Full wwPDB EM Validation Report ⓘ

Aug 28, 2022 – 07:15 am BST

PDB ID	:	7QTI
EMDB ID	:	EMD-14141
Title	:	SARS-CoV-2 S Omicron Spike B.1.1.529 - 3-P2G3 and 1-P5C3 Fabs (Global)
Authors	:	Ni, D.; Lau, K.; Turelli, P.; Fenwick, C.; Perez, L.; Pojer, F.; Stahlberg, H.; Pantaleo, G.; Trono, D.
Deposited on	:	2022-01-14
Resolution	:	3.04 Å(reported)
Based on initial model	:	7QO7

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:

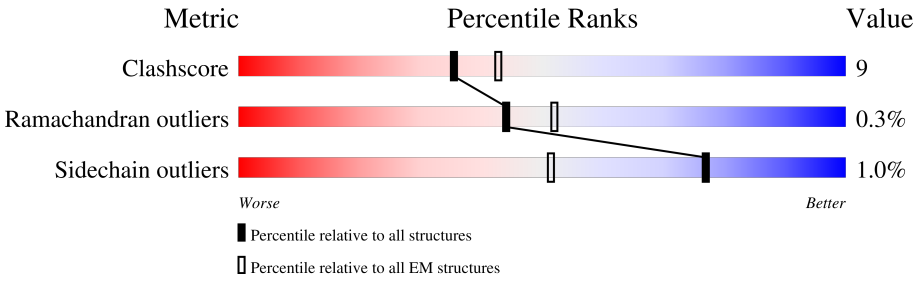
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.04 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=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	B	228	75% 25%
1	G	228	53% 79% 21%
1	I	228	20% 75% 25%
2	C	214	77% 21%
2	H	214	64% 80% 20%
2	J	214	29% 79% 21%
3	E	215	74% 26%
4	F	221	71% 29%

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Mol	Chain	Length	Quality of chain
5	A	1285	71% 14% 14%
5	D	1285	71% 14% 14%
5	K	1285	68% 16% 15%
6	L	2	100%
6	M	2	50% 50%
6	N	2	100%
6	O	2	50% 50%
6	P	2	100%
6	Q	2	50% 50%
6	R	2	50% 50%
6	S	2	50% 50%
6	T	2	100%
6	U	2	100%
6	V	2	100%
6	W	2	100%
6	Y	2	50% 50%
6	Z	2	100%
7	X	4	75% 25%
8	a	3	100%
8	b	3	100%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 40094 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 P2G3 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	228	Total	C	N	O	S	0	0
			1729	1090	296	337	6		
1	B	228	Total	C	N	O	S	0	0
			1729	1090	296	337	6		
1	I	228	Total	C	N	O	S	0	0
			1729	1090	296	337	6		

- Molecule 2 is a protein called P2G3 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	214	Total	C	N	O	S	0	0
			1640	1026	274	335	5		
2	C	214	Total	C	N	O	S	0	0
			1640	1026	274	335	5		
2	J	214	Total	C	N	O	S	0	0
			1640	1026	274	335	5		

- Molecule 3 is a protein called P5C3 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	215	Total	C	N	O	S	0	0
			1645	1028	279	333	5		

- Molecule 4 is a protein called P5C3 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	221	Total	C	N	O	S	0	0
			1637	1025	274	328	10		

- Molecule 5 is a protein called Spike glycoprotein,Envelope glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	1103	Total	C	N	O	S	0	0
			8623	5510	1442	1632	39		
5	K	1096	Total	C	N	O	S	0	0
			8589	5490	1435	1625	39		
5	A	1100	Total	C	N	O	S	0	0
			8609	5502	1439	1629	39		

There are 297 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	67	VAL	ALA	conflict	UNP P0DTC2
D	?	-	HIS	deletion	UNP P0DTC2
D	?	-	VAL	deletion	UNP P0DTC2
D	93	ILE	THR	conflict	UNP P0DTC2
D	?	-	GLY	deletion	UNP P0DTC2
D	?	-	VAL	deletion	UNP P0DTC2
D	?	-	TYR	deletion	UNP P0DTC2
D	140	ASP	TYR	conflict	UNP P0DTC2
D	206	ILE	-	insertion	UNP P0DTC2
D	207	VAL	-	insertion	UNP P0DTC2
D	208	ARG	ASN	conflict	UNP P0DTC2
D	209	GLU	LEU	conflict	UNP P0DTC2
D	210	PRO	VAL	conflict	UNP P0DTC2
D	211	GLU	ARG	conflict	UNP P0DTC2
D	336	ASP	GLY	conflict	UNP P0DTC2
D	368	LEU	SER	conflict	UNP P0DTC2
D	370	PRO	SER	conflict	UNP P0DTC2
D	372	PHE	SER	conflict	UNP P0DTC2
D	414	ASN	LYS	conflict	UNP P0DTC2
D	437	LYS	ASN	conflict	UNP P0DTC2
D	443	SER	GLY	conflict	UNP P0DTC2
D	474	ASN	SER	conflict	UNP P0DTC2
D	475	LYS	THR	conflict	UNP P0DTC2
D	481	ALA	GLU	conflict	UNP P0DTC2
D	490	ARG	GLN	conflict	UNP P0DTC2
D	493	SER	GLY	conflict	UNP P0DTC2
D	495	ARG	GLN	conflict	UNP P0DTC2
D	498	TYR	ASN	conflict	UNP P0DTC2
D	502	HIS	TYR	conflict	UNP P0DTC2
D	544	LYS	THR	conflict	UNP P0DTC2
D	611	GLY	ASP	conflict	UNP P0DTC2
D	652	TYR	HIS	conflict	UNP P0DTC2
D	676	LYS	ASN	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	678	HIS	PRO	conflict	UNP P0DTC2
D	679	GLY	ARG	conflict	UNP P0DTC2
D	680	SER	ARG	conflict	UNP P0DTC2
D	682	SER	ARG	conflict	UNP P0DTC2
D	761	LYS	ASN	conflict	UNP P0DTC2
D	793	TYR	ASP	conflict	UNP P0DTC2
D	853	LYS	ASN	conflict	UNP P0DTC2
D	951	HIS	GLN	conflict	UNP P0DTC2
D	966	LYS	ASN	conflict	UNP P0DTC2
D	978	PHE	LEU	conflict	UNP P0DTC2
D	983	PRO	LYS	conflict	UNP P0DTC2
D	984	PRO	VAL	conflict	UNP P0DTC2
D	1203	TYR	-	linker	UNP P0DTC2
D	1204	GLU	-	linker	UNP P0DTC2
D	1205	GLN	-	linker	UNP P0DTC2
D	1206	GLY	-	linker	UNP P0DTC2
D	1207	SER	-	linker	UNP P0DTC2
D	1236	ARG	SER	conflict	UNP M1E1E4
D	1238	LEU	-	expression tag	UNP M1E1E4
D	1239	GLU	-	expression tag	UNP M1E1E4
D	1240	VAL	-	expression tag	UNP M1E1E4
D	1241	LEU	-	expression tag	UNP M1E1E4
D	1242	PHE	-	expression tag	UNP M1E1E4
D	1243	GLN	-	expression tag	UNP M1E1E4
D	1244	GLY	-	expression tag	UNP M1E1E4
D	1245	PRO	-	expression tag	UNP M1E1E4
D	1246	GLY	-	expression tag	UNP M1E1E4
D	1247	HIS	-	expression tag	UNP M1E1E4
D	1248	HIS	-	expression tag	UNP M1E1E4
D	1249	HIS	-	expression tag	UNP M1E1E4
D	1250	HIS	-	expression tag	UNP M1E1E4
D	1251	HIS	-	expression tag	UNP M1E1E4
D	1252	HIS	-	expression tag	UNP M1E1E4
D	1253	HIS	-	expression tag	UNP M1E1E4
D	1254	HIS	-	expression tag	UNP M1E1E4
D	1255	SER	-	expression tag	UNP M1E1E4
D	1256	ALA	-	expression tag	UNP M1E1E4
D	1257	TRP	-	expression tag	UNP M1E1E4
D	1258	SER	-	expression tag	UNP M1E1E4
D	1259	HIS	-	expression tag	UNP M1E1E4
D	1260	PRO	-	expression tag	UNP M1E1E4
D	1261	GLN	-	expression tag	UNP M1E1E4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1262	PHE	-	expression tag	UNP M1E1E4
D	1263	GLU	-	expression tag	UNP M1E1E4
D	1264	LYS	-	expression tag	UNP M1E1E4
D	1265	GLY	-	expression tag	UNP M1E1E4
D	1266	GLY	-	expression tag	UNP M1E1E4
D	1267	GLY	-	expression tag	UNP M1E1E4
D	1268	SER	-	expression tag	UNP M1E1E4
D	1269	GLY	-	expression tag	UNP M1E1E4
D	1270	GLY	-	expression tag	UNP M1E1E4
D	1271	GLY	-	expression tag	UNP M1E1E4
D	1272	GLY	-	expression tag	UNP M1E1E4
D	1273	SER	-	expression tag	UNP M1E1E4
D	1274	GLY	-	expression tag	UNP M1E1E4
D	1275	GLY	-	expression tag	UNP M1E1E4
D	1276	SER	-	expression tag	UNP M1E1E4
D	1277	ALA	-	expression tag	UNP M1E1E4
D	1278	TRP	-	expression tag	UNP M1E1E4
D	1279	SER	-	expression tag	UNP M1E1E4
D	1280	HIS	-	expression tag	UNP M1E1E4
D	1281	PRO	-	expression tag	UNP M1E1E4
D	1282	GLN	-	expression tag	UNP M1E1E4
D	1283	PHE	-	expression tag	UNP M1E1E4
D	1284	GLU	-	expression tag	UNP M1E1E4
D	1285	LYS	-	expression tag	UNP M1E1E4
K	67	VAL	ALA	conflict	UNP P0DTC2
K	?	-	HIS	deletion	UNP P0DTC2
K	?	-	VAL	deletion	UNP P0DTC2
K	93	ILE	THR	conflict	UNP P0DTC2
K	?	-	GLY	deletion	UNP P0DTC2
K	?	-	VAL	deletion	UNP P0DTC2
K	?	-	TYR	deletion	UNP P0DTC2
K	140	ASP	TYR	conflict	UNP P0DTC2
K	206	ILE	-	insertion	UNP P0DTC2
K	207	VAL	-	insertion	UNP P0DTC2
K	208	ARG	ASN	conflict	UNP P0DTC2
K	209	GLU	LEU	conflict	UNP P0DTC2
K	210	PRO	VAL	conflict	UNP P0DTC2
K	211	GLU	ARG	conflict	UNP P0DTC2
K	336	ASP	GLY	conflict	UNP P0DTC2
K	368	LEU	SER	conflict	UNP P0DTC2
K	370	PRO	SER	conflict	UNP P0DTC2
K	372	PHE	SER	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
K	414	ASN	LYS	conflict	UNP P0DTC2
K	437	LYS	ASN	conflict	UNP P0DTC2
K	443	SER	GLY	conflict	UNP P0DTC2
K	474	ASN	SER	conflict	UNP P0DTC2
K	475	LYS	THR	conflict	UNP P0DTC2
K	481	ALA	GLU	conflict	UNP P0DTC2
K	490	ARG	GLN	conflict	UNP P0DTC2
K	493	SER	GLY	conflict	UNP P0DTC2
K	495	ARG	GLN	conflict	UNP P0DTC2
K	498	TYR	ASN	conflict	UNP P0DTC2
K	502	HIS	TYR	conflict	UNP P0DTC2
K	544	LYS	THR	conflict	UNP P0DTC2
K	611	GLY	ASP	conflict	UNP P0DTC2
K	652	TYR	HIS	conflict	UNP P0DTC2
K	676	LYS	ASN	conflict	UNP P0DTC2
K	678	HIS	PRO	conflict	UNP P0DTC2
K	679	GLY	ARG	conflict	UNP P0DTC2
K	680	SER	ARG	conflict	UNP P0DTC2
K	682	SER	ARG	conflict	UNP P0DTC2
K	761	LYS	ASN	conflict	UNP P0DTC2
K	793	TYR	ASP	conflict	UNP P0DTC2
K	853	LYS	ASN	conflict	UNP P0DTC2
K	951	HIS	GLN	conflict	UNP P0DTC2
K	966	LYS	ASN	conflict	UNP P0DTC2
K	978	PHE	LEU	conflict	UNP P0DTC2
K	983	PRO	LYS	conflict	UNP P0DTC2
K	984	PRO	VAL	conflict	UNP P0DTC2
K	1203	TYR	-	linker	UNP P0DTC2
K	1204	GLU	-	linker	UNP P0DTC2
K	1205	GLN	-	linker	UNP P0DTC2
K	1206	GLY	-	linker	UNP P0DTC2
K	1207	SER	-	linker	UNP P0DTC2
K	1236	ARG	SER	conflict	UNP M1E1E4
K	1238	LEU	-	expression tag	UNP M1E1E4
K	1239	GLU	-	expression tag	UNP M1E1E4
K	1240	VAL	-	expression tag	UNP M1E1E4
K	1241	LEU	-	expression tag	UNP M1E1E4
K	1242	PHE	-	expression tag	UNP M1E1E4
K	1243	GLN	-	expression tag	UNP M1E1E4
K	1244	GLY	-	expression tag	UNP M1E1E4
K	1245	PRO	-	expression tag	UNP M1E1E4
K	1246	GLY	-	expression tag	UNP M1E1E4

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1247	HIS	-	expression tag	UNP M1E1E4
K	1248	HIS	-	expression tag	UNP M1E1E4
K	1249	HIS	-	expression tag	UNP M1E1E4
K	1250	HIS	-	expression tag	UNP M1E1E4
K	1251	HIS	-	expression tag	UNP M1E1E4
K	1252	HIS	-	expression tag	UNP M1E1E4
K	1253	HIS	-	expression tag	UNP M1E1E4
K	1254	HIS	-	expression tag	UNP M1E1E4
K	1255	SER	-	expression tag	UNP M1E1E4
K	1256	ALA	-	expression tag	UNP M1E1E4
K	1257	TRP	-	expression tag	UNP M1E1E4
K	1258	SER	-	expression tag	UNP M1E1E4
K	1259	HIS	-	expression tag	UNP M1E1E4
K	1260	PRO	-	expression tag	UNP M1E1E4
K	1261	GLN	-	expression tag	UNP M1E1E4
K	1262	PHE	-	expression tag	UNP M1E1E4
K	1263	GLU	-	expression tag	UNP M1E1E4
K	1264	LYS	-	expression tag	UNP M1E1E4
K	1265	GLY	-	expression tag	UNP M1E1E4
K	1266	GLY	-	expression tag	UNP M1E1E4
K	1267	GLY	-	expression tag	UNP M1E1E4
K	1268	SER	-	expression tag	UNP M1E1E4
K	1269	GLY	-	expression tag	UNP M1E1E4
K	1270	GLY	-	expression tag	UNP M1E1E4
K	1271	GLY	-	expression tag	UNP M1E1E4
K	1272	GLY	-	expression tag	UNP M1E1E4
K	1273	SER	-	expression tag	UNP M1E1E4
K	1274	GLY	-	expression tag	UNP M1E1E4
K	1275	GLY	-	expression tag	UNP M1E1E4
K	1276	SER	-	expression tag	UNP M1E1E4
K	1277	ALA	-	expression tag	UNP M1E1E4
K	1278	TRP	-	expression tag	UNP M1E1E4
K	1279	SER	-	expression tag	UNP M1E1E4
K	1280	HIS	-	expression tag	UNP M1E1E4
K	1281	PRO	-	expression tag	UNP M1E1E4
K	1282	GLN	-	expression tag	UNP M1E1E4
K	1283	PHE	-	expression tag	UNP M1E1E4
K	1284	GLU	-	expression tag	UNP M1E1E4
K	1285	LYS	-	expression tag	UNP M1E1E4
A	67	VAL	ALA	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	93	ILE	THR	conflict	UNP P0DTC2
A	?	-	GLY	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	140	ASP	TYR	conflict	UNP P0DTC2
A	206	ILE	-	insertion	UNP P0DTC2
A	207	VAL	-	insertion	UNP P0DTC2
A	208	ARG	ASN	conflict	UNP P0DTC2
A	209	GLU	LEU	conflict	UNP P0DTC2
A	210	PRO	VAL	conflict	UNP P0DTC2
A	211	GLU	ARG	conflict	UNP P0DTC2
A	336	ASP	GLY	conflict	UNP P0DTC2
A	368	LEU	SER	conflict	UNP P0DTC2
A	370	PRO	SER	conflict	UNP P0DTC2
A	372	PHE	SER	conflict	UNP P0DTC2
A	414	ASN	LYS	conflict	UNP P0DTC2
A	437	LYS	ASN	conflict	UNP P0DTC2
A	443	SER	GLY	conflict	UNP P0DTC2
A	474	ASN	SER	conflict	UNP P0DTC2
A	475	LYS	THR	conflict	UNP P0DTC2
A	481	ALA	GLU	conflict	UNP P0DTC2
A	490	ARG	GLN	conflict	UNP P0DTC2
A	493	SER	GLY	conflict	UNP P0DTC2
A	495	ARG	GLN	conflict	UNP P0DTC2
A	498	TYR	ASN	conflict	UNP P0DTC2
A	502	HIS	TYR	conflict	UNP P0DTC2
A	544	LYS	THR	conflict	UNP P0DTC2
A	611	GLY	ASP	conflict	UNP P0DTC2
A	652	TYR	HIS	conflict	UNP P0DTC2
A	676	LYS	ASN	conflict	UNP P0DTC2
A	678	HIS	PRO	conflict	UNP P0DTC2
A	679	GLY	ARG	conflict	UNP P0DTC2
A	680	SER	ARG	conflict	UNP P0DTC2
A	682	SER	ARG	conflict	UNP P0DTC2
A	761	LYS	ASN	conflict	UNP P0DTC2
A	793	TYR	ASP	conflict	UNP P0DTC2
A	853	LYS	ASN	conflict	UNP P0DTC2
A	951	HIS	GLN	conflict	UNP P0DTC2
A	966	LYS	ASN	conflict	UNP P0DTC2
A	978	PHE	LEU	conflict	UNP P0DTC2
A	983	PRO	LYS	conflict	UNP P0DTC2
A	984	PRO	VAL	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1203	TYR	-	linker	UNP P0DTC2
A	1204	GLU	-	linker	UNP P0DTC2
A	1205	GLN	-	linker	UNP P0DTC2
A	1206	GLY	-	linker	UNP P0DTC2
A	1207	SER	-	linker	UNP P0DTC2
A	1236	ARG	SER	conflict	UNP M1E1E4
A	1238	LEU	-	expression tag	UNP M1E1E4
A	1239	GLU	-	expression tag	UNP M1E1E4
A	1240	VAL	-	expression tag	UNP M1E1E4
A	1241	LEU	-	expression tag	UNP M1E1E4
A	1242	PHE	-	expression tag	UNP M1E1E4
A	1243	GLN	-	expression tag	UNP M1E1E4
A	1244	GLY	-	expression tag	UNP M1E1E4
A	1245	PRO	-	expression tag	UNP M1E1E4
A	1246	GLY	-	expression tag	UNP M1E1E4
A	1247	HIS	-	expression tag	UNP M1E1E4
A	1248	HIS	-	expression tag	UNP M1E1E4
A	1249	HIS	-	expression tag	UNP M1E1E4
A	1250	HIS	-	expression tag	UNP M1E1E4
A	1251	HIS	-	expression tag	UNP M1E1E4
A	1252	HIS	-	expression tag	UNP M1E1E4
A	1253	HIS	-	expression tag	UNP M1E1E4
A	1254	HIS	-	expression tag	UNP M1E1E4
A	1255	SER	-	expression tag	UNP M1E1E4
A	1256	ALA	-	expression tag	UNP M1E1E4
A	1257	TRP	-	expression tag	UNP M1E1E4
A	1258	SER	-	expression tag	UNP M1E1E4
A	1259	HIS	-	expression tag	UNP M1E1E4
A	1260	PRO	-	expression tag	UNP M1E1E4
A	1261	GLN	-	expression tag	UNP M1E1E4
A	1262	PHE	-	expression tag	UNP M1E1E4
A	1263	GLU	-	expression tag	UNP M1E1E4
A	1264	LYS	-	expression tag	UNP M1E1E4
A	1265	GLY	-	expression tag	UNP M1E1E4
A	1266	GLY	-	expression tag	UNP M1E1E4
A	1267	GLY	-	expression tag	UNP M1E1E4
A	1268	SER	-	expression tag	UNP M1E1E4
A	1269	GLY	-	expression tag	UNP M1E1E4
A	1270	GLY	-	expression tag	UNP M1E1E4
A	1271	GLY	-	expression tag	UNP M1E1E4
A	1272	GLY	-	expression tag	UNP M1E1E4
A	1273	SER	-	expression tag	UNP M1E1E4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1274	GLY	-	expression tag	UNP M1E1E4
A	1275	GLY	-	expression tag	UNP M1E1E4
A	1276	SER	-	expression tag	UNP M1E1E4
A	1277	ALA	-	expression tag	UNP M1E1E4
A	1278	TRP	-	expression tag	UNP M1E1E4
A	1279	SER	-	expression tag	UNP M1E1E4
A	1280	HIS	-	expression tag	UNP M1E1E4
A	1281	PRO	-	expression tag	UNP M1E1E4
A	1282	GLN	-	expression tag	UNP M1E1E4
A	1283	PHE	-	expression tag	UNP M1E1E4
A	1284	GLU	-	expression tag	UNP M1E1E4
A	1285	LYS	-	expression tag	UNP M1E1E4

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

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

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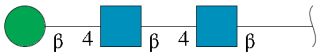
Mol	Chain	Residues	Atoms				AltConf	Trace
6	V	2	Total	C	N	O	0	0
			28	16	2	10		
6	W	2	Total	C	N	O	0	0
			28	16	2	10		
6	Y	2	Total	C	N	O	0	0
			28	16	2	10		
6	Z	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

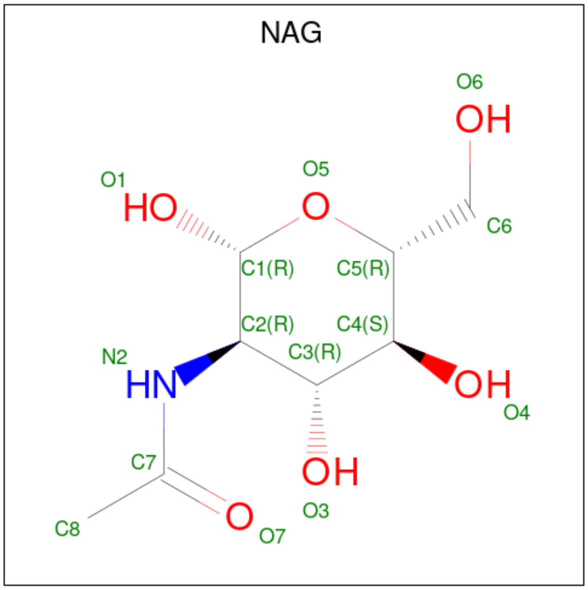
Mol	Chain	Residues	Atoms				AltConf	Trace
7	X	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
8	a	3	Total	C	N	O	0	0
			39	22	2	15		
8	b	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
9	D	1	Total 112	C 64	N 8	O 40	0
9	D	1	Total 112	C 64	N 8	O 40	0
9	D	1	Total 112	C 64	N 8	O 40	0
9	D	1	Total 112	C 64	N 8	O 40	0
9	D	1	Total 112	C 64	N 8	O 40	0
9	D	1	Total 112	C 64	N 8	O 40	0
9	D	1	Total 112	C 64	N 8	O 40	0
9	D	1	Total 112	C 64	N 8	O 40	0
9	K	1	Total 168	C 96	N 12	O 60	0
9	K	1	Total 168	C 96	N 12	O 60	0
9	K	1	Total 168	C 96	N 12	O 60	0
9	K	1	Total 168	C 96	N 12	O 60	0
9	K	1	Total 168	C 96	N 12	O 60	0
9	K	1	Total 168	C 96	N 12	O 60	0

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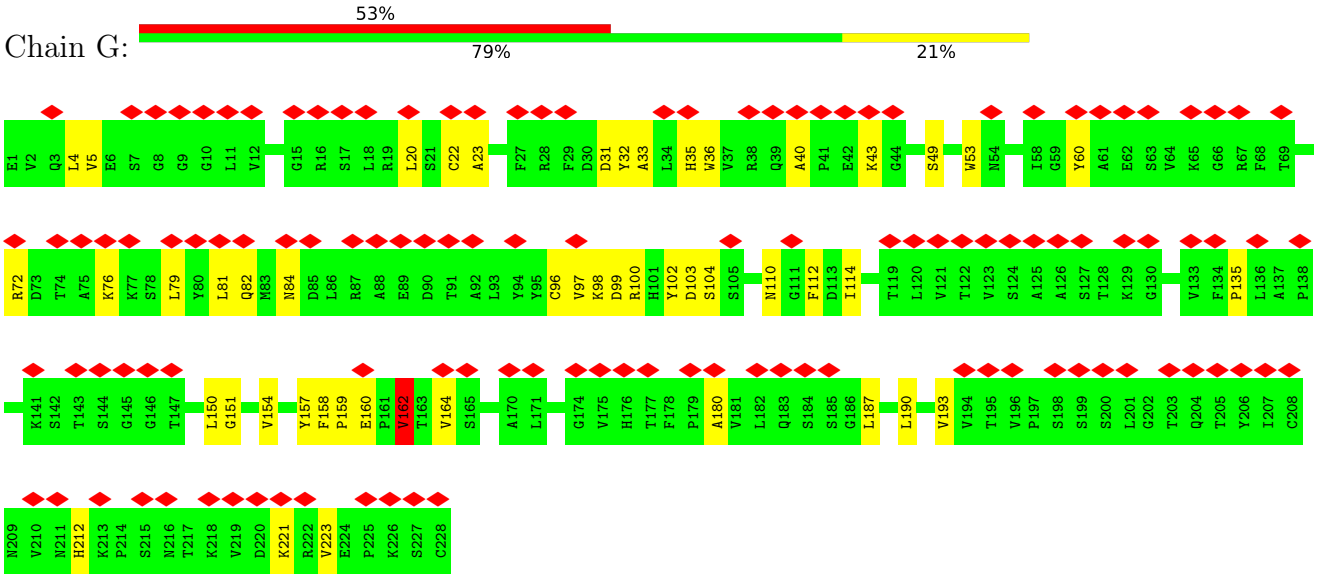
Mol	Chain	Residues	Atoms				AltConf
9	K	1	Total	C	N	O	0
			168	96	12	60	
9	K	1	Total	C	N	O	0
			168	96	12	60	
9	K	1	Total	C	N	O	0
			168	96	12	60	
9	K	1	Total	C	N	O	0
			168	96	12	60	
9	K	1	Total	C	N	O	0
			168	96	12	60	
9	K	1	Total	C	N	O	0
			168	96	12	60	
9	A	1	Total	C	N	O	0
			84	48	6	30	
9	A	1	Total	C	N	O	0
			84	48	6	30	
9	A	1	Total	C	N	O	0
			84	48	6	30	
9	A	1	Total	C	N	O	0
			84	48	6	30	
9	A	1	Total	C	N	O	0
			84	48	6	30	
9	A	1	Total	C	N	O	0
			84	48	6	30	

3 Residue-property plots (i)

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

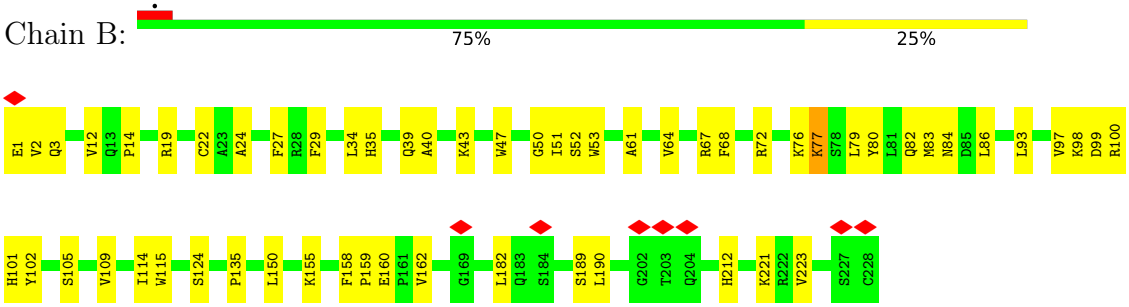
• Molecule 1: P2G3 Heavy Chain

Chain G:



