wwPDB EM Validation Summary Report (i)

Oct 26, 2026 – 01:05 PM JST

PDB ID	:	9XIB / pdb_00009xib
EMDB ID	:	EMD-66902
Title	:	SARS-CoV-2 Omicron LP.8.1 spike trimer (S-6P) in complex with 3 ZL58 Fabs and 3 ZL525 Fabs
Authors	:	Niu, C.; Liu, B.; Gao, X.; Li, Z.; He, J.; Xiong, X.
Deposited on	:	2025-11-02
Resolution	:	2.75 Å(reported)

This is a wwPDB EM Validation Summary 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 (i) 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 (i)) were used in the production of this report:

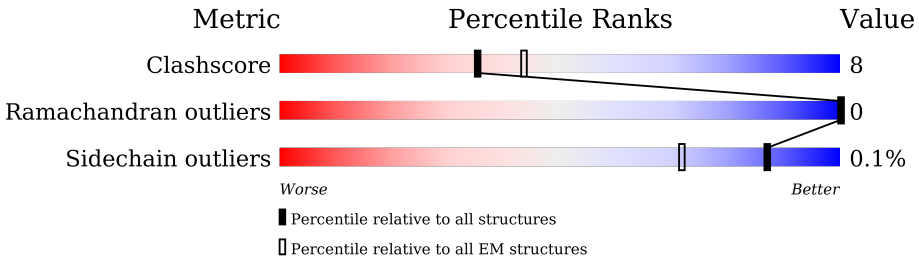
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

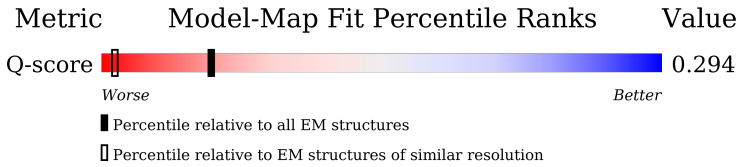
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.75 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10570 (2.25 - 3.25)

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	D	228	20% 73% 24% ·
1	E	228	21% 77% 20% ·
1	F	228	21% 76% 21% ·
2	G	217	25% 83% 17%

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Mol	Chain	Length	Quality of chain
2	H	217	24% 83% 17%
2	M	217	25% 85% 15%
3	I	221	24% 71% 25%
3	J	221	23% 71% 26%
3	d	221	23% 72% 24%
4	K	214	16% 78% 22%
4	L	214	16% 82% 18%
4	f	214	16% 79% 21%
5	A	1238	67% 15% 17%
5	B	1238	68% 15% 17%
5	C	1238	68% 15% 17%
6	N	2	100%
6	O	2	100%
6	P	2	50% 50%
6	Q	2	100%
6	R	2	100%
6	S	2	50% 50%
6	T	2	100%
6	U	2	100%
6	V	2	50% 50%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 43947 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 Heavy chain of ZL525 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	221	Total	C	N	O	S	0	0
			1645	1039	275	324	7		
1	D	221	Total	C	N	O	S	0	0
			1645	1039	275	324	7		
1	F	221	Total	C	N	O	S	0	0
			1645	1039	275	324	7		

- Molecule 2 is a protein called Light chain of ZL525 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	217	Total	C	N	O	S	0	0
			1610	1003	274	328	5		
2	G	217	Total	C	N	O	S	0	0
			1610	1003	274	328	5		
2	H	217	Total	C	N	O	S	0	0
			1610	1003	274	328	5		

- Molecule 3 is a protein called Heavy chain of ZL58 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	214	Total	C	N	O	S	0	0
			1584	995	267	316	6		
3	I	214	Total	C	N	O	S	0	0
			1584	995	267	316	6		
3	J	214	Total	C	N	O	S	0	0
			1584	995	267	316	6		

- Molecule 4 is a protein called Light chain of ZL58 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	f	214	Total	C	N	O	S	0	0
			1649	1031	272	339	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	214	Total	C	N	O	S	0	0
			1649	1031	272	339	7		
4	L	214	Total	C	N	O	S	0	0
			1649	1031	272	339	7		

- Molecule 5 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	1022	Total	C	N	O	S	0	0
			8007	5133	1321	1517	36		
5	B	1022	Total	C	N	O	S	0	0
			8007	5133	1321	1517	36		
5	C	1022	Total	C	N	O	S	0	0
			8007	5133	1321	1517	36		

There are 408 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLN	-	expression tag	UNP P0DTC2
A	11	CYS	-	expression tag	UNP P0DTC2
A	12	VAL	-	expression tag	UNP P0DTC2
A	13	MET	-	expression tag	UNP P0DTC2
A	14	PRO	-	expression tag	UNP P0DTC2
A	15	LEU	-	expression tag	UNP P0DTC2
A	16	PHE	-	expression tag	UNP P0DTC2
A	17	ASN	-	expression tag	UNP P0DTC2
A	18	LEU	-	expression tag	UNP P0DTC2
A	19	ILE	-	expression tag	UNP P0DTC2
A	20	THR	-	expression tag	UNP P0DTC2
A	21	THR	-	expression tag	UNP P0DTC2
A	22	THR	-	expression tag	UNP P0DTC2
A	23	GLN	-	expression tag	UNP P0DTC2
A	27	SER	-	expression tag	UNP P0DTC2
A	28	TYR	-	expression tag	UNP P0DTC2
A	29	THR	-	expression tag	UNP P0DTC2
A	30	ASN	-	expression tag	UNP P0DTC2
A	50	LEU	SER	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	127	PHE	VAL	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	157	SER	PHE	variant	UNP P0DTC2
A	158	GLY	ARG	variant	UNP P0DTC2
A	186	LEU	PHE	variant	UNP P0DTC2
A	190	SER	ARG	variant	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	212	ILE	LEU	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	216	PHE	LEU	variant	UNP P0DTC2
A	245	ASN	HIS	variant	UNP P0DTC2
A	264	ASP	ALA	variant	UNP P0DTC2
A	332	VAL	ILE	variant	UNP P0DTC2
A	339	HIS	GLY	variant	UNP P0DTC2
A	346	THR	ARG	variant	UNP P0DTC2
A	356	THR	LYS	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	403	LYS	ARG	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	445	ARG	VAL	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	450	ASP	ASN	variant	UNP P0DTC2
A	452	TRP	LEU	variant	UNP P0DTC2
A	455	SER	LEU	variant	UNP P0DTC2
A	456	LEU	PHE	variant	UNP P0DTC2
A	460	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	481	LYS	ASN	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	484	LYS	GLU	variant	UNP P0DTC2
A	486	PRO	PHE	variant	UNP P0DTC2
A	493	GLU	GLN	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	554	LYS	GLU	variant	UNP P0DTC2
A	570	VAL	ALA	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	614	GLY	ASP	variant	UNP P0DTC2
A	621	SER	PRO	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	670	VAL	ILE	variant	UNP P0DTC2
A	683	LYS	ASN	variant	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	939	PHE	SER	variant	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1143	LEU	PRO	variant	UNP P0DTC2
A	1212	GLY	-	expression tag	UNP P0DTC2
A	1213	SER	-	expression tag	UNP P0DTC2
A	1214	GLY	-	expression tag	UNP P0DTC2
A	1215	ARG	-	expression tag	UNP P0DTC2
A	1216	GLU	-	expression tag	UNP P0DTC2
A	1217	ASN	-	expression tag	UNP P0DTC2
A	1218	LEU	-	expression tag	UNP P0DTC2
A	1219	TYR	-	expression tag	UNP P0DTC2
A	1220	PHE	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	GLY	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	GLY	-	expression tag	UNP P0DTC2
A	1226	SER	-	expression tag	UNP P0DTC2
A	1227	GLY	-	expression tag	UNP P0DTC2
A	1228	TYR	-	expression tag	UNP P0DTC2
A	1229	ILE	-	expression tag	UNP P0DTC2
A	1230	PRO	-	expression tag	UNP P0DTC2
A	1231	GLU	-	expression tag	UNP P0DTC2
A	1232	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1233	PRO	-	expression tag	UNP P0DTC2
A	1234	ARG	-	expression tag	UNP P0DTC2
A	1235	ASP	-	expression tag	UNP P0DTC2
A	1236	GLY	-	expression tag	UNP P0DTC2
A	1237	GLN	-	expression tag	UNP P0DTC2
A	1238	ALA	-	expression tag	UNP P0DTC2
A	1239	TYR	-	expression tag	UNP P0DTC2
A	1240	VAL	-	expression tag	UNP P0DTC2
A	1241	ARG	-	expression tag	UNP P0DTC2
A	1242	LYS	-	expression tag	UNP P0DTC2
A	1243	ASP	-	expression tag	UNP P0DTC2
A	1244	GLY	-	expression tag	UNP P0DTC2
A	1245	GLU	-	expression tag	UNP P0DTC2
A	1246	TRP	-	expression tag	UNP P0DTC2
A	1247	VAL	-	expression tag	UNP P0DTC2
A	1248	LEU	-	expression tag	UNP P0DTC2
A	1249	LEU	-	expression tag	UNP P0DTC2
A	1250	SER	-	expression tag	UNP P0DTC2
A	1251	THR	-	expression tag	UNP P0DTC2
A	1252	PHE	-	expression tag	UNP P0DTC2
A	1253	LEU	-	expression tag	UNP P0DTC2
A	1254	GLY	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
A	1260	HIS	-	expression tag	UNP P0DTC2
B	10	GLN	-	expression tag	UNP P0DTC2
B	11	CYS	-	expression tag	UNP P0DTC2
B	12	VAL	-	expression tag	UNP P0DTC2
B	13	MET	-	expression tag	UNP P0DTC2
B	14	PRO	-	expression tag	UNP P0DTC2
B	15	LEU	-	expression tag	UNP P0DTC2
B	16	PHE	-	expression tag	UNP P0DTC2
B	17	ASN	-	expression tag	UNP P0DTC2
B	18	LEU	-	expression tag	UNP P0DTC2
B	19	ILE	-	expression tag	UNP P0DTC2
B	20	THR	-	expression tag	UNP P0DTC2
B	21	THR	-	expression tag	UNP P0DTC2
B	22	THR	-	expression tag	UNP P0DTC2
B	23	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	27	SER	-	expression tag	UNP P0DTC2
B	28	TYR	-	expression tag	UNP P0DTC2
B	29	THR	-	expression tag	UNP P0DTC2
B	30	ASN	-	expression tag	UNP P0DTC2
B	50	LEU	SER	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	127	PHE	VAL	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	157	SER	PHE	variant	UNP P0DTC2
B	158	GLY	ARG	variant	UNP P0DTC2
B	186	LEU	PHE	variant	UNP P0DTC2
B	190	SER	ARG	variant	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	212	ILE	LEU	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	216	PHE	LEU	variant	UNP P0DTC2
B	245	ASN	HIS	variant	UNP P0DTC2
B	264	ASP	ALA	variant	UNP P0DTC2
B	332	VAL	ILE	variant	UNP P0DTC2
B	339	HIS	GLY	variant	UNP P0DTC2
B	346	THR	ARG	variant	UNP P0DTC2
B	356	THR	LYS	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	403	LYS	ARG	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	445	ARG	VAL	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	450	ASP	ASN	variant	UNP P0DTC2
B	452	TRP	LEU	variant	UNP P0DTC2
B	455	SER	LEU	variant	UNP P0DTC2
B	456	LEU	PHE	variant	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	481	LYS	ASN	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	484	LYS	GLU	variant	UNP P0DTC2
B	486	PRO	PHE	variant	UNP P0DTC2
B	493	GLU	GLN	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	554	LYS	GLU	variant	UNP P0DTC2
B	570	VAL	ALA	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	621	SER	PRO	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	670	VAL	ILE	variant	UNP P0DTC2
B	683	LYS	ASN	variant	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	939	PHE	SER	variant	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1143	LEU	PRO	variant	UNP P0DTC2
B	1212	GLY	-	expression tag	UNP P0DTC2
B	1213	SER	-	expression tag	UNP P0DTC2
B	1214	GLY	-	expression tag	UNP P0DTC2
B	1215	ARG	-	expression tag	UNP P0DTC2
B	1216	GLU	-	expression tag	UNP P0DTC2
B	1217	ASN	-	expression tag	UNP P0DTC2
B	1218	LEU	-	expression tag	UNP P0DTC2
B	1219	TYR	-	expression tag	UNP P0DTC2
B	1220	PHE	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1223	GLY	-	expression tag	UNP P0DTC2
B	1224	GLY	-	expression tag	UNP P0DTC2
B	1225	GLY	-	expression tag	UNP P0DTC2
B	1226	SER	-	expression tag	UNP P0DTC2
B	1227	GLY	-	expression tag	UNP P0DTC2
B	1228	TYR	-	expression tag	UNP P0DTC2
B	1229	ILE	-	expression tag	UNP P0DTC2
B	1230	PRO	-	expression tag	UNP P0DTC2
B	1231	GLU	-	expression tag	UNP P0DTC2
B	1232	ALA	-	expression tag	UNP P0DTC2
B	1233	PRO	-	expression tag	UNP P0DTC2
B	1234	ARG	-	expression tag	UNP P0DTC2
B	1235	ASP	-	expression tag	UNP P0DTC2
B	1236	GLY	-	expression tag	UNP P0DTC2
B	1237	GLN	-	expression tag	UNP P0DTC2
B	1238	ALA	-	expression tag	UNP P0DTC2
B	1239	TYR	-	expression tag	UNP P0DTC2
B	1240	VAL	-	expression tag	UNP P0DTC2
B	1241	ARG	-	expression tag	UNP P0DTC2
B	1242	LYS	-	expression tag	UNP P0DTC2
B	1243	ASP	-	expression tag	UNP P0DTC2
B	1244	GLY	-	expression tag	UNP P0DTC2
B	1245	GLU	-	expression tag	UNP P0DTC2
B	1246	TRP	-	expression tag	UNP P0DTC2
B	1247	VAL	-	expression tag	UNP P0DTC2
B	1248	LEU	-	expression tag	UNP P0DTC2
B	1249	LEU	-	expression tag	UNP P0DTC2
B	1250	SER	-	expression tag	UNP P0DTC2
B	1251	THR	-	expression tag	UNP P0DTC2
B	1252	PHE	-	expression tag	UNP P0DTC2
B	1253	LEU	-	expression tag	UNP P0DTC2
B	1254	GLY	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
B	1260	HIS	-	expression tag	UNP P0DTC2
C	10	GLN	-	expression tag	UNP P0DTC2
C	11	CYS	-	expression tag	UNP P0DTC2
C	12	VAL	-	expression tag	UNP P0DTC2
C	13	MET	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	14	PRO	-	expression tag	UNP P0DTC2
C	15	LEU	-	expression tag	UNP P0DTC2
C	16	PHE	-	expression tag	UNP P0DTC2
C	17	ASN	-	expression tag	UNP P0DTC2
C	18	LEU	-	expression tag	UNP P0DTC2
C	19	ILE	-	expression tag	UNP P0DTC2
C	20	THR	-	expression tag	UNP P0DTC2
C	21	THR	-	expression tag	UNP P0DTC2
C	22	THR	-	expression tag	UNP P0DTC2
C	23	GLN	-	expression tag	UNP P0DTC2
C	27	SER	-	expression tag	UNP P0DTC2
C	28	TYR	-	expression tag	UNP P0DTC2
C	29	THR	-	expression tag	UNP P0DTC2
C	30	ASN	-	expression tag	UNP P0DTC2
C	50	LEU	SER	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	127	PHE	VAL	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	157	SER	PHE	variant	UNP P0DTC2
C	158	GLY	ARG	variant	UNP P0DTC2
C	186	LEU	PHE	variant	UNP P0DTC2
C	190	SER	ARG	variant	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	212	ILE	LEU	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	216	PHE	LEU	variant	UNP P0DTC2
C	245	ASN	HIS	variant	UNP P0DTC2
C	264	ASP	ALA	variant	UNP P0DTC2
C	332	VAL	ILE	variant	UNP P0DTC2
C	339	HIS	GLY	variant	UNP P0DTC2
C	346	THR	ARG	variant	UNP P0DTC2
C	356	THR	LYS	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	403	LYS	ARG	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	440	LYS	ASN	variant	UNP P0DTC2
C	445	ARG	VAL	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	450	ASP	ASN	variant	UNP P0DTC2
C	452	TRP	LEU	variant	UNP P0DTC2
C	455	SER	LEU	variant	UNP P0DTC2
C	456	LEU	PHE	variant	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	481	LYS	ASN	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	484	LYS	GLU	variant	UNP P0DTC2
C	486	PRO	PHE	variant	UNP P0DTC2
C	493	GLU	GLN	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	554	LYS	GLU	variant	UNP P0DTC2
C	570	VAL	ALA	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	621	SER	PRO	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	670	VAL	ILE	variant	UNP P0DTC2
C	683	LYS	ASN	variant	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	939	PHE	SER	variant	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1143	LEU	PRO	variant	UNP P0DTC2
C	1212	GLY	-	expression tag	UNP P0DTC2

