:HG23	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:65:PHE:O	7:W:69:VAL:HG12	1.98	0.62
7:X:34:ALA:HB1	7:X:52:PHE:HB3	1.81	0.62
3:C:335:LEU:HA	3:C:362:VAL:HB	1.81	0.62
7:W:37:TRP:HB2	7:W:49:MET:HG3	1.82	0.62
3:A:405:ASP:HA	3:A:408:ARG:HE	1.65	0.62
4:T:38:ARG:HH12	4:T:64:VAL:HG11	1.64	0.62
7:X:37:TRP:HB2	7:X:49:MET:HG3	1.81	0.62
7:P:37:TRP:HB2	7:P:49:MET:HG3	1.81	0.62
3:B:391:CYS:SG	3:B:522:ALA:CB	2.88	0.61
3:A:905:ARG:NH1	3:A:1049:LEU:O	2.31	0.61
5:V:91:SER:HA	5:V:96:ARG:HE	1.64	0.61
7:W:51:GLY:O	7:W:60:MET:N	2.33	0.61
3:B:718:PHE:CG	3:B:1067:TYR:CE1	2.88	0.61
7:X:51:GLY:O	7:X:60:MET:N	2.33	0.61
3:C:107:GLY:N	3:C:235:ILE:HG23	2.16	0.61
3:A:361:CYS:HB3	3:A:524:VAL:HG13	1.81	0.61
3:A:391:CYS:SG	3:A:522:ALA:CB	2.88	0.61
3:A:904:TYR:OH	3:C:1094:VAL:HG22	2.00	0.61
7:P:51:GLY:O	7:P:60:MET:N	2.33	0.61
3:C:391:CYS:SG	3:C:522:ALA:CB	2.88	0.61
3:A:335:LEU:HA	3:A:362:VAL:HB	1.81	0.61
7:P:68:ARG:HH22	7:P:88:ARG:HD3	1.66	0.61
3:C:361:CYS:HB3	3:C:524:VAL:HG13	1.81	0.61
3:A:108:THR:HA	3:A:236:THR:HG22	1.83	0.61
3:A:970:PHE:HD1	3:A:996:LEU:HD23	1.66	0.61
3:C:108:THR:HA	3:C:236:THR:HG22	1.83	0.61
3:B:720:ILE:HG13	3:B:923:ILE:HG23	1.83	0.61
3:C:763:LEU:HD22	3:C:1008:VAL:HG11	1.83	0.61
7:W:68:ARG:HH22	7:W:88:ARG:HD3	1.66	0.61
3:B:970:PHE:HD1	3:B:996:LEU:HD23	1.66	0.61
7:W:69:VAL:HG21	7:W:82:MET:HE3	1.82	0.61
1:H:10:GLN:HB3	1:H:103:LEU:HA	1.83	0.60
3:A:87:ASN:HB3	8:F:2:NAG:H82	1.82	0.60
3:A:107:GLY:H	3:A:235:ILE:HG23	1.66	0.60
3:A:135:PHE:HA	3:A:160:TYR:HA	1.82	0.60
2:L:102:ASP:OD2	3:A:408:ARG:NE	2.34	0.60
7:W:11:GLU:OE1	7:W:19:VAL:CG2	2.49	0.60
7:X:68:ARG:HH22	7:X:88:ARG:HD3	1.66	0.60
3:C:970:PHE:HD1	3:C:996:LEU:HD23	1.66	0.60
1:D:10:GLN:HB3	1:D:103:LEU:HA	1.83	0.60
3:B:331:ASN:OD1	3:B:527:PRO:HA	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:763:LEU:HD22	3:B:1008:VAL:HG11	1.83	0.60
3:C:135:PHE:HA	3:C:160:TYR:HA	1.82	0.60
3:C:330:PRO:C	3:C:332:ILE:H	2.10	0.60
3:C:720:ILE:HG13	3:C:923:ILE:HG23	1.83	0.60
3:C:1102:TRP:HB2	3:C:1135:ASN:HD22	1.65	0.60
3:A:718:PHE:CG	3:A:1067:TYR:CE1	2.90	0.60
3:B:108:THR:HA	3:B:236:THR:HG22	1.83	0.60
3:A:298:GLU:O	3:A:302:THR:HG23	2.02	0.60
3:C:391:CYS:SG	3:C:522:ALA:HB1	2.42	0.60
3:A:763:LEU:HD22	3:A:1008:VAL:HG11	1.83	0.60
1:E:10:GLN:HB3	1:E:103:LEU:HA	1.83	0.59
3:A:391:CYS:SG	3:A:522:ALA:HB1	2.42	0.59
3:C:578:ASP:OD1	3:C:580:GLN:N	2.35	0.59
3:B:391:CYS:SG	3:B:522:ALA:HB1	2.42	0.59
3:B:975:SER:O	3:B:1000:ARG:NH2	2.36	0.59
3:A:327:VAL:HG23	3:A:542:ASN:HD22	1.67	0.59
3:A:975:SER:O	3:A:1000:ARG:NH2	2.36	0.59
4:M:4:LEU:O	4:M:111:GLN:NE2	2.35	0.59
3:B:40:ASP:OD2	3:B:44:ARG:NH1	2.36	0.59
3:A:1102:TRP:HB2	3:A:1135:ASN:HD22	1.64	0.59
3:B:96:GLU:OE2	3:B:264:ALA:N	2.36	0.59
3:C:718:PHE:CG	3:C:1067:TYR:CE1	2.90	0.59
3:A:40:ASP:OD2	3:A:44:ARG:NH1	2.36	0.59
3:B:236:THR:HG23	3:B:237:ARG:HG3	1.84	0.59
3:B:298:GLU:O	3:B:302:THR:HG23	2.02	0.59
3:A:720:ILE:HG13	3:A:923:ILE:HG23	1.83	0.59
3:A:551:VAL:HG23	3:A:590:CYS:HB3	1.84	0.59
3:C:236:THR:HG23	3:C:237:ARG:HG3	1.84	0.59
3:C:551:VAL:HG23	3:C:590:CYS:HB3	1.84	0.59
3:C:975:SER:O	3:C:1000:ARG:NH2	2.36	0.59
6:S:5:THR:HB	6:S:23:SER:HB3	1.85	0.59
3:C:110:LEU:HB3	3:C:135:PHE:HD2	1.68	0.59
3:C:327:VAL:HG23	3:C:542:ASN:HD22	1.67	0.59
3:B:330:PRO:C	3:B:332:ILE:H	2.09	0.59
3:C:96:GLU:OE2	3:C:264:ALA:N	2.36	0.59
7:W:7:GLN:NE2	7:W:97:CYS:H	2.01	0.58
7:W:56:ASP:HB3	7:W:58:GLU:HG2	1.85	0.58
7:X:56:ASP:HB3	7:X:58:GLU:HG2	1.85	0.58
3:B:110:LEU:HB3	3:B:135:PHE:HD2	1.68	0.58
3:B:331:ASN:HA	3:B:526:GLY:O	2.03	0.58
3:C:40:ASP:OD2	3:C:44:ARG:NH1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:331:ASN:HA	3:C:526:GLY:O	2.03	0.58
3:A:110:LEU:HB3	3:A:135:PHE:HD2	1.68	0.58
3:A:330:PRO:C	3:A:332:ILE:H	2.09	0.58
3:B:551:VAL:HG23	3:B:590:CYS:HB3	1.84	0.58
3:B:578:ASP:OD1	3:B:580:GLN:N	2.36	0.58
3:C:298:GLU:O	3:C:302:THR:HG23	2.02	0.58
4:T:101:THR:OG1	3:B:484:GLU:OE1	2.20	0.58
7:P:7:GLN:NE2	7:P:97:CYS:H	2.01	0.58
3:C:191:GLU:O	3:C:205:SER:HA	2.04	0.58
2:L:93:VAL:HA	2:L:115:THR:HA	1.86	0.58
2:N:93:VAL:HA	2:N:115:THR:HA	1.86	0.58
3:A:96:GLU:OE2	3:A:264:ALA:N	2.36	0.58
5:K:94:THR:OG1	5:K:96:ARG:NH1	2.37	0.58
3:B:332:ILE:HG13	3:B:525:CYS:SG	2.44	0.58
7:P:44:LYS:HG2	7:P:45:GLY:H	1.69	0.58
2:N:87:ARG:NE	2:N:89:GLU:OE1	2.36	0.58
3:A:150:LYS:NZ	7:P:54:PRO:O	2.35	0.58
3:A:236:THR:HG23	3:A:237:ARG:HG3	1.84	0.58
6:R:86:ASP:HB3	6:R:106:LYS:HE2	1.86	0.58
3:C:106:PHE:HB3	3:C:235:ILE:CG2	2.32	0.58
3:A:578:ASP:OD1	3:A:580:GLN:N	2.35	0.58
3:B:191:GLU:O	3:B:205:SER:HA	2.04	0.58
6:S:86:ASP:HB3	6:S:106:LYS:HE2	1.86	0.58
6:R:5:THR:HB	6:R:23:SER:HB3	1.85	0.58
3:A:331:ASN:HA	3:A:526:GLY:O	2.03	0.57
3:A:644:GLN:NE2	3:A:645:THR:O	2.36	0.57
3:B:131:CYS:HA	3:B:166:CYS:HA	1.86	0.57
3:B:660:TYR:HE2	3:B:675:GLN:HE22	1.51	0.57
7:P:58:GLU:OE2	7:P:59:THR:O	2.21	0.57
2:L:67:ALA:HB3	2:L:84:SER:HB2	1.86	0.57
7:X:7:GLN:NE2	7:X:97:CYS:H	2.01	0.57
3:C:214:ARG:O	3:C:266:TYR:OH	2.20	0.57
3:C:398:ASP:OD2	3:C:423:TYR:OH	2.21	0.57
2:N:67:ALA:HB3	2:N:84:SER:HB2	1.86	0.57
3:A:191:GLU:O	3:A:205:SER:HA	2.04	0.57
2:O:93:VAL:HA	2:O:115:THR:HA	1.86	0.57
3:A:472:ILE:HA	3:A:491:PRO:HD3	1.86	0.57
5:U:94:THR:OG1	5:U:96:ARG:NH1	2.37	0.57
7:X:44:LYS:HG2	7:X:45:GLY:H	1.69	0.57
3:C:644:GLN:NE2	3:C:645:THR:O	2.36	0.57
2:O:87:ARG:NE	2:O:89:GLU:OE1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:5:THR:HB	6:Q:23:SER:HB3	1.84	0.57
2:L:87:ARG:NE	2:L:89:GLU:OE1	2.35	0.57
2:N:65:LYS:HE3	3:B:385:THR:HG21	1.86	0.57
7:W:44:LYS:HG2	7:W:45:GLY:H	1.68	0.57
7:X:52:PHE:HA	7:X:59:THR:HA	1.87	0.57
4:I:4:LEU:O	4:I:111:GLN:NE2	2.35	0.57
3:B:563:GLN:NE2	3:C:40:ASP:O	2.36	0.57
3:C:332:ILE:HG13	3:C:525:CYS:SG	2.43	0.57
2:O:67:ALA:HB3	2:O:84:SER:HB2	1.86	0.57
3:A:332:ILE:HD11	3:A:528:LYS:CE	2.35	0.57
3:C:356:LYS:HB2	3:C:397:ALA:HB3	1.87	0.57
3:A:405:ASP:CA	3:A:408:ARG:NE	2.64	0.57
3:B:326:ILE:O	3:B:542:ASN:N	2.38	0.57
3:B:472:ILE:HA	3:B:491:PRO:HD3	1.86	0.57
3:C:115:GLN:HB2	3:C:233:ILE:HD11	1.87	0.57
3:C:131:CYS:HA	3:C:166:CYS:HA	1.86	0.57
4:I:35:HIS:CD2	4:I:50:VAL:HG13	2.40	0.56
3:A:660:TYR:HE2	3:A:675:GLN:HE22	1.51	0.56
3:C:87:ASN:HB3	8:f:2:NAG:H82	1.87	0.56
3:C:326:ILE:O	3:C:542:ASN:N	2.38	0.56
3:A:131:CYS:HA	3:A:166:CYS:HA	1.86	0.56
4:M:35:HIS:CD2	4:M:50:VAL:HG13	2.41	0.56
5:K:33:LEU:HB3	5:K:51:ALA:HB2	1.88	0.56
3:B:180:GLU:HA	3:B:186:PHE:CE2	2.41	0.56
3:B:398:ASP:OD2	3:B:423:TYR:OH	2.21	0.56
6:Q:56:PRO:HD2	6:Q:59:ILE:HG13	1.87	0.56
3:C:564:GLN:NE2	3:C:577:ARG:HB3	2.21	0.56
3:A:502:GLY:O	3:A:506:GLN:N	2.38	0.56
7:P:52:PHE:HA	7:P:59:THR:HA	1.87	0.56
1:H:17:LYS:HA	1:H:75:ASN:HA	1.88	0.56
2:N:35:HIS:CD2	2:N:99:SER:HB2	2.41	0.56
3:A:326:ILE:O	3:A:542:ASN:N	2.38	0.56
7:W:117:LEU:HD21	7:W:118:VAL:O	2.06	0.56
3:C:180:GLU:HA	3:C:186:PHE:CE2	2.41	0.56
3:C:410:ILE:HD11	3:C:418:ILE:HG22	1.87	0.56
3:A:180:GLU:HA	3:A:186:PHE:CE2	2.41	0.56
4:T:35:HIS:CD2	4:T:50:VAL:HG13	2.40	0.56
3:C:660:TYR:HE2	3:C:675:GLN:HE22	1.51	0.56
2:O:47:TRP:O	2:O:61:ASN:ND2	2.34	0.56
5:U:33:LEU:HB3	5:U:51:ALA:HB2	1.88	0.56
4:T:4:LEU:O	4:T:111:GLN:NE2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:332:ILE:HD11	3:B:528:LYS:CE	2.36	0.56
6:R:56:PRO:HD2	6:R:59:ILE:HG13	1.87	0.56
7:W:52:PHE:HA	7:W:59:THR:HA	1.87	0.56
1:D:17:LYS:HA	1:D:75:ASN:HA	1.88	0.56
3:A:147:LYS:HE2	7:P:52:PHE:CE2	2.40	0.56
3:A:398:ASP:OD2	3:A:423:TYR:OH	2.21	0.56
3:A:564:GLN:NE2	3:A:577:ARG:HB3	2.21	0.56
3:A:650:LEU:HD11	3:A:666:ILE:HD13	1.87	0.56
3:B:502:GLY:O	3:B:506:GLN:N	2.38	0.56
3:C:1106:GLN:NE2	3:C:1111:GLU:OE1	2.39	0.56
6:S:56:PRO:HD2	6:S:59:ILE:HG13	1.87	0.56
6:Q:86:ASP:HB3	6:Q:106:LYS:HE2	1.86	0.56
2:O:35:HIS:CD2	2:O:99:SER:HB2	2.41	0.56
3:A:356:LYS:HB2	3:A:397:ALA:HB3	1.87	0.56
3:A:410:ILE:HD11	3:A:418:ILE:HG22	1.87	0.56
3:A:1106:GLN:NE2	3:A:1111:GLU:OE1	2.39	0.56
4:M:91:THR:HG23	4:M:116:THR:HA	1.88	0.56
6:S:84:GLU:HG2	6:S:109:VAL:H	1.71	0.56
3:C:332:ILE:HD11	3:C:528:LYS:CE	2.36	0.56
4:T:91:THR:HG23	4:T:116:THR:HA	1.88	0.55
4:I:60:TYR:HD2	4:I:65:LYS:HZ2	1.55	0.55
3:A:922:LEU:HD11	8:G:1:NAG:H5	1.88	0.55
5:U:9:SER:HG	5:U:100:GLN:HE21	1.53	0.55
3:B:410:ILE:HD11	3:B:418:ILE:HG22	1.87	0.55
3:C:472:ILE:HA	3:C:491:PRO:HD3	1.86	0.55
1:H:60:ARG:O	1:H:75:ASN:N	2.39	0.55
2:L:102:ASP:OD1	3:A:408:ARG:HG2	2.06	0.55
3:A:130:VAL:HB	3:A:168:PHE:HB3	1.89	0.55
3:A:146:HIS:CE1	3:A:148:ASN:HB2	2.42	0.55
3:B:564:GLN:NE2	3:B:577:ARG:HB3	2.21	0.55
3:C:502:GLY:O	3:C:506:GLN:N	2.38	0.55
5:V:33:LEU:HB3	5:V:51:ALA:HB2	1.88	0.55
3:B:644:GLN:NE2	3:B:645:THR:O	2.36	0.55
3:B:650:LEU:HD11	3:B:666:ILE:HD13	1.87	0.55
3:C:193:VAL:HG23	3:C:223:LEU:HD22	1.88	0.55
3:A:193:VAL:HG23	3:A:223:LEU:HD22	1.88	0.55
3:C:196:ASN:ND2	3:C:235:ILE:H	2.04	0.55
1:E:60:ARG:O	1:E:75:ASN:N	2.39	0.55
3:A:332:ILE:HG13	3:A:525:CYS:SG	2.47	0.55
2:L:35:HIS:CD2	2:L:99:SER:HB2	2.41	0.55
3:A:496:GLY:O	3:A:501:ASN:ND2	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:60:TYR:HD2	4:T:65:LYS:HZ2	1.54	0.55
3:B:1102:TRP:HB2	3:B:1135:ASN:HD22	1.66	0.55
3:C:546:LEU:HD21	3:C:573:THR:HG21	1.89	0.55
1:E:17:LYS:HA	1:E:75:ASN:HA	1.88	0.55
3:A:546:LEU:HD21	3:A:573:THR:HG21	1.89	0.55
7:X:13:LYS:HD2	7:X:17:ALA:HB3	1.89	0.55
4:I:91:THR:HG23	4:I:116:THR:HA	1.88	0.55
3:B:146:HIS:CE1	3:B:148:ASN:HB2	2.42	0.55
3:B:1106:GLN:NE2	3:B:1111:GLU:OE1	2.39	0.55
3:C:650:LEU:HD11	3:C:666:ILE:HD13	1.87	0.55
1:D:90:THR:OG1	1:D:91:ASN:N	2.33	0.55
3:A:405:ASP:HA	3:A:408:ARG:CD	2.37	0.55
3:B:356:LYS:HB2	3:B:397:ALA:HB3	1.87	0.55
3:B:546:LEU:HD21	3:B:573:THR:HG21	1.89	0.55
1:D:60:ARG:O	1:D:75:ASN:N	2.39	0.54
2:L:47:TRP:O	2:L:61:ASN:ND2	2.34	0.54
3:B:193:VAL:HG23	3:B:223:LEU:HD22	1.88	0.54
3:B:295:PRO:HB2	3:B:608:VAL:HG11	1.89	0.54
7:W:8:SER:OG	7:W:21:VAL:HA	2.08	0.54
7:W:13:LYS:HD2	7:W:17:ALA:HB3	1.89	0.54
7:P:8:SER:OG	7:P:21:VAL:HA	2.08	0.54
3:C:146:HIS:CE1	3:C:148:ASN:HB2	2.42	0.54
3:B:597:VAL:HG13	3:B:608:VAL:HG13	1.90	0.54
3:C:105:ILE:HD11	3:C:239:GLN:HB3	1.90	0.54
2:N:102:ASP:O	2:N:105:TYR:CE1	2.60	0.54
4:I:68:PHE:HA	4:I:82:GLN:O	2.08	0.54
3:C:597:VAL:HG13	3:C:608:VAL:HG13	1.90	0.54
2:O:102:ASP:O	2:O:105:TYR:CE1	2.61	0.54
3:C:130:VAL:HB	3:C:168:PHE:HB3	1.89	0.54
4:M:60:TYR:HD2	4:M:65:LYS:HZ2	1.54	0.54
7:P:13:LYS:HD2	7:P:17:ALA:HB3	1.89	0.54
3:A:597:VAL:HG13	3:A:608:VAL:HG13	1.90	0.54
6:R:84:GLU:HG2	6:R:109:VAL:H	1.73	0.54
7:P:117:LEU:HD21	7:P:118:VAL:O	2.06	0.54
7:W:35:MET:O	7:W:52:PHE:N	2.40	0.54
2:O:47:TRP:HZ2	2:O:50:TYR:HD1	1.56	0.53
4:T:68:PHE:HA	4:T:82:GLN:O	2.08	0.53
3:B:130:VAL:HB	3:B:168:PHE:HB3	1.88	0.53
3:C:391:CYS:SG	3:C:522:ALA:HB3	2.48	0.53
2:N:47:TRP:HZ2	2:N:50:TYR:HD1	1.56	0.53
3:A:391:CYS:SG	3:A:522:ALA:HB3	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:8:SER:OG	7:X:21:VAL:HA	2.08	0.53
3:C:186:PHE:HD2	3:C:187:LYS:H	1.57	0.53
2:N:30:SER:HA	2:N:53:PRO:HB2	1.91	0.53
3:A:186:PHE:HD2	3:A:187:LYS:H	1.57	0.53
3:A:533:LEU:HD21	3:A:585:LEU:HD21	1.90	0.53
3:B:186:PHE:HD2	3:B:187:LYS:H	1.57	0.53
7:X:30:LEU:N	7:X:78:ASP:OD1	2.41	0.53
6:Q:99:VAL:HG13	7:P:107:TYR:OH	2.07	0.53
7:P:35:MET:O	7:P:52:PHE:N	2.40	0.53
3:C:106:PHE:CB	3:C:235:ILE:HD13	2.37	0.53
3:C:295:PRO:HB2	3:C:608:VAL:HG11	1.90	0.53
2:O:13:LYS:CE	2:O:16:ALA:CB	2.81	0.53
3:A:278:LYS:HB3	3:A:287:ASP:HB3	1.91	0.53
3:B:139:PRO:HD2	3:B:239:GLN:HE22	1.74	0.53
3:B:496:GLY:O	3:B:501:ASN:ND2	2.33	0.53
3:B:533:LEU:HD21	3:B:585:LEU:HD21	1.90	0.53
7:X:35:MET:O	7:X:52:PHE:N	2.40	0.53
6:Q:66:SER:OG	6:Q:73:THR:OG1	2.26	0.53
6:Q:53:ASN:OD1	6:Q:54:LYS:HG2	2.08	0.53
2:L:33:TYR:HA	2:L:53:PRO:HD3	1.91	0.53
3:A:431:GLY:HA2	3:A:515:PHE:H	1.74	0.53
3:B:431:GLY:HA2	3:B:515:PHE:H	1.74	0.53
7:X:3:GLN:O	7:X:26:SER:OG	2.23	0.53
6:Q:84:GLU:HG2	6:Q:109:VAL:H	1.73	0.53
3:C:538:CYS:HA	3:C:550:GLY:O	2.09	0.53
7:X:37:TRP:CZ3	7:X:97:CYS:HB2	2.43	0.53
3:A:105:ILE:HD11	3:A:239:GLN:HB3	1.90	0.53
3:A:139:PRO:HD2	3:A:239:GLN:HE22	1.74	0.53
3:A:295:PRO:HB2	3:A:608:VAL:HG11	1.90	0.53
3:A:570:ALA:HB2	3:B:963:VAL:HG13	1.89	0.53
3:B:27:ALA:HB3	3:B:64:TRP:HE3	1.74	0.53
3:B:145:TYR:OH	3:B:150:LYS:HD2	2.09	0.53
7:P:37:TRP:CZ3	7:P:97:CYS:HB2	2.43	0.53
3:C:676:THR:OG1	3:C:689:SER:OG	2.27	0.53
3:A:1032:CYS:HB3	3:A:1043:CYS:SG	2.49	0.53
6:R:68:SER:HG	6:R:71:SER:HG	1.55	0.53
4:M:68:PHE:HA	4:M:82:GLN:O	2.08	0.53
3:B:391:CYS:SG	3:B:522:ALA:HB3	2.48	0.53
2:L:47:TRP:HZ2	2:L:50:TYR:HD1	1.56	0.52
3:B:538:CYS:HA	3:B:550:GLY:O	2.09	0.52
6:S:10:VAL:HG23	6:S:107:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:30:LEU:N	7:P:78:ASP:OD1	2.41	0.52
3:C:984:LEU:HD13	3:C:988:GLU:HG3	1.91	0.52
2:O:33:TYR:HA	2:O:53:PRO:HD3	1.91	0.52
4:I:47:TRP:HZ2	4:I:50:VAL:HG23	1.74	0.52
3:C:533:LEU:HD21	3:C:585:LEU:HD21	1.90	0.52
3:C:1032:CYS:HB3	3:C:1043:CYS:SG	2.49	0.52
3:B:278:LYS:HB3	3:B:287:ASP:HB3	1.91	0.52
7:W:37:TRP:CZ3	7:W:97:CYS:HB2	2.43	0.52
3:B:105:ILE:HD11	3:B:239:GLN:HB3	1.90	0.52
6:R:66:SER:OG	6:R:73:THR:OG1	2.26	0.52
3:C:27:ALA:HB3	3:C:64:TRP:HE3	1.74	0.52
3:C:145:TYR:OH	3:C:150:LYS:HD2	2.09	0.52
3:C:278:LYS:HB3	3:C:287:ASP:HB3	1.91	0.52
1:E:65:GLY:HA3	1:E:70:PHE:HA	1.92	0.52
3:A:145:TYR:CE2	7:P:103:PHE:HA	2.44	0.52
3:B:1032:CYS:HB3	3:B:1043:CYS:SG	2.49	0.52
3:C:213:VAL:HG23	3:C:214:ARG:H	1.75	0.52
1:H:79:ALA:HA	1:H:82:PHE:CE2	2.45	0.52
2:O:30:SER:HA	2:O:53:PRO:HB2	1.91	0.52
3:A:145:TYR:OH	3:A:150:LYS:HD2	2.09	0.52
3:A:405:ASP:HA	3:A:408:ARG:HG3	1.91	0.52
3:B:303:LEU:HD13	3:B:306:PHE:CE2	2.44	0.52
6:S:66:SER:OG	6:S:73:THR:OG1	2.26	0.52
7:X:110:ASP:HB2	7:X:111:PRO:HD3	1.92	0.52
3:A:676:THR:OG1	3:A:689:SER:OG	2.27	0.52
3:B:676:THR:OG1	3:B:689:SER:OG	2.27	0.52
7:X:49:MET:HE1	7:X:95:TYR:CE1	2.30	0.52
3:C:398:ASP:HB2	3:C:512:VAL:HB	1.91	0.52
3:A:27:ALA:HB3	3:A:64:TRP:HE3	1.74	0.52
3:A:303:LEU:HD13	3:A:306:PHE:CE2	2.45	0.52
3:A:538:CYS:HA	3:A:550:GLY:O	2.09	0.52
3:B:34:ARG:NH2	3:B:217:PRO:HG2	2.25	0.52
3:C:139:PRO:HD2	3:C:239:GLN:HE22	1.74	0.52
1:H:65:GLY:HA3	1:H:70:PHE:HA	1.92	0.52
1:E:79:ALA:HA	1:E:82:PHE:CE2	2.45	0.52
3:A:392:PHE:CD1	3:A:517:LEU:HG	2.45	0.52
5:V:25:ALA:O	5:V:69:THR:OG1	2.27	0.52
3:B:961:THR:CG2	3:C:762:GLN:HE21	2.21	0.52
6:Q:68:SER:HG	6:Q:71:SER:HG	1.54	0.52
3:A:278:LYS:HD3	3:A:287:ASP:HB3	1.92	0.52
3:A:1089:PHE:HE2	3:B:917:TYR:HD1	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:100:THR:HB	7:X:106:SER:OG	2.10	0.52
6:Q:99:VAL:HG13	7:P:107:TYR:CZ	2.45	0.52
2:L:30:SER:HA	2:L:53:PRO:HB2	1.91	0.51
3:A:34:ARG:NH2	3:A:217:PRO:HG2	2.25	0.51
3:A:105:ILE:HG12	3:A:239:GLN:O	2.10	0.51
3:A:180:GLU:O	3:A:182:LYS:N	2.43	0.51
4:T:47:TRP:HZ2	4:T:50:VAL:HG23	1.75	0.51
5:K:32:TYR:HD2	5:K:92:TYR:HA	1.75	0.51
3:B:106:PHE:HB3	3:B:235:ILE:HD13	1.91	0.51
3:B:214:ARG:O	3:B:266:TYR:OH	2.20	0.51
7:P:3:GLN:O	7:P:26:SER:OG	2.23	0.51
2:N:102:ASP:C	2:N:104:TYR:H	2.17	0.51
3:A:213:VAL:HG23	3:A:214:ARG:H	1.75	0.51
3:B:580:GLN:HG2	3:B:581:THR:H	1.75	0.51
3:B:984:LEU:HD13	3:B:988:GLU:HG3	1.91	0.51
3:C:303:LEU:HD13	3:C:306:PHE:CE2	2.44	0.51
3:C:974:SER:H	3:C:980:ILE:HD11	1.76	0.51
3:A:592:PHE:CZ	3:B:855:PHE:HA	2.46	0.51
3:A:762:GLN:HE21	3:C:961:THR:HG21	1.75	0.51
3:A:984:LEU:HD13	3:A:988:GLU:HG3	1.91	0.51
3:B:105:ILE:HG12	3:B:239:GLN:O	2.10	0.51
3:B:392:PHE:CD1	3:B:517:LEU:HG	2.45	0.51
3:B:398:ASP:HB2	3:B:512:VAL:HB	1.91	0.51
7:W:15:PRO:HA	7:W:87:LEU:HD23	1.93	0.51
3:C:180:GLU:O	3:C:182:LYS:N	2.43	0.51
3:C:580:GLN:HG2	3:C:581:THR:H	1.75	0.51
3:A:398:ASP:HB2	3:A:512:VAL:HB	1.91	0.51
3:A:580:GLN:HG2	3:A:581:THR:H	1.75	0.51
4:M:47:TRP:HZ2	4:M:50:VAL:HG23	1.74	0.51
4:T:51:ILE:HB	4:T:70:ILE:HG12	1.92	0.51
5:V:96:ARG:HH22	3:B:485:GLY:HA2	1.76	0.51
3:B:180:GLU:O	3:B:182:LYS:N	2.43	0.51
3:B:389:ASP:HB3	3:B:528:LYS:HA	1.92	0.51
3:B:568:ASP:HB3	3:C:854:LYS:NZ	2.25	0.51
7:P:38:VAL:HG11	7:P:46:LEU:HD23	1.92	0.51
1:D:65:GLY:HA3	1:D:70:PHE:HA	1.92	0.51
2:N:47:TRP:O	2:N:61:ASN:ND2	2.34	0.51
3:A:15:CYS:HB3	3:A:158:ARG:HA	1.92	0.51
5:K:25:ALA:O	5:K:69:THR:OG1	2.27	0.51
3:B:718:PHE:CD1	3:B:1067:TYR:CE1	2.98	0.51
7:W:30:LEU:N	7:W:78:ASP:OD1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:69:VAL:HG21	7:W:82:MET:HE2	1.92	0.51
2:O:102:ASP:C	2:O:104:TYR:H	2.19	0.51
3:C:15:CYS:HB3	3:C:158:ARG:HA	1.93	0.51
3:C:598:ILE:HG23	3:C:664:ILE:HG21	1.93	0.51
3:A:106:PHE:HB3	3:A:235:ILE:HD13	1.92	0.51
3:B:598:ILE:HG23	3:B:664:ILE:HG21	1.93	0.51
7:P:110:ASP:HB2	7:P:111:PRO:HD3	1.92	0.51
3:A:104:TRP:HB2	3:A:106:PHE:CE2	2.46	0.51
4:I:51:ILE:HB	4:I:70:ILE:HG12	1.92	0.51
3:B:1006:THR:O	3:B:1010:GLN:HG2	2.11	0.51
6:R:10:VAL:HG23	6:R:107:LEU:HD13	1.91	0.51
6:Q:10:VAL:HG23	6:Q:107:LEU:HD13	1.92	0.51
7:P:100:THR:HB	7:P:106:SER:OG	2.10	0.51
3:C:431:GLY:HA2	3:C:515:PHE:H	1.74	0.51
3:B:213:VAL:HG23	3:B:214:ARG:H	1.75	0.51
7:W:100:THR:HB	7:W:106:SER:OG	2.10	0.51
1:D:79:ALA:HA	1:D:82:PHE:CE2	2.45	0.51
2:N:33:TYR:HA	2:N:53:PRO:HD3	1.91	0.51
3:A:146:HIS:HB3	3:A:151:SER:HB3	1.93	0.51
5:V:7:SER:OG	5:V:22:THR:OG1	2.29	0.51
5:K:7:SER:OG	5:K:22:THR:OG1	2.29	0.51
7:W:110:ASP:HB2	7:W:111:PRO:HD3	1.92	0.51
7:X:8:SER:H	7:X:116:THR:HG21	1.76	0.51
7:X:15:PRO:HA	7:X:87:LEU:HD23	1.93	0.51
3:C:34:ARG:NH2	3:C:217:PRO:HG2	2.25	0.51
3:C:104:TRP:HB2	3:C:106:PHE:CE2	2.46	0.51
3:C:278:LYS:HD3	3:C:287:ASP:HB3	1.92	0.51
5:K:89:GLN:HG3	5:K:98:PHE:CE1	2.46	0.50
7:P:8:SER:H	7:P:116:THR:HG21	1.76	0.50
3:A:598:ILE:HG23	3:A:664:ILE:HG21	1.93	0.50
3:A:1006:THR:O	3:A:1010:GLN:HG2	2.11	0.50
4:M:51:ILE:HB	4:M:70:ILE:HG12	1.92	0.50
3:B:333:THR:OG1	3:B:361:CYS:O	2.29	0.50
3:B:644:GLN:NE2	3:B:648:GLY:O	2.44	0.50
6:S:37:TYR:HD1	6:S:47:LEU:HA	1.77	0.50
3:A:214:ARG:O	3:A:266:TYR:OH	2.20	0.50
3:A:389:ASP:HB3	3:A:528:LYS:HA	1.92	0.50
3:A:797:PHE:O	3:A:800:PHE:HD1	1.94	0.50
5:U:18:ARG:NH1	5:U:74:THR:HG22	2.27	0.50
5:U:35:TRP:HD1	5:U:48:ILE:HB	1.76	0.50
5:V:35:TRP:HD1	5:V:48:ILE:HB	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:354:ASN:HB2	3:C:399:SER:HB3	1.94	0.50
3:C:392:PHE:CD1	3:C:517:LEU:HG	2.45	0.50
3:A:57:PRO:HB2	3:A:60:SER:HB2	1.94	0.50
4:M:19:ARG:HD3	4:M:80:TYR:CD2	2.47	0.50
5:U:89:GLN:HG3	5:U:98:PHE:CE1	2.46	0.50
5:V:37:GLN:HB2	5:V:47:LEU:HD11	1.93	0.50
3:B:15:CYS:HB3	3:B:158:ARG:HA	1.93	0.50
5:V:89:GLN:HG3	5:V:98:PHE:CE1	2.46	0.50
4:I:2:GLN:HG2	4:I:26:GLY:HA3	1.94	0.50
3:B:104:TRP:HB2	3:B:106:PHE:CE2	2.46	0.50
7:W:29:THR:HG23	7:W:31:PRO:HD2	1.94	0.50
6:Q:39:GLN:HB3	6:Q:86:ASP:OD1	2.12	0.50
3:C:67:ALA:N	3:C:263:ALA:O	2.45	0.50
3:C:146:HIS:HB3	3:C:151:SER:HB3	1.93	0.50
7:X:38:VAL:HG11	7:X:46:LEU:HD23	1.92	0.50
3:C:105:ILE:HG12	3:C:239:GLN:O	2.10	0.50
3:C:385:THR:O	3:C:388:ASN:HB2	2.12	0.50
3:C:1006:THR:O	3:C:1010:GLN:HG2	2.10	0.50
6:S:39:GLN:HB3	6:S:86:ASP:OD1	2.12	0.50
3:C:93:ALA:HB1	3:C:189:LEU:HD11	1.94	0.50
3:C:328:ARG:NH1	3:C:533:LEU:HB2	2.26	0.50
1:E:15:LYS:HE2	1:E:78:GLU:CB	2.42	0.50
2:O:103:PRO:C	2:O:105:TYR:H	2.20	0.50
3:A:718:PHE:CD1	3:A:1067:TYR:CE1	2.99	0.50
3:A:974:SER:H	3:A:980:ILE:HD11	1.76	0.50
5:U:37:GLN:HB2	5:U:47:LEU:HD11	1.93	0.50
3:B:922:LEU:HD11	8:b:1:NAG:H5	1.94	0.50
3:C:142:GLY:HA3	3:C:158:ARG:HG3	1.94	0.50
3:C:736:VAL:HG12	3:C:858:LEU:HD23	1.94	0.50
1:D:15:LYS:HE2	1:D:78:GLU:CB	2.42	0.50
3:A:726:ILE:HG13	3:A:1061:VAL:HG22	1.94	0.50
3:B:328:ARG:NH1	3:B:533:LEU:HB2	2.27	0.50
3:B:974:SER:H	3:B:980:ILE:HD11	1.76	0.50
7:W:38:VAL:HG11	7:W:46:LEU:HD23	1.92	0.50
3:C:180:GLU:HA	3:C:186:PHE:CD2	2.47	0.50
2:O:103:PRO:HA	2:O:105:TYR:CZ	2.46	0.49
3:A:41:LYS:O	3:C:563:GLN:HB3	2.12	0.49
3:A:385:THR:O	3:A:388:ASN:HB2	2.12	0.49
3:A:1089:PHE:CE2	3:B:917:TYR:HD1	2.29	0.49
4:T:19:ARG:HD3	4:T:80:TYR:CD2	2.47	0.49
3:B:57:PRO:HB2	3:B:60:SER:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:354:ASN:HB2	3:B:399:SER:HB3	1.94	0.49
6:R:39:GLN:HB3	6:R:86:ASP:OD1	2.12	0.49
7:P:15:PRO:HA	7:P:87:LEU:HD23	1.93	0.49
3:C:34:ARG:HH21	3:C:217:PRO:HG2	1.77	0.49
3:A:41:LYS:HA	3:C:563:GLN:HG2	1.93	0.49
3:A:56:LEU:HD12	3:A:57:PRO:HD2	1.94	0.49
3:A:67:ALA:N	3:A:263:ALA:O	2.45	0.49
3:A:578:ASP:HB3	3:A:583:GLU:H	1.77	0.49
3:B:578:ASP:HB3	3:B:583:GLU:H	1.77	0.49
3:C:195:LYS:HG2	3:C:197:ILE:HG13	1.94	0.49
3:C:818:ILE:O	3:C:822:LEU:HG	2.12	0.49
2:O:39:GLN:HB3	2:O:93:VAL:HG13	1.94	0.49
3:A:34:ARG:HH21	3:A:217:PRO:HG2	1.77	0.49
3:A:180:GLU:HA	3:A:186:PHE:CD2	2.47	0.49
3:A:354:ASN:HB2	3:A:399:SER:HB3	1.94	0.49
3:A:644:GLN:NE2	3:A:648:GLY:O	2.44	0.49
3:B:56:LEU:HD12	3:B:57:PRO:HD2	1.94	0.49
3:B:146:HIS:HB3	3:B:151:SER:HB3	1.93	0.49
7:X:13:LYS:H	7:X:119:THR:HB	1.77	0.49
3:C:333:THR:HB	3:C:360:ASN:HA	1.94	0.49
1:H:15:LYS:HE2	1:H:78:GLU:CB	2.42	0.49
3:A:818:ILE:O	3:A:822:LEU:HG	2.12	0.49
5:K:35:TRP:HD1	5:K:48:ILE:HB	1.76	0.49
5:K:37:GLN:HB2	5:K:47:LEU:HD11	1.93	0.49
7:P:13:LYS:H	7:P:119:THR:HB	1.76	0.49
7:P:88:ARG:NH2	7:P:90:GLU:OE1	2.46	0.49
2:L:39:GLN:HB3	2:L:93:VAL:HG13	1.94	0.49
3:A:854:LYS:NZ	3:C:568:ASP:HB3	2.27	0.49
4:T:2:GLN:HG2	4:T:26:GLY:HA3	1.93	0.49
5:V:18:ARG:NH1	5:V:74:THR:HG22	2.27	0.49
5:V:32:TYR:HD2	5:V:92:TYR:HA	1.76	0.49
5:V:33:LEU:HA	5:V:89:GLN:O	2.13	0.49
3:B:67:ALA:N	3:B:263:ALA:O	2.45	0.49
3:B:180:GLU:HA	3:B:186:PHE:CD2	2.47	0.49
3:B:278:LYS:HD3	3:B:287:ASP:HB3	1.92	0.49
3:B:818:ILE:O	3:B:822:LEU:HG	2.12	0.49
6:R:37:TYR:HD1	6:R:47:LEU:HA	1.77	0.49
6:Q:37:TYR:HD1	6:Q:47:LEU:HA	1.77	0.49
3:C:56:LEU:HD12	3:C:57:PRO:HD2	1.94	0.49
3:C:115:GLN:HB2	3:C:233:ILE:HD12	1.91	0.49
3:C:984:LEU:HD12	3:C:992:GLN:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:33:TYR:CE1	2:L:101:TYR:CE1	3.00	0.49
3:A:93:ALA:HB1	3:A:189:LEU:HD11	1.94	0.49
5:U:32:TYR:HD2	5:U:92:TYR:HA	1.76	0.49
5:U:82:ASP:O	5:U:86:TYR:OH	2.29	0.49
3:B:736:VAL:HG12	3:B:858:LEU:HD23	1.94	0.49
3:C:389:ASP:HB3	3:C:528:LYS:HA	1.92	0.49
3:C:644:GLN:NE2	3:C:648:GLY:O	2.44	0.49
3:C:718:PHE:CD1	3:C:1067:TYR:CE1	3.00	0.49
5:K:33:LEU:HA	5:K:89:GLN:O	2.13	0.49
3:B:93:ALA:HB1	3:B:189:LEU:HD11	1.94	0.49
3:B:142:GLY:HA3	3:B:158:ARG:HG3	1.94	0.49
7:P:117:LEU:HD23	7:P:118:VAL:C	2.38	0.49
2:N:103:PRO:HA	2:N:105:TYR:CZ	2.48	0.49
3:B:328:ARG:O	3:B:579:PRO:HG3	2.13	0.49
3:B:385:THR:O	3:B:388:ASN:HB2	2.12	0.49
7:X:29:THR:HG23	7:X:31:PRO:HD2	1.94	0.49
3:A:328:ARG:NH1	3:A:533:LEU:HB2	2.27	0.49
5:U:7:SER:OG	5:U:22:THR:OG1	2.30	0.49
4:I:19:ARG:HD3	4:I:80:TYR:CD2	2.47	0.49
5:K:18:ARG:NH1	5:K:74:THR:HG22	2.27	0.49
7:W:13:LYS:H	7:W:119:THR:HB	1.77	0.49
3:C:57:PRO:HB2	3:C:60:SER:HB2	1.94	0.49
3:C:333:THR:OG1	3:C:361:CYS:O	2.29	0.49
3:A:984:LEU:HD12	3:A:992:GLN:HG3	1.94	0.49
3:A:1030:SER:OG	3:C:1041:ASP:HB3	2.13	0.49
4:T:29:PHE:HD1	4:T:34:MET:HE2	1.78	0.49
4:I:29:PHE:HD1	4:I:34:MET:HE2	1.78	0.49
7:W:8:SER:H	7:W:116:THR:HG21	1.76	0.49
3:C:726:ILE:HG13	3:C:1061:VAL:HG22	1.94	0.49
3:C:902:MET:HE1	3:C:1049:LEU:HD13	1.94	0.49
3:A:902:MET:HE1	3:A:1049:LEU:HD13	1.94	0.48
4:M:47:TRP:CZ2	4:M:50:VAL:HG23	2.48	0.48
4:T:103:MET:HE2	3:B:489:TYR:HB3	1.95	0.48
7:P:29:THR:HG23	7:P:31:PRO:HD2	1.94	0.48
1:D:83:GLY:O	1:D:103:LEU:N	2.45	0.48
2:N:39:GLN:HB3	2:N:93:VAL:HG13	1.94	0.48
3:A:178:ASP:OD1	3:A:178:ASP:N	2.45	0.48
3:A:736:VAL:HG12	3:A:858:LEU:HD23	1.94	0.48
5:V:29:ILE:N	5:V:68:GLY:O	2.43	0.48
4:I:47:TRP:CZ2	4:I:50:VAL:HG23	2.48	0.48
6:S:31:ASN:OD1	6:S:32:ASN:ND2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:VAL:HG22	3:C:77:LYS:HG2	1.96	0.48
3:C:182:LYS:HB2	3:C:186:PHE:HB2	1.96	0.48
3:A:170:TYR:CZ	3:A:172:SER:HB2	2.49	0.48
3:A:328:ARG:O	3:A:579:PRO:HG3	2.14	0.48
4:M:2:GLN:HG2	4:M:26:GLY:HA3	1.94	0.48
3:B:538:CYS:O	3:B:538:CYS:SG	2.72	0.48
3:B:726:ILE:HG13	3:B:1061:VAL:HG22	1.94	0.48
3:B:984:LEU:HD12	3:B:992:GLN:HG3	1.94	0.48
7:W:117:LEU:HD23	7:W:118:VAL:C	2.38	0.48
3:C:922:LEU:HD11	8:g:1:NAG:H5	1.95	0.48
5:U:39:LYS:HZ3	5:U:84:ALA:HB2	1.78	0.48
3:B:195:LYS:HG2	3:B:197:ILE:HG13	1.94	0.48
6:R:31:ASN:OD1	6:R:32:ASN:ND2	2.47	0.48
7:W:88:ARG:NH2	7:W:90:GLU:OE1	2.46	0.48
3:C:453:TYR:HB3	3:C:495:TYR:CZ	2.49	0.48
3:C:496:GLY:O	3:C:501:ASN:ND2	2.33	0.48
3:C:578:ASP:HB3	3:C:583:GLU:H	1.77	0.48
3:A:182:LYS:HB2	3:A:186:PHE:HB2	1.96	0.48
3:A:333:THR:HB	3:A:360:ASN:HA	1.94	0.48
3:B:34:ARG:HH21	3:B:217:PRO:HG2	1.77	0.48
3:B:70:VAL:HG22	3:B:77:LYS:HG2	1.96	0.48
3:B:170:TYR:CZ	3:B:172:SER:HB2	2.49	0.48
3:B:902:MET:HE1	3:B:1049:LEU:HD13	1.94	0.48
7:W:87:LEU:HD11	7:W:120:VAL:HG12	1.96	0.48
3:C:43:PHE:CE1	3:C:283:GLY:HA3	2.49	0.48
3:A:195:LYS:HG2	3:A:197:ILE:HG13	1.94	0.48
4:M:11:VAL:HA	4:M:116:THR:HB	1.96	0.48
5:K:21:ILE:HG21	5:K:102:THR:HG21	1.96	0.48
1:H:83:GLY:O	1:H:103:LEU:N	2.45	0.48
3:A:142:GLY:HA3	3:A:158:ARG:HG3	1.94	0.48
5:U:21:ILE:HG21	5:U:102:THR:HG21	1.96	0.48
3:B:392:PHE:HB3	3:B:516:GLU:O	2.14	0.48
6:Q:31:ASN:OD1	6:Q:32:ASN:ND2	2.47	0.48
7:P:87:LEU:HD11	7:P:120:VAL:HG12	1.96	0.48
3:C:328:ARG:O	3:C:579:PRO:HG3	2.14	0.48
3:C:715:PRO:HA	3:C:1071:GLN:O	2.14	0.48
3:A:792:PRO:O	3:A:795:LYS:NZ	2.37	0.48
3:B:43:PHE:CE1	3:B:283:GLY:HA3	2.49	0.48
3:B:182:LYS:HB2	3:B:186:PHE:HB2	1.96	0.48
3:A:405:ASP:CB	3:A:408:ARG:NE	2.76	0.48
3:A:1097:SER:HB2	3:A:1102:TRP:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:82:ASP:O	5:K:86:TYR:OH	2.30	0.48
3:B:244:LEU:HD22	3:B:259:THR:HA	1.96	0.48
3:A:70:VAL:HG22	3:A:77:LYS:HG2	1.95	0.48
3:A:86:PHE:HE2	3:A:196:ASN:HB2	1.79	0.48
3:A:392:PHE:HB3	3:A:516:GLU:O	2.14	0.48
3:A:538:CYS:SG	3:A:538:CYS:O	2.72	0.48
5:U:33:LEU:HA	5:U:89:GLN:O	2.13	0.48
6:R:11:SER:OG	6:R:108:THR:OG1	2.26	0.48
7:X:87:LEU:HD11	7:X:120:VAL:HG12	1.96	0.48
3:C:392:PHE:HB3	3:C:516:GLU:O	2.14	0.48
3:A:715:PRO:HA	3:A:1071:GLN:O	2.14	0.47
3:B:333:THR:HB	3:B:360:ASN:HA	1.94	0.47
3:B:453:TYR:HB3	3:B:495:TYR:CZ	2.49	0.47
3:B:901:GLN:HE22	3:B:905:ARG:HH21	1.62	0.47
7:X:88:ARG:NH2	7:X:90:GLU:OE1	2.46	0.47
3:C:170:TYR:CZ	3:C:172:SER:HB2	2.49	0.47
3:C:412:PRO:HG3	3:C:429:PHE:CD2	2.49	0.47
1:H:61:PHE:HA	1:H:74:ILE:HA	1.97	0.47
3:A:453:TYR:HB3	3:A:495:TYR:CZ	2.49	0.47
3:A:665:PRO:HA	3:A:671:CYS:SG	2.54	0.47
3:A:816:SER:HB2	3:A:819:GLU:HG3	1.96	0.47
3:C:115:GLN:NE2	3:C:165:ASN:O	2.45	0.47
2:L:35:HIS:HD1	2:L:50:TYR:HB3	1.80	0.47
2:N:13:LYS:CE	2:N:16:ALA:CB	2.81	0.47
2:N:40:ALA:HB3	2:N:43:LYS:HB2	1.96	0.47
3:A:43:PHE:CE1	3:A:283:GLY:HA3	2.49	0.47
4:M:32:TYR:CZ	4:M:106:LYS:HG3	2.49	0.47
5:V:21:ILE:HG21	5:V:102:THR:HG21	1.96	0.47
3:B:83:VAL:HG12	3:B:237:ARG:HB3	1.97	0.47
3:B:178:ASP:HB3	3:B:190:ARG:HH12	1.79	0.47
3:B:1097:SER:HB2	3:B:1102:TRP:CD2	2.50	0.47
7:P:49:MET:SD	7:P:82:MET:HE1	2.54	0.47
3:A:412:PRO:HG3	3:A:429:PHE:CD2	2.49	0.47
4:I:32:TYR:CZ	4:I:106:LYS:HG3	2.49	0.47
7:W:49:MET:SD	7:W:82:MET:HE1	2.54	0.47
3:C:244:LEU:HD22	3:C:259:THR:HA	1.96	0.47
3:C:374:PHE:HA	3:C:436:TRP:HB3	1.97	0.47
1:E:83:GLY:O	1:E:103:LEU:N	2.45	0.47
3:A:83:VAL:HG12	3:A:237:ARG:HB3	1.97	0.47
3:A:962:LEU:HD11	3:A:1007:TYR:CB	2.42	0.47
3:B:178:ASP:OD1	3:B:178:ASP:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:461:LEU:HD11	3:B:466:ARG:HA	1.96	0.47
7:W:96:TYR:HA	7:W:115:GLY:HA2	1.97	0.47
3:A:196:ASN:ND2	3:A:235:ILE:H	2.13	0.47
3:A:330:PRO:C	3:A:332:ILE:N	2.73	0.47
3:A:374:PHE:HA	3:A:436:TRP:HB3	1.97	0.47
4:T:11:VAL:HA	4:T:116:THR:HB	1.96	0.47
4:T:47:TRP:CZ2	4:T:50:VAL:HG23	2.49	0.47
3:B:86:PHE:HE2	3:B:196:ASN:HB2	1.79	0.47