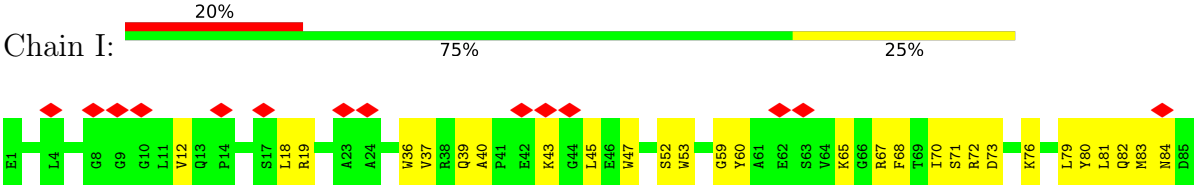
• Molecule 1: P2G3 Heavy Chain

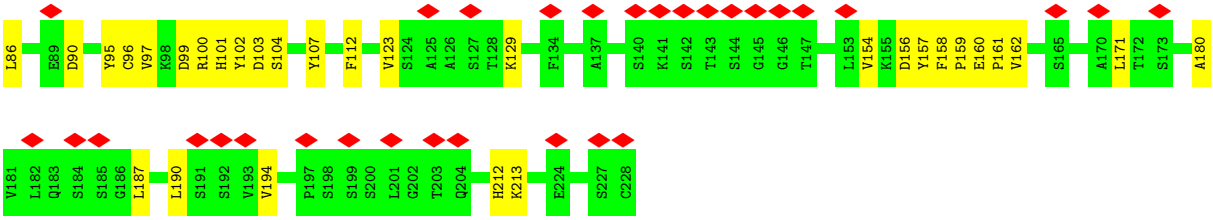
Chain B:



• Molecule 1: P2G3 Heavy Chain

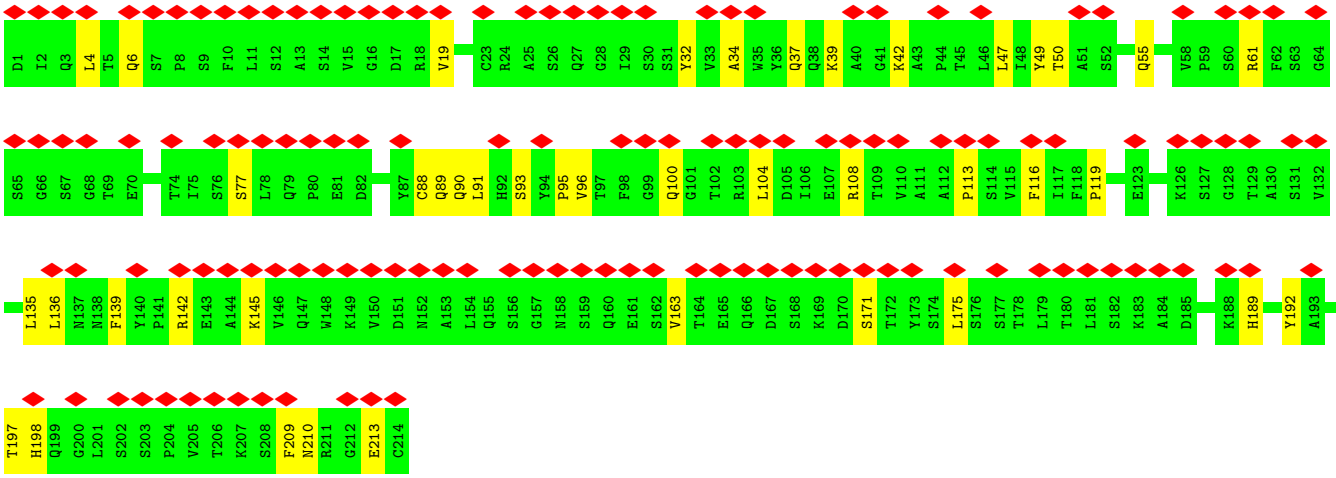
Chain I:





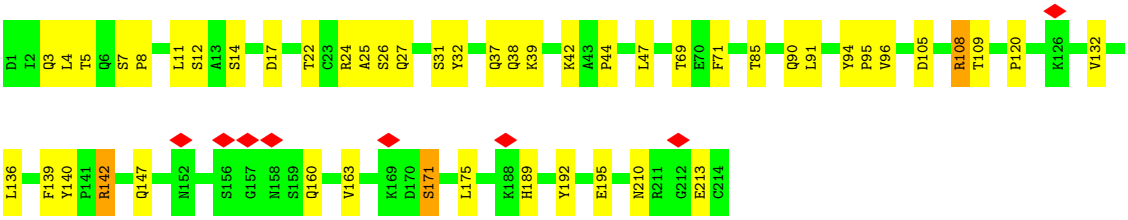
• Molecule 2: P2G3 Light Chain

Chain H:



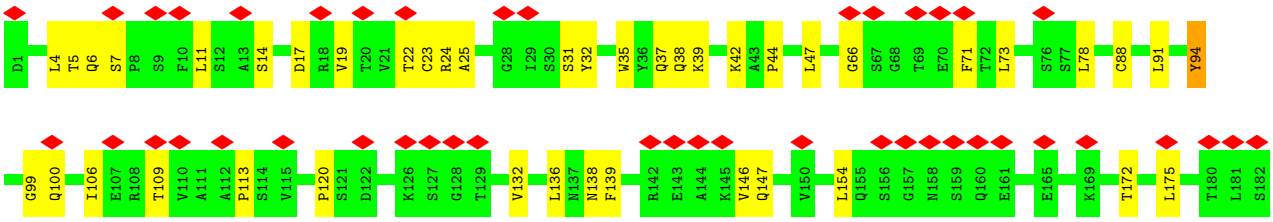
• Molecule 2: P2G3 Light Chain

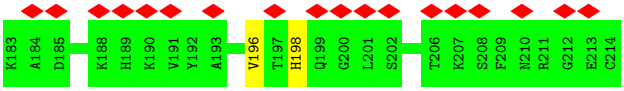
Chain C:



• Molecule 2: P2G3 Light Chain

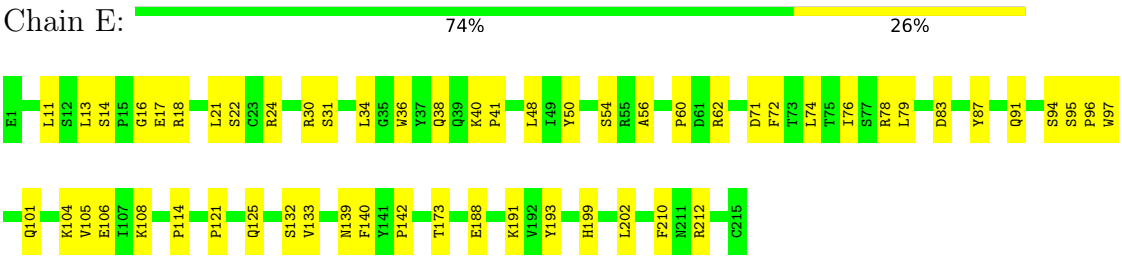
Chain J:





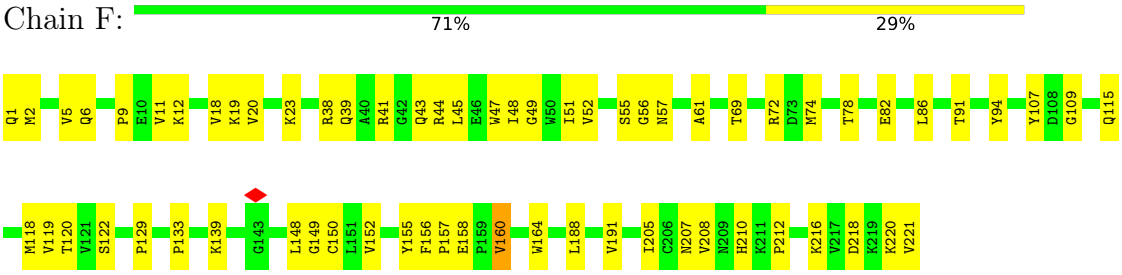
• Molecule 3: P5C3 Light Chain

Chain E:



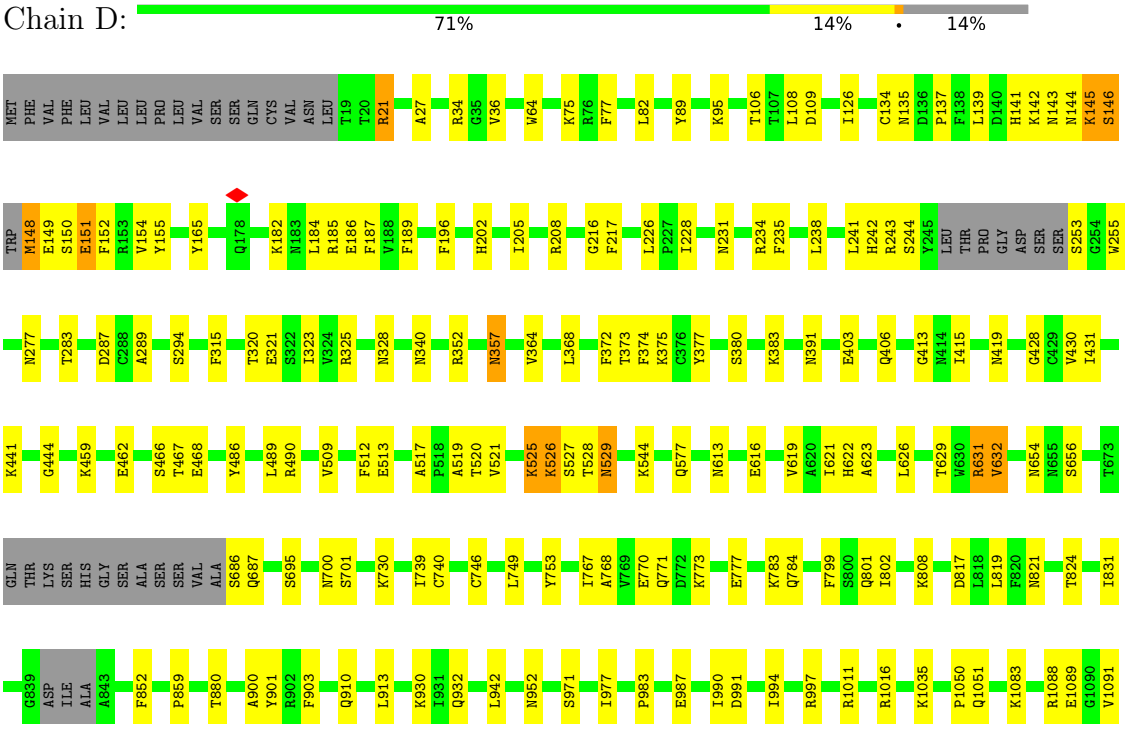
• Molecule 4: P5C3 Heavy Chain

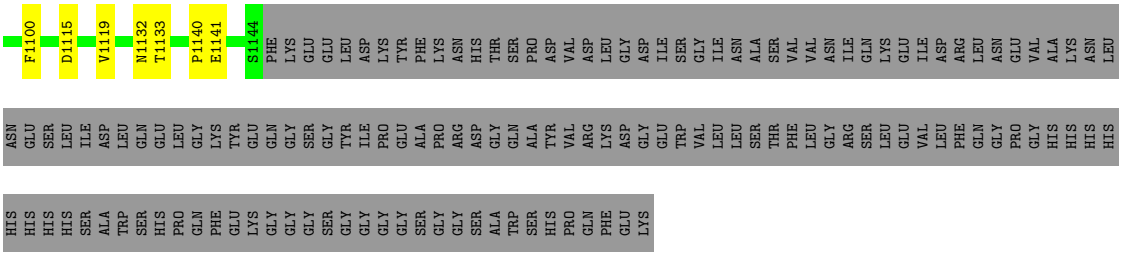
Chain F:



• Molecule 5: Spike glycoprotein,Envelope glycoprotein

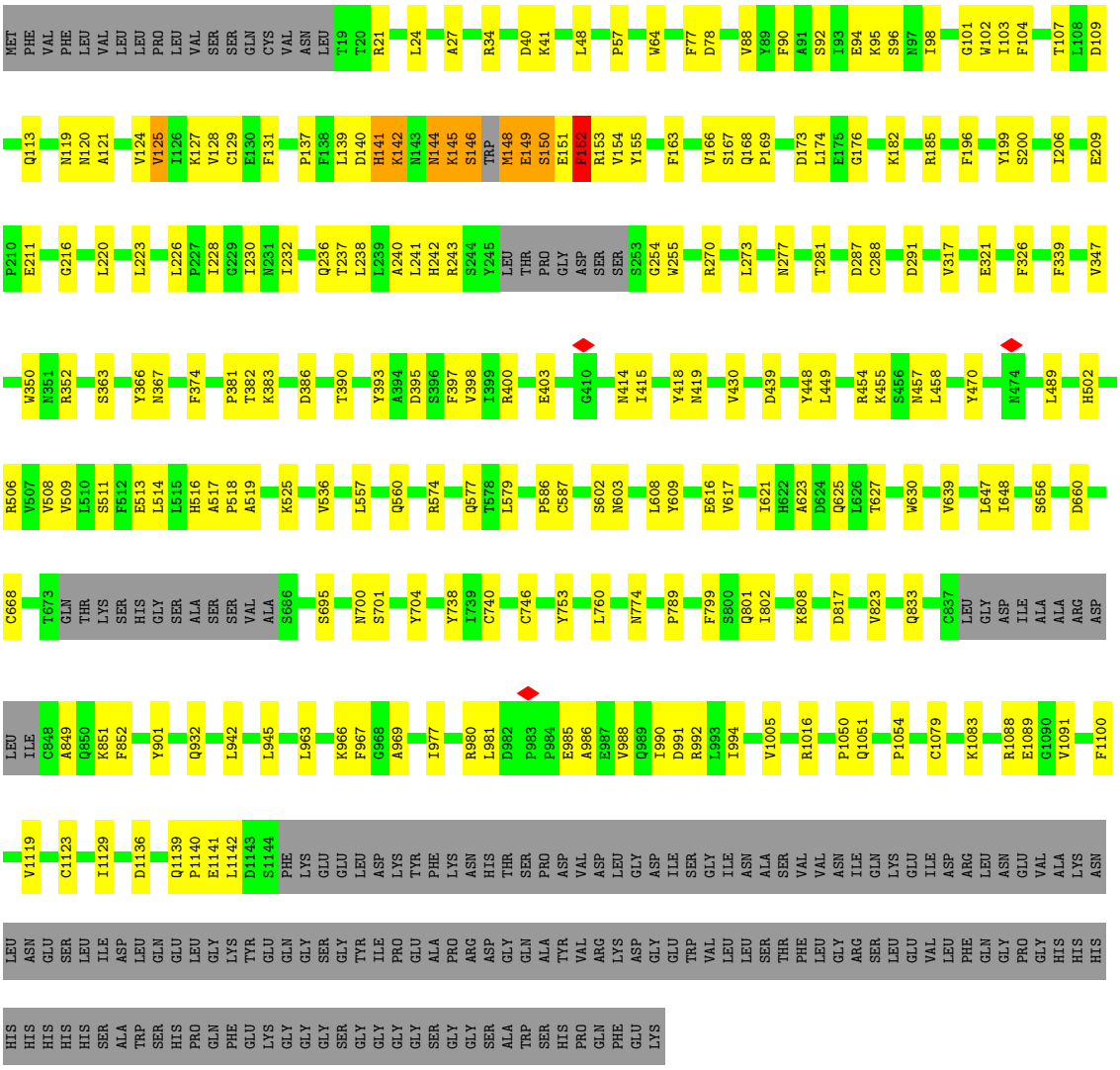
Chain D:





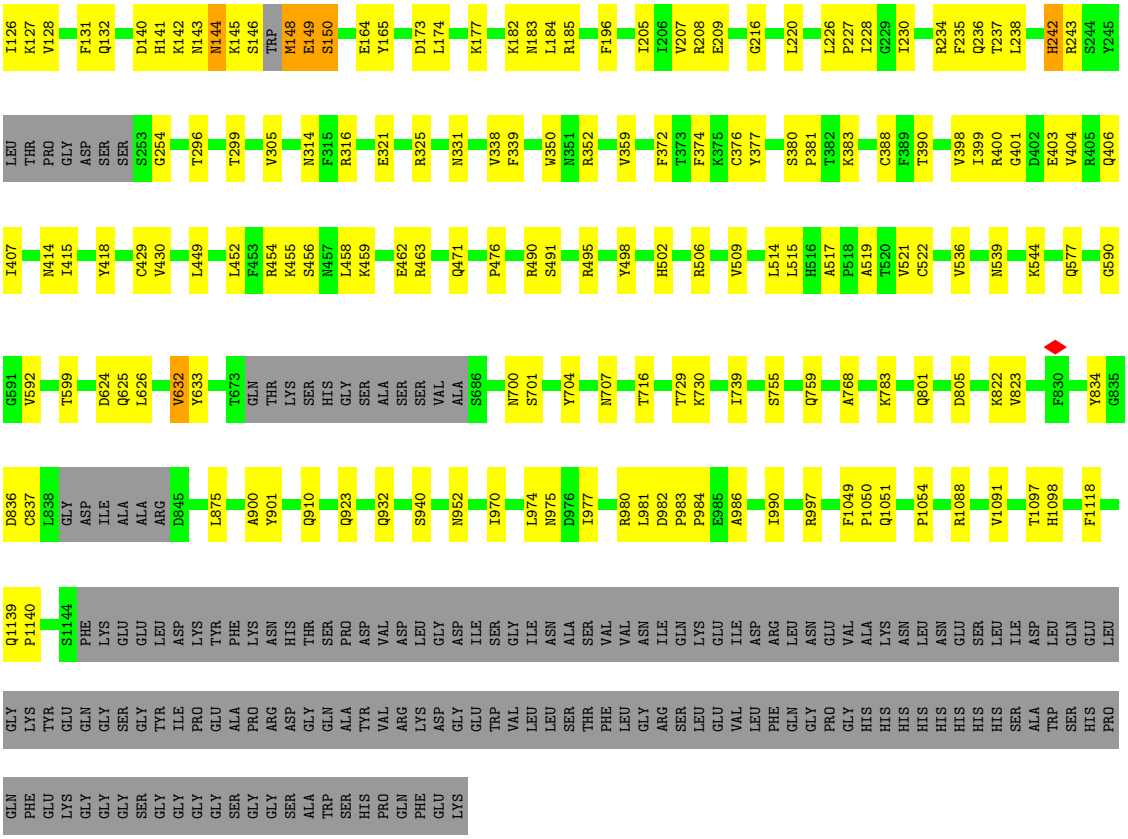
• Molecule 5: Spike glycoprotein,Envelope glycoprotein

Chain K:



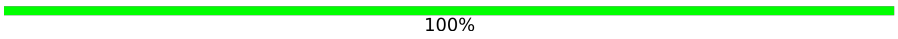
• Molecule 5: Spike glycoprotein,Envelope glycoprotein

Chain A:



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

Chain L:

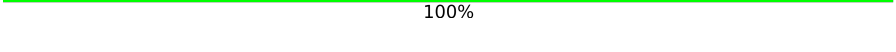


• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

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

Chain N:

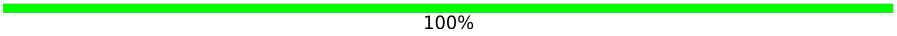


• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

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

Chain P:



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

Chain Q:

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

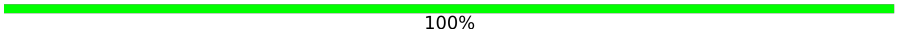
Chain R:

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

Chain S:

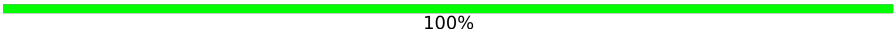
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



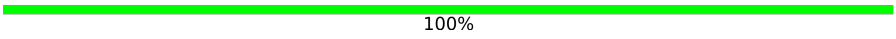
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



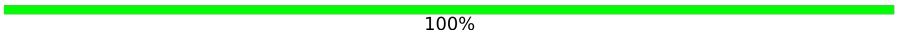
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



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

Chain W:

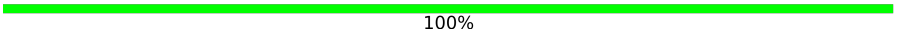


• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

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

Chain Z:

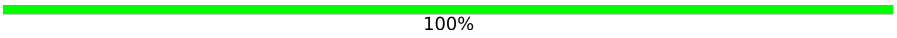


• Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:

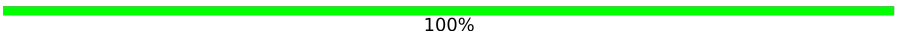
• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



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

Chain b:




NAG1
NAG2
BMA3

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28478	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.849	Depositor
Minimum map value	-0.390	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	415.0, 415.0, 415.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3833333, 1.3833333, 1.3833333	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	B	0.29	0/1771	0.54	0/2409
1	G	0.30	0/1771	0.53	0/2409
1	I	0.27	0/1771	0.52	0/2409
2	C	0.31	0/1675	0.55	0/2278
2	H	0.26	0/1675	0.49	0/2278
2	J	0.31	0/1675	0.52	0/2278
3	E	0.25	0/1682	0.50	0/2283
4	F	0.29	0/1674	0.51	0/2280
5	A	0.27	0/8813	0.49	0/11989
5	D	0.27	0/8827	0.49	0/12008
5	K	0.27	0/8793	0.49	0/11961
All	All	0.28	0/40127	0.50	0/54582

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1729	0	1684	40	0
1	G	1729	0	1684	32	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1729	0	1684	39	0
2	C	1640	0	1585	33	0
2	H	1640	0	1585	24	0
2	J	1640	0	1585	30	0
3	E	1645	0	1591	39	0
4	F	1637	0	1595	44	0
5	A	8609	0	8396	145	0
5	D	8623	0	8404	125	0
5	K	8589	0	8385	157	0
6	L	28	0	25	0	0
6	M	28	0	25	3	0
6	N	28	0	25	0	0
6	O	28	0	25	0	0
6	P	28	0	25	0	0
6	Q	28	0	25	1	0
6	R	28	0	25	1	0
6	S	28	0	25	1	0
6	T	28	0	25	0	0
6	U	28	0	25	0	0
6	V	28	0	25	0	0
6	W	28	0	25	0	0
6	Y	28	0	25	0	0
6	Z	28	0	25	0	0
7	X	50	0	43	0	0
8	a	39	0	34	0	0
8	b	39	0	34	0	0
9	A	84	0	78	1	0
9	D	112	0	104	2	0
9	K	168	0	156	3	0
All	All	40094	0	38977	680	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 9.

