



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 03:04 AM UTC

PDB ID : 7K8S / pdb_00007k8s
EMDB ID : EMD-22729
Title : Structure of the SARS-CoV-2 S 2P trimer in complex with the human neutralizing antibody Fab fragment, C002 (state 1)
Authors : Barnes, C.O.; Malyutin, A.G.; Bjorkman, P.J.
Deposited on : 2020-09-27
Resolution : 3.40 Å(reported)
Based on initial model : 6VXX

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:

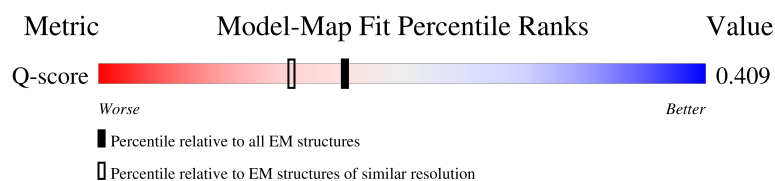
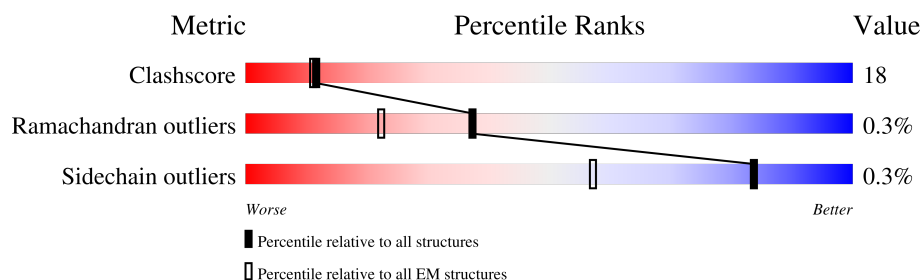
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.40 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.



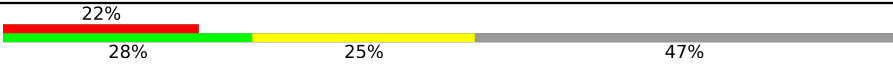
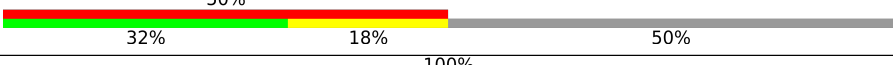
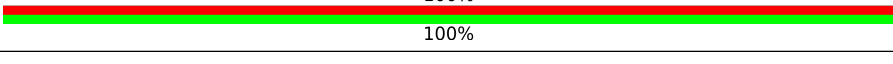
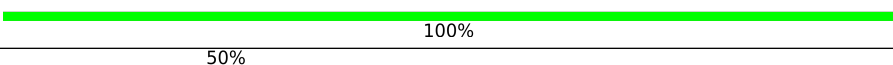
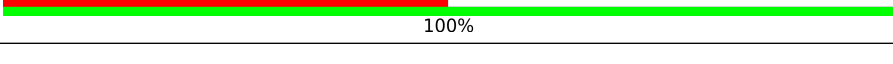
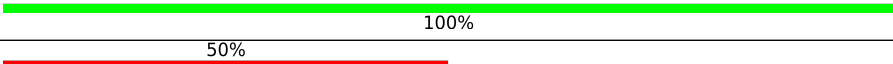
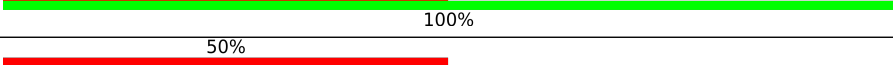
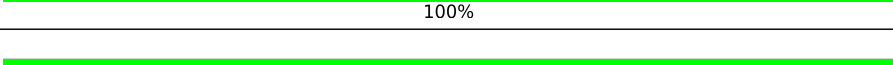
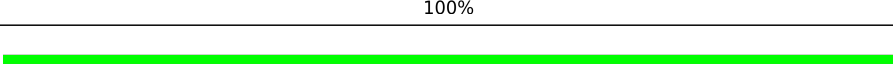
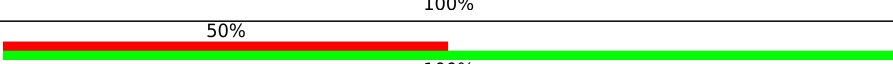
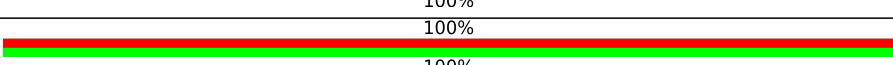
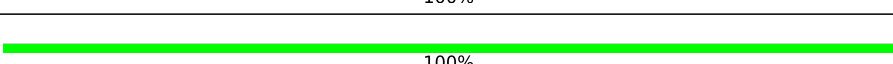
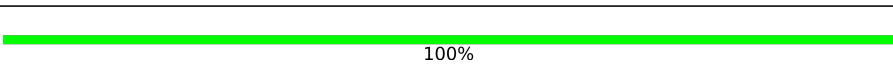
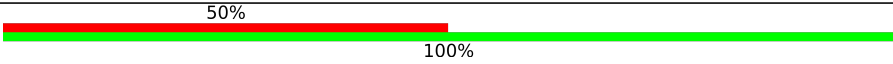
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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

Mol	Chain	Length	Quality of chain
1	A	1259	 11% 55% 24% 20%
1	B	1259	 11% 54% 25% 20%
1	C	1259	 11% 56% 23% 20%
2	H	236	 20% 25% 27% 47%

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Mol	Chain	Length	Quality of chain
2	M	236	
2	O	236	
3	L	214	
3	N	214	
3	P	214	
4	D	2	
4	E	2	
4	F	2	
4	G	2	
4	I	2	
4	J	2	
4	K	2	
4	Q	2	
4	R	2	
4	S	2	
4	T	2	
4	U	2	
4	V	2	
4	W	2	
4	X	2	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 29649 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1004	Total	C	N	O	S	0	0
			7845	5011	1305	1494	35		
1	B	1004	Total	C	N	O	S	0	0
			7845	5011	1305	1494	35		
1	C	1004	Total	C	N	O	S	0	0
			7845	5011	1305	1494	35		

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1214	SER	-	expression tag	UNP P0DTC2
A	1215	GLY	-	expression tag	UNP P0DTC2
A	1216	ARG	-	expression tag	UNP P0DTC2
A	1217	LEU	-	expression tag	UNP P0DTC2
A	1218	VAL	-	expression tag	UNP P0DTC2
A	1219	PRO	-	expression tag	UNP P0DTC2
A	1220	ARG	-	expression tag	UNP P0DTC2
A	1221	GLY	-	expression tag	UNP P0DTC2
A	1222	SER	-	expression tag	UNP P0DTC2
A	1223	PRO	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	SER	-	expression tag	UNP P0DTC2
A	1226	GLY	-	expression tag	UNP P0DTC2
A	1227	TYR	-	expression tag	UNP P0DTC2
A	1228	ILE	-	expression tag	UNP P0DTC2
A	1229	PRO	-	expression tag	UNP P0DTC2
A	1230	GLU	-	expression tag	UNP P0DTC2
A	1231	ALA	-	expression tag	UNP P0DTC2
A	1232	PRO	-	expression tag	UNP P0DTC2
A	1233	ARG	-	expression tag	UNP P0DTC2
A	1234	ASP	-	expression tag	UNP P0DTC2
A	1235	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1236	GLN	-	expression tag	UNP P0DTC2
A	1237	ALA	-	expression tag	UNP P0DTC2
A	1238	TYR	-	expression tag	UNP P0DTC2
A	1239	VAL	-	expression tag	UNP P0DTC2
A	1240	ARG	-	expression tag	UNP P0DTC2
A	1241	LYS	-	expression tag	UNP P0DTC2
A	1242	ASP	-	expression tag	UNP P0DTC2
A	1243	GLY	-	expression tag	UNP P0DTC2
A	1244	GLU	-	expression tag	UNP P0DTC2
A	1245	TRP	-	expression tag	UNP P0DTC2
A	1246	VAL	-	expression tag	UNP P0DTC2
A	1247	LEU	-	expression tag	UNP P0DTC2
A	1248	LEU	-	expression tag	UNP P0DTC2
A	1249	SER	-	expression tag	UNP P0DTC2
A	1250	THR	-	expression tag	UNP P0DTC2
A	1251	PHE	-	expression tag	UNP P0DTC2
A	1252	LEU	-	expression tag	UNP P0DTC2
A	1253	GLY	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1214	SER	-	expression tag	UNP P0DTC2
B	1215	GLY	-	expression tag	UNP P0DTC2
B	1216	ARG	-	expression tag	UNP P0DTC2
B	1217	LEU	-	expression tag	UNP P0DTC2
B	1218	VAL	-	expression tag	UNP P0DTC2
B	1219	PRO	-	expression tag	UNP P0DTC2
B	1220	ARG	-	expression tag	UNP P0DTC2
B	1221	GLY	-	expression tag	UNP P0DTC2
B	1222	SER	-	expression tag	UNP P0DTC2
B	1223	PRO	-	expression tag	UNP P0DTC2
B	1224	GLY	-	expression tag	UNP P0DTC2
B	1225	SER	-	expression tag	UNP P0DTC2
B	1226	GLY	-	expression tag	UNP P0DTC2
B	1227	TYR	-	expression tag	UNP P0DTC2
B	1228	ILE	-	expression tag	UNP P0DTC2
B	1229	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1230	GLU	-	expression tag	UNP P0DTC2
B	1231	ALA	-	expression tag	UNP P0DTC2
B	1232	PRO	-	expression tag	UNP P0DTC2
B	1233	ARG	-	expression tag	UNP P0DTC2
B	1234	ASP	-	expression tag	UNP P0DTC2
B	1235	GLY	-	expression tag	UNP P0DTC2
B	1236	GLN	-	expression tag	UNP P0DTC2
B	1237	ALA	-	expression tag	UNP P0DTC2
B	1238	TYR	-	expression tag	UNP P0DTC2
B	1239	VAL	-	expression tag	UNP P0DTC2
B	1240	ARG	-	expression tag	UNP P0DTC2
B	1241	LYS	-	expression tag	UNP P0DTC2
B	1242	ASP	-	expression tag	UNP P0DTC2
B	1243	GLY	-	expression tag	UNP P0DTC2
B	1244	GLU	-	expression tag	UNP P0DTC2
B	1245	TRP	-	expression tag	UNP P0DTC2
B	1246	VAL	-	expression tag	UNP P0DTC2
B	1247	LEU	-	expression tag	UNP P0DTC2
B	1248	LEU	-	expression tag	UNP P0DTC2
B	1249	SER	-	expression tag	UNP P0DTC2
B	1250	THR	-	expression tag	UNP P0DTC2
B	1251	PHE	-	expression tag	UNP P0DTC2
B	1252	LEU	-	expression tag	UNP P0DTC2
B	1253	GLY	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1214	SER	-	expression tag	UNP P0DTC2
C	1215	GLY	-	expression tag	UNP P0DTC2
C	1216	ARG	-	expression tag	UNP P0DTC2
C	1217	LEU	-	expression tag	UNP P0DTC2
C	1218	VAL	-	expression tag	UNP P0DTC2
C	1219	PRO	-	expression tag	UNP P0DTC2
C	1220	ARG	-	expression tag	UNP P0DTC2
C	1221	GLY	-	expression tag	UNP P0DTC2
C	1222	SER	-	expression tag	UNP P0DTC2
C	1223	PRO	-	expression tag	UNP P0DTC2

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

- Molecule 2 is a protein called C002 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	125	Total	C	N	O	S	0	0
			959	607	165	183	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	125	Total	C	N	O	S	0	0
			959	607	165	183	4		
2	O	125	Total	C	N	O	S	0	0
			959	607	165	183	4		

- Molecule 3 is a protein called C002 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	107	Total	C	N	O	S	0	0
			813	509	136	166	2		
3	N	107	Total	C	N	O	S	0	0
			813	509	136	166	2		
3	P	107	Total	C	N	O	S	0	0
			813	509	136	166	2		

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



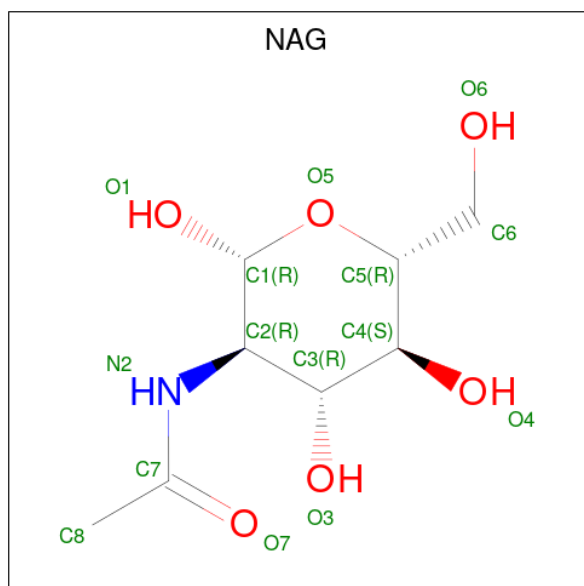
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		
4	W	2	Total	C	N	O	0	0
			28	16	2	10		
4	X	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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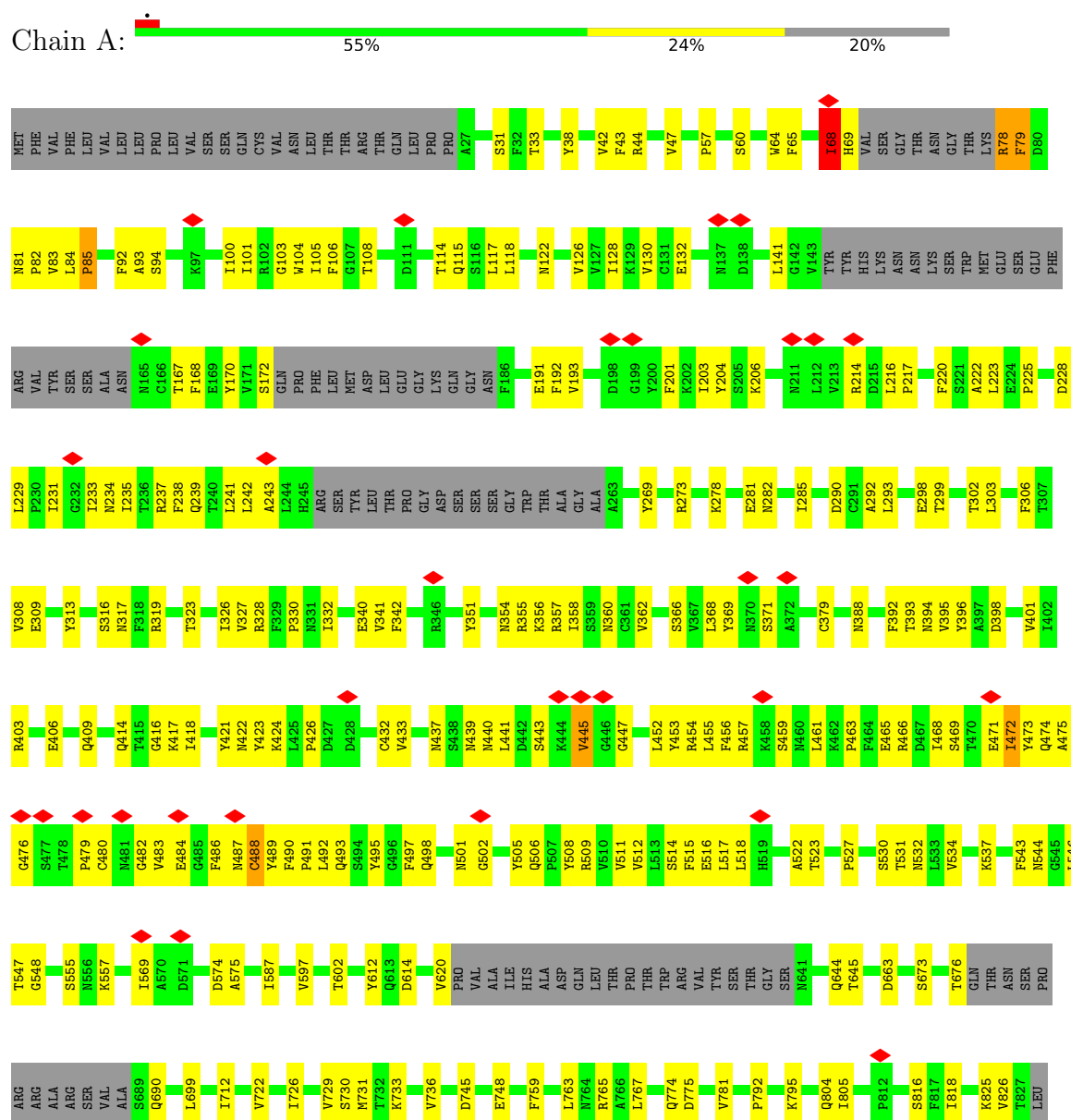
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	C	1	14	8	1	5	0

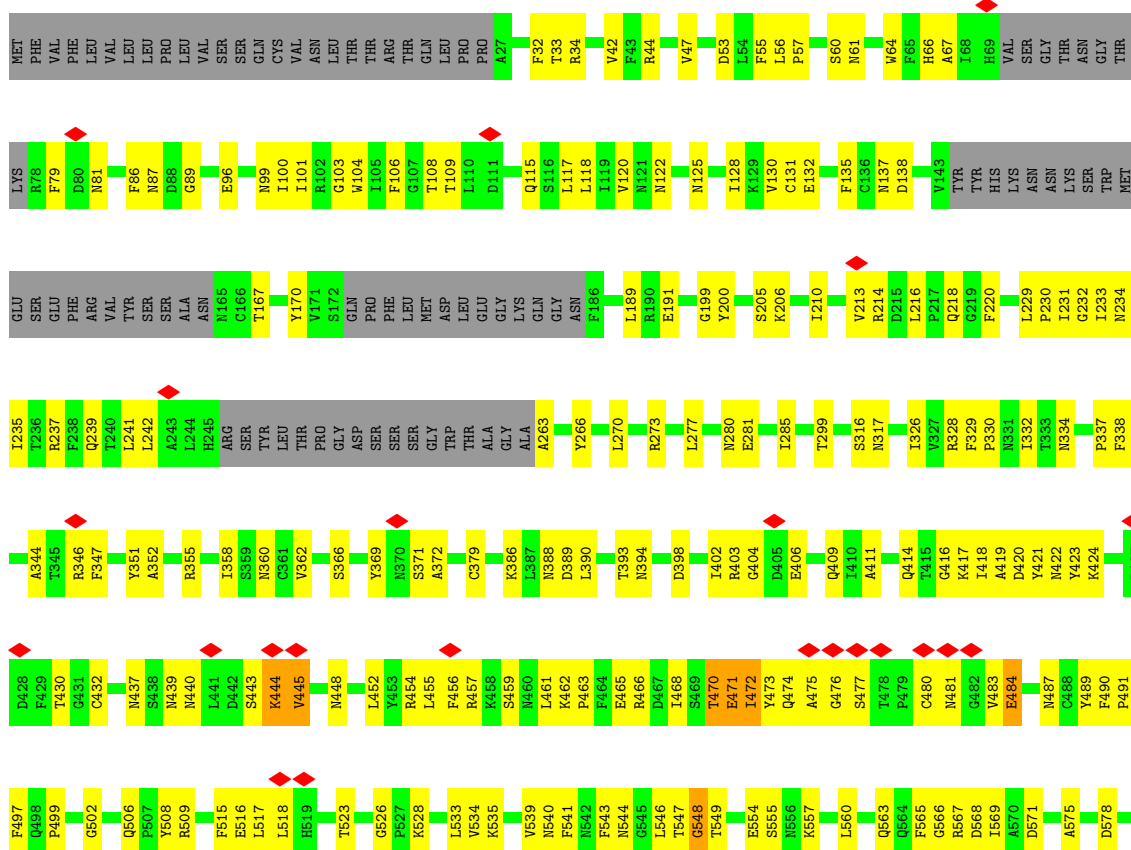
3 Residue-property plots

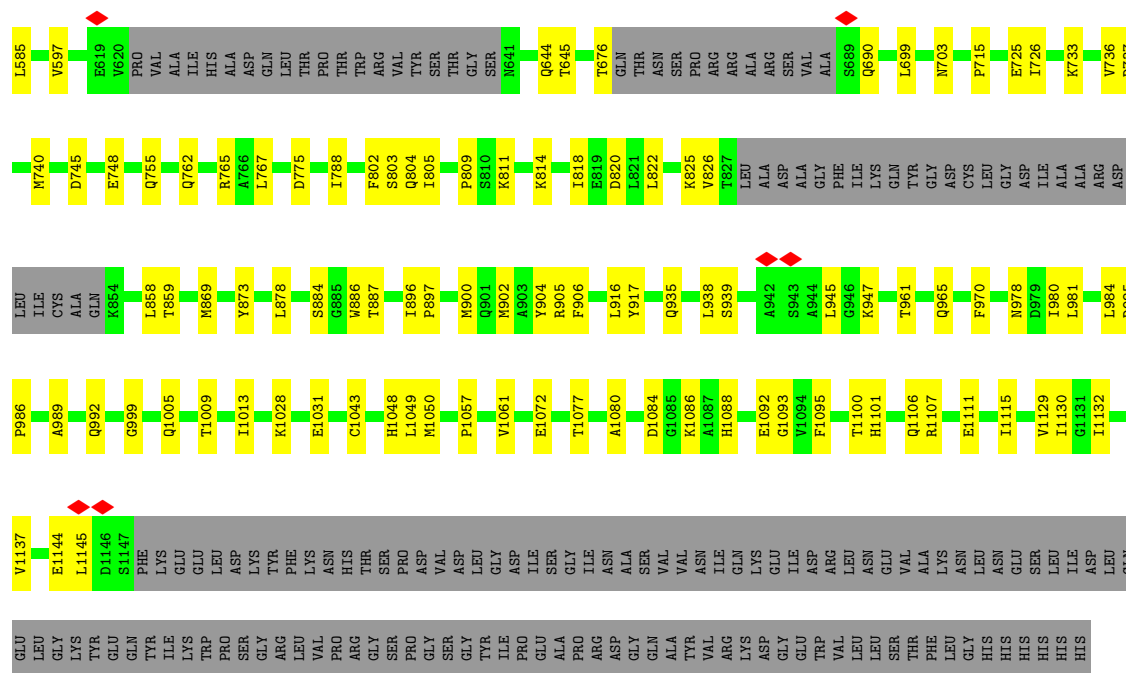
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Spike glycoprotein

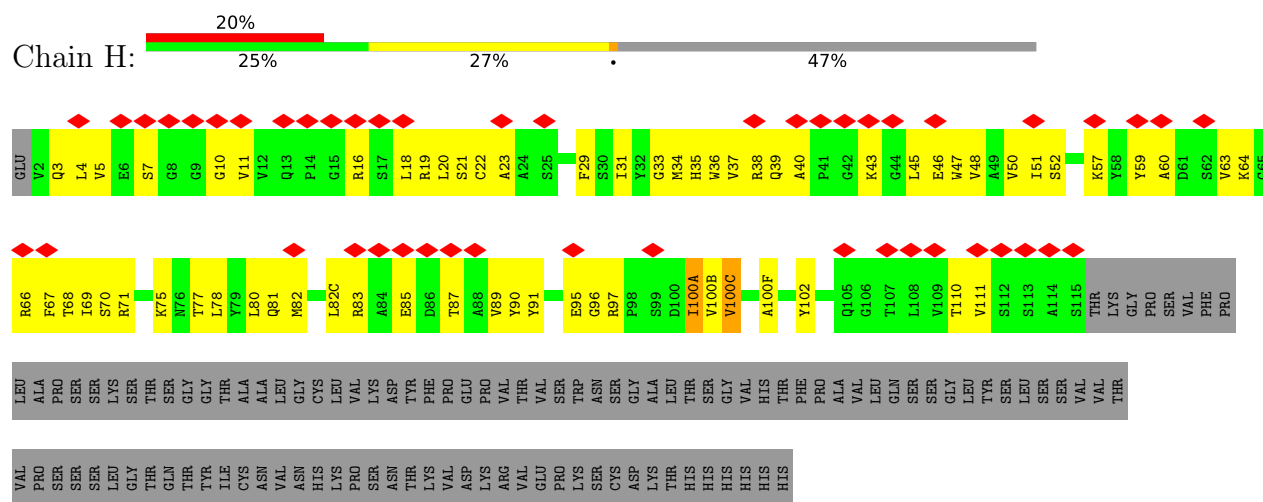


- Molecule 1: Spike glycoprotein

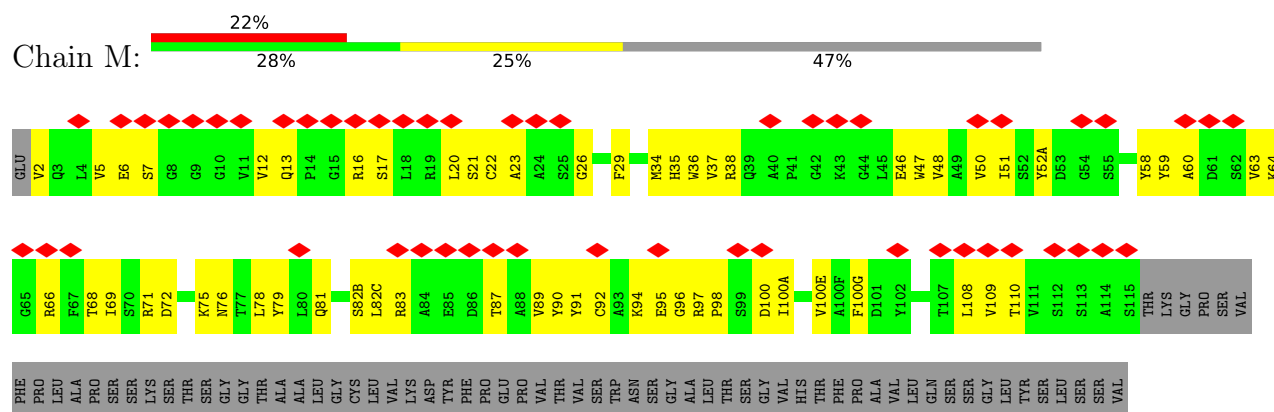




- Molecule 2: C002 Fab Heavy Chain



- Molecule 2: C002 Fab Heavy Chain



GLU
LYS
HIS
LYS
VAL
TVR
ALA
CYS
GLU
VAL
THR
HIS
GLN
GLY
LEU
SER
SER
PRO
VAL
THR
LYS
PHE
ASN
ARG
GLY
CYS

• Molecule 3: C002 Fab Light Chain

Chain P: 

D1 I2 Q3 I4 T5 Q6 S7 P8 S9 S10 L11 S12 S13 S14 V15 G16 D17 R18 V19 T20 I21 I22 C23 R24 A25 S26 Q27 S28 S29 I29 S30 S31 Y32 L33 N34 K35 Y36 Q37 Q38 K39 P40 G41 K42 A43 P44 K45 L46 L47 I48 Y49 A50 A51 S52 S53 L54 Q55 S56 G57 V58 P59 S60

R61 F62 S63 G64 S65 G66 S67 G68 T69 D70 F71 T72 L73 T74 I75 S76 S77 L78 Q79 P80 E81 D82 F83 A84 T85 Y86 Y87 C88 Q89 Q90 S91 Y92 S93 T94 P95 R96 T97 F98 G99 Q100 G101 T102 K103 V104 E105 I106 K107 ARG THR VAL ALA PRO VAL PHE ILE PHE PRO