3:B:540:ASN:ND2	3:B:549:THR:OG1	2.48	0.47
7:X:49:MET:SD	7:X:82:MET:HE1	2.54	0.47
6:Q:24:GLY:HA3	6:Q:29:ILE:HD12	1.97	0.47
3:C:538:CYS:SG	3:C:538:CYS:O	2.72	0.47
8:d:1:NAG:H61	8:d:2:NAG:H82	1.96	0.47
2:O:41:PRO:HG3	2:O:91:THR:O	2.15	0.47
3:A:128:ILE:HG21	3:A:229:LEU:HD13	1.97	0.47
3:A:244:LEU:HD22	3:A:259:THR:HA	1.96	0.47
3:A:540:ASN:ND2	3:A:549:THR:OG1	2.48	0.47
3:A:674:TYR:CZ	3:A:690:GLN:HB3	2.50	0.47
3:A:864:LEU:O	3:C:669:GLY:N	2.43	0.47
4:T:28:THR:HA	4:T:77:ASN:HD21	1.80	0.47
5:V:6:GLN:O	5:V:100:GLN:NE2	2.48	0.47
4:I:28:THR:HA	4:I:77:ASN:HD21	1.80	0.47
3:B:412:PRO:HG3	3:B:429:PHE:CD2	2.49	0.47
3:B:715:PRO:HA	3:B:1071:GLN:O	2.14	0.47
3:B:1094:VAL:HG22	3:C:904:TYR:OH	2.15	0.47
6:R:24:GLY:HA3	6:R:29:ILE:HD12	1.97	0.47
3:C:816:SER:HB2	3:C:819:GLU:HG3	1.96	0.47
4:M:29:PHE:HD1	4:M:34:MET:HE2	1.78	0.47
3:B:128:ILE:HG21	3:B:229:LEU:HD13	1.97	0.47
7:W:3:GLN:O	7:W:26:SER:OG	2.23	0.47
3:C:83:VAL:HG12	3:C:237:ARG:HB3	1.97	0.47
3:C:461:LEU:HD11	3:C:466:ARG:HA	1.96	0.47
3:C:901:GLN:HE22	3:C:905:ARG:HH21	1.62	0.47
2:L:41:PRO:HG3	2:L:91:THR:O	2.15	0.47
2:O:40:ALA:HB3	2:O:43:LYS:HB2	1.96	0.47
4:M:17:SER:OG	4:M:84:ASN:OD1	2.33	0.47
5:U:6:GLN:O	5:U:100:GLN:NE2	2.48	0.47
4:I:11:VAL:HA	4:I:116:THR:HB	1.96	0.47
3:B:674:TYR:CZ	3:B:690:GLN:HB3	2.50	0.47
3:A:792:PRO:HG3	3:C:707:TYR:HB3	1.95	0.47
5:V:34:ASN:HB3	5:V:46:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:196:ASN:ND2	3:B:235:ILE:H	2.13	0.47
3:B:665:PRO:HA	3:B:671:CYS:SG	2.54	0.47
6:S:24:GLY:HA3	6:S:29:ILE:HD12	1.97	0.47
7:P:49:MET:HE1	7:P:95:TYR:CE1	2.30	0.47
7:P:96:TYR:HA	7:P:115:GLY:HA2	1.97	0.47
3:C:328:ARG:NH1	3:C:533:LEU:CB	2.77	0.47
3:C:540:ASN:ND2	3:C:549:THR:OG1	2.47	0.47
3:C:665:PRO:HA	3:C:671:CYS:SG	2.54	0.47
3:C:1097:SER:HB2	3:C:1102:TRP:CD2	2.49	0.47
1:D:61:PHE:HA	1:D:74:ILE:HA	1.97	0.46
3:A:961:THR:HG21	3:B:762:GLN:HE21	1.80	0.46
3:B:15:CYS:H	3:B:158:ARG:HD3	1.80	0.46
3:B:816:SER:HB2	3:B:819:GLU:HG3	1.96	0.46
3:C:15:CYS:H	3:C:158:ARG:HD3	1.80	0.46
3:C:476:GLY:HA3	3:C:487:ASN:HB3	1.97	0.46
3:C:808:ASP:OD1	3:C:810:SER:OG	2.33	0.46
8:Y:1:NAG:H61	8:Y:2:NAG:H82	1.97	0.46
2:N:103:PRO:C	2:N:105:TYR:H	2.22	0.46
3:A:15:CYS:H	3:A:158:ARG:HD3	1.80	0.46
3:A:178:ASP:HB3	3:A:190:ARG:HH12	1.79	0.46
3:A:476:GLY:HA3	3:A:487:ASN:HB3	1.97	0.46
4:T:32:TYR:CZ	4:T:106:LYS:HG3	2.49	0.46
5:K:80:PRO:HA	5:K:83:PHE:CE2	2.51	0.46
3:B:273:ARG:HH12	3:B:290:ASP:CG	2.23	0.46
6:S:6:GLN:HE22	6:S:89:CYS:H	1.63	0.46
3:C:22:THR:OG1	3:C:78:ARG:HB3	2.16	0.46
3:C:178:ASP:HB3	3:C:190:ARG:HH12	1.79	0.46
3:C:662:CYS:HB2	3:C:671:CYS:HB3	1.70	0.46
2:N:41:PRO:HG3	2:N:91:THR:O	2.15	0.46
2:O:102:ASP:CG	2:O:103:PRO:CD	2.66	0.46
3:A:396:TYR:HB2	3:A:514:SER:OG	2.16	0.46
3:B:374:PHE:HA	3:B:436:TRP:HB3	1.97	0.46
3:C:145:TYR:CE2	3:C:147:LYS:HA	2.51	0.46
3:C:273:ARG:HH12	3:C:290:ASP:CG	2.23	0.46
2:L:93:VAL:HG13	2:L:95:TYR:HE1	1.80	0.46
2:N:35:HIS:HD1	2:N:50:TYR:HB3	1.80	0.46
2:N:93:VAL:HG13	2:N:95:TYR:HE1	1.80	0.46
5:U:80:PRO:HA	5:U:83:PHE:CE2	2.51	0.46
5:K:34:ASN:HB3	5:K:46:LEU:HD11	1.97	0.46
3:B:67:ALA:HA	3:B:80:ASP:HB3	1.98	0.46
3:B:412:PRO:HA	3:B:425:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:25:SER:OG	6:S:28:ASN:ND2	2.49	0.46
3:C:578:ASP:O	3:C:582:LEU:HD23	2.16	0.46
3:C:674:TYR:CZ	3:C:690:GLN:HB3	2.50	0.46
1:H:15:LYS:HA	1:H:76:SER:HA	1.98	0.46
1:D:15:LYS:HA	1:D:76:SER:HA	1.98	0.46
3:A:107:GLY:N	3:A:235:ILE:HG23	2.31	0.46
3:A:567:ARG:NH1	3:B:44:ARG:HH21	2.13	0.46
3:A:726:ILE:HB	3:A:947:LYS:HE3	1.97	0.46
4:I:17:SER:OG	4:I:84:ASN:OD1	2.33	0.46
3:C:804:GLN:HB3	3:C:935:GLN:HE21	1.81	0.46
2:L:91:THR:HA	2:L:116:VAL:O	2.16	0.46
3:A:67:ALA:HA	3:A:80:ASP:HB3	1.98	0.46
3:A:87:ASN:HB3	8:F:2:NAG:C8	2.46	0.46
3:A:558:LYS:HB3	3:A:558:LYS:HE3	1.75	0.46
5:K:96:ARG:HH22	3:C:485:GLY:HA2	1.80	0.46
3:B:145:TYR:CE2	3:B:147:LYS:HA	2.51	0.46
7:P:69:VAL:HG22	7:P:84:LEU:HD12	1.98	0.46
3:C:436:TRP:HZ3	3:C:511:VAL:HG12	1.81	0.46
2:L:40:ALA:HB3	2:L:43:LYS:HB2	1.96	0.46
3:A:461:LEU:HD11	3:A:466:ARG:HA	1.96	0.46
3:A:808:ASP:OD1	3:A:810:SER:OG	2.33	0.46
3:B:87:ASN:HB3	8:a:2:NAG:C8	2.45	0.46
3:B:563:GLN:HB3	3:C:41:LYS:O	2.15	0.46
3:B:726:ILE:HB	3:B:947:LYS:HE3	1.97	0.46
3:C:396:TYR:HB2	3:C:514:SER:OG	2.16	0.46
3:C:412:PRO:HA	3:C:425:LEU:HB3	1.97	0.46
3:C:748:GLU:OE1	3:C:748:GLU:N	2.43	0.46
1:E:15:LYS:HA	1:E:76:SER:HA	1.98	0.46
3:A:1040:VAL:O	3:B:1030:SER:OG	2.33	0.46
5:K:6:GLN:O	5:K:100:GLN:NE2	2.48	0.46
3:B:330:PRO:C	3:B:332:ILE:N	2.73	0.46
3:B:804:GLN:HB3	3:B:935:GLN:HE21	1.81	0.46
7:X:69:VAL:HG22	7:X:84:LEU:HD12	1.98	0.46
7:X:74:ASP:OD1	7:X:77:THR:OG1	2.29	0.46
6:Q:6:GLN:HE22	6:Q:89:CYS:H	1.63	0.46
3:C:67:ALA:HA	3:C:80:ASP:HB3	1.98	0.46
1:E:61:PHE:HA	1:E:74:ILE:HA	1.97	0.46
3:A:273:ARG:HH12	3:A:290:ASP:CG	2.23	0.46
3:A:804:GLN:HB3	3:A:935:GLN:HE21	1.81	0.46
3:A:901:GLN:HE22	3:A:905:ARG:HH21	1.62	0.46
3:A:907:ASN:HD21	3:A:913:GLN:HE21	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:22:THR:OG1	3:B:78:ARG:HB3	2.15	0.46
3:B:396:TYR:HB2	3:B:514:SER:OG	2.16	0.46
3:B:563:GLN:HG2	3:C:41:LYS:HA	1.98	0.46
7:X:64:LYS:HG3	7:X:65:PHE:CD2	2.51	0.46
7:X:96:TYR:HA	7:X:115:GLY:HA2	1.97	0.46
7:P:117:LEU:HD23	7:P:118:VAL:N	2.30	0.46
1:D:7:SER:C	1:D:99:GLN:HE22	2.23	0.46
1:E:7:SER:C	1:E:99:GLN:HE22	2.23	0.46
3:A:328:ARG:NH1	3:A:533:LEU:CB	2.79	0.46
3:A:1094:VAL:HG22	3:B:904:TYR:OH	2.16	0.46
5:U:34:ASN:HB3	5:U:46:LEU:HD11	1.97	0.46
3:B:808:ASP:OD1	3:B:810:SER:OG	2.33	0.46
7:W:117:LEU:HD23	7:W:118:VAL:N	2.30	0.46
7:P:64:LYS:HG3	7:P:65:PHE:CD2	2.51	0.46
3:C:86:PHE:HE2	3:C:196:ASN:HB2	1.79	0.46
3:C:461:LEU:HD23	3:C:462:LYS:O	2.16	0.46
1:H:7:SER:C	1:H:99:GLN:HE22	2.23	0.45
3:A:578:ASP:O	3:A:582:LEU:HD23	2.16	0.45
5:V:82:ASP:O	5:V:86:TYR:OH	2.30	0.45
5:K:29:ILE:N	5:K:68:GLY:O	2.43	0.45
3:B:539:VAL:O	3:B:549:THR:HA	2.16	0.45
7:W:64:LYS:HG3	7:W:65:PHE:CD2	2.51	0.45
3:C:533:LEU:HD23	3:C:535:LYS:HE3	1.98	0.45
2:O:39:GLN:O	2:O:92:ALA:HB1	2.16	0.45
2:O:91:THR:HA	2:O:116:VAL:O	2.16	0.45
3:B:436:TRP:HZ3	3:B:511:VAL:HG12	1.80	0.45
3:B:578:ASP:O	3:B:582:LEU:HD23	2.16	0.45
6:Q:25:SER:OG	6:Q:28:ASN:ND2	2.49	0.45
3:C:539:VAL:O	3:C:549:THR:HA	2.16	0.45
3:C:907:ASN:HD21	3:C:913:GLN:HE21	1.64	0.45
1:D:86:PHE:HA	1:D:100:GLY:HA2	1.98	0.45
2:N:39:GLN:O	2:N:92:ALA:HB1	2.16	0.45
2:N:91:THR:HA	2:N:116:VAL:O	2.16	0.45
3:A:27:ALA:HB3	3:A:64:TRP:CE3	2.51	0.45
3:A:145:TYR:CE2	3:A:147:LYS:HA	2.50	0.45
3:A:333:THR:OG1	3:A:361:CYS:O	2.29	0.45
3:A:533:LEU:HD23	3:A:535:LYS:HE3	1.98	0.45
3:A:539:VAL:O	3:A:549:THR:HA	2.16	0.45
3:A:789:TYR:HE2	3:C:703:ASN:HD22	1.64	0.45
4:T:17:SER:OG	4:T:84:ASN:OD1	2.33	0.45
5:V:91:SER:O	5:V:96:ARG:NH2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:273:ARG:HH11	3:B:292:ALA:HB3	1.81	0.45
3:B:643:PHE:CE2	3:B:645:THR:HG22	2.51	0.45
6:R:2:SER:OG	6:R:3:VAL:N	2.48	0.45
6:Q:62:ARG:NH2	6:Q:80:GLN:OE1	2.49	0.45
3:C:128:ILE:HG21	3:C:229:LEU:HD13	1.97	0.45
1:H:34:TRP:O	1:H:46:LEU:N	2.49	0.45
1:E:86:PHE:HA	1:E:100:GLY:HA2	1.99	0.45
3:A:22:THR:OG1	3:A:78:ARG:HB3	2.16	0.45
3:A:256:SER:OG	3:A:257:GLY:N	2.49	0.45
5:U:29:ILE:N	5:U:68:GLY:O	2.43	0.45
5:V:35:TRP:CE2	5:V:73:LEU:HB2	2.52	0.45
3:B:27:ALA:HB3	3:B:64:TRP:CE3	2.51	0.45
3:B:107:GLY:N	3:B:235:ILE:HG23	2.29	0.45
3:B:328:ARG:NH1	3:B:533:LEU:CB	2.78	0.45
3:B:533:LEU:HD23	3:B:535:LYS:HE3	1.98	0.45
6:Q:2:SER:OG	6:Q:3:VAL:N	2.48	0.45
3:A:436:TRP:HZ3	3:A:511:VAL:HG12	1.80	0.45
3:C:27:ALA:HB3	3:C:64:TRP:CE3	2.51	0.45
2:O:35:HIS:HD1	2:O:50:TYR:HB3	1.80	0.45
2:O:93:VAL:HG13	2:O:95:TYR:HE1	1.80	0.45
3:A:115:GLN:NE2	3:A:165:ASN:O	2.45	0.45
3:A:134:GLN:O	3:A:161:SER:N	2.47	0.45
4:M:28:THR:HA	4:M:77:ASN:HD21	1.80	0.45
4:I:57:ASN:HD21	3:C:483:VAL:CG2	2.29	0.45
3:B:476:GLY:HA3	3:B:487:ASN:HB3	1.97	0.45
3:B:591:SER:HB3	3:B:615:VAL:HG22	1.99	0.45
6:R:6:GLN:HE22	6:R:89:CYS:H	1.63	0.45
3:A:273:ARG:HH11	3:A:292:ALA:HB3	1.81	0.45
3:B:907:ASN:HD21	3:B:913:GLN:HE21	1.64	0.45
6:Q:60:PRO:HB2	6:Q:62:ARG:HG2	1.99	0.45
3:C:962:LEU:HD11	3:C:1007:TYR:CB	2.42	0.45
1:D:34:TRP:O	1:D:46:LEU:N	2.49	0.45
5:U:30:SER:OG	5:U:31:SER:N	2.50	0.45
5:V:80:PRO:HA	5:V:83:PHE:CE2	2.51	0.45
3:B:256:SER:OG	3:B:257:GLY:N	2.49	0.45
3:B:558:LYS:HE3	3:B:558:LYS:HB3	1.74	0.45
6:R:25:SER:OG	6:R:28:ASN:ND2	2.49	0.45
6:S:62:ARG:NH2	6:S:80:GLN:OE1	2.49	0.45
3:C:355:ARG:HE	3:C:396:TYR:HB3	1.82	0.45
2:L:39:GLN:O	2:L:92:ALA:HB1	2.16	0.45
1:E:34:TRP:O	1:E:46:LEU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:461:LEU:HD23	3:A:462:LYS:O	2.16	0.45
3:A:643:PHE:CE2	3:A:645:THR:HG22	2.51	0.45
3:B:461:LEU:HD23	3:B:462:LYS:O	2.16	0.45
3:C:87:ASN:HB3	8:f:2:NAG:C8	2.47	0.45
3:C:1093:GLY:HA3	3:C:1105:THR:O	2.17	0.45
3:A:412:PRO:HA	3:A:425:LEU:HB3	1.97	0.45
3:A:750:SER:O	3:A:754:LEU:HG	2.17	0.45
6:R:62:ARG:NH2	6:R:80:GLN:OE1	2.49	0.45
5:U:35:TRP:CE2	5:U:73:LEU:HB2	2.52	0.44
3:B:666:ILE:HD12	3:B:670:ILE:HG22	1.99	0.44
7:W:101:THR:HG22	7:W:106:SER:OG	2.18	0.44
7:X:83:GLU:OE2	7:X:83:GLU:N	2.50	0.44
7:X:101:THR:HG22	7:X:106:SER:OG	2.17	0.44
3:C:476:GLY:HA3	3:C:487:ASN:HD22	1.82	0.44
3:C:643:PHE:CE2	3:C:645:THR:HG22	2.51	0.44
3:C:797:PHE:O	3:C:800:PHE:HD1	1.99	0.44
8:i:1:NAG:H61	8:i:2:NAG:H82	1.98	0.44
2:N:108:ASP:OD1	2:N:109:TYR:N	2.50	0.44
4:M:28:THR:HA	4:M:77:ASN:ND2	2.33	0.44
3:B:115:GLN:NE2	3:B:165:ASN:O	2.45	0.44
3:B:461:LEU:HD21	3:B:465:GLU:O	2.17	0.44
3:B:476:GLY:HA3	3:B:487:ASN:HD22	1.82	0.44
7:W:112:TRP:HD1	7:W:114:GLN:H	1.65	0.44
2:L:5:VAL:O	2:L:22:CYS:HA	2.18	0.44
2:L:108:ASP:OD1	2:L:109:TYR:N	2.50	0.44
2:N:102:ASP:OD2	3:B:408:ARG:NE	2.45	0.44
3:A:461:LEU:HD21	3:A:465:GLU:O	2.17	0.44
3:A:484:GLU:OE1	4:M:101:THR:OG1	2.32	0.44
3:A:666:ILE:HD12	3:A:670:ILE:HG22	1.99	0.44
5:U:25:ALA:O	5:U:69:THR:OG1	2.27	0.44
5:V:33:LEU:HD13	5:V:71:PHE:CD2	2.52	0.44
5:V:88:CYS:O	5:V:99:GLY:N	2.45	0.44
5:K:8:PRO:HG2	5:K:11:LEU:HD23	2.00	0.44
3:C:330:PRO:C	3:C:332:ILE:N	2.73	0.44
3:C:726:ILE:HB	3:C:947:LYS:HE3	1.97	0.44
3:C:901:GLN:HE22	3:C:905:ARG:NH2	2.16	0.44
3:A:557:LYS:HB3	3:B:43:PHE:HB3	1.99	0.44
3:B:350:VAL:HG12	3:B:495:TYR:OH	2.17	0.44
3:B:568:ASP:HB3	3:C:854:LYS:HZ1	1.80	0.44
3:B:797:PHE:O	3:B:800:PHE:HD1	2.00	0.44
7:P:83:GLU:N	7:P:83:GLU:OE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:350:VAL:HG12	3:C:495:TYR:OH	2.17	0.44
3:C:461:LEU:HD21	3:C:465:GLU:O	2.17	0.44
2:N:5:VAL:O	2:N:22:CYS:HA	2.18	0.44
3:A:117:LEU:HD13	3:A:130:VAL:HG22	1.99	0.44
3:A:355:ARG:HE	3:A:396:TYR:HB3	1.82	0.44
3:A:738:CYS:HB3	3:A:760:CYS:HB2	1.58	0.44
3:B:134:GLN:O	3:B:161:SER:N	2.47	0.44
6:S:40:LEU:HB2	6:S:43:THR:OG1	2.17	0.44
7:X:39:ARG:HG2	7:X:95:TYR:CE1	2.52	0.44
3:C:117:LEU:HD13	3:C:130:VAL:HG22	1.99	0.44
1:H:86:PHE:HA	1:H:100:GLY:HA2	1.98	0.44
3:A:201:PHE:HB2	3:A:231:ILE:HG13	1.99	0.44
3:A:290:ASP:O	3:A:297:SER:HB3	2.18	0.44
5:K:35:TRP:CE2	5:K:73:LEU:HB2	2.52	0.44
5:K:39:LYS:HZ3	5:K:84:ALA:HB2	1.83	0.44
3:B:336:CYS:HB3	3:B:361:CYS:HA	2.00	0.44
3:B:750:SER:O	3:B:754:LEU:HG	2.17	0.44
3:B:1093:GLY:HA3	3:B:1105:THR:O	2.17	0.44
6:R:60:PRO:HB2	6:R:62:ARG:HG2	1.99	0.44
7:W:83:GLU:N	7:W:83:GLU:OE2	2.51	0.44
7:P:112:TRP:HD1	7:P:114:GLN:H	1.65	0.44
3:C:182:LYS:HG3	3:C:186:PHE:CD1	2.53	0.44
3:C:331:ASN:OD1	3:C:527:PRO:HA	2.18	0.44
5:V:39:LYS:HZ3	5:V:84:ALA:HB2	1.82	0.44
5:K:7:SER:HA	5:K:8:PRO:HA	1.81	0.44
7:P:39:ARG:HG2	7:P:95:TYR:CE1	2.52	0.44
3:A:591:SER:HB3	3:A:615:VAL:HG22	1.99	0.44
4:T:28:THR:HA	4:T:77:ASN:ND2	2.33	0.44
5:K:33:LEU:HD13	5:K:71:PHE:CD2	2.52	0.44
3:B:792:PRO:O	3:B:795:LYS:NZ	2.37	0.44
3:B:1045:LYS:HD3	3:C:786:LYS:HE2	1.99	0.44
7:W:49:MET:HE1	7:W:95:TYR:CE1	2.31	0.44
7:P:39:ARG:HG3	7:P:49:MET:SD	2.58	0.44
3:C:134:GLN:O	3:C:161:SER:N	2.47	0.44
3:C:273:ARG:HH11	3:C:292:ALA:HB3	1.81	0.44
2:L:13:LYS:CE	2:L:16:ALA:CB	2.81	0.44
3:A:197:ILE:HD12	3:A:202:LYS:HD2	2.00	0.44
3:A:476:GLY:HA3	3:A:487:ASN:HD22	1.82	0.44
3:A:900:MET:HE1	3:C:1094:VAL:HG13	2.00	0.44
3:A:1093:GLY:HA3	3:A:1105:THR:O	2.17	0.44
3:B:85:PRO:O	3:B:269:TYR:OH	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:412:PRO:HG3	3:B:429:PHE:HD2	1.83	0.44
3:B:718:PHE:HE1	3:B:720:ILE:HD11	1.83	0.44
6:S:60:PRO:HB2	6:S:62:ARG:HG2	1.99	0.44
7:X:112:TRP:HD1	7:X:114:GLN:H	1.65	0.44
3:C:28:TYR:HD1	3:C:61:ASN:HB3	1.83	0.44
2:L:33:TYR:OH	3:A:378:LYS:NZ	2.30	0.43
3:A:98:SER:O	3:A:100:ILE:N	2.49	0.43
3:A:350:VAL:HG12	3:A:495:TYR:OH	2.17	0.43
5:U:7:SER:HA	5:U:8:PRO:HA	1.82	0.43
6:R:40:LEU:HB2	6:R:43:THR:OG1	2.17	0.43
7:W:37:TRP:HD1	7:W:50:GLY:HA3	1.83	0.43
3:C:85:PRO:O	3:C:269:TYR:OH	2.35	0.43
3:C:611:LEU:HB2	3:C:650:LEU:HD23	2.00	0.43
3:A:332:ILE:HB	3:A:525:CYS:SG	2.58	0.43
3:A:374:PHE:HB2	3:A:377:PHE:HB2	2.00	0.43
3:A:901:GLN:HE22	3:A:905:ARG:NH2	2.16	0.43
5:V:30:SER:OG	5:V:31:SER:N	2.50	0.43
4:I:28:THR:HA	4:I:77:ASN:ND2	2.33	0.43
5:K:82:ASP:OD2	5:K:86:TYR:OH	2.34	0.43
3:B:117:LEU:HD13	3:B:130:VAL:HG22	1.99	0.43
3:B:201:PHE:HB2	3:B:231:ILE:HG13	2.00	0.43
3:B:901:GLN:HE22	3:B:905:ARG:NH2	2.16	0.43
3:C:374:PHE:HB2	3:C:377:PHE:HB2	2.00	0.43
3:C:666:ILE:HD12	3:C:670:ILE:HG22	1.99	0.43
3:A:182:LYS:HG3	3:A:186:PHE:CD1	2.53	0.43
5:U:33:LEU:HD13	5:U:71:PHE:CD2	2.52	0.43
3:B:197:ILE:HD12	3:B:202:LYS:HD2	2.00	0.43
7:P:101:THR:HG22	7:P:106:SER:OG	2.18	0.43
3:C:290:ASP:O	3:C:297:SER:HB3	2.18	0.43
3:B:152:TRP:CZ2	7:W:103:PHE:HZ	2.36	0.43
3:B:290:ASP:O	3:B:297:SER:HB3	2.18	0.43
3:B:656:VAL:HG12	3:B:658:ASN:H	1.84	0.43
3:B:901:GLN:HE22	3:B:905:ARG:HE	1.67	0.43
3:C:197:ILE:HD12	3:C:202:LYS:HD2	2.00	0.43
3:A:708:SER:HB2	3:A:711:SER:HB3	2.00	0.43
4:I:57:ASN:HD21	3:C:483:VAL:HG23	1.82	0.43
5:K:30:SER:OG	5:K:31:SER:N	2.50	0.43
3:C:750:SER:O	3:C:754:LEU:HG	2.18	0.43
4:I:35:HIS:HD2	4:I:50:VAL:HG13	1.84	0.43
3:B:182:LYS:HG3	3:B:186:PHE:CD1	2.53	0.43
3:B:718:PHE:CE1	3:B:720:ILE:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:47:LEU:HD22	7:W:108:TRP:HB2	2.00	0.43
7:X:39:ARG:HG3	7:X:49:MET:SD	2.58	0.43
3:C:738:CYS:HB3	3:C:760:CYS:HB2	1.58	0.43
3:C:901:GLN:HE22	3:C:905:ARG:HE	1.67	0.43
3:A:1050:MET:HE2	3:A:1050:MET:HB3	1.90	0.43
3:B:24:LEU:HD11	3:B:78:ARG:HB2	2.01	0.43
3:B:355:ARG:HE	3:B:396:TYR:HB3	1.82	0.43
3:B:738:CYS:HB3	3:B:760:CYS:HB2	1.58	0.43
6:R:39:GLN:O	6:R:85:ALA:HB1	2.19	0.43
7:X:53:ASP:HB3	7:X:55:GLU:O	2.19	0.43
3:C:591:SER:HB3	3:C:615:VAL:HG22	1.99	0.43
2:N:18:VAL:HG12	2:N:86:LEU:HD21	2.01	0.43
3:A:897:PRO:HD3	3:C:711:SER:O	2.19	0.43
3:B:327:VAL:O	3:B:531:THR:HG22	2.18	0.43
6:R:28:ASN:O	6:R:32:ASN:HB2	2.19	0.43
6:S:2:SER:OG	6:S:3:VAL:N	2.48	0.43
3:C:327:VAL:O	3:C:531:THR:HG22	2.18	0.43
3:C:1051:SER:HG	3:C:1064:HIS:HD1	1.63	0.43
2:O:5:VAL:O	2:O:22:CYS:HA	2.18	0.43
2:O:108:ASP:OD1	2:O:109:TYR:N	2.50	0.43
3:A:901:GLN:HE22	3:A:905:ARG:HE	1.67	0.43
7:W:39:ARG:HG3	7:W:49:MET:SD	2.58	0.43
6:Q:99:VAL:HG13	7:P:107:TYR:CE1	2.54	0.43
2:L:18:VAL:HG12	2:L:86:LEU:HD21	2.01	0.43
2:N:102:ASP:C	2:N:104:TYR:N	2.77	0.43
3:B:150:LYS:NZ	7:W:54:PRO:O	2.52	0.43
3:B:643:PHE:CZ	3:B:655:HIS:CD2	3.07	0.43
6:R:13:ALA:HB3	6:R:16:GLN:HG2	2.01	0.43
3:C:433:VAL:HG22	3:C:512:VAL:HG13	2.01	0.43
3:C:558:LYS:HE3	3:C:558:LYS:HB3	1.75	0.43
1:E:85:TYR:O	1:E:101:THR:N	2.52	0.42
2:O:35:HIS:ND1	2:O:50:TYR:HB3	2.34	0.42
3:A:24:LEU:HD11	3:A:78:ARG:HB2	2.01	0.42
3:A:1053:PRO:O	3:A:1054:GLN:NE2	2.53	0.42
5:V:82:ASP:OD2	5:V:86:TYR:OH	2.34	0.42
7:P:37:TRP:HD1	7:P:50:GLY:HA3	1.83	0.42
3:C:98:SER:O	3:C:100:ILE:N	2.49	0.42
3:C:256:SER:OG	3:C:257:GLY:N	2.49	0.42
1:D:31:ASN:OD1	1:D:32:LEU:N	2.52	0.42
3:A:85:PRO:O	3:A:269:TYR:OH	2.35	0.42
3:A:273:ARG:NH1	3:A:292:ALA:HB3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:327:VAL:O	3:A:531:THR:HG22	2.19	0.42
3:A:336:CYS:HB3	3:A:361:CYS:HA	2.00	0.42
3:B:718:PHE:CG	3:B:1067:TYR:HE1	2.35	0.42
3:B:1082:CYS:HB2	3:B:1126:CYS:HB2	1.86	0.42
6:R:37:TYR:HE2	6:R:101:PHE:CE1	2.37	0.42
6:R:37:TYR:O	6:R:87:TYR:HA	2.20	0.42
7:W:74:ASP:OD1	7:W:77:THR:OG1	2.29	0.42
6:Q:28:ASN:O	6:Q:32:ASN:HB2	2.19	0.42
3:C:336:CYS:HB3	3:C:361:CYS:HA	2.00	0.42
2:N:6:GLN:HE21	2:N:111:GLY:HA3	1.84	0.42
3:A:412:PRO:HG3	3:A:429:PHE:HD2	1.83	0.42
3:A:643:PHE:CZ	3:A:655:HIS:CD2	3.07	0.42
3:B:1053:PRO:O	3:B:1054:GLN:NE2	2.53	0.42
6:S:13:ALA:HB3	6:S:16:GLN:HG2	2.01	0.42
7:P:53:ASP:HB3	7:P:55:GLU:O	2.19	0.42
3:C:412:PRO:HG3	3:C:429:PHE:HD2	1.83	0.42
2:L:35:HIS:ND1	2:L:50:TYR:HB3	2.34	0.42
2:N:6:GLN:H	2:N:112:GLN:NE2	2.17	0.42
2:O:6:GLN:HE21	2:O:111:GLY:HA3	1.84	0.42
2:O:18:VAL:HG12	2:O:86:LEU:HD21	2.01	0.42
3:A:97:LYS:HG3	3:A:98:SER:H	1.85	0.42
4:M:53:TYR:CD1	4:M:72:ARG:HD3	2.55	0.42
5:V:8:PRO:HG2	5:V:11:LEU:HD23	2.00	0.42
4:I:53:TYR:CD1	4:I:72:ARG:HD3	2.55	0.42
3:B:37:TYR:O	3:B:39:PRO:HD3	2.20	0.42
3:B:246:ARG:NH2	7:W:102:PRO:HG3	2.34	0.42
6:S:28:ASN:O	6:S:32:ASN:HB2	2.19	0.42
6:S:37:TYR:O	6:S:87:TYR:HA	2.19	0.42
7:X:37:TRP:HD1	7:X:50:GLY:HA3	1.83	0.42
7:P:103:PHE:O	7:P:104:SER:OG	2.33	0.42
3:C:431:GLY:HA3	3:C:514:SER:HA	2.02	0.42
3:C:432:CYS:HB2	3:C:515:PHE:CE2	2.55	0.42
3:C:1053:PRO:O	3:C:1054:GLN:NE2	2.53	0.42
3:A:855:PHE:CG	3:C:589:PRO:HG2	2.54	0.42
3:A:1041:ASP:HB3	3:B:1030:SER:OG	2.20	0.42
4:T:60:TYR:HE1	4:T:70:ILE:HG22	1.84	0.42
5:K:37:GLN:HG3	5:K:86:TYR:HE1	1.84	0.42
3:B:273:ARG:NH1	3:B:292:ALA:HB3	2.34	0.42
7:W:70:THR:HG22	7:W:83:GLU:HB2	2.02	0.42
6:S:39:GLN:O	6:S:85:ALA:HB1	2.19	0.42
6:Q:37:TYR:HE2	6:Q:101:PHE:CE1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:39:GLN:O	6:Q:85:ALA:HB1	2.19	0.42
3:C:273:ARG:NH1	3:C:292:ALA:HB3	2.35	0.42
3:C:656:VAL:HG12	3:C:658:ASN:H	1.83	0.42
1:H:31:ASN:OD1	1:H:32:LEU:N	2.52	0.42
3:A:144:TYR:CE2	3:A:155:SER:HB3	2.55	0.42
3:A:405:ASP:HA	3:A:408:ARG:CG	2.49	0.42
3:A:543:PHE:HB3	3:A:565:PHE:CZ	2.54	0.42
3:A:656:VAL:HG12	3:A:658:ASN:H	1.83	0.42
3:B:743:CYS:HB3	3:B:977:LEU:HD12	2.02	0.42
3:C:743:CYS:HB3	3:C:977:LEU:HD12	2.01	0.42
3:A:438:SER:OG	3:A:442:ASP:OD2	2.31	0.42
3:A:611:LEU:HB2	3:A:650:LEU:HD23	2.00	0.42
5:U:88:CYS:O	5:U:99:GLY:N	2.45	0.42
3:B:73:THR:OG1	3:B:74:ASN:N	2.52	0.42
3:B:433:VAL:HG22	3:B:512:VAL:HG13	2.01	0.42
3:B:543:PHE:HB3	3:B:565:PHE:CZ	2.54	0.42
7:X:21:VAL:HB	7:X:82:MET:HB3	2.02	0.42
7:P:21:VAL:HB	7:P:82:MET:HB3	2.02	0.42
3:C:73:THR:OG1	3:C:74:ASN:N	2.52	0.42
3:C:201:PHE:HB2	3:C:231:ILE:HG13	2.00	0.42
3:C:970:PHE:CD1	3:C:996:LEU:HD23	2.51	0.42
1:D:85:TYR:O	1:D:101:THR:N	2.52	0.42
2:N:35:HIS:ND1	2:N:50:TYR:HB3	2.34	0.42
2:O:6:GLN:H	2:O:112:GLN:NE2	2.17	0.42
3:A:584:ILE:C	3:A:585:LEU:HD12	2.45	0.42
3:A:748:GLU:OE1	3:A:748:GLU:N	2.43	0.42
3:A:894:LEU:HD22	3:C:1072:GLU:HG2	2.02	0.42
5:V:39:LYS:NZ	5:V:84:ALA:HB2	2.35	0.42
5:V:62:PHE:HD1	5:V:73:LEU:HD11	1.85	0.42
3:B:28:TYR:HD1	3:B:61:ASN:HB3	1.83	0.42
6:S:18:VAL:HG12	6:S:79:LEU:HD11	2.02	0.42
3:C:97:LYS:HG3	3:C:98:SER:H	1.85	0.42
3:C:144:TYR:CE2	3:C:155:SER:HB3	2.55	0.42
3:C:643:PHE:CZ	3:C:655:HIS:CD2	3.07	0.42
2:N:4:LEU:HB3	2:N:22:CYS:SG	2.60	0.42
2:N:11:VAL:HG13	2:N:117:THR:HB	2.02	0.42
2:O:4:LEU:HB3	2:O:22:CYS:SG	2.60	0.42
4:M:60:TYR:HE1	4:M:70:ILE:HG22	1.84	0.42
3:B:432:CYS:HB2	3:B:515:PHE:CE2	2.55	0.42
3:B:611:LEU:HB2	3:B:650:LEU:HD23	2.00	0.42
6:S:37:TYR:HE2	6:S:101:PHE:CE1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:333:THR:OG1	3:C:361:CYS:N	2.53	0.42
1:E:31:ASN:OD1	1:E:32:LEU:N	2.52	0.42
3:A:28:TYR:HD1	3:A:61:ASN:HB3	1.83	0.42
3:A:129:LYS:HB3	3:A:131:CYS:SG	2.60	0.42
3:A:333:THR:OG1	3:A:361:CYS:N	2.53	0.42
3:A:433:VAL:HG22	3:A:512:VAL:HG13	2.01	0.42
5:K:39:LYS:NZ	5:K:84:ALA:HB2	2.35	0.42
3:B:962:LEU:HD11	3:B:1007:TYR:CB	2.42	0.42
7:W:53:ASP:HB3	7:W:55:GLU:O	2.19	0.42
6:S:28:ASN:OD1	6:S:29:ILE:HG13	2.20	0.42
3:C:24:LEU:HD11	3:C:78:ARG:HB2	2.01	0.42
3:C:121:ASN:ND2	3:C:176:LEU:HB2	2.35	0.42
2:N:24:VAL:HG11	2:N:29:PHE:CD1	2.55	0.41
3:A:73:THR:OG1	3:A:74:ASN:N	2.52	0.41
3:A:121:ASN:ND2	3:A:176:LEU:HB2	2.35	0.41
3:A:718:PHE:CG	3:A:1067:TYR:HE1	2.36	0.41
5:K:62:PHE:HD1	5:K:73:LEU:HD11	1.85	0.41
3:B:97:LYS:HG3	3:B:98:SER:H	1.85	0.41
6:R:28:ASN:OD1	6:R:29:ILE:HG13	2.20	0.41
7:W:21:VAL:HB	7:W:82:MET:HB3	2.02	0.41
6:Q:13:ALA:HB3	6:Q:16:GLN:HG2	2.01	0.41
6:Q:37:TYR:O	6:Q:87:TYR:HA	2.19	0.41
3:C:246:ARG:HA	3:C:257:GLY:O	2.20	0.41
3:C:792:PRO:O	3:C:795:LYS:NZ	2.37	0.41
2:L:51:ILE:HG13	2:L:58:THR:HG22	2.02	0.41
2:N:102:ASP:CG	2:N:103:PRO:CD	2.66	0.41
5:U:37:GLN:HG3	5:U:86:TYR:HE1	1.84	0.41
4:I:47:TRP:CZ3	5:K:95:PRO:HB3	2.54	0.41
3:B:91:TYR:OH	3:B:191:GLU:OE2	2.31	0.41
3:B:178:ASP:HB3	3:B:190:ARG:NH1	2.36	0.41
3:B:246:ARG:HA	3:B:257:GLY:O	2.21	0.41
3:B:333:THR:OG1	3:B:361:CYS:N	2.53	0.41
3:B:351:TYR:CE1	3:B:452:LEU:HB2	2.55	0.41
7:W:68:ARG:HH12	7:W:88:ARG:HG2	1.86	0.41
3:C:543:PHE:HB3	3:C:565:PHE:CZ	2.55	0.41
2:L:6:GLN:H	2:L:112:GLN:NE2	2.17	0.41
2:O:24:VAL:HG11	2:O:29:PHE:CD1	2.55	0.41
2:O:102:ASP:C	2:O:104:TYR:N	2.78	0.41
3:A:431:GLY:HA3	3:A:514:SER:HA	2.02	0.41
3:A:825:LYS:HD2	3:A:942:ALA:HA	2.02	0.41
4:M:24:ALA:HB3	4:M:77:ASN:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:37:GLN:HG3	5:V:86:TYR:HE1	1.84	0.41
3:B:129:LYS:HB3	3:B:131:CYS:SG	2.60	0.41
2:L:11:VAL:HG13	2:L:117:THR:HB	2.02	0.41
3:A:37:TYR:O	3:A:39:PRO:HD3	2.20	0.41
3:A:718:PHE:CE1	3:A:720:ILE:HD11	2.56	0.41
4:I:24:ALA:HB3	4:I:77:ASN:OD1	2.20	0.41
4:I:60:TYR:HE1	4:I:70:ILE:HG22	1.84	0.41
3:B:144:TYR:CE2	3:B:155:SER:HB3	2.55	0.41
3:B:374:PHE:HB2	3:B:377:PHE:HB2	2.00	0.41
7:W:103:PHE:O	7:W:104:SER:OG	2.33	0.41
3:C:37:TYR:O	3:C:39:PRO:HD3	2.20	0.41
3:C:151:SER:OG	3:C:152:TRP:N	2.54	0.41
3:C:351:TYR:CE1	3:C:452:LEU:HB2	2.55	0.41
2:O:101:TYR:OH	3:C:414:GLN:NE2	2.54	0.41
5:U:47:LEU:HD13	5:U:62:PHE:CE1	2.56	0.41
3:B:128:ILE:HD11	3:B:175:PHE:CZ	2.55	0.41
3:B:1094:VAL:HG13	3:C:900:MET:HE1	2.03	0.41
6:Q:18:VAL:HG12	6:Q:79:LEU:HD11	2.02	0.41
6:Q:28:ASN:OD1	6:Q:29:ILE:HG13	2.20	0.41
3:C:584:ILE:C	3:C:585:LEU:HD12	2.45	0.41
3:C:657:ASN:OD1	3:C:657:ASN:N	2.52	0.41
3:C:718:PHE:CG	3:C:1067:TYR:HE1	2.37	0.41
3:C:825:LYS:HD2	3:C:942:ALA:HA	2.02	0.41
3:A:128:ILE:HD11	3:A:175:PHE:CZ	2.55	0.41
3:A:864:LEU:HG	3:A:865:LEU:HD12	2.03	0.41
5:U:39:LYS:NZ	5:U:84:ALA:HB2	2.35	0.41
5:U:62:PHE:HD1	5:U:73:LEU:HD11	1.85	0.41
3:B:864:LEU:HG	3:B:865:LEU:HD12	2.03	0.41
7:P:68:ARG:HH12	7:P:88:ARG:HG2	1.86	0.41
3:C:416:GLY:O	3:C:420:ASP:N	2.54	0.41
3:C:864:LEU:HG	3:C:865:LEU:HD12	2.03	0.41
3:B:151:SER:OG	3:B:152:TRP:N	2.54	0.41
3:B:431:GLY:HA3	3:B:514:SER:HA	2.02	0.41
3:B:584:ILE:C	3:B:585:LEU:HD12	2.45	0.41
1:H:85:TYR:O	1:H:101:THR:N	2.53	0.41
2:L:6:GLN:HE21	2:L:111:GLY:HA3	1.84	0.41
1:E:34:TRP:HB2	1:E:47:ILE:HB	2.03	0.41
3:A:151:SER:OG	3:A:152:TRP:N	2.54	0.41
3:A:432:CYS:HB2	3:A:515:PHE:CE2	2.55	0.41
3:A:743:CYS:HB3	3:A:977:LEU:HD12	2.02	0.41
4:T:24:ALA:HB3	4:T:77:ASN:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:53:TYR:CD1	4:T:72:ARG:HD3	2.55	0.41
3:B:102:ARG:HA	3:B:102:ARG:HD3	1.89	0.41
2:L:4:LEU:HB3	2:L:22:CYS:SG	2.60	0.41
3:A:808:ASP:HB3	3:A:811:LYS:HE3	2.03	0.41
3:A:984:LEU:HD23	3:A:984:LEU:HA	1.93	0.41
4:I:58:LYS:HD3	4:I:60:TYR:OH	2.21	0.41
3:B:350:VAL:HG13	3:B:422:ASN:CB	2.51	0.41
3:B:722:VAL:HG12	3:B:1065:VAL:HG22	2.03	0.41
6:R:18:VAL:HG12	6:R:79:LEU:HD11	2.02	0.41
6:Q:43:THR:CG2	6:Q:44:ALA:N	2.62	0.41
3:C:129:LYS:HB3	3:C:131:CYS:SG	2.60	0.41
3:C:178:ASP:HB3	3:C:190:ARG:NH1	2.36	0.41
3:C:438:SER:OG	3:C:442:ASP:OD2	2.31	0.41
3:C:961:THR:O	3:C:965:GLN:HG2	2.21	0.41
3:A:103:GLY:HA3	3:A:119:ILE:O	2.21	0.41
3:A:1139:ASP:O	3:A:1143:PRO:HD2	2.21	0.41
4:M:35:HIS:HD2	4:M:50:VAL:HG13	1.84	0.41
4:T:29:PHE:N	4:T:77:ASN:OD1	2.53	0.41
5:V:47:LEU:HD13	5:V:62:PHE:CE1	2.56	0.41
3:B:57:PRO:HA	3:B:273:ARG:HH21	1.85	0.41
3:B:589:PRO:HG2	3:C:855:PHE:CG	2.56	0.41
3:C:106:PHE:HB2	3:C:117:LEU:HB3	2.02	0.41
2:N:51:ILE:HG13	2:N:58:THR:HG22	2.02	0.40
2:O:11:VAL:HG13	2:O:117:THR:HB	2.02	0.40
3:A:178:ASP:HB3	3:A:190:ARG:NH1	2.36	0.40
3:A:416:GLY:O	3:A:420:ASP:N	2.54	0.40
3:A:718:PHE:HE1	3:A:720:ILE:HD11	1.86	0.40
3:A:1039:ARG:NE	3:B:1031:GLU:OE2	2.43	0.40
4:T:39:GLN:O	4:T:92:ALA:HB1	2.21	0.40
3:B:98:SER:O	3:B:100:ILE:N	2.49	0.40
3:B:106:PHE:HB2	3:B:117:LEU:HB3	2.02	0.40
3:C:332:ILE:HB	3:C:525:CYS:SG	2.61	0.40
3:C:724:THR:HG23	3:C:934:ILE:HD12	2.03	0.40
2:L:24:VAL:HG11	2:L:29:PHE:CD1	2.55	0.40
2:O:51:ILE:HG13	2:O:58:THR:HG22	2.02	0.40
3:A:22:THR:HG21	3:A:78:ARG:HH11	1.87	0.40
3:A:90:VAL:HG21	3:A:238:PHE:CE2	2.57	0.40
3:A:246:ARG:HA	3:A:257:GLY:O	2.21	0.40
3:A:351:TYR:CE1	3:A:452:LEU:HB2	2.55	0.40
3:A:357:ARG:CG	3:A:394:ASN:HB3	2.51	0.40
4:M:39:GLN:O	4:M:92:ALA:HB1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:58:LYS:HD3	4:M:60:TYR:OH	2.21	0.40
4:I:29:PHE:N	4:I:77:ASN:OD1	2.53	0.40
3:B:25:PRO:HA	3:B:26:PRO:HD3	1.88	0.40
3:B:121:ASN:ND2	3:B:176:LEU:HB2	2.35	0.40
3:B:825:LYS:HD2	3:B:942:ALA:HA	2.02	0.40
7:X:68:ARG:HH12	7:X:88:ARG:HG2	1.86	0.40
7:P:25:VAL:CG1	7:P:78:ASP:HB3	2.47	0.40
3:C:103:GLY:HA3	3:C:119:ILE:O	2.21	0.40
3:C:718:PHE:CE1	3:C:720:ILE:HD11	2.55	0.40
3:C:718:PHE:HE1	3:C:720:ILE:HD11	1.86	0.40
2:O:36:TRP:HB3	2:O:48:ILE:HD11	2.04	0.40
3:A:106:PHE:HB2	3:A:117:LEU:HB3	2.02	0.40
3:A:722:VAL:HG12	3:A:1065:VAL:HG22	2.03	0.40
3:B:416:GLY:O	3:B:420:ASP:N	2.54	0.40
3:A:68:ILE:H	3:A:263:ALA:HB3	1.87	0.40
3:B:22:THR:HG21	3:B:78:ARG:HH11	1.86	0.40
3:B:90:VAL:HG21	3:B:238:PHE:CE2	2.57	0.40
3:B:324:GLU:OE2	3:B:539:VAL:HG11	2.22	0.40
3:B:802:PHE:CD2	3:B:805:ILE:HD11	2.57	0.40
3:C:68:ILE:H	3:C:263:ALA:HB3	1.87	0.40
3:C:128:ILE:HD11	3:C:175:PHE:CZ	2.55	0.40
3:C:722:VAL:HG12	3:C:1065:VAL:HG22	2.03	0.40
3:C:1139:ASP:O	3:C:1143:PRO:HD2	2.21	0.40
2:L:65:LYS:HA	2:L:65:LYS:HD3	1.82	0.40
1:D:34:TRP:HB2	1:D:47:ILE:HB	2.03	0.40
3:A:421:TYR:O	3:A:454:ARG:HD2	2.22	0.40
3:A:429:PHE:CE1	3:A:464:PHE:HZ	2.40	0.40
4:T:58:LYS:HD3	4:T:60:TYR:OH	2.21	0.40
5:K:18:ARG:CZ	5:K:76:SER:HB3	2.52	0.40
5:K:47:LEU:HD13	5:K:62:PHE:CE1	2.56	0.40
3:B:429:PHE:CE1	3:B:464:PHE:HZ	2.40	0.40
3:C:128:ILE:HD13	3:C:229:LEU:HD11	2.03	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	D	103/210 (49%)	89 (86%)	14 (14%)	0	100	100
1	E	103/210 (49%)	89 (86%)	14 (14%)	0	100	100
1	H	103/210 (49%)	89 (86%)	14 (14%)	0	100	100
2	L	118/223 (53%)	109 (92%)	9 (8%)	0	100	100
2	N	118/223 (53%)	109 (92%)	8 (7%)	1 (1%)	16	49
2	O	118/223 (53%)	109 (92%)	8 (7%)	1 (1%)	16	49
3	A	1062/1281 (83%)	955 (90%)	105 (10%)	2 (0%)	43	72
3	B	1062/1281 (83%)	956 (90%)	104 (10%)	2 (0%)	43	72
3	C	1055/1281 (82%)	949 (90%)	104 (10%)	2 (0%)	43	72
4	I	118/120 (98%)	109 (92%)	9 (8%)	0	100	100
4	M	118/120 (98%)	109 (92%)	9 (8%)	0	100	100
4	T	118/120 (98%)	109 (92%)	9 (8%)	0	100	100
5	K	106/108 (98%)	99 (93%)	7 (7%)	0	100	100
5	U	106/108 (98%)	99 (93%)	7 (7%)	0	100	100
5	V	106/108 (98%)	99 (93%)	7 (7%)	0	100	100
6	Q	90/109 (83%)	87 (97%)	3 (3%)	0	100	100
6	R	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
6	S	83/109 (76%)	79 (95%)	4 (5%)	0	100	100
7	P	118/120 (98%)	108 (92%)	10 (8%)	0	100	100
7	W	118/120 (98%)	108 (92%)	10 (8%)	0	100	100
7	X	106/120 (88%)	97 (92%)	9 (8%)	0	100	100
All	All	5136/6513 (79%)	4659 (91%)	469 (9%)	8 (0%)	44	72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	181	GLY
3	B	181	GLY
3	C	181	GLY
2	N	103	PRO
2	O	103	PRO