All (680) 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)
5:A:146:SER:HB2	5:A:150:SER:H	1.45	0.82
2:J:24:ARG:NH2	2:J:71:PHE:O	2.15	0.78
5:D:415:ILE:HA	5:D:419:ASN:HD22	1.47	0.77
2:J:6:GLN:NE2	2:J:88:CYS:SG	2.59	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:364:VAL:HG12	6:M:1:NAG:H83	1.68	0.75
2:H:6:GLN:NE2	2:H:88:CYS:SG	2.59	0.75
5:A:242:HIS:HD2	5:A:243:ARG:HB2	1.53	0.74
3:E:101:GLN:O	4:F:44:ARG:NH1	2.21	0.74
5:D:196:PHE:HB3	5:D:226:LEU:HB3	1.69	0.74
5:K:141:HIS:HB3	5:K:240:ALA:HB1	1.70	0.74
3:E:16:GLY:H	3:E:79:LEU:HB2	1.53	0.74
3:E:210:PHE:HB2	4:F:139:LYS:HD3	1.70	0.73
1:I:101:HIS:O	1:I:101:HIS:ND1	2.21	0.73
2:H:32:TYR:HB3	2:H:91:LEU:HB3	1.71	0.72
5:A:144:ASN:HA	5:A:242:HIS:CE1	2.24	0.72
1:I:103:ASP:HB3	1:I:107:TYR:HE2	1.54	0.72
5:A:116:LEU:HD21	5:A:127:LYS:HB3	1.72	0.72
1:G:159:PRO:HB2	1:G:212:HIS:HE2	1.53	0.72
5:K:196:PHE:HB3	5:K:226:LEU:HB3	1.72	0.71
5:K:236:GLN:NE2	5:K:237:THR:O	2.23	0.71
5:D:520:THR:HG23	5:D:521:VAL:HG23	1.72	0.71
5:K:403:GLU:HG3	5:K:415:ILE:HG13	1.72	0.71
1:I:18:LEU:H	1:I:83:MET:HB2	1.56	0.71
5:K:616:GLU:HG2	5:K:617:VAL:HG23	1.71	0.70
5:K:980:ARG:HH21	5:A:544:LYS:HZ1	1.38	0.70
1:G:154:VAL:HG12	1:G:157:TYR:CE1	2.27	0.70
1:B:12:VAL:HG21	1:B:86:LEU:HD13	1.74	0.69
1:I:52:SER:O	1:I:72:ARG:NH2	2.25	0.69
2:C:7:SER:OG	2:C:24:ARG:NH1	2.22	0.69
1:B:22:CYS:HB3	1:B:79:LEU:HB3	1.74	0.68
5:A:70:GLY:HA2	5:A:76:ARG:HH21	1.58	0.68
1:I:107:TYR:CZ	5:D:441:LYS:HE3	2.28	0.68
5:D:528:THR:HG22	5:D:529:ASN:H	1.58	0.68
5:K:150:SER:HB2	5:K:152:PHE:CZ	2.29	0.68
5:K:774:ASN:OD1	5:K:1016:ARG:NH1	2.25	0.68
5:A:374:PHE:HE2	5:A:381:PRO:HB3	1.59	0.68
2:H:39:LYS:HB2	2:H:42:LYS:HB3	1.75	0.68
5:K:382:THR:HG23	5:K:383:LYS:HG3	1.76	0.68
5:A:142:LYS:HB2	5:A:242:HIS:ND1	2.08	0.68
5:D:773:LYS:NZ	5:D:777:GLU:OE2	2.27	0.68
5:D:621:ILE:HG22	5:D:622:HIS:H	1.58	0.67
2:H:113:PRO:HB3	2:H:139:PHE:HB3	1.76	0.67
1:B:115:TRP:HZ3	2:C:44:PRO:HB2	1.59	0.67
5:K:142:LYS:HB2	5:K:242:HIS:CG	2.29	0.67
5:A:146:SER:C	5:A:148:MET:HA	2.15	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:37:GLN:HB2	2:C:47:LEU:HD11	1.77	0.67
3:E:38:GLN:HB2	3:E:48:LEU:HD11	1.78	0.66
5:K:621:ILE:HG22	5:K:623:ALA:H	1.61	0.66
2:C:136:LEU:HB2	2:C:175:LEU:HB3	1.77	0.66
5:K:150:SER:HB2	5:K:152:PHE:CE1	2.31	0.66
4:F:152:VAL:HG11	4:F:160:VAL:HG11	1.78	0.65
2:C:108:ARG:HG3	2:C:171:SER:HB2	1.76	0.65
5:D:544:LYS:HB2	5:A:975:ASN:HB3	1.78	0.65
5:A:454:ARG:HD2	5:A:455:LYS:H	1.62	0.64
2:J:113:PRO:HB3	2:J:139:PHE:HB3	1.79	0.64
5:K:967:PHE:O	5:K:992:ARG:NH1	2.30	0.64
5:A:376:CYS:HB3	5:A:381:PRO:HG3	1.79	0.64
1:G:159:PRO:HB2	1:G:212:HIS:NE2	2.13	0.64
5:D:34:ARG:NH1	5:D:216:GLY:O	2.31	0.64
5:K:326:PHE:O	5:K:577:GLN:NE2	2.31	0.64
2:J:24:ARG:NH2	2:J:71:PHE:H	1.95	0.64
1:I:97:VAL:HG21	1:I:112:PHE:HB3	1.79	0.63
5:K:140:ASP:HB2	5:K:151:GLU:OE2	1.97	0.63
5:A:40:ASP:OD2	5:A:44:ARG:NH2	2.31	0.63
1:G:33:ALA:HB3	1:G:99:ASP:HB3	1.81	0.63
2:H:198:HIS:O	3:E:78:ARG:NH1	2.28	0.63
5:A:207:VAL:HG22	5:A:209:GLU:H	1.64	0.63
5:A:716:THR:HA	5:A:923:GLN:HE22	1.64	0.63
5:K:226:LEU:HD23	5:K:228:ILE:H	1.63	0.63
4:F:38:ARG:HB2	4:F:48:ILE:HD11	1.80	0.62
5:D:95:LYS:HB2	5:D:182:LYS:HG2	1.82	0.62
1:I:40:ALA:HB3	1:I:43:LYS:HB3	1.82	0.62
4:F:107:TYR:HD1	4:F:109:GLY:H	1.48	0.62
2:C:142:ARG:HH12	2:C:163:VAL:HG21	1.65	0.62
2:H:136:LEU:HD13	2:H:175:LEU:HD23	1.81	0.61
4:F:18:VAL:HB	4:F:86:LEU:HD11	1.82	0.61
5:K:574:ARG:HH11	5:K:579:LEU:HD12	1.65	0.61
5:A:632:VAL:HG12	5:A:633:TYR:H	1.65	0.61
5:A:126:ILE:HB	5:A:165:TYR:HB3	1.82	0.61
5:A:399:ILE:HG22	5:A:400:ARG:H	1.63	0.61
5:A:34:ARG:NH1	5:A:216:GLY:O	2.34	0.61
5:A:141:HIS:ND1	5:A:142:LYS:HG3	2.16	0.61
5:A:146:SER:C	5:A:149:GLU:H	2.03	0.61
1:B:182:LEU:O	2:C:160:GLN:NE2	2.34	0.61
4:F:43:GLN:HG2	4:F:44:ARG:H	1.66	0.61
5:D:150:SER:O	5:D:152:PHE:N	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:317:VAL:HG22	5:K:625:GLN:HG2	1.82	0.60
5:D:770:GLU:OE2	5:D:1016:ARG:NH1	2.32	0.60
5:K:21:ARG:HH22	5:K:24:LEU:HB2	1.65	0.60
5:D:613:ASN:HB2	5:D:616:GLU:HB3	1.84	0.60
4:F:149:GLY:HA2	4:F:164:TRP:HH2	1.66	0.60
5:A:321:GLU:HB2	5:A:536:VAL:HG12	1.82	0.60
1:I:159:PRO:HD2	1:I:212:HIS:HE1	1.67	0.60
5:D:952:ASN:OD1	5:D:1011:ARG:NH2	2.35	0.60
5:K:557:LEU:HB2	5:K:560:GLN:HG3	1.84	0.60
3:E:139:ASN:HA	3:E:173:THR:HB	1.83	0.60
5:K:363:SER:O	5:K:367:ASN:ND2	2.35	0.60
1:G:150:LEU:HD13	1:G:223:VAL:HG21	1.84	0.59
5:A:196:PHE:HB3	5:A:226:LEU:HB2	1.83	0.59
5:K:151:GLU:C	5:K:153:ARG:H	2.05	0.59
5:K:517:ALA:HB3	5:K:518:PRO:HD3	1.84	0.59
5:K:243:ARG:NH1	5:K:254:GLY:O	2.36	0.59
1:I:161:PRO:O	1:I:212:HIS:HD2	1.85	0.58
5:A:140:ASP:CB	5:A:144:ASN:HB2	2.33	0.58
3:E:14:SER:N	3:E:17:GLU:OE1	2.37	0.58
5:D:368:LEU:HB2	6:M:1:NAG:H82	1.84	0.58
5:A:146:SER:CB	5:A:150:SER:H	2.16	0.58
1:G:151:GLY:HA3	1:G:193:VAL:HG12	1.86	0.58
5:A:350:TRP:N	5:A:463:ARG:HH12	2.01	0.58
4:F:157:PRO:HD2	4:F:210:HIS:CE1	2.39	0.58
5:D:831:ILE:HG21	5:D:859:PRO:HB3	1.85	0.58
5:K:374:PHE:HE2	5:K:381:PRO:HB3	1.68	0.58
5:A:350:TRP:HZ3	5:A:352:ARG:HB2	1.68	0.58
1:G:20:LEU:HD12	1:G:81:LEU:HD23	1.86	0.58
3:E:13:LEU:O	3:E:108:LYS:N	2.36	0.58
1:I:39:GLN:HB2	1:I:45:LEU:HD23	1.86	0.58
5:K:449:LEU:HD21	5:K:489:LEU:HD13	1.86	0.58
3:E:34:LEU:HD23	3:E:91:GLN:HA	1.86	0.58
2:J:4:LEU:HD11	2:J:23:CYS:SG	2.43	0.58
5:K:173:ASP:HB2	5:K:185:ARG:HH21	1.68	0.58
5:D:901:TYR:OH	5:K:1091:VAL:HG12	2.05	0.57
5:A:350:TRP:H	5:A:463:ARG:HH12	1.51	0.57
5:D:27:ALA:HB3	5:D:64:TRP:HB3	1.85	0.57
5:D:184:LEU:HB2	5:D:205:ILE:HD11	1.85	0.57
5:K:639:VAL:HG12	5:K:648:ILE:HG12	1.86	0.57
5:K:1100:PHE:HZ	6:R:1:NAG:H62	1.68	0.57
4:F:133:PRO:HA	4:F:150:CYS:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ARG:NH2	1:B:83:MET:O	2.38	0.57
5:K:95:LYS:HD3	5:K:182:LYS:HE3	1.85	0.57
1:B:35:HIS:HA	1:B:50:GLY:HA2	1.86	0.57
1:I:159:PRO:HD2	1:I:212:HIS:CE1	2.39	0.57
5:D:375:LYS:NZ	5:D:377:TYR:OH	2.37	0.57
2:J:147:GLN:HB3	2:J:154:LEU:HD11	1.85	0.57
5:K:660:ASP:H	5:K:668:CYS:HB3	1.70	0.57
4:F:91:THR:HG23	4:F:120:THR:HA	1.86	0.56
5:D:801:GLN:NE2	5:D:932:GLN:OE1	2.27	0.56
5:D:352:ARG:NH1	5:A:227:PRO:O	2.38	0.56
5:K:151:GLU:O	5:K:153:ARG:N	2.36	0.56
5:A:401:GLY:O	5:A:404:VAL:HG22	2.04	0.56
1:B:80:TYR:HB3	1:B:82:GLN:HE22	1.70	0.56
5:K:386:ASP:OD1	5:K:525:LYS:NZ	2.33	0.56
5:K:449:LEU:HD11	5:K:489:LEU:HB3	1.86	0.56
5:A:314:ASN:HB2	5:A:590:GLY:HA3	1.87	0.56
5:K:393:TYR:HB2	5:K:511:SER:HB3	1.88	0.56
3:E:95:SER:OG	3:E:96:PRO:HD3	2.06	0.56
6:S:1:NAG:O4	6:S:1:NAG:N2	2.37	0.56
1:B:135:PRO:HD3	1:B:221:LYS:HE2	1.88	0.56
5:K:141:HIS:H	5:K:141:HIS:CD2	2.24	0.56
4:F:152:VAL:HG12	4:F:155:TYR:CE1	2.41	0.55
5:D:1088:ARG:NH1	5:D:1115:ASP:O	2.38	0.55
5:K:400:ARG:HD2	5:K:502:HIS:HA	1.88	0.55
5:K:277:ASN:OD1	5:K:281:THR:N	2.34	0.55
5:K:1136:ASP:OD2	5:K:1139:GLN:NE2	2.35	0.55
5:A:982:ASP:OD1	5:A:984:PRO:HD2	2.07	0.55
2:H:49:TYR:HE1	2:H:55:GLN:HA	1.72	0.55
1:B:53:TRP:HA	1:B:72:ARG:HH12	1.72	0.55
5:D:226:LEU:HD23	5:D:228:ILE:H	1.70	0.55
5:K:1050:PRO:O	5:K:1051:GLN:NE2	2.32	0.55
1:G:40:ALA:HB3	1:G:43:LYS:HD3	1.89	0.55
1:B:39:GLN:NE2	1:B:40:ALA:O	2.38	0.55
5:K:146:SER:HG	5:K:148:MET:N	2.05	0.55
5:D:799:PHE:HD1	5:D:802:ILE:HD11	1.72	0.55
1:I:156:ASP:HA	1:I:187:LEU:HB3	1.88	0.55
5:D:525:LYS:C	5:D:526:LYS:HG2	2.27	0.55
1:G:157:TYR:HB2	1:G:212:HIS:HE1	1.72	0.54
2:C:22:THR:HG22	2:C:24:ARG:HH11	1.72	0.54
5:D:149:GLU:HB3	5:D:151:GLU:HG3	1.88	0.54
5:A:380:SER:HB3	5:A:383:LYS:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1050:PRO:O	5:A:1051:GLN:NE2	2.35	0.54
5:D:150:SER:C	5:D:152:PHE:N	2.59	0.54
5:K:129:CYS:HB2	5:K:131:PHE:CE1	2.43	0.54
5:A:120:ASN:HD21	5:A:149:GLU:CD	2.11	0.54
5:A:403:GLU:HG2	5:A:415:ILE:HD13	1.89	0.54
5:D:150:SER:C	5:D:152:PHE:H	2.10	0.54
5:D:244:SER:HG	5:D:253:SER:N	2.05	0.54
9:K:1303:NAG:H83	9:K:1303:NAG:H3	1.88	0.54
5:D:106:THR:OG1	5:D:231:ASN:O	2.25	0.54
5:A:376:CYS:HA	5:A:429:CYS:HB2	1.89	0.54
1:B:67:ARG:NE	1:B:84:ASN:O	2.30	0.54
2:J:7:SER:HB2	2:J:22:THR:HB	1.89	0.54
5:A:140:ASP:HB2	5:A:144:ASN:HB2	1.89	0.54
2:J:37:GLN:HB2	2:J:47:LEU:HD11	1.88	0.54
5:D:126:ILE:HB	5:D:165:TYR:HB3	1.89	0.54
5:D:320:THR:OG1	5:D:321:GLU:OE1	2.25	0.54
5:K:27:ALA:HB3	5:K:64:TRP:HE1	1.72	0.54
5:A:783:LYS:HE3	5:A:783:LYS:HA	1.89	0.54
5:D:325:ARG:HH21	5:D:577:GLN:HB2	1.72	0.54
5:A:305:VAL:HG22	5:A:599:THR:HG23	1.90	0.54
5:D:467:THR:HG22	5:D:489:LEU:HD11	1.90	0.54
1:G:22:CYS:HB3	1:G:79:LEU:HB3	1.89	0.53
5:D:315:PHE:HA	5:D:626:LEU:HB2	1.90	0.53
4:F:160:VAL:HG13	4:F:208:VAL:HG13	1.90	0.53
5:K:141:HIS:HB3	5:K:240:ALA:CB	2.38	0.53
5:K:801:GLN:OE1	5:K:932:GLN:NE2	2.31	0.53
5:K:990:ILE:O	5:K:994:ILE:HD12	2.07	0.53
1:B:97:VAL:HG22	1:B:115:TRP:CD1	2.43	0.53
5:A:79:ASN:HD22	5:A:237:THR:HG23	1.73	0.53
3:E:121:PRO:HD3	3:E:133:VAL:HG22	1.91	0.53
5:D:185:ARG:HA	5:D:202:HIS:HD2	1.73	0.53
5:K:347:VAL:HA	5:K:397:PHE:HB2	1.90	0.53
2:H:210:ASN:HB3	2:H:213:GLU:HB2	1.91	0.53
5:A:403:GLU:HA	5:A:406:GLN:HB2	1.90	0.53
5:D:383:LYS:HZ1	5:A:983:PRO:HD3	1.74	0.53
5:D:990:ILE:O	5:D:994:ILE:HG12	2.08	0.53
5:A:113:GLN:HB2	5:A:230:ILE:HD13	1.91	0.53
5:A:184:LEU:HD21	5:A:205:ILE:HD12	1.90	0.53
1:G:4:LEU:HD21	1:G:96:CYS:HB3	1.90	0.53
2:H:4:LEU:HD11	2:H:90:GLN:HB3	1.91	0.53
3:E:21:LEU:HB2	3:E:74:LEU:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:36:VAL:HG21	5:D:217:PHE:CZ	2.44	0.53
5:D:134:CYS:HB3	5:D:137:PRO:HG3	1.91	0.53
5:D:517:ALA:HB1	5:A:41:LYS:HG2	1.91	0.53
4:F:69:THR:HB	4:F:82:GLU:HB2	1.89	0.52
1:I:12:VAL:HG11	1:I:86:LEU:HD13	1.91	0.52
5:D:182:LYS:H	5:D:208:ARG:NH2	2.06	0.52
5:K:415:ILE:HA	5:K:419:ASN:HD22	1.74	0.52
5:A:146:SER:CA	5:A:148:MET:HA	2.39	0.52
1:G:53:TRP:HB3	1:G:102:TYR:HB2	1.91	0.52
1:B:99:ASP:OD1	1:B:100:ARG:N	2.32	0.52
4:F:149:GLY:HA3	4:F:191:VAL:HG12	1.91	0.52
5:D:108:LEU:HD12	5:D:234:ARG:HE	1.73	0.52
5:A:374:PHE:CE2	5:A:381:PRO:HB3	2.42	0.52
5:A:449:LEU:HA	5:A:491:SER:HA	1.90	0.52
1:I:103:ASP:HB3	1:I:107:TYR:CE2	2.39	0.52
1:I:129:LYS:NZ	1:I:156:ASP:HB3	2.23	0.52
5:K:107:THR:OG1	5:K:109:ASP:OD1	2.27	0.52
5:A:242:HIS:C	5:A:242:HIS:CD2	2.82	0.52
5:D:900:ALA:HB1	5:D:910:GLN:HB2	1.92	0.52
5:K:430:VAL:HG12	5:K:509:VAL:HG22	1.91	0.52
2:J:146:VAL:HG12	2:J:196:VAL:HG22	1.91	0.52
5:K:88:VAL:HG12	5:K:90:PHE:H	1.74	0.52
5:A:624:ASP:OD1	5:A:625:GLN:N	2.42	0.52
5:A:296:THR:HA	5:A:299:THR:HG22	1.91	0.52
4:F:207:ASN:HB3	4:F:216:LYS:HZ2	1.74	0.52
1:B:40:ALA:HB3	1:B:43:LYS:HD3	1.90	0.52
1:I:103:ASP:OD1	1:I:104:SER:N	2.38	0.52
5:D:486:TYR:HB3	5:D:490:ARG:HH22	1.75	0.52
5:K:418:TYR:HA	5:K:454:ARG:HH22	1.75	0.52
1:B:61:ALA:HB3	1:B:64:VAL:HG22	1.91	0.52
5:A:128:VAL:HG21	5:A:228:ILE:HG21	1.92	0.52
5:A:242:HIS:HD2	5:A:243:ARG:CB	2.23	0.52
5:A:388:CYS:HA	5:A:522:CYS:HB3	1.91	0.52
5:K:34:ARG:NH1	5:K:216:GLY:O	2.42	0.51
4:F:41:ARG:HH12	4:F:91:THR:HG22	1.75	0.51
5:D:983:PRO:O	5:D:987:GLU:HG2	2.09	0.51
5:A:403:GLU:O	5:A:407:ILE:HG12	2.11	0.51
4:F:148:LEU:HD13	4:F:221:VAL:HG11	1.92	0.51
5:D:383:LYS:NZ	5:A:981:LEU:O	2.42	0.51
5:K:350:TRP:HZ3	5:K:352:ARG:HB2	1.74	0.51
3:E:18:ARG:NH1	3:E:76:ILE:O	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:144:ASN:HB2	5:D:149:GLU:HA	1.92	0.51
5:D:149:GLU:C	5:D:151:GLU:H	2.12	0.51
5:D:783:LYS:HG3	5:D:784:GLN:HG2	1.93	0.51
5:K:241:LEU:HB3	5:K:255:TRP:HB3	1.92	0.51
5:A:388:CYS:HA	5:A:522:CYS:CB	2.40	0.51
5:A:801:GLN:NE2	5:A:932:GLN:OE1	2.43	0.51
1:B:35:HIS:HE1	1:B:99:ASP:HB2	1.75	0.51
3:E:40:LYS:HG3	3:E:41:PRO:HD2	1.93	0.51
2:H:163:VAL:HG22	2:H:175:LEU:HD13	1.92	0.51
3:E:60:PRO:HB2	3:E:62:ARG:HG2	1.93	0.51
1:G:5:VAL:HB	1:G:23:ALA:HB3	1.92	0.51
1:B:39:GLN:N	1:B:93:LEU:O	2.41	0.51
5:D:403:GLU:O	5:D:403:GLU:HG2	2.11	0.51
5:K:516:HIS:O	5:K:516:HIS:ND1	2.44	0.51
2:C:142:ARG:NH1	2:C:163:VAL:HG21	2.26	0.51
5:A:141:HIS:CD2	5:A:242:HIS:H	2.29	0.51
5:A:495:ARG:NH1	5:A:498:TYR:OH	2.44	0.51
1:B:105:SER:OG	2:C:91:LEU:O	2.28	0.51
5:D:971:SER:HB3	5:D:977:ILE:HD11	1.93	0.51
5:K:119:ASN:HD21	5:K:169:PRO:HB3	1.76	0.51
5:K:1140:PRO:HG2	5:K:1141:GLU:OE1	2.11	0.51
1:B:77:LYS:HD2	1:B:77:LYS:O	2.12	0.50
1:I:37:VAL:HG12	1:I:47:TRP:HA	1.93	0.50
5:D:328:ASN:OD1	9:D:1301:NAG:N2	2.44	0.50
5:A:455:LYS:NZ	5:A:471:GLN:O	2.44	0.50
5:K:1123:CYS:HB2	5:K:1129:ILE:HD13	1.93	0.50
1:G:35:HIS:HE2	1:G:104:SER:HA	1.76	0.50
1:G:157:TYR:HB2	1:G:212:HIS:CE1	2.46	0.50
3:E:21:LEU:HD13	3:E:74:LEU:HD23	1.94	0.50
5:D:380:SER:HB2	5:A:982:ASP:HB2	1.93	0.50
5:D:880:THR:HG23	5:K:704:TYR:HB2	1.93	0.50
5:K:125:VAL:HA	5:K:166:VAL:HG12	1.93	0.50
4:F:149:GLY:HA2	4:F:164:TRP:CH2	2.46	0.50
5:K:753:TYR:OH	5:K:991:ASP:OD1	2.23	0.50
5:A:316:ARG:HD2	5:A:626:LEU:HD21	1.93	0.50
2:C:147:GLN:HB2	2:C:195:GLU:HB2	1.93	0.50
5:K:48:LEU:HD12	5:K:273:LEU:HD21	1.94	0.50
1:G:162:VAL:O	1:G:164:VAL:HG23	2.12	0.50
5:D:75:LYS:HD2	5:D:255:TRP:HD1	1.76	0.50
5:D:154:VAL:HG23	5:D:155:TYR:HD1	1.75	0.50
1:I:71:SER:N	1:I:80:TYR:O	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:7:SER:HG	2:C:24:ARG:HH12	1.57	0.50
2:C:139:PHE:HZ	2:C:175:LEU:HB2	1.77	0.49
4:F:47:TRP:HE3	4:F:61:ALA:HB2	1.77	0.49
5:A:372:PHE:HB2	5:A:374:PHE:H	1.76	0.49
5:D:490:ARG:HD2	5:A:372:PHE:CE2	2.46	0.49
5:K:969:ALA:N	5:K:992:ARG:HH12	2.10	0.49
5:A:974:LEU:HD21	5:A:997:ARG:HH12	1.77	0.49
1:G:110:ASN:HB2	2:H:91:LEU:HD21	1.93	0.49
4:F:218:ASP:OD1	4:F:218:ASP:N	2.45	0.49
1:I:37:VAL:HG23	1:I:95:TYR:HB2	1.94	0.49
1:G:180:ALA:HB2	1:G:190:LEU:HD23	1.93	0.49
2:H:19:VAL:HG11	2:H:104:LEU:HD21	1.94	0.49
2:C:11:LEU:O	2:C:105:ASP:N	2.39	0.49
5:A:243:ARG:NH1	5:A:254:GLY:O	2.46	0.49
1:G:180:ALA:HA	1:G:190:LEU:HB3	1.93	0.49
2:J:66:GLY:HA3	2:J:71:PHE:HA	1.94	0.49
5:K:398:VAL:HG22	5:K:506:ARG:HG2	1.94	0.49
5:A:144:ASN:HA	5:A:242:HIS:ND1	2.27	0.49
5:A:242:HIS:CD2	5:A:243:ARG:HB2	2.39	0.49
1:B:159:PRO:HD2	1:B:212:HIS:HE1	1.76	0.49
5:D:656:SER:HB3	5:D:695:SER:HB3	1.94	0.49
5:D:753:TYR:OH	5:D:991:ASP:OD1	2.29	0.49
5:D:145:LYS:O	5:D:146:SER:HB2	2.13	0.49
5:A:390:THR:HG21	5:A:515:LEU:HB2	1.94	0.49
2:J:22:THR:HG23	2:J:24:ARG:NH1	2.28	0.49
5:D:82:LEU:O	5:D:235:PHE:N	2.37	0.49
3:E:101:GLN:OE1	4:F:44:ARG:NH1	2.45	0.48
1:I:180:ALA:HA	1:I:190:LEU:HB3	1.95	0.48
5:A:110:SER:HB2	5:A:132:GLN:HB2	1.94	0.48
3:E:91:GLN:HG3	3:E:97:TRP:HA	1.95	0.48
3:E:188:GLU:O	3:E:212:ARG:NH1	2.44	0.48
1:I:70:ILE:HA	1:I:81:LEU:HA	1.95	0.48
5:K:350:TRP:CZ3	5:K:352:ARG:HB2	2.48	0.48
5:A:390:THR:HG23	5:A:517:ALA:HB3	1.95	0.48
3:E:142:PRO:HD2	3:E:199:HIS:CE1	2.47	0.48
5:K:103:ILE:H	5:K:103:ILE:HD12	1.78	0.48
5:K:141:HIS:CD2	5:K:141:HIS:N	2.81	0.48
5:K:627:THR:HB	5:K:630:TRP:HB3	1.95	0.48
5:D:739:ILE:O	5:D:997:ARG:NH1	2.46	0.48
4:F:205:ILE:HD11	4:F:220:LYS:HE2	1.96	0.48
4:F:207:ASN:HB3	4:F:216:LYS:NZ	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:525:LYS:HB2	5:K:525:LYS:HE2	1.66	0.48
1:I:60:TYR:HB2	1:I:65:LYS:HB3	1.95	0.48
5:K:137:PRO:HB2	5:K:154:VAL:HG12	1.95	0.48
5:K:851:LYS:HG3	5:K:852:PHE:H	1.78	0.48
5:A:174:LEU:O	5:A:177:LYS:NZ	2.47	0.48
3:E:16:GLY:HA2	3:E:78:ARG:HG2	1.96	0.48
4:F:19:LYS:NZ	4:F:20:VAL:O	2.47	0.48
5:K:942:LEU:HD23	5:K:945:LEU:HD12	1.96	0.48
5:K:174:LEU:HG	5:K:176:GLY:H	1.79	0.47
5:K:700:ASN:OD1	5:K:701:SER:N	2.47	0.47
5:D:374:PHE:HD1	5:D:431:ILE:HG13	1.79	0.47
5:A:101:GLY:HA3	5:A:238:LEU:HD12	1.95	0.47
5:A:376:CYS:HA	5:A:429:CYS:CB	2.44	0.47
1:G:53:TRP:O	1:G:72:ARG:NH1	2.47	0.47
2:C:25:ALA:O	2:C:69:THR:OG1	2.32	0.47
5:D:1088:ARG:HB3	5:D:1089:GLU:OE1	2.14	0.47
5:A:458:LEU:HD23	5:A:462:GLU:HB3	1.96	0.47
5:A:459:LYS:HG2	5:A:462:GLU:OE1	2.15	0.47
2:H:6:GLN:HB2	2:H:100:GLN:NE2	2.29	0.47
1:B:2:VAL:HG13	1:B:27:PHE:HD2	1.79	0.47
1:B:52:SER:O	1:B:72:ARG:NH1	2.47	0.47
5:D:1100:PHE:HZ	6:Q:1:NAG:H62	1.78	0.47
5:K:390:THR:HB	5:K:513:GLU:OE2	2.15	0.47
5:A:900:ALA:HB1	5:A:910:GLN:HB2	1.96	0.47
5:K:760:LEU:HD22	5:K:1005:VAL:HG21	1.96	0.47
1:I:90:ASP:HB2	1:I:123:VAL:HG21	1.95	0.47
5:K:287:ASP:OD1	5:K:288:CYS:N	2.47	0.47
5:K:418:TYR:HA	5:K:454:ARG:NH2	2.29	0.47
5:A:78:ASP:OD1	5:A:78:ASP:N	2.45	0.47
4:F:6:GLN:H	4:F:115:GLN:HE22	1.63	0.47
5:D:144:ASN:H	5:D:149:GLU:HG2	1.79	0.47
5:K:317:VAL:HB	5:K:587:CYS:SG	2.54	0.47
4:F:39:GLN:HB2	4:F:45:LEU:HD23	1.96	0.47
4:F:155:TYR:OH	4:F:188:LEU:HD23	2.15	0.47
5:A:970:ILE:HG21	5:A:980:ARG:HH21	1.80	0.47
1:B:1:GLU:HB3	1:B:3:GLN:HE22	1.79	0.47
5:D:89:TYR:OH	5:D:186:GLU:OE1	2.17	0.47
5:D:900:ALA:HB2	5:D:913:LEU:HD23	1.96	0.47
5:K:113:GLN:HB3	5:K:230:ILE:HG12	1.96	0.47
5:K:823:VAL:HB	5:K:1054:PRO:HG2	1.96	0.47
5:A:140:ASP:HB3	5:A:242:HIS:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:TRP:CG	2:C:96:VAL:HG13	2.50	0.47
4:F:129:PRO:HD3	4:F:210:HIS:ND1	2.30	0.47
5:K:121:ALA:HB3	9:K:1310:NAG:O3	2.14	0.47
5:K:150:SER:C	5:K:152:PHE:H	2.17	0.47
5:K:808:LYS:NZ	5:K:817:ASP:OD2	2.33	0.47
2:C:14:SER:OG	2:C:17:ASP:OD2	2.30	0.46
3:E:30:ARG:HG2	3:E:31:SER:H	1.80	0.46
5:K:141:HIS:H	5:K:141:HIS:HD2	1.63	0.46
5:K:199:TYR:HB3	5:K:220:LEU:HG	1.96	0.46
5:K:656:SER:HB3	5:K:695:SER:HB3	1.97	0.46
5:A:94:GLU:OE2	5:A:185:ARG:NH1	2.48	0.46
5:D:441:LYS:HB3	5:D:444:GLY:H	1.80	0.46
5:D:1132:ASN:OD1	5:D:1133:THR:N	2.39	0.46
5:K:449:LEU:HG	5:K:489:LEU:HD22	1.98	0.46
2:H:49:TYR:HD2	2:H:50:THR:HG23	1.80	0.46
2:J:6:GLN:HE22	2:J:99:GLY:HA3	1.80	0.46
2:J:120:PRO:HD3	2:J:132:VAL:HG22	1.97	0.46
5:A:205:ILE:O	5:A:208:ARG:NH2	2.47	0.46
5:A:730:LYS:HD2	5:A:768:ALA:HB1	1.97	0.46
2:C:32:TYR:HB3	2:C:91:LEU:HB2	1.97	0.46
2:J:11:LEU:HD23	2:J:19:VAL:HG13	1.98	0.46
5:D:730:LYS:HD2	5:D:768:ALA:HB1	1.96	0.46
5:D:459:LYS:HB2	5:D:462:GLU:OE1	2.15	0.46
5:D:466:SER:OG	5:D:468:GLU:OE1	2.31	0.46
5:D:686:SER:OG	5:D:687:GLN:N	2.47	0.46
5:K:151:GLU:C	5:K:153:ARG:N	2.68	0.46
5:D:340:ASN:ND2	6:M:1:NAG:H61	2.31	0.46
5:A:141:HIS:CE1	5:A:142:LYS:HG3	2.51	0.46
2:J:14:SER:OG	2:J:17:ASP:OD2	2.31	0.46
5:K:139:LEU:O	5:K:241:LEU:N	2.48	0.46
5:A:173:ASP:HB2	5:A:185:ARG:HH21	1.81	0.46
3:E:94:SER:OG	3:E:96:PRO:O	2.30	0.46
5:K:1079:CYS:HB2	5:K:1123:CYS:HB2	1.92	0.46
1:G:31:ASP:O	1:G:32:TYR:CD1	2.69	0.46
2:H:116:PHE:O	2:H:135:LEU:N	2.39	0.46
1:B:68:PHE:CE1	1:B:83:MET:HG3	2.51	0.46
1:B:115:TRP:CZ3	2:C:44:PRO:HB2	2.46	0.46
5:K:738:TYR:CE1	5:K:963:LEU:HD11	2.51	0.46
5:A:144:ASN:O	5:A:145:LYS:HB2	2.16	0.46
5:A:146:SER:HA	5:A:148:MET:HA	1.98	0.46
4:F:23:LYS:HA	4:F:78:THR:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:1140:PRO:HG2	5:D:1141:GLU:OE1	2.15	0.45
5:K:980:ARG:NH2	5:A:544:LYS:HZ1	2.08	0.45
1:G:36:TRP:CD2	1:G:81:LEU:HD22	2.51	0.45
1:G:157:TYR:N	1:G:187:LEU:HB3	2.31	0.45
1:B:150:LEU:HB2	1:B:223:VAL:HG11	1.99	0.45
2:C:31:SER:HA	2:C:71:PHE:HZ	1.80	0.45
5:D:372:PHE:O	5:D:374:PHE:N	2.50	0.45
5:K:40:ASP:OD1	5:K:41:LYS:N	2.50	0.45
5:K:124:VAL:HG22	5:K:167:SER:H	1.81	0.45
5:K:154:VAL:HG23	5:K:155:TYR:HD1	1.81	0.45
5:A:823:VAL:HB	5:A:1054:PRO:HG2	1.98	0.45
5:A:974:LEU:O	5:A:977:ILE:HG22	2.15	0.45
2:C:39:LYS:HB3	2:C:42:LYS:HE3	1.99	0.45
3:E:104:LYS:NZ	3:E:106:GLU:OE1	2.49	0.45
4:F:155:TYR:HD2	4:F:157:PRO:O	1.99	0.45
1:I:73:ASP:HB3	1:I:76:LYS:NZ	2.32	0.45
2:J:138:ASN:HA	2:J:172:THR:HB	1.98	0.45
5:K:149:GLU:O	5:K:150:SER:C	2.55	0.45
5:K:609:TYR:HE2	5:K:648:ILE:HD12	1.82	0.45
2:H:139:PHE:HE2	2:H:142:ARG:HA	1.82	0.45
4:F:156:PHE:HB3	4:F:157:PRO:HD3	1.99	0.45
2:H:145:LYS:HB3	2:H:197:THR:HB	1.98	0.45
2:C:39:LYS:HB2	2:C:42:LYS:HB2	1.99	0.45
5:D:1091:VAL:HG12	5:A:901:TYR:OH	2.15	0.45
5:A:377:TYR:H	5:A:429:CYS:HB3	1.81	0.45
1:B:155:LYS:HD3	1:B:189:SER:HB2	1.97	0.45
1:B:162:VAL:HG11	1:B:190:LEU:HD21	1.99	0.45
2:C:120:PRO:HD3	2:C:132:VAL:HG22	1.98	0.45
4:F:52:VAL:HG12	4:F:55:SER:H	1.80	0.45
5:D:142:LYS:HB2	5:D:242:HIS:CG	2.52	0.45
5:K:145:LYS:HA	5:K:145:LYS:HD3	1.48	0.45
5:A:82:LEU:O	5:A:235:PHE:N	2.44	0.45
2:C:7:SER:HB2	2:C:8:PRO:HD3	1.98	0.45
3:E:36:TRP:CE2	3:E:74:LEU:HB2	2.52	0.45
5:K:167:SER:OG	5:K:168:GLN:N	2.50	0.45
5:A:986:ALA:O	5:A:990:ILE:HG12	2.17	0.45
5:K:220:LEU:HD12	5:K:220:LEU:HA	1.85	0.45
5:A:121:ALA:HB3	9:A:1305:NAG:H81	1.99	0.45
1:B:72:ARG:HB2	1:B:79:LEU:HD12	1.98	0.44
2:C:3:GLN:HE22	2:C:5:THR:HG22	1.82	0.44
5:K:92:SER:OG	5:K:94:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:142:LYS:HB2	5:K:242:HIS:CD2	2.52	0.44
5:K:985:GLU:O	5:K:988:VAL:HG12	2.17	0.44
5:A:143:ASN:O	5:A:146:SER:OG	2.34	0.44
5:A:449:LEU:HG	5:A:491:SER:HB3	1.99	0.44
2:J:19:VAL:HG23	2:J:78:LEU:HD11	2.00	0.44
5:D:808:LYS:HE3	5:D:817:ASP:OD2	2.18	0.44
5:D:1050:PRO:O	5:D:1051:GLN:NE2	2.35	0.44
5:K:1142:LEU:HD23	5:K:1142:LEU:HA	1.84	0.44
5:A:430:VAL:HG12	5:A:509:VAL:HG22	1.99	0.44
2:J:136:LEU:HB2	2:J:175:LEU:HB3	1.99	0.44
5:D:406:GLN:NE2	5:D:413:GLY:HA3	2.32	0.44
5:A:454:ARG:HD2	5:A:455:LYS:N	2.30	0.44
1:B:64:VAL:HB	1:B:68:PHE:CD2	2.52	0.44
5:K:977:ILE:O	5:K:981:LEU:HB3	2.17	0.44
5:A:107:THR:HA	5:A:234:ARG:HH11	1.82	0.44
1:I:213:LYS:HB2	1:I:213:LYS:HE2	1.75	0.44
5:A:331:ASN:O	5:A:359:VAL:HG12	2.17	0.44
5:A:739:ILE:O	5:A:997:ARG:NH1	2.48	0.44
3:E:24:ARG:HH21	3:E:72:PHE:H	1.66	0.44
3:E:191:LYS:HA	3:E:212:ARG:HD3	2.00	0.44
5:K:291:ASP:OD1	5:K:291:ASP:N	2.50	0.44
5:A:37:TYR:HB3	5:A:220:LEU:HB2	2.00	0.44
1:B:35:HIS:CE1	1:B:99:ASP:HB2	2.52	0.44
5:D:654:ASN:OD1	9:D:1303:NAG:N2	2.51	0.44
5:K:101:GLY:HA3	5:K:238:LEU:HD12	1.99	0.44
5:A:399:ILE:HG22	5:A:400:ARG:N	2.31	0.44
5:A:521:VAL:HG12	5:A:521:VAL:O	2.17	0.44
2:H:90:GLN:NE2	2:H:95:PRO:O	2.51	0.44
5:K:414:ASN:OD1	5:K:415:ILE:N	2.49	0.44
5:A:729:THR:HB	5:A:952:ASN:ND2	2.33	0.44
1:G:82:GLN:HE21	1:G:84:ASN:HD21	1.66	0.44
1:G:99:ASP:OD1	1:G:100:ARG:N	2.46	0.44
4:F:72:ARG:HD2	4:F:74:MET:HE3	1.99	0.44
5:D:196:PHE:N	5:D:226:LEU:O	2.49	0.44
1:B:76:LYS:O	1:B:77:LYS:HG3	2.18	0.43
5:D:391:ASN:HB2	5:D:513:GLU:OE1	2.18	0.43
5:D:1083:LYS:HD3	5:D:1119:VAL:HG11	1.99	0.43
5:K:153:ARG:HH11	5:K:153:ARG:HB3	1.83	0.43
1:G:49:SER:HB2	1:G:60:TYR:CE1	2.53	0.43
1:B:101:HIS:ND1	1:B:109:VAL:O	2.48	0.43
5:D:821:ASN:O	5:D:824:THR:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:740:CYS:HB3	5:K:746:CYS:HB3	1.93	0.43
5:A:127:LYS:HD2	5:A:164:GLU:OE1	2.18	0.43
5:A:700:ASN:OD1	5:A:701:SER:N	2.51	0.43
3:E:71:ASP:OD1	3:E:71:ASP:N	2.51	0.43
2:J:39:LYS:HB2	2:J:42:LYS:HB2	2.00	0.43
5:D:767:ILE:O	5:D:771:GLN:HG2	2.18	0.43
5:K:454:ARG:CZ	5:K:458:LEU:HG	2.48	0.43
4:F:1:GLN:NE2	4:F:2:MET:O	2.52	0.43
5:D:1035:LYS:HE2	5:D:1035:LYS:HB3	1.81	0.43
5:K:148:MET:HE2	5:K:148:MET:HB3	1.89	0.43
2:C:142:ARG:O	2:C:142:ARG:HD3	2.19	0.43
3:E:22:SER:HB3	3:E:24:ARG:NH1	2.34	0.43
5:D:490:ARG:HH11	5:A:372:PHE:HE2	1.65	0.43
5:K:104:PHE:HB3	5:K:232:ILE:HD12	2.00	0.43
5:K:144:ASN:HB2	5:K:149:GLU:HB3	2.00	0.43
5:K:339:PHE:HE1	5:K:508:VAL:HG11	1.84	0.43
5:K:454:ARG:NH2	5:K:458:LEU:HG	2.34	0.43
5:K:1083:LYS:HD2	5:K:1119:VAL:HG11	2.00	0.43
4:F:12:LYS:HD2	4:F:12:LYS:HA	1.79	0.43
5:D:141:HIS:CD2	5:D:142:LYS:HG2	2.54	0.43
5:A:1139:GLN:HG3	5:A:1140:PRO:HD3	1.99	0.43
5:D:621:ILE:HG22	5:D:622:HIS:N	2.31	0.43
5:A:325:ARG:HH21	5:A:577:GLN:HB2	1.84	0.43
5:A:454:ARG:HE	5:A:456:SER:H	1.67	0.43
3:E:24:ARG:HH21	3:E:72:PHE:N	2.17	0.43
4:F:11:VAL:HG22	4:F:120:THR:HB	1.99	0.43
1:I:70:ILE:HD11	1:I:79:LEU:HD21	2.00	0.43
5:D:357:ASN:O	5:D:357:ASN:ND2	2.36	0.43
5:K:514:LEU:H	5:K:514:LEU:HD23	1.83	0.43
1:I:104:SER:HB2	2:J:94:TYR:CE1	2.53	0.43
5:D:521:VAL:HG12	5:D:521:VAL:O	2.19	0.43
5:K:986:ALA:O	5:K:990:ILE:HD12	2.18	0.43
2:C:139:PHE:CZ	2:C:175:LEU:HB2	2.53	0.43
4:F:56:GLY:HA2	4:F:72:ARG:HE	1.84	0.43
5:D:109:ASP:OD1	5:D:109:ASP:N	2.51	0.43
5:D:134:CYS:SG	5:D:135:ASN:N	2.92	0.43
5:D:819:LEU:HD22	5:D:942:LEU:HD21	2.01	0.43
2:H:108:ARG:HE	2:H:171:SER:HB2	1.82	0.42
3:E:50:TYR:HE1	3:E:56:ALA:HA	1.83	0.42
5:K:128:VAL:HG13	5:K:128:VAL:O	2.19	0.42
5:K:163:PHE:CG	5:K:228:ILE:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:115:LEU:HD21	5:A:228:ILE:HD12	2.01	0.42
5:A:805:ASP:OD1	5:A:805:ASP:N	2.51	0.42
3:E:125:GLN:HE22	3:E:132:SER:HB2	1.83	0.42
3:E:193:TYR:HB2	3:E:210:PHE:CE1	2.54	0.42
2:J:4:LEU:HD13	2:J:25:ALA:HB2	2.00	0.42
2:J:31:SER:HA	2:J:71:PHE:HZ	1.84	0.42
5:K:966:LYS:HE2	5:K:966:LYS:HB2	1.73	0.42
2:H:37:GLN:HB2	2:H:47:LEU:HD11	2.01	0.42
5:A:103:ILE:HG13	5:A:236:GLN:HB3	2.01	0.42
5:A:822:LYS:HZ2	5:A:940:SER:HB3	1.85	0.42
5:A:836:ASP:OD1	5:A:836:ASP:N	2.50	0.42
5:D:277:ASN:HB3	5:D:283:THR:HG23	2.01	0.42
5:D:325:ARG:HA	5:D:325:ARG:HD2	1.90	0.42
5:K:454:ARG:HH21	5:K:457:ASN:HA	1.85	0.42
5:A:707:ASN:OD1	5:A:707:ASN:N	2.52	0.42
2:J:31:SER:HA	2:J:71:PHE:CZ	2.54	0.42
5:K:98:ILE:O	5:K:240:ALA:N	2.52	0.42
5:A:755:SER:O	5:A:759:GLN:NE2	2.46	0.42
3:E:50:TYR:O	3:E:54:SER:OG	2.25	0.42
5:D:148:MET:HB2	5:D:149:GLU:H	1.64	0.42
5:D:631:ARG:H	5:D:631:ARG:HD3	1.83	0.42
5:D:749:LEU:HG	5:D:990:ILE:HD11	2.00	0.42
5:D:930:LYS:HE2	5:D:930:LYS:HB2	1.84	0.42
5:K:21:ARG:HG2	5:K:77:PHE:CE1	2.55	0.42
5:K:243:ARG:HD2	5:K:243:ARG:HA	1.90	0.42
5:K:363:SER:HA	5:K:366:TYR:CE2	2.55	0.42
1:I:18:LEU:HB3	1:I:83:MET:HG3	2.02	0.42
1:I:171:LEU:HD21	1:I:194:VAL:HG21	2.00	0.42
5:K:602:SER:OG	5:K:603:ASN:N	2.53	0.42
5:K:789:PRO:HG2	5:A:704:TYR:HB3	2.01	0.42
5:K:901:TYR:OH	5:A:1091:VAL:HG12	2.18	0.42
1:G:76:LYS:HB3	1:G:76:LYS:HE3	1.82	0.42
1:B:34:LEU:O	1:B:51:ILE:N	2.52	0.42
5:K:1088:ARG:HB3	5:K:1089:GLU:OE1	2.19	0.42
5:A:182:LYS:H	5:A:208:ARG:HH12	1.68	0.42
1:G:97:VAL:HG21	1:G:112:PHE:CD2	2.54	0.42
2:H:34:ALA:HB3	2:H:89:GLN:HE21	1.85	0.42
2:J:4:LEU:HD12	2:J:5:THR:H	1.85	0.42
5:D:700:ASN:OD1	5:D:701:SER:N	2.52	0.42
2:C:26:SER:OG	2:C:27:GLN:OE1	2.35	0.42
2:C:38:GLN:HB3	2:C:85:THR:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:740:CYS:HB3	5:D:746:CYS:HB3	1.82	0.42
1:G:98:LYS:HB3	1:G:114:ILE:HG22	2.02	0.41
1:G:154:VAL:HG11	1:G:162:VAL:HG11	2.01	0.41
2:C:189:HIS:HB2	2:C:192:TYR:OH	2.19	0.41
3:E:83:ASP:O	3:E:87:TYR:OH	2.29	0.41
1:I:67:ARG:O	1:I:84:ASN:HB2	2.20	0.41
5:D:631:ARG:HG2	5:D:632:VAL:N	2.35	0.41
5:K:209:GLU:O	5:K:211:GLU:N	2.51	0.41
5:K:242:HIS:CG	5:K:243:ARG:N	2.88	0.41
5:A:1097:THR:OG1	5:A:1098:HIS:ND1	2.45	0.41
1:B:53:TRP:CD1	1:B:102:TYR:HB2	2.55	0.41
2:C:4:LEU:HD11	2:C:90:GLN:HB3	2.02	0.41
2:C:94:TYR:N	2:C:95:PRO:HD3	2.35	0.41
3:E:142:PRO:HD2	3:E:199:HIS:NE2	2.35	0.41
5:D:21:ARG:HE	5:D:77:PHE:HB3	1.84	0.41
5:D:187:PHE:HB3	5:D:189:PHE:CE1	2.55	0.41
5:D:852:PHE:CD1	5:K:586:PRO:HG2	2.55	0.41
5:K:120:ASN:HD22	9:K:1310:NAG:H61	1.85	0.41
5:A:834:TYR:HD1	5:A:837:CYS:HB3	1.83	0.41
5:K:78:ASP:N	5:K:78:ASP:OD1	2.52	0.41
5:K:455:LYS:HD2	5:K:470:TYR:CD1	2.55	0.41
5:K:833:GLN:NE2	5:K:849:ALA:HB3	2.35	0.41
5:A:19:THR:N	5:A:75:LYS:HE3	2.36	0.41
5:A:338:VAL:HG23	5:A:339:PHE:CD1	2.54	0.41
1:G:33:ALA:HB2	1:G:103:ASP:N	2.35	0.41
2:H:189:HIS:HB2	2:H:192:TYR:OH	2.21	0.41
1:B:14:PRO:HD3	1:B:124:SER:O	2.21	0.41
1:B:98:LYS:HD3	1:B:114:ILE:HB	2.03	0.41
4:F:47:TRP:CZ2	4:F:49:GLY:HA2	2.55	0.41
2:J:35:TRP:CE2	2:J:73:LEU:HB2	2.55	0.41
5:D:430:VAL:HG12	5:D:509:VAL:HG22	2.03	0.41
5:D:490:ARG:HD2	5:A:372:PHE:HE2	1.84	0.41
5:K:57:PRO:HB3	5:K:270:ARG:HE	1.84	0.41
5:A:414:ASN:OD1	5:A:414:ASN:N	2.54	0.41
3:E:114:PRO:HB3	3:E:140:PHE:CD1	2.55	0.41
1:I:68:PHE:HB3	1:I:81:LEU:HD21	2.01	0.41
1:I:154:VAL:HG12	1:I:157:TYR:CE1	2.55	0.41
5:D:903:PHE:CD2	5:D:913:LEU:HB2	2.55	0.41
5:K:439:ASP:HB3	5:K:448:TYR:HE2	1.85	0.41
1:I:59:GLY:HA3	2:J:94:TYR:CE2	2.55	0.41
1:I:82:GLN:NE2	1:I:84:ASN:HD21	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:287:ASP:O	5:D:294:SER:HB3	2.21	0.41
5:K:127:LYS:HE3	5:K:131:PHE:HZ	1.86	0.41
5:K:200:SER:HB3	5:K:223:LEU:HD11	2.02	0.41
5:A:430:VAL:HG12	5:A:509:VAL:HG13	2.02	0.41
4:F:5:VAL:HB	4:F:23:LYS:HE3	2.03	0.41
1:I:18:LEU:HG	1:I:19:ARG:H	1.86	0.41
1:I:53:TRP:CD1	1:I:102:TYR:HD1	2.37	0.41
1:I:99:ASP:OD1	1:I:100:ARG:N	2.47	0.41
5:D:528:THR:HG22	5:D:529:ASN:N	2.32	0.41
5:K:321:GLU:HG3	5:K:536:VAL:HG23	2.03	0.41
5:K:347:VAL:HG22	5:K:419:ASN:HB3	2.01	0.41
5:K:608:LEU:HB2	5:K:647:LEU:HD13	2.03	0.41
5:A:182:LYS:HG3	5:A:208:ARG:HH11	1.85	0.41
5:A:1088:ARG:HE	5:A:1118:PHE:HB3	1.86	0.41
3:E:11:LEU:HD23	3:E:105:VAL:HG22	2.03	0.41
5:D:137:PRO:HB2	5:D:238:LEU:HD22	2.03	0.41
5:D:372:PHE:CD2	5:D:374:PHE:HB2	2.55	0.41
5:K:102:TRP:HB3	5:K:104:PHE:CZ	2.56	0.41
5:A:398:VAL:HG22	5:A:506:ARG:HG2	2.03	0.41
5:A:471:GLN:NE2	5:A:476:PRO:HA	2.36	0.41
2:H:61:ARG:HD2	2:H:77:SER:O	2.20	0.41
4:F:9:PRO:HB3	4:F:118:MET:HB2	2.02	0.41
5:D:289:ALA:O	5:D:629:THR:HB	2.21	0.41
5:D:323:ILE:HG23	5:D:529:ASN:O	2.21	0.41
5:D:428:GLY:HA2	5:D:512:PHE:CD2	2.56	0.41
5:K:393:TYR:O	5:K:511:SER:N	2.46	0.41
5:K:833:GLN:HE22	5:K:849:ALA:HB3	1.86	0.41
5:A:101:GLY:HA3	5:A:238:LEU:HB2	2.03	0.41
5:A:539:ASN:HA	5:A:544:LYS:HG2	2.03	0.41
5:A:875:LEU:HD21	5:A:1049:PHE:HB3	2.03	0.41
4:F:51:ILE:HG13	4:F:57:ASN:O	2.20	0.41
2:J:6:GLN:H	2:J:100:GLN:NE2	2.19	0.41
2:J:32:TYR:HD2	2:J:91:LEU:O	2.03	0.41
2:J:38:GLN:HA	2:J:44:PRO:HA	2.03	0.41
5:D:242:HIS:O	5:D:243:ARG:HG3	2.21	0.41
5:K:168:GLN:H	5:K:168:GLN:CD	2.24	0.41
5:A:93:ILE:HA	5:A:183:ASN:O	2.21	0.41
5:A:127:LYS:HG2	5:A:131:PHE:HZ	1.86	0.41
1:B:24:ALA:HB3	1:B:29:PHE:CZ	2.56	0.40
4:F:122:SER:HB3	4:F:156:PHE:CE1	2.56	0.40
5:D:619:VAL:O	5:D:621:ILE:HD12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:395:ASP:HB2	5:K:509:VAL:HB	2.03	0.40
5:K:799:PHE:HD1	5:K:802:ILE:HD11	1.86	0.40
5:A:89:TYR:CG	5:A:89:TYR:O	2.74	0.40
5:A:400:ARG:HE	5:A:502:HIS:HA	1.85	0.40
1:I:36:TRP:CZ3	1:I:96:CYS:HB3	2.56	0.40
5:D:139:LEU:O	5:D:241:LEU:N	2.54	0.40
5:K:339:PHE:CE1	5:K:508:VAL:HG11	2.57	0.40
5:K:738:TYR:HE1	5:K:963:LEU:HD11	1.87	0.40
5:A:452:LEU:HD11	5:A:490:ARG:HB3	2.03	0.40
2:H:119:PRO:HB3	2:H:209:PHE:CE2	2.56	0.40
3:E:114:PRO:HD2	3:E:202:LEU:HG	2.03	0.40
2:J:113:PRO:HD3	2:J:198:HIS:ND1	2.37	0.40
5:A:514:LEU:C	5:A:515:LEU:HD12	2.41	0.40
1:B:64:VAL:HB	1:B:68:PHE:CE2	2.56	0.40
1:G:135:PRO:HD3	1:G:221:LYS:HE2	2.04	0.40
2:C:210:ASN:HB3	2:C:213:GLU:HB2	2.03	0.40
4:F:94:TYR:HE2	4:F:119:VAL:HB	1.86	0.40
1:I:18:LEU:N	1:I:83:MET:HB2	2.30	0.40
5:K:94:GLU:HB3	5:K:96:SER:O	2.21	0.40
5:A:414:ASN:O	5:A:418:TYR:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	226/228 (99%)	214 (95%)	11 (5%)	1 (0%)	34 69
1	G	226/228 (99%)	216 (96%)	9 (4%)	1 (0%)	34 69
1	I	226/228 (99%)	218 (96%)	8 (4%)	0	100 100
2	C	212/214 (99%)	199 (94%)	13 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	212/214 (99%)	201 (95%)	11 (5%)	0	100	100
2	J	212/214 (99%)	198 (93%)	14 (7%)	0	100	100
3	E	213/215 (99%)	204 (96%)	9 (4%)	0	100	100
4	F	219/221 (99%)	211 (96%)	7 (3%)	1 (0%)	29	65
5	A	1090/1285 (85%)	1027 (94%)	60 (6%)	3 (0%)	41	74
5	D	1093/1285 (85%)	1021 (93%)	66 (6%)	6 (0%)	29	65
5	K	1086/1285 (84%)	1014 (93%)	68 (6%)	4 (0%)	34	69
All	All	5015/5617 (89%)	4723 (94%)	276 (6%)	16 (0%)	44	74