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

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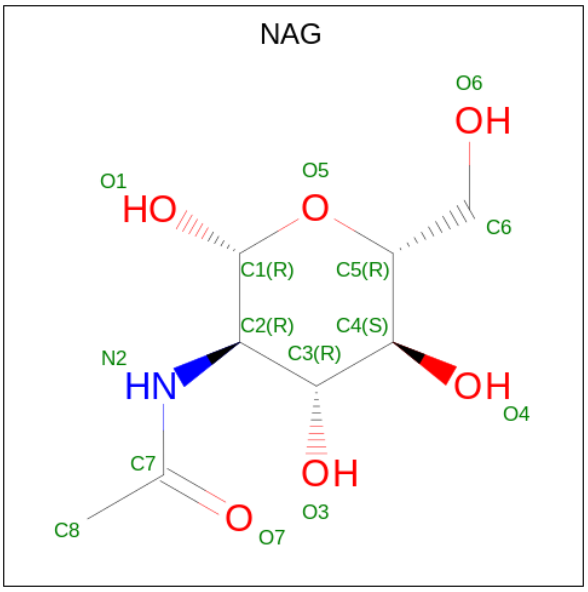
Chain	Residue	Modelled	Actual	Comment	Reference
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	HIS	-	expression tag	UNP P0DTC2
C	1259	HIS	-	expression tag	UNP P0DTC2
C	1260	HIS	-	expression tag	UNP P0DTC2

- 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	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		
6	V	2	Total	C	N	O	0	0
			28	16	2	10		

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



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

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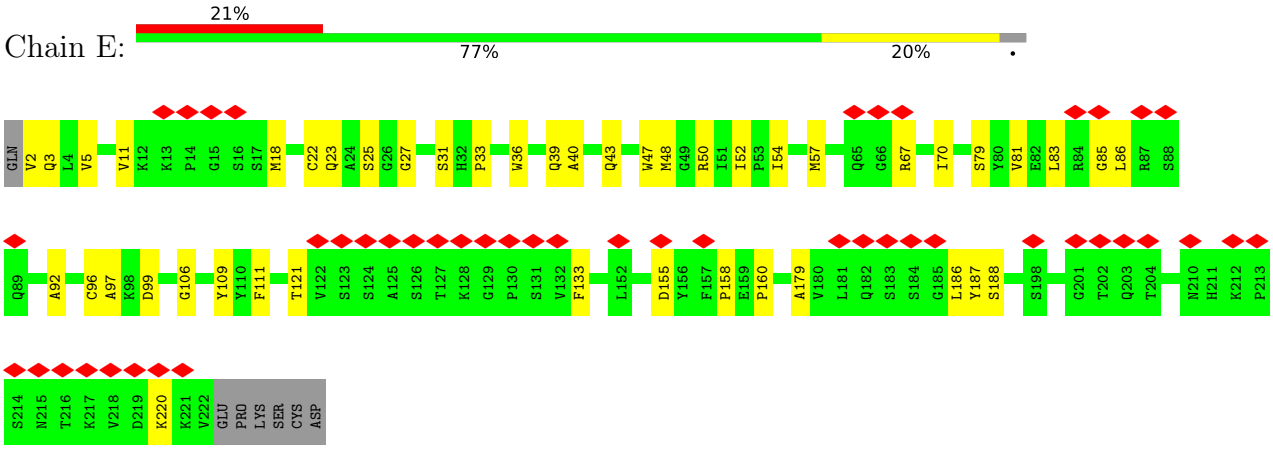
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Mol	Chain	Residues	Atoms				AltConf
7	C	1	Total	C	N	O	0
			14	8	1	5	

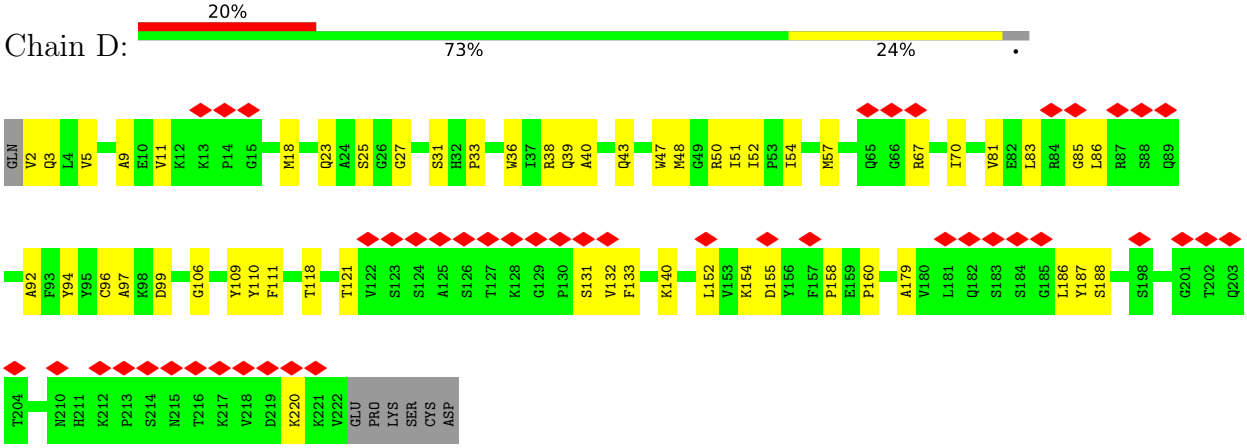
3 Residue-property plots (i)

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.