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Mol	Chain	Res	Type
3	A	1099	GLY
3	B	1099	GLY
3	C	1099	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	60/189 (32%)	60 (100%)	0	100	100
1	E	60/189 (32%)	60 (100%)	0	100	100
1	H	60/189 (32%)	60 (100%)	0	100	100
2	L	92/190 (48%)	91 (99%)	1 (1%)	65	74
2	N	92/190 (48%)	91 (99%)	1 (1%)	65	74
2	O	92/190 (48%)	91 (99%)	1 (1%)	65	74
3	A	930/1106 (84%)	929 (100%)	1 (0%)	88	87
3	B	930/1106 (84%)	929 (100%)	1 (0%)	88	87
3	C	930/1106 (84%)	929 (100%)	1 (0%)	88	87
4	I	96/98 (98%)	95 (99%)	1 (1%)	68	75
4	M	96/98 (98%)	95 (99%)	1 (1%)	68	75
4	T	96/98 (98%)	95 (99%)	1 (1%)	68	75
5	K	93/93 (100%)	92 (99%)	1 (1%)	65	74
5	U	93/93 (100%)	92 (99%)	1 (1%)	65	74
5	V	93/93 (100%)	92 (99%)	1 (1%)	65	74
6	Q	88/88 (100%)	87 (99%)	1 (1%)	65	74
6	R	88/88 (100%)	87 (99%)	1 (1%)	65	74
6	S	88/88 (100%)	87 (99%)	1 (1%)	65	74
7	P	101/101 (100%)	101 (100%)	0	100	100
7	W	101/101 (100%)	100 (99%)	1 (1%)	68	75
7	X	101/101 (100%)	101 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	4380/5595 (78%)	4364 (100%)	16 (0%)	81	81

