Full wwPDB EM Validation Report ⓘ

Nov 8, 2022 – 09:45 AM EST

PDB ID	:	6DZL
EMDB ID	:	EMD-8935
Title	:	Ebola virus Makona variant GP (mucin-deleted) in complex with pan-ebolavirus human antibody ADI-15878 Fab
Authors	:	Murin, C.D.; Ward, A.B.
Deposited on	:	2018-07-05
Resolution	:	4.14 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

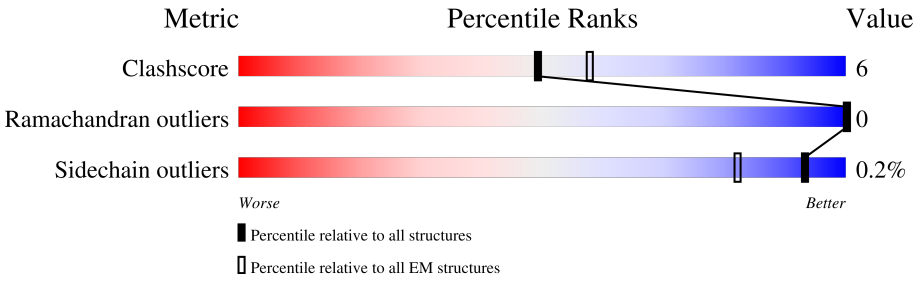
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.14 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	A	321	11% 58% 8% 34%
1	B	321	11% 57% 9% 34%
1	C	321	11% 58% 8% 34%
2	D	166	10% 46% 7% 46%
2	E	166	10% 48% 5% 46%
2	F	166	10% 48% 6% 46%
3	J	106	12% 84% 15%
3	K	106	12% 83% 16%

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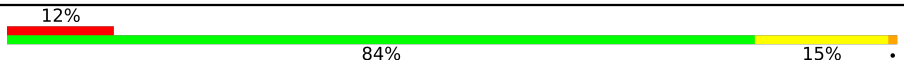
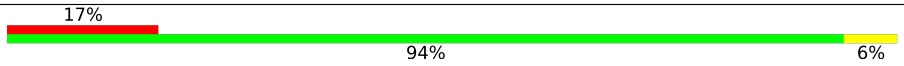
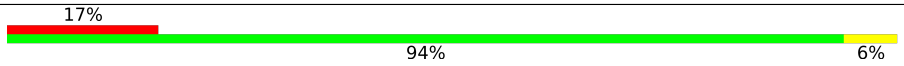
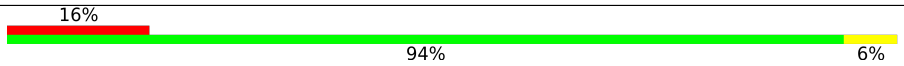
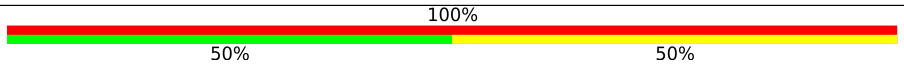
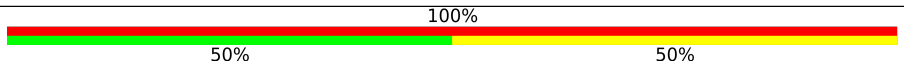
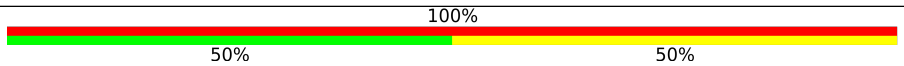
Mol	Chain	Length	Quality of chain
3	L	106	
4	G	121	
4	H	121	
4	I	121	
5	M	2	
5	O	2	
5	Q	2	
6	N	6	
6	P	6	
6	R	6	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12693 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 Ebola virus Makona GP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	213	Total	C	N	O	S	0	0
			1664	1061	281	317	5		
1	B	213	Total	C	N	O	S	0	0
			1664	1061	281	317	5		
1	C	213	Total	C	N	O	S	0	0
			1664	1061	281	317	5		

There are 123 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	312	ASN	-	expression tag	UNP A0A0F7IM40
A	313	ASN	-	expression tag	UNP A0A0F7IM40
A	314	ASN	-	expression tag	UNP A0A0F7IM40
A	315	THR	-	expression tag	UNP A0A0F7IM40
A	316	HIS	-	expression tag	UNP A0A0F7IM40
A	317	HIS	-	expression tag	UNP A0A0F7IM40
A	318	GLN	-	expression tag	UNP A0A0F7IM40
A	319	ASP	-	expression tag	UNP A0A0F7IM40
A	320	THR	-	expression tag	UNP A0A0F7IM40
A	321	GLY	-	expression tag	UNP A0A0F7IM40
A	322	GLU	-	expression tag	UNP A0A0F7IM40
A	323	GLU	-	expression tag	UNP A0A0F7IM40
A	324	SER	-	expression tag	UNP A0A0F7IM40
A	325	ALA	-	expression tag	UNP A0A0F7IM40
A	326	SER	-	expression tag	UNP A0A0F7IM40
A	327	SER	-	expression tag	UNP A0A0F7IM40
A	328	GLY	-	expression tag	UNP A0A0F7IM40
A	329	LYS	-	expression tag	UNP A0A0F7IM40
A	330	LEU	-	expression tag	UNP A0A0F7IM40
A	331	GLY	-	expression tag	UNP A0A0F7IM40
A	332	LEU	-	expression tag	UNP A0A0F7IM40
A	333	ILE	-	expression tag	UNP A0A0F7IM40
A	334	THR	-	expression tag	UNP A0A0F7IM40
A	335	ASN	-	expression tag	UNP A0A0F7IM40