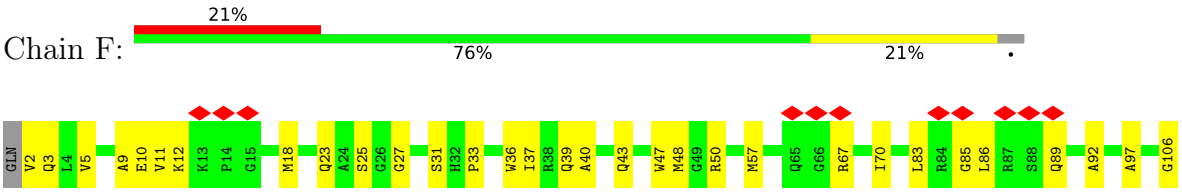
• Molecule 1: Heavy chain of ZL525 Fab

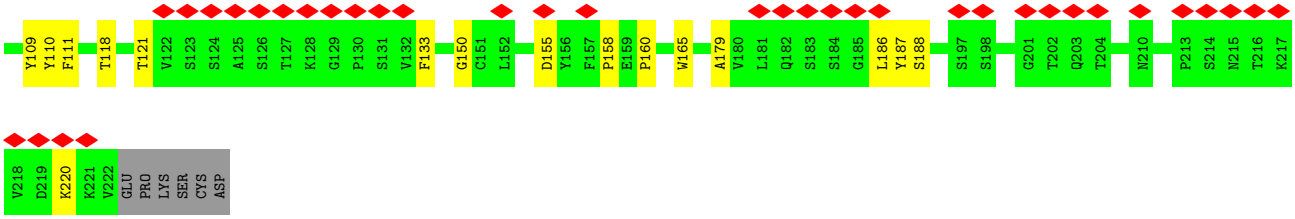


• Molecule 1: Heavy chain of ZL525 Fab

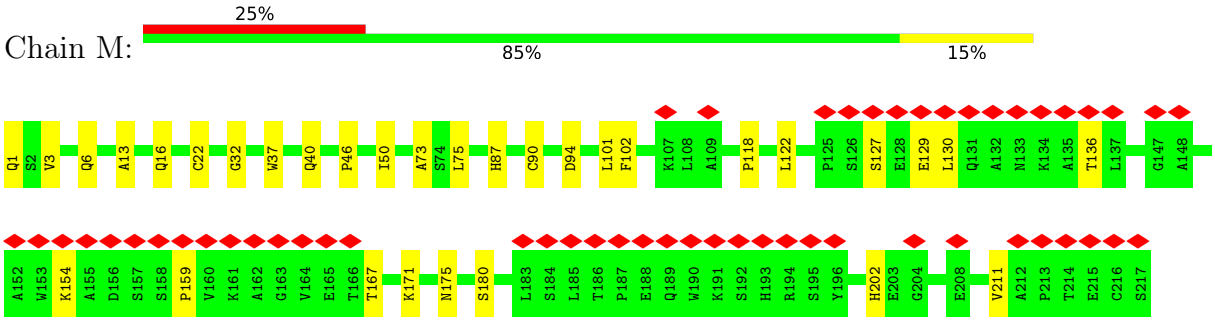


• Molecule 1: Heavy chain of ZL525 Fab

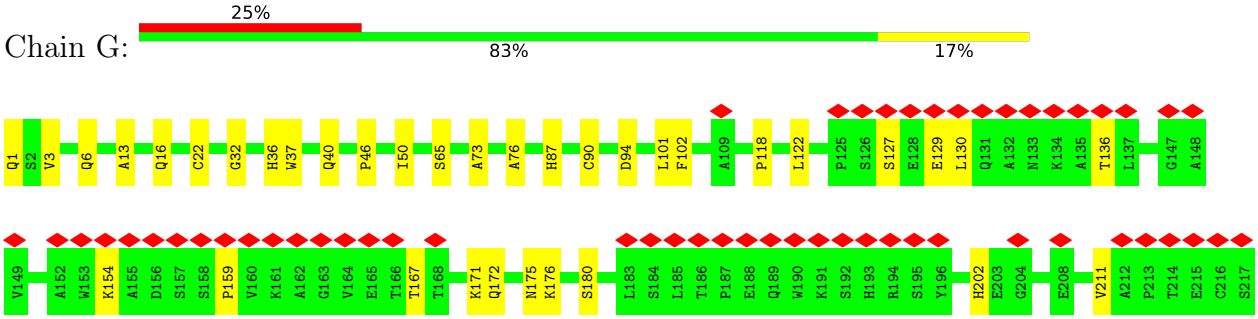




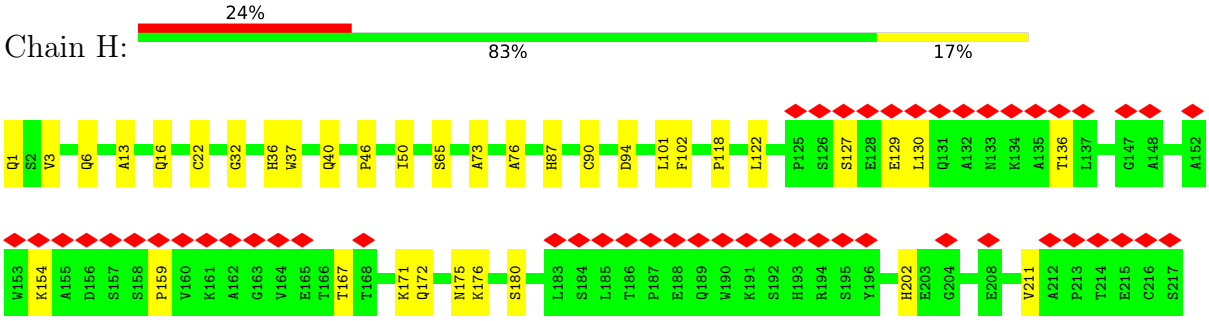
• Molecule 2: Light chain of ZL525 Fab



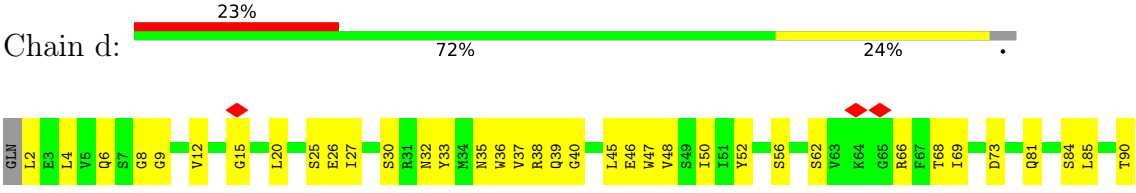
• Molecule 2: Light chain of ZL525 Fab

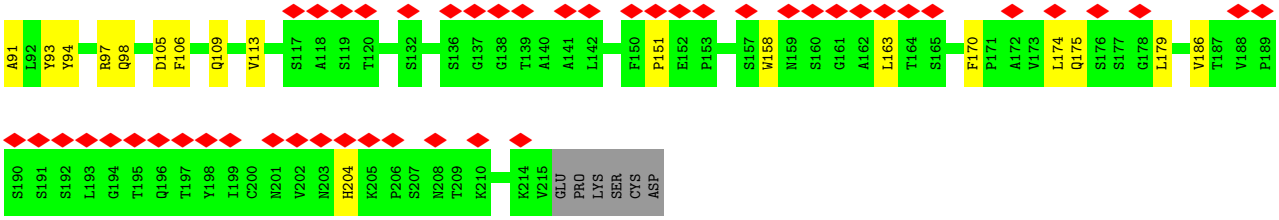


• Molecule 2: Light chain of ZL525 Fab

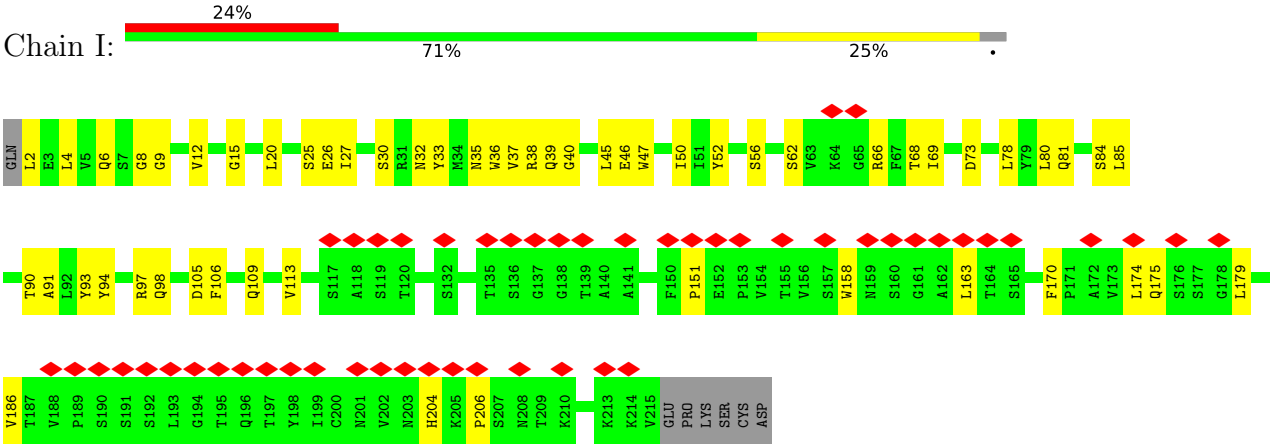


• Molecule 3: Heavy chain of ZL58 Fab

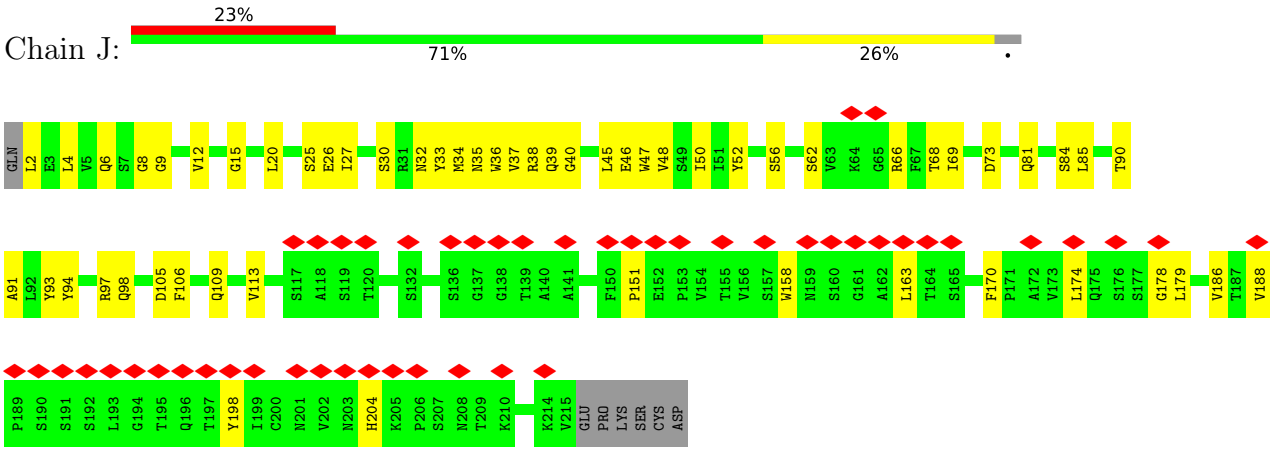




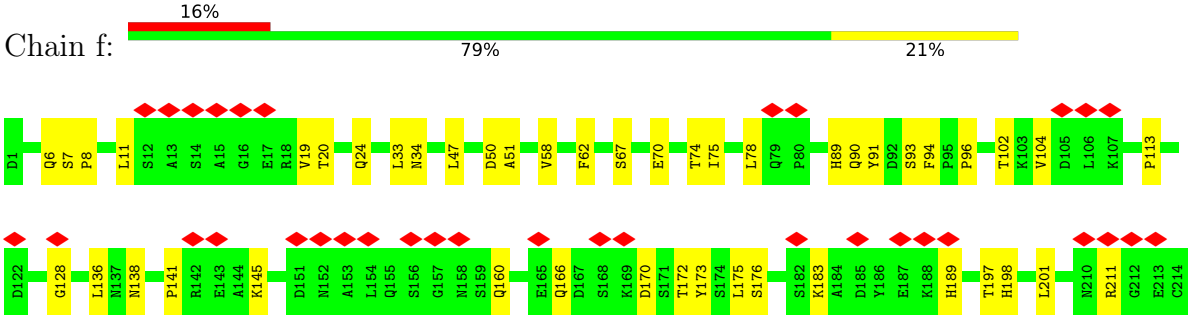
• Molecule 3: Heavy chain of ZL58 Fab



• Molecule 3: Heavy chain of ZL58 Fab

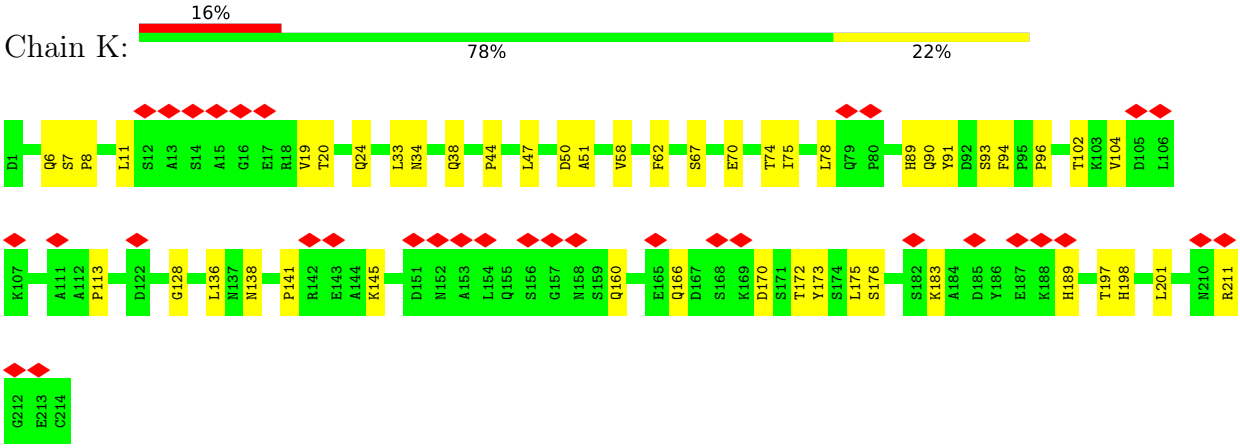


• Molecule 4: Light chain of ZL58 Fab



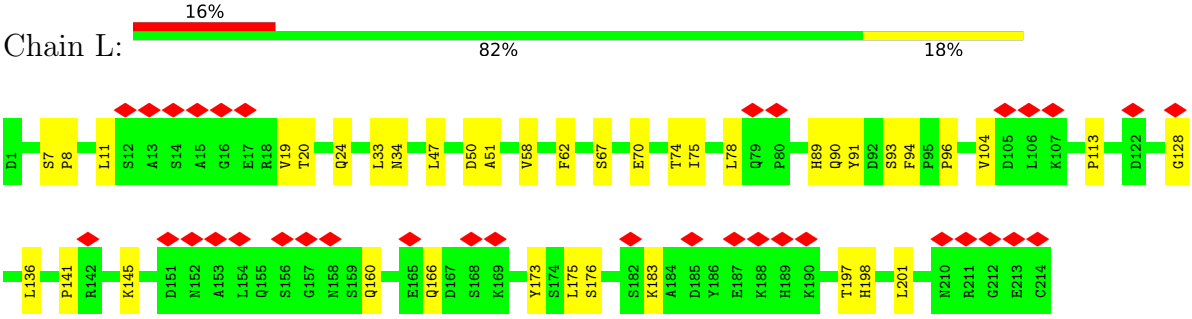
• Molecule 4: Light chain of ZL58 Fab

Chain K:



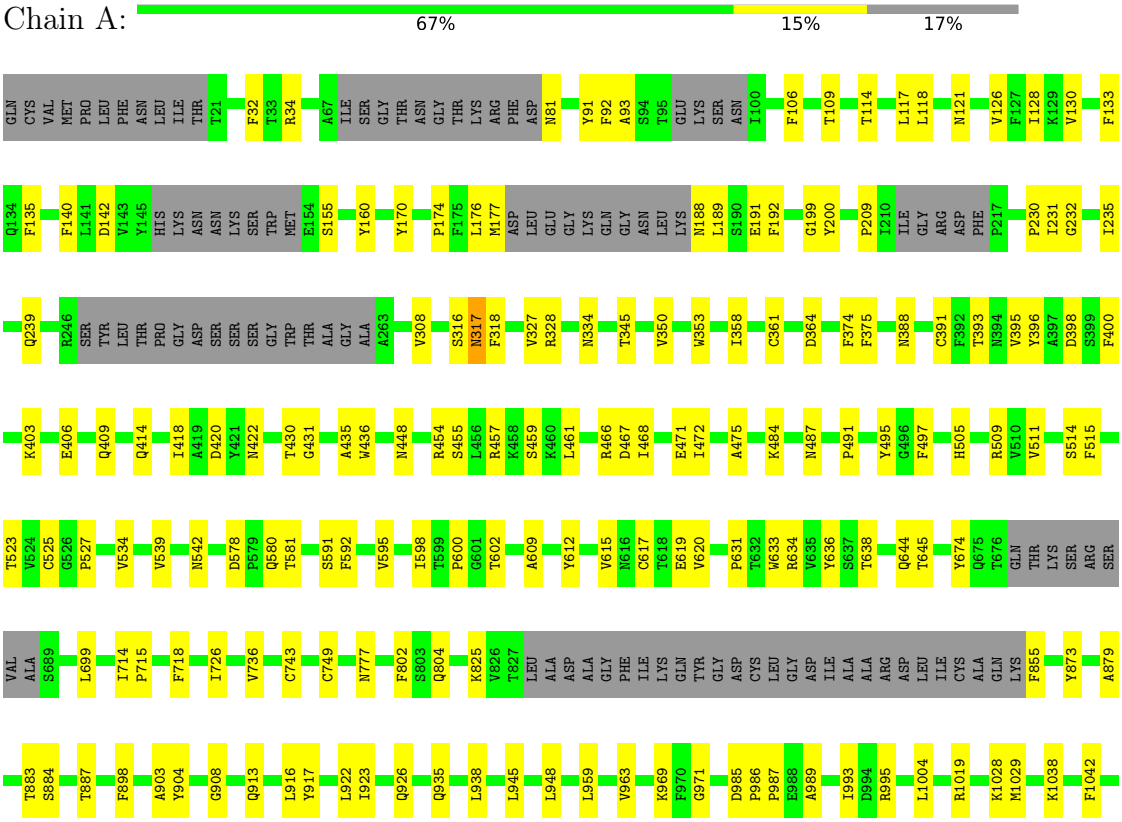
• Molecule 4: Light chain of ZL58 Fab

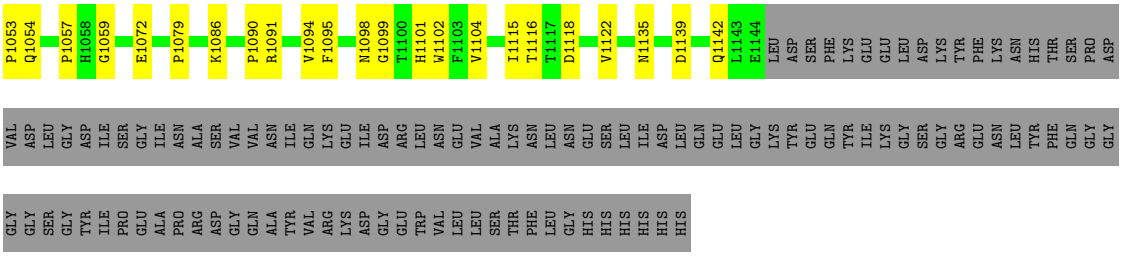
Chain L:



• Molecule 5: Spike glycoprotein

Chain A:

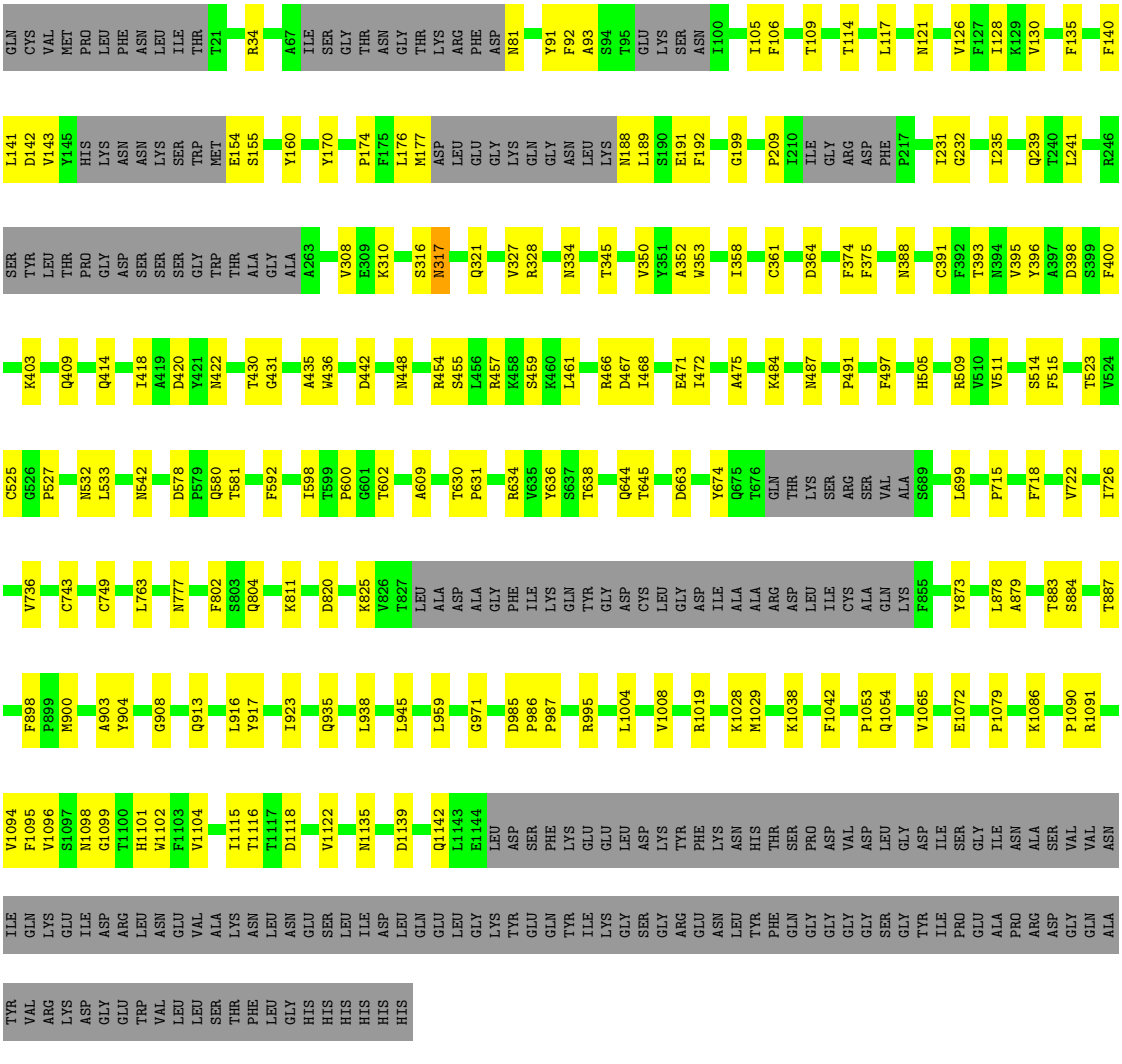




• Molecule 5: Spike glycoprotein

Chain B:



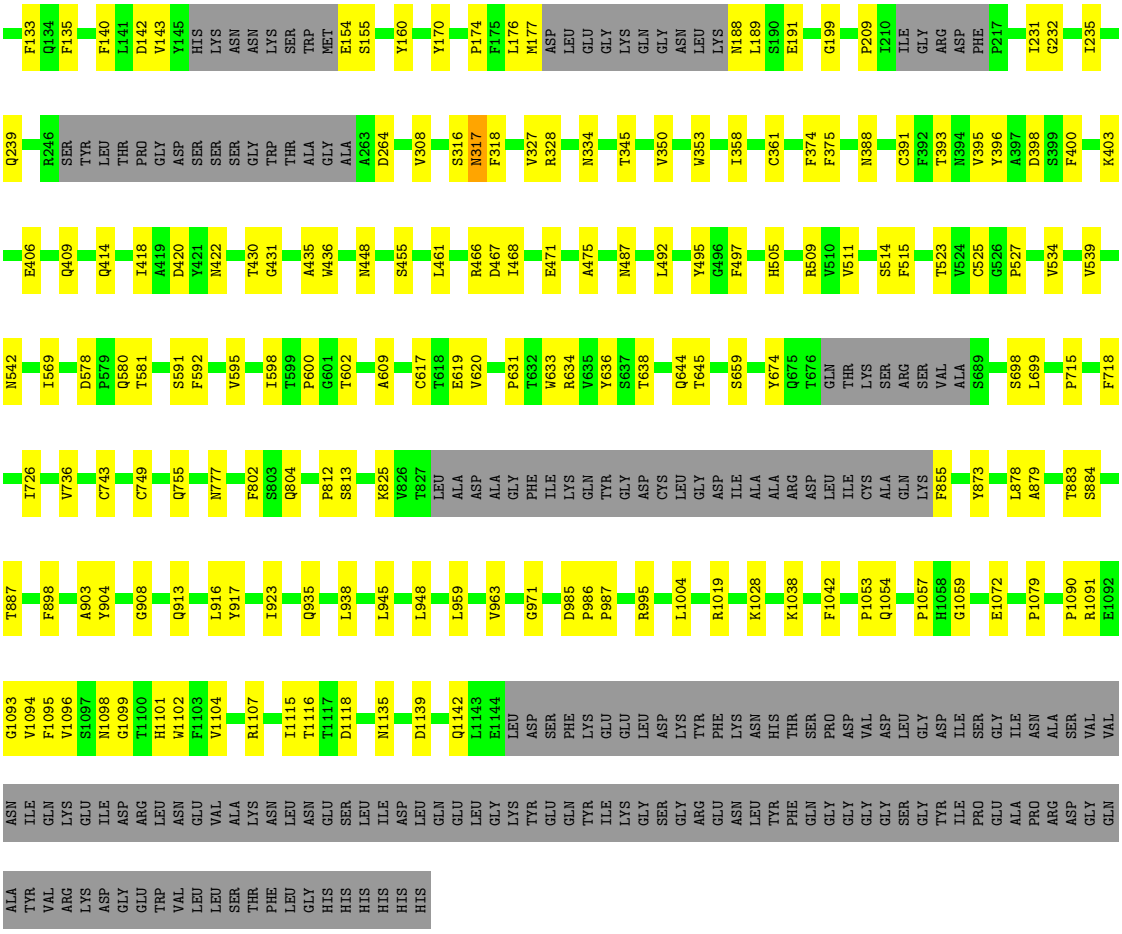


• Molecule 5: Spike glycoprotein

Chain C:

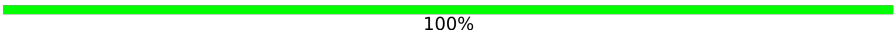






• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

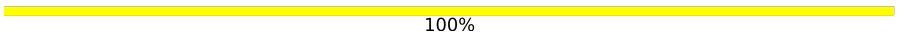
Chain N:





• 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

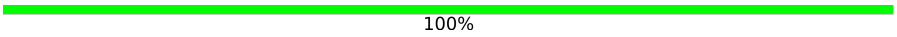
Chain P:





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

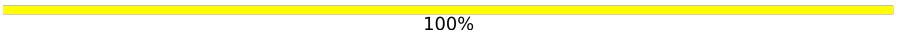
Chain Q:





• 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

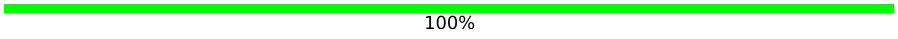
Chain S:





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

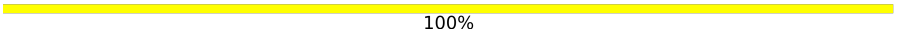
Chain T:





• 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:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	174630	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.750	Depositor
Minimum map value	-0.326	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	373.752, 373.752, 373.752	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0382, 1.0382, 1.0382	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	D	0.09	0/1686	0.24	0/2295
1	E	0.10	0/1686	0.25	0/2295
1	F	0.09	0/1686	0.24	0/2295
2	G	0.08	0/1649	0.23	0/2248
2	H	0.08	0/1649	0.23	0/2248
2	M	0.08	0/1649	0.22	0/2248
3	I	0.07	0/1620	0.22	0/2208
3	J	0.08	0/1620	0.23	0/2208
3	d	0.07	0/1620	0.22	0/2208
4	K	0.07	0/1686	0.23	0/2289
4	L	0.07	0/1686	0.23	0/2289
4	f	0.08	0/1686	0.23	0/2289
5	A	0.15	0/8200	0.29	0/11164
5	B	0.15	0/8200	0.29	0/11164
5	C	0.15	0/8200	0.29	0/11164
All	All	0.12	0/44523	0.26	0/60612

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1645	0	1610	40	0
1	E	1645	0	1610	34	0
1	F	1645	0	1610	34	0
2	G	1610	0	1561	24	0
2	H	1610	0	1561	24	0
2	M	1610	0	1561	22	0
3	I	1584	0	1551	40	0
3	J	1584	0	1551	39	0
3	d	1584	0	1551	36	0
4	K	1649	0	1584	30	0
4	L	1649	0	1584	24	0
4	f	1649	0	1584	28	0
5	A	8007	0	7814	126	0
5	B	8007	0	7814	123	0
5	C	8007	0	7814	120	0
6	N	28	0	25	0	0
6	O	28	0	25	1	0
6	P	28	0	25	0	0
6	Q	28	0	25	0	0
6	R	28	0	25	1	0
6	S	28	0	25	0	0
6	T	28	0	25	0	0
6	U	28	0	25	1	0
6	V	28	0	25	0	0
7	A	70	0	65	0	0
7	B	70	0	65	0	0
7	C	70	0	65	0	0
All	All	43947	0	42780	688	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 8.