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	5	VAL
2	N	5	VAL
2	O	5	VAL
3	A	503	VAL
4	M	115	VAL
5	U	15	VAL
4	T	115	VAL
5	V	15	VAL
4	I	115	VAL
5	K	15	VAL
3	B	503	VAL
6	R	3	VAL
7	W	33	VAL
6	S	3	VAL
6	Q	3	VAL
3	C	503	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	6	GLN
2	N	6	GLN
2	O	6	GLN
3	A	66	HIS
3	A	121	ASN
3	A	125	ASN
3	A	196	ASN
3	A	207	HIS
3	A	239	GLN
3	A	334	ASN
3	A	409	GLN
3	A	414	GLN
3	A	487	ASN
3	A	540	ASN
3	A	542	ASN
3	A	655	HIS

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Mol	Chain	Res	Type
3	A	675	GLN
3	A	762	GLN
3	A	804	GLN
3	A	901	GLN
3	A	907	ASN
3	A	935	GLN
3	A	954	GLN
3	A	957	GLN
3	A	1054	GLN
4	M	3	GLN
5	U	3	GLN
4	T	3	GLN
4	I	3	GLN
4	I	74	ASN
3	B	66	HIS
3	B	121	ASN
3	B	125	ASN
3	B	207	HIS
3	B	239	GLN
3	B	334	ASN
3	B	409	GLN
3	B	414	GLN
3	B	487	ASN
3	B	540	ASN
3	B	655	HIS
3	B	675	GLN
3	B	762	GLN
3	B	777	ASN
3	B	787	GLN
3	B	804	GLN
3	B	901	GLN
3	B	907	ASN
3	B	926	GLN
3	B	935	GLN
3	B	954	GLN
3	B	1054	GLN
6	R	6	GLN
6	R	28	ASN
6	R	32	ASN
6	R	52	ASN
6	S	6	GLN
6	S	28	ASN