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Chain	Residue	Modelled	Actual	Comment	Reference
A	336	THR	-	expression tag	UNP A0A0F7IM40
A	337	ILE	-	expression tag	UNP A0A0F7IM40
A	338	ALA	-	expression tag	UNP A0A0F7IM40
A	339	GLY	-	expression tag	UNP A0A0F7IM40
A	340	VAL	-	expression tag	UNP A0A0F7IM40
A	341	ALA	-	expression tag	UNP A0A0F7IM40
A	342	GLY	-	expression tag	UNP A0A0F7IM40
A	343	LEU	-	expression tag	UNP A0A0F7IM40
A	344	ILE	-	expression tag	UNP A0A0F7IM40
A	345	THR	-	expression tag	UNP A0A0F7IM40
A	346	GLY	-	expression tag	UNP A0A0F7IM40
A	347	GLY	-	expression tag	UNP A0A0F7IM40
A	348	ARG	-	expression tag	UNP A0A0F7IM40
A	349	ARG	-	expression tag	UNP A0A0F7IM40
A	350	THR	-	expression tag	UNP A0A0F7IM40
A	351	ARG	-	expression tag	UNP A0A0F7IM40
A	352	ARG	-	expression tag	UNP A0A0F7IM40
B	312	ASN	-	expression tag	UNP A0A0F7IM40
B	313	ASN	-	expression tag	UNP A0A0F7IM40
B	314	ASN	-	expression tag	UNP A0A0F7IM40
B	315	THR	-	expression tag	UNP A0A0F7IM40
B	316	HIS	-	expression tag	UNP A0A0F7IM40
B	317	HIS	-	expression tag	UNP A0A0F7IM40
B	318	GLN	-	expression tag	UNP A0A0F7IM40
B	319	ASP	-	expression tag	UNP A0A0F7IM40
B	320	THR	-	expression tag	UNP A0A0F7IM40
B	321	GLY	-	expression tag	UNP A0A0F7IM40
B	322	GLU	-	expression tag	UNP A0A0F7IM40
B	323	GLU	-	expression tag	UNP A0A0F7IM40
B	324	SER	-	expression tag	UNP A0A0F7IM40
B	325	ALA	-	expression tag	UNP A0A0F7IM40
B	326	SER	-	expression tag	UNP A0A0F7IM40
B	327	SER	-	expression tag	UNP A0A0F7IM40
B	328	GLY	-	expression tag	UNP A0A0F7IM40
B	329	LYS	-	expression tag	UNP A0A0F7IM40
B	330	LEU	-	expression tag	UNP A0A0F7IM40
B	331	GLY	-	expression tag	UNP A0A0F7IM40
B	332	LEU	-	expression tag	UNP A0A0F7IM40
B	333	ILE	-	expression tag	UNP A0A0F7IM40
B	334	THR	-	expression tag	UNP A0A0F7IM40
B	335	ASN	-	expression tag	UNP A0A0F7IM40
B	336	THR	-	expression tag	UNP A0A0F7IM40

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Chain	Residue	Modelled	Actual	Comment	Reference
B	337	ILE	-	expression tag	UNP A0A0F7IM40
B	338	ALA	-	expression tag	UNP A0A0F7IM40
B	339	GLY	-	expression tag	UNP A0A0F7IM40
B	340	VAL	-	expression tag	UNP A0A0F7IM40
B	341	ALA	-	expression tag	UNP A0A0F7IM40
B	342	GLY	-	expression tag	UNP A0A0F7IM40
B	343	LEU	-	expression tag	UNP A0A0F7IM40
B	344	ILE	-	expression tag	UNP A0A0F7IM40
B	345	THR	-	expression tag	UNP A0A0F7IM40
B	346	GLY	-	expression tag	UNP A0A0F7IM40
B	347	GLY	-	expression tag	UNP A0A0F7IM40
B	348	ARG	-	expression tag	UNP A0A0F7IM40
B	349	ARG	-	expression tag	UNP A0A0F7IM40
B	350	THR	-	expression tag	UNP A0A0F7IM40
B	351	ARG	-	expression tag	UNP A0A0F7IM40
B	352	ARG	-	expression tag	UNP A0A0F7IM40
C	312	ASN	-	expression tag	UNP A0A0F7IM40
C	313	ASN	-	expression tag	UNP A0A0F7IM40
C	314	ASN	-	expression tag	UNP A0A0F7IM40
C	315	THR	-	expression tag	UNP A0A0F7IM40
C	316	HIS	-	expression tag	UNP A0A0F7IM40
C	317	HIS	-	expression tag	UNP A0A0F7IM40
C	318	GLN	-	expression tag	UNP A0A0F7IM40
C	319	ASP	-	expression tag	UNP A0A0F7IM40
C	320	THR	-	expression tag	UNP A0A0F7IM40
C	321	GLY	-	expression tag	UNP A0A0F7IM40
C	322	GLU	-	expression tag	UNP A0A0F7IM40
C	323	GLU	-	expression tag	UNP A0A0F7IM40
C	324	SER	-	expression tag	UNP A0A0F7IM40
C	325	ALA	-	expression tag	UNP A0A0F7IM40
C	326	SER	-	expression tag	UNP A0A0F7IM40
C	327	SER	-	expression tag	UNP A0A0F7IM40
C	328	GLY	-	expression tag	UNP A0A0F7IM40
C	329	LYS	-	expression tag	UNP A0A0F7IM40
C	330	LEU	-	expression tag	UNP A0A0F7IM40
C	331	GLY	-	expression tag	UNP A0A0F7IM40
C	332	LEU	-	expression tag	UNP A0A0F7IM40
C	333	ILE	-	expression tag	UNP A0A0F7IM40
C	334	THR	-	expression tag	UNP A0A0F7IM40
C	335	ASN	-	expression tag	UNP A0A0F7IM40
C	336	THR	-	expression tag	UNP A0A0F7IM40
C	337	ILE	-	expression tag	UNP A0A0F7IM40

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Chain	Residue	Modelled	Actual	Comment	Reference
C	338	ALA	-	expression tag	UNP A0A0F7IM40
C	339	GLY	-	expression tag	UNP A0A0F7IM40
C	340	VAL	-	expression tag	UNP A0A0F7IM40
C	341	ALA	-	expression tag	UNP A0A0F7IM40
C	342	GLY	-	expression tag	UNP A0A0F7IM40
C	343	LEU	-	expression tag	UNP A0A0F7IM40
C	344	ILE	-	expression tag	UNP A0A0F7IM40
C	345	THR	-	expression tag	UNP A0A0F7IM40
C	346	GLY	-	expression tag	UNP A0A0F7IM40
C	347	GLY	-	expression tag	UNP A0A0F7IM40
C	348	ARG	-	expression tag	UNP A0A0F7IM40
C	349	ARG	-	expression tag	UNP A0A0F7IM40
C	350	THR	-	expression tag	UNP A0A0F7IM40
C	351	ARG	-	expression tag	UNP A0A0F7IM40
C	352	ARG	-	expression tag	UNP A0A0F7IM40

- Molecule 2 is a protein called Ebola virus Makona GP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	89	Total	C	N	O	S	0	0
			712	458	124	127	3		
2	E	89	Total	C	N	O	S	0	0
			712	458	124	127	3		
2	F	89	Total	C	N	O	S	0	0
			712	458	124	127	3		