The worst 5 of 688 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:C:1104:VAL:HG23	5:C:1115:ILE:HG12	1.68	0.75
5:B:1104:VAL:HG23	5:B:1115:ILE:HG12	1.69	0.74
5:A:1104:VAL:HG23	5:A:1115:ILE:HG12	1.68	0.73
5:C:358:ILE:HB	5:C:395:VAL:HB	1.70	0.73
5:A:358:ILE:HB	5:A:395:VAL:HB	1.71	0.72

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	219/228 (96%)	210 (96%)	9 (4%)	0	100	100
1	E	219/228 (96%)	210 (96%)	9 (4%)	0	100	100
1	F	219/228 (96%)	210 (96%)	9 (4%)	0	100	100
2	G	215/217 (99%)	205 (95%)	10 (5%)	0	100	100
2	H	215/217 (99%)	205 (95%)	10 (5%)	0	100	100
2	M	215/217 (99%)	205 (95%)	10 (5%)	0	100	100
3	I	212/221 (96%)	206 (97%)	6 (3%)	0	100	100
3	J	212/221 (96%)	208 (98%)	4 (2%)	0	100	100
3	d	212/221 (96%)	206 (97%)	6 (3%)	0	100	100
4	K	212/214 (99%)	201 (95%)	11 (5%)	0	100	100
4	L	212/214 (99%)	200 (94%)	12 (6%)	0	100	100
4	f	212/214 (99%)	200 (94%)	12 (6%)	0	100	100
5	A	1004/1238 (81%)	968 (96%)	36 (4%)	0	100	100
5	B	1004/1238 (81%)	968 (96%)	36 (4%)	0	100	100
5	C	1004/1238 (81%)	966 (96%)	38 (4%)	0	100	100
All	All	5586/6354 (88%)	5368 (96%)	218 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	D	184/191 (96%)	184 (100%)	0	100	100
1	E	184/191 (96%)	184 (100%)	0	100	100
1	F	184/191 (96%)	184 (100%)	0	100	100
2	G	180/180 (100%)	180 (100%)	0	100	100
2	H	180/180 (100%)	180 (100%)	0	100	100
2	M	180/180 (100%)	180 (100%)	0	100	100
3	I	179/186 (96%)	179 (100%)	0	100	100
3	J	179/186 (96%)	179 (100%)	0	100	100
3	d	179/186 (96%)	179 (100%)	0	100	100
4	K	189/189 (100%)	189 (100%)	0	100	100
4	L	189/189 (100%)	189 (100%)	0	100	100
4	f	189/189 (100%)	189 (100%)	0	100	100
5	A	898/1078 (83%)	897 (100%)	1 (0%)	88	95
5	B	898/1078 (83%)	897 (100%)	1 (0%)	88	95
5	C	898/1078 (83%)	897 (100%)	1 (0%)	88	95
All	All	4890/5472 (89%)	4887 (100%)	3 (0%)	87	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	317	ASN
5	B	317	ASN
5	C	317	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
3	I	81	GLN
5	C	414	GLN
5	B	505	HIS
5	C	409	GLN
5	C	919	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

18 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	N	1	6,5	14,14,15	0.22	0	17,19,21	0.48	0
6	NAG	N	2	6	14,14,15	0.22	0	17,19,21	0.43	0
6	NAG	O	1	6,5	14,14,15	0.29	0	17,19,21	0.46	0
6	NAG	O	2	6	14,14,15	0.20	0	17,19,21	0.41	0
6	NAG	P	1	6,5	14,14,15	1.25	1 (7%)	17,19,21	1.13	1 (5%)
6	NAG	P	2	6	14,14,15	0.24	0	17,19,21	0.48	0
6	NAG	Q	1	6,5	14,14,15	0.24	0	17,19,21	0.47	0
6	NAG	Q	2	6	14,14,15	0.21	0	17,19,21	0.41	0
6	NAG	R	1	6,5	14,14,15	0.27	0	17,19,21	0.46	0
6	NAG	R	2	6	14,14,15	0.19	0	17,19,21	0.41	0
6	NAG	S	1	6,5	14,14,15	1.24	1 (7%)	17,19,21	1.11	1 (5%)
6	NAG	S	2	6	14,14,15	0.24	0	17,19,21	0.47	0
6	NAG	T	1	6,5	14,14,15	0.22	0	17,19,21	0.49	0
6	NAG	T	2	6	14,14,15	0.21	0	17,19,21	0.42	0
6	NAG	U	1	6,5	14,14,15	0.29	0	17,19,21	0.46	0
6	NAG	U	2	6	14,14,15	0.19	0	17,19,21	0.41	0
6	NAG	V	1	6,5	14,14,15	1.22	1 (7%)	17,19,21	1.10	1 (5%)
6	NAG	V	2	6	14,14,15	0.27	0	17,19,21	0.48	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	N	1	6,5	-	0/6/23/26	0/1/1/1

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	1	NAG	O5-C1	-4.37	1.36	1.43
6	S	1	NAG	O5-C1	-4.32	1.36	1.43
6	V	1	NAG	O5-C1	-4.28	1.36	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	P	1	NAG	C3-C4-C5	3.11	115.78	110.24
6	S	1	NAG	C3-C4-C5	3.02	115.63	110.24
6	V	1	NAG	C3-C4-C5	2.97	115.54	110.24

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	P	1	NAG	O5-C5-C6-O6
6	S	1	NAG	C4-C5-C6-O6
6	O	2	NAG	O5-C5-C6-O6

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

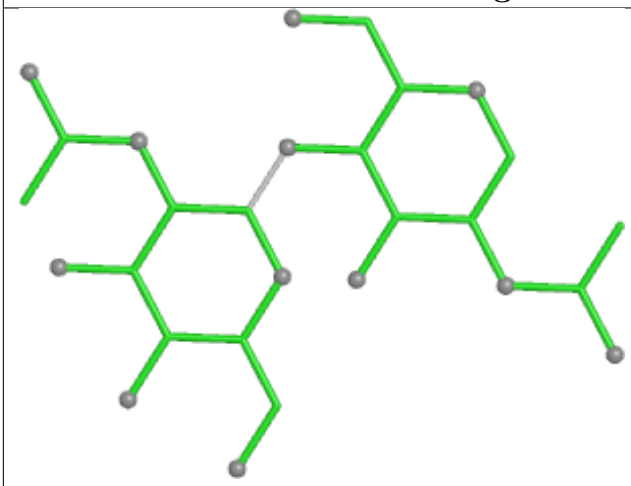
There are no ring outliers.

6 monomers are involved in 3 short contacts:

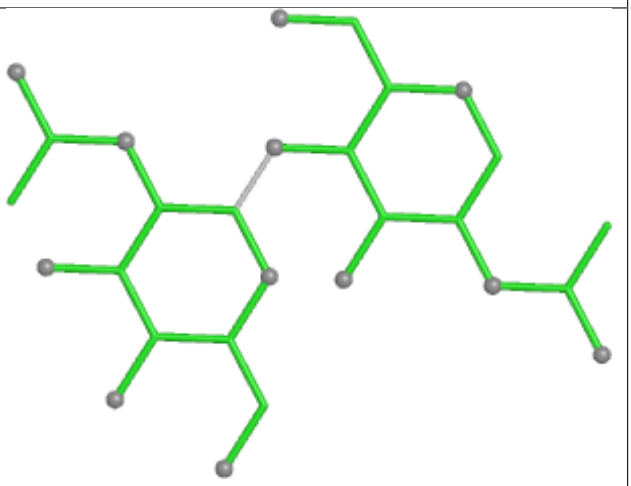
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	U	1	NAG	1	0
6	U	2	NAG	1	0
6	R	2	NAG	1	0
6	O	2	NAG	1	0
6	R	1	NAG	1	0
6	O	1	NAG	1	0