SER ASP GLU GLN LEU LYS SER GLY THR ALA SER VAL VAL CYS LEU LEU ASN PHE TYR PRO ARG GLU ALA LYS VAL GLN SER GLY ASN SER GLN SER VAL THR GLU GLN ASP LYS ASP SER THR TYR LEU SER THR

LEU SER LYS ALA TVR LYS HIS VAL VAL THR ALA CYS VAL VAL THR HIS GLN GLY LEU SER PRO VAL THR LYS SER PHE ASN ARG GLY CYS

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

Chain D: 

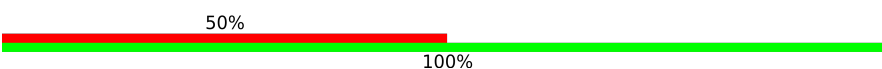
MAG1
MAG2

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

Chain E: 

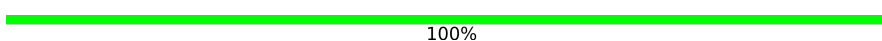
MAG1
MAG2

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

Chain F: 

MAG1
MAG2

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

Chain G: 

MAG1
MAG2

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



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



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



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



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



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

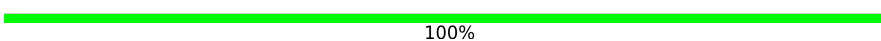


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T: 

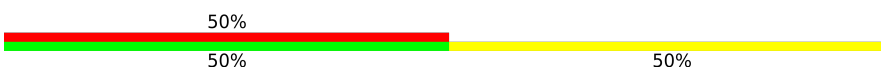


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U: 

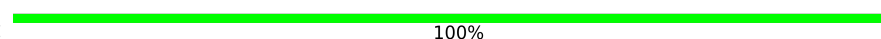


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V: 



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

Chain W: 



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

Chain X: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	51915	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)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.599	Depositor
Minimum map value	-0.309	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	361.152, 361.152, 361.152	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.836, 0.836, 0.836	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.42	0/8022	0.56	3/10915 (0.0%)
1	B	0.41	1/8022 (0.0%)	0.56	1/10915 (0.0%)
1	C	0.42	0/8022	0.54	3/10915 (0.0%)
2	H	0.20	0/980	0.50	0/1329
2	M	0.23	0/980	0.51	0/1329
2	O	0.19	0/980	0.53	0/1329
3	L	0.18	0/830	0.45	0/1126
3	N	0.18	0/830	0.45	0/1126
3	P	0.16	0/830	0.46	0/1126
All	All	0.39	1/29496 (0.0%)	0.54	7/40110 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
2	H	0	3
2	M	0	1
2	O	0	2
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	67	ALA	C-N	7.68	1.42	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	548	GLY	CA-C-O	-5.72	118.28	122.23
1	A	471	GLU	CA-C-O	-5.58	114.96	120.82
1	B	548	GLY	CA-C-O	-5.51	118.34	122.37
1	A	548	GLY	CA-C-O	-5.41	118.42	122.37
1	C	444	LYS	CA-C-O	-5.17	115.39	120.82
1	C	471	GLU	CA-C-O	-5.05	115.52	120.82
1	A	471	GLU	O-C-N	5.04	127.26	122.07