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	162	VAL
5	D	151	GLU
5	D	519	ALA
5	K	519	ALA
4	F	160	VAL
5	D	373	THR
5	D	623	ALA
5	A	592	VAL
5	A	632	VAL
1	B	160	GLU
5	D	145	LYS
5	K	152	PHE
5	A	519	ALA
5	K	125	VAL
5	D	632	VAL
5	K	206	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	192/192 (100%)	190 (99%)	2 (1%)	76 91
1	G	192/192 (100%)	189 (98%)	3 (2%)	62 85
1	I	192/192 (100%)	189 (98%)	3 (2%)	62 85
2	C	187/187 (100%)	181 (97%)	6 (3%)	39 72
2	H	187/187 (100%)	185 (99%)	2 (1%)	73 90
2	J	187/187 (100%)	184 (98%)	3 (2%)	62 85
3	E	185/185 (100%)	185 (100%)	0	100 100
4	F	186/186 (100%)	184 (99%)	2 (1%)	73 90
5	A	956/1113 (86%)	951 (100%)	5 (0%)	88 95
5	D	956/1113 (86%)	946 (99%)	10 (1%)	76 91
5	K	956/1113 (86%)	947 (99%)	9 (1%)	78 91
All	All	4376/4847 (90%)	4331 (99%)	45 (1%)	77 91

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	158	PHE
1	G	160	GLU
1	G	162	VAL
2	H	93	SER
2	H	96	VAL
1	B	77	LYS
1	B	158	PHE
2	C	12	SER
2	C	108	ARG
2	C	109	THR
2	C	140	TYR
2	C	142	ARG
2	C	171	SER
4	F	158	GLU
4	F	212	PRO
1	I	158	PHE
1	I	160	GLU
1	I	162	VAL
2	J	94	TYR
2	J	106	ILE
2	J	109	THR
5	D	21	ARG
5	D	143	ASN

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Mol	Chain	Res	Type
5	D	146	SER
5	D	148	MET
5	D	357	ASN
5	D	525	LYS
5	D	526	LYS
5	D	527	SER
5	D	529	ASN
5	D	631	ARG
5	K	141	HIS
5	K	142	LYS
5	K	144	ASN
5	K	145	LYS
5	K	146	SER
5	K	148	MET
5	K	149	GLU
5	K	150	SER
5	K	152	PHE
5	A	144	ASN
5	A	148	MET
5	A	149	GLU
5	A	150	SER
5	A	242	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	84	ASN
1	B	35	HIS
1	B	82	GLN
3	E	125	GLN
4	F	209	ASN
1	I	84	ASN
5	D	419	ASN
5	A	141	HIS
5	A	242	HIS
5	A	471	GLN
5	A	923	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