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Mol	Chain	Res	Type
6	S	32	ASN
6	S	52	ASN
6	Q	6	GLN
6	Q	28	ASN
6	Q	32	ASN
6	Q	52	ASN
7	P	114	GLN
3	C	121	ASN
3	C	125	ASN
3	C	207	HIS
3	C	239	GLN
3	C	245	HIS
3	C	334	ASN
3	C	409	GLN
3	C	414	GLN
3	C	487	ASN
3	C	540	ASN
3	C	542	ASN
3	C	655	HIS
3	C	675	GLN
3	C	703	ASN
3	C	762	GLN
3	C	777	ASN
3	C	787	GLN
3	C	804	GLN
3	C	901	GLN
3	C	913	GLN
3	C	926	GLN
3	C	935	GLN
3	C	954	GLN
3	C	1054	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

30 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	NAG	F	1	3,8	14,14,15	0.27	0	17,19,21	0.67	0
8	NAG	F	2	8	14,14,15	0.27	0	17,19,21	0.66	0
8	NAG	G	1	3,8	14,14,15	0.28	0	17,19,21	0.68	0
8	NAG	G	2	8	14,14,15	0.27	0	17,19,21	0.70	0
8	NAG	J	1	3,8	14,14,15	0.26	0	17,19,21	0.62	0
8	NAG	J	2	8	14,14,15	0.28	0	17,19,21	0.64	0
8	NAG	Y	1	3,8	14,14,15	0.27	0	17,19,21	0.64	0
8	NAG	Y	2	8	14,14,15	0.28	0	17,19,21	0.67	0
8	NAG	Z	1	3,8	14,14,15	0.27	0	17,19,21	0.64	0
8	NAG	Z	2	8	14,14,15	0.27	0	17,19,21	0.64	0
8	NAG	a	1	3,8	14,14,15	0.27	0	17,19,21	0.64	0
8	NAG	a	2	8	14,14,15	0.28	0	17,19,21	0.66	0
8	NAG	b	1	3,8	14,14,15	0.27	0	17,19,21	0.67	0
8	NAG	b	2	8	14,14,15	0.27	0	17,19,21	0.67	0
8	NAG	c	1	3,8	14,14,15	0.26	0	17,19,21	0.63	0
8	NAG	c	2	8	14,14,15	0.27	0	17,19,21	0.64	0
8	NAG	d	1	3,8	14,14,15	0.27	0	17,19,21	0.62	0
8	NAG	d	2	8	14,14,15	0.27	0	17,19,21	0.67	0
8	NAG	e	1	3,8	14,14,15	0.28	0	17,19,21	0.64	0
8	NAG	e	2	8	14,14,15	0.26	0	17,19,21	0.64	0
8	NAG	f	1	3,8	14,14,15	0.27	0	17,19,21	0.64	0
8	NAG	f	2	8	14,14,15	0.27	0	17,19,21	0.63	0
8	NAG	g	1	3,8	14,14,15	0.28	0	17,19,21	0.66	0
8	NAG	g	2	8	14,14,15	0.28	0	17,19,21	0.68	0
8	NAG	h	1	3,8	14,14,15	0.26	0	17,19,21	0.63	0
8	NAG	h	2	8	14,14,15	0.27	0	17,19,21	0.65	0
8	NAG	i	1	3,8	14,14,15	0.28	0	17,19,21	0.63	0
8	NAG	i	2	8	14,14,15	0.28	0	17,19,21	0.66	0
8	NAG	j	1	3,8	14,14,15	0.27	0	17,19,21	0.64	0
8	NAG	j	2	8	14,14,15	0.27	0	17,19,21	0.66	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
8	NAG	F	1	3,8	-	0/6/23/26	0/1/1/1
8	NAG	F	2	8	-	2/6/23/26	0/1/1/1
8	NAG	G	1	3,8	-	0/6/23/26	0/1/1/1
8	NAG	G	2	8	-	0/6/23/26	0/1/1/1
8	NAG	J	1	3,8	-	0/6/23/26	0/1/1/1
8	NAG	J	2	8	-	0/6/23/26	0/1/1/1
8	NAG	Y	1	3,8	-	0/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	2/6/23/26	0/1/1/1
8	NAG	Z	1	3,8	-	0/6/23/26	0/1/1/1
8	NAG	Z	2	8	-	0/6/23/26	0/1/1/1
8	NAG	a	1	3,8	-	0/6/23/26	0/1/1/1
8	NAG	a	2	8	-	2/6/23/26	0/1/1/1
8	NAG	b	1	3,8	-	0/6/23/26	0/1/1/1
8	NAG	b	2	8	-	0/6/23/26	0/1/1/1
8	NAG	c	1	3,8	-	0/6/23/26	0/1/1/1
8	NAG	c	2	8	-	0/6/23/26	0/1/1/1
8	NAG	d	1	3,8	-	0/6/23/26	0/1/1/1
8	NAG	d	2	8	-	2/6/23/26	0/1/1/1
8	NAG	e	1	3,8	-	0/6/23/26	0/1/1/1
8	NAG	e	2	8	-	0/6/23/26	0/1/1/1
8	NAG	f	1	3,8	-	2/6/23/26	0/1/1/1
8	NAG	f	2	8	-	2/6/23/26	0/1/1/1
8	NAG	g	1	3,8	-	0/6/23/26	0/1/1/1
8	NAG	g	2	8	-	0/6/23/26	0/1/1/1
8	NAG	h	1	3,8	-	0/6/23/26	0/1/1/1
8	NAG	h	2	8	-	0/6/23/26	0/1/1/1
8	NAG	i	1	3,8	-	0/6/23/26	0/1/1/1
8	NAG	i	2	8	-	2/6/23/26	0/1/1/1
8	NAG	j	1	3,8	-	0/6/23/26	0/1/1/1
8	NAG	j	2	8	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

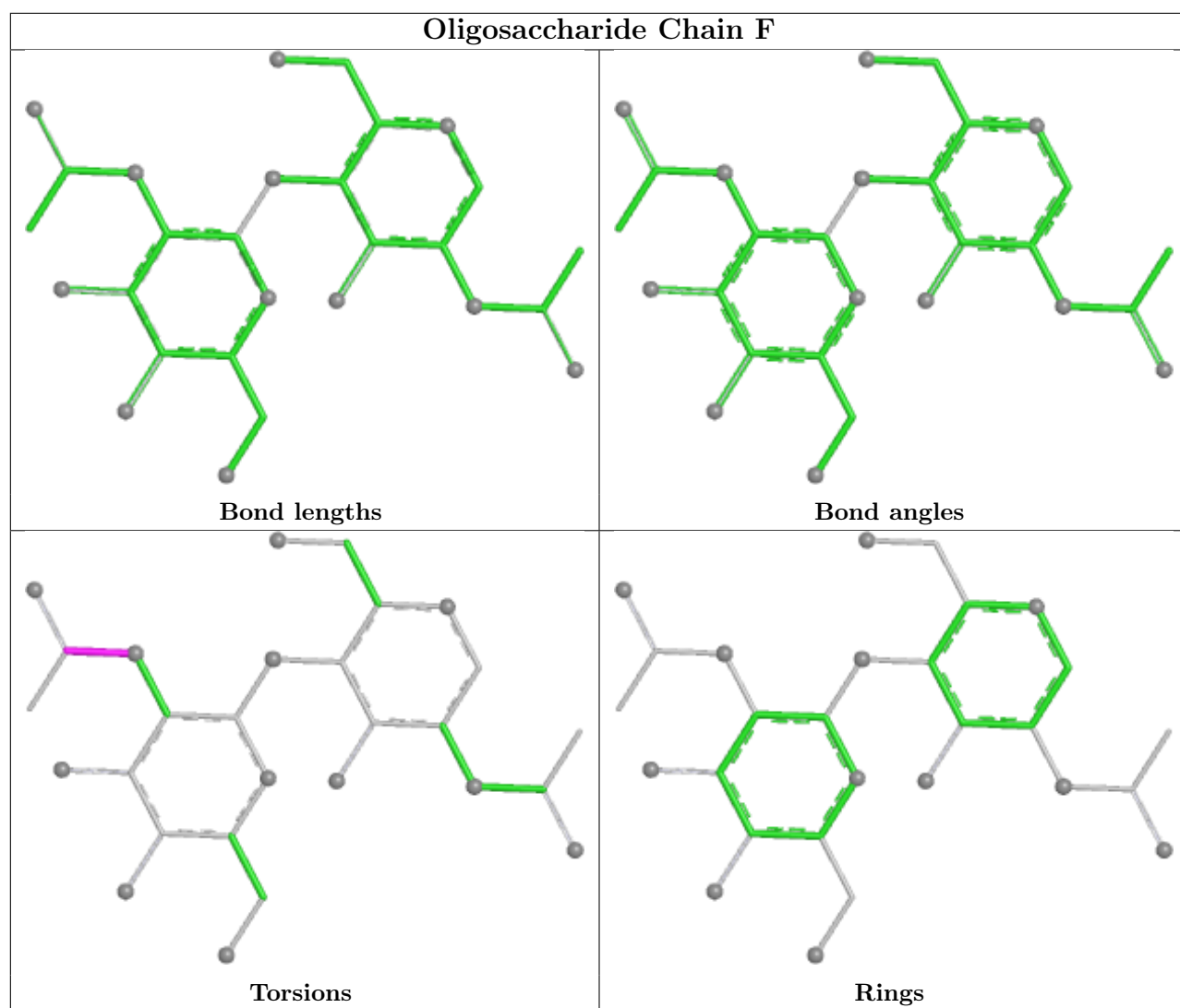
Mol	Chain	Res	Type	Atoms
8	F	2	NAG	C8-C7-N2-C2
8	F	2	NAG	O7-C7-N2-C2
8	a	2	NAG	C8-C7-N2-C2
8	a	2	NAG	O7-C7-N2-C2
8	f	2	NAG	C8-C7-N2-C2
8	f	2	NAG	O7-C7-N2-C2
8	d	2	NAG	C8-C7-N2-C2
8	Y	2	NAG	C8-C7-N2-C2
8	d	2	NAG	O7-C7-N2-C2
8	i	2	NAG	C8-C7-N2-C2
8	Y	2	NAG	O7-C7-N2-C2
8	f	1	NAG	C8-C7-N2-C2
8	i	2	NAG	O7-C7-N2-C2
8	f	1	NAG	O7-C7-N2-C2

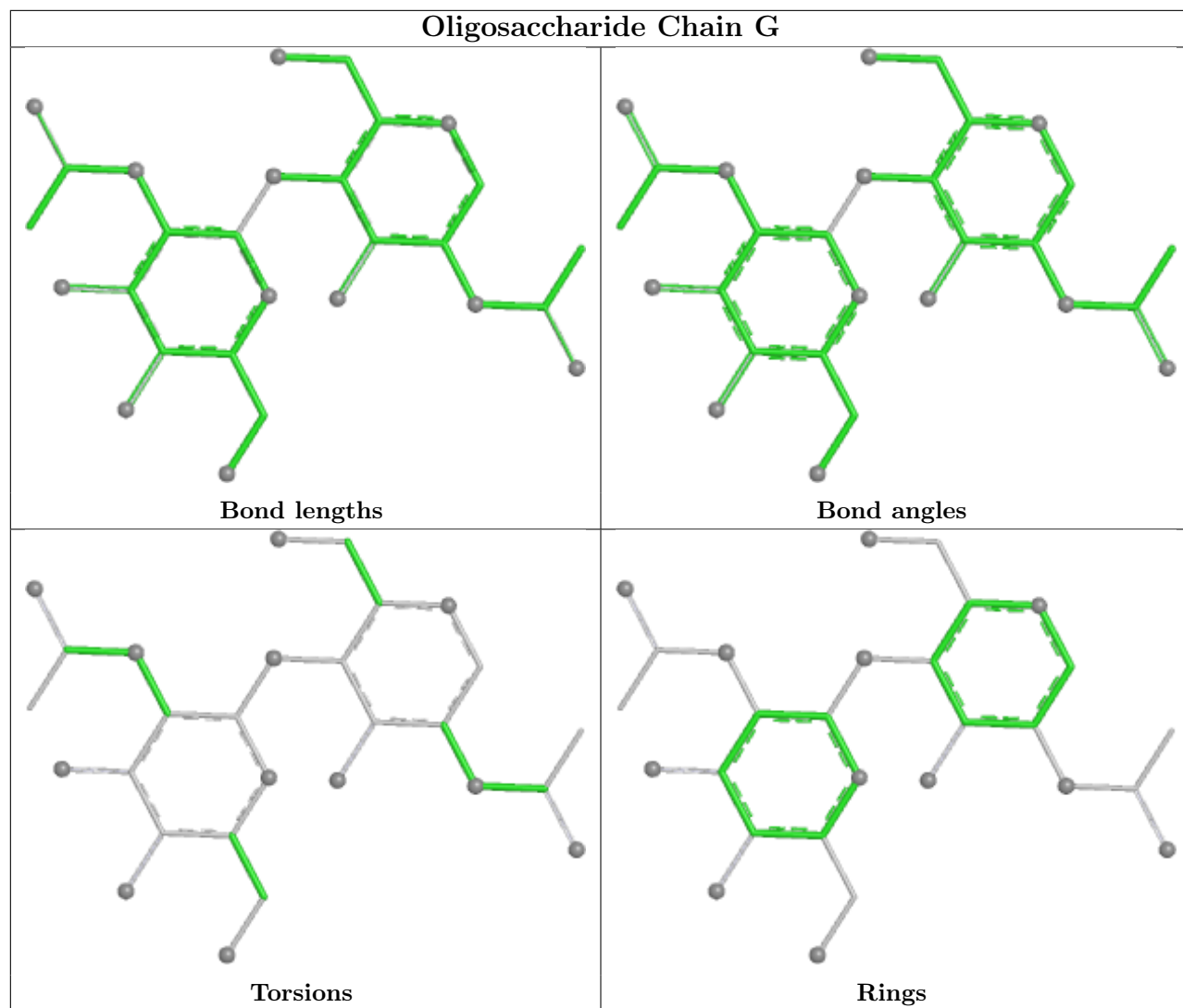
There are no ring outliers.