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

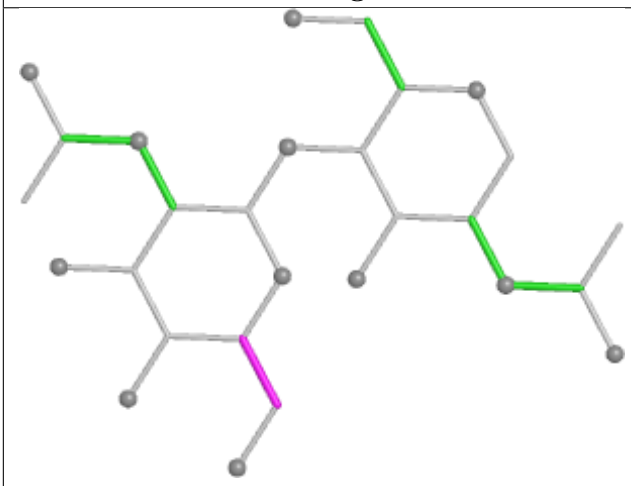
Oligosaccharide Chain N



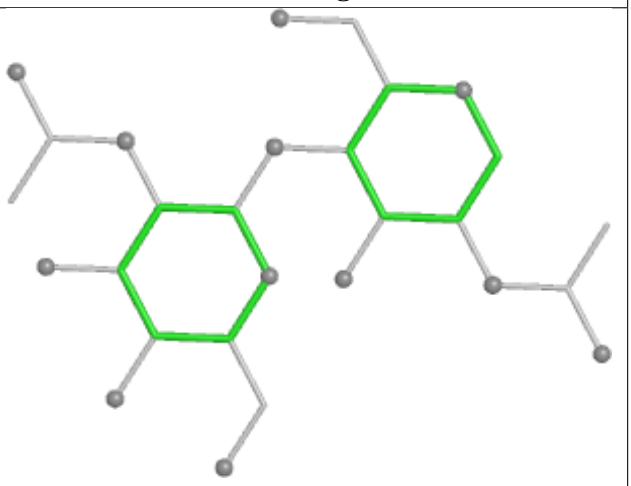
Bond lengths



Bond angles

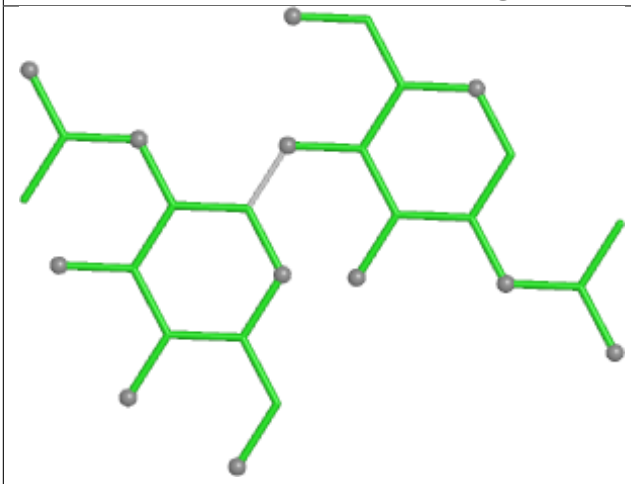


Torsions

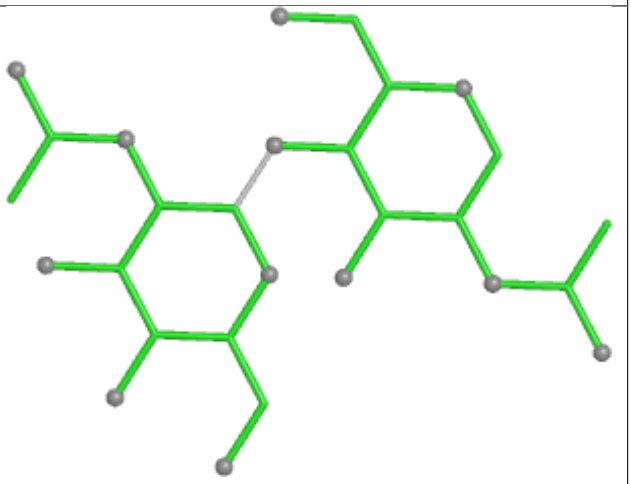


Rings

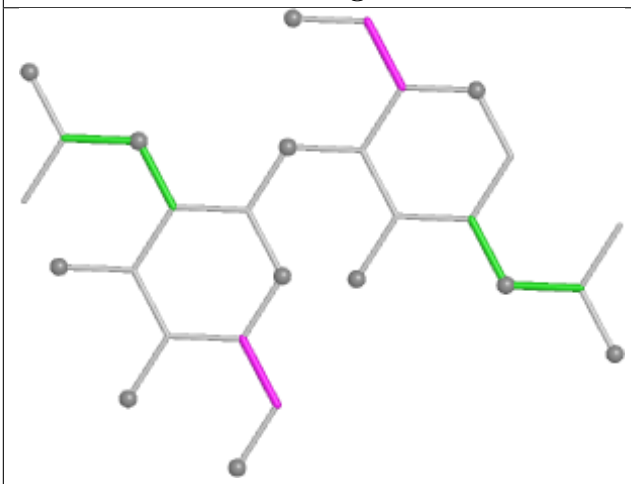
Oligosaccharide Chain O



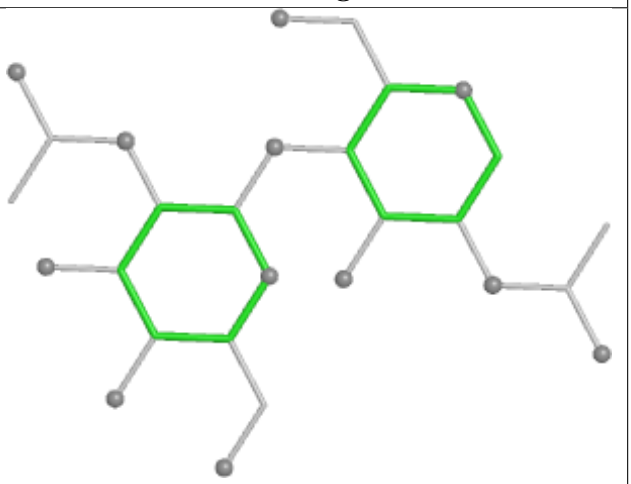
Bond lengths



Bond angles

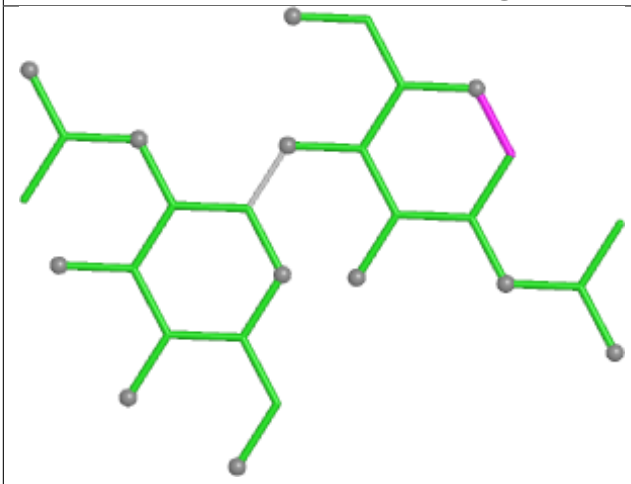


Torsions

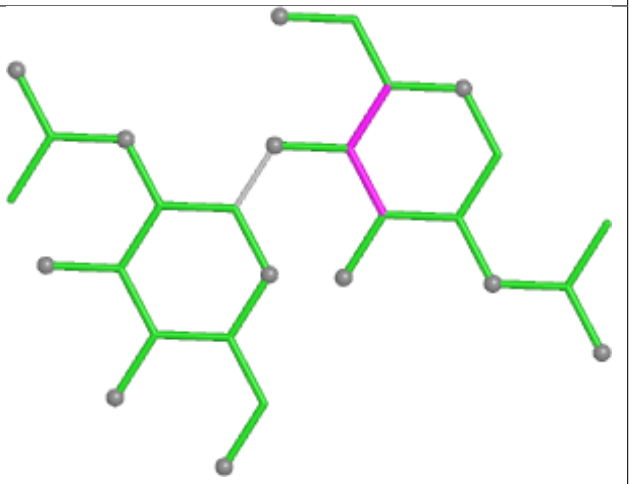


Rings

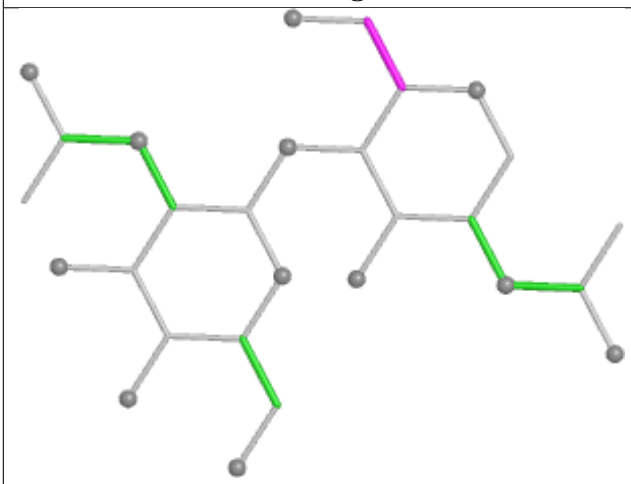
Oligosaccharide Chain P



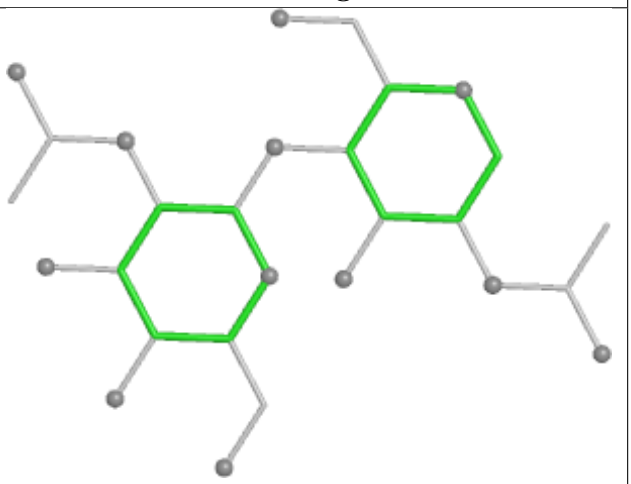
Bond lengths



Bond angles

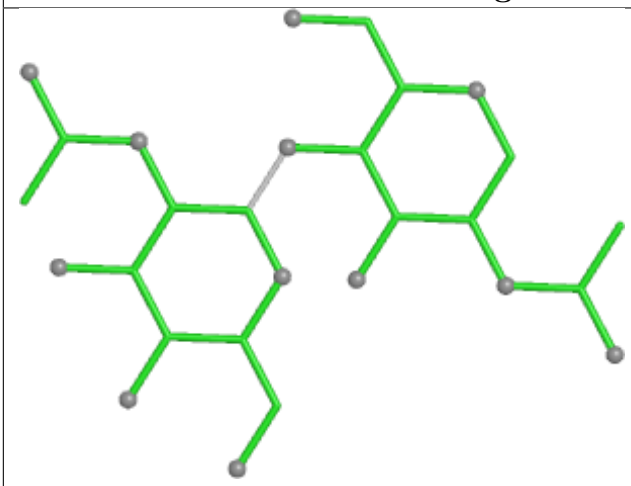


Torsions

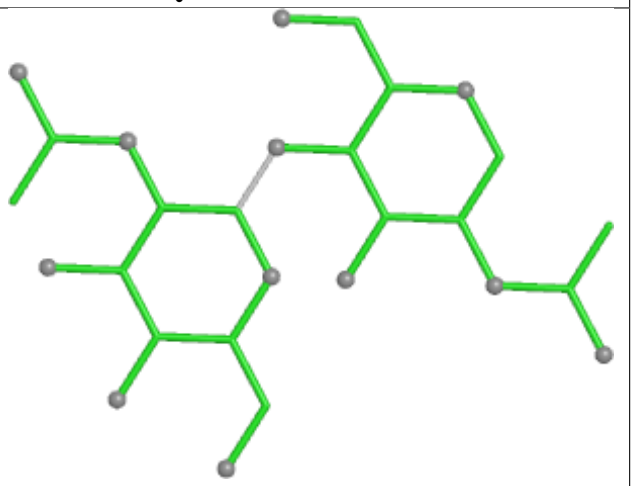


Rings

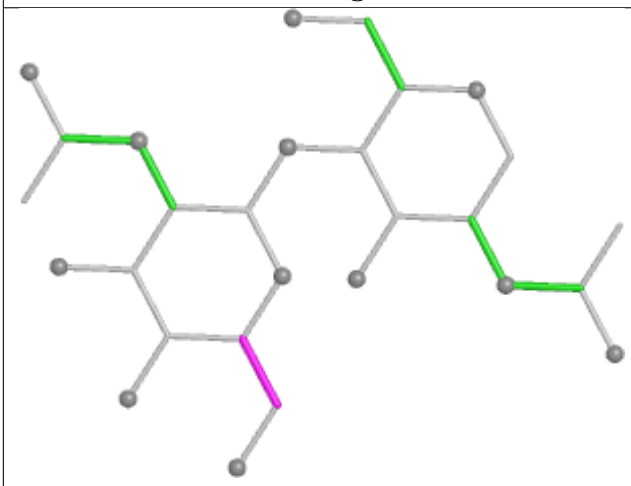
Oligosaccharide Chain Q



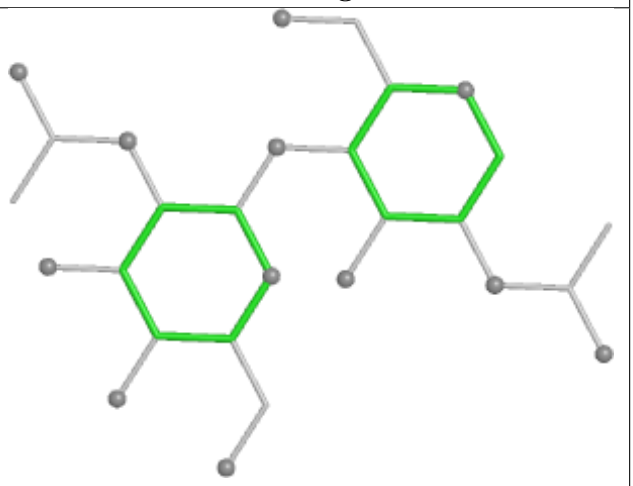
Bond lengths



Bond angles

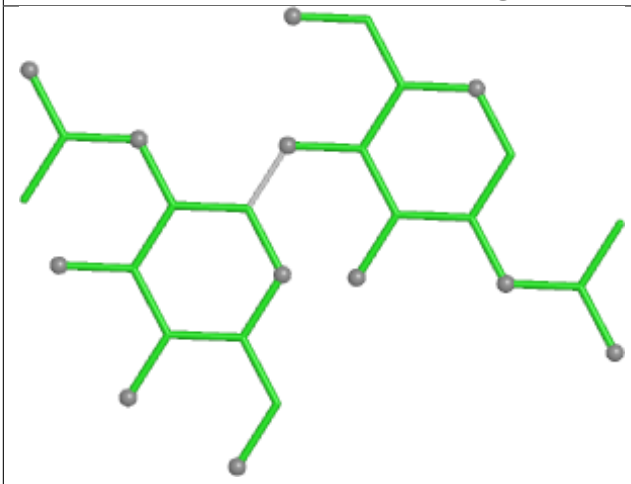


Torsions

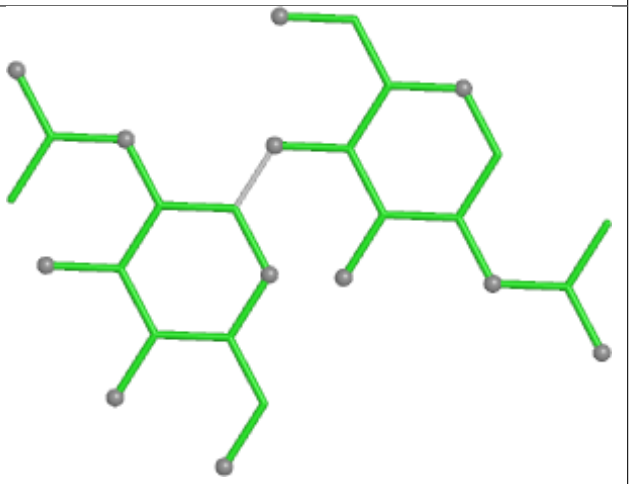


Rings

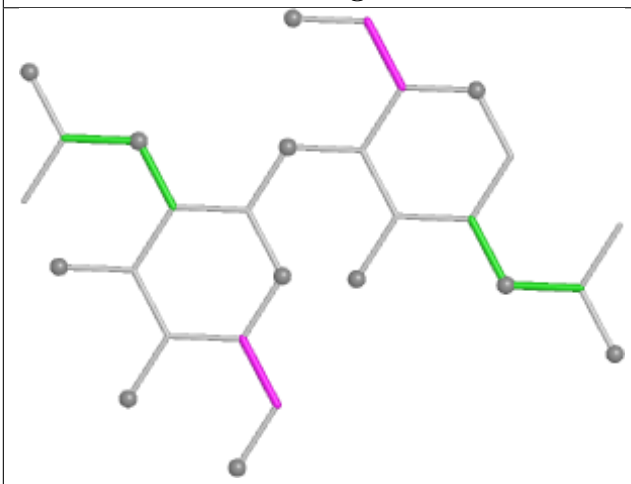
Oligosaccharide Chain R



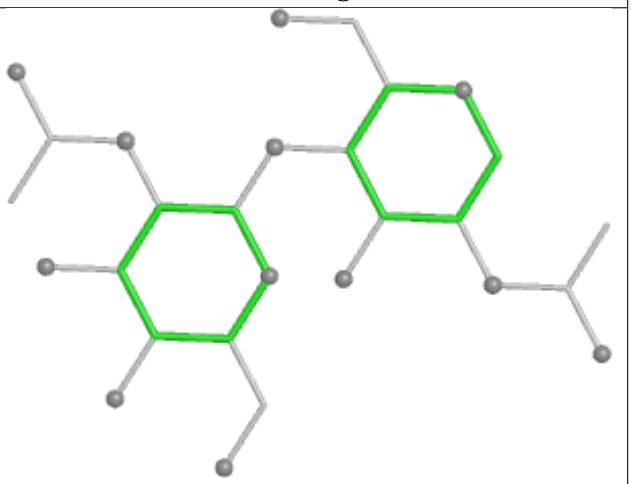
Bond lengths



Bond angles

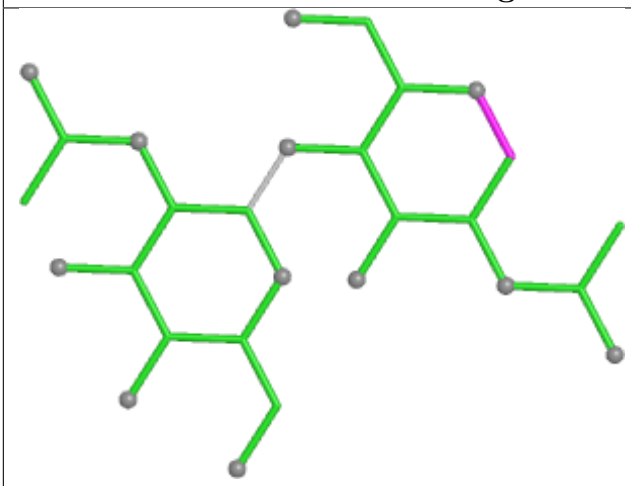


Torsions

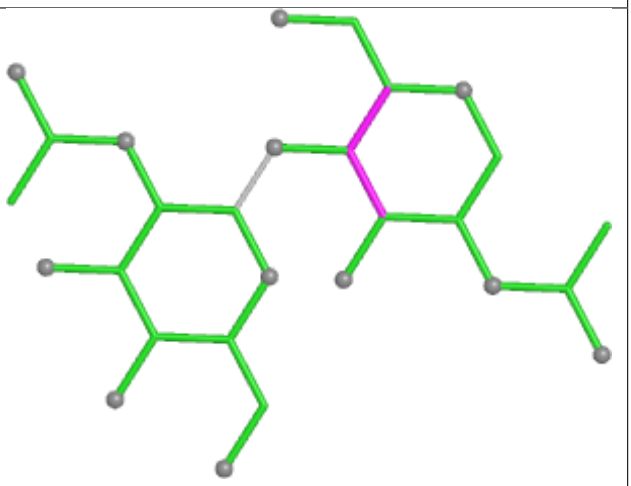


Rings

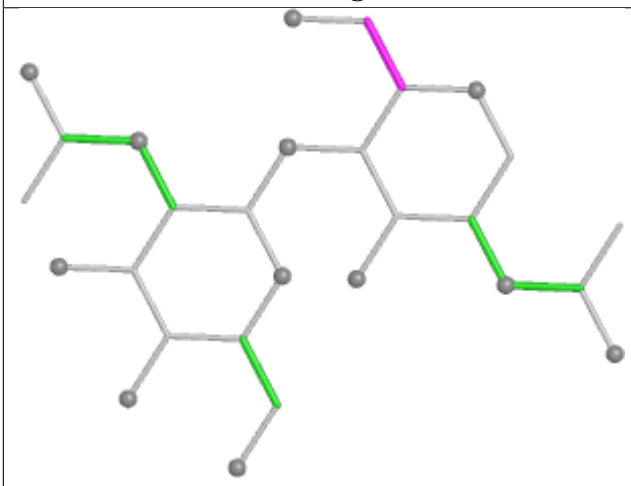
Oligosaccharide Chain S



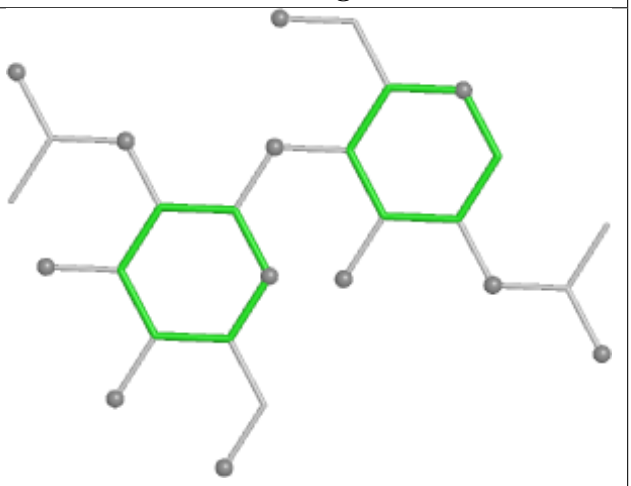
Bond lengths



Bond angles

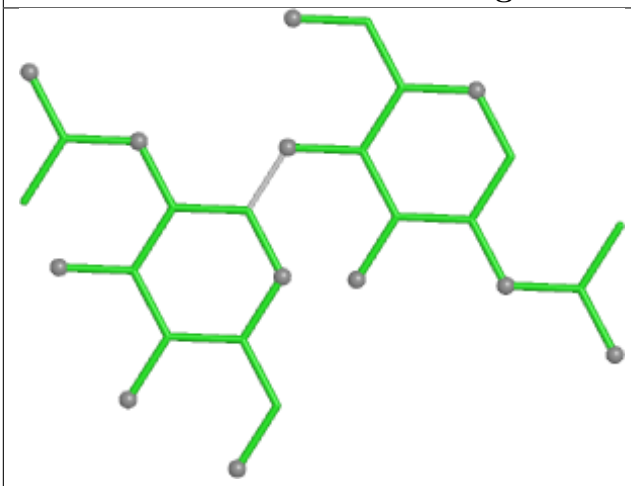


Torsions

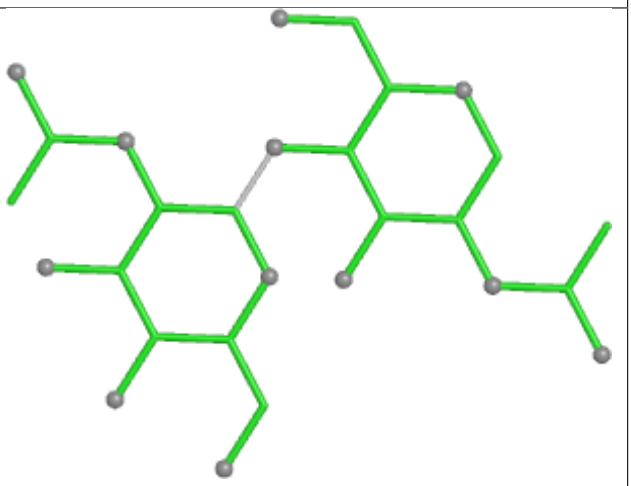


Rings

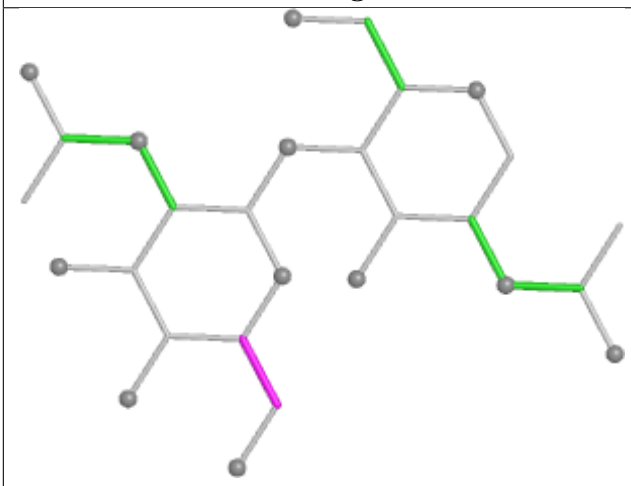
Oligosaccharide Chain T



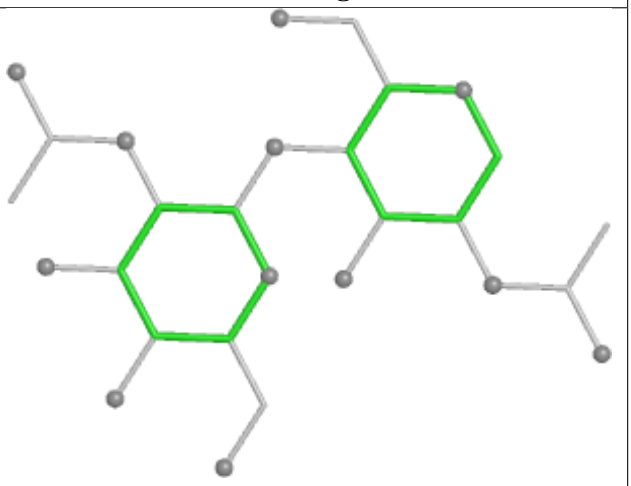
Bond lengths



Bond angles

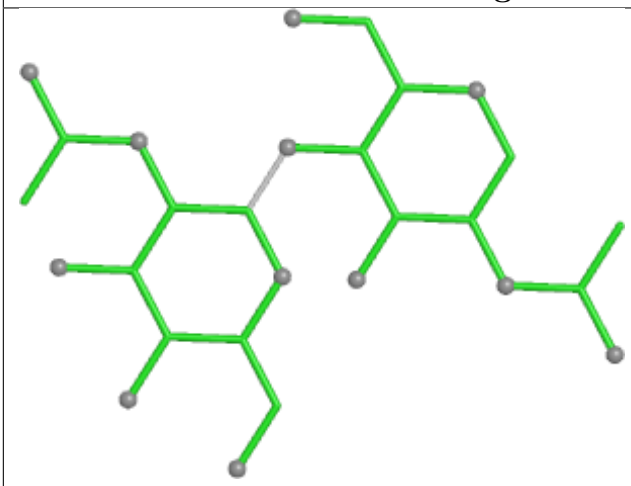


Torsions

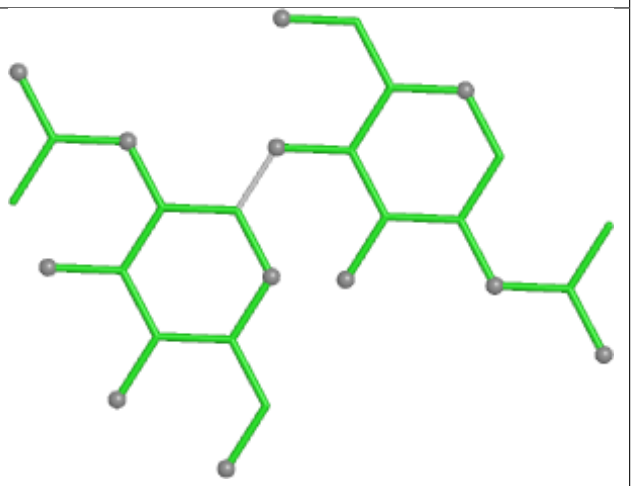


Rings

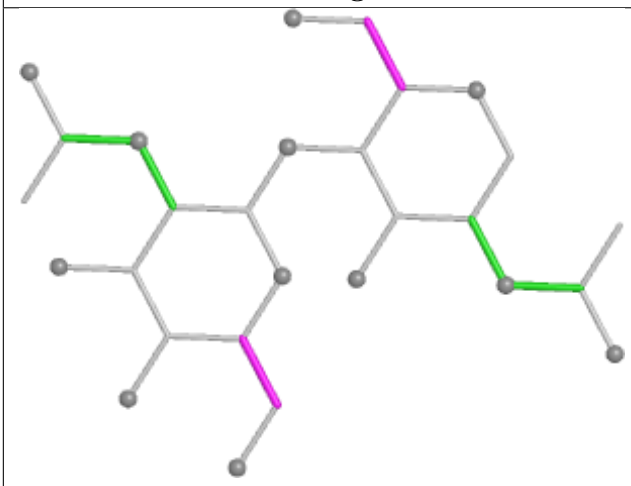
Oligosaccharide Chain U



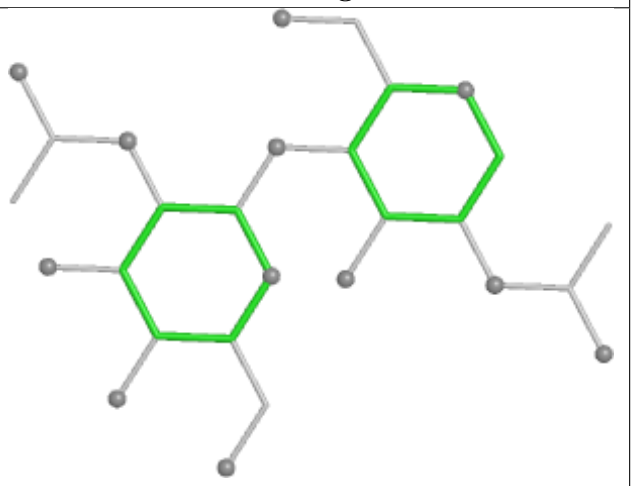
Bond lengths



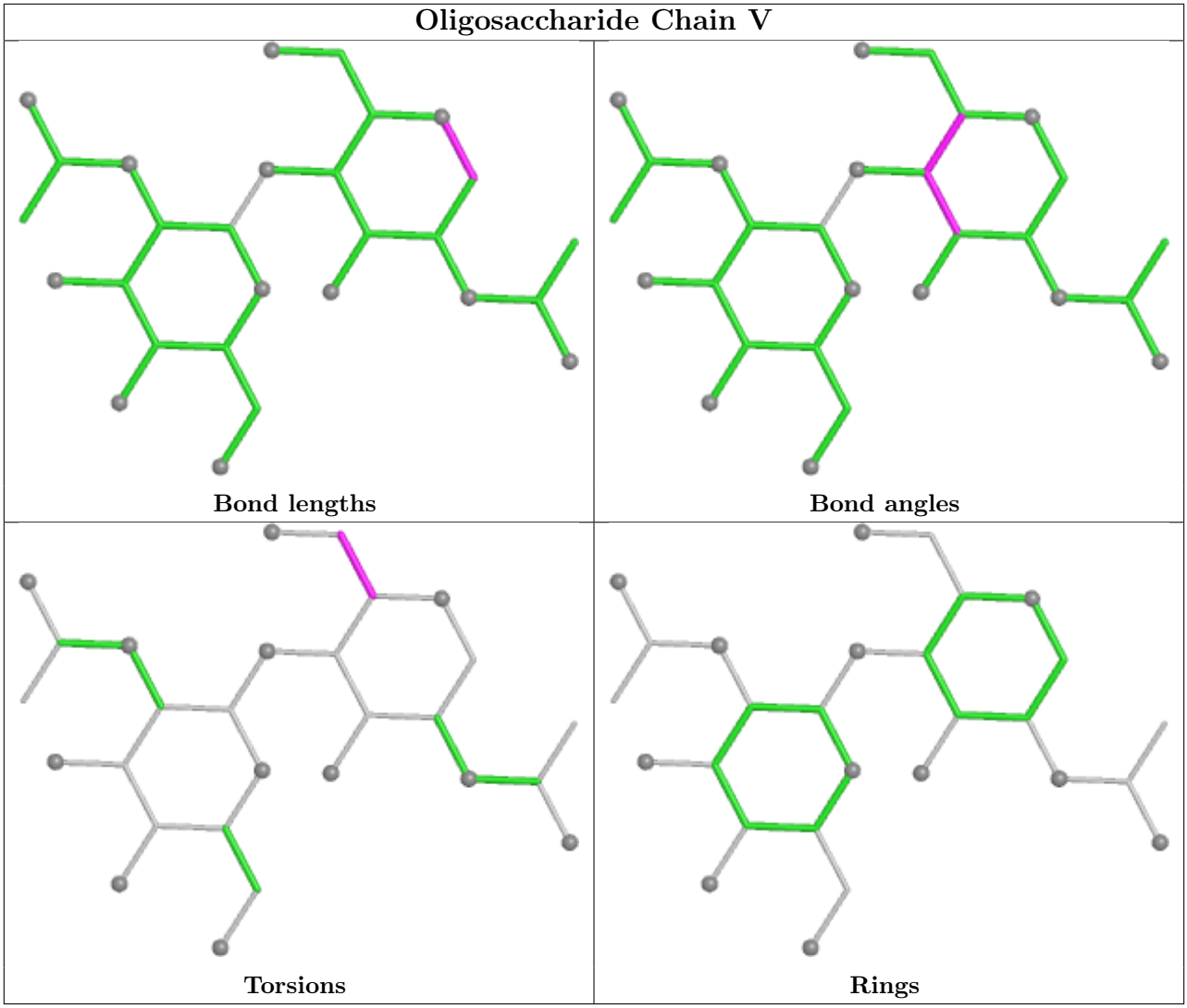
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	C	1302	5	14,14,15	0.22	0	17,19,21	0.54	0
7	NAG	B	1301	5	14,14,15	0.28	0	17,19,21	0.58	0
7	NAG	A	1302	5	14,14,15	0.22	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	C	1305	5	14,14,15	0.21	0	17,19,21	0.46	0