38 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	L	1	6,5	14,14,15	0.38	0	17,19,21	0.71	0
6	NAG	L	2	6	14,14,15	0.41	0	17,19,21	0.51	0
6	NAG	M	1	6,5	14,14,15	0.54	0	17,19,21	1.21	1 (5%)
6	NAG	M	2	6	14,14,15	0.24	0	17,19,21	0.43	0
6	NAG	N	1	6,5	14,14,15	0.31	0	17,19,21	0.48	0
6	NAG	N	2	6	14,14,15	0.52	0	17,19,21	0.44	0
6	NAG	O	1	6,5	14,14,15	0.57	0	17,19,21	1.00	1 (5%)
6	NAG	O	2	6	14,14,15	0.33	0	17,19,21	0.41	0
6	NAG	P	1	6,5	14,14,15	0.23	0	17,19,21	0.48	0
6	NAG	P	2	6	14,14,15	0.24	0	17,19,21	0.38	0
6	NAG	Q	1	6,5	14,14,15	0.22	0	17,19,21	0.52	0
6	NAG	Q	2	6	14,14,15	0.23	0	17,19,21	0.44	0
6	NAG	R	1	6,5	14,14,15	0.21	0	17,19,21	0.48	0
6	NAG	R	2	6	14,14,15	0.21	0	17,19,21	0.42	0
6	NAG	S	1	6,5	14,14,15	1.17	1 (7%)	17,19,21	2.52	1 (5%)
6	NAG	S	2	6	14,14,15	0.22	0	17,19,21	0.48	0
6	NAG	T	1	6,5	14,14,15	0.26	0	17,19,21	0.47	0
6	NAG	T	2	6	14,14,15	0.24	0	17,19,21	0.51	0
6	NAG	U	1	6,5	14,14,15	0.23	0	17,19,21	0.46	0
6	NAG	U	2	6	14,14,15	0.23	0	17,19,21	0.44	0
6	NAG	V	1	6,5	14,14,15	0.28	0	17,19,21	0.41	0
6	NAG	V	2	6	14,14,15	0.22	0	17,19,21	0.43	0
6	NAG	W	1	6,5	14,14,15	0.20	0	17,19,21	0.42	0
6	NAG	W	2	6	14,14,15	0.25	0	17,19,21	0.43	0
7	NAG	X	1	7,5	14,14,15	0.27	0	17,19,21	0.44	0
7	NAG	X	2	7	14,14,15	0.20	0	17,19,21	0.37	0
7	BMA	X	3	7	11,11,12	0.61	0	15,15,17	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	MAN	X	4	7	11,11,12	0.68	0	15,15,17	0.97	2 (13%)
6	NAG	Y	1	6,5	14,14,15	0.24	0	17,19,21	0.70	0
6	NAG	Y	2	6	14,14,15	1.16	1 (7%)	17,19,21	1.27	1 (5%)
6	NAG	Z	1	6,5	14,14,15	0.23	0	17,19,21	0.51	0
6	NAG	Z	2	6	14,14,15	0.28	0	17,19,21	0.52	0
8	NAG	a	1	8,5	14,14,15	0.22	0	17,19,21	0.47	0
8	NAG	a	2	8	14,14,15	0.22	0	17,19,21	0.38	0
8	BMA	a	3	8	11,11,12	0.60	0	15,15,17	0.73	0
8	NAG	b	1	8,5	14,14,15	0.33	0	17,19,21	0.48	0
8	NAG	b	2	8	14,14,15	0.24	0	17,19,21	0.49	0
8	BMA	b	3	8	11,11,12	0.57	0	15,15,17	0.80	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	L	1	6,5	-	1/6/23/26	0/1/1/1
6	NAG	L	2	6	-	1/6/23/26	0/1/1/1
6	NAG	M	1	6,5	-	2/6/23/26	0/1/1/1
6	NAG	M	2	6	-	2/6/23/26	0/1/1/1
6	NAG	N	1	6,5	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	0/6/23/26	0/1/1/1
6	NAG	O	1	6,5	-	2/6/23/26	0/1/1/1
6	NAG	O	2	6	-	1/6/23/26	0/1/1/1
6	NAG	P	1	6,5	-	1/6/23/26	0/1/1/1
6	NAG	P	2	6	-	1/6/23/26	0/1/1/1
6	NAG	Q	1	6,5	-	3/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	0/6/23/26	0/1/1/1
6	NAG	R	1	6,5	-	3/6/23/26	0/1/1/1
6	NAG	R	2	6	-	2/6/23/26	0/1/1/1
6	NAG	S	1	6,5	-	4/6/23/26	0/1/1/1
6	NAG	S	2	6	-	0/6/23/26	0/1/1/1
6	NAG	T	1	6,5	-	0/6/23/26	0/1/1/1
6	NAG	T	2	6	-	1/6/23/26	0/1/1/1
6	NAG	U	1	6,5	-	0/6/23/26	0/1/1/1
6	NAG	U	2	6	-	4/6/23/26	0/1/1/1
6	NAG	V	1	6,5	-	2/6/23/26	0/1/1/1
6	NAG	V	2	6	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	W	1	6,5	-	0/6/23/26	0/1/1/1
6	NAG	W	2	6	-	2/6/23/26	0/1/1/1
7	NAG	X	1	7,5	-	2/6/23/26	0/1/1/1
7	NAG	X	2	7	-	1/6/23/26	0/1/1/1
7	BMA	X	3	7	-	0/2/19/22	0/1/1/1
7	MAN	X	4	7	-	0/2/19/22	0/1/1/1
6	NAG	Y	1	6,5	-	3/6/23/26	0/1/1/1
6	NAG	Y	2	6	-	4/6/23/26	0/1/1/1
6	NAG	Z	1	6,5	-	3/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	1/6/23/26	0/1/1/1
8	NAG	a	1	8,5	-	0/6/23/26	0/1/1/1
8	NAG	a	2	8	-	1/6/23/26	0/1/1/1
8	BMA	a	3	8	-	0/2/19/22	0/1/1/1
8	NAG	b	1	8,5	-	2/6/23/26	0/1/1/1
8	NAG	b	2	8	-	1/6/23/26	0/1/1/1
8	BMA	b	3	8	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	S	1	NAG	O5-C1	4.17	1.50	1.43
6	Y	2	NAG	O5-C1	4.15	1.50	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	S	1	NAG	C1-O5-C5	9.95	125.67	112.19
6	Y	2	NAG	C1-O5-C5	4.97	118.93	112.19
6	M	1	NAG	C1-O5-C5	4.41	118.17	112.19
6	O	1	NAG	C1-O5-C5	3.46	116.88	112.19
7	X	4	MAN	O2-C2-C3	-2.26	105.61	110.14
7	X	4	MAN	C1-O5-C5	2.06	114.98	112.19

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	b	1	NAG	O5-C5-C6-O6
6	M	2	NAG	O5-C5-C6-O6
6	Y	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	b	1	NAG	C4-C5-C6-O6
6	Y	2	NAG	O5-C5-C6-O6
6	S	1	NAG	C8-C7-N2-C2
6	S	1	NAG	O7-C7-N2-C2
6	U	2	NAG	C8-C7-N2-C2
6	U	2	NAG	O7-C7-N2-C2
6	Y	2	NAG	C8-C7-N2-C2
6	Y	2	NAG	O7-C7-N2-C2
6	S	1	NAG	O5-C5-C6-O6
6	W	2	NAG	O5-C5-C6-O6
6	V	2	NAG	O5-C5-C6-O6
6	Y	2	NAG	C4-C5-C6-O6
6	Y	1	NAG	O5-C5-C6-O6
6	S	1	NAG	C4-C5-C6-O6
6	M	1	NAG	C4-C5-C6-O6
6	U	2	NAG	O5-C5-C6-O6
6	V	2	NAG	C4-C5-C6-O6
7	X	1	NAG	O5-C5-C6-O6
6	W	2	NAG	C4-C5-C6-O6
6	V	1	NAG	O5-C5-C6-O6
6	U	2	NAG	C4-C5-C6-O6
6	V	1	NAG	C4-C5-C6-O6
7	X	1	NAG	C4-C5-C6-O6
6	Q	1	NAG	C4-C5-C6-O6
6	P	1	NAG	O5-C5-C6-O6
7	X	2	NAG	O5-C5-C6-O6
6	O	1	NAG	O5-C5-C6-O6
6	P	2	NAG	O5-C5-C6-O6
6	O	2	NAG	O5-C5-C6-O6
6	M	2	NAG	C4-C5-C6-O6
6	R	1	NAG	C4-C5-C6-O6
6	N	1	NAG	C4-C5-C6-O6
6	Q	1	NAG	O5-C5-C6-O6
6	M	1	NAG	O5-C5-C6-O6
6	R	2	NAG	C4-C5-C6-O6
6	N	1	NAG	O5-C5-C6-O6
6	Z	1	NAG	C4-C5-C6-O6
6	R	1	NAG	O5-C5-C6-O6
6	L	2	NAG	C3-C2-N2-C7
6	Q	1	NAG	C3-C2-N2-C7
6	R	1	NAG	C3-C2-N2-C7
6	T	2	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
6	Y	1	NAG	C3-C2-N2-C7
6	Z	2	NAG	C3-C2-N2-C7
8	b	2	NAG	C3-C2-N2-C7
6	Z	1	NAG	O5-C5-C6-O6
6	R	2	NAG	O5-C5-C6-O6
8	a	2	NAG	O5-C5-C6-O6
6	L	1	NAG	C3-C2-N2-C7
6	O	1	NAG	C3-C2-N2-C7
6	Z	1	NAG	C3-C2-N2-C7

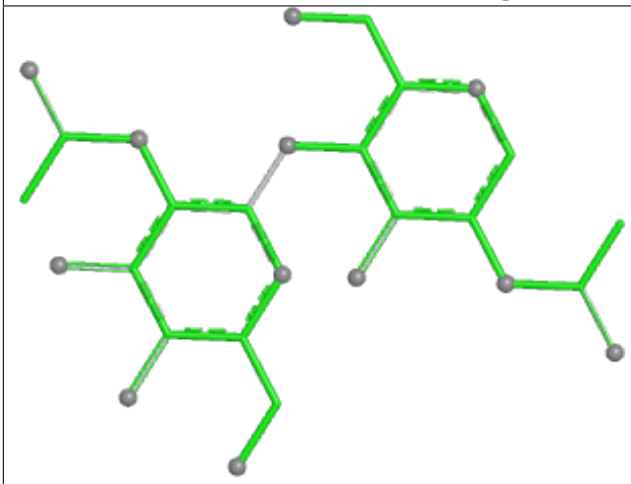
There are no ring outliers.

4 monomers are involved in 6 short contacts:

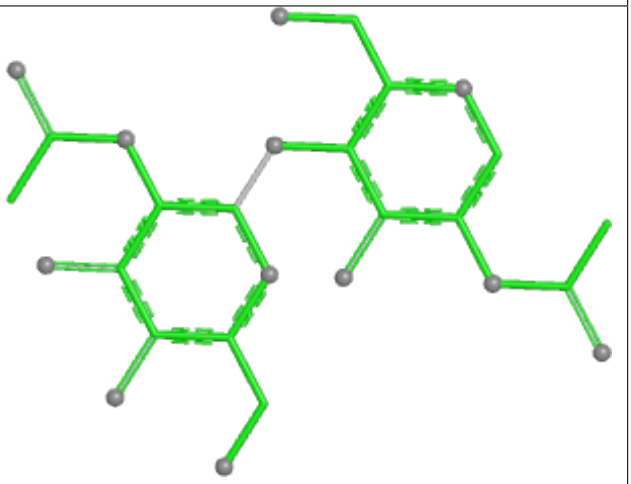
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	S	1	NAG	1	0
6	R	1	NAG	1	0
6	M	1	NAG	3	0
6	Q	1	NAG	1	0

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

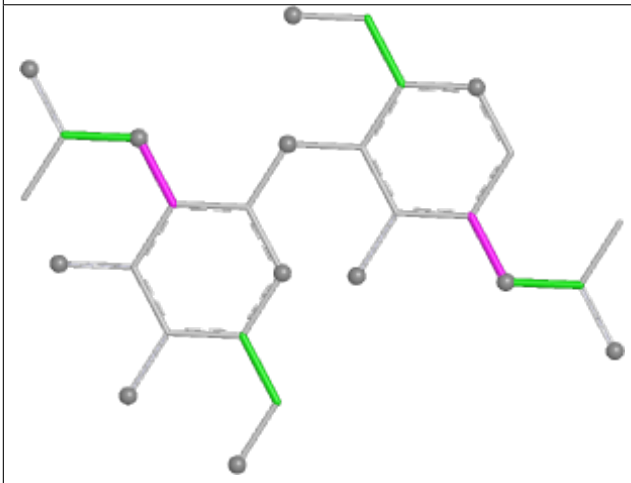
Oligosaccharide Chain L



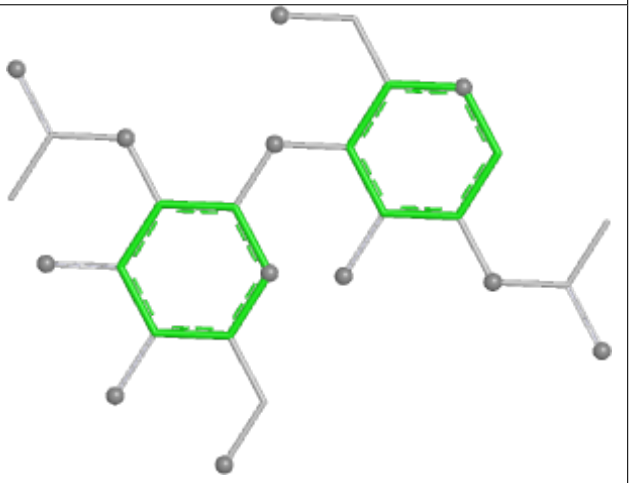
Bond lengths



Bond angles

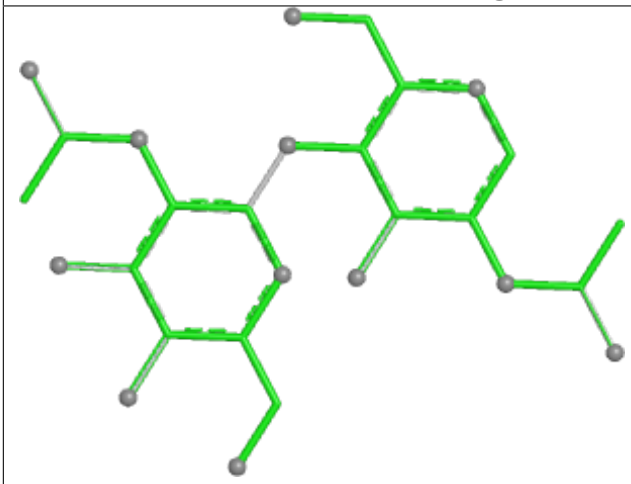


Torsions

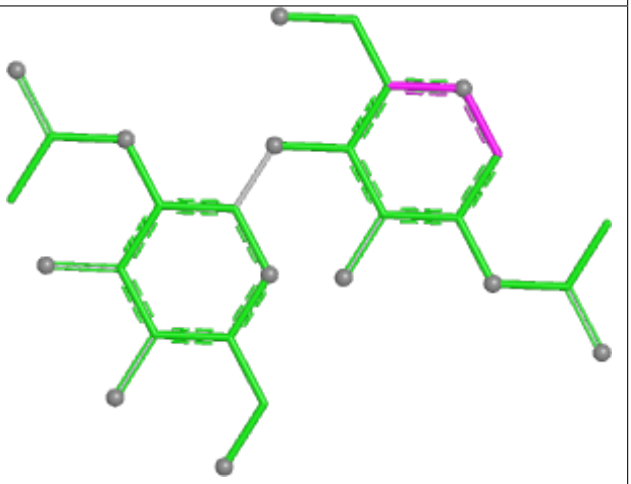


Rings

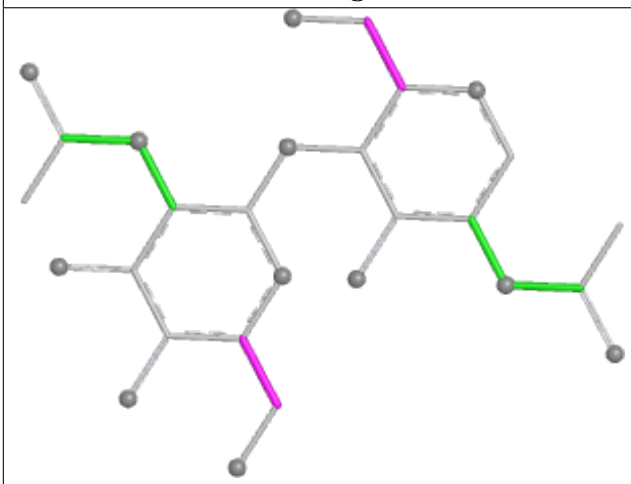
Oligosaccharide Chain M



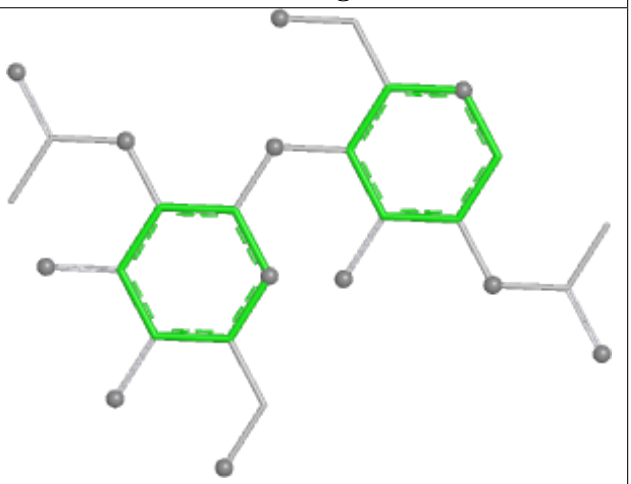
Bond lengths



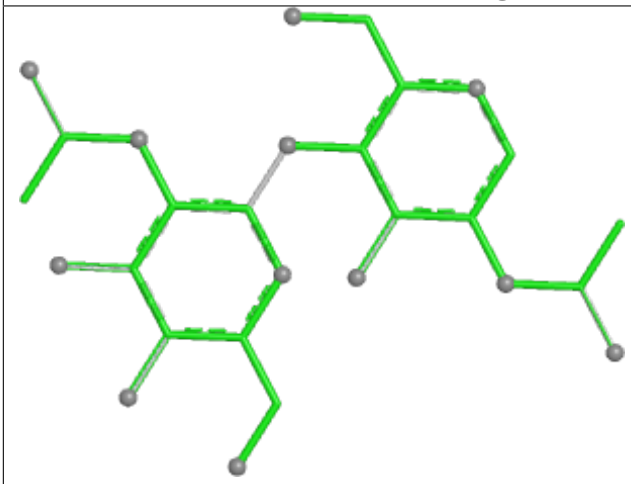
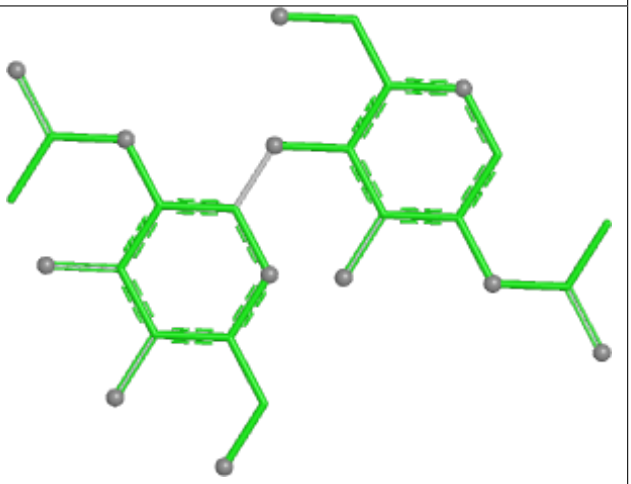
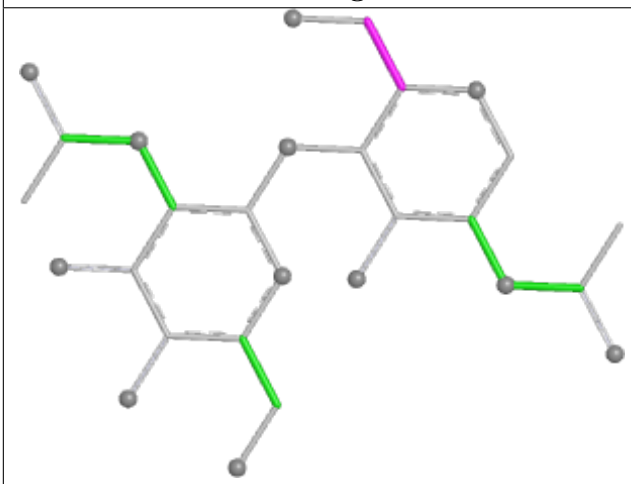
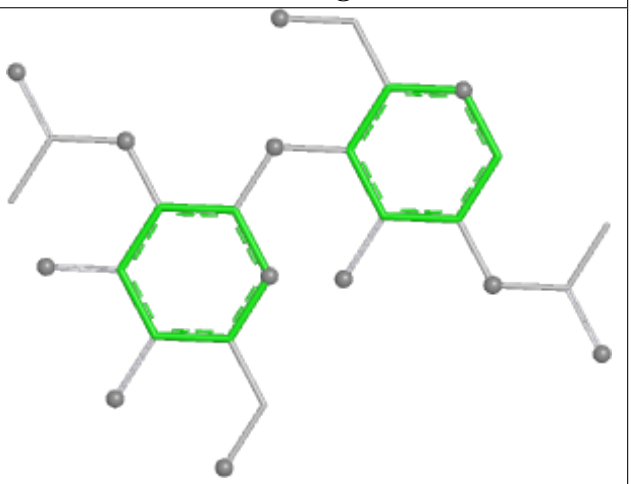
Bond angles