There are 123 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	502	GLU	-	expression tag	UNP P87666
D	503	VAL	-	expression tag	UNP P87666
D	517	PHE	TYR	conflict	UNP P87666
D	630	VAL	-	expression tag	UNP P87666
D	631	GLU	-	expression tag	UNP P87666
D	632	VAL	-	expression tag	UNP P87666
D	633	ASP	-	expression tag	UNP P87666
D	634	ASP	-	expression tag	UNP P87666
D	635	ASP	-	expression tag	UNP P87666
D	636	ASP	-	expression tag	UNP P87666
D	637	LYS	-	expression tag	UNP P87666
D	638	ALA	-	expression tag	UNP P87666
D	639	GLY	-	expression tag	UNP P87666

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Chain	Residue	Modelled	Actual	Comment	Reference
D	640	TRP	-	expression tag	UNP P87666
D	641	SER	-	expression tag	UNP P87666
D	642	HIS	-	expression tag	UNP P87666
D	643	PRO	-	expression tag	UNP P87666
D	644	GLN	-	expression tag	UNP P87666
D	645	PHE	-	expression tag	UNP P87666
D	646	GLU	-	expression tag	UNP P87666
D	647	LYS	-	expression tag	UNP P87666
D	648	GLY	-	expression tag	UNP P87666
D	649	GLY	-	expression tag	UNP P87666
D	650	GLY	-	expression tag	UNP P87666
D	651	SER	-	expression tag	UNP P87666
D	652	GLY	-	expression tag	UNP P87666
D	653	GLY	-	expression tag	UNP P87666
D	654	GLY	-	expression tag	UNP P87666
D	655	SER	-	expression tag	UNP P87666
D	656	GLY	-	expression tag	UNP P87666
D	657	GLY	-	expression tag	UNP P87666
D	658	GLY	-	expression tag	UNP P87666
D	659	SER	-	expression tag	UNP P87666
D	660	TRP	-	expression tag	UNP P87666
D	661	SER	-	expression tag	UNP P87666
D	662	HIS	-	expression tag	UNP P87666
D	663	PRO	-	expression tag	UNP P87666
D	664	GLN	-	expression tag	UNP P87666
D	665	PHE	-	expression tag	UNP P87666
D	666	GLU	-	expression tag	UNP P87666
D	667	LYS	-	expression tag	UNP P87666
E	502	GLU	-	expression tag	UNP P87666
E	503	VAL	-	expression tag	UNP P87666
E	517	PHE	TYR	conflict	UNP P87666
E	630	VAL	-	expression tag	UNP P87666
E	631	GLU	-	expression tag	UNP P87666
E	632	VAL	-	expression tag	UNP P87666
E	633	ASP	-	expression tag	UNP P87666
E	634	ASP	-	expression tag	UNP P87666
E	635	ASP	-	expression tag	UNP P87666
E	636	ASP	-	expression tag	UNP P87666
E	637	LYS	-	expression tag	UNP P87666
E	638	ALA	-	expression tag	UNP P87666
E	639	GLY	-	expression tag	UNP P87666
E	640	TRP	-	expression tag	UNP P87666

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Chain	Residue	Modelled	Actual	Comment	Reference
E	641	SER	-	expression tag	UNP P87666
E	642	HIS	-	expression tag	UNP P87666
E	643	PRO	-	expression tag	UNP P87666
E	644	GLN	-	expression tag	UNP P87666
E	645	PHE	-	expression tag	UNP P87666
E	646	GLU	-	expression tag	UNP P87666
E	647	LYS	-	expression tag	UNP P87666
E	648	GLY	-	expression tag	UNP P87666
E	649	GLY	-	expression tag	UNP P87666
E	650	GLY	-	expression tag	UNP P87666
E	651	SER	-	expression tag	UNP P87666
E	652	GLY	-	expression tag	UNP P87666
E	653	GLY	-	expression tag	UNP P87666
E	654	GLY	-	expression tag	UNP P87666
E	655	SER	-	expression tag	UNP P87666
E	656	GLY	-	expression tag	UNP P87666
E	657	GLY	-	expression tag	UNP P87666
E	658	GLY	-	expression tag	UNP P87666
E	659	SER	-	expression tag	UNP P87666
E	660	TRP	-	expression tag	UNP P87666
E	661	SER	-	expression tag	UNP P87666
E	662	HIS	-	expression tag	UNP P87666
E	663	PRO	-	expression tag	UNP P87666
E	664	GLN	-	expression tag	UNP P87666
E	665	PHE	-	expression tag	UNP P87666
E	666	GLU	-	expression tag	UNP P87666
E	667	LYS	-	expression tag	UNP P87666
F	502	GLU	-	expression tag	UNP P87666
F	503	VAL	-	expression tag	UNP P87666
F	517	PHE	TYR	conflict	UNP P87666
F	630	VAL	-	expression tag	UNP P87666
F	631	GLU	-	expression tag	UNP P87666
F	632	VAL	-	expression tag	UNP P87666
F	633	ASP	-	expression tag	UNP P87666
F	634	ASP	-	expression tag	UNP P87666
F	635	ASP	-	expression tag	UNP P87666
F	636	ASP	-	expression tag	UNP P87666
F	637	LYS	-	expression tag	UNP P87666
F	638	ALA	-	expression tag	UNP P87666
F	639	GLY	-	expression tag	UNP P87666
F	640	TRP	-	expression tag	UNP P87666
F	641	SER	-	expression tag	UNP P87666

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Chain	Residue	Modelled	Actual	Comment	Reference
F	642	HIS	-	expression tag	UNP P87666
F	643	PRO	-	expression tag	UNP P87666
F	644	GLN	-	expression tag	UNP P87666
F	645	PHE	-	expression tag	UNP P87666
F	646	GLU	-	expression tag	UNP P87666
F	647	LYS	-	expression tag	UNP P87666
F	648	GLY	-	expression tag	UNP P87666
F	649	GLY	-	expression tag	UNP P87666
F	650	GLY	-	expression tag	UNP P87666
F	651	SER	-	expression tag	UNP P87666
F	652	GLY	-	expression tag	UNP P87666
F	653	GLY	-	expression tag	UNP P87666
F	654	GLY	-	expression tag	UNP P87666
F	655	SER	-	expression tag	UNP P87666
F	656	GLY	-	expression tag	UNP P87666
F	657	GLY	-	expression tag	UNP P87666
F	658	GLY	-	expression tag	UNP P87666
F	659	SER	-	expression tag	UNP P87666
F	660	TRP	-	expression tag	UNP P87666
F	661	SER	-	expression tag	UNP P87666
F	662	HIS	-	expression tag	UNP P87666
F	663	PRO	-	expression tag	UNP P87666
F	664	GLN	-	expression tag	UNP P87666
F	665	PHE	-	expression tag	UNP P87666
F	666	GLU	-	expression tag	UNP P87666
F	667	LYS	-	expression tag	UNP P87666