7	NAG	A	1303	5	14,14,15	0.28	0	17,19,21	0.35	0
7	NAG	A	1305	5	14,14,15	0.21	0	17,19,21	0.46	0
7	NAG	B	1303	5	14,14,15	0.28	0	17,19,21	0.36	0
7	NAG	B	1304	5	14,14,15	0.24	0	17,19,21	0.48	0
7	NAG	A	1304	5	14,14,15	0.25	0	17,19,21	0.50	0
7	NAG	B	1302	5	14,14,15	0.24	0	17,19,21	0.48	0
7	NAG	A	1301	5	14,14,15	0.23	0	17,19,21	0.49	0
7	NAG	C	1301	5	14,14,15	0.22	0	17,19,21	0.46	0
7	NAG	B	1305	5	14,14,15	0.21	0	17,19,21	0.46	0
7	NAG	C	1303	5	14,14,15	0.28	0	17,19,21	0.36	0
7	NAG	C	1304	5	14,14,15	0.24	0	17,19,21	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	1302	5	-	2/6/23/26	0/1/1/1
7	NAG	B	1301	5	-	2/6/23/26	0/1/1/1
7	NAG	A	1302	5	-	2/6/23/26	0/1/1/1
7	NAG	C	1305	5	-	2/6/23/26	0/1/1/1
7	NAG	A	1303	5	-	3/6/23/26	0/1/1/1
7	NAG	A	1305	5	-	2/6/23/26	0/1/1/1
7	NAG	B	1303	5	-	3/6/23/26	0/1/1/1
7	NAG	B	1304	5	-	2/6/23/26	0/1/1/1
7	NAG	A	1304	5	-	2/6/23/26	0/1/1/1
7	NAG	B	1302	5	-	2/6/23/26	0/1/1/1
7	NAG	A	1301	5	-	2/6/23/26	0/1/1/1
7	NAG	C	1301	5	-	2/6/23/26	0/1/1/1
7	NAG	B	1305	5	-	2/6/23/26	0/1/1/1
7	NAG	C	1303	5	-	3/6/23/26	0/1/1/1
7	NAG	C	1304	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

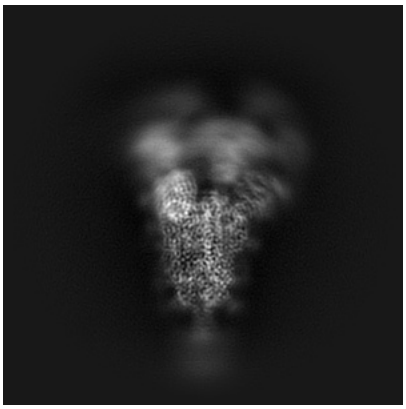
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-66902. These allow visual inspection of the internal detail of the map and identification of artifacts.

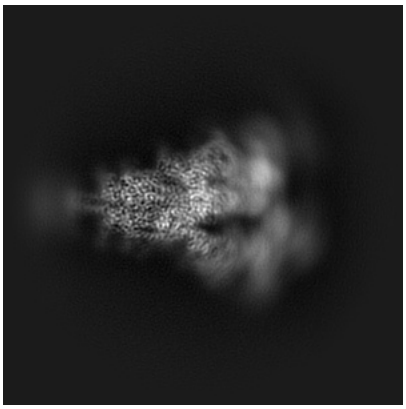
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

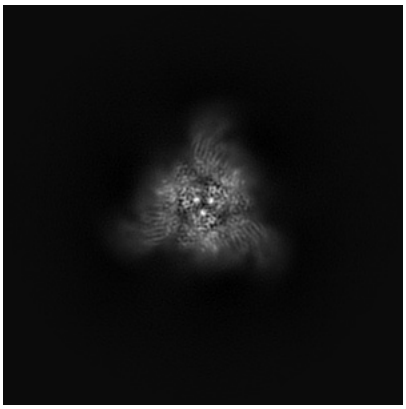
6.1.1 Primary map



X

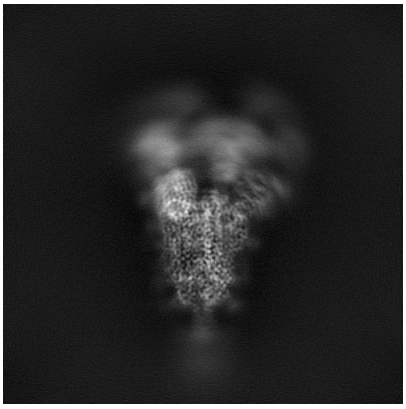


Y

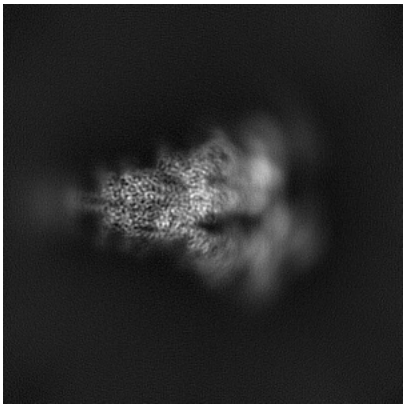


Z

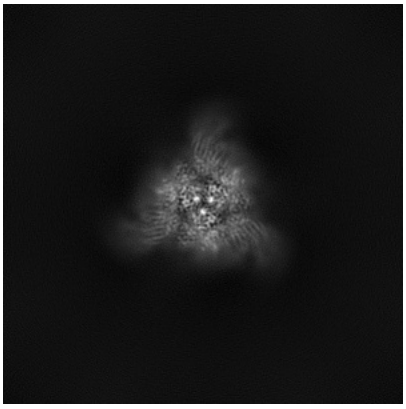
6.1.2 Raw map



X



Y



Z

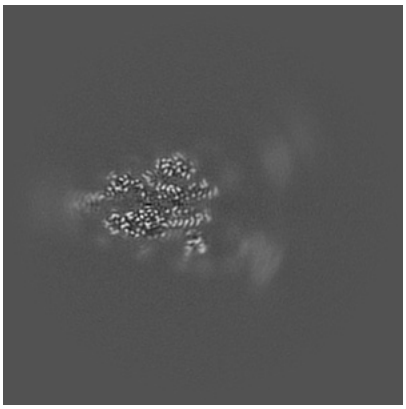
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

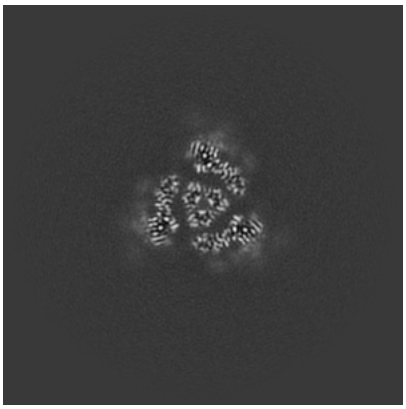
6.2.1 Primary map



X Index: 180

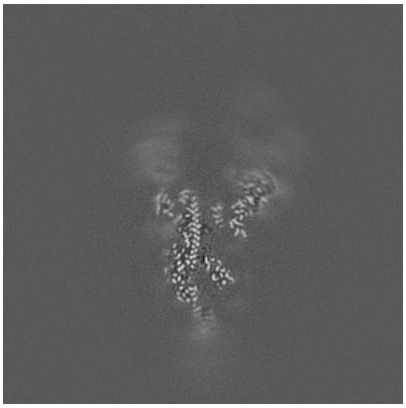


Y Index: 180

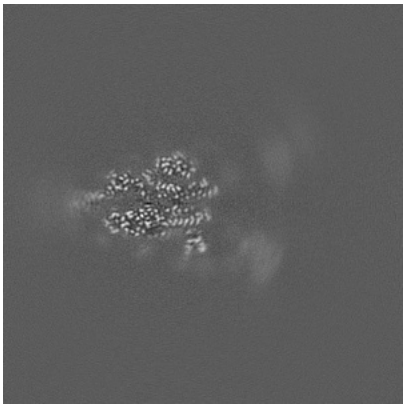


Z Index: 180

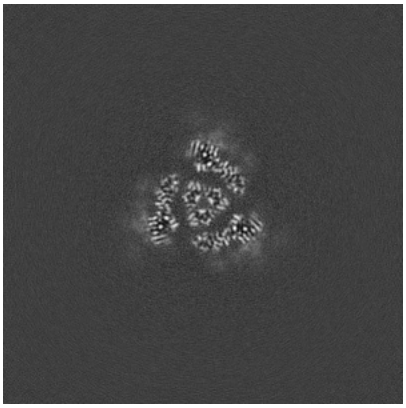
6.2.2 Raw map



X Index: 180



Y Index: 180



Z Index: 180

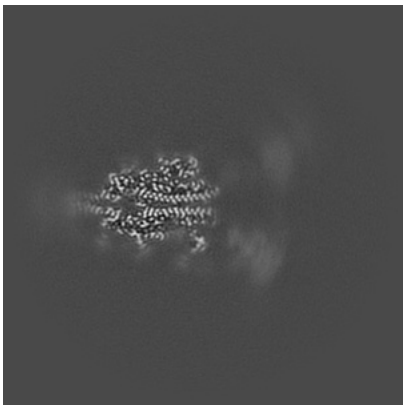
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