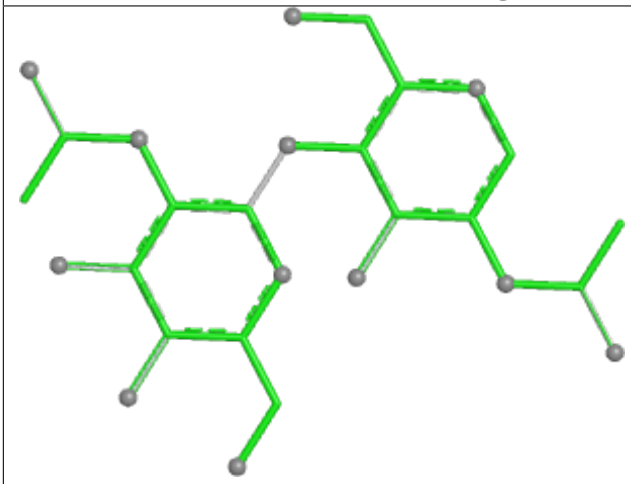
Torsions



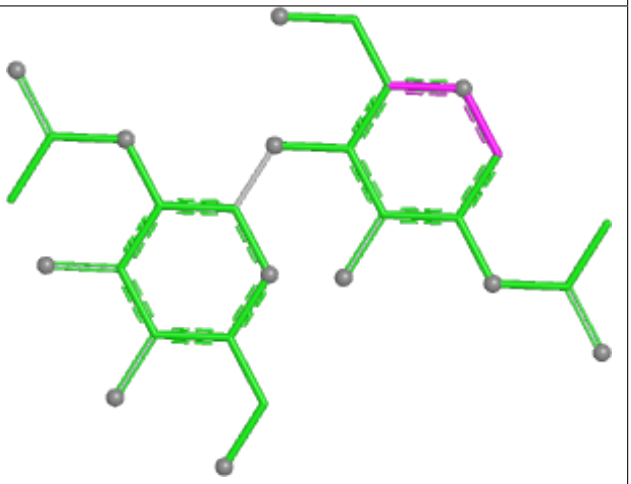
Rings

Oligosaccharide Chain N	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

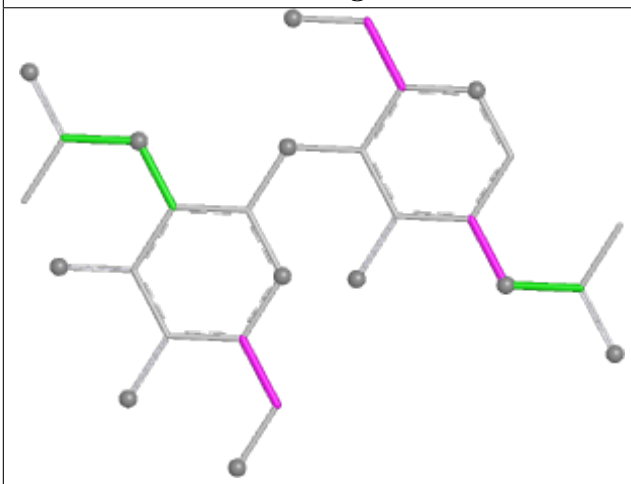
Oligosaccharide Chain O



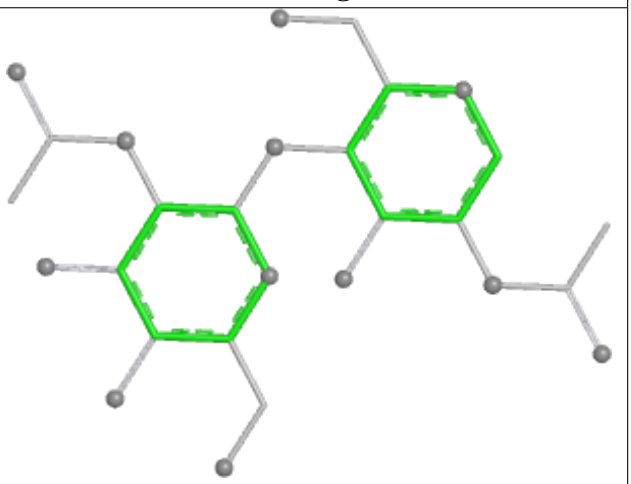
Bond lengths



Bond angles

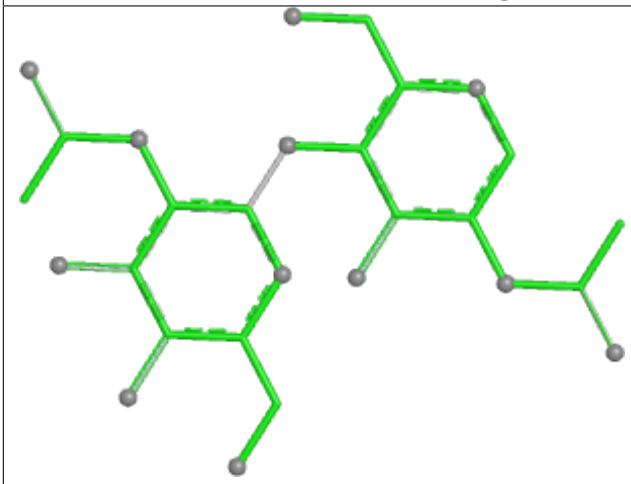


Torsions

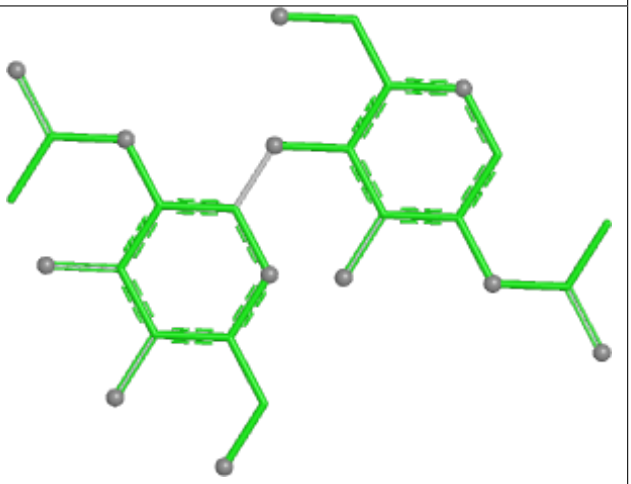


Rings

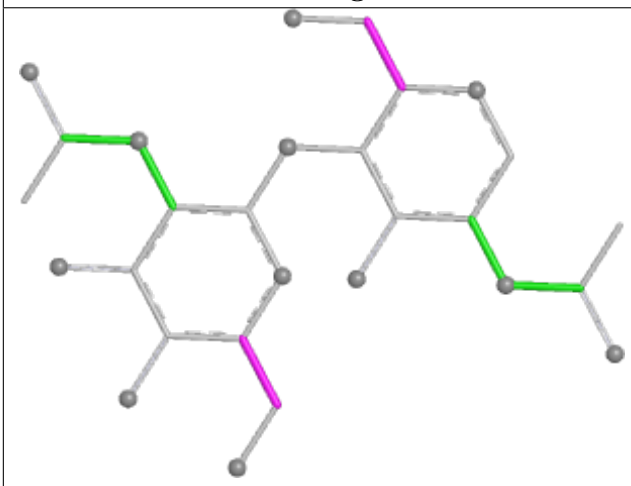
Oligosaccharide Chain P



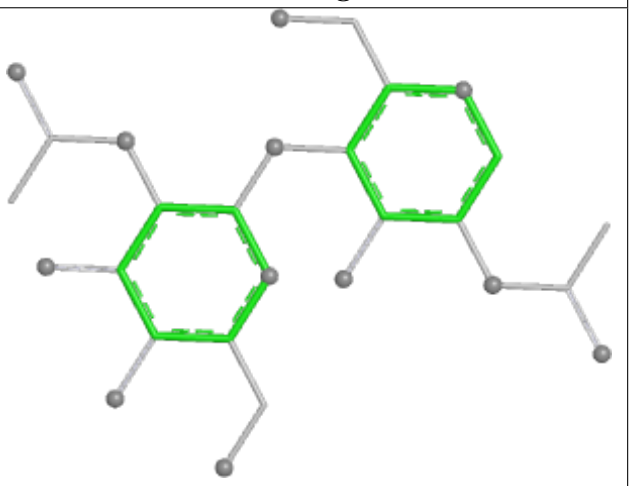
Bond lengths



Bond angles

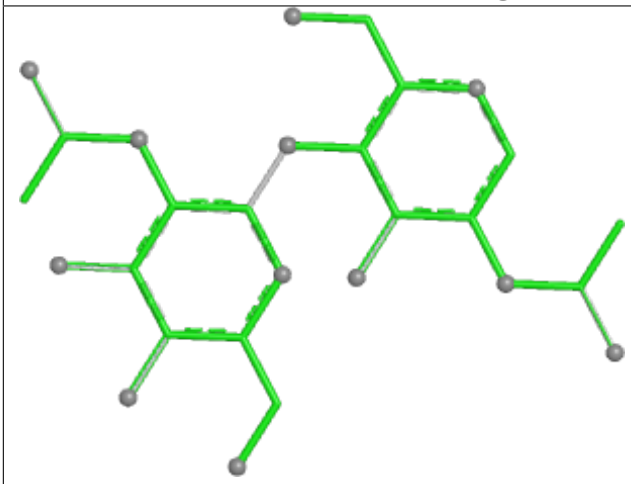


Torsions

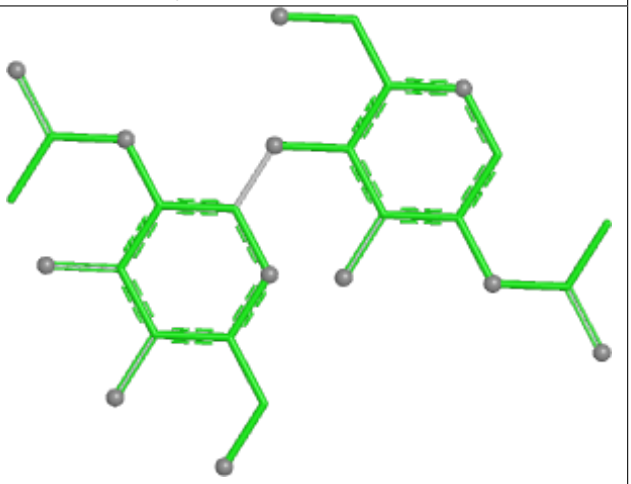


Rings

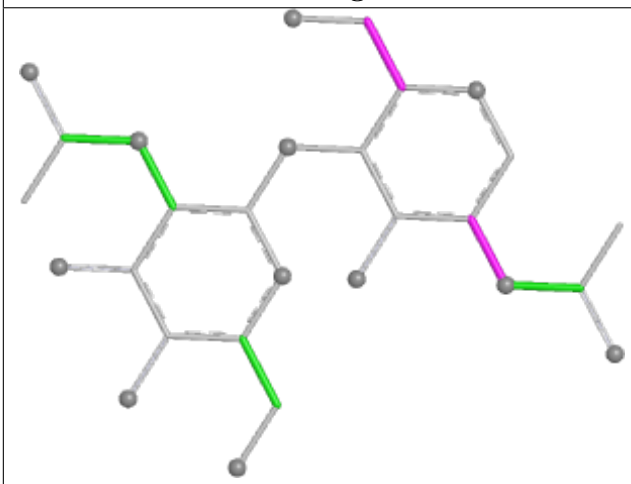
Oligosaccharide Chain Q



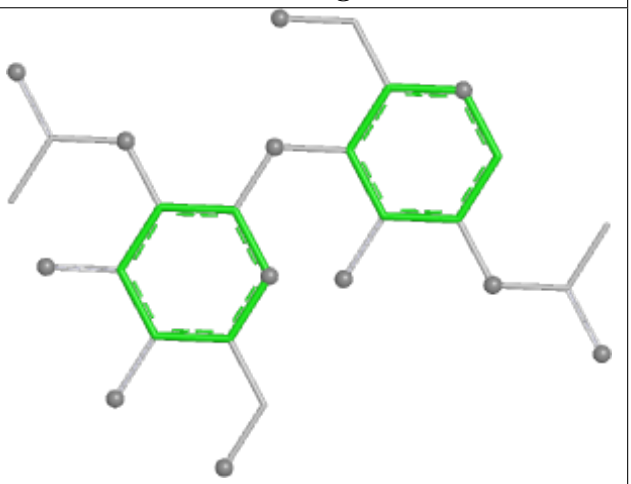
Bond lengths



Bond angles

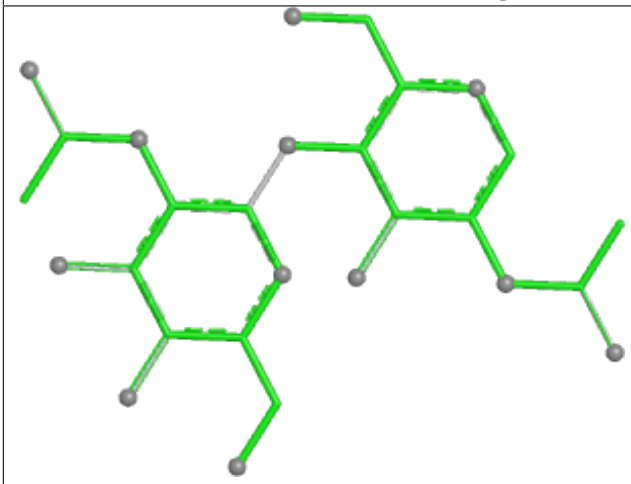


Torsions

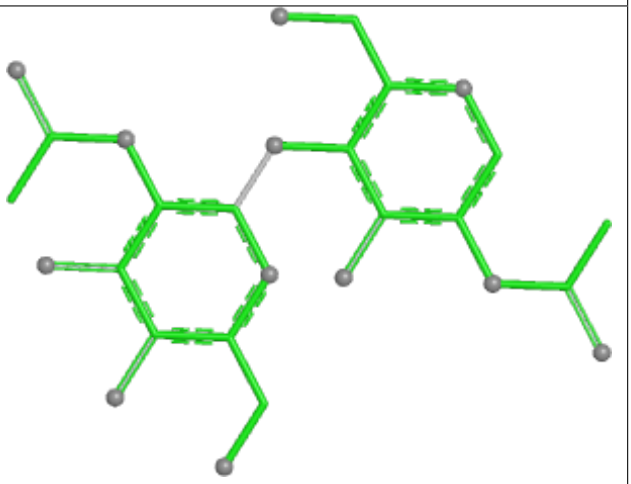


Rings

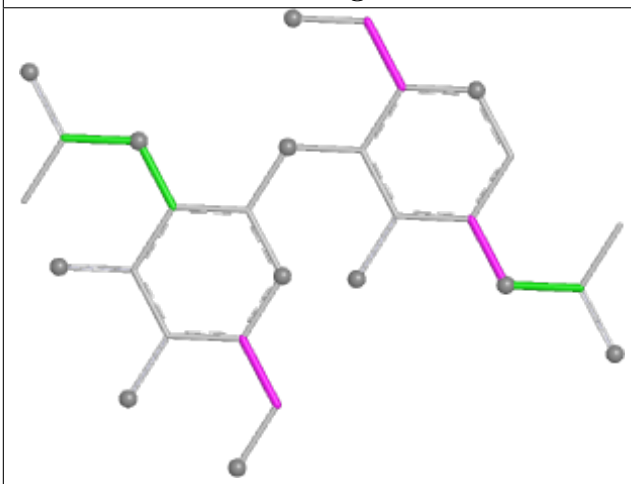
Oligosaccharide Chain R



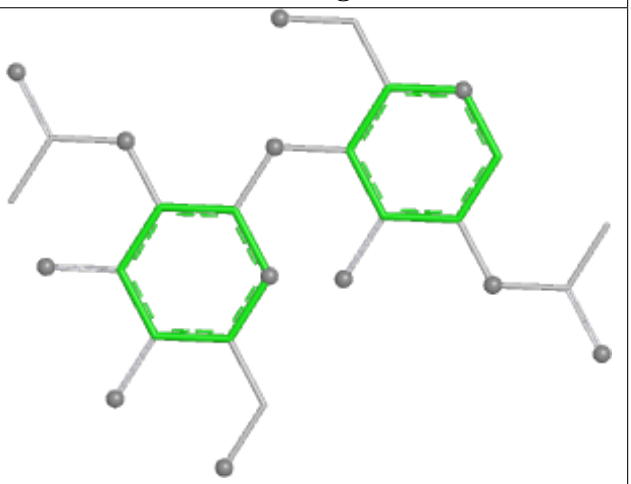
Bond lengths



Bond angles

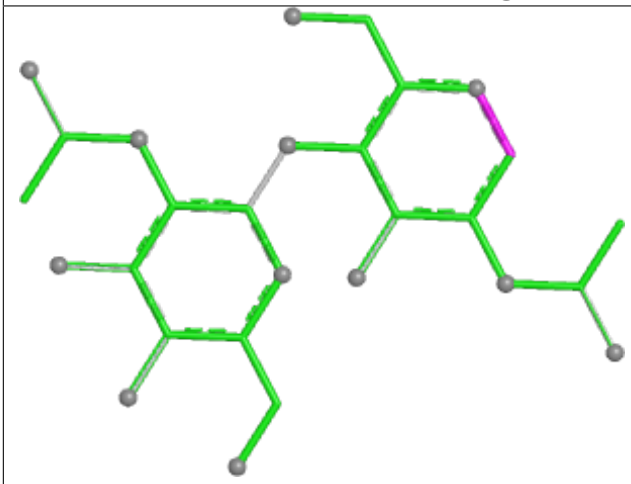


Torsions

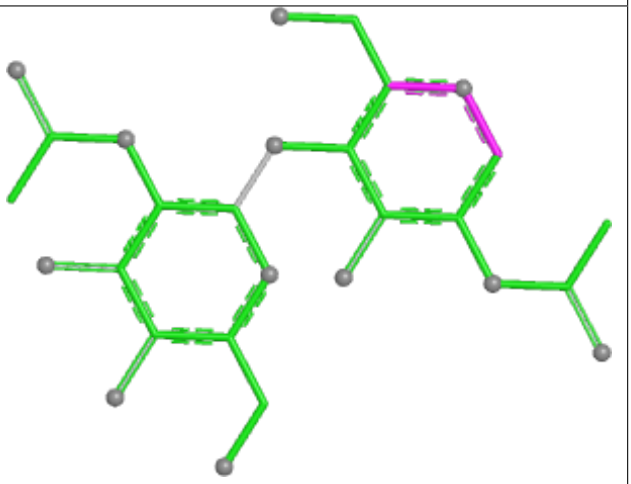


Rings

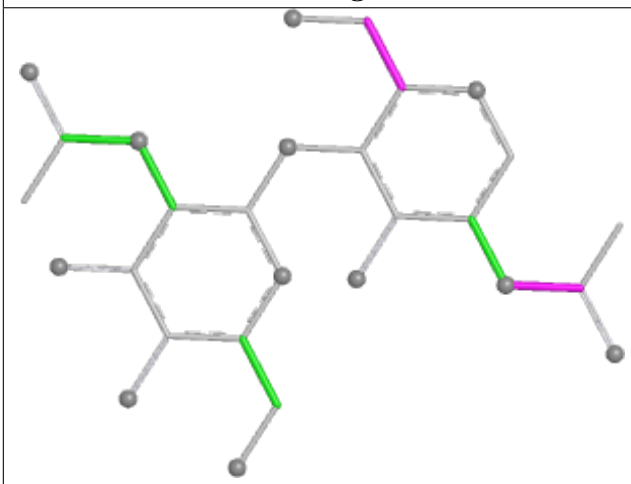
Oligosaccharide Chain S



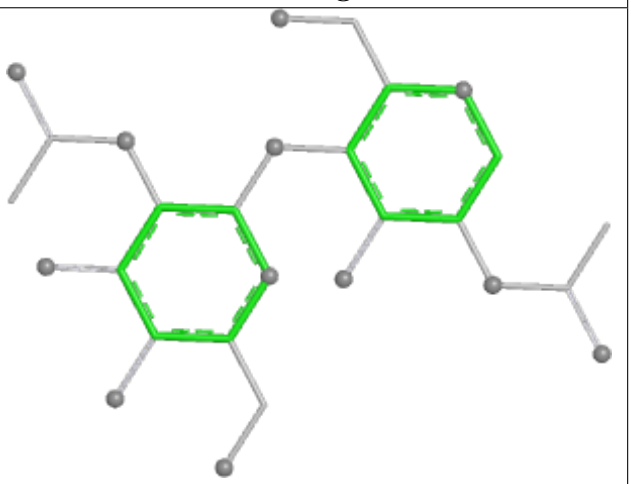
Bond lengths



Bond angles

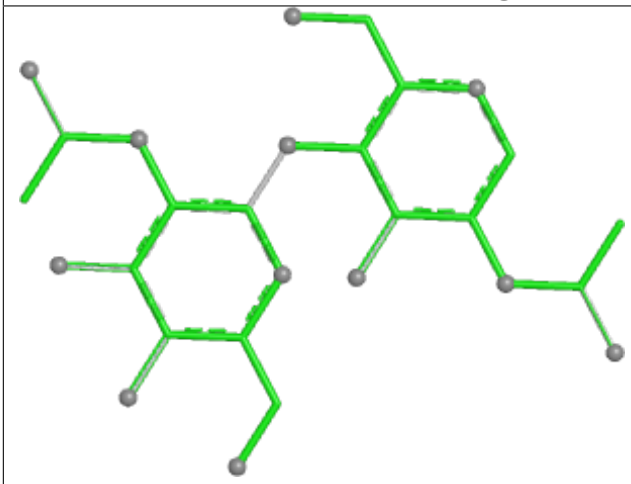


Torsions

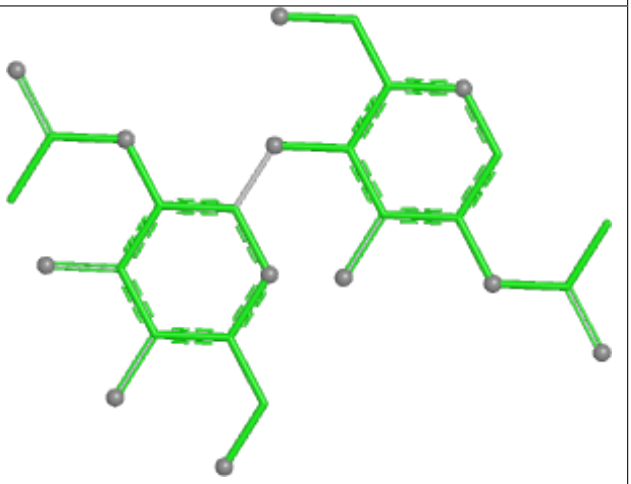


Rings

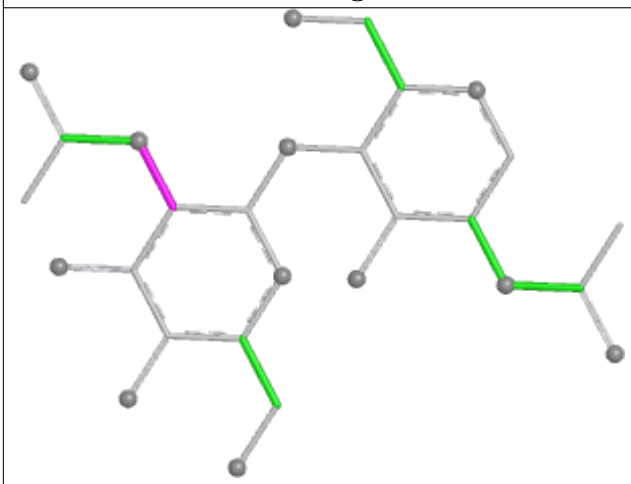
Oligosaccharide Chain T



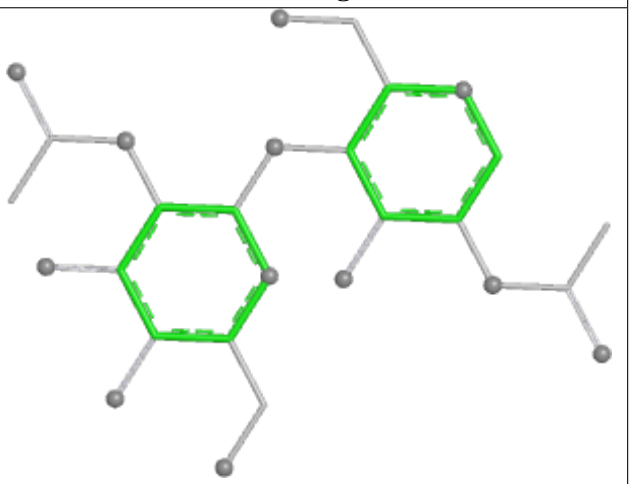
Bond lengths



Bond angles

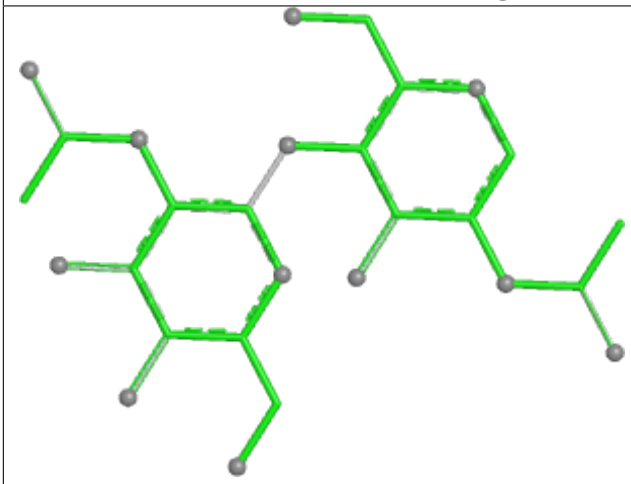


Torsions

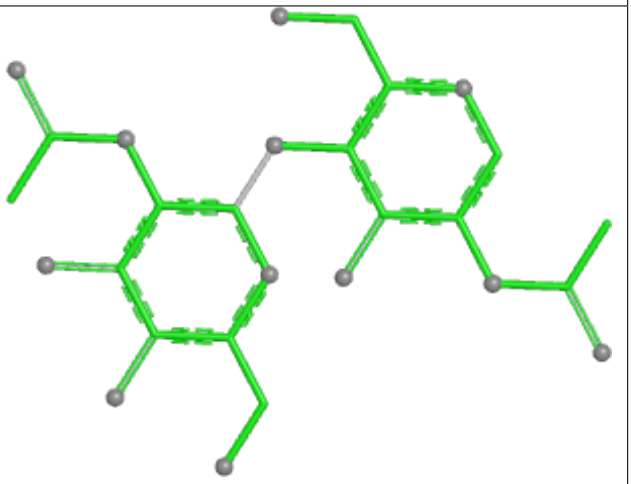


Rings

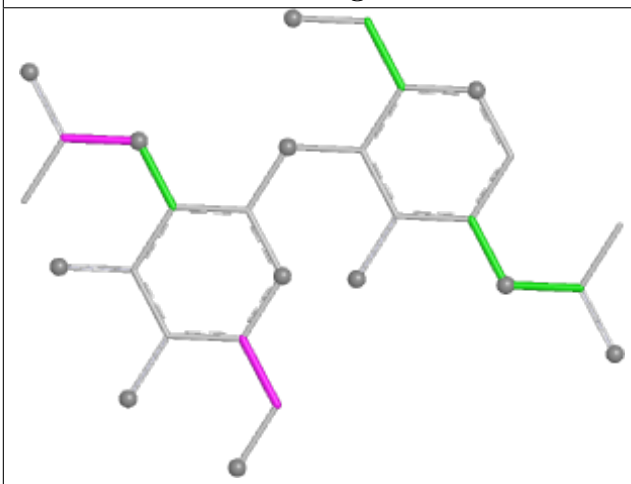
Oligosaccharide Chain U



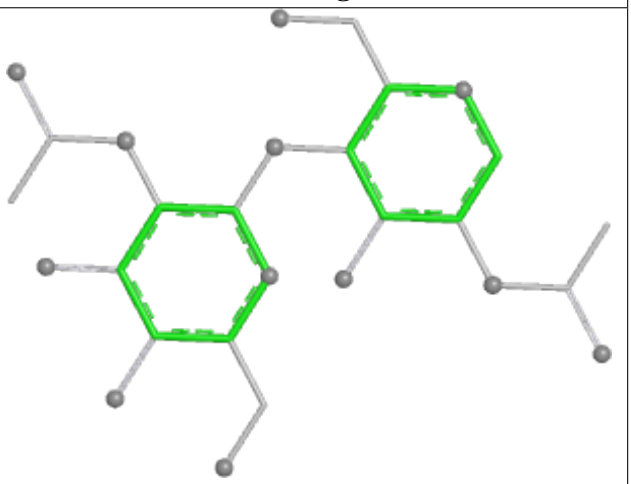
Bond lengths



Bond angles

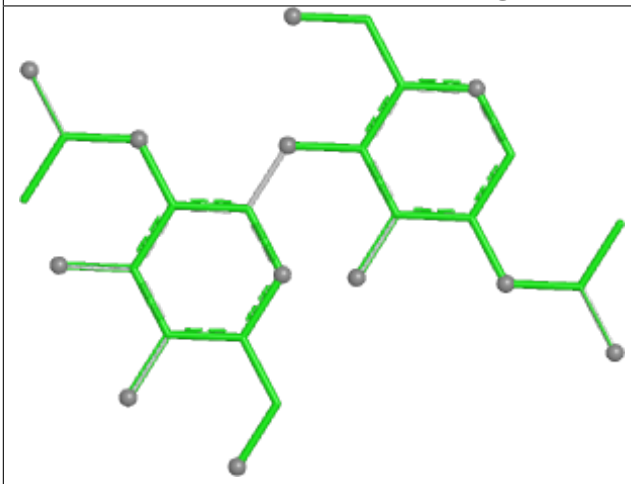


Torsions

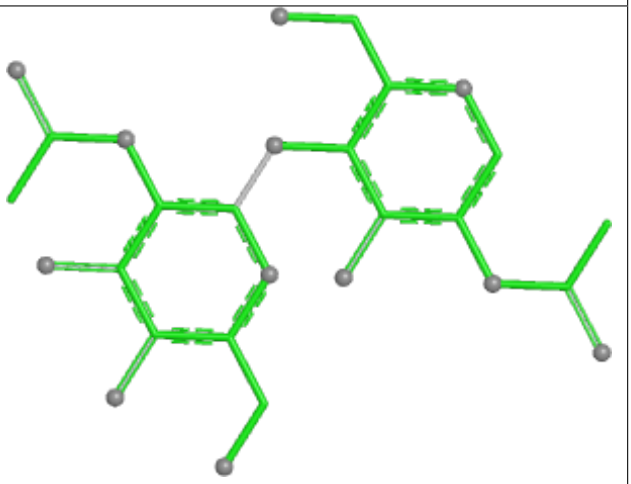


Rings

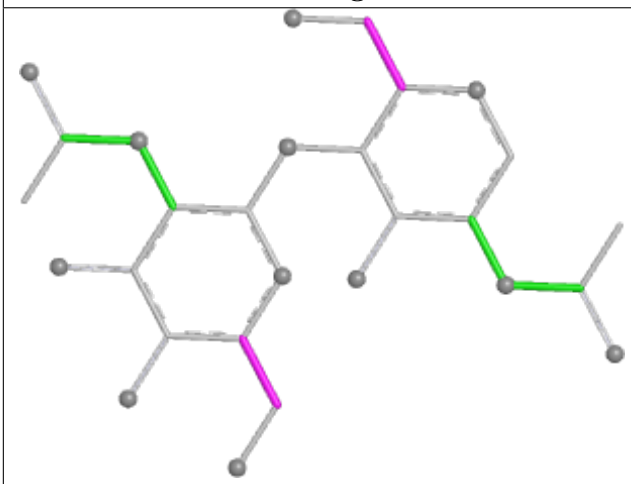
Oligosaccharide Chain V



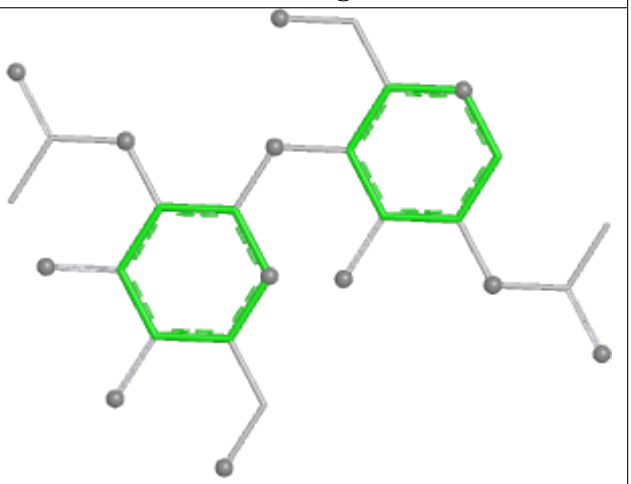
Bond lengths



Bond angles

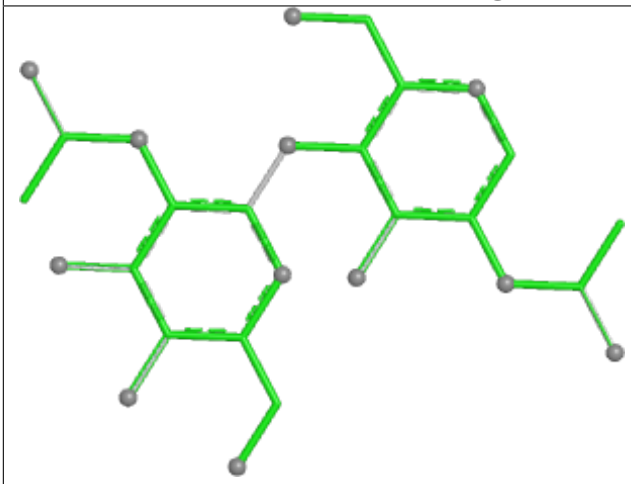


Torsions

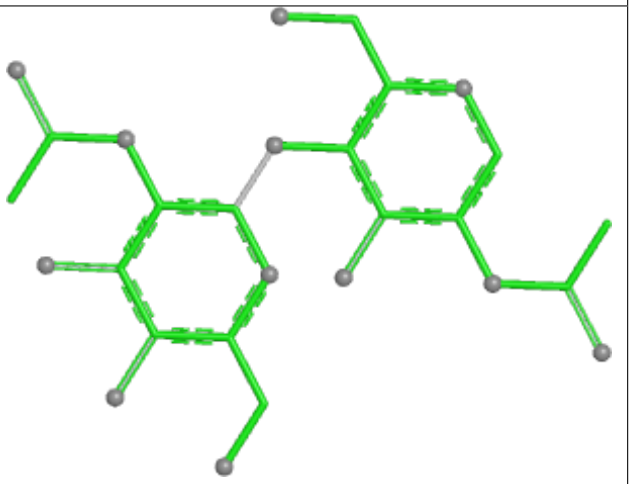


Rings

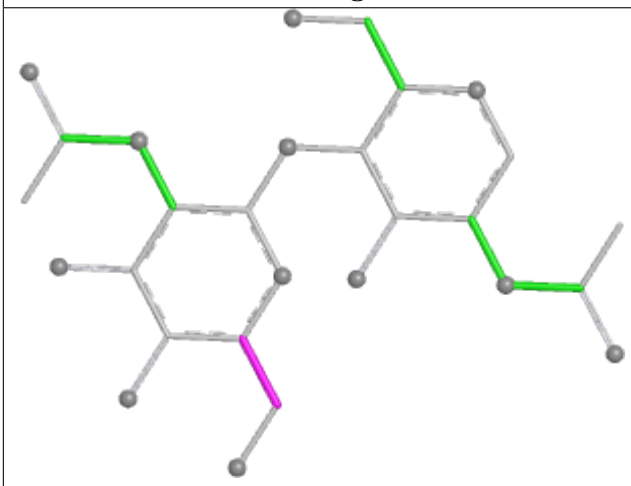
Oligosaccharide Chain W



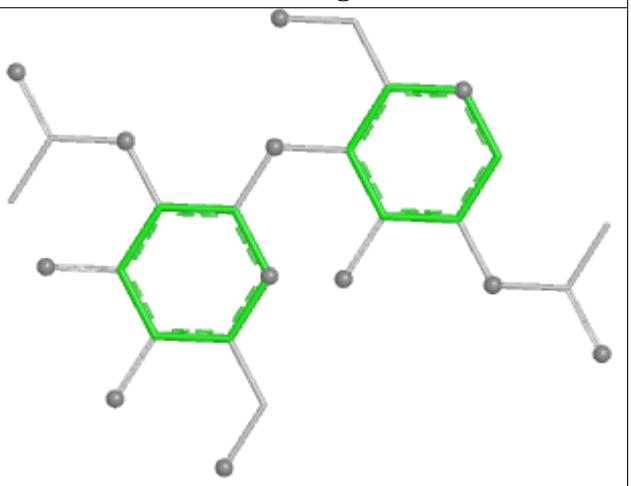
Bond lengths



Bond angles

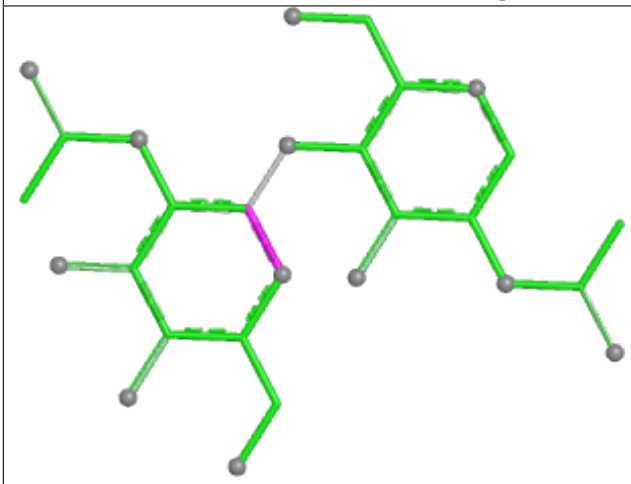


Torsions

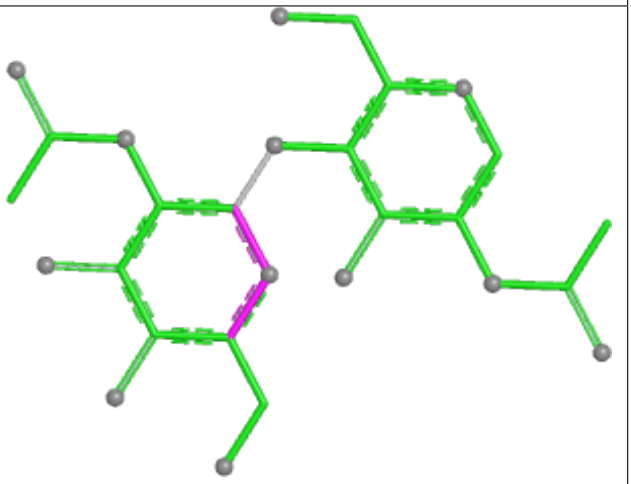


Rings

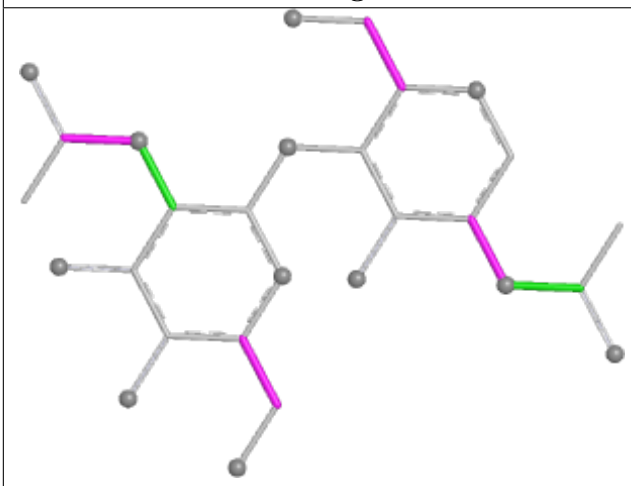
Oligosaccharide Chain Y



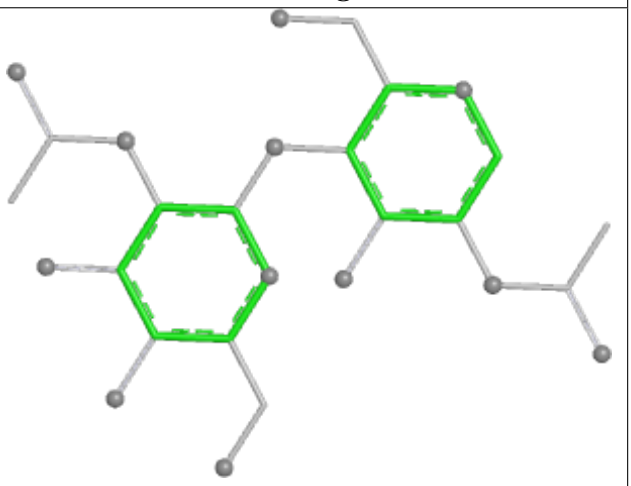
Bond lengths



Bond angles

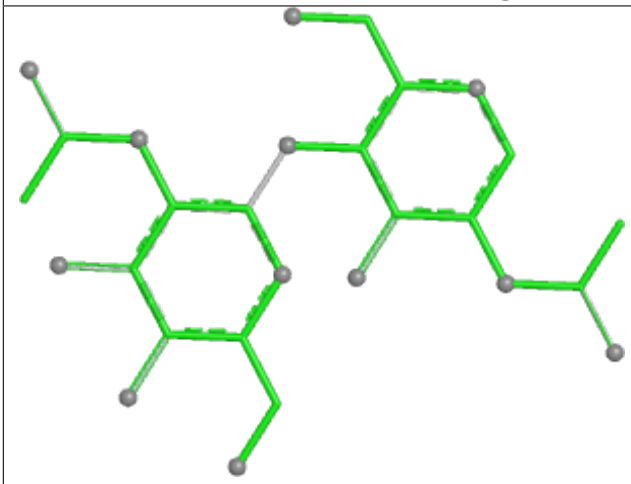


Torsions

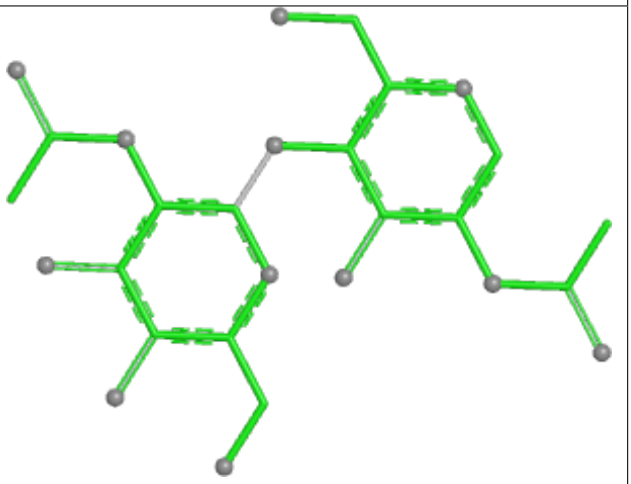


Rings

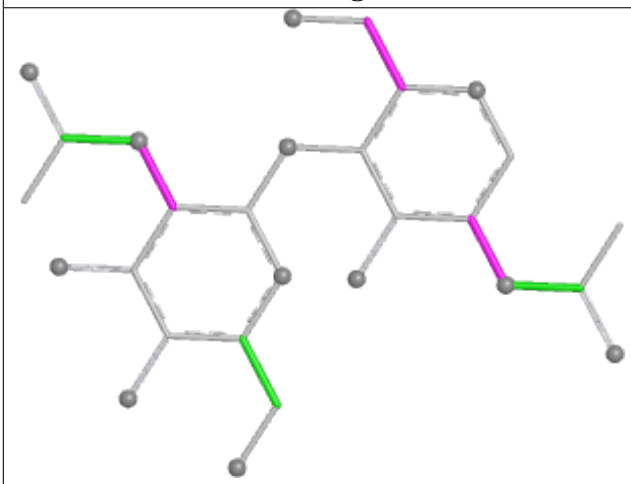
Oligosaccharide Chain Z



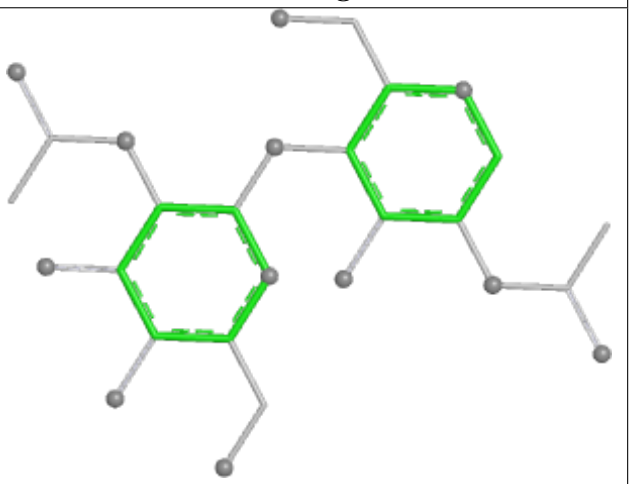
Bond lengths



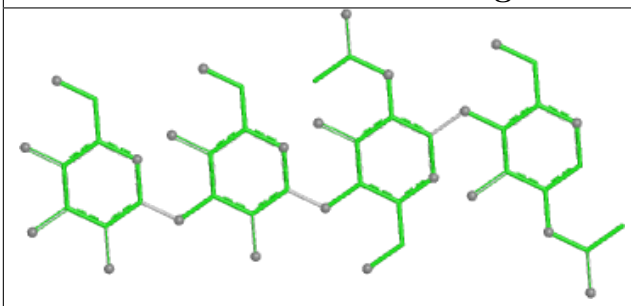
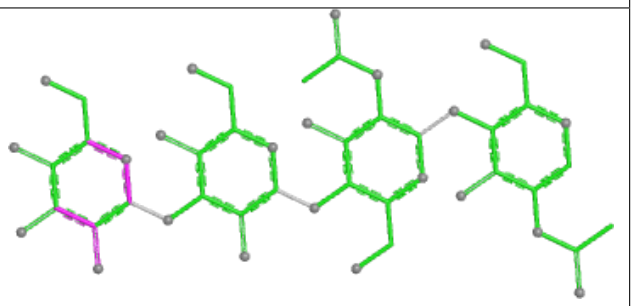
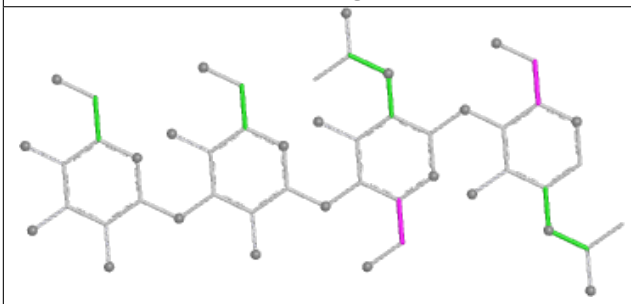
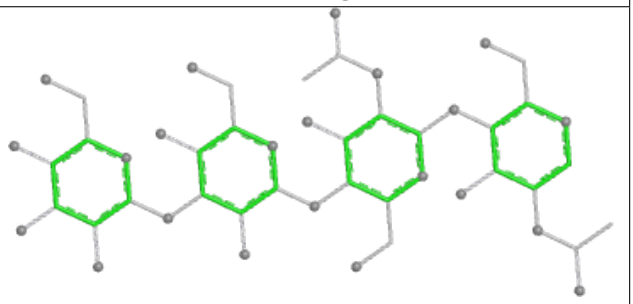
Bond angles

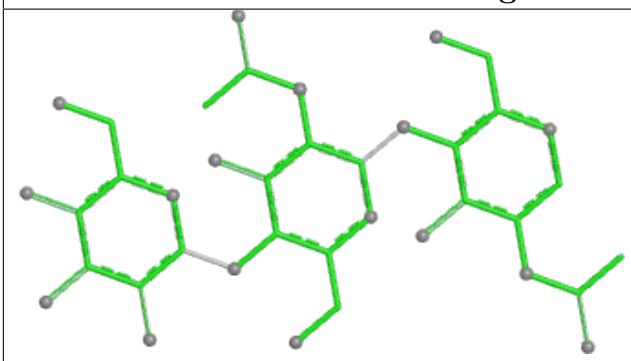
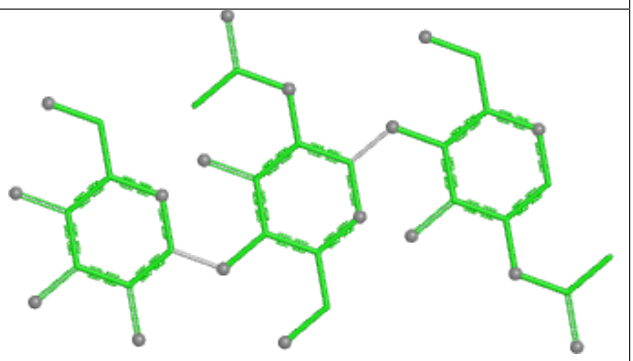
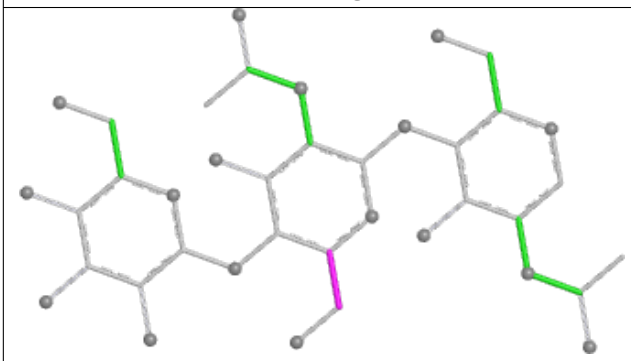
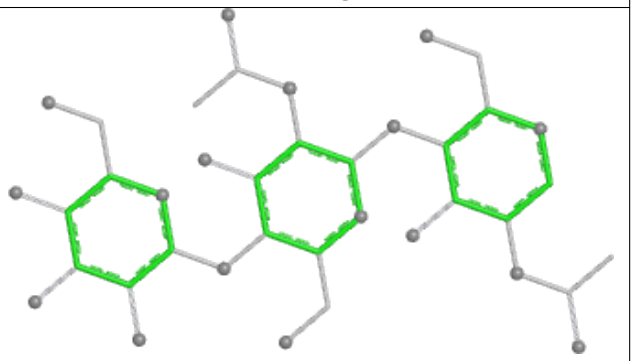


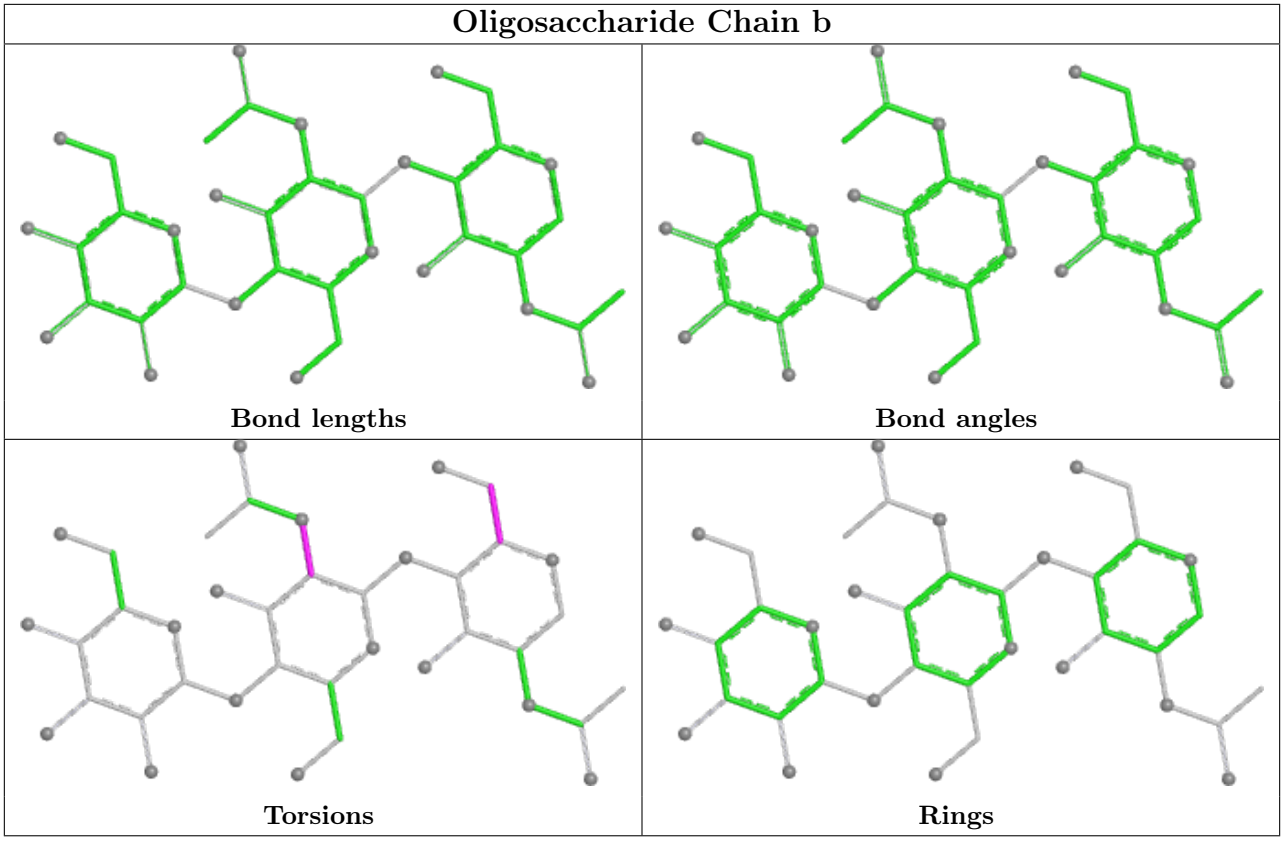
Torsions



Rings

Oligosaccharide Chain X	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain a	
 Bond lengths	 Bond angles
 Torsions	 Rings



5.6 Ligand geometry (i)

26 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	$\#\|Z\| > 2$
9	NAG	K	1303	5	14,14,15	0.44	0	17,19,21	1.25	1 (5%)
9	NAG	A	1305	5	14,14,15	0.25	0	17,19,21	0.59	0
9	NAG	A	1306	5	14,14,15	0.42	0	17,19,21	0.45	0
9	NAG	K	1302	5	14,14,15	0.31	0	17,19,21	0.56	0
9	NAG	D	1306	5	14,14,15	0.32	0	17,19,21	0.52	0
9	NAG	A	1302	5	14,14,15	0.23	0	17,19,21	0.41	0
9	NAG	K	1305	5	14,14,15	0.20	0	17,19,21	0.42	0
9	NAG	K	1308	5	14,14,15	0.21	0	17,19,21	0.45	0
9	NAG	K	1310	5	14,14,15	0.35	0	17,19,21	1.27	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	NAG	A	1304	5	14,14,15	0.19	0	17,19,21	0.44	0
9	NAG	K	1307	5	14,14,15	0.31	0	17,19,21	0.43	0
9	NAG	D	1304	5	14,14,15	0.18	0	17,19,21	0.43	0