- Molecule 3 is a protein called Fv domain of ADI-15878 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	106	Total	C	N	O	S	0	0
			798	501	128	167	2		
3	K	106	Total	C	N	O	S	0	0
			798	501	128	167	2		
3	L	106	Total	C	N	O	S	0	0
			798	501	128	167	2		

- Molecule 4 is a protein called Fv domain of ADI-15878 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	121	Total	C	N	O	S	0	0
			929	588	161	176	4		

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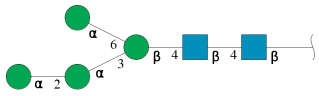
Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	121	Total	C	N	O	S	0	0
			929	588	161	176	4		
4	I	121	Total	C	N	O	S	0	0
			929	588	161	176	4		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

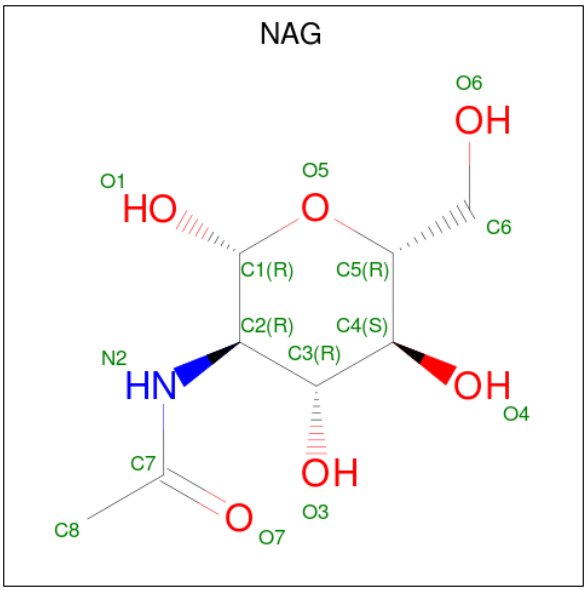
Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	2	Total	C	N	O	0	0
			28	16	2	10		
5	O	2	Total	C	N	O	0	0
			28	16	2	10		
5	Q	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
6	N	6	Total	C	N	O	0	0
			72	40	2	30		
6	P	6	Total	C	N	O	0	0
			72	40	2	30		
6	R	6	Total	C	N	O	0	0
			72	40	2	30		

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



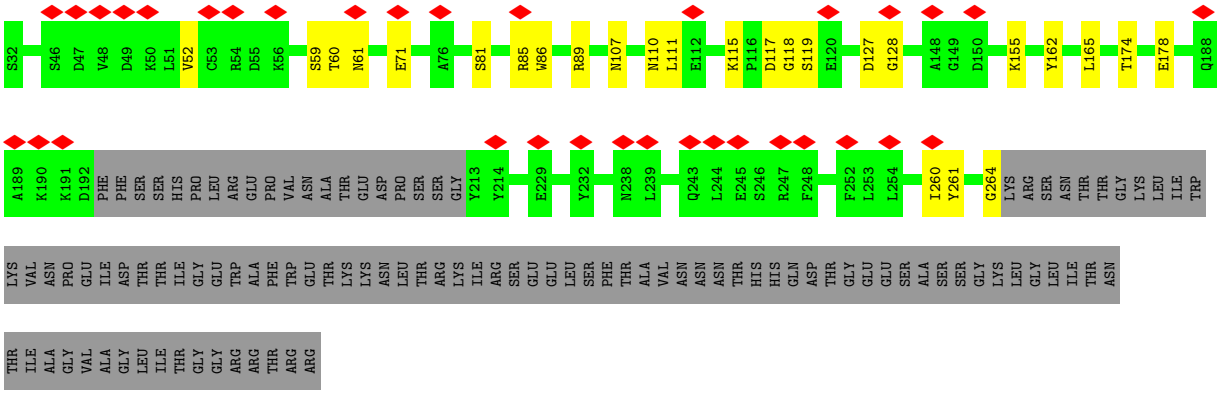
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			28	16	2	10	
7	A	1	Total	C	N	O	0
			28	16	2	10	
7	B	1	Total	C	N	O	0
			28	16	2	10	
7	B	1	Total	C	N	O	0
			28	16	2	10	
7	C	1	Total	C	N	O	0
			28	16	2	10	
7	C	1	Total	C	N	O	0
			28	16	2	10	

3 Residue-property plots (i)

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

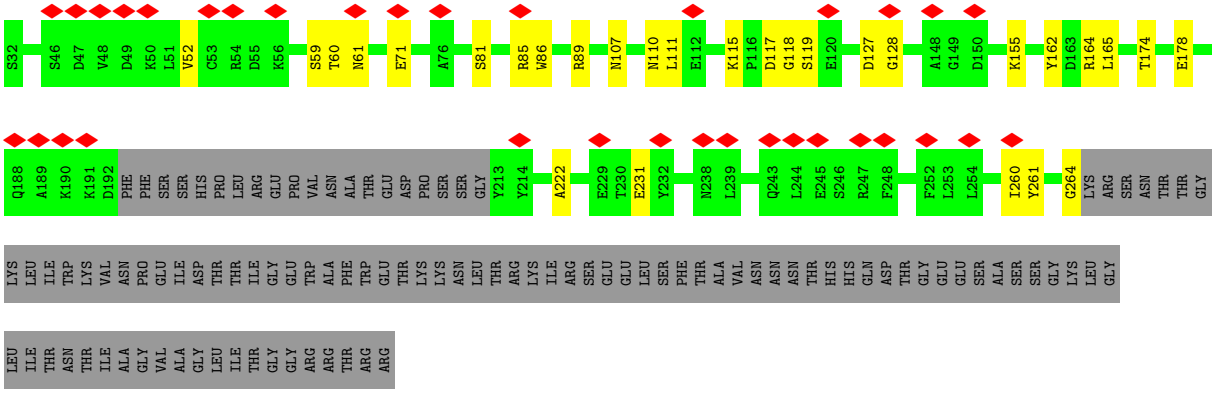
• Molecule 1: Ebola virus Makona GP1

Chain A:



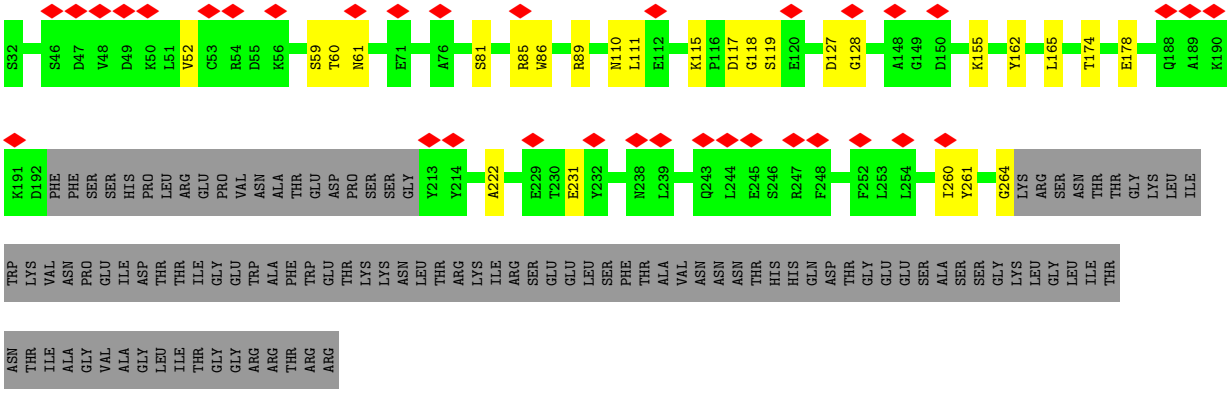
• Molecule 1: Ebola virus Makona GP1

Chain B:

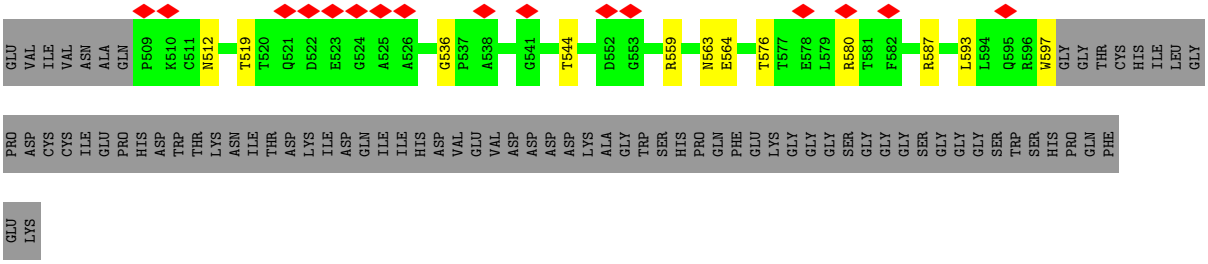


• Molecule 1: Ebola virus Makona GP1

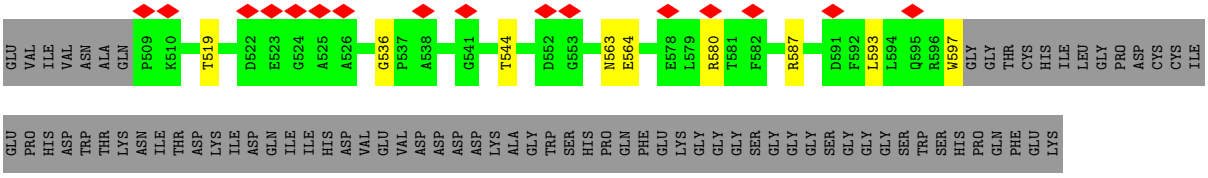
Chain C:



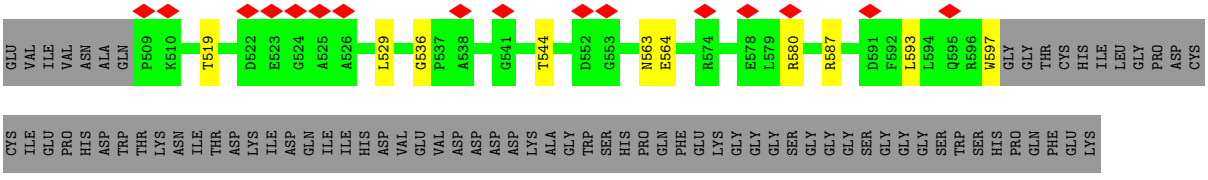
• Molecule 2: Ebola virus Makona GP2



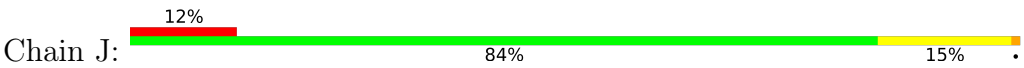
• Molecule 2: Ebola virus Makona GP2

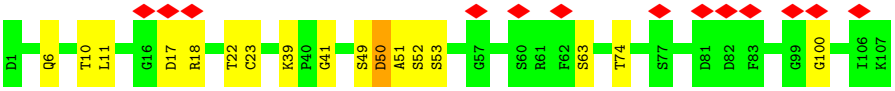


• Molecule 2: Ebola virus Makona GP2

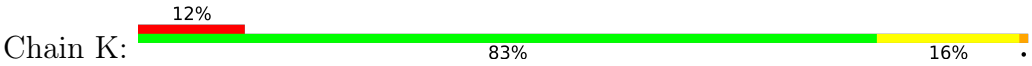


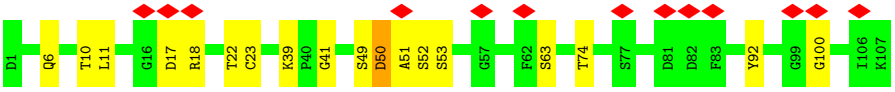
• Molecule 3: Fv domain of ADI-15878 Fab light chain



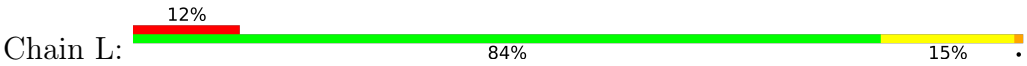


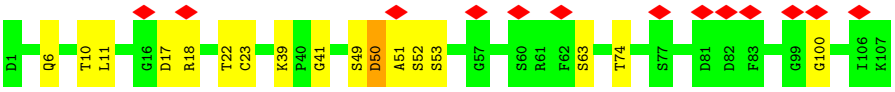
• Molecule 3: Fv domain of ADI-15878 Fab light chain