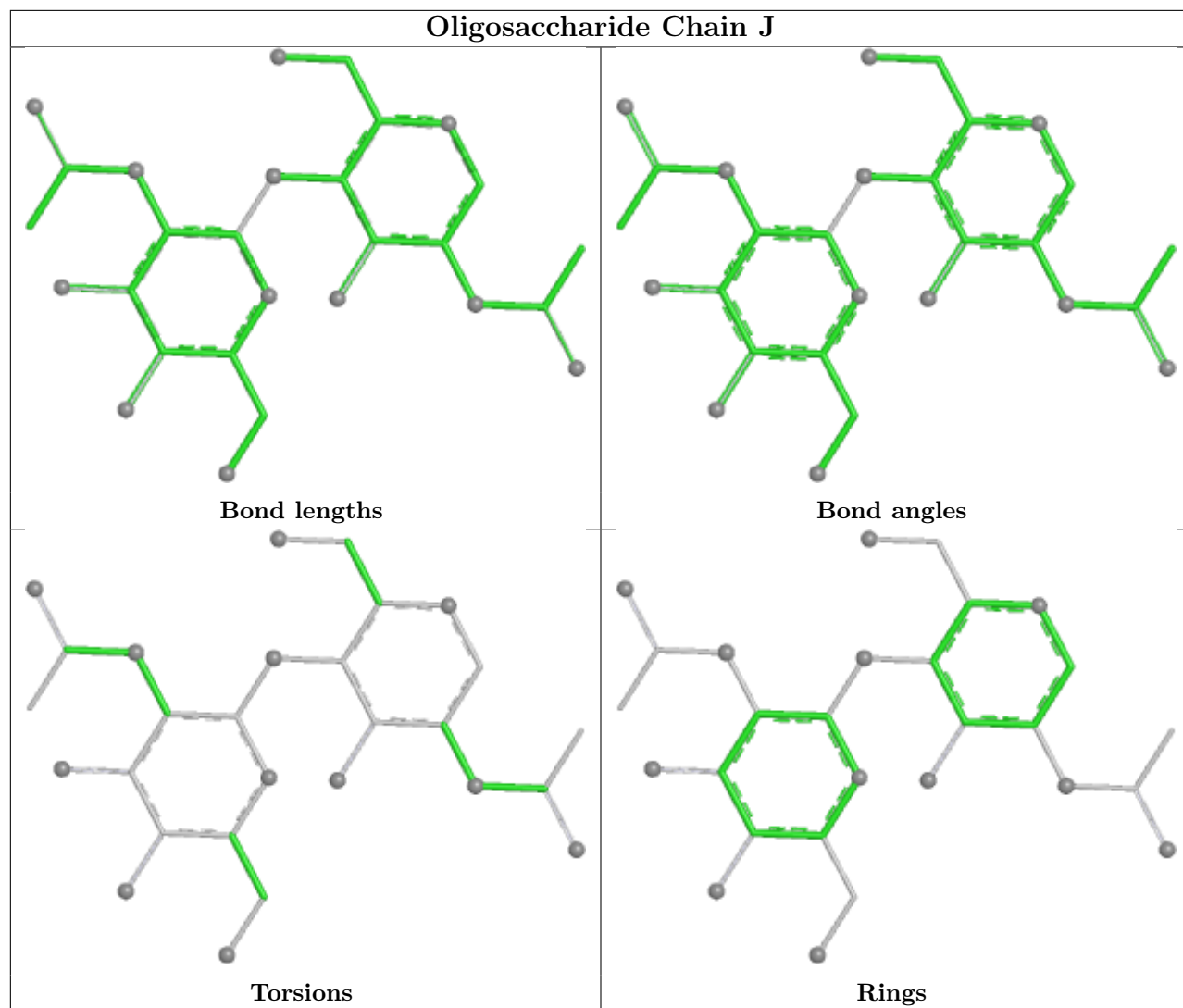
12 monomers are involved in 12 short contacts:

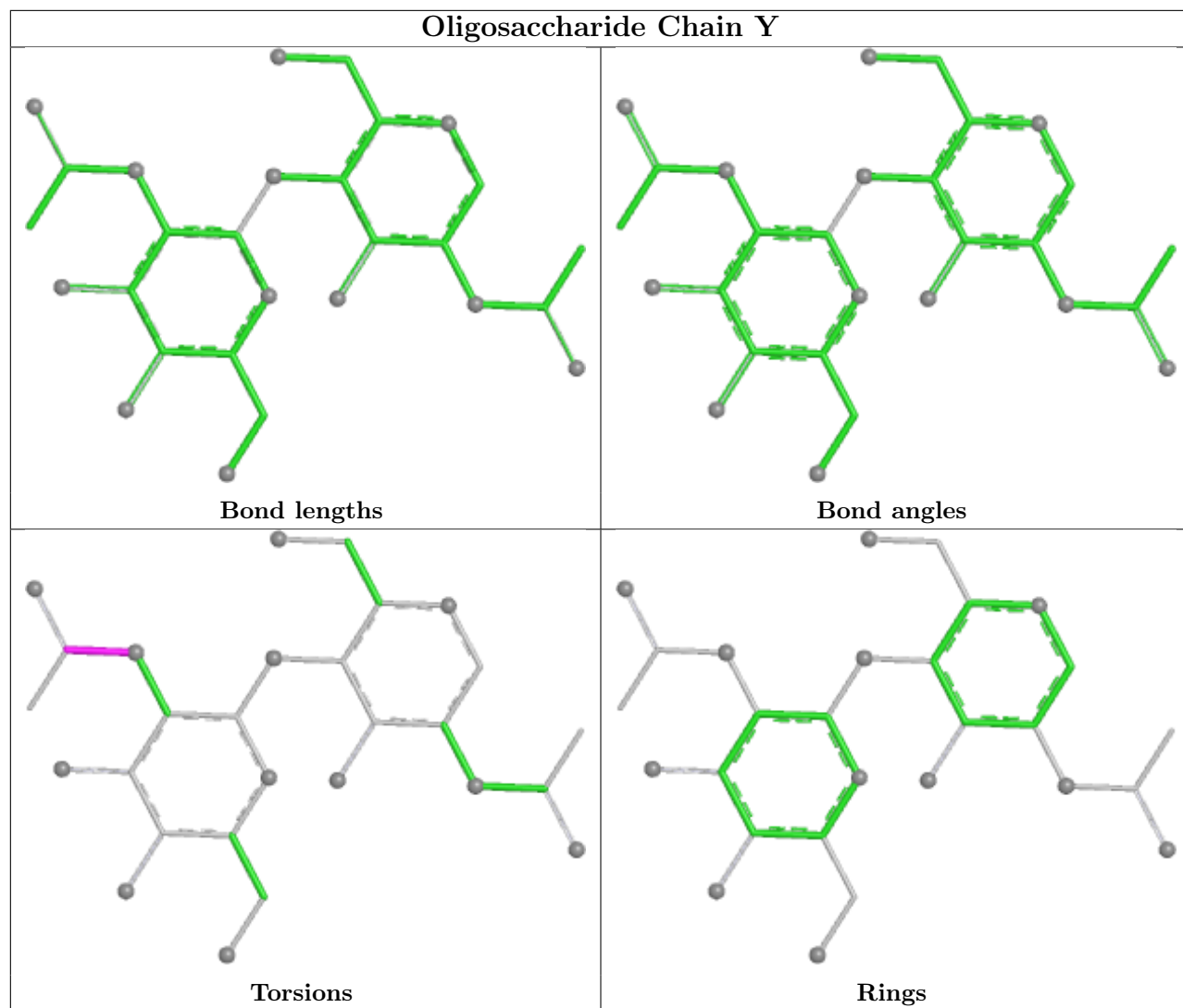
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	d	1	NAG	1	0
8	F	2	NAG	2	0
8	f	2	NAG	2	0
8	Y	2	NAG	1	0
8	a	2	NAG	2	0
8	i	2	NAG	1	0
8	d	2	NAG	1	0
8	G	1	NAG	1	0
8	i	1	NAG	1	0
8	Y	1	NAG	1	0
8	b	1	NAG	1	0
8	g	1	NAG	1	0

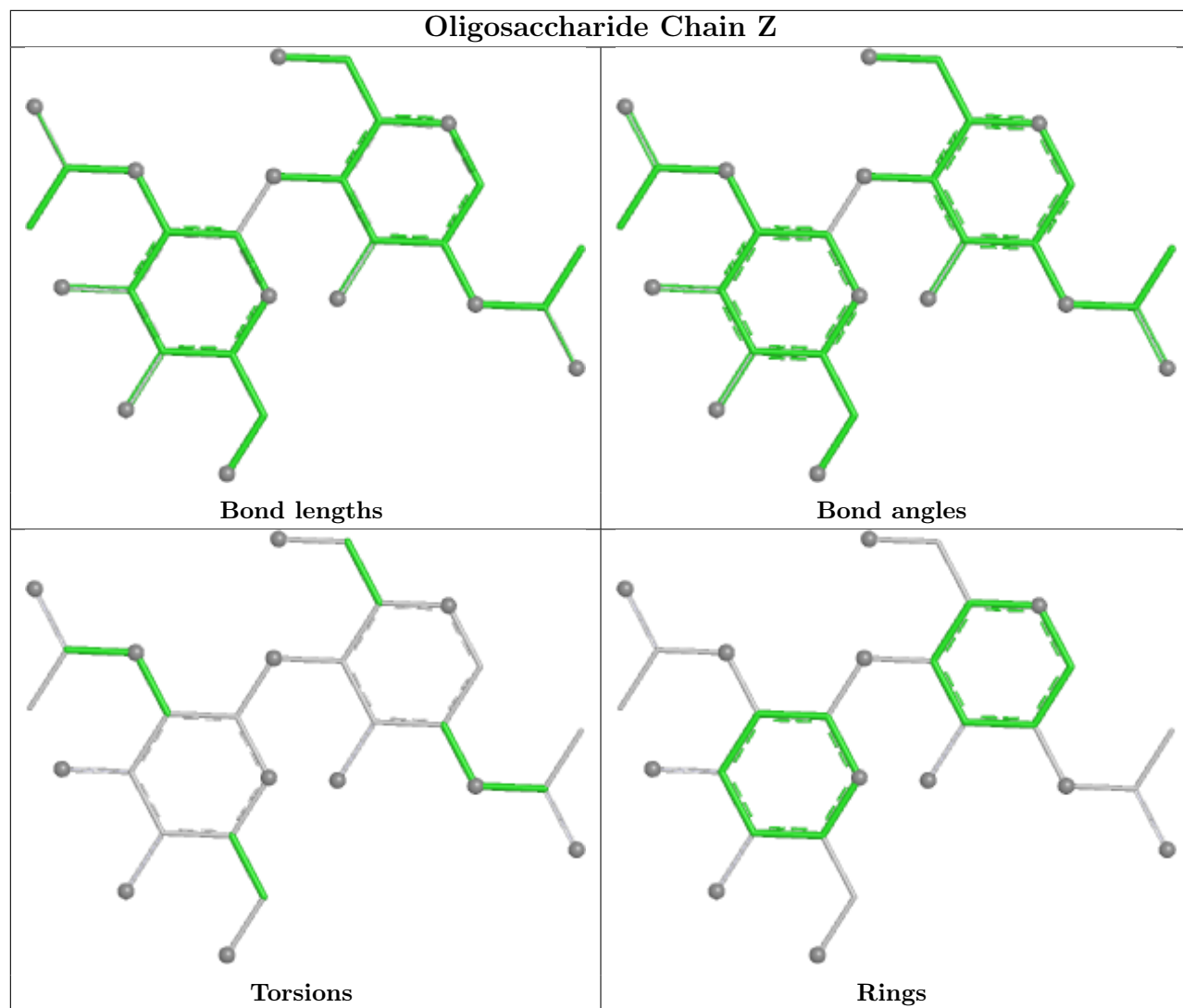
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