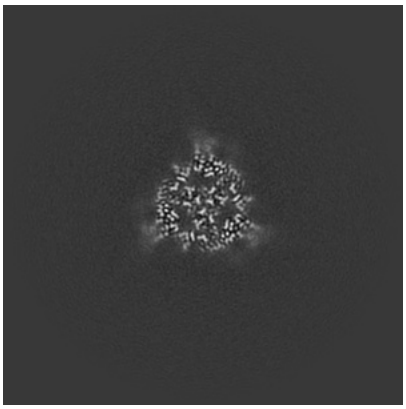
6.3.1 Primary map



X Index: 189

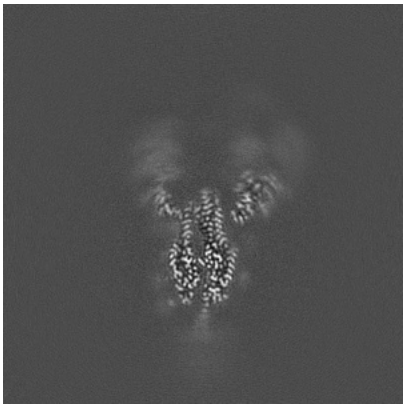


Y Index: 184

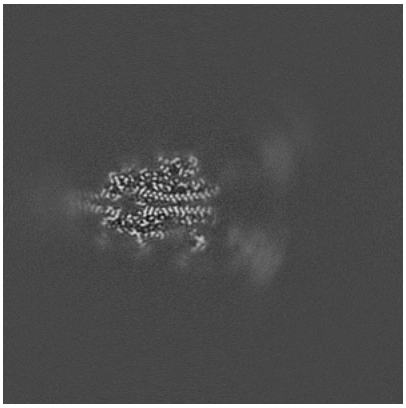


Z Index: 170

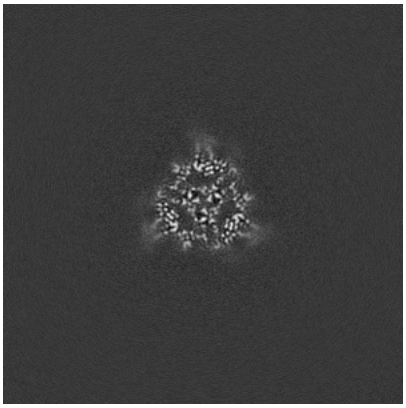
6.3.2 Raw map



X Index: 189



Y Index: 184

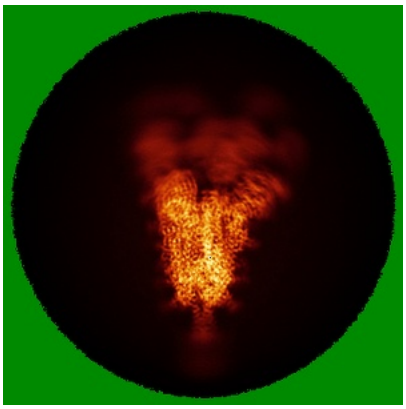


Z Index: 169

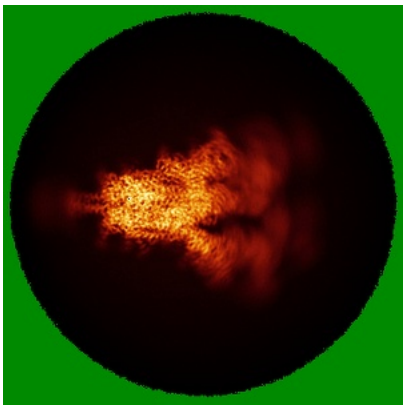
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

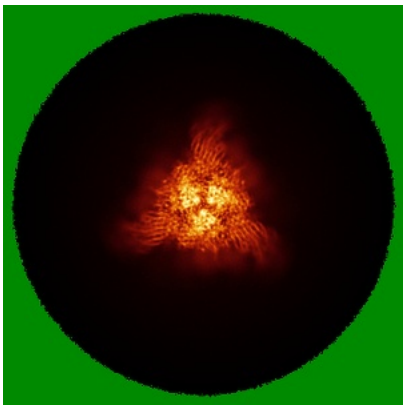
6.4.1 Primary map



X

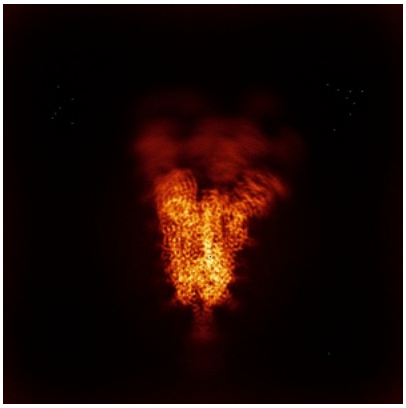


Y

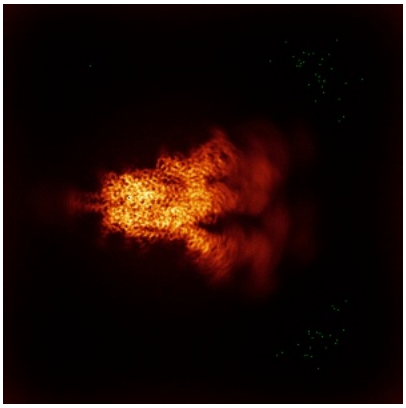


Z

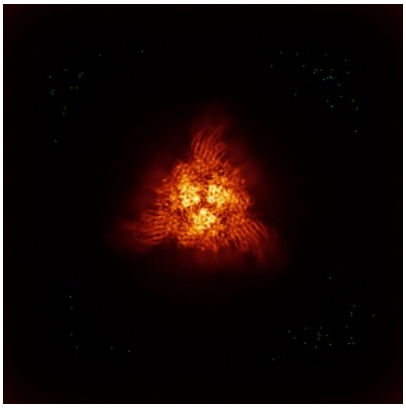
6.4.2 Raw map



X



Y

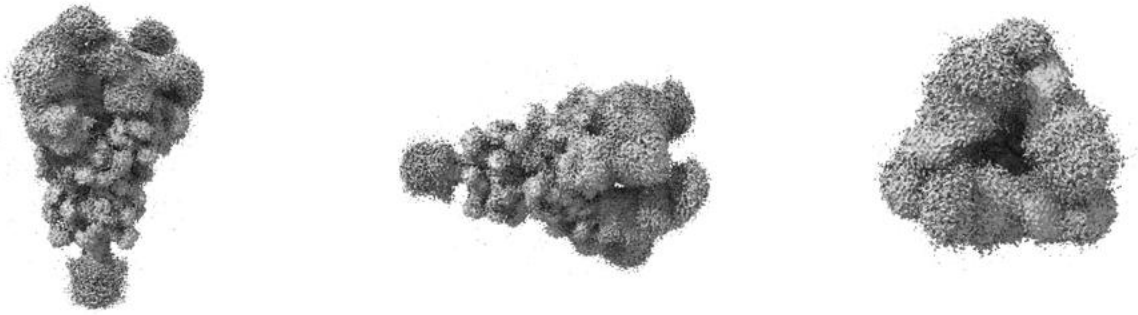


Z

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

6.5 Orthogonal surface views (i)

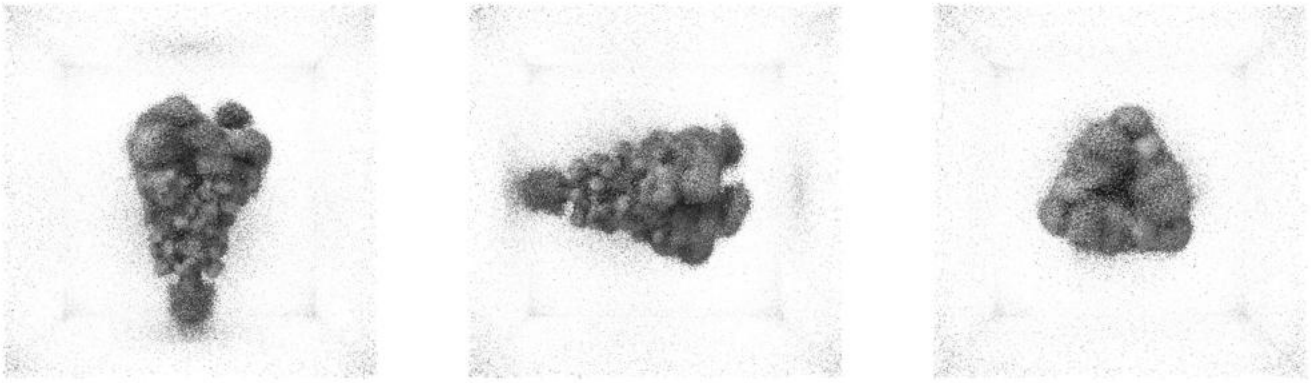
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

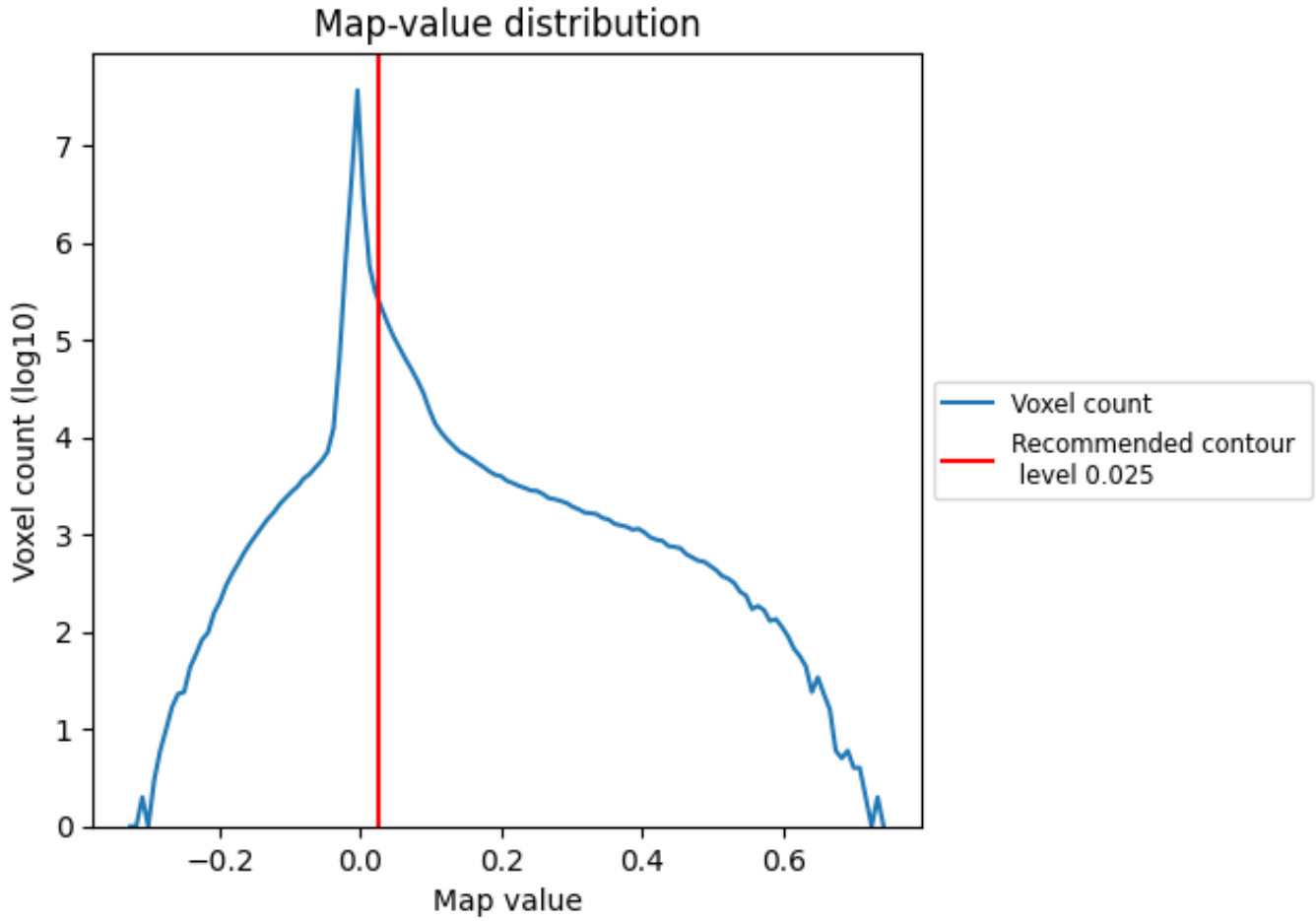
6.6 Mask visualisation (i)

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

7 Map analysis

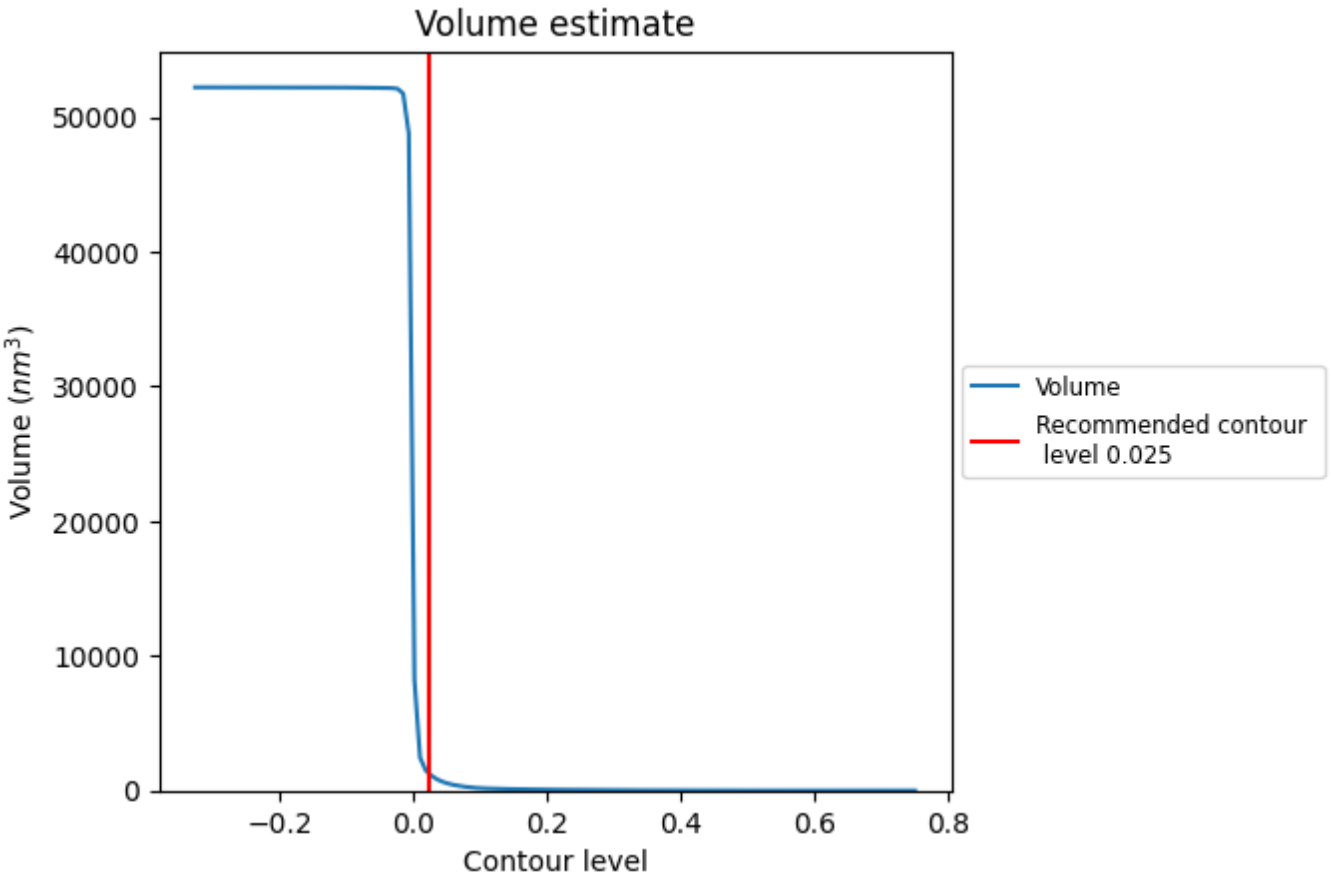
This section contains the results of statistical analysis of the map.

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.