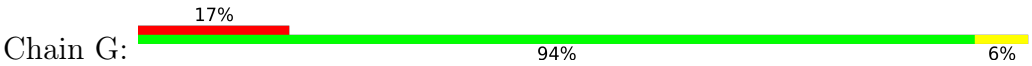


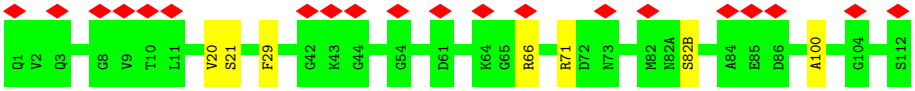
• Molecule 3: Fv domain of ADI-15878 Fab light chain



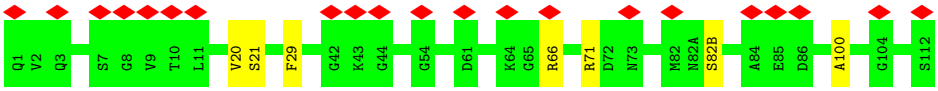


• Molecule 4: Fv domain of ADI-15878 Fab heavy chain

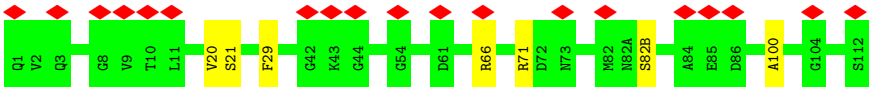




• Molecule 4: Fv domain of ADI-15878 Fab heavy chain



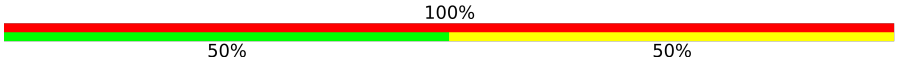
• Molecule 4: Fv domain of ADI-15878 Fab heavy chain



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

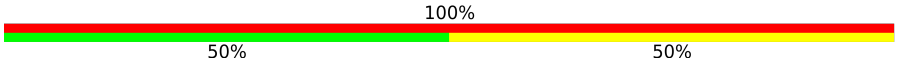
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



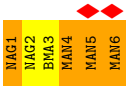
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



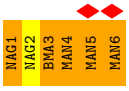
• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



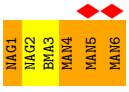
• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	157861	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	43478	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.111	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0455	Depositor
Map size (Å)	460.0, 460.0, 460.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.61	0/1703	0.62	0/2313
1	B	0.61	0/1703	0.62	0/2313
1	C	0.61	0/1703	0.62	0/2313
2	D	0.55	0/730	0.62	0/992
2	E	0.55	0/730	0.62	0/992
2	F	0.55	0/730	0.62	0/992
3	J	0.56	0/816	0.64	0/1109
3	K	0.56	0/816	0.64	0/1109
3	L	0.56	0/816	0.64	0/1109
4	G	0.58	0/952	0.60	0/1291
4	H	0.58	0/952	0.60	0/1291
4	I	0.58	0/952	0.60	0/1291
All	All	0.58	0/12603	0.62	0/17115

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	A	1664	0	1616	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1664	0	1616	19	0
1	C	1664	0	1616	17	0
2	D	712	0	698	9	0
2	E	712	0	698	7	0
2	F	712	0	698	8	0
3	J	798	0	770	16	0
3	K	798	0	770	17	0
3	L	798	0	770	16	0
4	G	929	0	892	4	0
4	H	929	0	892	4	0
4	I	929	0	892	4	0
5	M	28	0	25	1	0
5	O	28	0	25	1	0
5	Q	28	0	25	1	0
6	N	72	0	61	12	0
6	P	72	0	61	12	0
6	R	72	0	61	12	0
7	A	28	0	26	0	0
7	B	28	0	26	0	0
7	C	28	0	26	0	0
All	All	12693	0	12264	151	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 6.