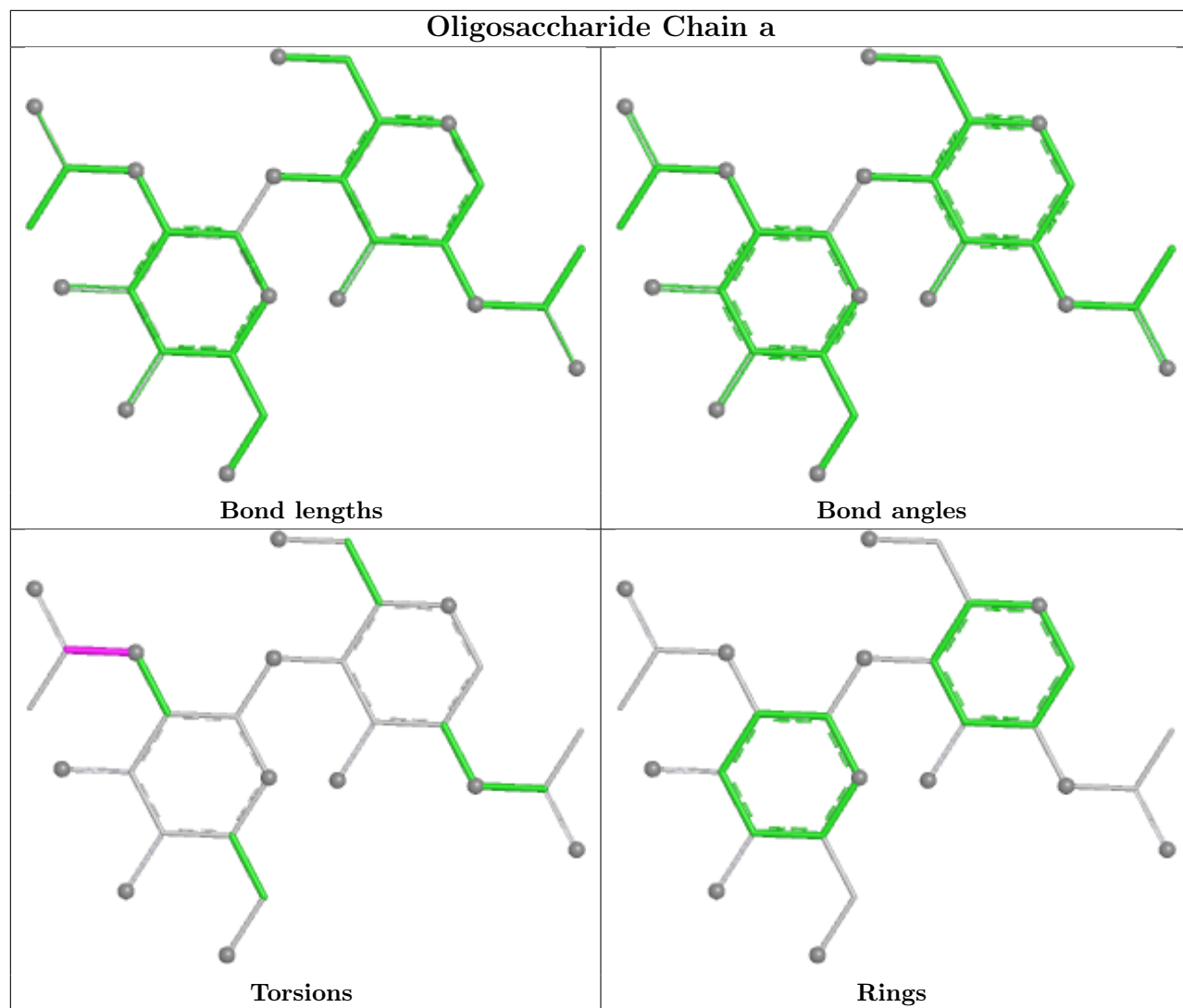


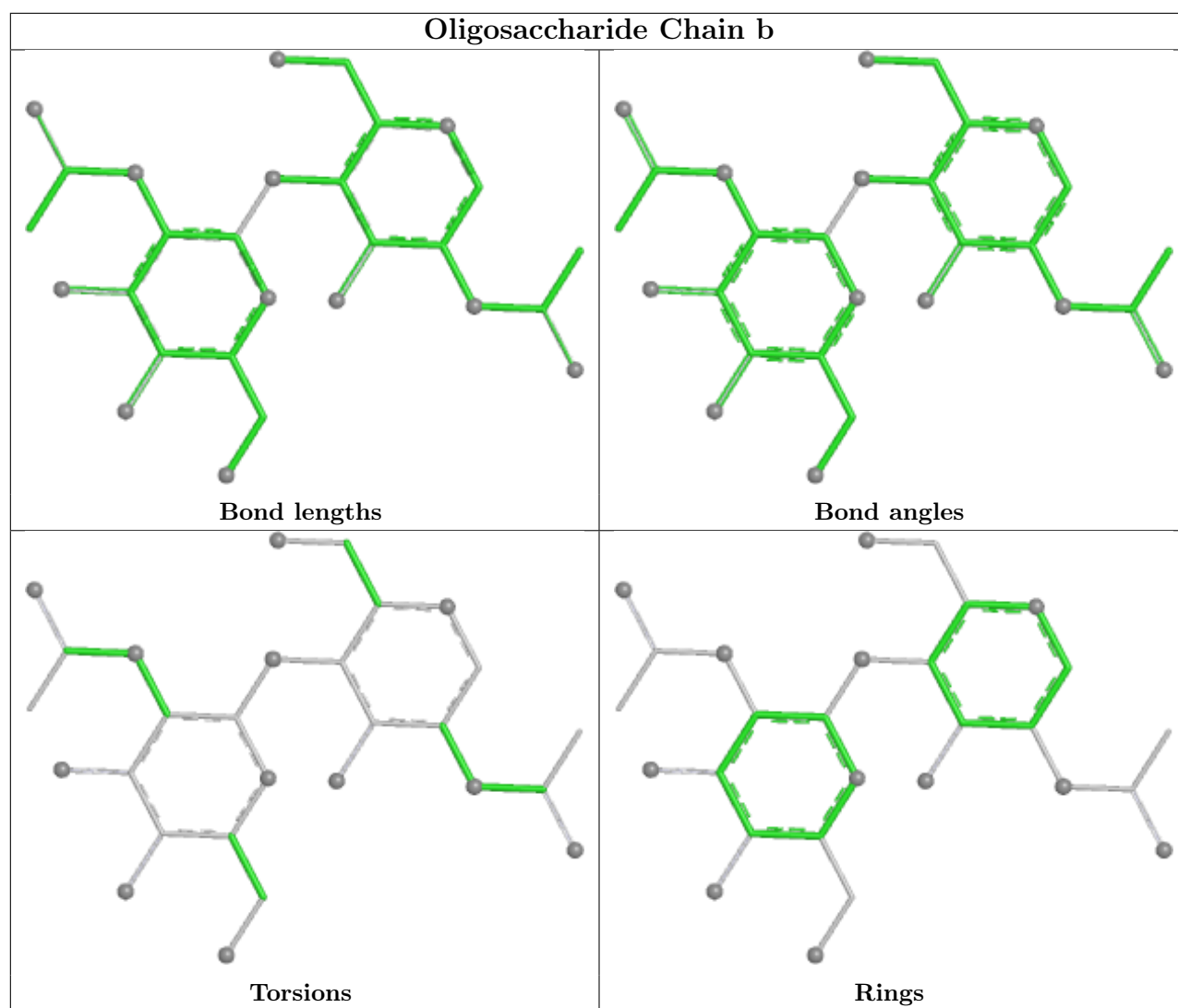


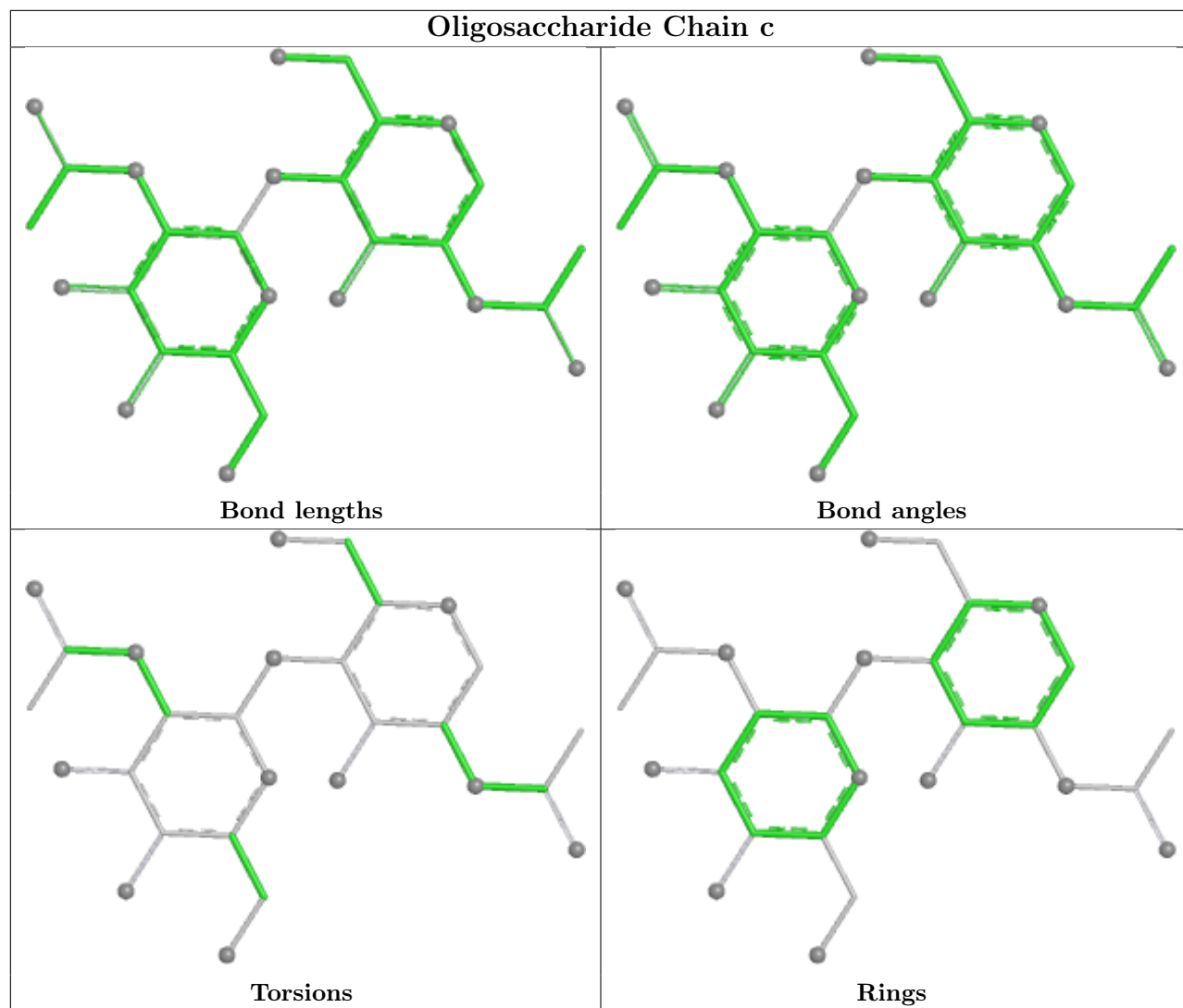


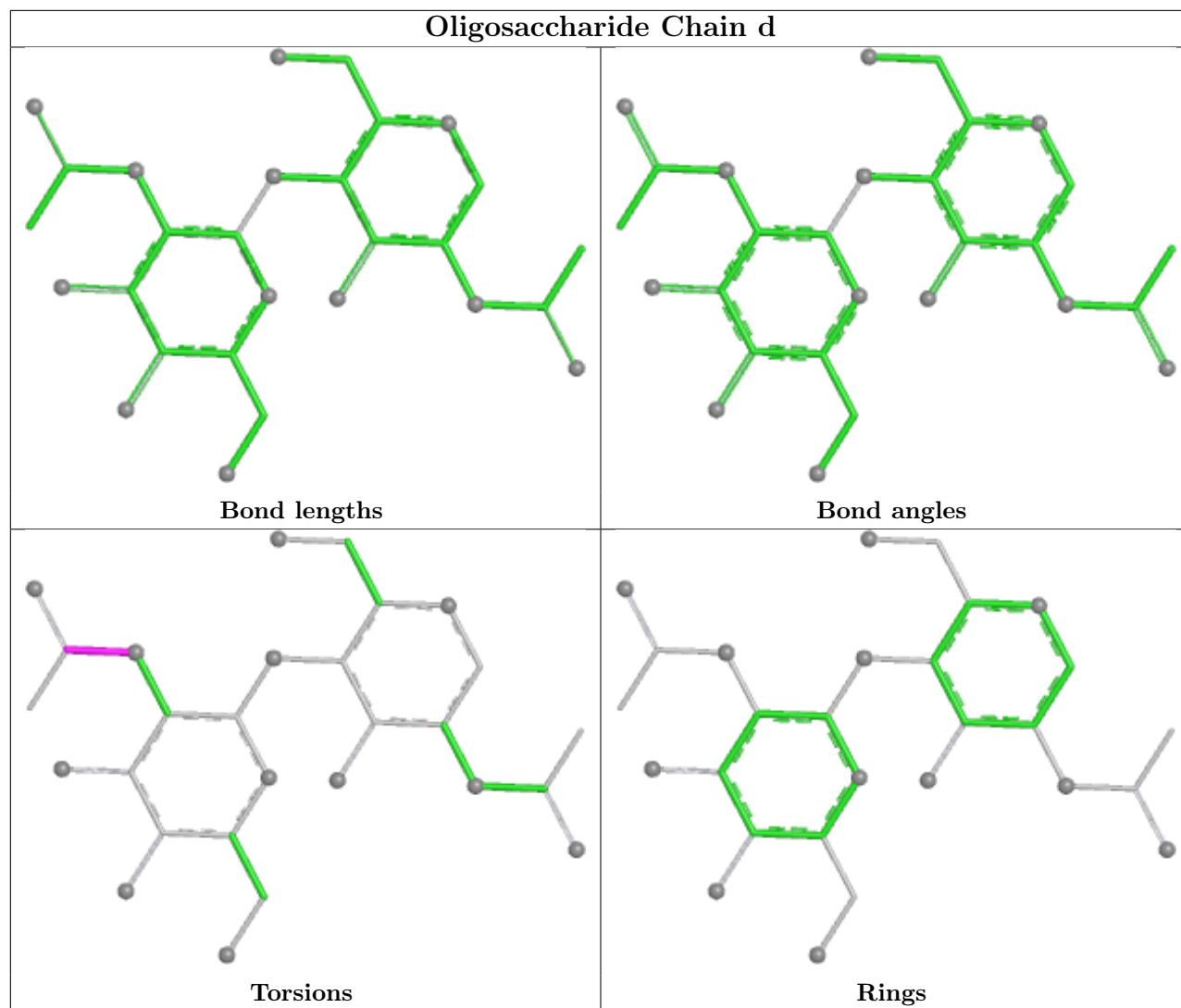


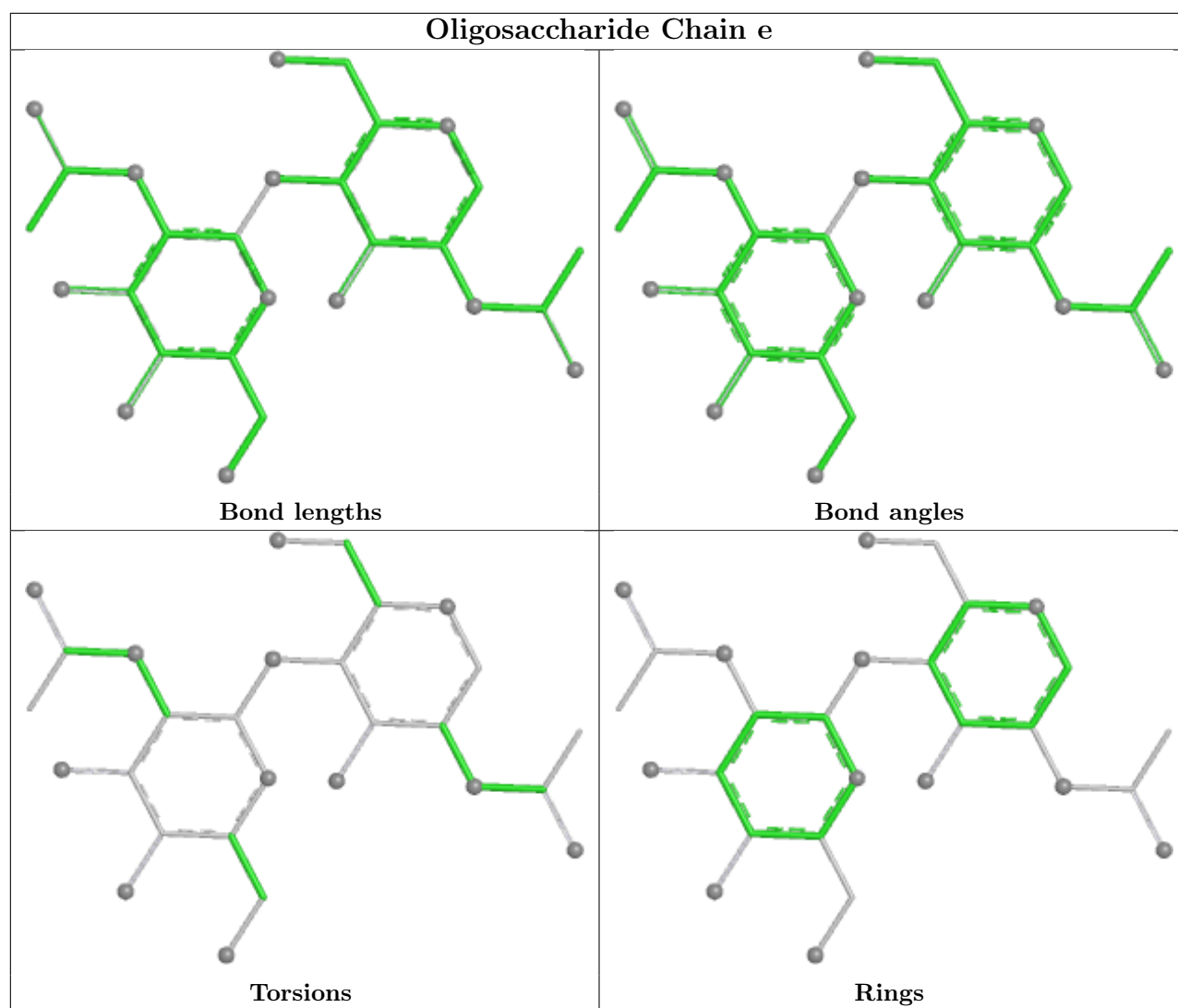


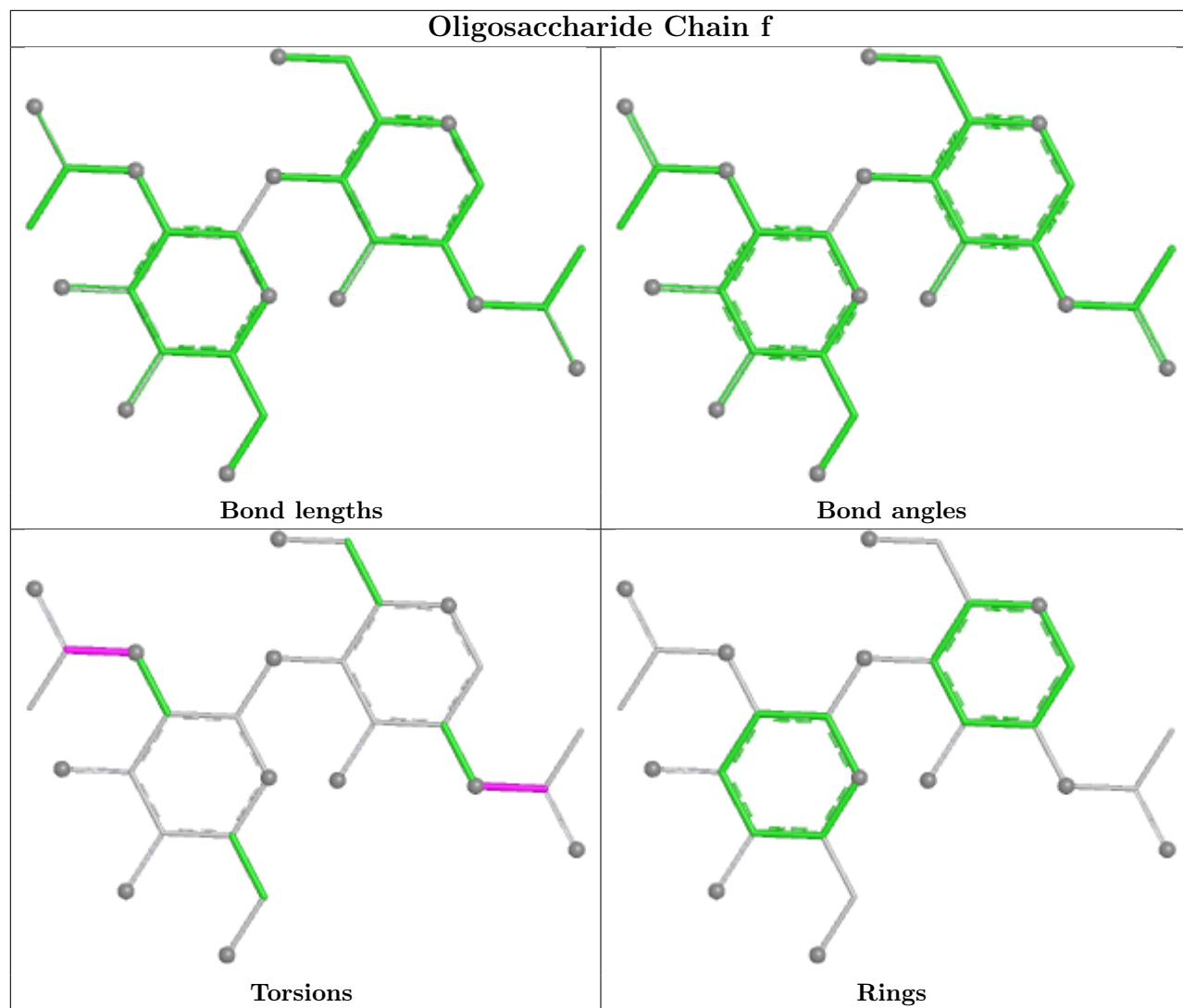


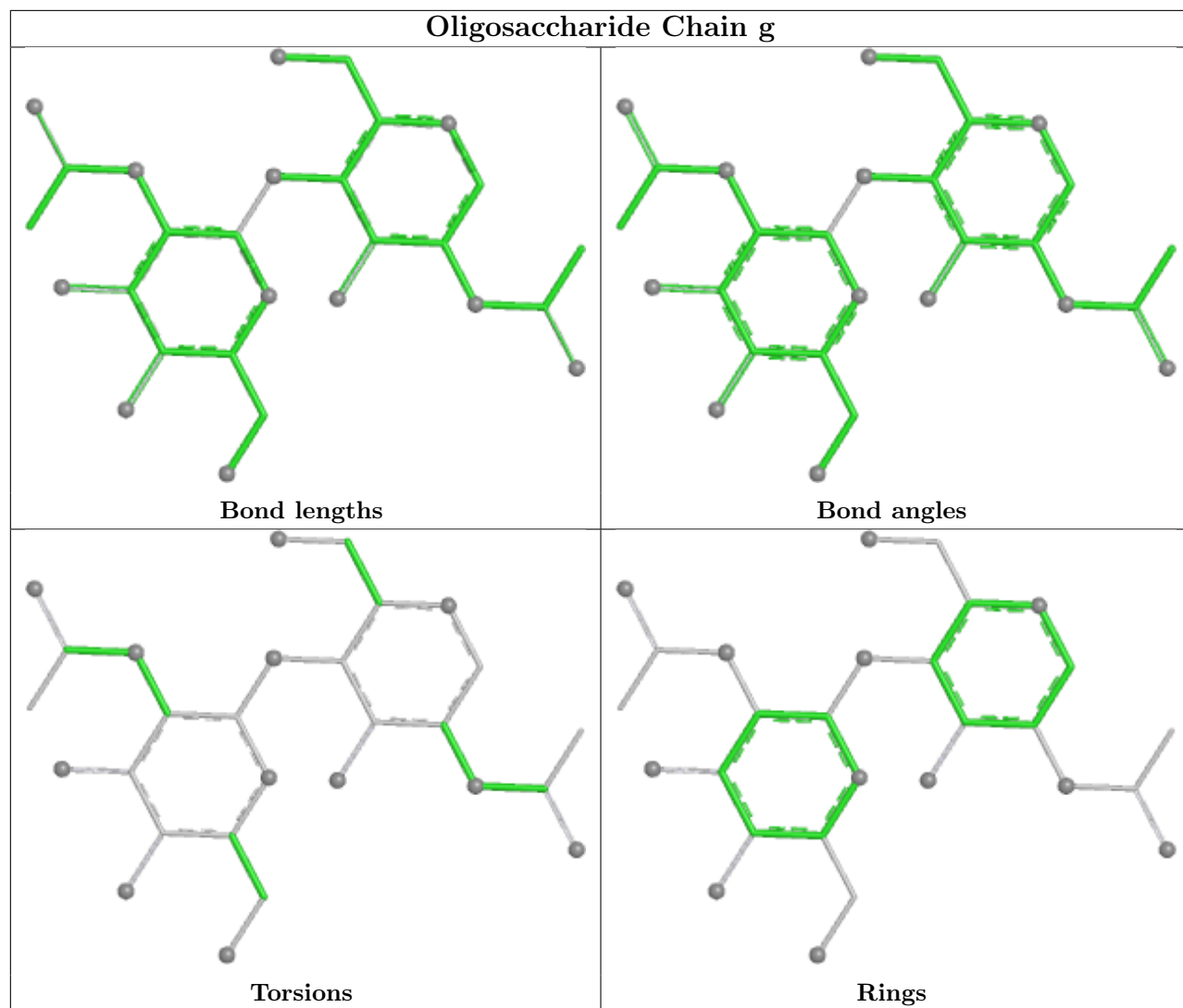


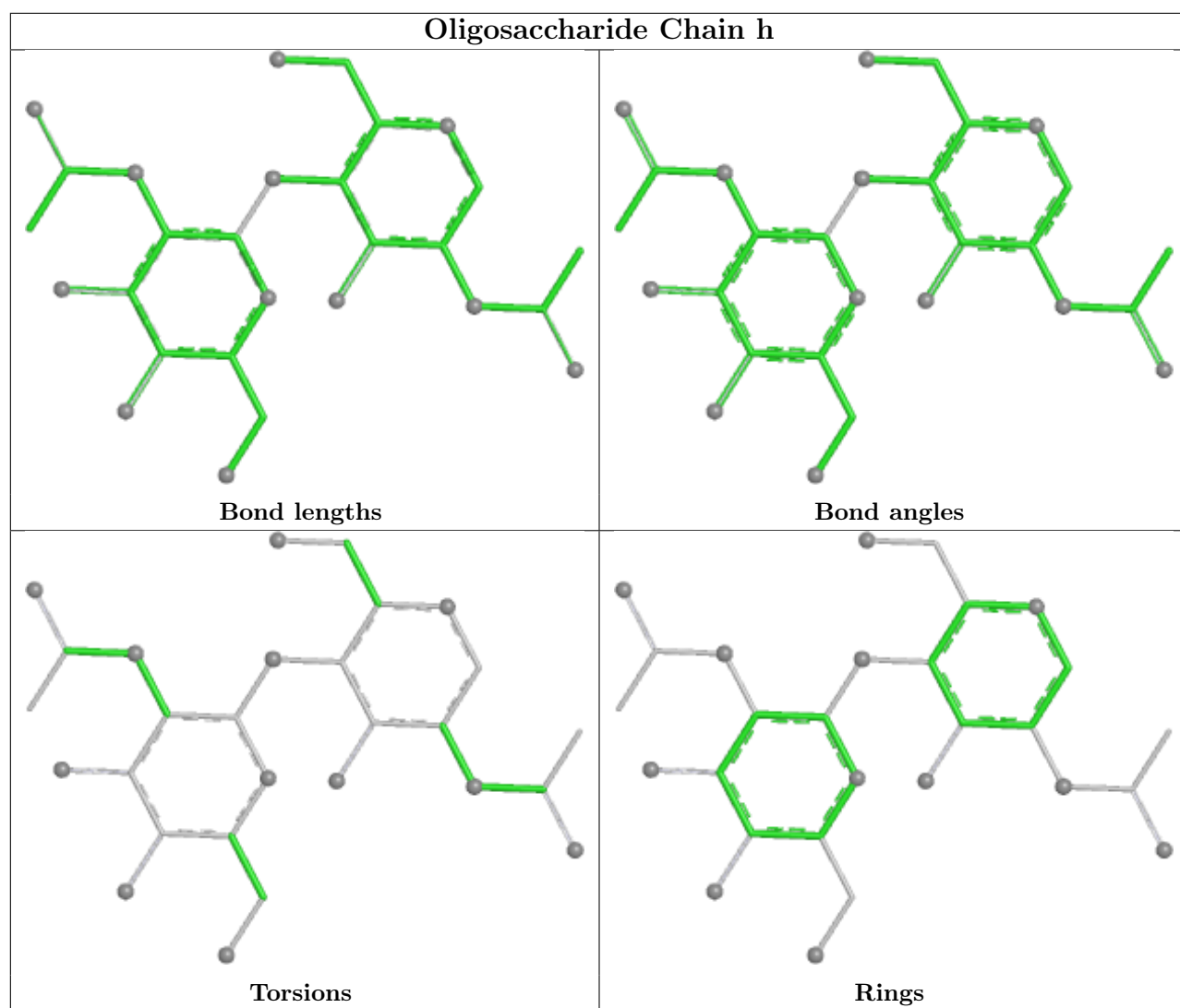


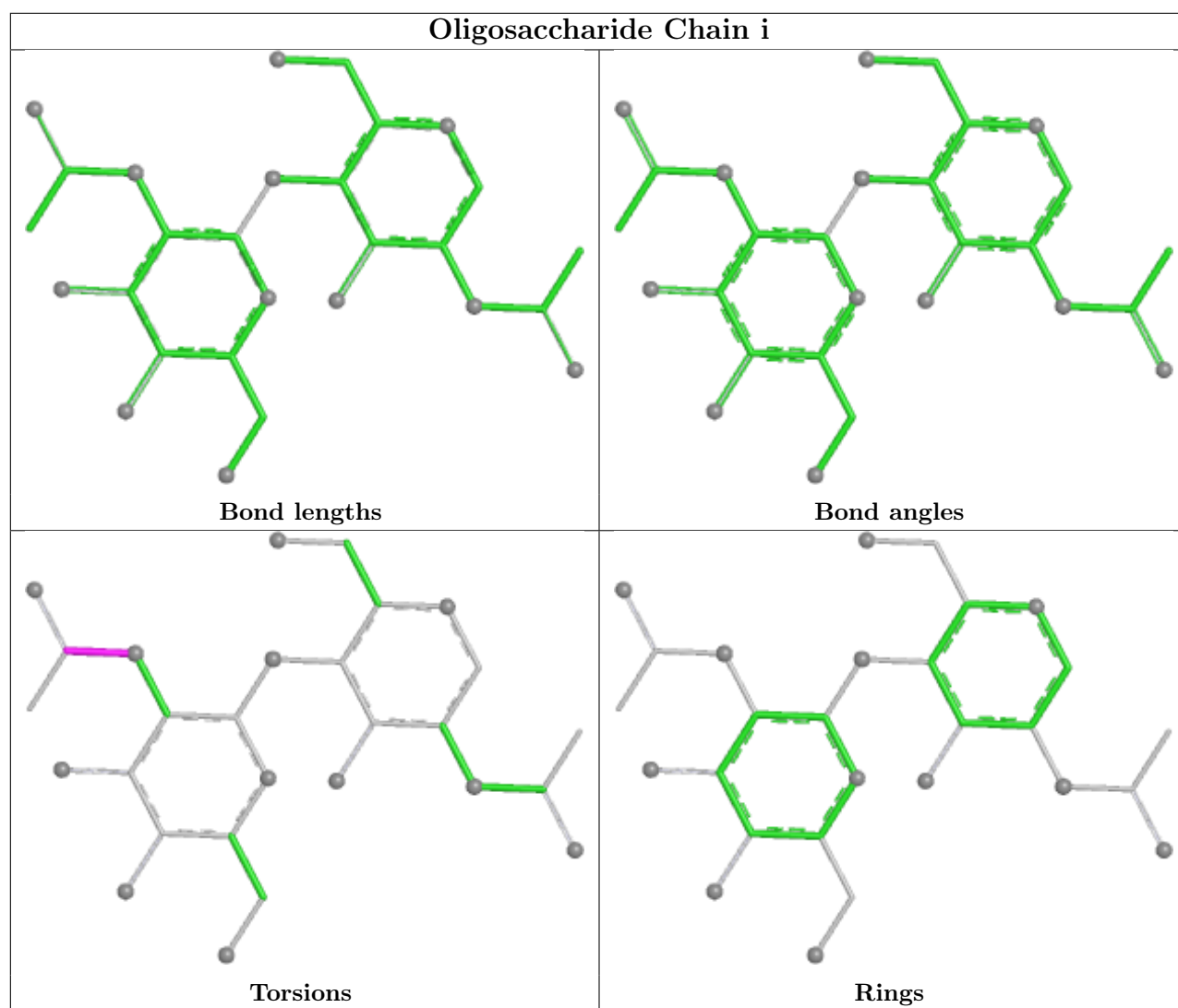


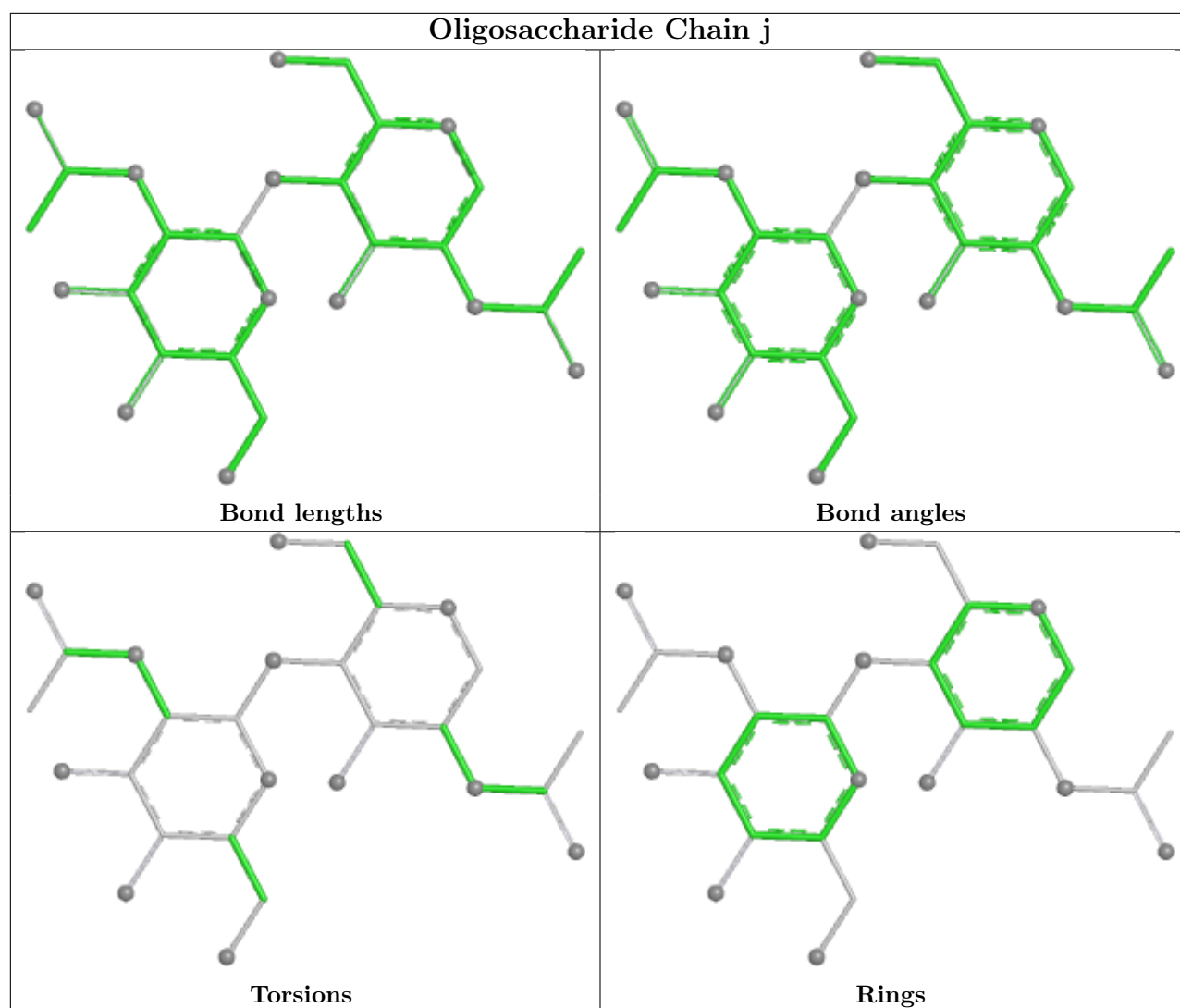












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

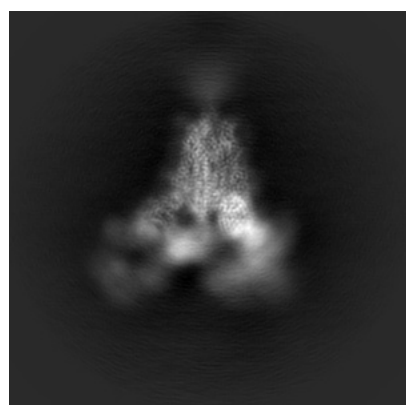
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30993. These allow visual inspection of the internal detail of the map and identification of artifacts.