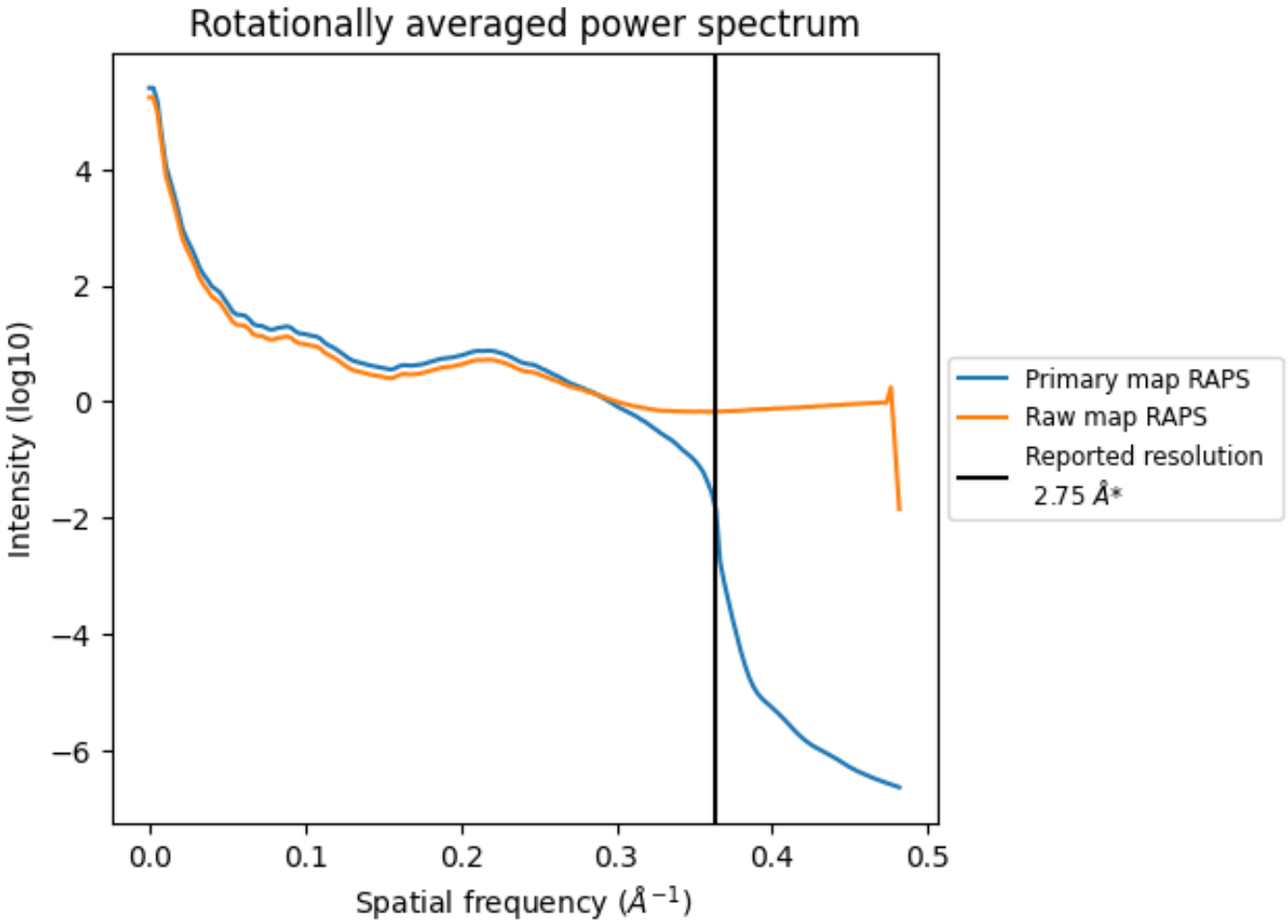
7.2 Volume estimate (i)



The volume at the recommended contour level is 1204 nm^3; this corresponds to an approximate mass of 1088 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)

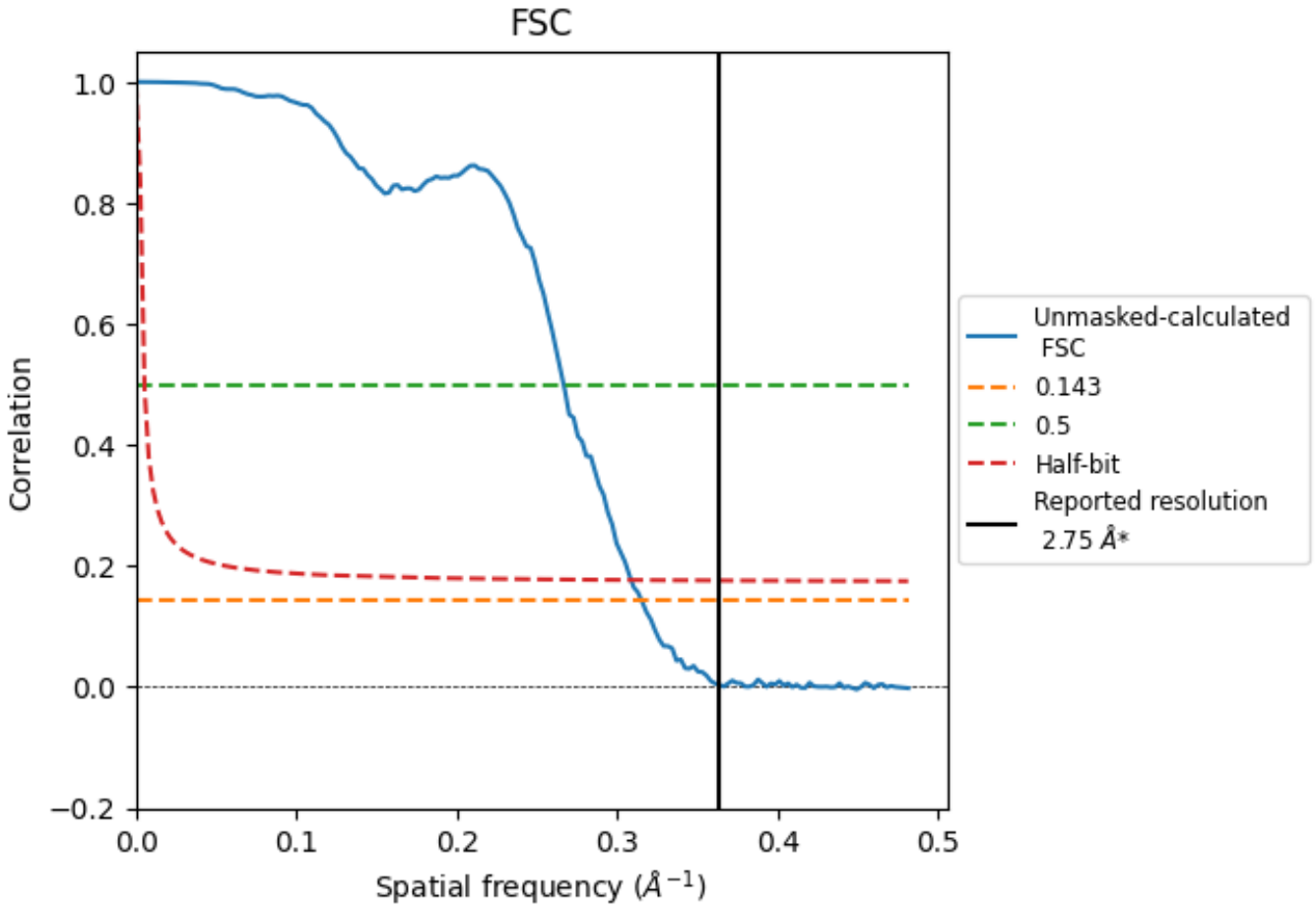


*Reported resolution corresponds to spatial frequency of 0.364 Å^{-1}

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 0.364 Å^{-1}

8.2 Resolution estimates (i)

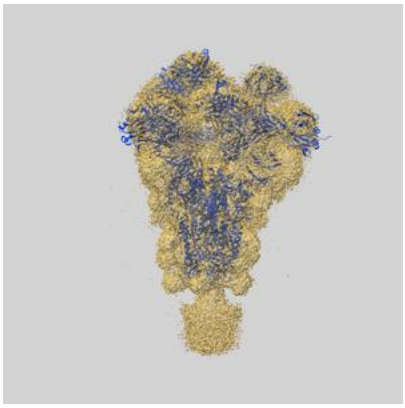
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.75	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.17	3.75	3.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.17 differs from the reported value 2.75 by more than 10 %

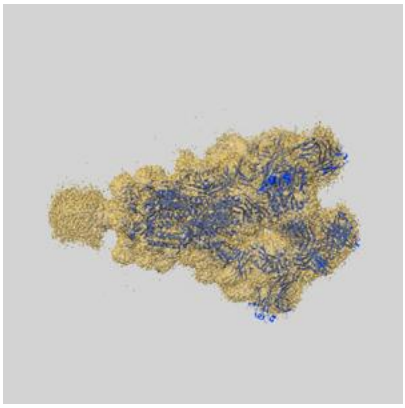
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-66902 and PDB model 9XIB. Per-residue inclusion information can be found in section 3 on page 18.

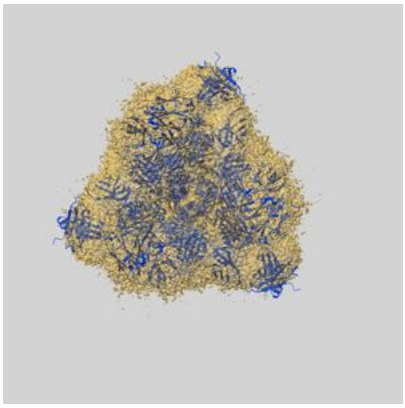
9.1 Map-model overlay



X



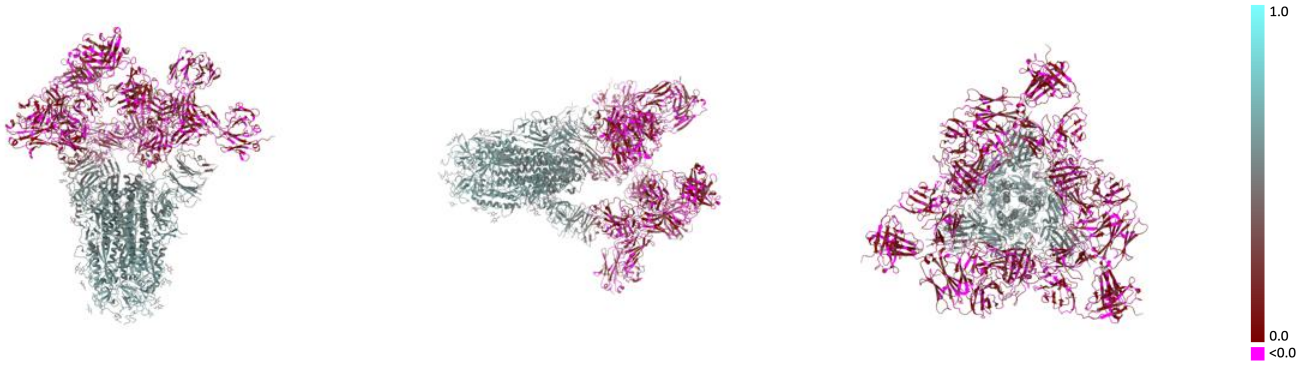
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

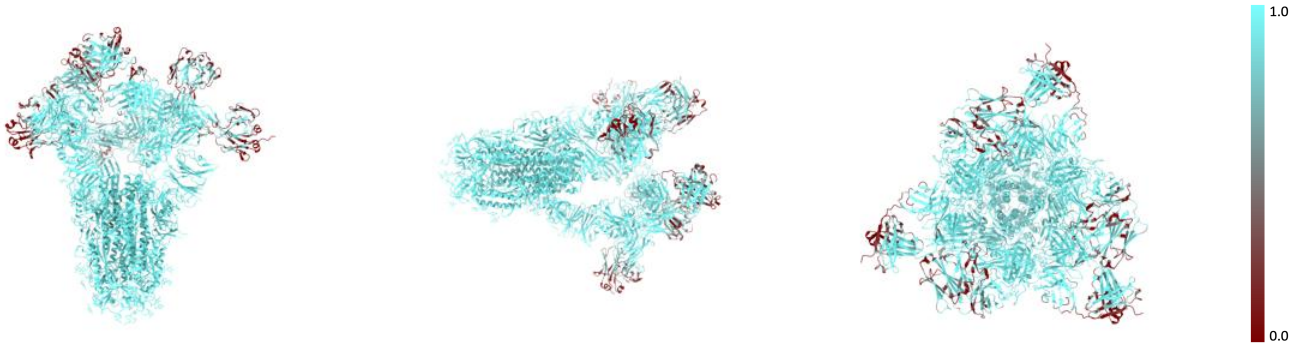
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

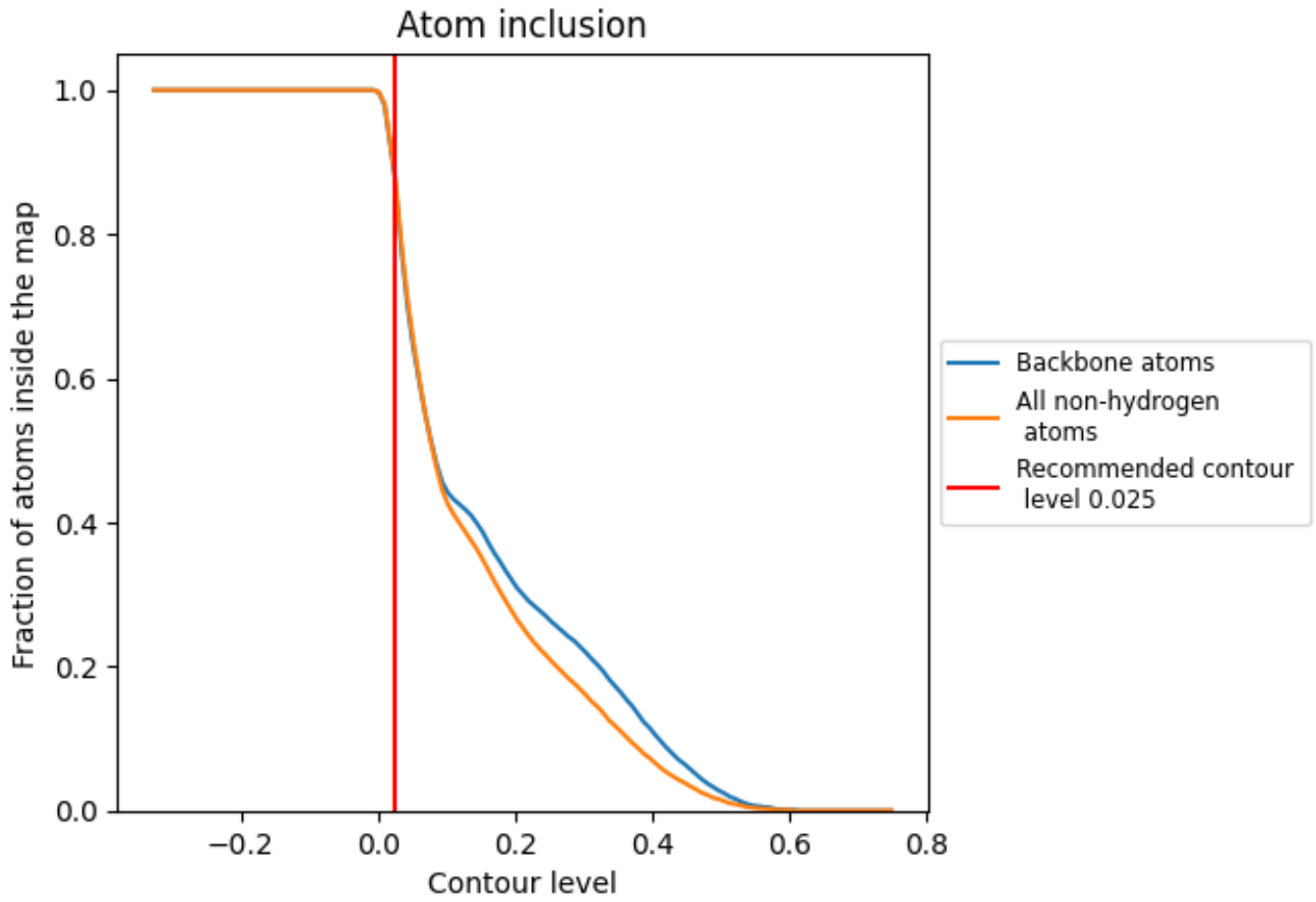
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8840	0.2940
A	0.9970	0.4660
B	0.9970	0.4660
C	0.9970	0.4660
D	0.7560	0.0740
E	0.7590	0.0700
F	0.7570	0.0740
G	0.7170	0.0740
H	0.7220	0.0750
I	0.7310	0.0630
J	0.7310	0.0660
K	0.7640	0.1020
L	0.7650	0.0980
M	0.7210	0.0730
N	1.0000	0.5520
O	0.9640	0.4420
P	1.0000	0.4730
Q	1.0000	0.5400
R	0.9640	0.4470
S	1.0000	0.4740
T	1.0000	0.5300
U	0.9640	0.4520
V	1.0000	0.4810
d	0.7300	0.0650
f	0.7660	0.1000