All (151) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:50:ASP:OD1	3:K:53:SER:CB	2.26	0.84
3:J:50:ASP:OD1	3:J:53:SER:CB	2.26	0.83
3:L:50:ASP:OD1	3:L:53:SER:CB	2.26	0.83
6:R:3:BMA:H2	6:R:4:MAN:H5	1.65	0.79
3:K:50:ASP:OD1	3:K:53:SER:HB2	1.82	0.79
6:P:3:BMA:H2	6:P:4:MAN:H5	1.65	0.78
6:N:3:BMA:H4	6:N:6:MAN:H5	1.64	0.78
6:N:3:BMA:H2	6:N:4:MAN:H5	1.64	0.78
6:R:3:BMA:H4	6:R:6:MAN:H5	1.64	0.78
3:L:50:ASP:OD1	3:L:53:SER:HB2	1.82	0.78
3:J:50:ASP:OD1	3:J:53:SER:HB2	1.82	0.78
6:P:3:BMA:H4	6:P:6:MAN:H5	1.64	0.77
3:L:49:SER:O	3:L:50:ASP:OD1	2.07	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:49:SER:O	3:K:50:ASP:OD1	2.07	0.72
3:J:49:SER:O	3:J:50:ASP:OD1	2.07	0.72
3:K:50:ASP:O	3:K:51:ALA:HB3	1.89	0.72
3:L:49:SER:O	3:L:50:ASP:CG	2.29	0.71
3:J:50:ASP:O	3:J:51:ALA:HB3	1.89	0.71
3:L:50:ASP:O	3:L:51:ALA:HB3	1.89	0.71
3:K:49:SER:O	3:K:50:ASP:CG	2.29	0.70
3:J:49:SER:O	3:J:50:ASP:CG	2.29	0.70
3:J:50:ASP:OD1	3:J:53:SER:HB3	1.93	0.68
3:L:50:ASP:OD1	3:L:53:SER:HB3	1.93	0.67
3:K:50:ASP:OD1	3:K:53:SER:HB3	1.94	0.67
4:H:66:ARG:NH2	4:H:82(B):SER:O	2.27	0.67
4:I:66:ARG:NH2	4:I:82(B):SER:O	2.27	0.67
4:G:66:ARG:NH2	4:G:82(B):SER:O	2.27	0.66
3:J:49:SER:C	3:J:50:ASP:CG	2.55	0.65
1:C:155:LYS:NZ	6:R:4:MAN:O3	2.30	0.65
3:K:49:SER:C	3:K:50:ASP:CG	2.55	0.65
1:A:155:LYS:NZ	6:N:4:MAN:O3	2.30	0.65
1:B:155:LYS:NZ	6:P:4:MAN:O3	2.30	0.64
3:L:49:SER:C	3:L:50:ASP:CG	2.55	0.63
1:A:260:ILE:O	1:A:264:GLY:N	2.33	0.62
3:K:52:SER:HG	6:P:5:MAN:HO6	1.48	0.62
1:B:260:ILE:O	1:B:264:GLY:N	2.33	0.61
2:D:536:GLY:O	1:C:89:ARG:NH1	2.33	0.61
3:L:52:SER:HG	6:R:5:MAN:HO6	1.44	0.61
1:C:260:ILE:O	1:C:264:GLY:N	2.33	0.61
1:A:89:ARG:NH1	2:E:536:GLY:O	2.33	0.60
2:D:593:LEU:O	2:D:597:TRP:N	2.34	0.60
1:B:89:ARG:NH1	2:F:536:GLY:O	2.33	0.60
2:F:593:LEU:O	2:F:597:TRP:N	2.34	0.60
2:E:593:LEU:O	2:E:597:TRP:N	2.34	0.60
4:H:29:PHE:O	4:H:71:ARG:NH2	2.36	0.59
3:J:22:THR:HG22	3:J:23:CYS:N	2.18	0.59
2:E:563:ASN:OD1	6:P:1:NAG:N2	2.36	0.58
3:K:22:THR:HG22	3:K:23:CYS:N	2.18	0.58
2:F:563:ASN:OD1	6:R:1:NAG:N2	2.36	0.58
4:I:29:PHE:O	4:I:71:ARG:NH2	2.36	0.58
3:L:63:SER:O	3:L:74:THR:N	2.37	0.58
4:G:29:PHE:O	4:G:71:ARG:NH2	2.36	0.58
3:K:63:SER:O	3:K:74:THR:N	2.37	0.58
1:A:81:SER:O	1:A:85:ARG:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:563:ASN:OD1	6:N:1:NAG:N2	2.36	0.57
3:L:22:THR:HG22	3:L:23:CYS:N	2.18	0.57
3:J:63:SER:O	3:J:74:THR:N	2.37	0.56
3:K:50:ASP:O	3:K:51:ALA:CB	2.53	0.56
3:J:50:ASP:O	3:J:51:ALA:CB	2.53	0.56
6:R:1:NAG:H62	6:R:2:NAG:H82	1.88	0.56
1:C:81:SER:O	1:C:85:ARG:N	2.37	0.56
6:P:1:NAG:H62	6:P:2:NAG:H82	1.88	0.56
1:B:81:SER:O	1:B:85:ARG:N	2.37	0.55
6:R:1:NAG:H62	6:R:2:NAG:N2	2.21	0.55
6:N:1:NAG:H62	6:N:2:NAG:N2	2.21	0.55
6:N:1:NAG:H62	6:N:2:NAG:H82	1.88	0.55
1:B:110:ASN:OD1	1:B:111:LEU:N	2.40	0.55
3:L:50:ASP:O	3:L:51:ALA:CB	2.53	0.55
3:J:52:SER:HG	6:N:5:MAN:HO6	1.49	0.54
1:C:115:LYS:N	1:C:119:SER:O	2.40	0.54
6:P:1:NAG:H62	6:P:2:NAG:N2	2.21	0.54
1:C:110:ASN:OD1	1:C:111:LEU:N	2.40	0.54
1:A:110:ASN:OD1	1:A:111:LEU:N	2.40	0.54
1:A:115:LYS:N	1:A:119:SER:O	2.40	0.54
1:B:115:LYS:N	1:B:119:SER:O	2.40	0.54
3:L:17:ASP:OD1	3:L:18:ARG:N	2.42	0.53
3:K:17:ASP:OD1	3:K:18:ARG:N	2.42	0.53
3:J:17:ASP:OD1	3:J:18:ARG:N	2.42	0.53
6:R:1:NAG:H62	6:R:2:NAG:C7	2.40	0.52
1:B:127:ASP:O	2:E:580:ARG:NH2	2.42	0.52
1:A:127:ASP:O	2:D:580:ARG:NH2	2.42	0.52
6:N:3:BMA:C2	6:N:4:MAN:H5	2.38	0.52
3:K:6:GLN:OE1	3:K:100:GLY:N	2.44	0.51
6:N:1:NAG:H62	6:N:2:NAG:C7	2.40	0.51
6:P:1:NAG:H62	6:P:2:NAG:C7	2.40	0.51
1:C:127:ASP:O	2:F:580:ARG:NH2	2.42	0.51
3:J:6:GLN:OE1	3:J:100:GLY:N	2.43	0.50
3:L:6:GLN:OE1	3:L:100:GLY:N	2.43	0.50
3:J:39:LYS:O	3:J:41:GLY:N	2.45	0.50
6:R:3:BMA:C2	6:R:4:MAN:H5	2.38	0.49
1:A:127:ASP:OD1	1:A:128:GLY:N	2.46	0.49
3:K:39:LYS:O	3:K:41:GLY:N	2.45	0.49
3:L:39:LYS:O	3:L:41:GLY:N	2.45	0.49
1:B:127:ASP:OD1	1:B:128:GLY:N	2.46	0.48
6:P:3:BMA:H4	6:P:6:MAN:C5	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:ASP:OD1	1:C:128:GLY:N	2.45	0.48
2:D:564:GLU:HG2	4:G:100:ALA:HB3	1.96	0.47
2:F:564:GLU:HG2	4:I:100:ALA:HB3	1.96	0.47
6:P:3:BMA:C2	6:P:4:MAN:H5	2.38	0.47
3:J:22:THR:CG2	3:J:23:CYS:N	2.78	0.47