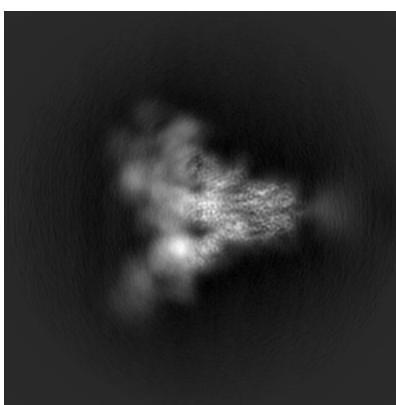
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

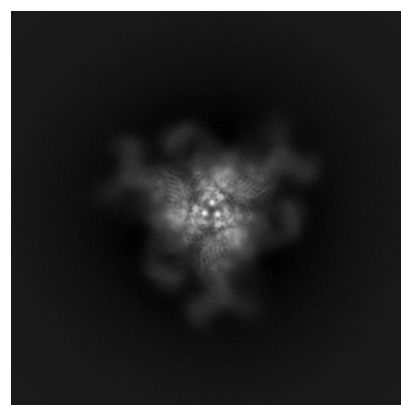
6.1.1 Primary map



X



Y

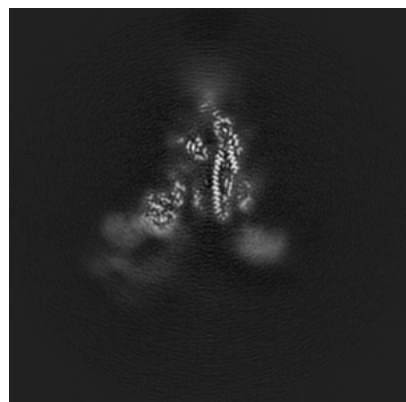


Z

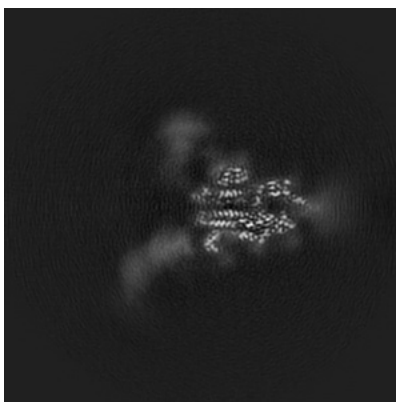
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

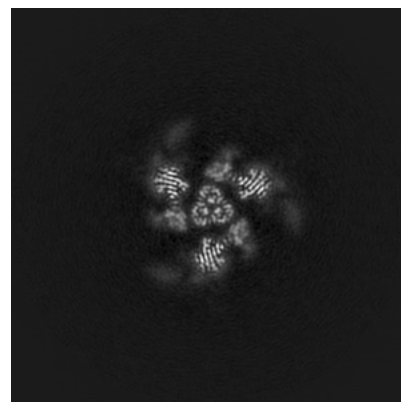
6.2.1 Primary map



X Index: 200



Y Index: 200

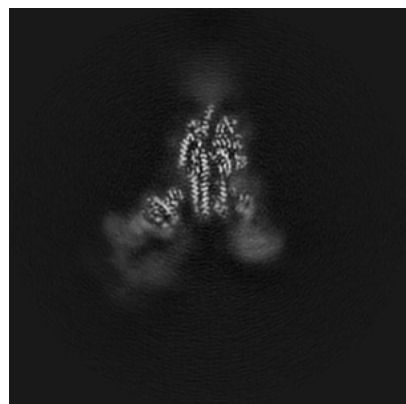


Z Index: 200

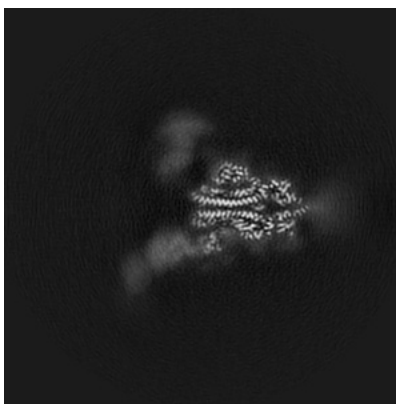
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

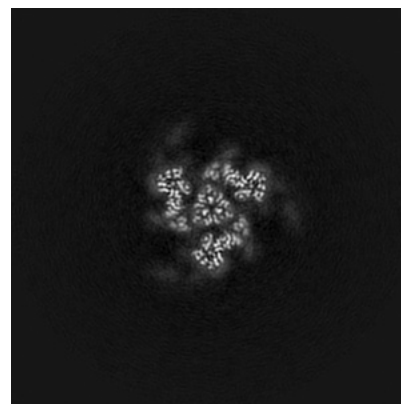
6.3.1 Primary map



X Index: 207



Y Index: 196

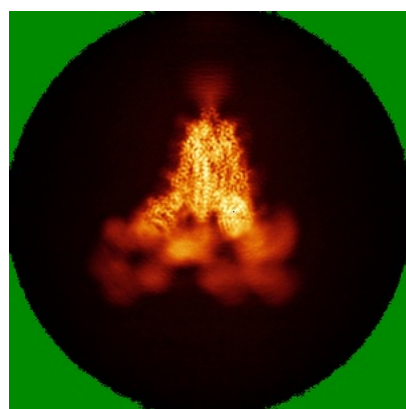


Z Index: 204

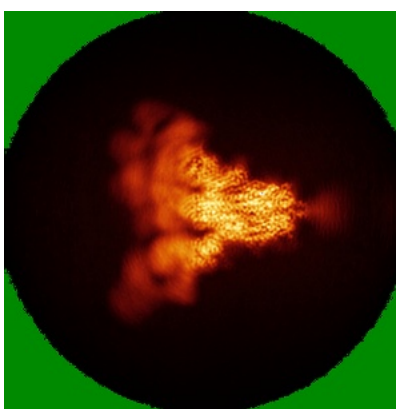
The images above show the largest variance slices of the map in three orthogonal directions.

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

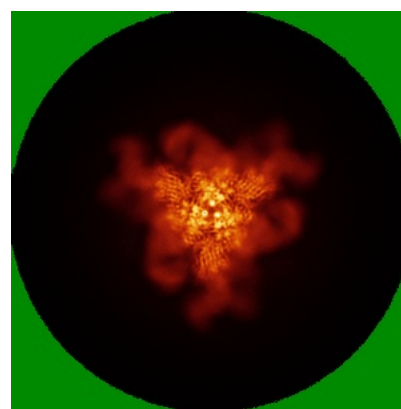
6.4.1 Primary map



X



Y

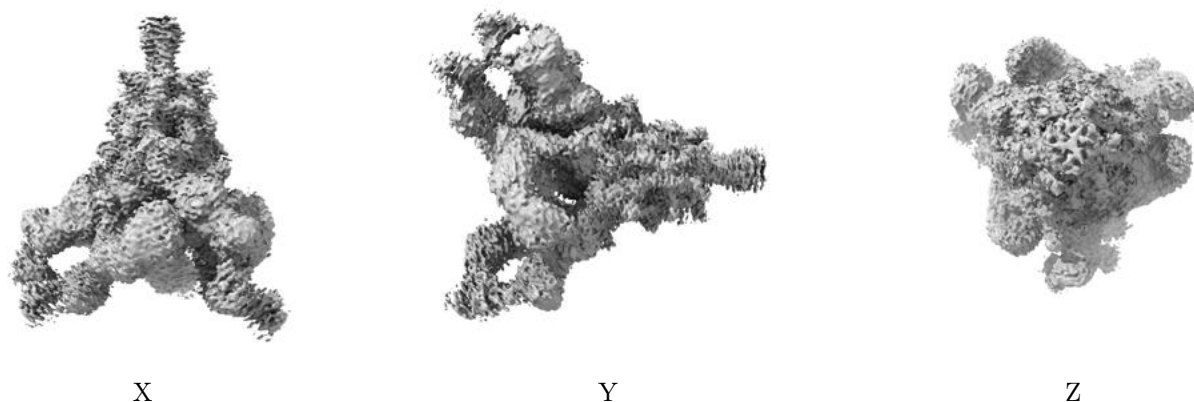


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

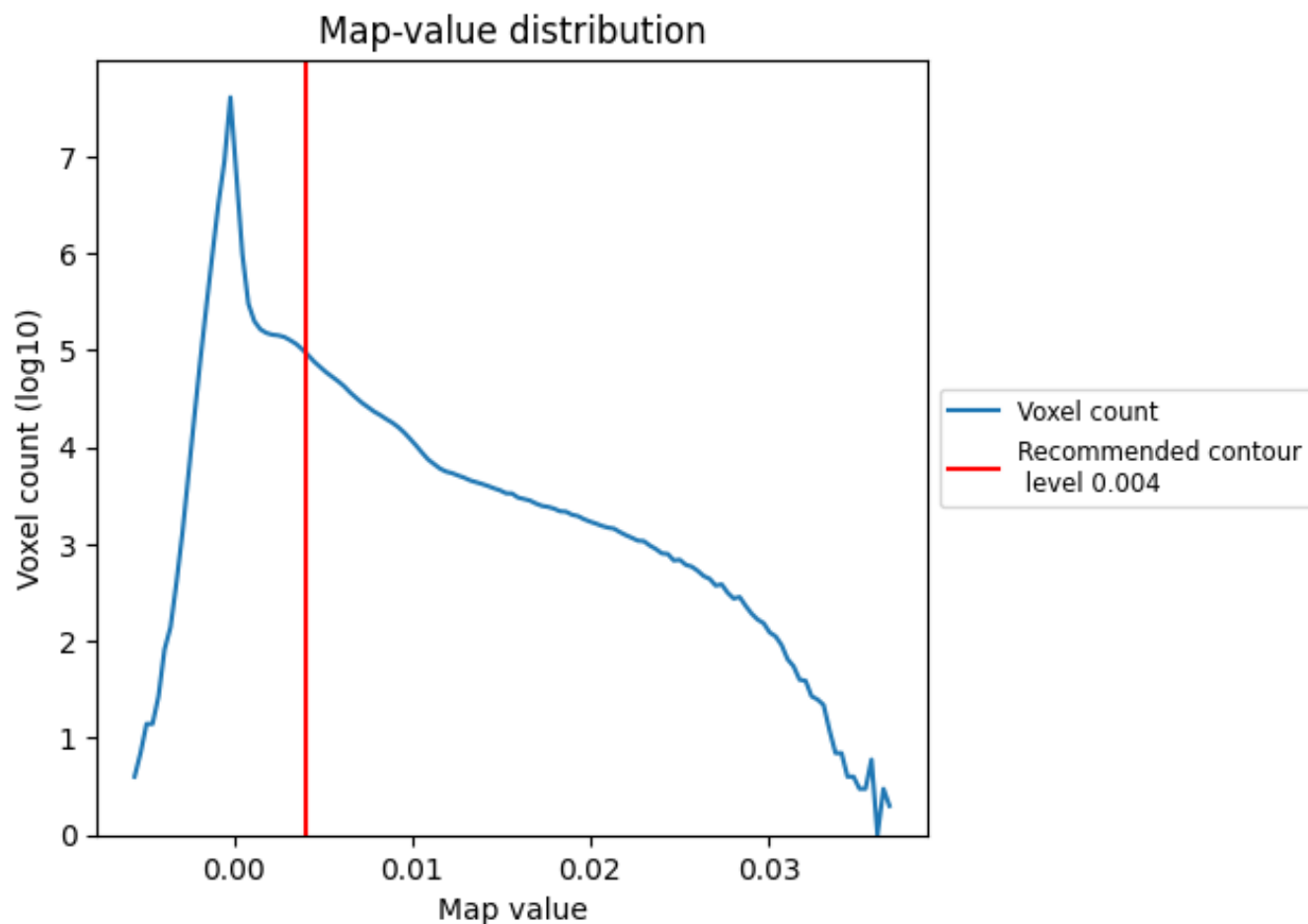
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

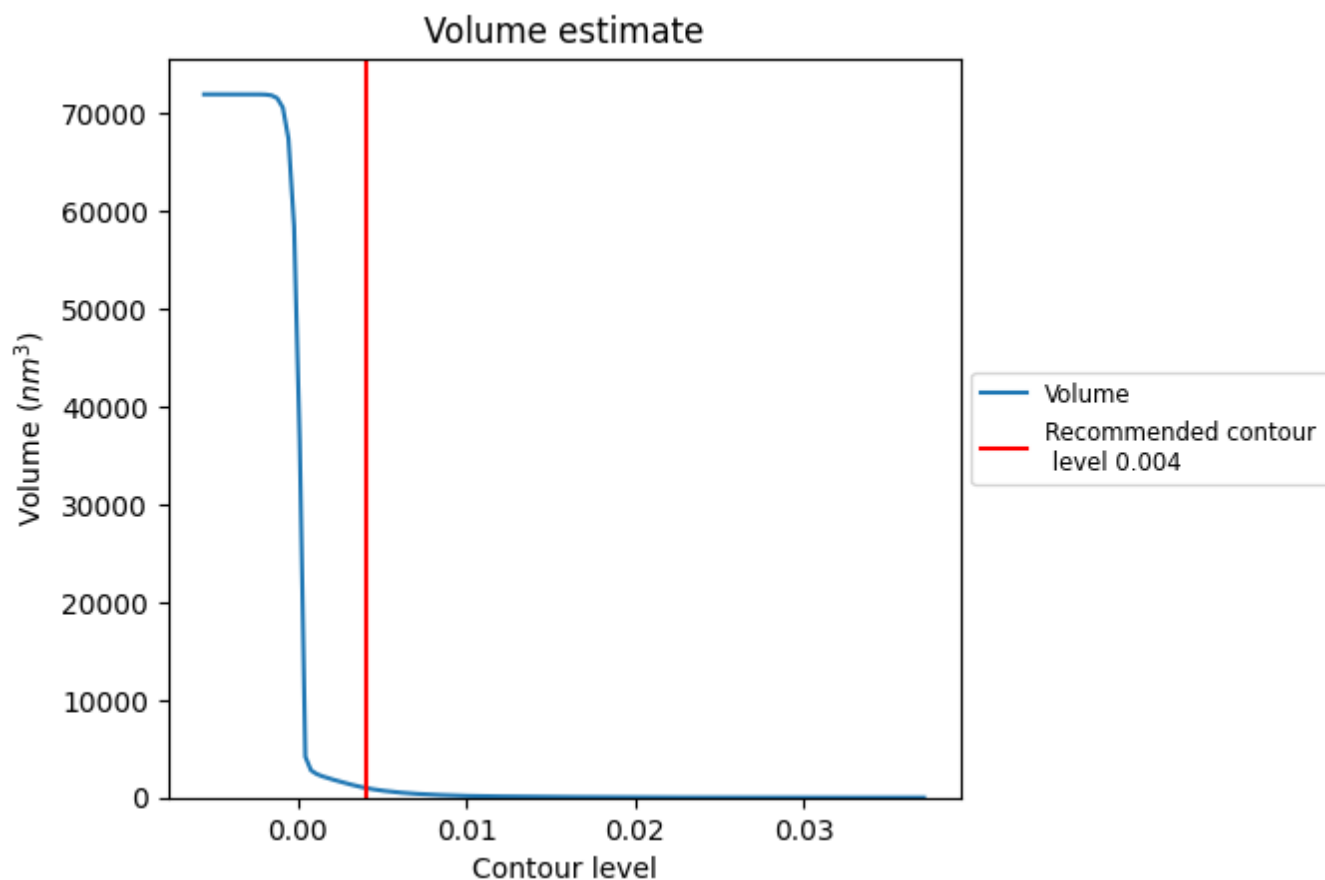
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

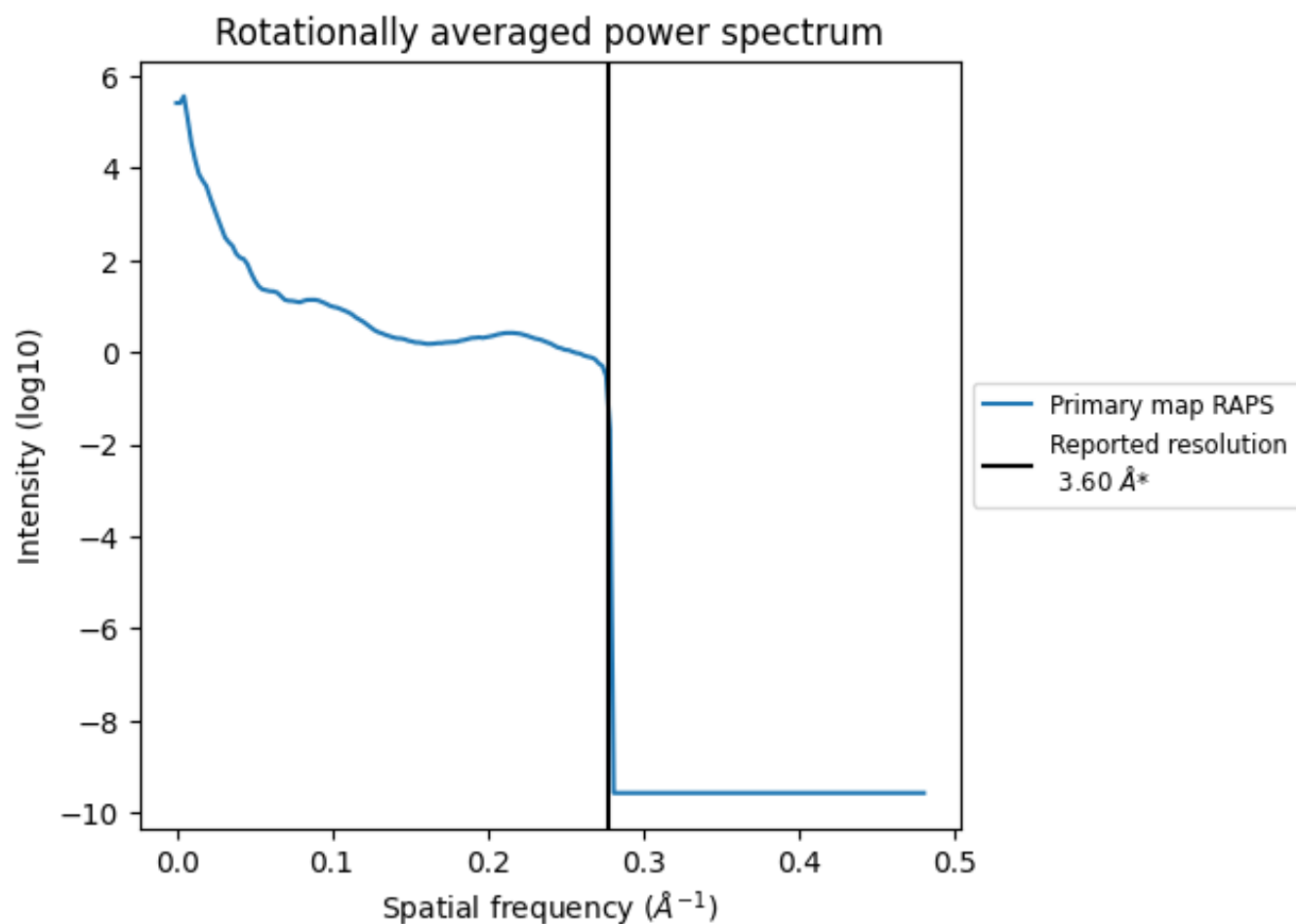
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 989 nm³; this corresponds to an approximate mass of 893 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.278 $\text{\AA}^{-1}$

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

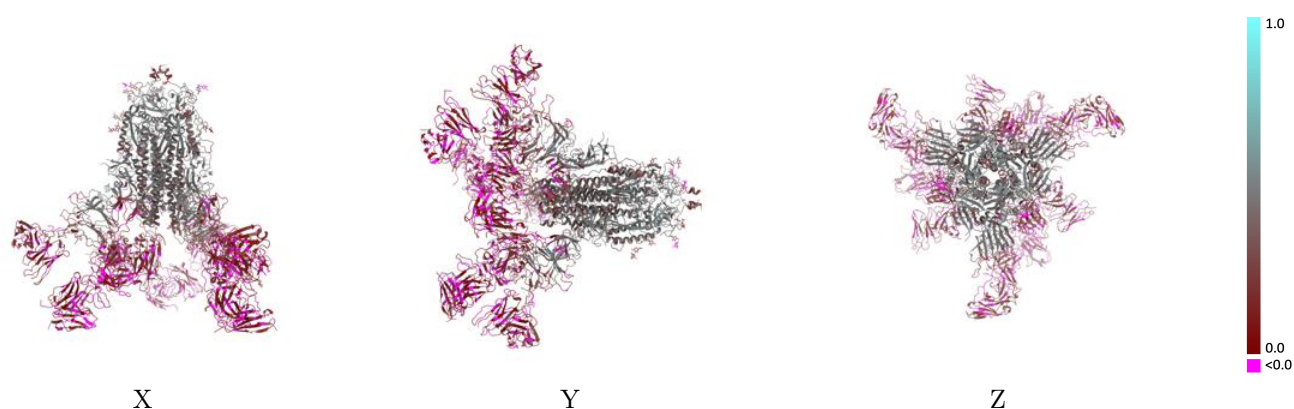
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30993 and PDB model 7E5R. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)

This section was not generated.

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

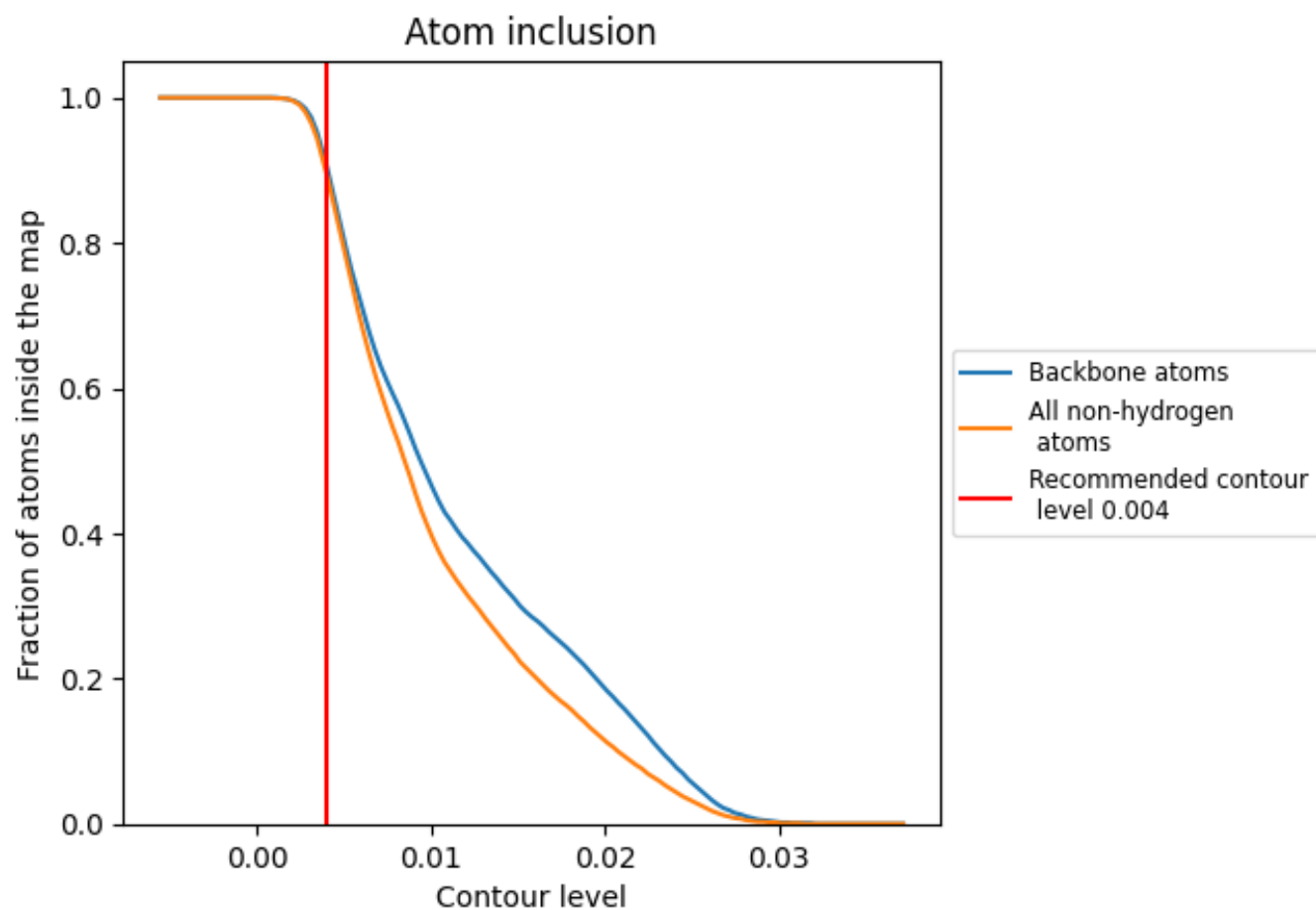


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8930	 0.2400
A	 0.9760	 0.3330
B	 0.9770	 0.3310
C	 0.9760	 0.3330
D	 0.9410	 0.0910
E	 0.9490	 0.0940
F	 0.1430	 0.0020
G	 0.9640	 0.3050
H	 0.9310	 0.0690
I	 0.6880	 0.0740
J	 0.9640	 0.1670
K	 0.6630	 0.0920
L	 0.9580	 0.1090
M	 0.6390	 0.0710
N	 0.9610	 0.1180
O	 0.9490	 0.0990
P	 0.6860	 0.0750
Q	 0.6720	 0.1070
R	 0.6490	 0.0900
S	 0.6520	 0.0950
T	 0.6330	 0.0770
U	 0.6420	 0.0720
V	 0.6500	 0.0820
W	 0.7620	 0.0990
X	 0.7270	 0.0920
Y	 0.8210	 0.2310
Z	 0.7860	 0.0950
a	 0.1430	 0.0240
b	 0.9290	 0.2740
c	 0.8930	 0.1640
d	 0.8210	 0.2510
e	 0.7140	 0.1120
f	 0.2140	 0.0770
g	 0.9290	 0.3030
h	 0.8930	 0.1560



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Chain	Atom inclusion	Q-score
i	 0.8930	 0.2730
j	 0.7860	 0.1090