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	ASN	Peptide
1	A	484	GLU	Peptide
1	B	122	ASN	Peptide
1	B	233	ILE	Peptide
1	C	122	ASN	Peptide
1	C	484	GLU	Peptide
2	H	100(A)	ILE	Peptide
2	H	100(B)	VAL	Peptide
2	H	100(C)	VAL	Peptide
2	M	100(A)	ILE	Peptide
2	O	100(A)	ILE	Peptide
2	O	100(B)	VAL	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7845	0	7652	265	0
1	B	7845	0	7652	289	0
1	C	7845	0	7652	275	0
2	H	959	0	932	62	0
2	M	959	0	932	55	0
2	O	959	0	932	51	0
3	L	813	0	797	43	0
3	N	813	0	797	41	0
3	P	813	0	797	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	28	0	25	0	0
4	E	28	0	25	0	0
4	F	28	0	25	0	0
4	G	28	0	25	0	0
4	I	28	0	25	0	0
4	J	28	0	25	2	0
4	K	28	0	25	0	0
4	Q	28	0	25	0	0
4	R	28	0	25	0	0
4	S	28	0	25	0	0
4	T	28	0	25	0	0
4	U	28	0	25	0	0
4	V	28	0	25	0	0
4	W	28	0	25	0	0
4	X	28	0	25	0	0
5	A	126	0	117	0	0
5	B	126	0	117	2	0
5	C	126	0	117	2	0
All	All	29649	0	28869	1038	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (1038) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:HIS:CB	1:C:79:PHE:CE2	1.84	1.57
1:C:66:HIS:HB2	1:C:79:PHE:CE2	0.94	1.46
1:A:443:SER:OG	1:A:497:PHE:HB3	1.35	1.25
1:B:443:SER:O	1:B:499:PRO:HD3	1.39	1.23
1:B:543:PHE:O	1:B:546:LEU:HD13	1.33	1.22
1:A:472:ILE:HG12	1:A:488:CYS:SG	1.80	1.20
1:C:66:HIS:HB2	1:C:79:PHE:CZ	1.79	1.17
1:A:85:PRO:HD2	1:A:269:TYR:OH	1.40	1.16
1:B:443:SER:HB3	1:B:497:PHE:HB3	1.36	1.06
1:C:66:HIS:CB	1:C:79:PHE:HE2	1.35	1.06
1:C:66:HIS:CB	1:C:79:PHE:CZ	2.39	1.03
1:A:472:ILE:CG1	1:A:488:CYS:SG	2.48	1.01
1:C:470:THR:HG21	1:C:492:LEU:HD11	1.05	1.01
1:C:543:PHE:O	1:C:546:LEU:HG	1.62	1.00
1:C:470:THR:HG21	1:C:492:LEU:CD1	1.92	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:PHE:O	1:B:546:LEU:CD1	2.11	0.99
2:H:20:LEU:HG	2:H:82:MET:HE1	1.46	0.98
1:B:470:THR:HG22	1:B:492:LEU:HD11	1.45	0.97
1:B:804:GLN:NE2	1:B:935:GLN:OE1	1.97	0.96
1:B:470:THR:HG22	1:B:492:LEU:CD1	1.96	0.95
1:A:406:GLU:OE1	1:A:409:GLN:NE2	2.01	0.93
1:C:389:ASP:OD1	1:C:528:LYS:NZ	2.01	0.93
1:B:542:ASN:CG	1:B:547:THR:HG22	1.93	0.92
1:C:540:ASN:HA	1:C:549:THR:HG22	1.48	0.91
1:C:444:LYS:H	1:C:444:LYS:HD2	1.34	0.90
1:C:443:SER:HB3	1:C:497:PHE:HB3	1.54	0.90
3:P:33:LEU:HD11	3:P:88:CYS:HB2	1.52	0.90
1:C:472:ILE:CD1	1:C:483:VAL:HG23	2.02	0.90
2:O:22:CYS:HB3	2:O:78:LEU:HB3	1.56	0.88
1:A:43:PHE:HB2	1:B:563:GLN:HE22	1.39	0.86
1:C:484:GLU:OE2	3:N:96:ARG:NH2	2.09	0.86
1:A:443:SER:HG	1:A:497:PHE:HB3	1.41	0.85
1:B:379:CYS:HA	1:B:432:CYS:HB3	1.59	0.84
1:C:66:HIS:HB3	1:C:79:PHE:CE2	2.11	0.84
2:M:22:CYS:HB3	2:M:78:LEU:HB3	1.57	0.84
1:C:115:GLN:NE2	1:C:130:VAL:O	2.10	0.83
1:B:737:ASP:OD2	1:C:317:ASN:ND2	2.11	0.83
1:A:905:ARG:HH12	1:A:1050:MET:HB3	1.43	0.82
3:P:33:LEU:HB3	3:P:51:ALA:HB2	1.61	0.82
2:O:38:ARG:HH12	2:O:86:ASP:HA	1.44	0.82
2:O:100(B):VAL:HG23	2:O:100(C):VAL:H	1.45	0.82
1:C:462:LYS:HE3	1:C:465:GLU:HB2	1.61	0.81
2:O:17:SER:OG	2:O:81:GLN:NE2	2.14	0.80
1:C:472:ILE:HD13	1:C:483:VAL:CG2	2.11	0.80
1:C:493:GLN:OE1	2:M:97:ARG:NH2	2.14	0.80
1:A:69:HIS:C	1:A:79:PHE:CE2	2.61	0.79
1:A:1144:GLU:HB3	1:B:1145:LEU:HD21	1.65	0.79
1:C:541:PHE:HE2	1:C:549:THR:O	1.64	0.79
1:B:443:SER:O	1:B:499:PRO:CD	2.29	0.78
1:B:462:LYS:HE3	1:B:465:GLU:HB2	1.63	0.78
2:O:29:PHE:O	2:O:71:ARG:NH2	2.17	0.78
1:C:546:LEU:HD21	1:C:565:PHE:CZ	2.19	0.78
1:A:1145:LEU:HD21	1:C:1144:GLU:HB3	1.65	0.78
1:C:470:THR:CG2	1:C:492:LEU:HD11	2.01	0.77
1:C:811:LYS:NZ	1:C:820:ASP:OD2	2.15	0.77
2:H:37:VAL:HG22	2:H:47:TRP:HA	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:983:ARG:HH11	1:C:517:LEU:HD13	1.49	0.77
1:C:108:THR:OG1	1:C:234:ASN:O	2.02	0.77
1:B:437:ASN:HA	1:B:508:TYR:HA	1.67	0.77
2:H:22:CYS:HB3	2:H:78:LEU:HB3	1.67	0.76
1:C:448:ASN:HB3	1:C:497:PHE:HB2	1.68	0.76
3:N:33:LEU:HD11	3:N:88:CYS:HB2	1.67	0.76
1:C:106:PHE:HB2	1:C:117:LEU:HB3	1.67	0.76
2:M:35:HIS:CE1	2:M:50:VAL:HG23	2.21	0.75
2:M:5:VAL:HB	2:M:23:ALA:HB3	1.66	0.75
1:B:542:ASN:HA	1:B:547:THR:HA	1.67	0.75
1:B:430:THR:OG1	1:B:515:PHE:O	2.04	0.75
1:A:81:ASN:O	1:A:239:GLN:NE2	2.18	0.75
1:A:479:PRO:O	1:A:487:ASN:OD1	2.05	0.75
1:C:411:ALA:HB3	1:C:414:GLN:HG3	1.68	0.75
3:L:89:GLN:NE2	3:L:90:GLN:O	2.20	0.75
1:A:85:PRO:CD	1:A:269:TYR:OH	2.29	0.74
1:B:453:TYR:HD1	1:B:495:TYR:HE1	1.35	0.74
1:B:86:PHE:O	1:B:87:ASN:ND2	2.20	0.74
1:C:330:PRO:HD3	1:C:544:ASN:HD22	1.50	0.74
3:L:49:TYR:O	3:L:53:SER:OG	2.04	0.74
1:B:457:ARG:NH1	1:B:459:SER:O	2.20	0.74
1:C:454:ARG:HH11	1:C:470:THR:HG22	1.51	0.74
1:B:323:THR:OG1	1:B:537:LYS:NZ	2.21	0.73
1:B:546:LEU:HD21	1:B:565:PHE:CZ	2.23	0.73
1:A:69:HIS:C	1:A:79:PHE:CD2	2.67	0.73
1:A:905:ARG:NH1	1:A:1049:LEU:O	2.22	0.73
1:B:456:PHE:HZ	1:B:489:TYR:HB2	1.53	0.73
1:C:568:ASP:OD1	1:C:569:ILE:N	2.20	0.73
1:C:444:LYS:H	1:C:444:LYS:CD	2.03	0.72
1:C:540:ASN:CA	1:C:549:THR:HG22	2.20	0.72
1:C:472:ILE:HD13	1:C:483:VAL:HG23	1.71	0.72
1:C:444:LYS:HD2	1:C:444:LYS:N	2.04	0.72
3:N:3:GLN:H	3:N:26:SER:HB3	1.54	0.71
1:A:905:ARG:NH1	1:A:1050:MET:HB3	2.04	0.71
1:B:351:TYR:CE1	1:B:452:LEU:HB2	2.25	0.71
3:N:37:GLN:HB2	3:N:47:LEU:HD11	1.73	0.71
3:N:85:THR:OG1	3:N:103:LYS:NZ	2.23	0.71
1:B:117:LEU:HD12	1:B:231:ILE:HG21	1.70	0.71
1:C:379:CYS:HA	1:C:432:CYS:CB	2.20	0.71
2:H:82:MET:HG3	2:H:82(C):LEU:HD21	1.73	0.71
1:A:340:GLU:OE2	1:A:356:LYS:NZ	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:PHE:O	1:B:580:GLN:NE2	2.23	0.71
1:C:277:LEU:HD23	1:C:285:ILE:HD13	1.73	0.71
1:B:454:ARG:NH2	1:B:467:ASP:OD2	2.21	0.70
2:O:5:VAL:HA	2:O:105:GLN:HE22	1.55	0.70
1:C:130:VAL:HG23	1:C:167:THR:HG23	1.73	0.70
1:A:502:GLY:O	1:A:506:GLN:NE2	2.24	0.70
1:B:418:ILE:HG13	1:B:422:ASN:HD22	1.56	0.70
3:N:49:TYR:O	3:N:53:SER:OG	2.09	0.70
2:M:29:PHE:O	2:M:71:ARG:NH2	2.24	0.70
1:B:126:VAL:HB	1:B:172:SER:HB2	1.73	0.69
1:B:411:ALA:HB3	1:B:414:GLN:HG3	1.74	0.69
1:C:337:PRO:HD2	1:C:358:ILE:HD12	1.75	0.69
1:A:379:CYS:HA	1:A:432:CYS:CB	2.22	0.69
1:B:546:LEU:N	1:B:546:LEU:HD12	2.08	0.69
1:A:93:ALA:HA	1:A:191:GLU:HA	1.75	0.69
1:C:472:ILE:HD11	1:C:483:VAL:HG23	1.73	0.69
2:M:37:VAL:HG12	2:M:47:TRP:HA	1.74	0.69
1:A:825:LYS:NZ	1:A:938:LEU:O	2.22	0.69
1:A:869:MET:HG2	1:B:699:LEU:HD21	1.74	0.69
1:C:472:ILE:CD1	1:C:483:VAL:CG2	2.70	0.69
1:A:457:ARG:NH1	1:A:459:SER:O	2.26	0.69
1:A:971:GLY:O	1:A:995:ARG:NE	2.25	0.69
1:B:805:ILE:HG13	1:B:878:LEU:HD21	1.75	0.68
2:O:61:ASP:HA	2:O:64:LYS:HG2	1.75	0.68
2:M:34:MET:HB3	2:M:78:LEU:HD22	1.74	0.68
2:M:34:MET:HE1	2:M:94:LYS:HA	1.75	0.68
1:A:473:TYR:O	1:A:488:CYS:HA	1.92	0.68
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.76	0.68
1:C:379:CYS:HA	1:C:432:CYS:HB3	1.76	0.68
2:M:95:GLU:HG3	2:M:96:GLY:H	1.57	0.68
1:B:564:GLN:HA	1:B:577:ARG:HD3	1.75	0.68
1:B:409:GLN:OE1	1:B:419:ALA:N	2.26	0.68
3:P:78:LEU:HD21	3:P:83:PHE:HE1	1.57	0.68
1:B:480:CYS:SG	1:B:481:ASN:N	2.67	0.68
2:O:16:ARG:HG3	2:O:17:SER:H	1.59	0.68
3:L:90:GLN:HE21	3:L:97:THR:H	1.41	0.67
1:A:326:ILE:HD11	1:A:534:VAL:HG22	1.75	0.67
1:B:825:LYS:NZ	1:B:938:LEU:O	2.16	0.67
1:C:418:ILE:HG23	1:C:422:ASN:HB2	1.75	0.67
1:B:503:VAL:O	1:B:508:TYR:OH	2.12	0.67
3:N:90:GLN:HE21	3:N:97:THR:H	1.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:33:LEU:HD11	3:L:88:CYS:HB2	1.77	0.67
1:A:569:ILE:HG12	1:C:47:VAL:HG22	1.77	0.67
3:P:34:ASN:ND2	3:P:91:SER:OG	2.27	0.67
1:A:454:ARG:NH1	1:A:469:SER:O	2.27	0.67
1:B:418:ILE:HG23	1:B:422:ASN:HB2	1.77	0.67
1:A:493:GLN:OE1	2:H:97:ARG:NH2	2.26	0.66
2:H:19:ARG:HD2	2:H:81:GLN:HE21	1.61	0.66
1:B:277:LEU:HD23	1:B:285:ILE:HD13	1.76	0.66
1:A:731:MET:H	1:A:774:GLN:NE2	1.94	0.66
1:A:379:CYS:HA	1:A:432:CYS:HB3	1.78	0.66
1:A:516:GLU:OE2	1:C:200:TYR:OH	2.11	0.66
1:C:404:GLY:HA2	1:C:508:TYR:HD1	1.60	0.66
1:A:489:TYR:CZ	2:H:100(C):VAL:HG21	2.31	0.66
1:C:404:GLY:HA2	1:C:508:TYR:CD1	2.31	0.66
1:C:502:GLY:O	1:C:506:GLN:NE2	2.29	0.66
1:B:128:ILE:HD11	1:B:170:TYR:HB3	1.78	0.65
2:H:38:ARG:O	2:H:46:GLU:N	2.28	0.65
3:L:3:GLN:H	3:L:26:SER:HB3	1.61	0.65
1:C:418:ILE:HG12	1:C:422:ASN:HD22	1.61	0.65
1:A:676:THR:HA	1:A:690:GLN:HA	1.77	0.65
1:A:712:ILE:HD13	1:A:1094:VAL:HG11	1.77	0.65
1:B:438:SER:N	1:B:507:PRO:O	2.25	0.65
1:B:992:GLN:OE1	1:B:995:ARG:NH2	2.29	0.65
2:M:82(B):SER:O	2:M:83:ARG:NH2	2.29	0.65
1:A:805:ILE:HG22	1:A:818:ILE:HD12	1.78	0.65
1:C:86:PHE:O	1:C:87:ASN:ND2	2.30	0.65
1:B:323:THR:OG1	1:B:324:GLU:OE1	2.13	0.65
2:O:36:TRP:HD1	2:O:69:ILE:HD12	1.60	0.65
1:B:448:ASN:HB3	1:B:497:PHE:HB2	1.78	0.65
2:M:87:THR:HG23	2:M:110:THR:HA	1.79	0.65
1:B:542:ASN:ND2	1:B:547:THR:HG22	2.12	0.65
1:C:644:GLN:NE2	1:C:645:THR:O	2.30	0.65
1:A:43:PHE:HB2	1:B:563:GLN:NE2	2.11	0.64
1:C:66:HIS:CG	1:C:79:PHE:CZ	2.84	0.64
1:C:421:TYR:CD1	1:C:457:ARG:HG2	2.33	0.64
2:O:44:GLY:HA2	3:P:87:TYR:HE1	1.63	0.64
1:A:501:ASN:HB3	1:A:505:TYR:HB2	1.78	0.64
1:B:456:PHE:CZ	1:B:489:TYR:HB2	2.32	0.64
1:C:299:THR:OG1	1:C:597:VAL:HG21	1.96	0.64
1:C:456:PHE:HZ	1:C:489:TYR:HB2	1.63	0.64
1:B:108:THR:OG1	1:B:234:ASN:O	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:983:ARG:HG2	1:C:390:LEU:HD11	1.80	0.64
1:B:355:ARG:HB2	1:B:466:ARG:HH12	1.63	0.64
1:B:568:ASP:OD1	1:B:569:ILE:N	2.28	0.64
1:A:1107:ARG:NE	1:C:904:TYR:CZ	2.63	0.64
1:A:443:SER:OG	1:A:497:PHE:CB	2.29	0.64
1:A:968:SER:OG	1:C:755:GLN:O	2.16	0.64
1:A:971:GLY:HA3	1:A:995:ARG:HH21	1.61	0.63
1:A:985:ASP:HB2	1:A:986:PRO:HD2	1.79	0.63
1:B:424:LYS:HB3	1:B:463:PRO:HA	1.80	0.63
1:A:644:GLN:NE2	1:A:645:THR:O	2.32	0.63
1:B:676:THR:HA	1:B:690:GLN:HA	1.80	0.63
1:B:873:TYR:CZ	1:C:699:LEU:HD22	2.33	0.63
1:B:917:TYR:HB3	1:C:1129:VAL:HG13	1.80	0.63
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.79	0.63
1:C:480:CYS:SG	1:C:481:ASN:N	2.72	0.63
2:H:11:VAL:HA	2:H:110:THR:HB	1.79	0.63
1:A:418:ILE:HA	1:A:422:ASN:ND2	2.14	0.63
1:A:437:ASN:HA	1:A:508:TYR:HA	1.80	0.63
1:B:365:TYR:HD2	1:B:387:LEU:HB3	1.62	0.63
1:B:731:MET:HG2	1:B:774:GLN:HE22	1.64	0.63
3:L:20:THR:HG23	3:L:74:THR:HG22	1.80	0.63
2:O:19:ARG:HD3	2:O:81:GLN:OE1	1.98	0.63
1:A:731:MET:H	1:A:774:GLN:HE21	1.46	0.63
1:B:328:ARG:NH2	1:B:578:ASP:OD2	2.32	0.62
1:C:457:ARG:NH1	1:C:459:SER:O	2.32	0.62
1:C:541:PHE:O	1:C:548:GLY:O	2.16	0.62
1:A:65:PHE:CE1	1:A:84:LEU:HD21	2.34	0.62
1:A:455:LEU:HG	1:A:456:PHE:H	1.64	0.62
1:B:379:CYS:HA	1:B:432:CYS:CB	2.28	0.62
3:N:33:LEU:HB3	3:N:51:ALA:HB2	1.81	0.62
3:L:33:LEU:HB3	3:L:51:ALA:HB2	1.80	0.62
3:N:79:GLN:N	3:N:82:ASP:OD2	2.32	0.62
1:A:935:GLN:O	1:A:939:SER:N	2.30	0.62
1:C:805:ILE:HG13	1:C:878:LEU:HD21	1.80	0.62
3:L:90:GLN:NE2	3:L:96:ARG:HA	2.14	0.62
1:A:108:THR:O	1:A:237:ARG:NH2	2.33	0.62
1:C:328:ARG:NH2	1:C:578:ASP:OD1	2.32	0.62
1:B:546:LEU:CD2	1:B:565:PHE:CE1	2.82	0.62
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.82	0.62
1:A:395:VAL:HG12	1:A:515:PHE:HD2	1.63	0.61
1:C:89:GLY:HA3	1:C:270:LEU:HD12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:59:TYR:HB2	2:H:64:LYS:HE2	1.82	0.61
2:M:66:ARG:HD2	2:M:83:ARG:HH22	1.64	0.61
3:P:82:ASP:O	3:P:86:TYR:OH	2.13	0.61
3:P:89:GLN:NE2	3:P:90:GLN:O	2.33	0.61
2:M:6:GLU:OE2	2:M:92:CYS:N	2.26	0.61
1:B:273:ARG:NH1	1:B:290:ASP:OD2	2.33	0.61
1:B:906:PHE:CD2	1:B:916:LEU:HB2	2.35	0.61
1:C:803:SER:OG	1:C:804:GLN:OE1	2.15	0.61
1:C:406:GLU:OE1	1:C:409:GLN:NE2	2.34	0.61
2:M:34:MET:HE3	2:M:34:MET:HA	1.82	0.61
1:B:89:GLY:HA3	1:B:270:LEU:HD12	1.82	0.61
1:A:332:ILE:HG13	1:A:362:VAL:HG23	1.83	0.61
1:B:902:MET:HE3	1:B:1049:LEU:HD13	1.81	0.61
1:C:567:ARG:NH1	1:C:571:ASP:OD1	2.29	0.61
1:A:360:ASN:H	1:A:523:THR:HB	1.65	0.61
3:P:49:TYR:O	3:P:53:SER:OG	2.18	0.61
1:A:421:TYR:CD1	1:A:457:ARG:HG2	2.35	0.60
1:A:804:GLN:NE2	1:A:935:GLN:HE22	1.98	0.60
1:C:455:LEU:HG	1:C:456:PHE:H	1.66	0.60
2:O:2:VAL:HA	2:O:26:GLY:HA3	1.84	0.60
2:O:35:HIS:NE2	2:O:95:GLU:OE1	2.34	0.60
1:C:108:THR:O	1:C:237:ARG:NH1	2.35	0.60
3:L:39:LYS:HD3	3:L:84:ALA:HB2	1.83	0.60
1:B:563:GLN:HG2	1:B:564:GLN:N	2.16	0.60
1:C:338:PHE:HE2	1:C:358:ILE:HG21	1.67	0.60
1:C:472:ILE:HD13	1:C:483:VAL:HG21	1.81	0.60
2:H:33:GLY:O	2:H:34:MET:HE2	2.01	0.60
2:O:35:HIS:CE1	2:O:50:VAL:HG23	2.37	0.60
1:A:472:ILE:HG13	1:A:488:CYS:SG	2.41	0.60
1:B:985:ASP:HB2	1:B:986:PRO:HD2	1.84	0.60
1:C:100:ILE:HG22	1:C:242:LEU:HD12	1.84	0.60
1:C:366:SER:HA	1:C:369:TYR:CE1	2.37	0.60
3:N:39:LYS:HD2	3:N:84:ALA:HB2	1.82	0.59
2:M:35:HIS:NE2	2:M:95:GLU:OE1	2.34	0.59
2:O:59:TYR:HB2	2:O:64:LYS:HD2	1.84	0.59
1:A:319:ARG:HH12	1:C:745:ASP:HB3	1.67	0.59
2:O:38:ARG:NH2	2:O:85:GLU:O	2.36	0.59
1:C:66:HIS:CA	1:C:79:PHE:CE2	2.82	0.59
1:C:402:ILE:HD12	1:C:406:GLU:HB2	1.84	0.59
1:C:422:ASN:OD1	1:C:454:ARG:HB3	2.02	0.59
1:B:170:TYR:OH	1:B:172:SER:OG	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:3:GLN:H	3:P:26:SER:HB3	1.67	0.59
1:A:733:LYS:NZ	1:A:775:ASP:OD2	2.29	0.59
3:N:61:ARG:NH1	3:N:82:ASP:OD1	2.35	0.59
1:A:323:THR:HB	1:A:537:LYS:NZ	2.18	0.59
1:B:388:ASN:OD1	1:B:527:PRO:HD2	2.02	0.59
1:B:973:ILE:HD12	1:B:983:ARG:HH21	1.68	0.59
2:M:37:VAL:HG23	2:M:91:TYR:HB2	1.84	0.59
3:P:59:PRO:HB2	3:P:61:ARG:HG2	1.83	0.59
1:A:745:ASP:OD2	1:B:319:ARG:NH2	2.36	0.58
1:B:984:LEU:HD12	1:B:988:GLU:HG2	1.84	0.58
1:A:1006:THR:OG1	1:C:1005:GLN:NE2	2.30	0.58
1:B:452:LEU:HA	1:B:494:SER:HA	1.85	0.58
1:B:453:TYR:CD1	1:B:495:TYR:HE1	2.20	0.58
1:A:409:GLN:OE1	1:A:416:GLY:HA3	2.03	0.58
2:M:35:HIS:HD2	2:M:100(G):PHE:CZ	2.21	0.58
1:B:805:ILE:HG22	1:B:818:ILE:HD12	1.85	0.58
1:C:540:ASN:CB	1:C:549:THR:HG22	2.32	0.58
1:C:980:ILE:HD13	1:C:992:GLN:HB3	1.85	0.58
2:H:95:GLU:HG3	2:H:96:GLY:H	1.68	0.58
3:L:14:SER:N	3:L:17:ASP:OD2	2.36	0.58
1:B:83:VAL:HG11	1:B:237:ARG:HH21	1.67	0.58
2:H:87:THR:HG22	2:H:111:VAL:H	1.66	0.58
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.86	0.58
1:B:117:LEU:HD23	1:B:118:LEU:N	2.18	0.58
2:H:36:TRP:HD1	2:H:69:ILE:HD12	1.69	0.58
1:C:346:ARG:HA	1:C:346:ARG:HH11	1.68	0.58
2:M:63:VAL:HG12	2:M:66:ARG:HH21	1.68	0.58
1:C:905:ARG:HD3	1:C:1049:LEU:O	2.04	0.58
1:A:736:VAL:HG21	1:A:1004:LEU:HD11	1.86	0.58
1:B:226:LEU:HG	1:B:227:VAL:HG23	1.84	0.58
1:C:555:SER:HB2	1:C:557:LYS:HG2	1.86	0.58
1:B:137:ASN:OD1	1:B:138:ASP:N	2.37	0.57
1:A:403:ARG:HD2	1:A:505:TYR:CD1	2.40	0.57
1:B:403:ARG:NH1	1:B:505:TYR:O	2.38	0.57
1:C:540:ASN:CG	1:C:549:THR:HG22	2.29	0.57
1:A:805:ILE:HG13	1:A:878:LEU:HD21	1.86	0.57
1:B:408:ARG:HG2	1:B:408:ARG:HH11	1.69	0.57
2:H:29:PHE:O	2:H:71:ARG:NH2	2.37	0.57
1:A:108:THR:OG1	1:A:234:ASN:O	2.20	0.57
1:A:873:TYR:CE1	1:B:699:LEU:HD12	2.40	0.57
1:B:973:ILE:HG23	1:B:992:GLN:NE2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:HIS:CA	1:C:79:PHE:HE2	2.12	0.57
1:A:826:VAL:HB	1:A:1057:PRO:HG2	1.86	0.56
1:B:117:LEU:HD12	1:B:231:ILE:HD13	1.87	0.56
1:A:906:PHE:CD2	1:A:916:LEU:HB2	2.40	0.56
1:B:328:ARG:HD2	1:B:580:GLN:OE1	2.05	0.56
1:B:331:ASN:HB2	1:B:580:GLN:HG3	1.87	0.56
1:C:360:ASN:H	1:C:523:THR:HB	1.70	0.56
2:M:91:TYR:CE2	3:N:44:PRO:HD3	2.39	0.56
1:A:421:TYR:HD1	1:A:457:ARG:HG2	1.69	0.56
1:B:396:TYR:HB2	1:B:514:SER:OG	2.05	0.56
1:A:317:ASN:ND2	1:C:737:ASP:OD2	2.38	0.56
1:B:731:MET:CG	1:B:774:GLN:HE22	2.17	0.56
1:B:982:SER:O	1:C:386:LYS:HD3	2.06	0.56
1:B:351:TYR:HE1	1:B:452:LEU:HB2	1.71	0.56
1:B:973:ILE:HD12	1:B:983:ARG:NH2	2.21	0.56
3:L:6:GLN:OE1	3:L:101:GLY:N	2.38	0.56
1:B:360:ASN:H	1:B:523:THR:HB	1.70	0.56
1:C:379:CYS:HA	1:C:432:CYS:HB2	1.88	0.56
1:C:900:MET:HG2	1:C:917:TYR:OH	2.06	0.56
1:B:231:ILE:HG13	1:B:232:GLY:N	2.21	0.56
1:B:310:LYS:HG2	1:B:664:ILE:HD11	1.87	0.56
2:O:40:ALA:HA	2:O:88:ALA:HA	1.88	0.56
1:C:421:TYR:HD1	1:C:457:ARG:HG2	1.71	0.55
1:C:101:ILE:HG13	1:C:242:LEU:HD11	1.87	0.55
1:C:1106:GLN:NE2	1:C:1111:GLU:OE2	2.38	0.55
2:O:100(B):VAL:HG23	2:O:100(C):VAL:N	2.17	0.55
2:H:3:GLN:HE22	2:H:5:VAL:HG22	1.71	0.55
1:A:115:GLN:CD	1:A:115:GLN:H	2.15	0.55
1:B:210:ILE:HG21	1:B:217:PRO:HG2	1.89	0.55
1:C:906:PHE:CD2	1:C:916:LEU:HB2	2.42	0.55
1:C:1100:THR:HG23	1:C:1101:HIS:ND1	2.21	0.55
1:A:439:ASN:HD21	1:A:506:GLN:HG2	1.71	0.55
3:N:89:GLN:NE2	3:N:90:GLN:O	2.39	0.55
2:O:20:LEU:HG	2:O:82:MET:HE1	1.89	0.55
2:O:47:TRP:HZ2	2:O:50:VAL:HB	1.71	0.55
1:B:546:LEU:HD21	1:B:565:PHE:CE1	2.41	0.55
1:C:533:LEU:HD21	1:C:585:LEU:HD11	1.87	0.55
1:B:417:LYS:HG2	1:B:453:TYR:OH	2.06	0.55
1:C:332:ILE:HG13	1:C:362:VAL:HG23	1.89	0.55
1:C:471:GLU:O	2:M:52(A):TYR:OH	2.20	0.55
1:B:236:THR:HG23	1:B:237:ARG:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:80:LEU:HG	2:O:82:MET:SD	2.47	0.55
1:A:379:CYS:HA	1:A:432:CYS:HB2	1.89	0.55
1:B:81:ASN:HD22	1:B:242:LEU:HD12	1.71	0.55
1:B:484:GLU:HG2	3:P:96:ARG:NH2	2.22	0.55
1:B:980:ILE:HD12	1:B:980:ILE:H	1.72	0.55
1:A:393:THR:HG21	1:A:518:LEU:HB2	1.88	0.55
1:B:186:PHE:HE1	1:B:263:ALA:HA	1.72	0.55
1:C:316:SER:OG	1:C:317:ASN:N	2.40	0.55
3:P:6:GLN:OE1	3:P:101:GLY:N	2.40	0.55
1:B:983:ARG:NH1	1:C:517:LEU:HD13	2.21	0.54
1:C:985:ASP:HB2	1:C:986:PRO:HD2	1.89	0.54
1:A:917:TYR:HB3	1:B:1129:VAL:HG13	1.87	0.54
1:B:555:SER:HB3	1:B:586:ASP:CG	2.33	0.54
2:H:59:TYR:CE1	2:H:69:ILE:HG22	2.42	0.54
1:C:406:GLU:HG3	1:C:418:ILE:HD12	1.88	0.54
2:M:82(B):SER:OG	2:M:83:ARG:NH2	2.40	0.54
1:C:96:GLU:CD	1:C:100:ILE:H	2.15	0.54
2:O:45:LEU:HD21	3:P:38:GLN:HE22	1.73	0.54
2:O:37:VAL:HG13	2:O:91:TYR:HB2	1.88	0.54
1:A:126:VAL:HB	1:A:172:SER:HB3	1.90	0.54
1:A:466:ARG:HG2	1:A:468:ILE:HD11	1.89	0.54
1:B:900:MET:HE1	1:C:1077:THR:HG21	1.90	0.54
1:C:66:HIS:CG	1:C:79:PHE:CE2	2.85	0.54
1:B:546:LEU:HD22	1:B:565:PHE:CE1	2.43	0.54
1:C:118:LEU:HD12	1:C:135:PHE:HZ	1.73	0.54
1:C:355:ARG:HG3	1:C:398:ASP:OD1	2.07	0.54
1:A:281:GLU:HG2	1:A:282:ASN:N	2.23	0.53
1:A:43:PHE:CE1	1:B:559:PHE:HA	2.43	0.53
1:A:81:ASN:OD1	1:A:242:LEU:HG	2.08	0.53
1:C:541:PHE:HE2	1:C:549:THR:C	2.16	0.53
1:C:541:PHE:CE2	1:C:549:THR:C	2.86	0.53
1:A:57:PRO:HG3	1:A:273:ARG:HD2	1.90	0.53
1:A:804:GLN:CD	1:A:935:GLN:HE22	2.17	0.53
1:B:792:PRO:O	1:B:795:LYS:NZ	2.35	0.53
1:A:906:PHE:CE2	1:A:916:LEU:HD12	2.42	0.53
1:B:34:ARG:HD2	1:B:191:GLU:OE2	2.08	0.53
1:B:338:PHE:CZ	1:B:365:TYR:HE1	2.26	0.53
1:B:439:ASN:HD21	1:B:506:GLN:HG2	1.73	0.53
1:A:1019:ARG:HG2	1:A:1019:ARG:HH11	1.74	0.53
2:H:5:VAL:O	2:H:22:CYS:HA	2.08	0.53
2:O:95:GLU:HG3	2:O:96:GLY:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:63:VAL:HG12	2:H:66:ARG:HH21	1.73	0.53
1:A:748:GLU:H	1:A:748:GLU:CD	2.16	0.53
1:A:1039:ARG:NH2	1:C:1031:GLU:OE2	2.39	0.53
1:C:477:SER:HB3	1:C:487:ASN:ND2	2.23	0.53
1:B:433:VAL:HG12	1:B:512:VAL:HG23	1.89	0.53
3:L:80:PRO:HA	3:L:83:PHE:HE2	1.73	0.53
3:N:90:GLN:NE2	3:N:96:ARG:HA	2.24	0.53
1:A:517:LEU:C	1:A:518:LEU:HD12	2.34	0.53
2:O:87:THR:HG22	2:O:111:VAL:H	1.73	0.53
3:L:32:TYR:HB3	3:L:91:SER:H	1.74	0.53
2:M:72:ASP:O	2:M:76:ASN:N	2.42	0.53
2:O:59:TYR:CE1	2:O:69:ILE:HG22	2.44	0.53
1:A:33:THR:HG22	1:A:220:PHE:HD1	1.72	0.52
1:A:1106:GLN:HE21	1:A:1109:PHE:HB3	1.73	0.52
1:B:388:ASN:O	1:B:526:GLY:HA3	2.07	0.52
2:H:38:ARG:HG2	2:H:46:GLU:HB3	1.91	0.52
1:A:1094:VAL:HG22	1:C:904:TYR:OH	2.09	0.52
1:C:748:GLU:CD	1:C:748:GLU:H	2.17	0.52
2:M:7:SER:OG	2:M:21:SER:OG	2.21	0.52
1:A:1089:PHE:HE2	1:C:917:TYR:HD1	1.58	0.52
1:B:470:THR:HG22	1:B:492:LEU:HD12	1.87	0.52
1:B:1097:SER:HB2	1:B:1102:TRP:CD2	2.45	0.52
1:A:555:SER:OG	1:A:557:LYS:HG2	2.10	0.52
1:B:443:SER:CB	1:B:497:PHE:HB3	2.23	0.52
1:B:552:LEU:HD22	1:B:587:ILE:HG22	1.90	0.52
1:B:904:TYR:CE2	1:C:1107:ARG:HD3	2.44	0.52
2:M:75:LYS:HE2	2:M:75:LYS:HA	1.91	0.52
1:A:101:ILE:HG12	1:A:242:LEU:HD22	1.91	0.52
1:C:822:LEU:HD21	1:C:1061:VAL:HG21	1.91	0.52
1:C:1111:GLU:O	1:C:1111:GLU:HG3	2.10	0.52
2:H:40:ALA:HB3	2:H:43:LYS:HB3	1.90	0.52
3:L:7:SER:HB2	3:L:24:ARG:HH12	1.73	0.52
3:L:34:ASN:N	3:L:89:GLN:O	2.42	0.52
3:P:32:TYR:O	3:P:91:SER:N	2.42	0.52
1:A:418:ILE:HG23	1:A:422:ASN:HD22	1.74	0.52
1:A:759:PHE:HD2	1:A:1001:LEU:HD21	1.75	0.52
1:B:327:VAL:HG12	1:B:327:VAL:O	2.09	0.52
1:B:447:GLY:N	1:B:498:GLN:OE1	2.43	0.52
1:A:309:GLU:O	1:A:313:TYR:OH	2.19	0.52
1:A:357:ARG:HD2	1:A:396:TYR:HE1	1.74	0.52
1:A:117:LEU:HD23	1:A:118:LEU:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873:TYR:CZ	1:B:699:LEU:HD12	2.44	0.52
1:C:409:GLN:OE1	1:C:416:GLY:HA3	2.10	0.52
1:C:809:PRO:O	1:C:814:LYS:NZ	2.42	0.52
2:H:52:SER:O	2:H:71:ARG:NH1	2.43	0.52
2:M:51:ILE:HD12	2:M:71:ARG:HD2	1.91	0.52
1:B:100:ILE:HD12	1:B:263:ALA:HB2	1.91	0.52
1:B:309:GLU:O	1:B:313:TYR:OH	2.23	0.52
1:B:472:ILE:HG13	1:B:473:TYR:N	2.24	0.52
1:B:546:LEU:CD1	1:B:546:LEU:N	2.73	0.52
3:N:17:ASP:HB2	3:N:78:LEU:HD12	1.91	0.52
3:P:83:PHE:CE2	3:P:106:ILE:HB	2.45	0.52
3:N:83:PHE:CD1	3:N:104:VAL:HG12	2.45	0.52
1:C:424:LYS:HB3	1:C:463:PRO:HA	1.92	0.51
1:C:726:ILE:HD13	1:C:945:LEU:HD12	1.92	0.51
2:M:35:HIS:HD2	2:M:100(G):PHE:CE2	2.28	0.51
2:O:40:ALA:H	2:O:43:LYS:HE3	1.75	0.51
1:A:31:SER:OG	1:A:60:SER:N	2.42	0.51
1:A:290:ASP:HB3	1:A:293:LEU:HB2	1.90	0.51
1:B:78:ARG:N	1:B:78:ARG:CZ	2.73	0.51
1:B:130:VAL:HG22	1:B:168:PHE:O	2.10	0.51
1:B:869:MET:HB3	1:C:699:LEU:HD11	1.93	0.51
2:M:36:TRP:HD1	2:M:69:ILE:HD12	1.76	0.51
1:A:854:LYS:HE2	1:A:855:PHE:CE1	2.46	0.51
1:B:417:LYS:HG2	1:B:453:TYR:CZ	2.45	0.51
1:B:988:GLU:OE2	1:B:988:GLU:N	2.39	0.51
2:M:68:THR:OG1	2:M:81:GLN:HB3	2.10	0.51
3:P:78:LEU:HD21	3:P:83:PHE:CE1	2.42	0.51
1:A:47:VAL:HG22	1:B:569:ILE:HG22	1.93	0.51
1:B:502:GLY:O	1:B:506:GLN:NE2	2.42	0.51
1:C:131:CYS:SG	1:C:132:GLU:N	2.84	0.51
2:M:59:TYR:CE1	2:M:69:ILE:HG22	2.46	0.51
1:A:278:LYS:HB2	1:A:306:PHE:CE2	2.46	0.51
1:A:531:THR:HG23	1:A:531:THR:O	2.10	0.51
1:B:394:ASN:OD1	1:B:395:VAL:N	2.43	0.51
1:B:935:GLN:O	1:B:939:SER:N	2.42	0.51
1:C:42:VAL:HG21	1:C:44:ARG:NH1	2.25	0.51
3:P:105:GLU:HG2	3:P:106:ILE:N	2.26	0.51
1:B:409:GLN:NE2	1:B:416:GLY:HA3	2.25	0.51
1:C:418:ILE:HG12	1:C:422:ASN:ND2	2.26	0.51
2:O:63:VAL:HG12	2:O:66:ARG:HH21	1.76	0.50
1:C:534:VAL:HG23	1:C:539:VAL:HG11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:986:PRO:HA	1:C:989:ALA:HB3	1.93	0.50
3:P:105:GLU:HG2	3:P:106:ILE:H	1.76	0.50
1:A:233:ILE:HB	1:A:235:ILE:HG13	1.94	0.50
1:A:316:SER:OG	1:A:317:ASN:N	2.42	0.50
1:A:433:VAL:HG12	1:A:512:VAL:HG23	1.93	0.50
1:A:440:ASN:OD1	1:A:441:LEU:N	2.44	0.50
1:A:1077:THR:HG21	1:C:900:MET:HE1	1.91	0.50
1:C:96:GLU:OE2	1:C:100:ILE:HG12	2.11	0.50
1:C:805:ILE:HG22	1:C:818:ILE:HD13	1.94	0.50
2:M:38:ARG:HE	2:M:48:VAL:HG22	1.76	0.50
1:A:403:ARG:HD2	1:A:505:TYR:HD1	1.77	0.50
1:B:66:HIS:ND1	1:B:68:ILE:HD11	2.26	0.50
1:C:372:ALA:O	2:H:100(A):ILE:HD11	2.11	0.50
1:A:65:PHE:HE1	1:A:84:LEU:HD21	1.75	0.50
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.93	0.50
1:B:418:ILE:HG13	1:B:422:ASN:ND2	2.25	0.50
1:B:770:ILE:HD11	1:B:1012:LEU:HA	1.94	0.50
3:N:6:GLN:OE1	3:N:101:GLY:N	2.44	0.50
1:C:66:HIS:HB3	1:C:79:PHE:CZ	2.39	0.50
2:O:34:MET:HA	2:O:34:MET:HE3	1.94	0.50
2:O:51:ILE:HD11	2:O:71:ARG:HD2	1.94	0.50
1:C:398:ASP:OD2	1:C:423:TYR:OH	2.28	0.50
1:A:103:GLY:HA3	1:A:241:LEU:HD12	1.94	0.50
3:L:63:SER:O	3:L:73:LEU:HD12	2.12	0.50
1:A:736:VAL:HG12	1:A:858:LEU:HD22	1.94	0.50
1:C:540:ASN:HA	1:C:549:THR:CG2	2.33	0.50
4:J:1:NAG:O7	4:J:1:NAG:O3	2.29	0.50
1:A:342:PHE:CE1	1:A:511:VAL:HG11	2.47	0.49
1:B:431:GLY:HA2	1:B:515:PHE:CD1	2.47	0.49
1:B:980:ILE:HG23	1:B:984:LEU:HD21	1.94	0.49
1:C:417:LYS:HD2	1:C:455:LEU:HD12	1.93	0.49
2:H:16:ARG:O	2:H:82(C):LEU:HG	2.12	0.49
1:A:452:LEU:HD12	1:A:492:LEU:HB3	1.94	0.49
1:A:473:TYR:CE2	1:A:475:ALA:HB2	2.47	0.49
1:B:353:TRP:O	1:B:466:ARG:NH1	2.37	0.49
1:A:327:VAL:O	1:A:327:VAL:HG12	2.11	0.49
1:A:489:TYR:CE1	2:H:100(C):VAL:HG21	2.47	0.49
1:A:1097:SER:HB2	1:A:1102:TRP:CE3	2.48	0.49
1:C:676:THR:HA	1:C:690:GLN:HA	1.93	0.49
3:P:2:ILE:HA	3:P:26:SER:OG	2.13	0.49
1:A:903:ALA:HA	1:A:916:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:ARG:NE	1:C:191:GLU:OE2	2.29	0.49
2:H:91:TYR:HE1	3:L:44:PRO:HD3	1.77	0.49
2:O:69:ILE:HB	2:O:80:LEU:HD13	1.93	0.49
1:A:699:LEU:HD22	1:C:873:TYR:CE1	2.47	0.49