9	NAG	K	1311	5	14,14,15	0.21	0	17,19,21	0.39	0
9	NAG	D	1301	5	14,14,15	0.32	0	17,19,21	0.47	0
9	NAG	K	1312	5	14,14,15	0.30	0	17,19,21	0.49	0
9	NAG	K	1306	5	14,14,15	0.21	0	17,19,21	0.47	0
9	NAG	D	1302	5	14,14,15	0.20	0	17,19,21	0.46	0
9	NAG	K	1304	5	14,14,15	0.19	0	17,19,21	0.44	0
9	NAG	D	1305	5	14,14,15	0.22	0	17,19,21	0.45	0
9	NAG	D	1303	5	14,14,15	0.30	0	17,19,21	0.41	0
9	NAG	D	1307	5	14,14,15	0.70	1 (7%)	17,19,21	0.74	1 (5%)
9	NAG	D	1308	5	14,14,15	0.21	0	17,19,21	0.41	0
9	NAG	K	1301	5	14,14,15	0.21	0	17,19,21	0.50	0
9	NAG	A	1303	5	14,14,15	0.21	0	17,19,21	0.46	0
9	NAG	A	1301	5	14,14,15	0.20	0	17,19,21	0.42	0
9	NAG	K	1309	5	14,14,15	0.19	0	17,19,21	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	K	1303	5	-	3/6/23/26	0/1/1/1
9	NAG	A	1305	5	-	3/6/23/26	0/1/1/1
9	NAG	A	1306	5	-	3/6/23/26	0/1/1/1
9	NAG	K	1302	5	-	0/6/23/26	0/1/1/1
9	NAG	D	1306	5	-	4/6/23/26	0/1/1/1
9	NAG	A	1302	5	-	2/6/23/26	0/1/1/1
9	NAG	K	1305	5	-	2/6/23/26	0/1/1/1
9	NAG	K	1308	5	-	1/6/23/26	0/1/1/1
9	NAG	K	1310	5	-	6/6/23/26	0/1/1/1
9	NAG	A	1304	5	-	2/6/23/26	0/1/1/1
9	NAG	K	1307	5	-	4/6/23/26	0/1/1/1
9	NAG	D	1304	5	-	0/6/23/26	0/1/1/1
9	NAG	K	1311	5	-	2/6/23/26	0/1/1/1
9	NAG	D	1301	5	-	2/6/23/26	0/1/1/1
9	NAG	K	1312	5	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	K	1306	5	-	2/6/23/26	0/1/1/1
9	NAG	D	1302	5	-	2/6/23/26	0/1/1/1
9	NAG	K	1304	5	-	2/6/23/26	0/1/1/1
9	NAG	D	1305	5	-	2/6/23/26	0/1/1/1
9	NAG	D	1303	5	-	1/6/23/26	0/1/1/1
9	NAG	D	1307	5	-	3/6/23/26	0/1/1/1
9	NAG	D	1308	5	-	2/6/23/26	0/1/1/1
9	NAG	K	1301	5	-	3/6/23/26	0/1/1/1
9	NAG	A	1303	5	-	2/6/23/26	0/1/1/1
9	NAG	A	1301	5	-	2/6/23/26	0/1/1/1
9	NAG	K	1309	5	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	1307	NAG	C1-C2	2.28	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	K	1303	NAG	C2-N2-C7	4.26	128.97	122.90
9	K	1310	NAG	C1-O5-C5	2.66	115.80	112.19
9	K	1310	NAG	O5-C1-C2	-2.62	107.15	111.29
9	D	1307	NAG	C1-O5-C5	2.60	115.71	112.19
9	K	1310	NAG	O5-C5-C6	2.23	110.70	107.20

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	K	1307	NAG	C4-C5-C6-O6
9	K	1310	NAG	C8-C7-N2-C2
9	K	1310	NAG	O7-C7-N2-C2
9	K	1307	NAG	O5-C5-C6-O6
9	A	1303	NAG	O5-C5-C6-O6
9	K	1301	NAG	C4-C5-C6-O6
9	A	1305	NAG	C4-C5-C6-O6
9	K	1304	NAG	C4-C5-C6-O6
9	K	1305	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	D	1306	NAG	O5-C5-C6-O6
9	K	1310	NAG	O5-C5-C6-O6
9	K	1309	NAG	O5-C5-C6-O6
9	K	1312	NAG	C4-C5-C6-O6
9	K	1301	NAG	O5-C5-C6-O6
9	A	1305	NAG	O5-C5-C6-O6
9	K	1304	NAG	O5-C5-C6-O6
9	K	1310	NAG	C1-C2-N2-C7
9	D	1307	NAG	C4-C5-C6-O6
9	A	1303	NAG	C4-C5-C6-O6
9	D	1306	NAG	C8-C7-N2-C2
9	D	1306	NAG	O7-C7-N2-C2
9	D	1308	NAG	C8-C7-N2-C2
9	D	1308	NAG	O7-C7-N2-C2
9	K	1303	NAG	C8-C7-N2-C2
9	K	1303	NAG	O7-C7-N2-C2
9	K	1307	NAG	C8-C7-N2-C2
9	K	1307	NAG	O7-C7-N2-C2
9	A	1304	NAG	C8-C7-N2-C2
9	A	1304	NAG	O7-C7-N2-C2
9	D	1305	NAG	O5-C5-C6-O6
9	K	1312	NAG	O5-C5-C6-O6
9	K	1305	NAG	C4-C5-C6-O6
9	K	1309	NAG	C4-C5-C6-O6
9	K	1308	NAG	O5-C5-C6-O6
9	D	1307	NAG	O5-C5-C6-O6
9	D	1305	NAG	C4-C5-C6-O6
9	A	1302	NAG	O5-C5-C6-O6
9	K	1310	NAG	C4-C5-C6-O6
9	A	1302	NAG	C4-C5-C6-O6
9	K	1311	NAG	C4-C5-C6-O6
9	A	1306	NAG	O5-C5-C6-O6
9	A	1306	NAG	C1-C2-N2-C7
9	D	1302	NAG	C4-C5-C6-O6
9	K	1311	NAG	O5-C5-C6-O6
9	D	1306	NAG	C4-C5-C6-O6
9	A	1301	NAG	C4-C5-C6-O6
9	K	1306	NAG	C4-C5-C6-O6
9	D	1302	NAG	O5-C5-C6-O6
9	D	1301	NAG	C4-C5-C6-O6
9	K	1306	NAG	O5-C5-C6-O6
9	D	1307	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
9	K	1312	NAG	C3-C2-N2-C7
9	A	1305	NAG	C3-C2-N2-C7
9	D	1301	NAG	O5-C5-C6-O6
9	A	1301	NAG	O5-C5-C6-O6
9	K	1301	NAG	C3-C2-N2-C7
9	K	1303	NAG	C3-C2-N2-C7
9	K	1310	NAG	C3-C2-N2-C7
9	A	1306	NAG	C3-C2-N2-C7
9	D	1303	NAG	C1-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	K	1303	NAG	1	0
9	A	1305	NAG	1	0
9	K	1310	NAG	2	0
9	D	1301	NAG	1	0
9	D	1303	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

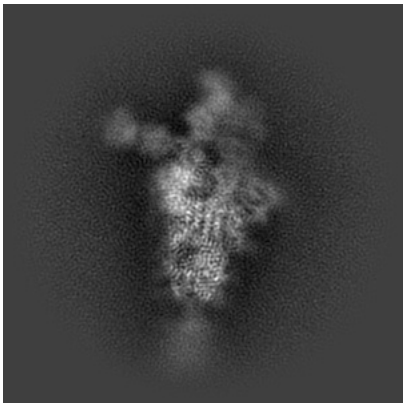
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14141. These allow visual inspection of the internal detail of the map and identification of artifacts.

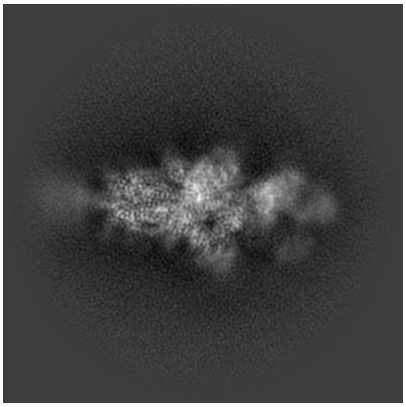
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

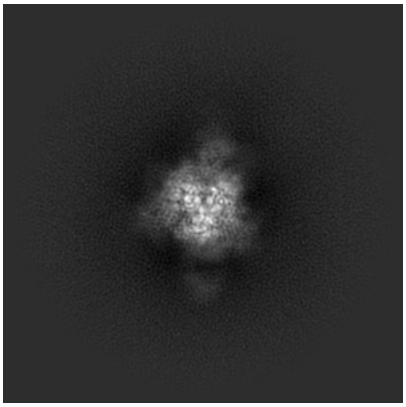
6.1.1 Primary map



X



Y

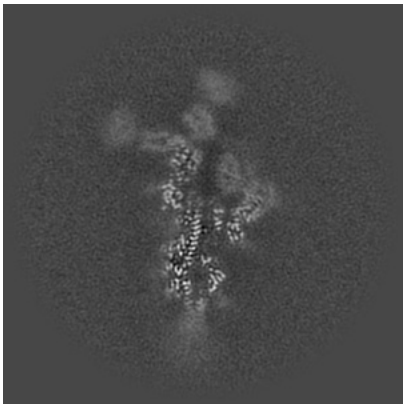


Z

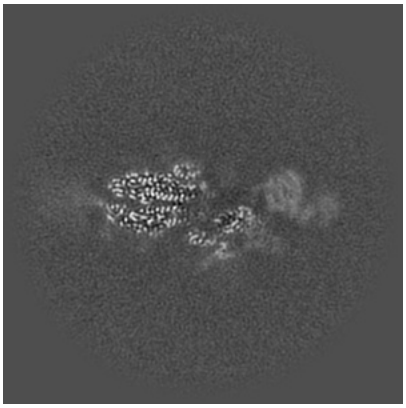
The images above show the map projected in three orthogonal directions.

6.2 Central slices

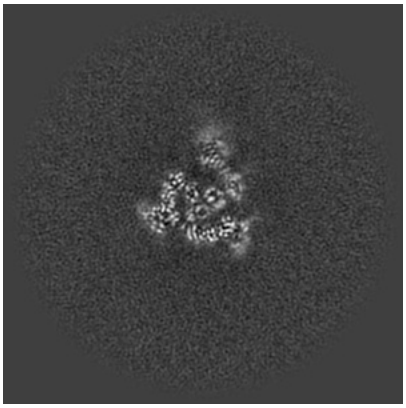
6.2.1 Primary map



X Index: 150



Y Index: 150

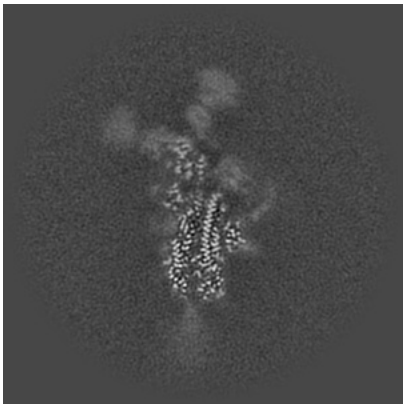


Z Index: 150

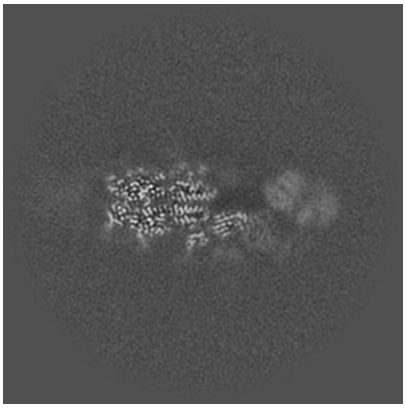
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

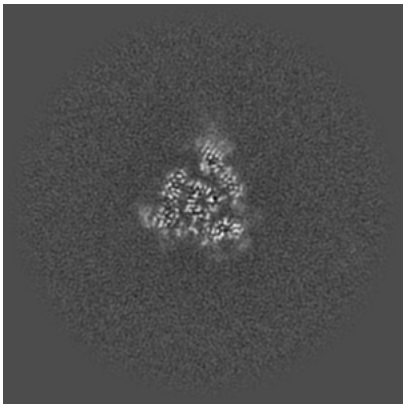
6.3.1 Primary map



X Index: 145



Y Index: 154

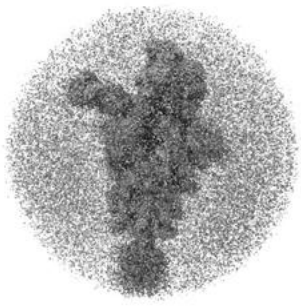


Z Index: 146

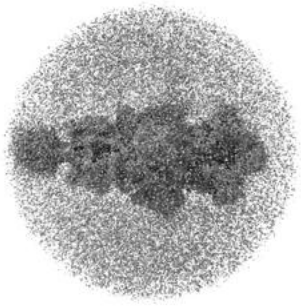
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

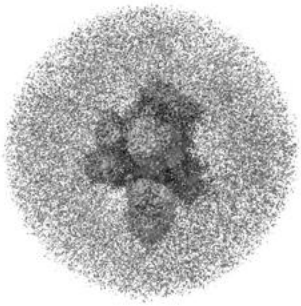
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

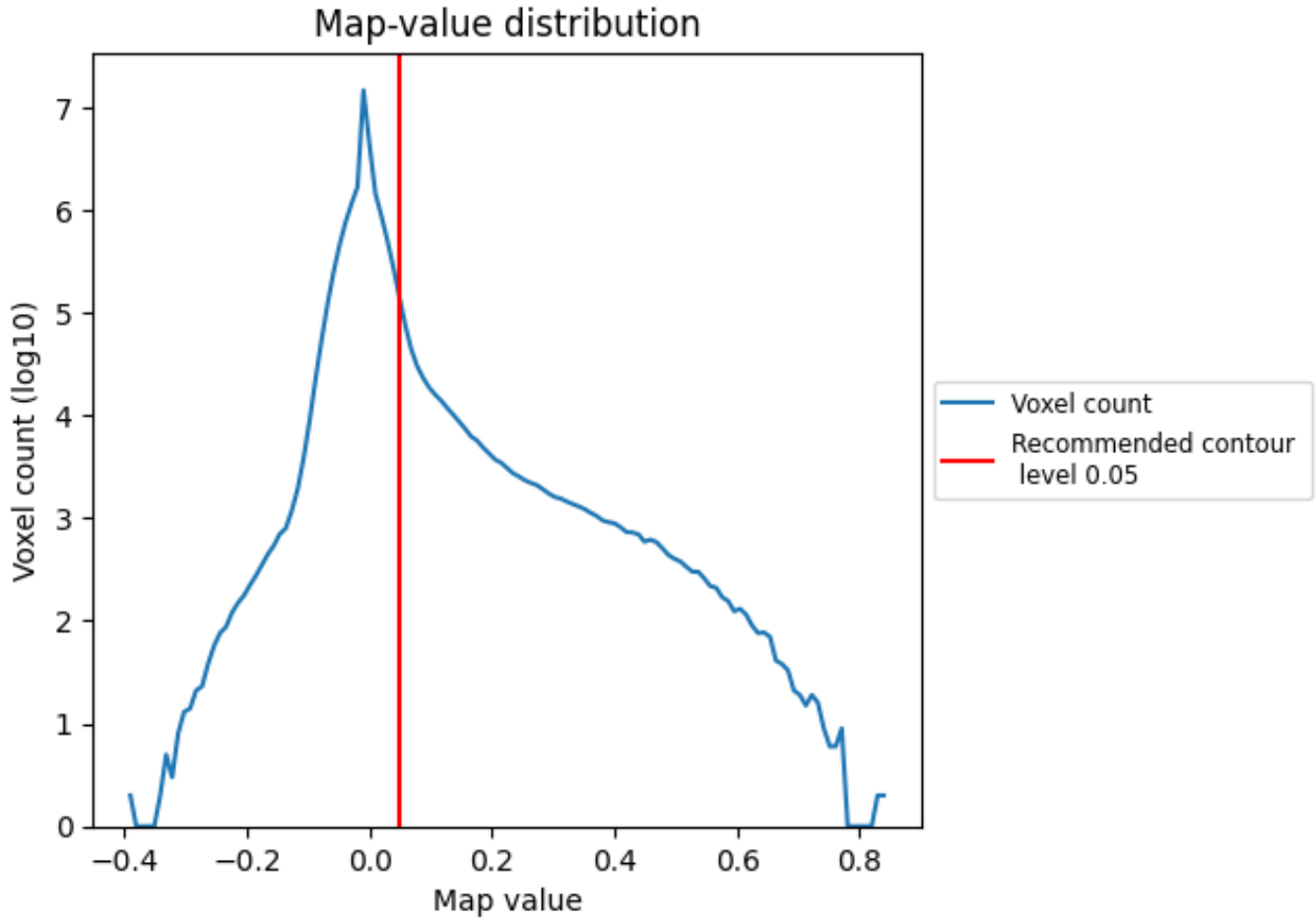
6.5 Mask visualisation (i)

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

7 Map analysis

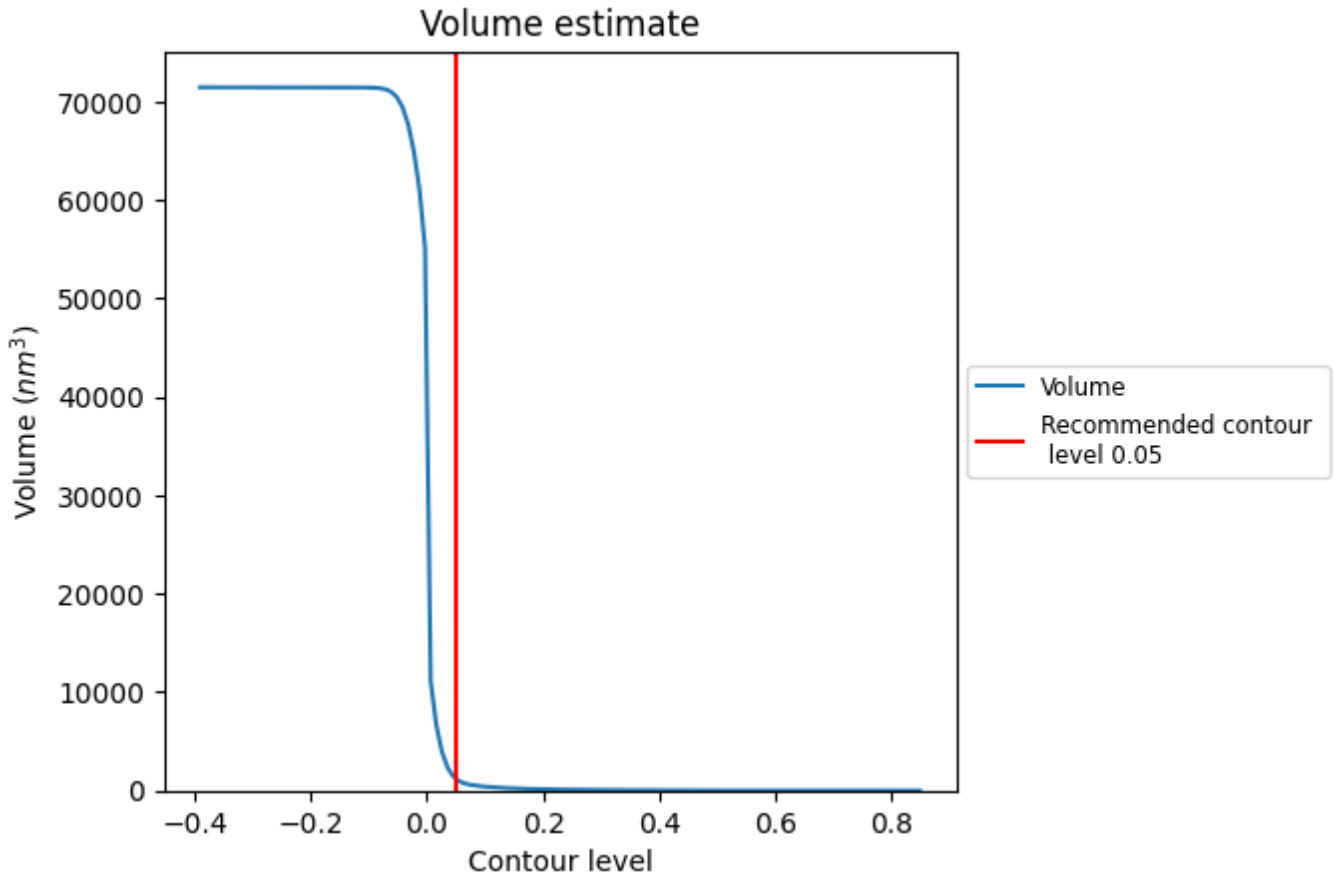
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

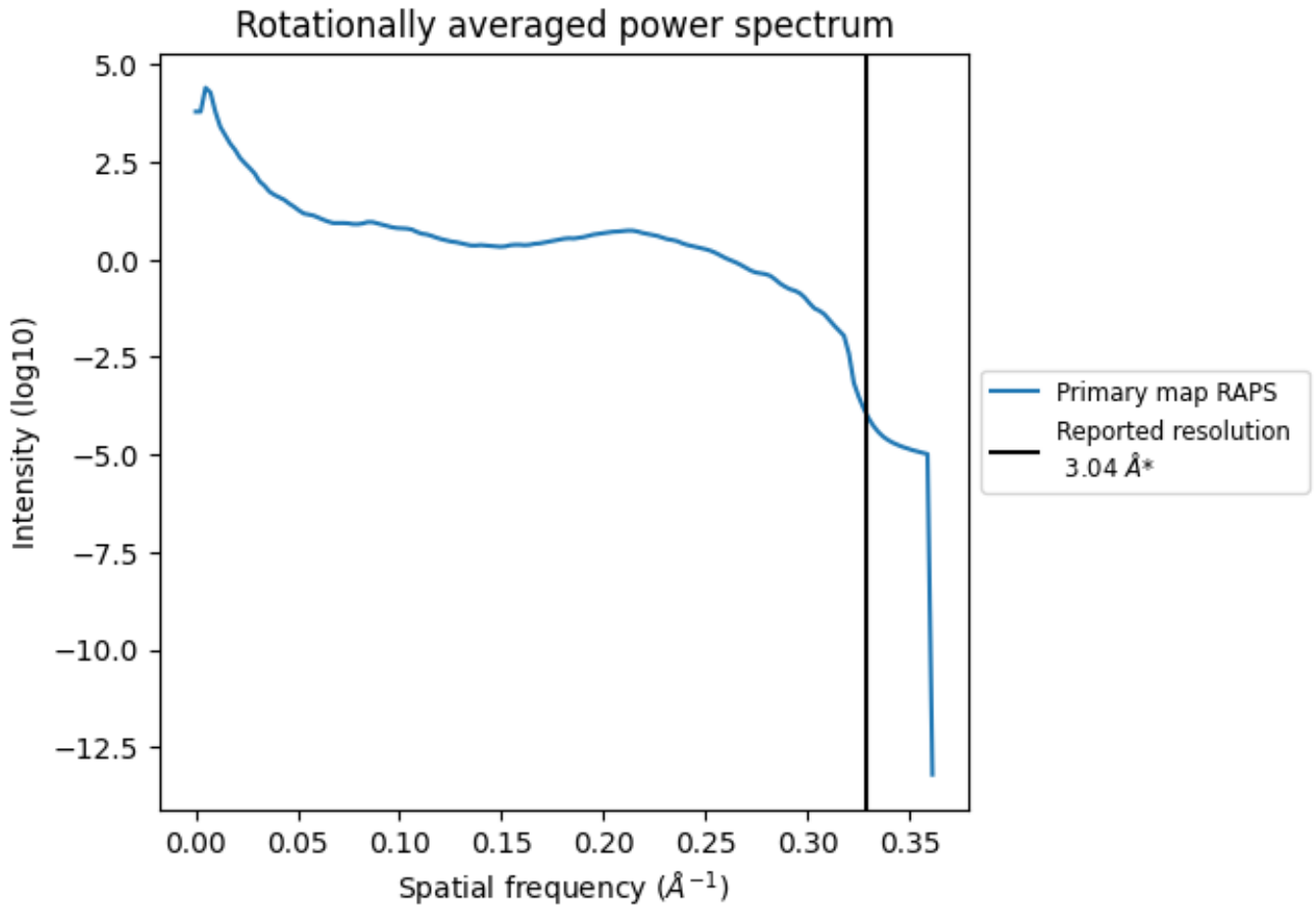
7.2 Volume estimate



The volume at the recommended contour level is 1222 nm^3; this corresponds to an approximate mass of 1104 kDa.

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

7.3 Rotationally averaged power spectrum (i)

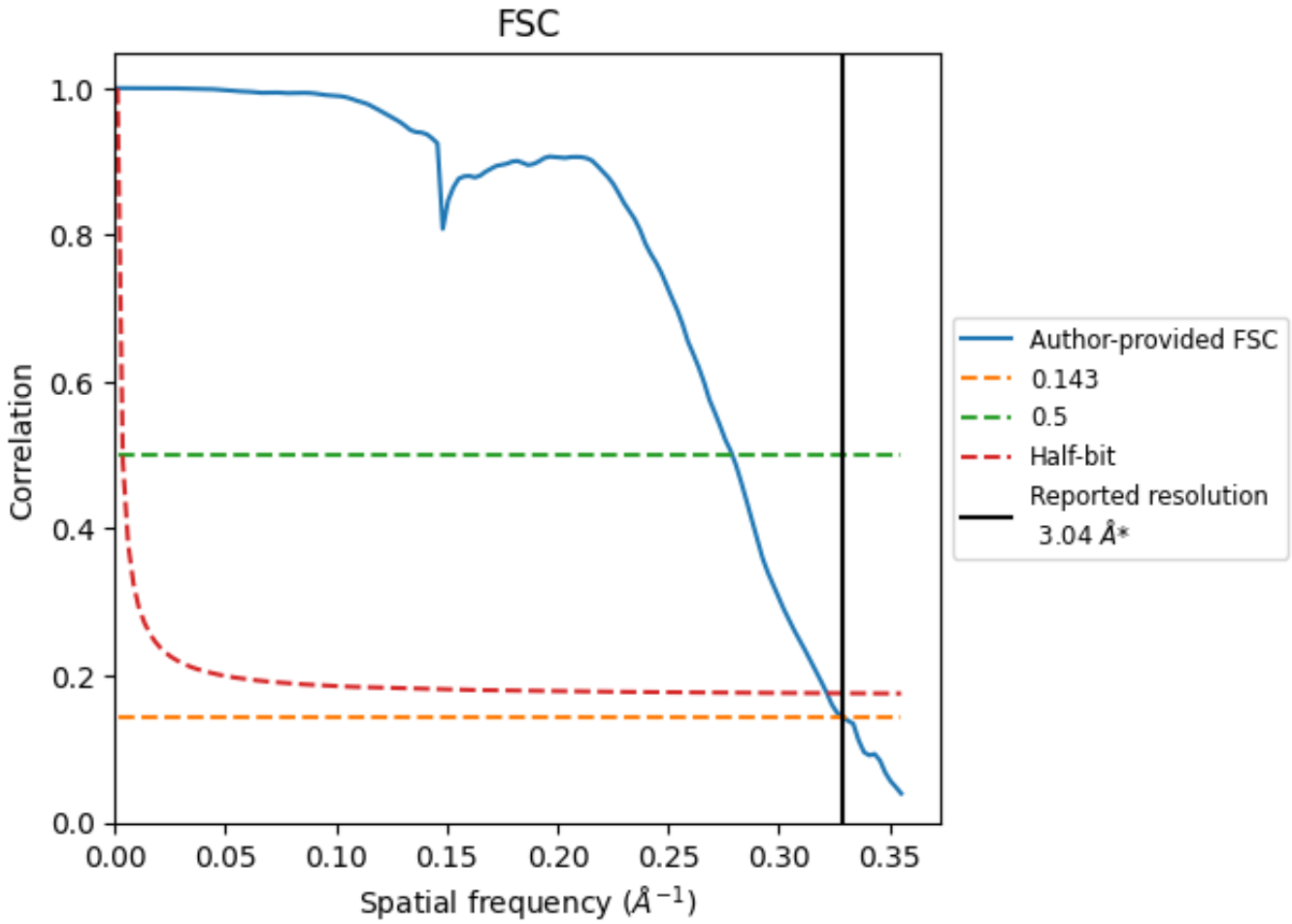


*Reported resolution corresponds to spatial frequency of 0.329 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.329 Å^{-1}

8.2 Resolution estimates (i)

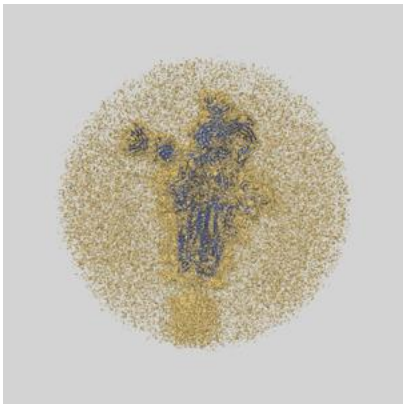
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	3.04	3.58	3.11
Unmasked-calculated*	-	-	-

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

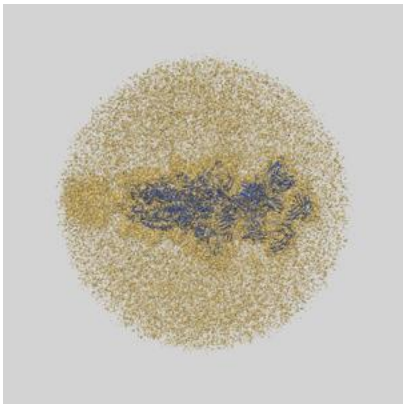
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14141 and PDB model 7QTI. Per-residue inclusion information can be found in section 3 on page 16.

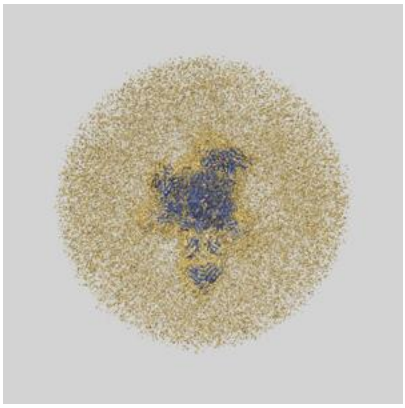
9.1 Map-model overlay



X



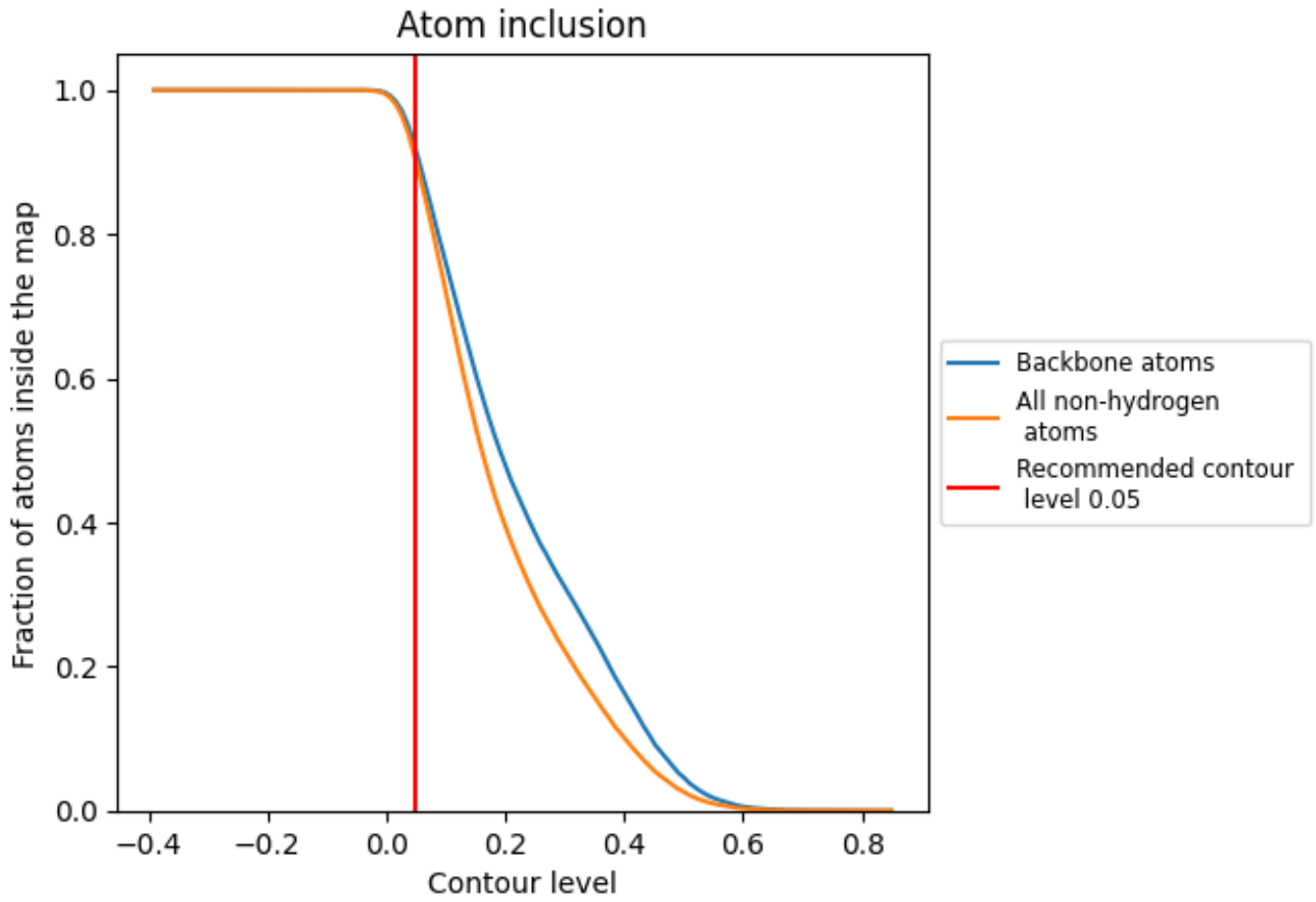
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.