1:B:186:PHE:CE1	1:B:263:ALA:HA	2.46	0.49
3:N:97:THR:HG22	3:N:98:PHE:H	1.77	0.49
1:A:355:ARG:HG3	1:A:398:ASP:OD1	2.12	0.49
1:A:574:ASP:O	1:A:587:ILE:N	2.32	0.49
1:B:729:VAL:HG12	1:B:1059:GLY:HA2	1.94	0.49
2:M:2:VAL:HA	2:M:26:GLY:HA3	1.94	0.49
2:H:67:PHE:CE1	2:H:82:MET:HB2	2.48	0.49
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.95	0.49
1:C:214:ARG:CZ	1:C:214:ARG:HA	2.43	0.49
2:H:5:VAL:HB	2:H:23:ALA:HB3	1.95	0.49
2:M:38:ARG:NE	2:M:46:GLU:OE1	2.46	0.49
3:N:34:ASN:N	3:N:89:GLN:O	2.46	0.49
1:A:85:PRO:HG2	1:A:269:TYR:HE1	1.78	0.49
1:A:394:ASN:OD1	1:A:395:VAL:N	2.45	0.49
1:A:424:LYS:HB3	1:A:463:PRO:HA	1.95	0.49
1:B:186:PHE:N	1:B:213:VAL:HG12	2.28	0.49
1:B:978:ASN:O	1:B:982:SER:N	2.44	0.49
1:C:220:PHE:HE2	1:C:285:ILE:HG22	1.78	0.49
1:C:231:ILE:HD12	1:C:233:ILE:HD12	1.94	0.49
1:C:483:VAL:O	1:C:483:VAL:HG13	2.12	0.49
2:H:38:ARG:HB3	2:H:90:TYR:CE2	2.47	0.49
1:B:328:ARG:HH12	1:B:533:LEU:HG	1.78	0.48
1:C:897:PRO:HD2	1:C:900:MET:HE3	1.94	0.48
2:M:87:THR:HA	2:M:109:VAL:O	2.13	0.48
1:B:905:ARG:HD3	1:B:1049:LEU:O	2.13	0.48
1:A:299:THR:OG1	1:A:597:VAL:HG21	2.13	0.48
1:C:96:GLU:OE2	1:C:99:ASN:N	2.46	0.48
1:C:443:SER:O	1:C:499:PRO:HD3	2.13	0.48
3:L:18:ARG:HA	3:L:75:ILE:O	2.14	0.48
1:A:330:PRO:HD3	1:A:544:ASN:OD1	2.13	0.48
1:B:106:PHE:HB3	1:B:235:ILE:HD13	1.94	0.48
1:C:906:PHE:CE2	1:C:916:LEU:HB2	2.49	0.48
3:L:81:GLU:N	3:L:81:GLU:OE1	2.45	0.48
1:A:42:VAL:HG21	1:A:44:ARG:NH1	2.28	0.48
1:A:406:GLU:CD	1:A:418:ILE:HD13	2.38	0.48
1:A:973:ILE:CG2	1:A:980:ILE:HD13	2.43	0.48
1:C:541:PHE:CE2	1:C:549:THR:O	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:6:GLN:H	3:L:100:GLN:HE22	1.61	0.48
1:B:78:ARG:N	1:B:78:ARG:NE	2.60	0.48
1:B:355:ARG:HH22	1:B:464:PHE:HD2	1.62	0.48
1:B:726:ILE:HD13	1:B:945:LEU:HD12	1.94	0.48
1:A:900:MET:HE1	1:B:1077:THR:OG1	2.14	0.48
1:B:462:LYS:HD2	1:B:463:PRO:O	2.13	0.48
2:M:97:ARG:HG2	2:M:100(E):VAL:HA	1.96	0.48
1:A:663:ASP:HB3	1:A:673:SER:HB3	1.96	0.48
2:H:39:GLN:N	2:H:89:VAL:O	2.43	0.48
2:M:17:SER:OG	2:M:81:GLN:NE2	2.42	0.48
1:A:461:LEU:HD11	1:A:465:GLU:HG3	1.96	0.48
1:A:543:PHE:O	1:A:546:LEU:HB2	2.14	0.48
1:B:555:SER:OG	1:B:584:ILE:HG22	2.13	0.48
1:B:748:GLU:CD	1:B:748:GLU:H	2.21	0.48
1:A:69:HIS:C	1:A:79:PHE:HE2	2.16	0.48
1:B:324:GLU:OE1	1:B:537:LYS:NZ	2.42	0.48
3:P:38:GLN:HA	3:P:44:PRO:HA	1.96	0.48
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.95	0.47
1:B:335:LEU:HD23	1:B:336:CYS:O	2.14	0.47
1:C:81:ASN:O	1:C:239:GLN:NE2	2.36	0.47
1:B:281:GLU:HB2	5:B:1303:NAG:H82	1.96	0.47
1:B:384:PRO:HA	1:B:387:LEU:HD23	1.96	0.47
1:C:344:ALA:HB3	1:C:347:PHE:HE1	1.79	0.47
1:C:902:MET:HE1	1:C:1050:MET:HE3	1.96	0.47
3:L:6:GLN:H	3:L:100:GLN:NE2	2.12	0.47
2:O:17:SER:HA	2:O:82:MET:O	2.14	0.47
1:A:396:TYR:HB2	1:A:514:SER:OG	2.14	0.47
1:B:973:ILE:HG23	1:B:992:GLN:HE22	1.78	0.47
1:C:535:LYS:HE3	1:C:554:GLU:OE2	2.14	0.47
3:P:30:SER:HA	3:P:68:GLY:H	1.80	0.47
1:A:201:PHE:HE2	1:A:203:ILE:HD11	1.79	0.47
1:C:541:PHE:CD2	1:C:548:GLY:O	2.68	0.47
1:A:105:ILE:HD11	1:A:241:LEU:HD11	1.95	0.47
1:A:474:GLN:HG2	1:A:480:CYS:SG	2.55	0.47
1:A:763:LEU:HD11	1:A:1005:GLN:OE1	2.12	0.47
1:B:104:TRP:O	1:B:105:ILE:HD13	2.13	0.47
1:B:403:ARG:HG3	1:B:505:TYR:HA	1.96	0.47
1:C:214:ARG:HA	1:C:214:ARG:NE	2.29	0.47
2:O:4:LEU:HD12	2:O:23:ALA:O	2.14	0.47
1:A:351:TYR:HB2	1:A:454:ARG:HB2	1.95	0.47
1:A:574:ASP:OD1	1:A:575:ALA:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:PRO:HG3	1:C:273:ARG:HD2	1.97	0.47
1:C:546:LEU:HD21	1:C:565:PHE:CE2	2.48	0.47
2:H:7:SER:OG	2:H:21:SER:OG	2.15	0.47
1:A:323:THR:HB	1:A:537:LYS:HZ1	1.79	0.47
1:A:490:PHE:HZ	2:H:31:ILE:HD11	1.79	0.47
1:B:326:ILE:HG23	1:B:539:VAL:HG21	1.96	0.47
1:B:1144:GLU:HB3	1:C:1145:LEU:HD21	1.97	0.47
1:C:490:PHE:HE2	1:C:492:LEU:HB2	1.79	0.47
1:C:543:PHE:O	1:C:546:LEU:CG	2.48	0.47
1:C:568:ASP:OD1	1:C:569:ILE:HG22	2.15	0.47
1:C:825:LYS:NZ	1:C:938:LEU:O	2.22	0.47
3:N:35:TRP:CE2	3:N:73:LEU:HB2	2.49	0.47
2:O:19:ARG:HH21	2:O:79:TYR:CB	2.27	0.47
2:O:38:ARG:N	2:O:46:GLU:O	2.43	0.47
2:O:51:ILE:CD1	2:O:71:ARG:HD2	2.45	0.47
3:P:83:PHE:HE2	3:P:106:ILE:HB	1.80	0.47
1:A:43:PHE:CB	1:B:563:GLN:HE22	2.19	0.47
1:A:83:VAL:HG21	1:A:237:ARG:HD2	1.97	0.47
1:B:66:HIS:CE1	1:B:68:ILE:HD11	2.50	0.47
1:B:866:THR:OG1	1:B:869:MET:HE2	2.15	0.47
1:A:222:ALA:HB2	1:A:285:ILE:HB	1.97	0.47
1:A:447:GLY:HA2	1:A:497:PHE:O	2.15	0.47
1:A:805:ILE:O	1:A:816:SER:OG	2.21	0.47
1:B:453:TYR:N	1:B:493:GLN:O	2.47	0.47
1:C:64:TRP:CD1	1:C:266:TYR:CE2	3.03	0.47
1:C:329:PHE:HB3	1:C:330:PRO:HD2	1.97	0.47
3:L:55:GLN:NE2	3:L:56:SER:O	2.43	0.47
1:B:767:LEU:HD23	1:B:767:LEU:HA	1.77	0.46
1:C:884:SER:O	1:C:887:THR:OG1	2.28	0.46
3:L:90:GLN:HE22	3:L:96:ARG:HA	1.78	0.46
2:M:6:GLU:HG2	2:M:92:CYS:SG	2.56	0.46
3:N:17:ASP:O	3:N:78:LEU:HG	2.14	0.46
1:A:358:ILE:HB	1:A:395:VAL:HG23	1.97	0.46
2:H:22:CYS:N	2:H:78:LEU:O	2.45	0.46
3:P:91:SER:HA	3:P:96:ARG:HD2	1.97	0.46
1:A:614:ASP:OD2	1:C:859:THR:OG1	2.34	0.46
1:A:961:THR:HG21	1:C:762:GLN:NE2	2.31	0.46
1:A:1005:GLN:NE2	1:B:1006:THR:OG1	2.48	0.46
1:A:1080:ALA:C	1:A:1132:ILE:HG13	2.40	0.46
1:B:954:GLN:HB3	1:B:1014:ARG:NH1	2.31	0.46
1:C:351:TYR:HE2	1:C:468:ILE:HG13	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:63:VAL:HG12	2:M:66:ARG:NH2	2.30	0.46
1:A:94:SER:OG	1:A:101:ILE:HD12	2.16	0.46
1:A:792:PRO:O	1:A:795:LYS:NZ	2.41	0.46
1:B:559:PHE:HZ	1:B:575:ALA:HB1	1.80	0.46
1:B:725:GLU:CD	1:B:1028:LYS:HE2	2.40	0.46
1:C:326:ILE:HD11	1:C:534:VAL:HG22	1.97	0.46
3:N:90:GLN:HE22	3:N:96:ARG:HA	1.80	0.46
1:B:67:ALA:HB3	1:B:263:ALA:N	2.31	0.46
2:H:48:VAL:O	2:H:60:ALA:N	2.41	0.46
2:H:75:LYS:HB2	2:H:75:LYS:HE2	1.66	0.46
1:A:44:ARG:HB3	1:A:47:VAL:HB	1.95	0.46
1:A:84:LEU:N	1:A:84:LEU:HD12	2.31	0.46
1:A:398:ASP:OD2	1:A:423:TYR:OH	2.31	0.46
1:B:878:LEU:O	1:B:882:ILE:HG13	2.15	0.46
1:C:443:SER:HA	1:C:448:ASN:HB2	1.97	0.46
2:H:97:ARG:HD2	2:H:100(C):VAL:O	2.16	0.46
1:A:168:PHE:CZ	1:A:170:TYR:HB2	2.51	0.46
1:A:193:VAL:HG23	1:A:223:LEU:HD22	1.97	0.46
1:A:228:ASP:C	1:A:229:LEU:HD12	2.40	0.46
1:A:228:ASP:OD1	1:A:229:LEU:N	2.48	0.46
1:A:328:ARG:HA	1:A:530:SER:HB2	1.98	0.46
1:A:699:LEU:HD22	1:C:873:TYR:CZ	2.50	0.46
1:C:118:LEU:HD21	1:C:120:VAL:HG23	1.98	0.46
1:A:64:TRP:HH2	1:A:214:ARG:HH12	1.62	0.46
1:A:357:ARG:HD2	1:A:396:TYR:CE1	2.50	0.46
1:B:91:TYR:CZ	1:B:93:ALA:HB2	2.51	0.46
1:C:490:PHE:CE2	1:C:492:LEU:HB2	2.50	0.46
2:H:4:LEU:HD12	2:H:23:ALA:O	2.14	0.46
3:L:39:LYS:NZ	3:L:83:PHE:O	2.46	0.46
2:O:68:THR:OG1	2:O:81:GLN:HB3	2.16	0.46
1:B:578:ASP:HB3	1:B:581:THR:O	2.16	0.46
1:B:873:TYR:CE1	1:C:699:LEU:HD22	2.51	0.46
1:B:1127:ASP:OD1	1:B:1128:VAL:N	2.49	0.46
1:A:546:LEU:O	1:A:546:LEU:HD23	2.16	0.46
1:C:33:THR:HG22	1:C:220:PHE:HD1	1.81	0.46
2:H:23:ALA:HA	2:H:77:THR:HG23	1.98	0.46
2:M:12:VAL:HG11	2:M:82(C):LEU:HD13	1.98	0.46
3:N:14:SER:N	3:N:17:ASP:OD2	2.49	0.46
1:A:130:VAL:HG23	1:A:167:THR:OG1	2.16	0.45
1:B:334:ASN:OD1	1:B:361:CYS:HA	2.16	0.45
1:B:453:TYR:HD2	1:B:455:LEU:HD12	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:GLU:HG2	3:P:96:ARG:HH22	1.82	0.45
1:B:544:ASN:HB2	1:B:546:LEU:CD1	2.47	0.45
1:C:229:LEU:HA	1:C:230:PRO:HD3	1.84	0.45
3:L:39:LYS:NZ	3:L:81:GLU:O	2.45	0.45
3:P:81:GLU:N	3:P:81:GLU:OE1	2.49	0.45
1:A:92:PHE:O	1:A:192:PHE:N	2.39	0.45
1:C:205:SER:OG	1:C:206:LYS:N	2.50	0.45
1:A:354:ASN:OD1	1:A:355:ARG:N	2.50	0.45
1:A:699:LEU:HD21	1:C:869:MET:HE2	1.99	0.45
1:B:200:TYR:OH	1:C:394:ASN:ND2	2.44	0.45
1:B:439:ASN:OD1	1:B:506:GLN:HB3	2.16	0.45
1:C:66:HIS:CG	1:C:79:PHE:HZ	2.32	0.45
1:C:1093:GLY:HA2	1:C:1107:ARG:HG2	1.98	0.45
2:O:45:LEU:HD21	3:P:38:GLN:NE2	2.32	0.45
3:P:32:TYR:HD2	3:P:92:TYR:HD1	1.65	0.45
3:P:37:GLN:HB2	3:P:47:LEU:HD11	1.99	0.45
1:A:38:TYR:CE2	1:A:285:ILE:HG12	2.52	0.45
1:A:409:GLN:HA	1:A:414:GLN:HG2	1.97	0.45
1:A:1089:PHE:CE2	1:C:917:TYR:HD1	2.35	0.45
1:B:342:PHE:CZ	1:B:368:LEU:HD21	2.52	0.45
1:C:560:LEU:HB2	1:C:563:GLN:CD	2.42	0.45
1:C:961:THR:O	1:C:965:GLN:HG2	2.16	0.45
2:H:96:GLY:O	2:H:100(F):ALA:N	2.48	0.45
3:L:1:ASP:OD1	3:L:2:ILE:N	2.40	0.45
1:A:1031:GLU:OE2	1:B:1039:ARG:NE	2.49	0.45
1:B:443:SER:HB2	1:B:498:GLN:N	2.32	0.45
1:C:347:PHE:CE2	1:C:509:ARG:HB3	2.52	0.45
2:H:35:HIS:CE1	2:H:50:VAL:HG23	2.51	0.45
3:N:21:ILE:HD11	3:N:102:THR:HG21	1.99	0.45
3:P:48:ILE:HD13	3:P:54:LEU:HA	1.99	0.45
1:A:369:TYR:C	1:A:371:SER:H	2.24	0.45
1:B:440:ASN:OD1	3:N:52:SER:HB2	2.17	0.45
1:B:984:LEU:HD23	1:B:984:LEU:H	1.82	0.45
2:H:51:ILE:HD12	2:H:71:ARG:HB2	1.98	0.45
2:O:100(D):VAL:HG12	3:P:32:TYR:CE1	2.51	0.45
1:A:498:GLN:HB2	1:A:501:ASN:OD1	2.17	0.45
1:A:966:LEU:HD23	1:A:966:LEU:HA	1.67	0.45
2:H:69:ILE:HB	2:H:80:LEU:HD13	1.98	0.45
1:A:417:LYS:HA	1:A:417:LYS:HD3	1.79	0.45
1:A:426:PRO:HG3	1:A:463:PRO:HB3	1.99	0.45
1:A:1031:GLU:CD	1:B:1039:ARG:HE	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:THR:OG1	1:B:215:ASP:OD2	2.21	0.45
1:B:229:LEU:HA	1:B:230:PRO:HD3	1.85	0.45
1:B:472:ILE:HG13	1:B:473:TYR:H	1.81	0.45
1:C:818:ILE:H	1:C:818:ILE:HD12	1.82	0.45
4:J:1:NAG:H62	4:J:2:NAG:HN2	1.81	0.45
1:A:101:ILE:HG12	1:A:242:LEU:CD2	2.47	0.44
1:B:1097:SER:HB2	1:B:1102:TRP:CE3	2.51	0.44
1:C:67:ALA:HB3	1:C:263:ALA:O	2.16	0.44
3:L:39:LYS:HB2	3:L:42:LYS:HE2	1.99	0.44
1:A:546:LEU:HD23	1:A:546:LEU:C	2.42	0.44
1:A:904:TYR:CE1	1:B:1107:ARG:NE	2.78	0.44
1:B:83:VAL:HG11	1:B:237:ARG:NH2	2.30	0.44
1:B:201:PHE:HD2	1:B:229:LEU:HD21	1.82	0.44
1:C:53:ASP:HB3	1:C:55:PHE:CE1	2.51	0.44
1:C:802:PHE:HD2	1:C:805:ILE:HD11	1.82	0.44
2:H:68:THR:O	2:H:81:GLN:N	2.45	0.44
3:N:35:TRP:HB2	3:N:48:ILE:HB	1.99	0.44
1:A:486:PHE:HB2	3:L:92:TYR:O	2.16	0.44
1:B:42:VAL:HG12	1:B:44:ARG:HG3	2.00	0.44
1:B:228:ASP:OD1	1:B:229:LEU:N	2.51	0.44
1:B:662:CYS:HB2	1:B:697:MET:SD	2.57	0.44
1:C:213:VAL:HG23	1:C:214:ARG:NH1	2.33	0.44
1:C:231:ILE:HG13	1:C:232:GLY:N	2.32	0.44
3:L:36:TYR:HD1	3:L:46:LEU:HA	1.82	0.44
2:M:94:LYS:HG2	2:M:95:GLU:O	2.17	0.44
1:A:81:ASN:HD21	1:A:242:LEU:HD11	1.82	0.44
1:A:878:LEU:O	1:A:882:ILE:HG13	2.17	0.44
1:B:1043:CYS:HB3	1:B:1048:HIS:CD2	2.52	0.44
1:C:980:ILE:HG23	1:C:984:LEU:HD21	1.99	0.44
2:H:34:MET:HB2	2:H:51:ILE:HG12	2.00	0.44
3:N:59:PRO:HG2	3:N:61:ARG:NH2	2.32	0.44
1:A:85:PRO:HD2	1:A:269:TYR:HH	1.71	0.44
1:A:988:GLU:O	1:A:991:VAL:HG12	2.18	0.44
1:B:788:ILE:HD11	1:C:699:LEU:HB2	2.00	0.44
1:C:233:ILE:HG22	1:C:234:ASN:N	2.33	0.44
2:M:36:TRP:O	2:M:48:VAL:HB	2.18	0.44
3:N:34:ASN:OD1	3:N:49:TYR:HA	2.17	0.44
1:B:42:VAL:HG12	1:B:43:PHE:N	2.33	0.44
1:B:81:ASN:ND2	1:B:242:LEU:HD12	2.33	0.44
1:B:406:GLU:OE1	1:B:409:GLN:NE2	2.51	0.44
1:C:273:ARG:HG3	1:C:273:ARG:HH11	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:68:THR:OG1	2:H:81:GLN:HB2	2.17	0.44
1:A:959:LEU:HD23	1:A:959:LEU:HA	1.82	0.44
1:B:408:ARG:HG2	1:B:408:ARG:NH1	2.31	0.44
1:B:503:VAL:HA	1:B:506:GLN:NE2	2.33	0.44
1:B:970:PHE:CD2	1:B:999:GLY:HA3	2.53	0.44
1:C:906:PHE:CE2	1:C:916:LEU:HD12	2.53	0.44
2:H:38:ARG:HA	2:H:90:TYR:HA	1.99	0.44
2:M:37:VAL:HA	2:M:48:VAL:HG23	1.99	0.44
1:A:392:PHE:HD1	1:A:517:LEU:HD21	1.83	0.44
1:C:403:ARG:HG3	1:C:406:GLU:HG2	1.99	0.44
1:C:826:VAL:HB	1:C:1057:PRO:HG2	2.00	0.44
2:M:38:ARG:HB3	2:M:90:TYR:CE2	2.53	0.44
1:A:128:ILE:HD13	1:A:170:TYR:CD2	2.53	0.44
1:B:454:ARG:HA	1:B:492:LEU:HD23	2.00	0.44
1:C:109:THR:C	1:C:237:ARG:HH22	2.25	0.44
1:C:733:LYS:NZ	1:C:775:ASP:OD2	2.48	0.44
1:C:1092:GLU:N	1:C:1092:GLU:OE1	2.51	0.44
1:B:426:PRO:HD2	1:B:429:PHE:CD1	2.53	0.43
1:C:128:ILE:HD13	1:C:170:TYR:HD2	1.82	0.43
1:C:970:PHE:CG	1:C:999:GLY:HA3	2.53	0.43
2:H:19:ARG:HD2	2:H:81:GLN:NE2	2.30	0.43
2:M:89:VAL:HA	2:M:108:LEU:HA	1.99	0.43
1:A:273:ARG:NH1	1:A:273:ARG:HG2	2.33	0.43
1:A:298:GLU:O	1:A:302:THR:HG23	2.18	0.43
1:B:344:ALA:HB3	1:B:347:PHE:HE1	1.83	0.43
1:B:398:ASP:OD2	1:B:423:TYR:OH	2.35	0.43
1:C:104:TRP:HB3	1:C:106:PHE:CE2	2.53	0.43
3:P:14:SER:N	3:P:17:ASP:OD1	2.51	0.43
1:A:480:CYS:C	1:A:482:GLY:H	2.25	0.43
1:B:453:TYR:HD1	1:B:495:TYR:CE1	2.24	0.43
1:C:329:PHE:CE2	1:C:528:LYS:HB2	2.53	0.43
1:C:352:ALA:HA	1:C:466:ARG:HG3	2.00	0.43
1:C:406:GLU:O	1:C:409:GLN:HB2	2.19	0.43
1:A:278:LYS:HB2	1:A:306:PHE:HE2	1.82	0.43
1:A:866:THR:H	1:A:869:MET:CE	2.31	0.43
1:B:991:VAL:HG12	1:B:995:ARG:HH12	1.82	0.43
1:C:715:PRO:HA	1:C:1072:GLU:HA	2.01	0.43
2:O:51:ILE:HG22	2:O:57:LYS:HB3	2.00	0.43
1:B:115:GLN:OE1	1:B:130:VAL:O	2.37	0.43
1:B:206:LYS:HD2	1:B:206:LYS:HA	1.82	0.43
1:B:417:LYS:HD3	1:B:421:TYR:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:439:ASN:OD1	1:C:506:GLN:HB3	2.17	0.43
3:L:61:ARG:O	3:L:75:ILE:HA	2.18	0.43
3:P:6:GLN:NE2	3:P:99:GLY:HA3	2.33	0.43
1:A:453:TYR:CD1	1:A:495:TYR:HE1	2.36	0.43
1:B:405:ASP:OD1	1:B:406:GLU:N	2.51	0.43
1:C:137:ASN:OD1	1:C:138:ASP:N	2.52	0.43
1:C:473:TYR:HE2	1:C:475:ALA:HB2	1.84	0.43
1:C:725:GLU:OE2	1:C:1028:LYS:HE2	2.17	0.43
1:A:479:PRO:HG2	1:A:487:ASN:HD21	1.84	0.43
1:A:1106:GLN:NE2	1:A:1109:PHE:HB3	2.34	0.43
1:B:43:PHE:CE2	1:C:557:LYS:HD3	2.54	0.43
1:C:220:PHE:CE2	1:C:285:ILE:HG22	2.54	0.43
1:A:996:LEU:HD23	1:A:996:LEU:HA	1.82	0.43
1:B:737:ASP:OD1	1:B:738:CYS:N	2.52	0.43
1:C:430:THR:OG1	1:C:515:PHE:O	2.37	0.43
2:H:18:LEU:O	2:H:82:MET:HE3	2.18	0.43
3:L:35:TRP:HB2	3:L:48:ILE:HB	2.01	0.43
1:A:303:LEU:HD23	1:A:303:LEU:HA	1.83	0.43
1:A:490:PHE:CE2	1:A:492:LEU:HB2	2.53	0.43
1:B:42:VAL:CG1	1:B:44:ARG:HG3	2.48	0.43
1:B:197:ILE:HG23	1:B:198:ASP:OD1	2.19	0.43
1:B:353:TRP:HZ3	1:B:355:ARG:HB2	1.83	0.43
1:C:416:GLY:O	1:C:420:ASP:N	2.36	0.43
2:H:3:GLN:HA	2:H:102:TYR:OH	2.18	0.43
3:L:27:GLN:C	3:L:69:THR:HG22	2.44	0.43
1:A:493:GLN:CD	2:H:97:ARG:HH21	2.24	0.43
1:C:330:PRO:HD3	1:C:544:ASN:ND2	2.25	0.43
1:C:767:LEU:HD23	1:C:767:LEU:HA	1.72	0.43
1:A:85:PRO:HG2	1:A:269:TYR:CE1	2.54	0.42
1:A:342:PHE:HE2	1:A:368:LEU:HD21	1.84	0.42
1:A:490:PHE:CD1	1:A:491:PRO:HD2	2.53	0.42
1:B:56:LEU:HD12	1:B:57:PRO:HD2	2.00	0.42
1:C:32:PHE:CD1	1:C:218:GLN:HG3	2.54	0.42
1:C:437:ASN:HB3	1:C:508:TYR:CE2	2.54	0.42
1:A:357:ARG:HH22	1:C:200:TYR:HE1	1.66	0.42
1:A:765:ARG:NH1	1:B:957:GLN:HE22	2.17	0.42
1:C:566:GLY:N	1:C:575:ALA:O	2.50	0.42
1:C:737:ASP:OD2	1:C:740:MET:HE3	2.19	0.42
1:C:1088:HIS:CD2	1:C:1137:VAL:HG21	2.54	0.42
2:M:51:ILE:CD1	2:M:71:ARG:HD2	2.49	0.42
3:N:82:ASP:O	3:N:86:TYR:OH	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:767:LEU:HA	1:A:767:LEU:HD23	1.84	0.42
1:B:544:ASN:HB2	1:B:546:LEU:HD11	2.01	0.42
1:C:452:LEU:HD12	1:C:492:LEU:HB3	2.01	0.42
1:C:978:ASN:HA	1:C:981:LEU:HD12	2.01	0.42
2:M:69:ILE:HD11	2:M:78:LEU:HD11	2.00	0.42
3:N:19:VAL:HG12	3:N:75:ILE:HB	2.01	0.42
2:O:34:MET:HE1	2:O:94:LYS:HA	2.00	0.42
1:A:699:LEU:HB2	1:C:788:ILE:HD11	2.02	0.42
1:B:392:PHE:O	1:B:524:VAL:HG12	2.19	0.42
1:C:541:PHE:HD2	1:C:549:THR:HA	1.83	0.42
2:M:35:HIS:O	2:M:92:CYS:HA	2.19	0.42
1:A:104:TRP:O	1:A:105:ILE:HD13	2.19	0.42
1:A:712:ILE:HG13	1:C:896:ILE:HG12	2.00	0.42
1:B:117:LEU:HD21	1:B:119:ILE:HG13	2.02	0.42
1:B:461:LEU:HD11	1:B:465:GLU:HG3	2.01	0.42
1:B:993:ILE:O	1:B:996:LEU:N	2.53	0.42
1:B:1014:ARG:HE	1:B:1014:ARG:HB2	1.65	0.42
1:C:473:TYR:CE2	1:C:475:ALA:HB2	2.54	0.42
2:H:18:LEU:HD12	2:H:19:ARG:H	1.84	0.42
1:A:612:TYR:HE2	1:A:620:VAL:HG23	1.84	0.42
1:A:866:THR:OG1	1:A:869:MET:HE2	2.20	0.42
1:A:957:GLN:HE22	1:C:765:ARG:CZ	2.32	0.42
1:B:487:ASN:HA	1:B:489:TYR:CE1	2.54	0.42
1:B:966:LEU:HD23	1:B:966:LEU:HA	1.86	0.42
1:C:189:LEU:HB2	1:C:210:ILE:HD13	2.01	0.42
2:M:69:ILE:HG13	2:M:79:TYR:O	2.20	0.42
1:A:64:TRP:HH2	1:A:214:ARG:NH1	2.18	0.42
1:B:131:CYS:HB2	1:B:133:PHE:CZ	2.54	0.42
1:B:394:ASN:HB3	1:B:516:GLU:OE2	2.19	0.42
1:B:498:GLN:OE1	1:B:498:GLN:HA	2.20	0.42
1:C:103:GLY:HA3	1:C:241:LEU:HD12	2.01	0.42
1:A:216:LEU:HA	1:A:217:PRO:HD3	1.95	0.42
1:A:437:ASN:HB3	1:A:508:TYR:CZ	2.54	0.42
1:B:328:ARG:HD3	1:B:530:SER:HB2	2.01	0.42
1:B:378:LYS:O	1:B:378:LYS:HG3	2.19	0.42
1:B:406:GLU:CD	1:B:418:ILE:HD13	2.44	0.42
1:B:676:THR:HG22	1:B:690:GLN:HG2	2.01	0.42
1:B:904:TYR:CZ	1:C:1107:ARG:NH1	2.87	0.42
1:B:986:PRO:HA	1:B:989:ALA:HB3	2.01	0.42
1:B:1018:ILE:HD13	1:B:1018:ILE:HA	1.82	0.42
1:C:34:ARG:HD3	1:C:216:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:SER:HB2	1:C:388:ASN:HB2	2.01	0.42
1:C:736:VAL:HG12	1:C:858:LEU:HB3	2.01	0.42
2:H:69:ILE:HD11	2:H:78:LEU:HD11	2.02	0.42
3:L:36:TYR:CD1	3:L:46:LEU:HA	2.55	0.42
1:A:474:GLN:HE22	1:A:476:GLY:C	2.28	0.42
1:B:187:LYS:HD3	1:B:210:ILE:O	2.20	0.42
1:C:388:ASN:O	1:C:526:GLY:HA3	2.20	0.42
1:C:454:ARG:HA	1:C:492:LEU:HD23	2.01	0.42
2:H:35:HIS:NE2	2:H:95:GLU:OE1	2.53	0.42
2:M:98:PRO:O	2:M:100:ASP:N	2.53	0.42
1:A:204:TYR:CE2	1:A:225:PRO:HB3	2.55	0.42
1:A:308:VAL:HG12	1:A:602:THR:HG23	2.00	0.42
1:A:869:MET:HE3	1:A:869:MET:HB2	1.96	0.42
1:B:84:LEU:O	1:B:238:PHE:HB3	2.20	0.42
1:B:1080:ALA:C	1:B:1132:ILE:HG13	2.45	0.42
1:C:125:ASN:HD22	5:C:1302:NAG:C7	2.31	0.42
1:C:541:PHE:CD2	1:C:549:THR:HA	2.54	0.42
1:C:676:THR:HG22	1:C:690:GLN:HG2	2.01	0.42
2:H:82:MET:HG3	2:H:82(C):LEU:CD2	2.46	0.42
3:L:12:SER:OG	3:L:105:GLU:HB2	2.19	0.42
2:M:13:GLN:HB2	2:M:16:ARG:HH11	1.84	0.42
3:N:83:PHE:HD1	3:N:104:VAL:HG12	1.82	0.42
2:O:82:MET:SD	2:O:82:MET:N	2.92	0.42
1:A:141:LEU:O	1:A:243:ALA:HA	2.20	0.41
1:A:358:ILE:HB	1:A:395:VAL:CG2	2.50	0.41
1:A:388:ASN:OD1	1:A:527:PRO:HD2	2.20	0.41
1:A:394:ASN:HB3	1:A:516:GLU:OE2	2.20	0.41
1:B:323:THR:HG1	1:B:324:GLU:CD	2.24	0.41
1:B:353:TRP:HE3	1:B:354:ASN:O	2.03	0.41
1:C:1095:PHE:CE2	1:C:1115:ILE:HD12	2.55	0.41
1:B:216:LEU:HA	1:B:217:PRO:HD3	1.93	0.41
1:C:125:ASN:ND2	5:C:1302:NAG:H81	2.34	0.41
1:C:199:GLY:O	1:C:200:TYR:HD1	2.03	0.41
2:H:83:ARG:HD2	2:H:85:GLU:OE2	2.19	0.41
2:M:100(G):PHE:HB2	3:N:36:TYR:OH	2.20	0.41
1:A:78:ARG:HB2	1:A:79:PHE:H	1.73	0.41
1:B:717:ASN:OD1	1:B:718:PHE:N	2.52	0.41
1:C:206:LYS:HA	1:C:206:LYS:HD2	1.81	0.41
1:C:455:LEU:N	1:C:491:PRO:O	2.46	0.41
1:C:543:PHE:HB2	1:C:546:LEU:HD12	2.02	0.41
1:C:947:LYS:HB2	1:C:947:LYS:HE3	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1080:ALA:O	1:C:1132:ILE:HG13	2.21	0.41
2:M:47:TRP:HZ2	2:M:50:VAL:HB	1.85	0.41
3:N:19:VAL:HG11	3:N:78:LEU:HD21	2.02	0.41
2:O:82:MET:HE2	2:O:82:MET:HB2	1.97	0.41
1:A:114:THR:C	1:A:132:GLU:HG2	2.45	0.41
1:A:273:ARG:HG2	1:A:273:ARG:HH11	1.84	0.41
1:B:546:LEU:CD2	1:B:565:PHE:CZ	2.97	0.41
1:C:56:LEU:HD12	1:C:57:PRO:HD2	2.02	0.41
3:N:24:ARG:HA	3:N:69:THR:O	2.20	0.41
1:A:206:LYS:HA	1:A:206:LYS:HD2	1.76	0.41
1:A:231:ILE:HG22	1:A:233:ILE:HG13	2.01	0.41
1:B:36:VAL:HB	1:B:220:PHE:CE1	2.55	0.41
1:B:311:GLY:HA2	1:B:664:ILE:HD12	2.03	0.41
1:B:787:GLN:OE1	1:C:703:ASN:ND2	2.41	0.41
1:C:416:GLY:N	1:C:419:ALA:HB3	2.36	0.41
3:L:29:ILE:HG13	3:L:30:SER:N	2.36	0.41
3:N:29:ILE:HG13	3:N:30:SER:N	2.36	0.41
3:N:97:THR:HG22	3:N:98:PHE:N	2.35	0.41
1:A:453:TYR:CD1	1:A:495:TYR:CE1	3.08	0.41
1:A:517:LEU:HD23	1:A:517:LEU:HA	1.83	0.41
1:A:1018:ILE:HD13	1:A:1018:ILE:HA	1.81	0.41
1:B:119:ILE:HG12	1:B:128:ILE:HG22	2.02	0.41
1:B:493:GLN:HG3	1:B:494:SER:O	2.21	0.41
1:B:529:LYS:HG3	1:B:529:LYS:O	2.21	0.41
1:B:1127:ASP:OD1	1:B:1128:VAL:HG23	2.21	0.41
1:C:470:THR:CG2	1:C:492:LEU:CD1	2.81	0.41
1:C:474:GLN:HE22	1:C:476:GLY:C	2.29	0.41
2:M:50:VAL:CG1	2:M:58:TYR:HB2	2.51	0.41
2:O:19:ARG:HH21	2:O:79:TYR:HB3	1.85	0.41
1:A:68:ILE:H	1:A:68:ILE:HG12	1.62	0.41
1:B:455:LEU:N	1:B:491:PRO:O	2.35	0.41
1:B:763:LEU:HD23	1:B:1004:LEU:HD22	2.02	0.41
1:C:60:SER:OG	1:C:61:ASN:N	2.54	0.41
1:C:334:ASN:OD1	1:C:334:ASN:O	2.39	0.41
1:C:440:ASN:OD1	3:L:52:SER:HB2	2.20	0.41
2:H:45:LEU:HD11	3:L:98:PHE:CG	2.55	0.41
3:N:4:LEU:HB2	3:N:98:PHE:O	2.21	0.41
3:N:4:LEU:HD23	3:N:4:LEU:HA	1.88	0.41
3:N:54:LEU:HD23	3:N:55:GLN:O	2.21	0.41
2:O:39:GLN:O	2:O:89:VAL:N	2.48	0.41
2:O:61:ASP:HA	2:O:64:LYS:CG	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:VAL:HG23	1:A:781:VAL:HG21	2.01	0.41
1:A:730:SER:O	1:A:1058:HIS:HB3	2.20	0.41
1:A:908:GLY:O	1:A:1038:LYS:NZ	2.54	0.41
1:B:897:PRO:HD2	1:B:900:MET:HE3	2.02	0.41
1:B:945:LEU:HD11	1:B:948:LEU:HD12	2.03	0.41
1:C:1084:ASP:HB2	1:C:1086:LYS:NZ	2.36	0.41
3:L:78:LEU:HD21	3:L:83:PHE:CE1	2.55	0.41
3:P:34:ASN:HB2	3:P:89:GLN:HB3	2.03	0.41
1:A:100:ILE:HD13	1:A:100:ILE:HA	1.92	0.41
1:A:104:TRP:HD1	1:A:238:PHE:HE1	1.69	0.41
1:A:216:LEU:HA	1:A:216:LEU:HD23	1.80	0.41
1:A:437:ASN:HB3	1:A:508:TYR:CE1	2.55	0.41
1:A:473:TYR:HB3	1:A:489:TYR:O	2.21	0.41
1:B:91:TYR:HD1	1:B:193:VAL:HG22	1.86	0.41
1:B:108:THR:OG1	1:B:234:ASN:OD1	2.39	0.41
1:B:130:VAL:HG23	1:B:167:THR:OG1	2.21	0.41
1:B:206:LYS:HG3	1:B:208:THR:HG23	2.03	0.41
1:B:296:LEU:HB2	1:B:608:VAL:HG21	2.02	0.41
1:B:443:SER:HB2	1:B:497:PHE:C	2.45	0.41
1:B:477:SER:C	1:B:479:PRO:HD2	2.46	0.41
1:C:394:ASN:O	1:C:516:GLU:HG2	2.21	0.41
1:C:394:ASN:HB3	1:C:516:GLU:OE2	2.21	0.41
3:L:2:ILE:HA	3:L:26:SER:OG	2.20	0.41
3:L:85:THR:HA	3:L:103:LYS:HA	2.02	0.41
2:M:60:ALA:O	2:M:64:LYS:HG3	2.21	0.41
3:N:29:ILE:HG13	3:N:30:SER:H	1.86	0.41
1:A:393:THR:HA	1:A:522:ALA:HA	2.03	0.41
1:A:401:VAL:HG22	1:A:509:ARG:HG2	2.02	0.41
1:A:921:LYS:HE2	1:A:921:LYS:HB2	1.89	0.41
1:A:973:ILE:HG21	1:A:980:ILE:HD13	2.04	0.41
1:B:328:ARG:NH1	1:B:531:THR:O	2.50	0.41
1:B:599:THR:OG1	1:B:600:PRO:O	2.37	0.41
1:B:920:GLN:CD	1:C:1130:ILE:HD11	2.46	0.41
1:C:280:ASN:OD1	1:C:281:GLU:N	2.49	0.41
1:C:393:THR:HG21	1:C:518:LEU:HB2	2.03	0.41
1:C:461:LEU:HD11	1:C:465:GLU:HG3	2.03	0.41
1:C:1043:CYS:HB3	1:C:1048:HIS:CD2	2.55	0.41
2:H:31:ILE:O	2:H:31:ILE:HG13	2.21	0.41
2:H:51:ILE:HG22	2:H:57:LYS:HB2	2.03	0.41
2:H:70:SER:O	2:H:78:LEU:HD12	2.20	0.41
2:O:52:SER:OG	2:O:56:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ILE:HG13	1:B:232:GLY:H	1.85	0.40
1:B:906:PHE:HD2	1:B:916:LEU:HB2	1.85	0.40
1:C:935:GLN:O	1:C:939:SER:N	2.40	0.40
2:H:34:MET:HB3	2:H:78:LEU:HD22	2.03	0.40
2:M:75:LYS:O	2:M:75:LYS:HD3	2.20	0.40
3:N:5:THR:HG21	3:N:24:ARG:HH22	1.86	0.40
2:O:50:VAL:CG1	2:O:58:TYR:HB2	2.51	0.40
3:P:32:TYR:CD2	3:P:92:TYR:HA	2.57	0.40
1:A:474:GLN:OE1	1:A:476:GLY:N	2.53	0.40
1:A:483:VAL:HG23	1:A:483:VAL:O	2.22	0.40
1:B:280:ASN:ND2	5:B:1303:NAG:H81	2.36	0.40
1:C:233:ILE:HB	1:C:235:ILE:HG13	2.02	0.40
1:C:886:TRP:CH2	1:C:904:TYR:HD2	2.39	0.40
2:H:38:ARG:HB3	2:H:90:TYR:CD2	2.57	0.40
2:M:20:LEU:O	2:M:79:TYR:HA	2.21	0.40
2:O:31:ILE:HG13	2:O:31:ILE:O	2.21	0.40
2:O:39:GLN:N	2:O:89:VAL:O	2.38	0.40
1:A:237:ARG:HH11	1:A:237:ARG:HG3	1.86	0.40
1:A:340:GLU:OE2	1:A:341:VAL:HG23	2.22	0.40
1:B:141:LEU:O	1:B:243:ALA:HA	2.21	0.40
1:B:365:TYR:CD2	1:B:387:LEU:HB3	2.50	0.40
1:B:392:PHE:CE2	1:B:517:LEU:HD12	2.55	0.40
1:B:401:VAL:HG22	1:B:509:ARG:HA	2.02	0.40
3:L:33:LEU:HD21	3:L:88:CYS:HB2	2.03	0.40
3:L:74:THR:O	3:L:75:ILE:HD13	2.22	0.40
1:A:82:PRO:O	1:A:84:LEU:HD12	2.21	0.40
1:A:805:ILE:HB	1:A:1054:GLN:NE2	2.36	0.40
1:B:204:TYR:CE2	1:B:225:PRO:HB3	2.56	0.40
1:B:287:ASP:OD2	1:B:288:ALA:N	2.54	0.40
1:C:344:ALA:HB3	1:C:347:PHE:CE1	2.56	0.40
1:C:369:TYR:C	1:C:371:SER:H	2.28	0.40
1:C:1009:THR:O	1:C:1013:ILE:HG12	2.21	0.40
2:H:10:GLY:O	2:H:110:THR:N	2.33	0.40
2:O:36:TRP:CD1	2:O:80:LEU:HD22	2.56	0.40
1:A:273:ARG:HH21	1:A:292:ALA:HB3	1.86	0.40
1:A:366:SER:HA	1:A:369:TYR:CE1	2.57	0.40
1:B:902:MET:HB3	1:B:916:LEU:HD11	2.03	0.40
1:B:921:LYS:HE2	1:B:921:LYS:HB3	1.83	0.40
1:B:973:ILE:HG12	1:B:992:GLN:HE21	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	988/1259 (78%)	914 (92%)	67 (7%)	7 (1%)	18	47
1	B	988/1259 (78%)	923 (93%)	63 (6%)	2 (0%)	43	71
1	C	988/1259 (78%)	923 (93%)	63 (6%)	2 (0%)	43	71
2	H	123/236 (52%)	108 (88%)	15 (12%)	0	100	100
2	M	123/236 (52%)	110 (89%)	13 (11%)	0	100	100
2	O	123/236 (52%)	114 (93%)	9 (7%)	0	100	100
3	L	105/214 (49%)	101 (96%)	4 (4%)	0	100	100
3	N	105/214 (49%)	100 (95%)	5 (5%)	0	100	100
3	P	105/214 (49%)	100 (95%)	5 (5%)	0	100	100
All	All	3648/5127 (71%)	3393 (93%)	244 (7%)	11 (0%)	37	65

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	472	ILE
1	C	445	VAL
1	A	68	ILE
1	A	445	VAL
1	B	471	GLU
1	A	488	CYS
1	A	532	ASN
1	A	79	PHE
1	B	445	VAL
1	C	472	ILE
1	A	85	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	878/1096 (80%)	873 (99%)	5 (1%)	78	80
1	B	878/1096 (80%)	875 (100%)	3 (0%)	86	84
1	C	878/1096 (80%)	875 (100%)	3 (0%)	86	84
2	H	102/200 (51%)	102 (100%)	0	100	100
2	M	102/200 (51%)	102 (100%)	0	100	100
2	O	102/200 (51%)	102 (100%)	0	100	100
3	L	93/189 (49%)	93 (100%)	0	100	100
3	N	93/189 (49%)	93 (100%)	0	100	100
3	P	93/189 (49%)	93 (100%)	0	100	100
All	All	3219/4455 (72%)	3208 (100%)	11 (0%)	84	84

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ILE
1	A	78	ARG
1	A	445	VAL
1	A	547	THR
1	A	895	GLN
1	B	68	ILE
1	B	78	ARG
1	B	445	VAL
1	C	445	VAL
1	C	470	THR
1	C	547	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	207	HIS

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Mol	Chain	Res	Type
1	A	422	ASN
1	A	544	ASN
1	A	644	GLN
1	A	690	GLN
1	A	774	GLN
1	A	935	GLN
1	A	955	ASN
1	A	1005	GLN
1	A	1011	GLN
1	A	1036	GLN
1	B	87	ASN
1	B	115	GLN
1	B	317	ASN
1	B	437	ASN
1	B	439	ASN
1	B	532	ASN
1	B	563	GLN
1	B	564	GLN
1	B	804	GLN
1	B	901	GLN
1	B	914	ASN
1	B	935	GLN
1	B	1005	GLN
1	C	69	HIS
1	C	87	ASN
1	C	125	ASN
1	C	544	ASN
1	C	644	GLN
1	C	690	GLN
1	C	762	GLN
1	C	901	GLN
1	C	1011	GLN
2	H	81	GLN
3	L	38	GLN
3	L	90	GLN
2	M	35	HIS
2	M	56	ASN
3	N	90	GLN
2	O	39	GLN
2	O	81	GLN
3	P	34	ASN
3	P	55	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	$\# Z > 2$
4	NAG	D	1	4,1	14,14,15	0.22	0	17,19,21	0.39	0
4	NAG	D	2	4	14,14,15	0.39	0	17,19,21	0.51	0
4	NAG	E	1	4,1	14,14,15	0.50	0	17,19,21	0.52	0
4	NAG	E	2	4	14,14,15	0.19	0	17,19,21	0.48	0
4	NAG	F	1	4,1	14,14,15	0.47	0	17,19,21	0.44	0
4	NAG	F	2	4	14,14,15	0.19	0	17,19,21	0.45	0
4	NAG	G	1	4,1	14,14,15	0.29	0	17,19,21	0.51	0
4	NAG	G	2	4	14,14,15	0.22	0	17,19,21	0.36	0
4	NAG	I	1	4,1	14,14,15	0.29	0	17,19,21	0.47	0
4	NAG	I	2	4	14,14,15	0.15	0	17,19,21	0.55	0
4	NAG	J	1	4,1	14,14,15	0.49	0	17,19,21	0.79	1 (5%)
4	NAG	J	2	4	14,14,15	0.30	0	17,19,21	0.52	0
4	NAG	K	1	4,1	14,14,15	0.50	0	17,19,21	0.53	0
4	NAG	K	2	4	14,14,15	0.23	0	17,19,21	0.36	0
4	NAG	Q	1	4,1	14,14,15	0.52	0	17,19,21	0.40	0
4	NAG	Q	2	4	14,14,15	0.18	0	17,19,21	0.44	0
4	NAG	R	1	4,1	14,14,15	0.50	0	17,19,21	0.53	0
4	NAG	R	2	4	14,14,15	0.23	0	17,19,21	0.37	0
4	NAG	S	1	4,1	14,14,15	0.24	0	17,19,21	0.44	0
4	NAG	S	2	4	14,14,15	0.20	0	17,19,21	0.43	0
4	NAG	T	1	4,1	14,14,15	0.40	0	17,19,21	0.69	0
4	NAG	T	2	4	14,14,15	0.22	0	17,19,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	U	1	4,1	14,14,15	0.58	0	17,19,21	0.57	0
4	NAG	U	2	4	14,14,15	0.19	0	17,19,21	0.37	0
4	NAG	V	1	4,1	14,14,15	0.60	1 (7%)	17,19,21	0.45	0
4	NAG	V	2	4	14,14,15	0.20	0	17,19,21	0.45	0
4	NAG	W	1	4,1	14,14,15	0.22	0	17,19,21	0.50	0
4	NAG	W	2	4	14,14,15	0.23	0	17,19,21	0.37	0
4	NAG	X	1	4,1	14,14,15	0.19	0	17,19,21	0.55	0
4	NAG	X	2	4	14,14,15	0.37	0	17,19,21	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	NAG	I	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	NAG	J	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	1/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
4	NAG	S	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
4	NAG	T	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1
4	NAG	U	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	U	2	4	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	V	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1
4	NAG	W	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	W	2	4	-	2/6/23/26	0/1/1/1
4	NAG	X	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	X	2	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	1	NAG	O5-C1	-2.04	1.40	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	1	NAG	C1-O5-C5	2.58	115.64	112.19

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	X	1	NAG	O5-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	X	1	NAG	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6
4	V	1	NAG	C4-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	W	2	NAG	C4-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6

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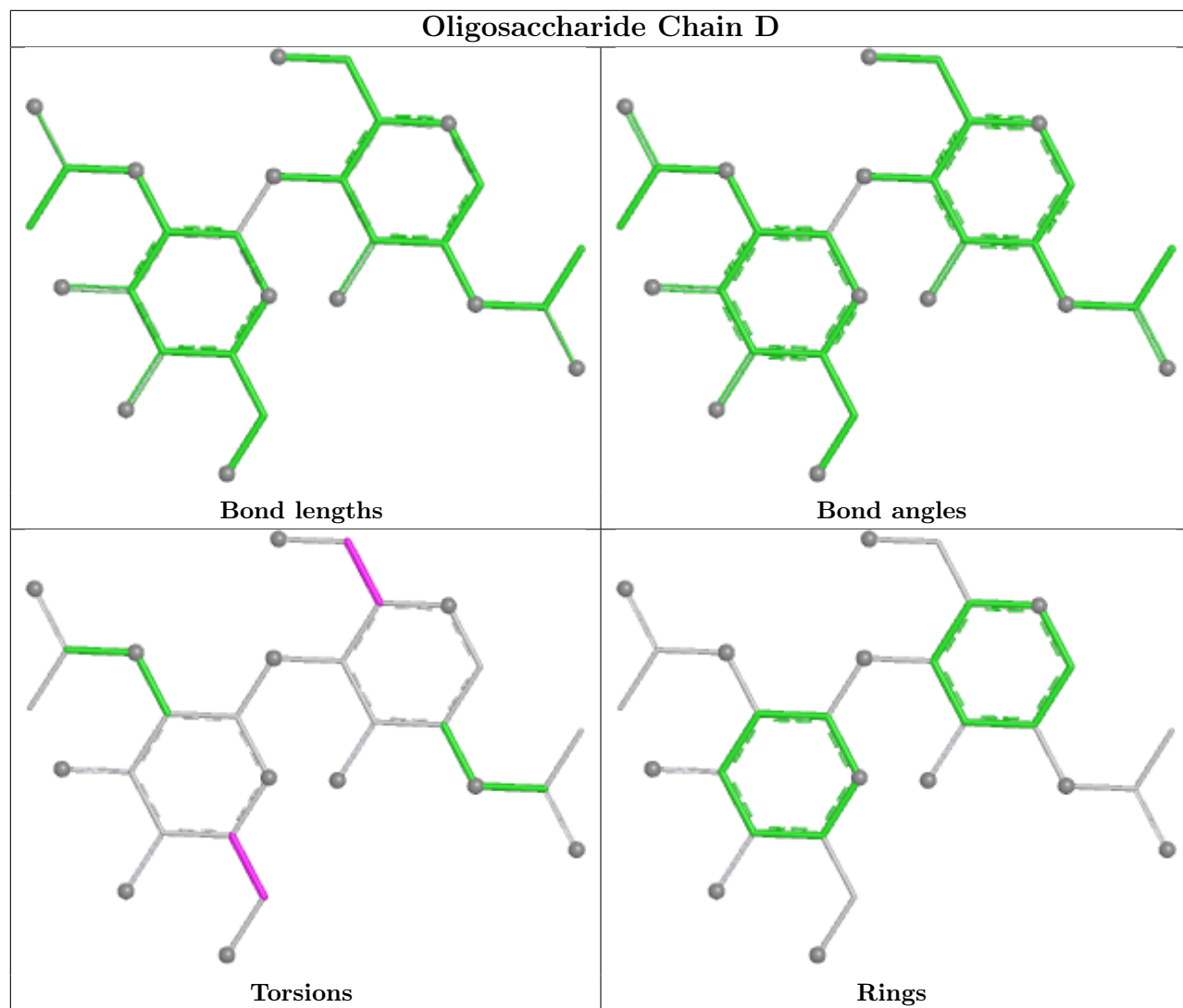
Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C4-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
4	V	2	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
4	J	1	NAG	C3-C2-N2-C7
4	J	2	NAG	C4-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6

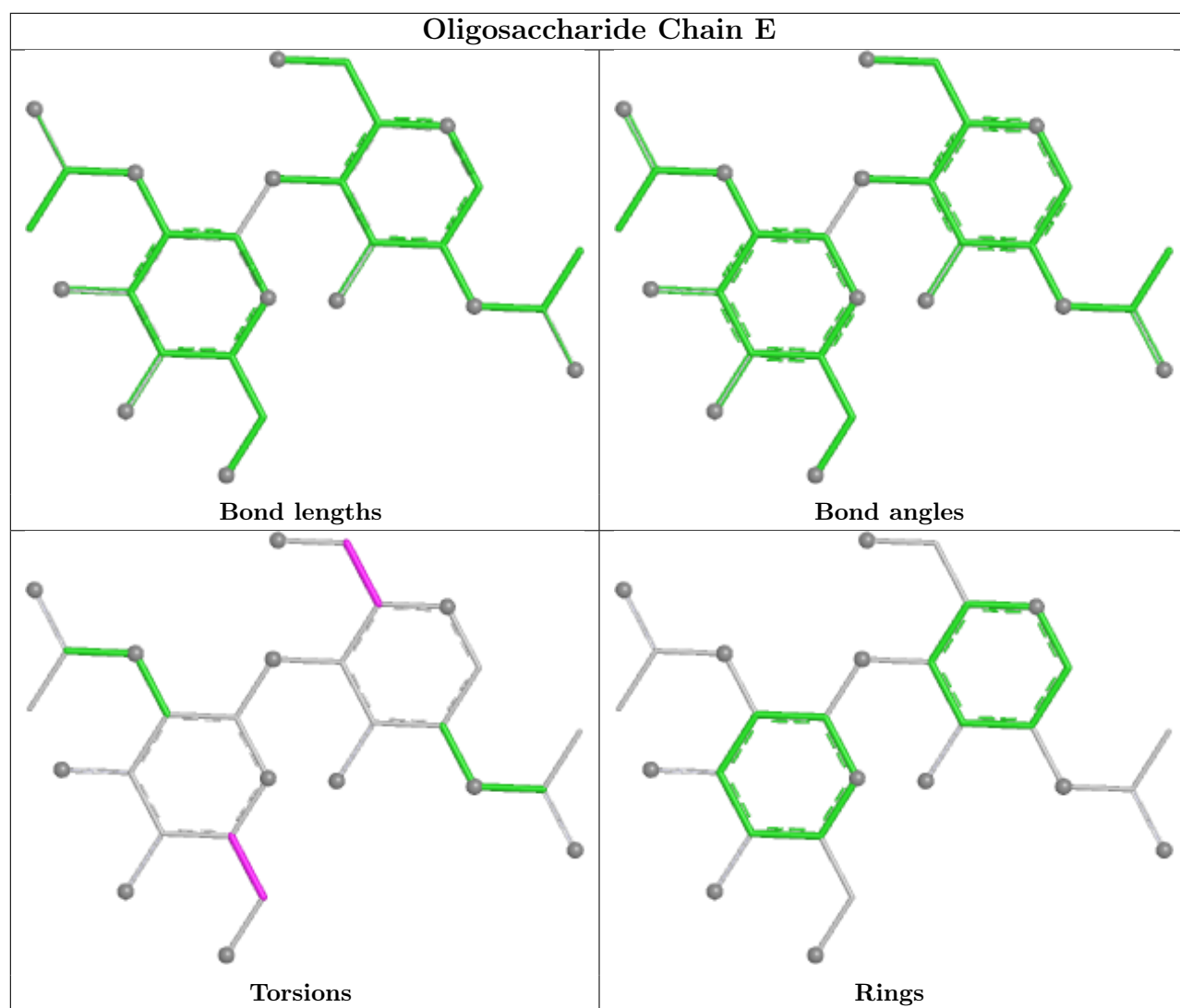
There are no ring outliers.

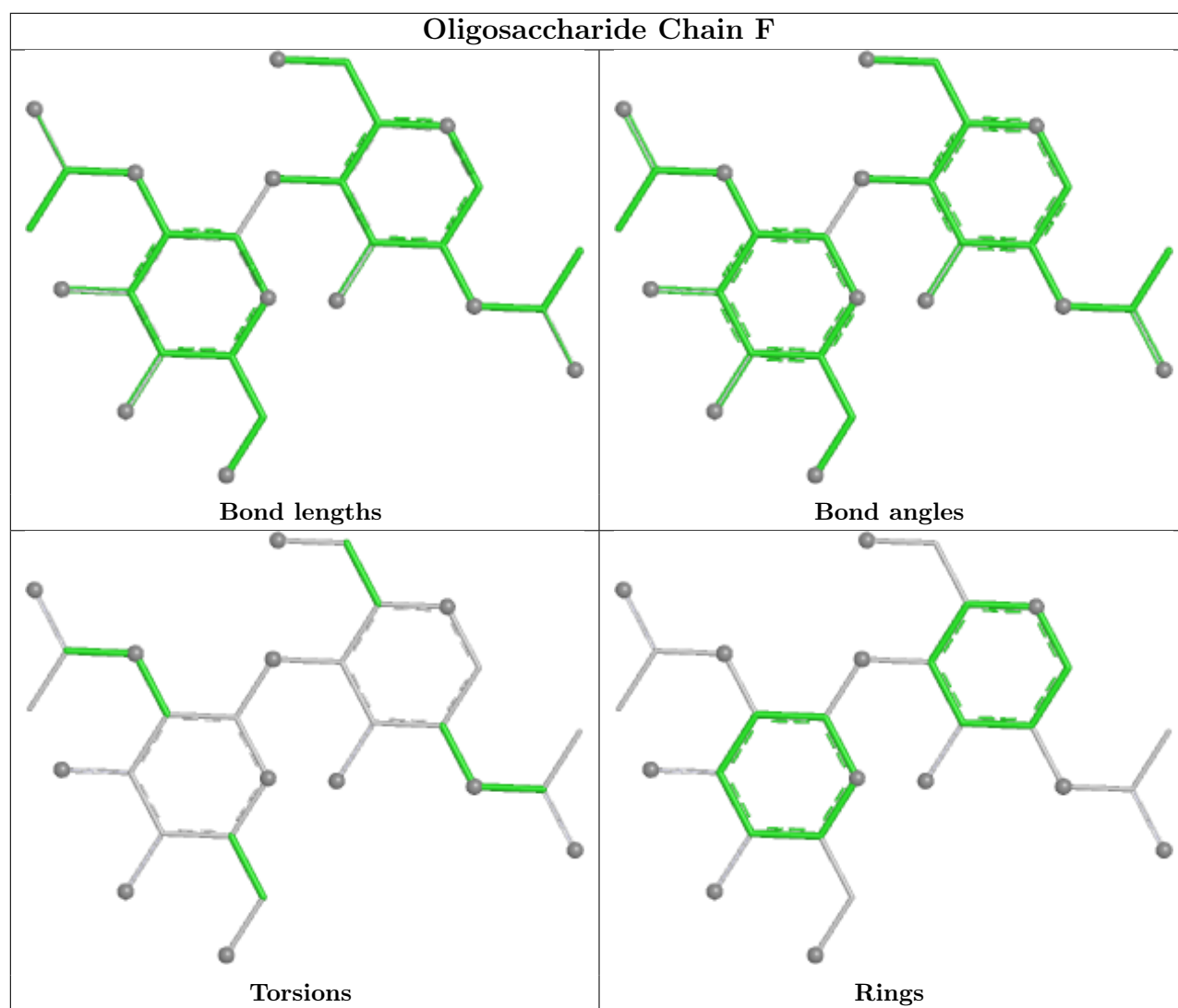
2 monomers are involved in 2 short contacts:

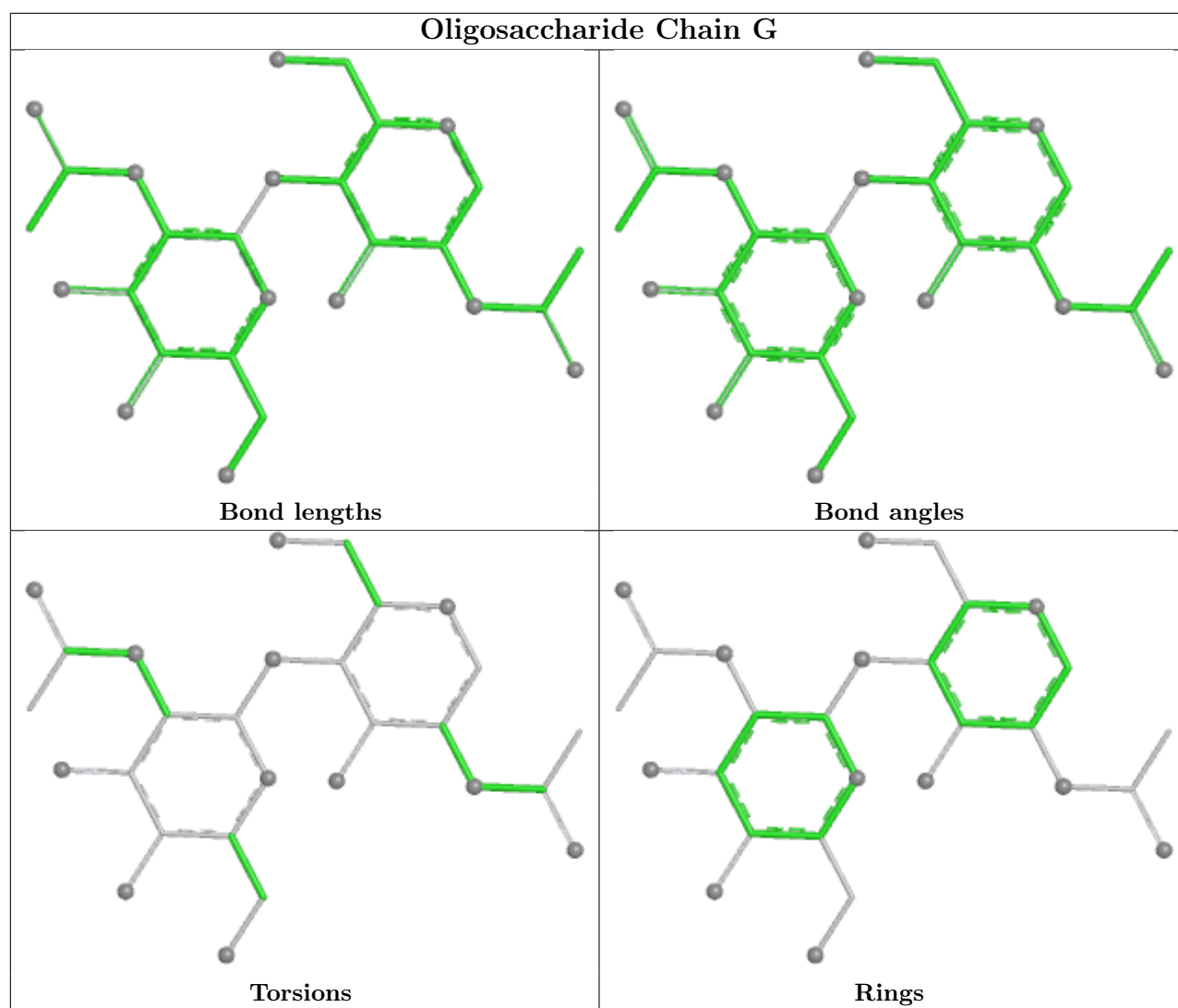
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	2	NAG	1	0
4	J	1	NAG	2	0

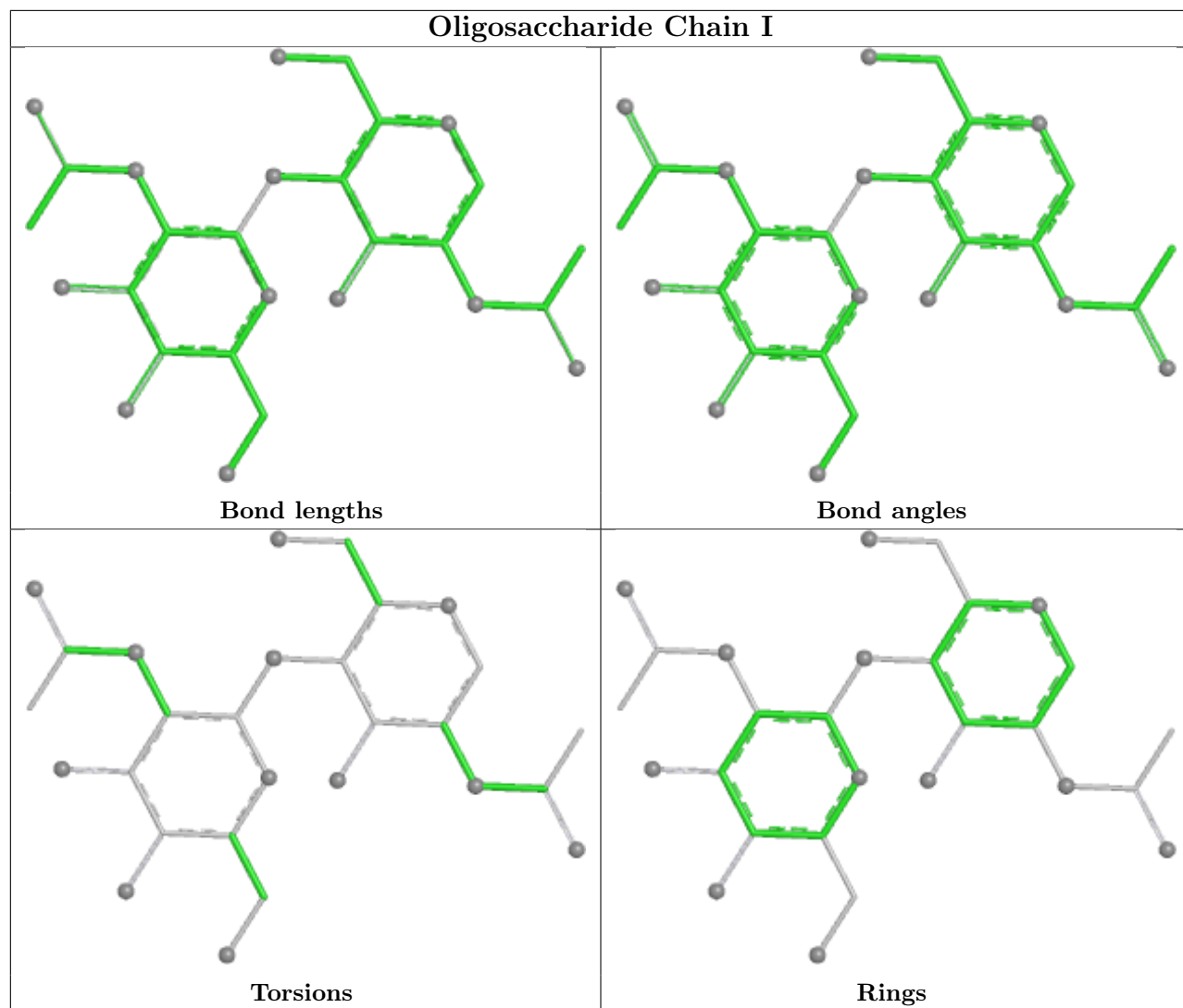
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

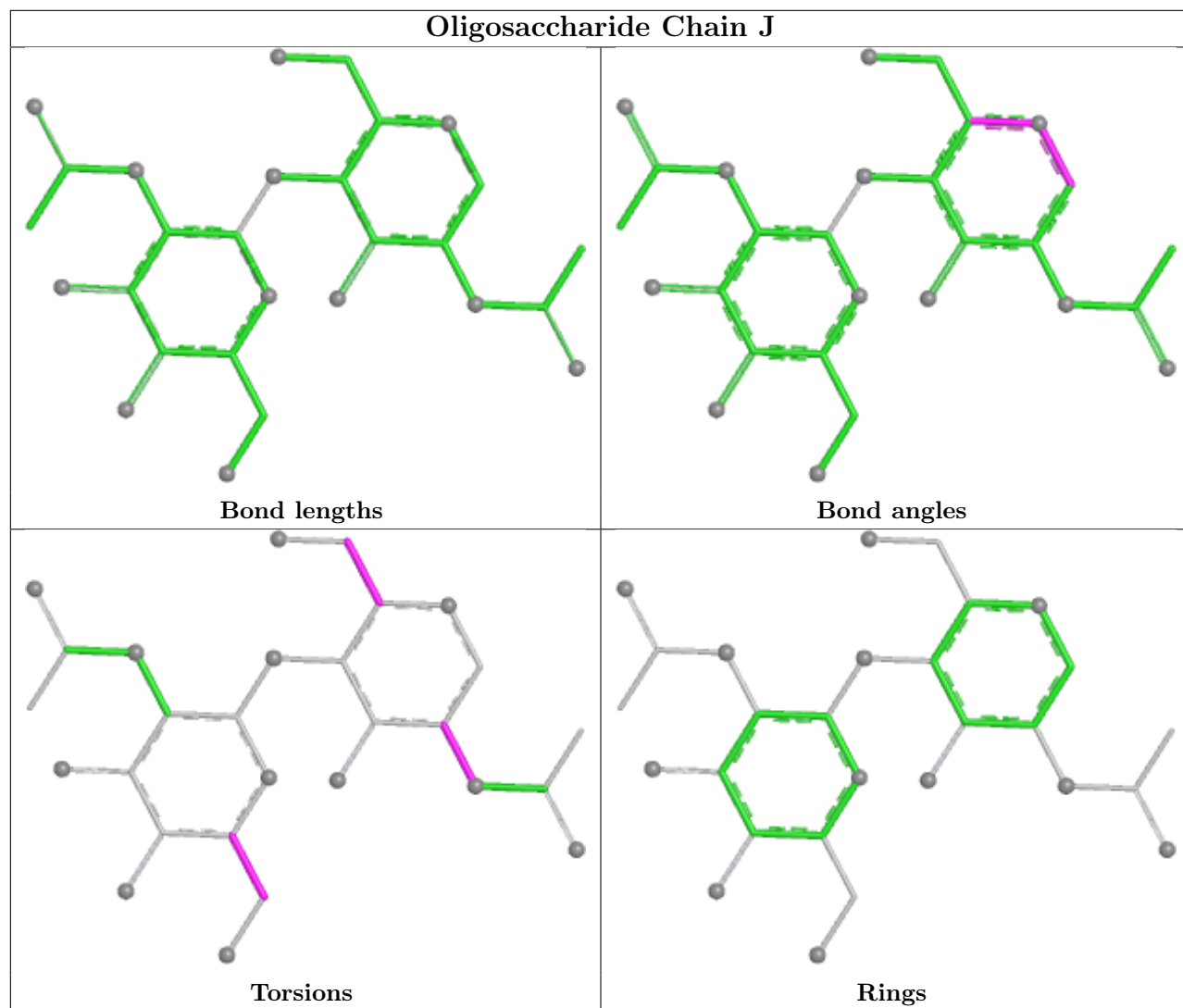


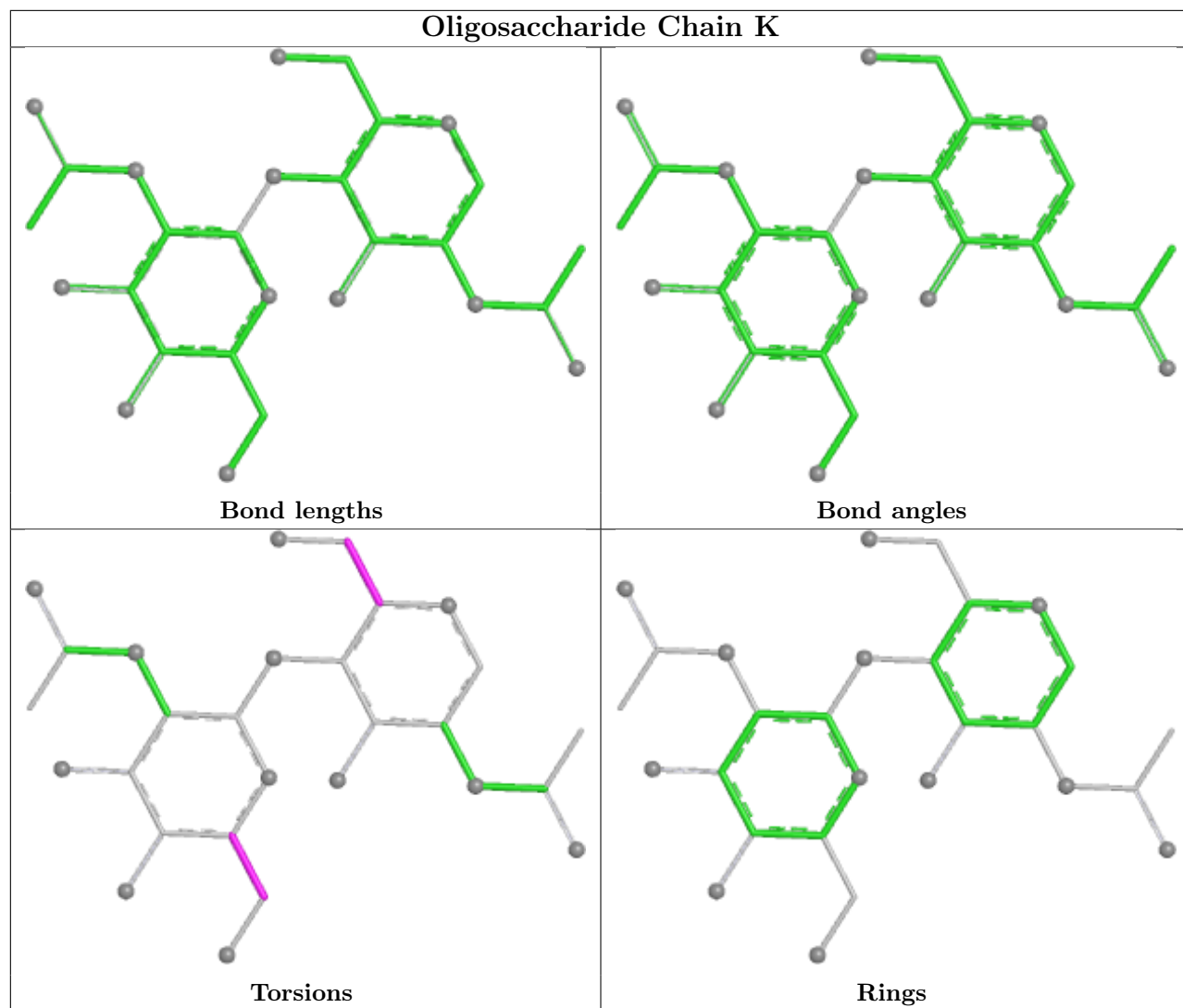


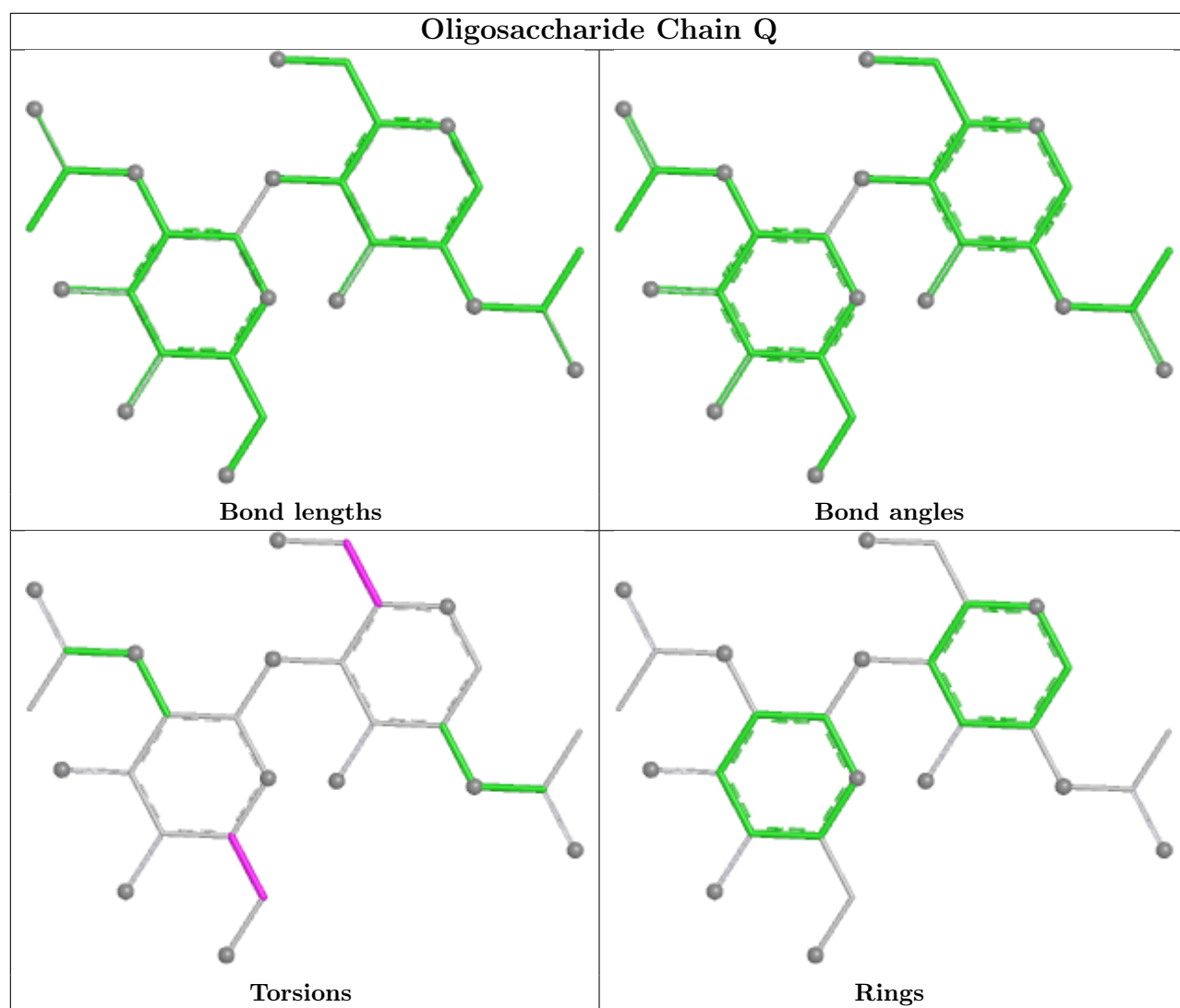


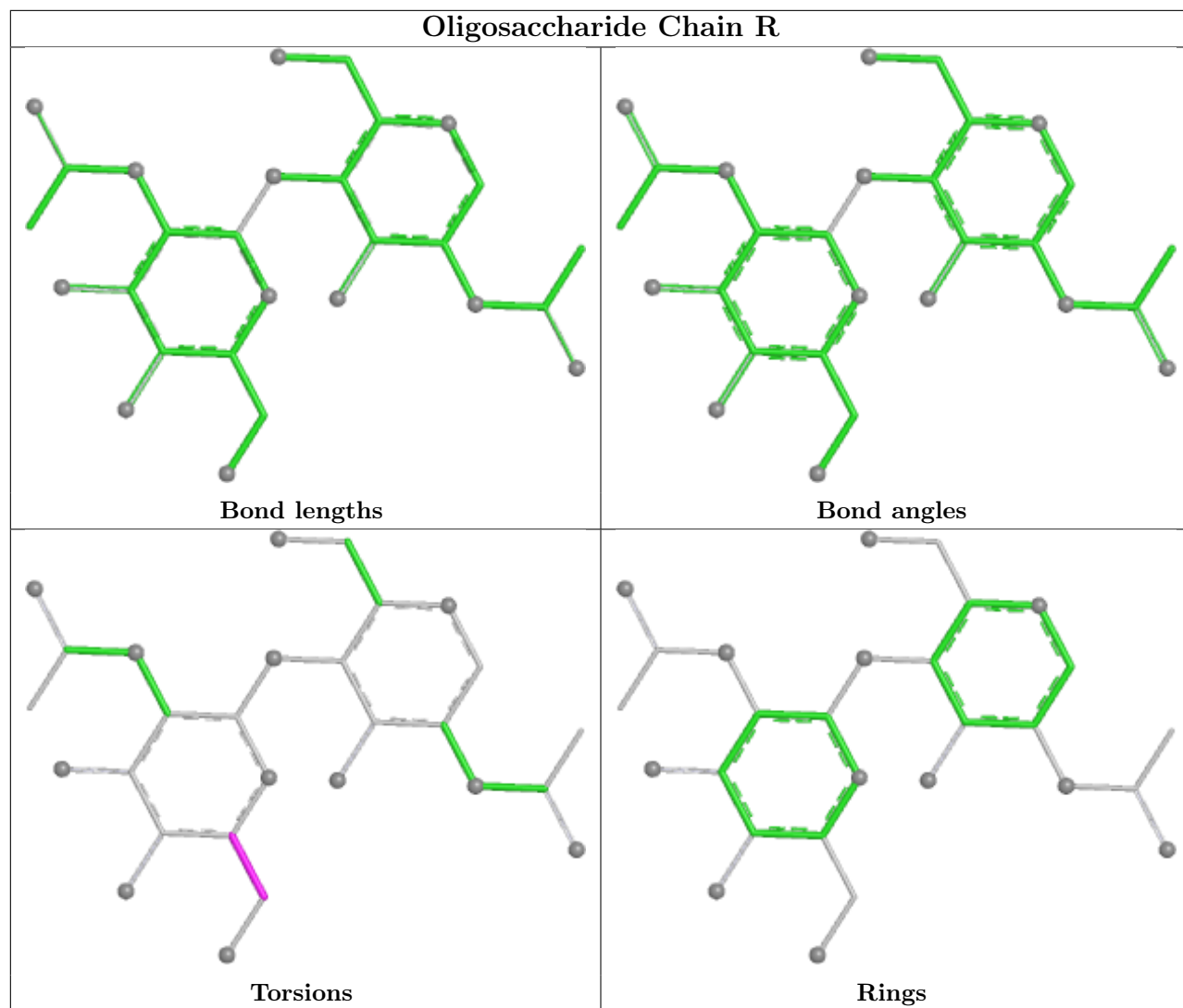


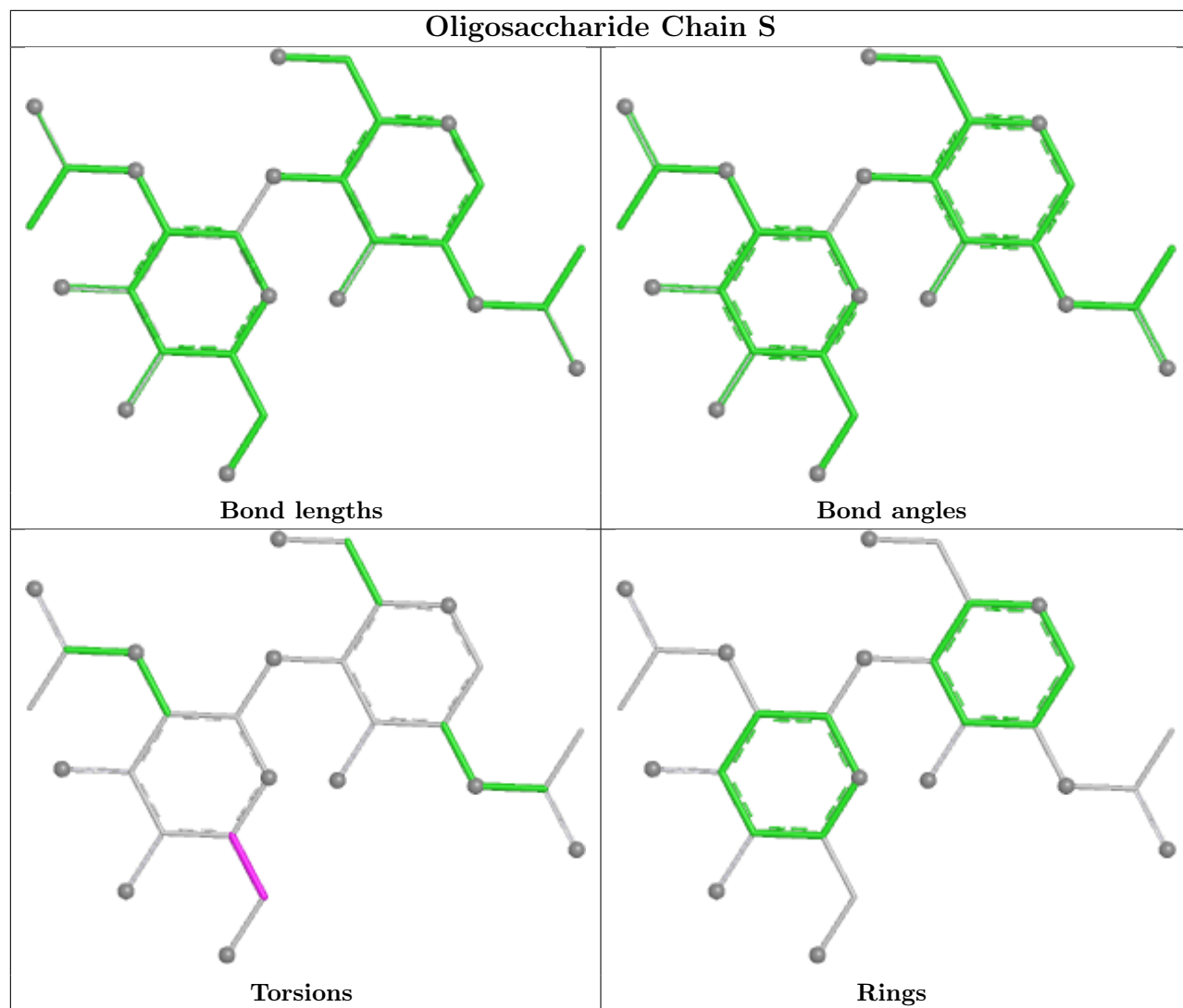


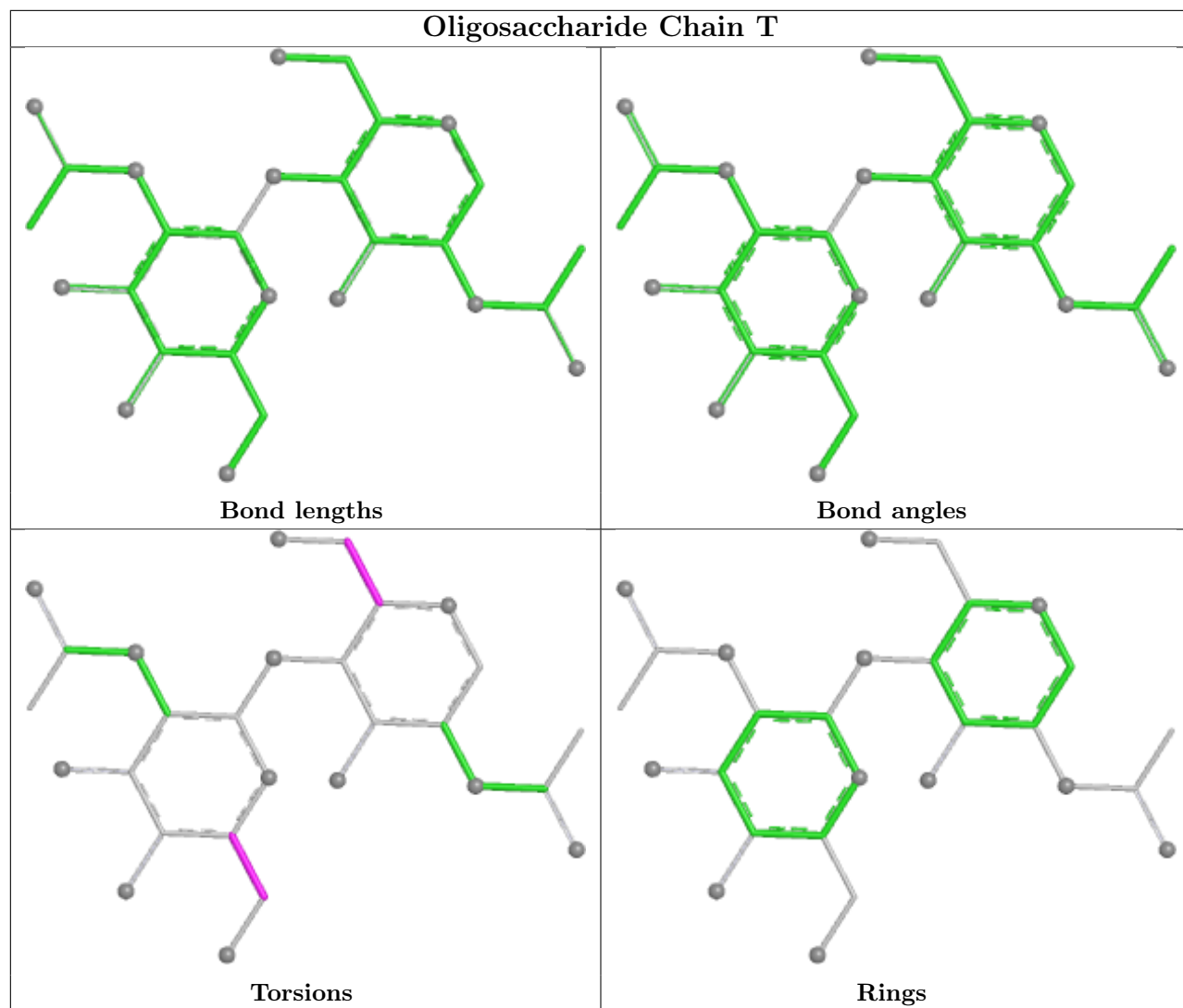


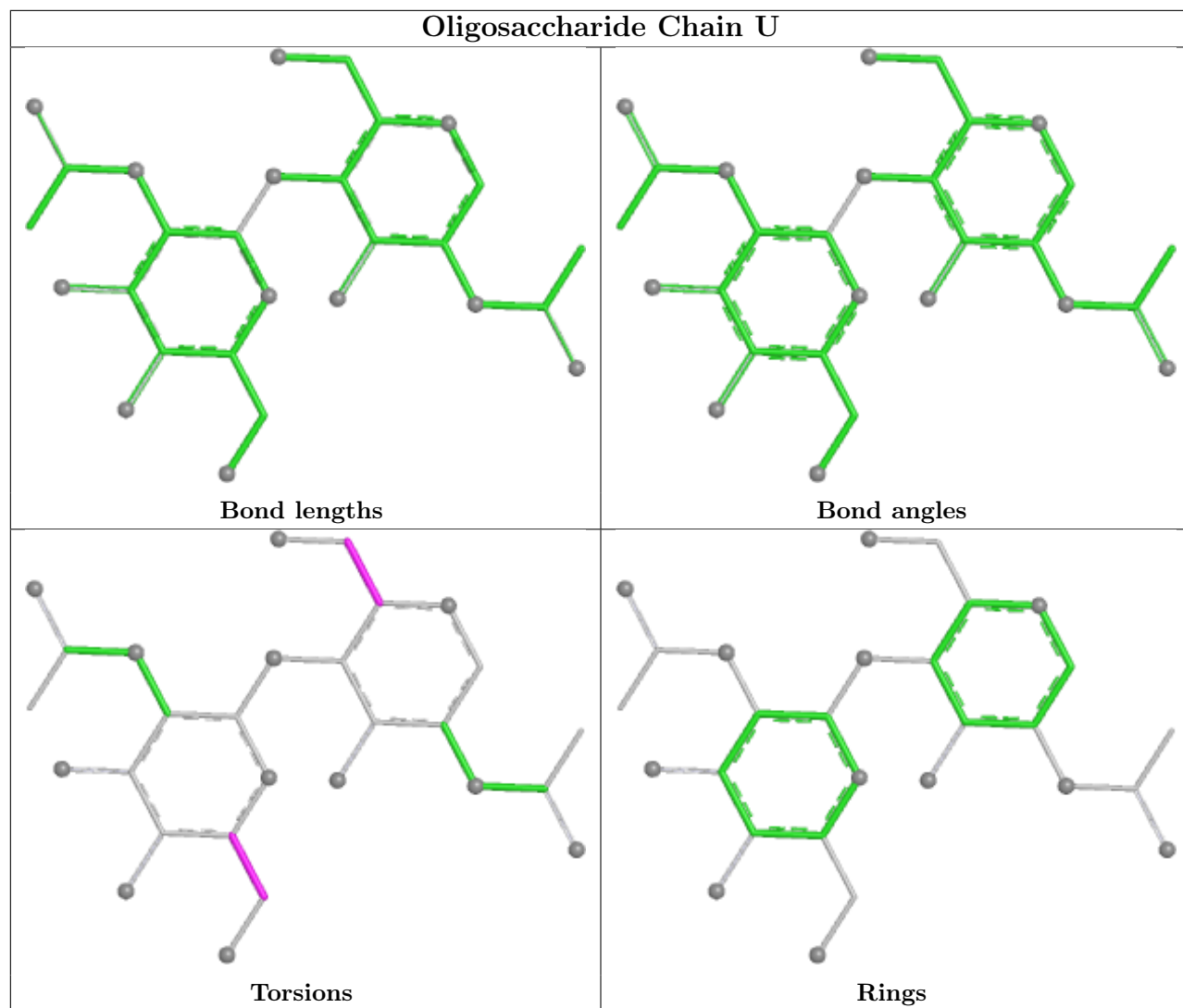


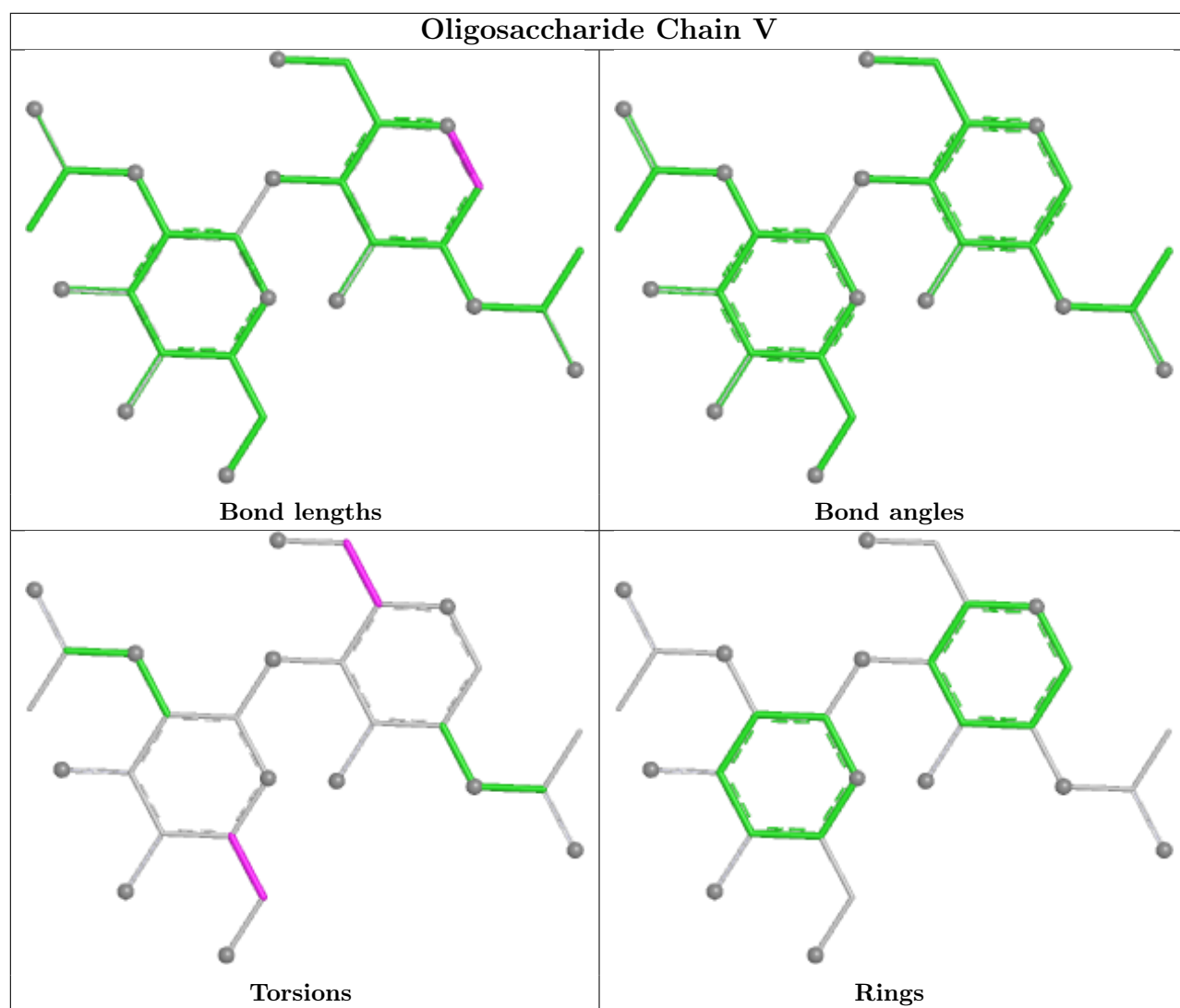


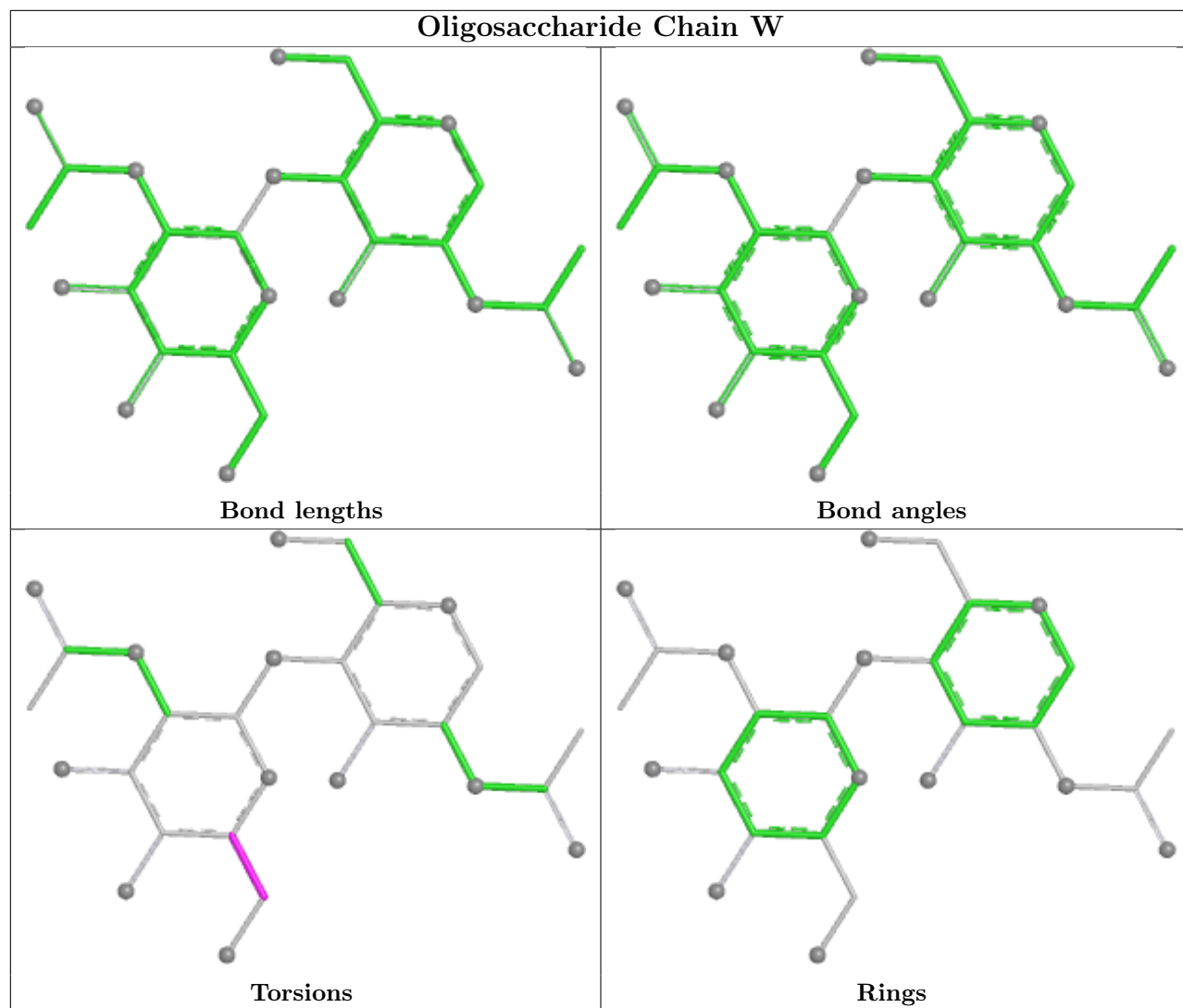


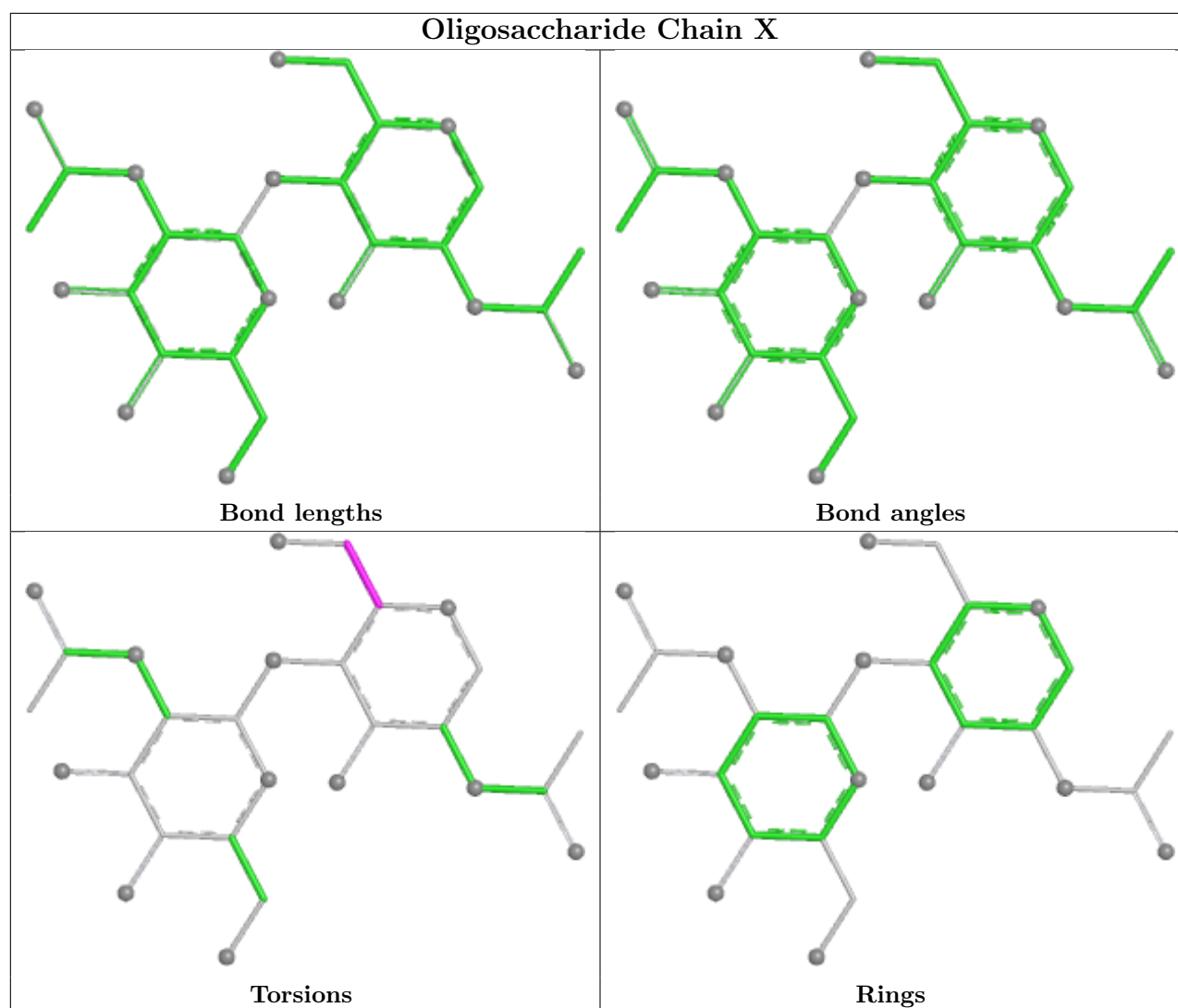












5.6 Ligand geometry [i](#)

27 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	C	1304	1	14,14,15	0.24	0	17,19,21	0.44	0
5	NAG	C	1302	1	14,14,15	0.19	0	17,19,21	0.52	0
5	NAG	A	1303	1	14,14,15	0.19	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1309	1	14,14,15	0.20	0	17,19,21	0.55	0
5	NAG	B	1308	1	14,14,15	0.19	0	17,19,21	0.53	0
5	NAG	C	1303	1	14,14,15	0.16	0	17,19,21	0.45	0
5	NAG	B	1301	1	14,14,15	0.21	0	17,19,21	0.50	0
5	NAG	B	1303	1	14,14,15	0.22	0	17,19,21	0.45	0
5	NAG	C	1307	1	14,14,15	0.27	0	17,19,21	0.41	0
5	NAG	C	1308	1	14,14,15	0.23	0	17,19,21	0.59	0
5	NAG	A	1302	1	14,14,15	0.38	0	17,19,21	0.61	0
5	NAG	C	1309	1	14,14,15	0.22	0	17,19,21	0.47	0
5	NAG	A	1305	1	14,14,15	0.15	0	17,19,21	0.54	0
5	NAG	C	1305	1	14,14,15	0.23	0	17,19,21	0.51	0
5	NAG	C	1301	1	14,14,15	0.30	0	17,19,21	0.39	0
5	NAG	A	1304	1	14,14,15	0.17	0	17,19,21	0.51	0
5	NAG	C	1306	1	14,14,15	0.15	0	17,19,21	0.58	0
5	NAG	B	1306	1	14,14,15	0.26	0	17,19,21	0.40	0
5	NAG	B	1309	1	14,14,15	0.31	0	17,19,21	0.49	0
5	NAG	A	1301	1	14,14,15	0.31	0	17,19,21	0.40	0
5	NAG	B	1307	1	14,14,15	0.25	0	17,19,21	0.39	0
5	NAG	A	1308	1	14,14,15	0.26	0	17,19,21	0.48	0
5	NAG	B	1305	1	14,14,15	0.21	0	17,19,21	0.55	0
5	NAG	A	1306	1	14,14,15	0.16	0	17,19,21	0.49	0
5	NAG	B	1302	1	14,14,15	0.38	0	17,19,21	0.52	0
5	NAG	A	1307	1	14,14,15	0.25	0	17,19,21	0.38	0
5	NAG	B	1304	1	14,14,15	0.45	0	17,19,21	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1309	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1307	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1308	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1302	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1309	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1308	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1304	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1306	NAG	O5-C5-C6-O6
5	C	1304	NAG	O5-C5-C6-O6
5	A	1307	NAG	O5-C5-C6-O6
5	B	1308	NAG	O5-C5-C6-O6
5	C	1308	NAG	O5-C5-C6-O6
5	A	1303	NAG	O5-C5-C6-O6
5	A	1307	NAG	C4-C5-C6-O6
5	B	1307	NAG	C4-C5-C6-O6
5	C	1306	NAG	C4-C5-C6-O6
5	C	1305	NAG	O5-C5-C6-O6
5	A	1304	NAG	C4-C5-C6-O6
5	C	1304	NAG	C4-C5-C6-O6
5	C	1305	NAG	C4-C5-C6-O6
5	A	1304	NAG	O5-C5-C6-O6
5	B	1307	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	C	1309	NAG	O5-C5-C6-O6
5	A	1303	NAG	C4-C5-C6-O6
5	B	1308	NAG	C4-C5-C6-O6
5	C	1309	NAG	C4-C5-C6-O6
5	C	1307	NAG	C4-C5-C6-O6
5	C	1308	NAG	C4-C5-C6-O6
5	B	1303	NAG	O5-C5-C6-O6
5	B	1306	NAG	O5-C5-C6-O6
5	B	1309	NAG	O5-C5-C6-O6
5	A	1302	NAG	O5-C5-C6-O6
5	C	1307	NAG	O5-C5-C6-O6
5	A	1306	NAG	O5-C5-C6-O6
5	A	1308	NAG	O5-C5-C6-O6
5	C	1302	NAG	O5-C5-C6-O6
5	A	1309	NAG	O5-C5-C6-O6
5	C	1303	NAG	O5-C5-C6-O6
5	B	1302	NAG	O5-C5-C6-O6
5	B	1303	NAG	C4-C5-C6-O6
5	B	1306	NAG	C4-C5-C6-O6
5	A	1302	NAG	C1-C2-N2-C7
5	C	1302	NAG	C1-C2-N2-C7
5	B	1302	NAG	C3-C2-N2-C7
5	A	1302	NAG	C4-C5-C6-O6
5	A	1306	NAG	C4-C5-C6-O6
5	B	1304	NAG	O5-C5-C6-O6
5	B	1302	NAG	C1-C2-N2-C7
5	C	1307	NAG	C1-C2-N2-C7
5	A	1302	NAG	C3-C2-N2-C7
5	C	1302	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1302	NAG	2	0
5	B	1303	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

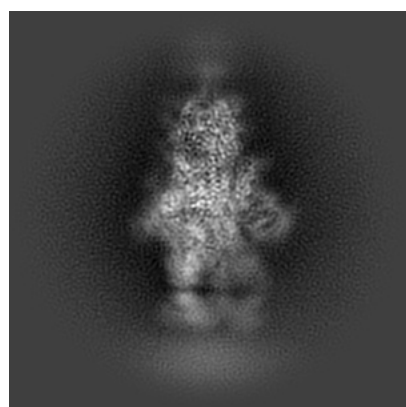
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22729. These allow visual inspection of the internal detail of the map and identification of artifacts.

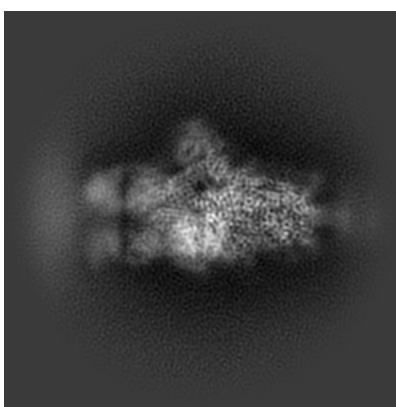
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

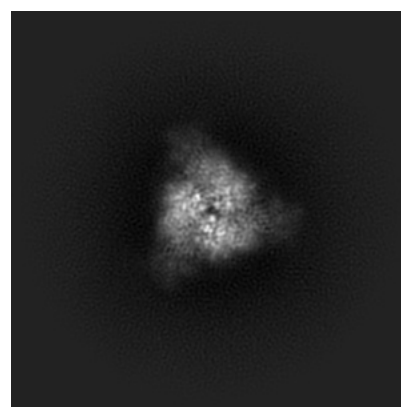
6.1.1 Primary map



X



Y

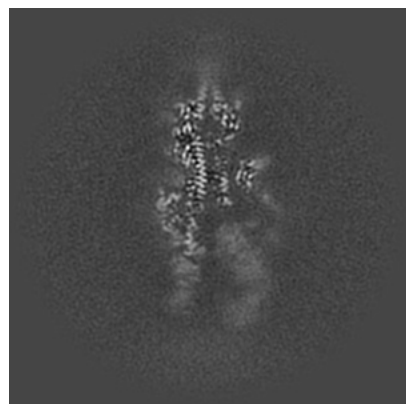


Z

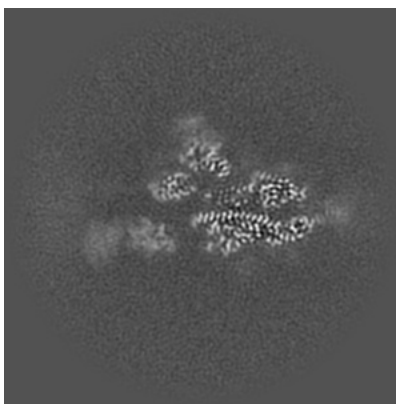
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

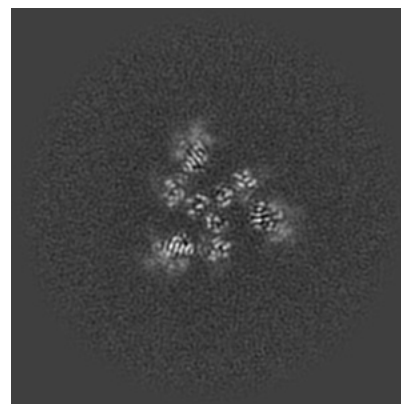
6.2.1 Primary map



X Index: 216



Y Index: 216

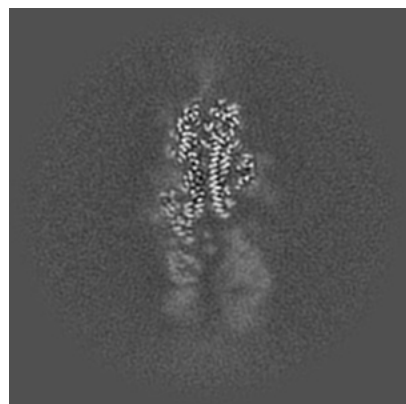


Z Index: 216

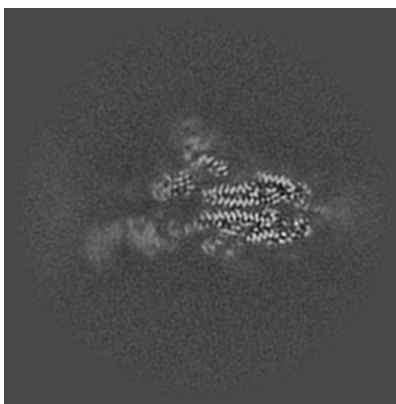
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

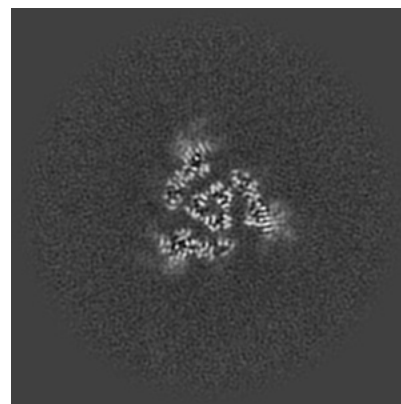
6.3.1 Primary map



X Index: 223



Y Index: 220

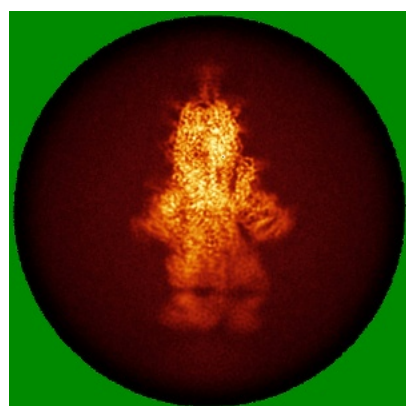


Z Index: 221

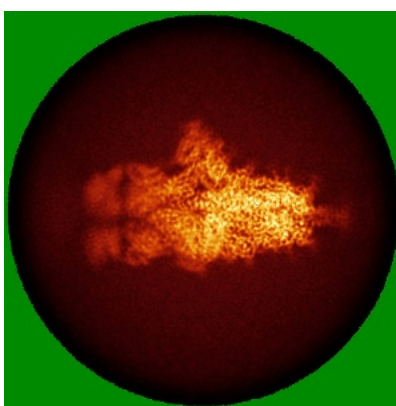
The images above show the largest variance slices of the map in three orthogonal directions.

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

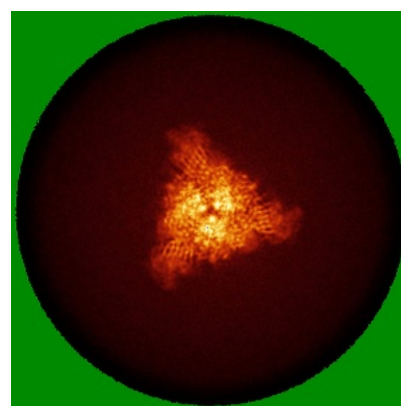
6.4.1 Primary map



X



Y

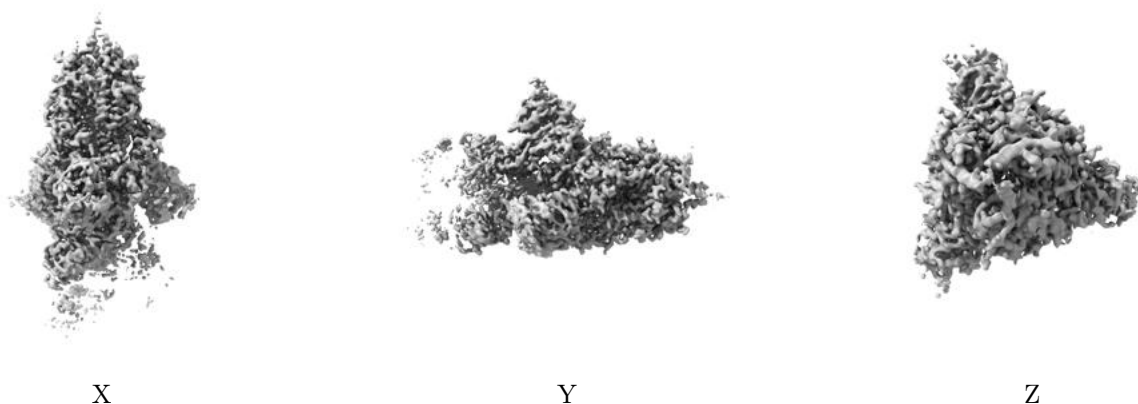


Z

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 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

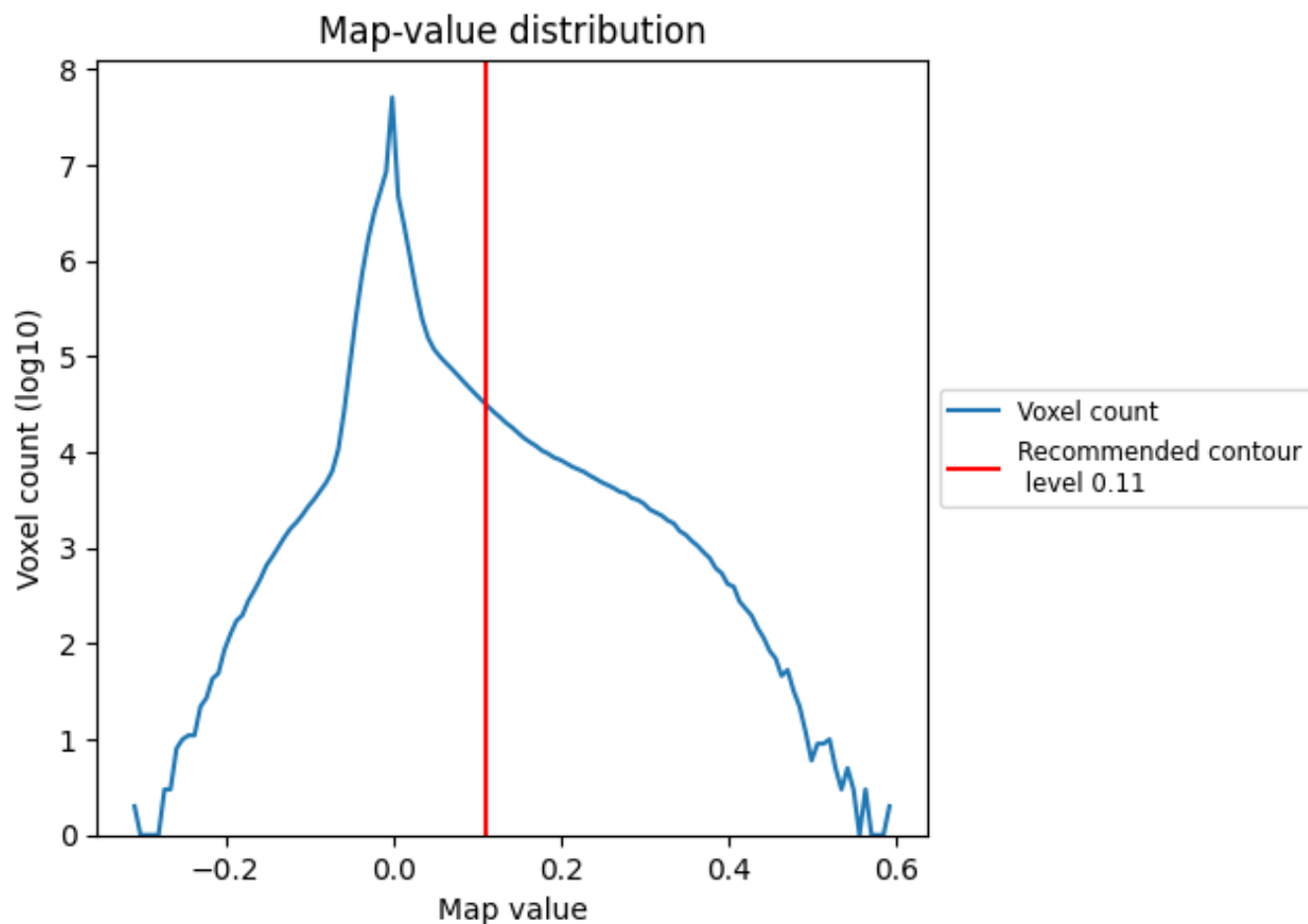
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

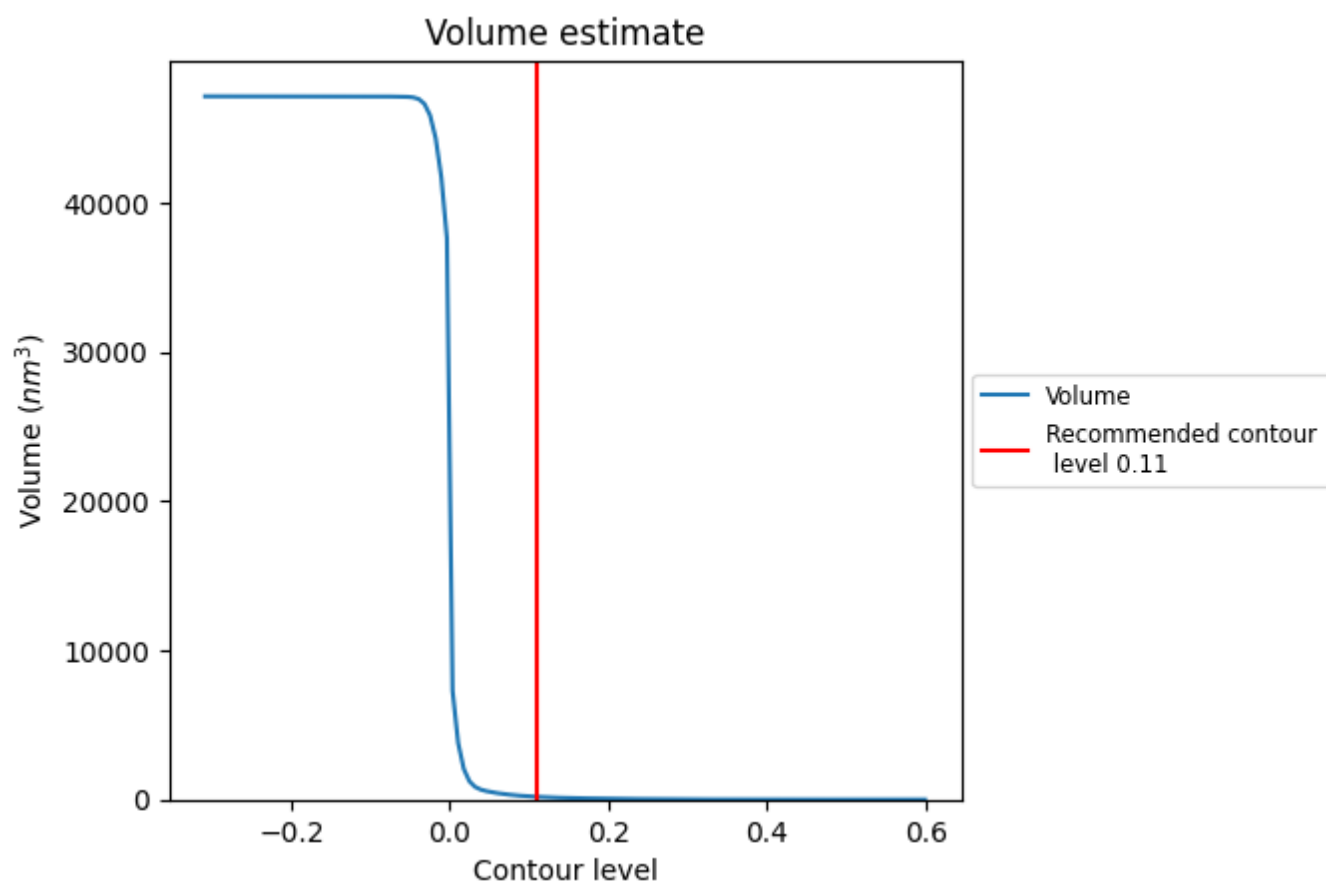
This section contains the results of statistical analysis of the map.

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.

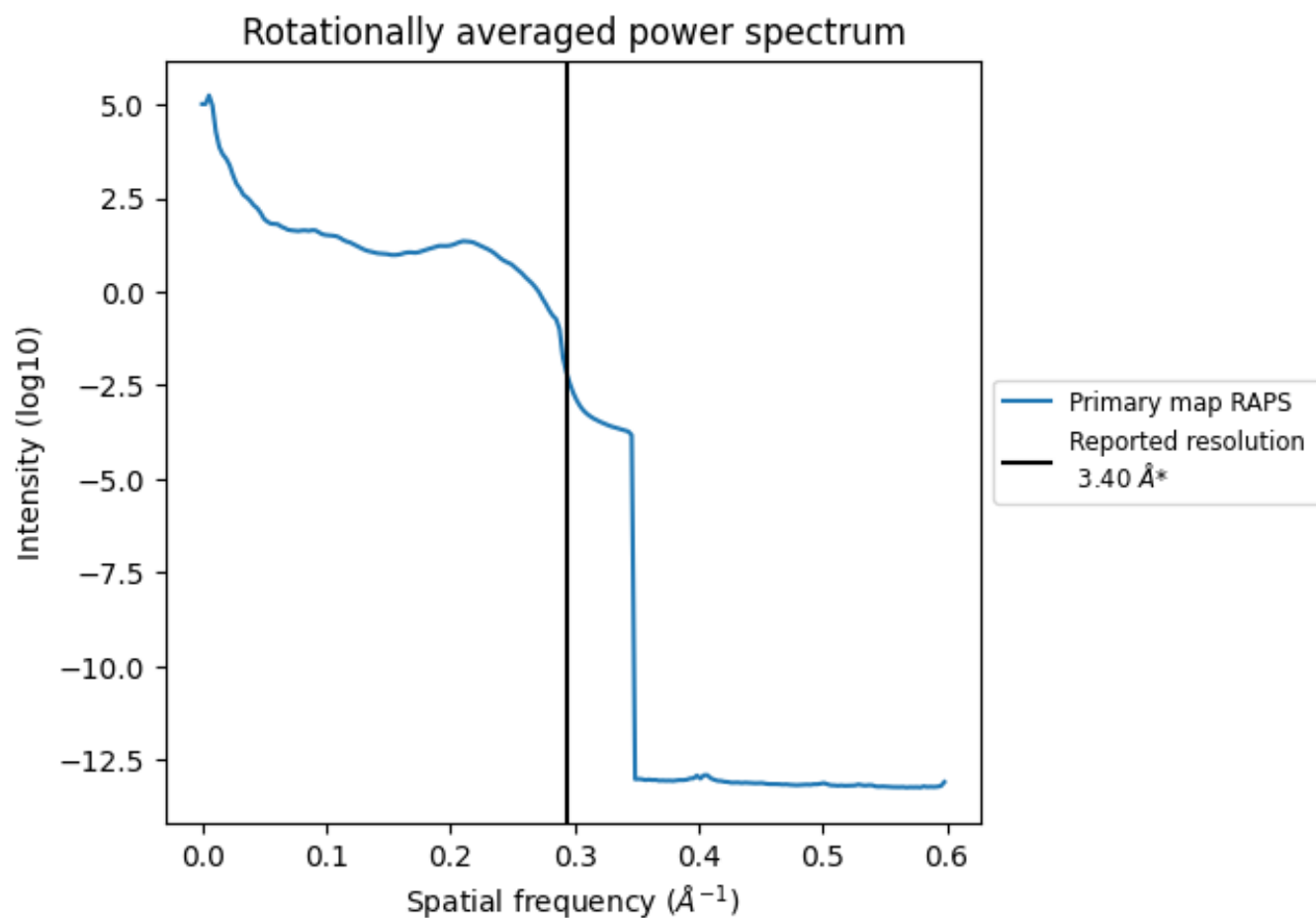
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 183 nm³; this corresponds to an approximate mass of 165 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 ⓘ

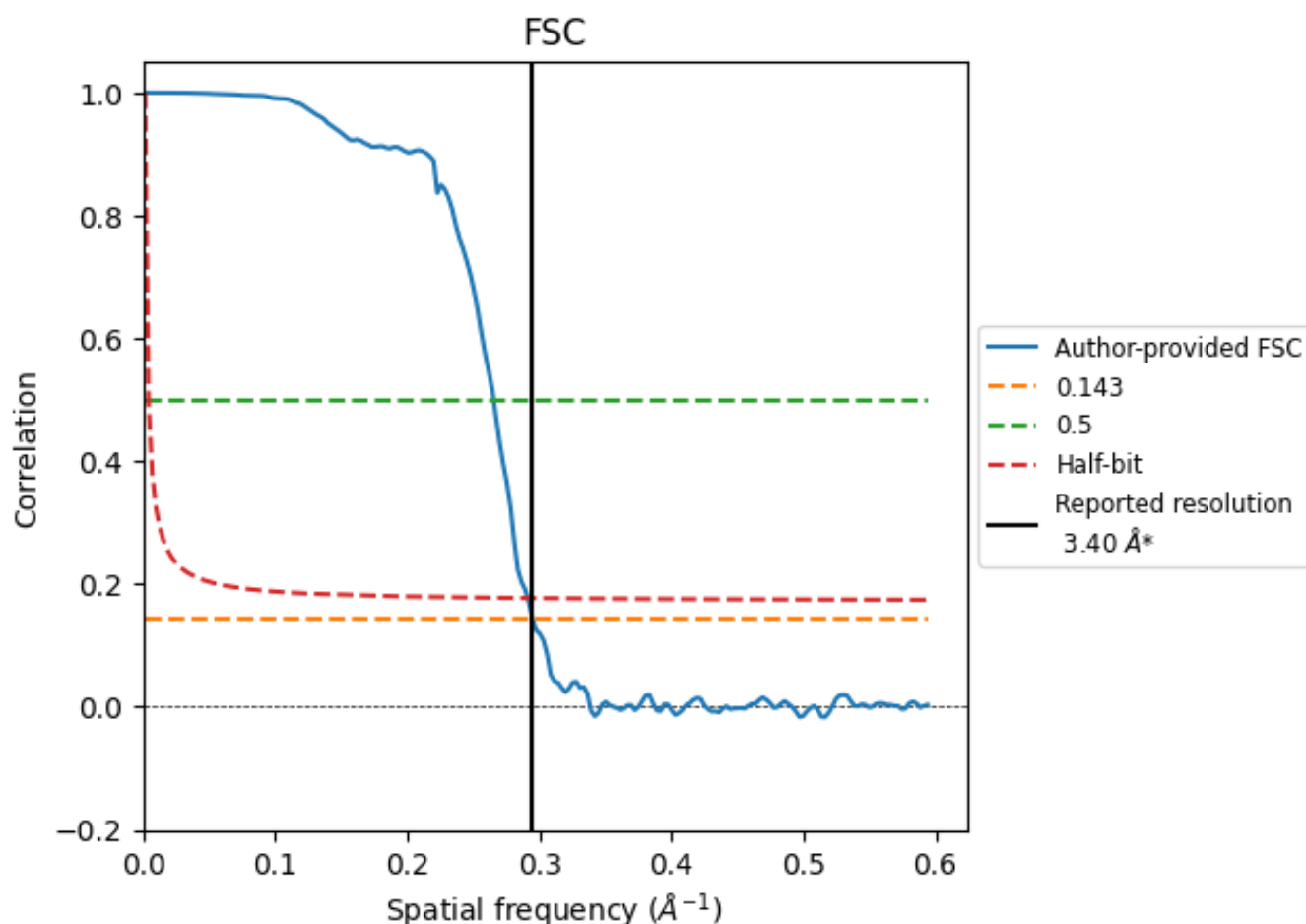


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

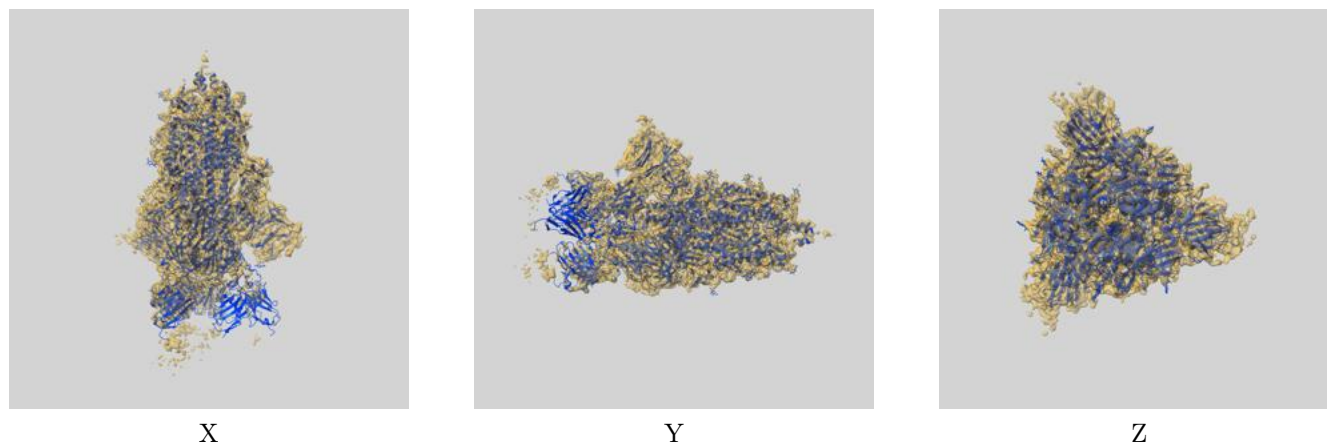
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	3.77	3.43
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

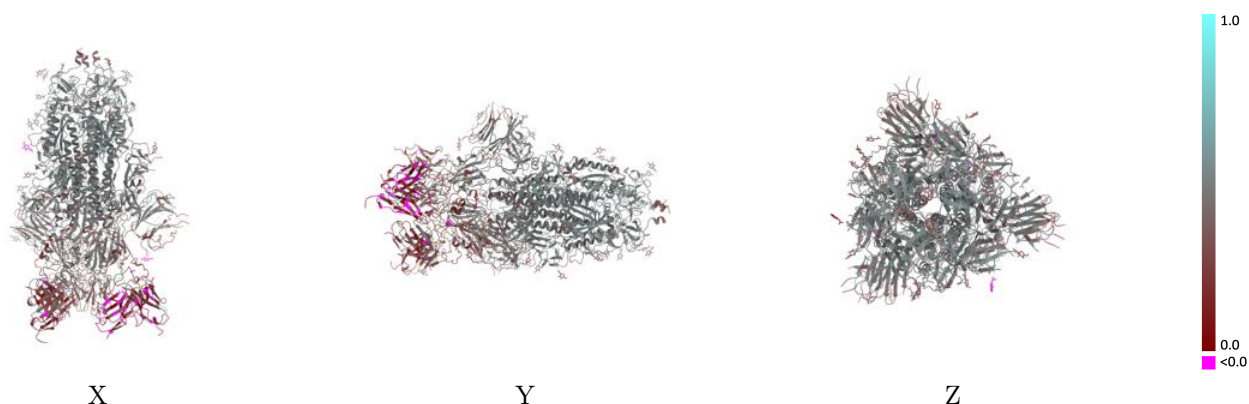
This section contains information regarding the fit between EMDB map EMD-22729 and PDB model 7K8S. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



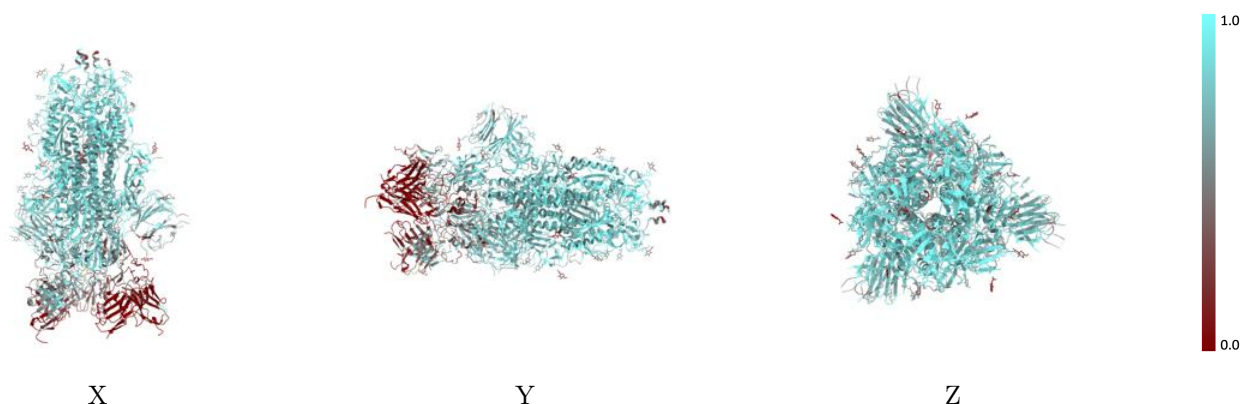
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



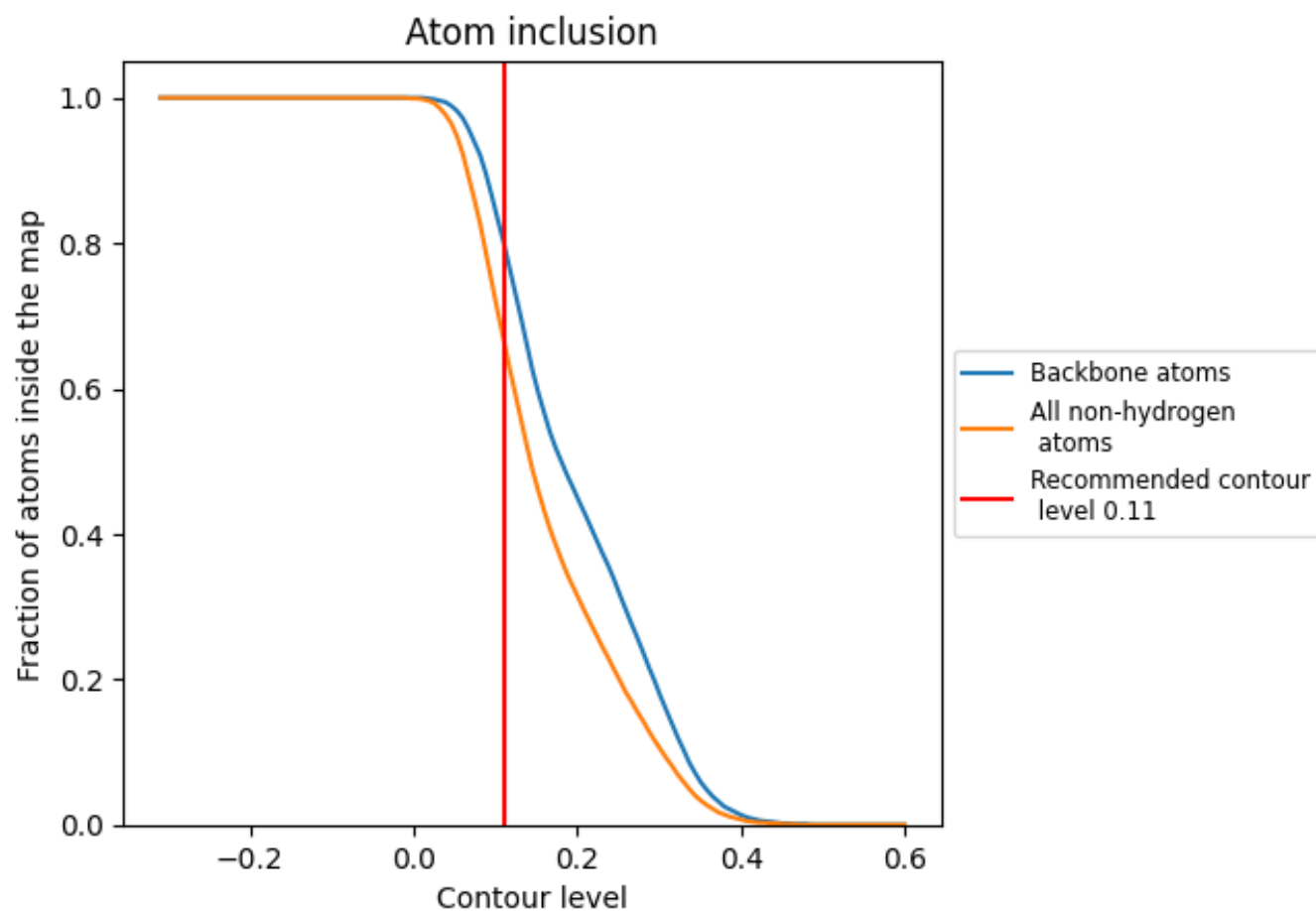
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.11).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 67% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6670	 0.4090
A	 0.7750	 0.4560
B	 0.7070	 0.4350
C	 0.7850	 0.4620
D	 0.0360	 0.1140
E	 0.7140	 0.4780
F	 0.5000	 0.3040
G	 0.7140	 0.4540
H	 0.4690	 0.2900
I	 0.5710	 0.3660
J	 0.2860	 0.1450
K	 0.7860	 0.5070
L	 0.3710	 0.2710
M	 0.4270	 0.2740
N	 0.3150	 0.2690
O	 0.0290	 0.1230
P	 0.0150	 0.1040
Q	 0.6070	 0.3840
R	 0.6430	 0.4040
S	 0.5710	 0.3950
T	 0.0710	 0.2080
U	 0.7860	 0.4530
V	 0.5000	 0.3730
W	 0.6790	 0.4250
X	 0.5710	 0.3800