2:E:564:GLU:HG2	4:H:100:ALA:HB3	1.96	0.47
3:K:22:THR:CG2	3:K:23:CYS:N	2.78	0.47
2:D:519:THR:O	2:D:544:THR:N	2.49	0.46
2:E:519:THR:O	2:E:544:THR:N	2.49	0.46
2:F:519:THR:O	2:F:544:THR:N	2.49	0.46
1:C:110:ASN:OD1	1:C:174:THR:N	2.49	0.46
1:B:110:ASN:OD1	1:B:174:THR:N	2.49	0.46
6:R:1:NAG:C6	6:R:2:NAG:H82	2.47	0.45
6:P:1:NAG:C6	6:P:2:NAG:H82	2.47	0.45
6:N:1:NAG:C6	6:N:2:NAG:H82	2.46	0.45
1:A:110:ASN:OD1	1:A:174:THR:N	2.49	0.45
3:L:22:THR:CG2	3:L:23:CYS:N	2.78	0.45
1:C:261:TYR:OH	5:Q:2:NAG:H82	2.17	0.45
3:K:10:THR:OG1	3:K:11:LEU:N	2.50	0.44
6:N:3:BMA:H4	6:N:6:MAN:C5	2.40	0.44
1:A:261:TYR:OH	5:M:2:NAG:H82	2.17	0.44
1:C:86:TRP:NE1	1:C:178:GLU:OE2	2.51	0.44
3:J:10:THR:OG1	3:J:11:LEU:N	2.50	0.44
1:C:117:ASP:OD1	1:C:118:GLY:N	2.51	0.44
3:L:10:THR:OG1	3:L:11:LEU:N	2.50	0.44
2:D:587:ARG:NH2	1:B:61:ASN:OD1	2.51	0.43
2:E:587:ARG:NH2	1:C:61:ASN:OD1	2.51	0.43
1:B:86:TRP:NE1	1:B:178:GLU:OE2	2.51	0.43
1:A:117:ASP:OD1	1:A:118:GLY:N	2.51	0.43
1:A:61:ASN:OD1	2:F:587:ARG:NH2	2.51	0.43
1:B:117:ASP:OD1	1:B:118:GLY:N	2.51	0.43
1:B:261:TYR:OH	5:O:2:NAG:H82	2.17	0.43
3:K:92:TYR:O	2:F:529:LEU:N	2.49	0.43
6:N:1:NAG:H62	6:N:2:NAG:C8	2.49	0.43
6:R:3:BMA:H4	6:R:6:MAN:C5	2.41	0.43
1:C:162:TYR:N	1:C:165:LEU:O	2.51	0.42
1:B:162:TYR:N	1:B:165:LEU:O	2.51	0.42
1:B:222:ALA:HB1	1:B:231:GLU:O	2.20	0.42
2:D:512:ASN:O	2:D:559:ARG:NH1	2.46	0.42
6:P:1:NAG:H62	6:P:2:NAG:C8	2.49	0.42
1:A:86:TRP:NE1	1:A:178:GLU:OE2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:SER:OG	1:A:60:THR:N	2.53	0.41
4:G:20:VAL:HG12	4:G:21:SER:N	2.35	0.41
4:H:20:VAL:HG12	4:H:21:SER:N	2.35	0.41
1:C:59:SER:OG	1:C:60:THR:N	2.54	0.41
1:B:59:SER:OG	1:B:60:THR:N	2.53	0.41
1:C:222:ALA:HB1	1:C:231:GLU:O	2.20	0.41
4:I:20:VAL:HG12	4:I:21:SER:N	2.35	0.41
1:A:162:TYR:N	1:A:165:LEU:O	2.51	0.41
1:B:71:GLU:OE2	1:B:107:ASN:N	2.54	0.41
1:C:52:VAL:HG23	1:C:52:VAL:O	2.21	0.40
6:R:1:NAG:H62	6:R:2:NAG:C8	2.49	0.40
1:A:71:GLU:OE2	1:A:107:ASN:N	2.54	0.40
1:A:52:VAL:HG23	1:A:52:VAL:O	2.21	0.40
2:D:576:THR:O	1:B:164:ARG:NH2	2.55	0.40
1:B:52:VAL:O	1:B:52:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	209/321 (65%)	180 (86%)	29 (14%)	0	100	100
1	B	209/321 (65%)	180 (86%)	29 (14%)	0	100	100
1	C	209/321 (65%)	180 (86%)	29 (14%)	0	100	100
2	D	87/166 (52%)	78 (90%)	9 (10%)	0	100	100
2	E	87/166 (52%)	78 (90%)	9 (10%)	0	100	100
2	F	87/166 (52%)	78 (90%)	9 (10%)	0	100	100
3	J	104/106 (98%)	88 (85%)	16 (15%)	0	100	100
3	K	104/106 (98%)	88 (85%)	16 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	104/106 (98%)	88 (85%)	16 (15%)	0	100	100
4	G	119/121 (98%)	107 (90%)	12 (10%)	0	100	100
4	H	119/121 (98%)	107 (90%)	12 (10%)	0	100	100
4	I	119/121 (98%)	107 (90%)	12 (10%)	0	100	100
All	All	1557/2142 (73%)	1359 (87%)	198 (13%)	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	A	180/272 (66%)	180 (100%)	0	100	100
1	B	180/272 (66%)	180 (100%)	0	100	100
1	C	180/272 (66%)	180 (100%)	0	100	100
2	D	73/135 (54%)	73 (100%)	0	100	100
2	E	73/135 (54%)	73 (100%)	0	100	100
2	F	73/135 (54%)	73 (100%)	0	100	100
3	J	91/91 (100%)	90 (99%)	1 (1%)	73	84
3	K	91/91 (100%)	90 (99%)	1 (1%)	73	84
3	L	91/91 (100%)	90 (99%)	1 (1%)	73	84
4	G	96/96 (100%)	96 (100%)	0	100	100
4	H	96/96 (100%)	96 (100%)	0	100	100
4	I	96/96 (100%)	96 (100%)	0	100	100
All	All	1320/1782 (74%)	1317 (100%)	3 (0%)	93	96

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

Mol	Chain	Res	Type
3	J	50	ASP

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Mol	Chain	Res	Type
3	K	50	ASP
3	L	50	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

24 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	$\#\|Z\| > 2$
5	NAG	M	1	5,1	14,14,15	0.16	0	17,19,21	0.41	0
5	NAG	M	2	5	14,14,15	0.23	0	17,19,21	0.45	0
6	NAG	N	1	2,6	14,14,15	0.65	1 (7%)	17,19,21	0.64	0
6	NAG	N	2	6	14,14,15	0.29	0	17,19,21	0.55	0
6	BMA	N	3	6	11,11,12	0.56	0	15,15,17	0.91	0
6	MAN	N	4	6	11,11,12	0.88	0	15,15,17	1.43	2 (13%)
6	MAN	N	5	6	11,11,12	0.57	0	15,15,17	0.99	1 (6%)
6	MAN	N	6	6	11,11,12	0.59	0	15,15,17	1.02	2 (13%)
5	NAG	O	1	5,1	14,14,15	0.16	0	17,19,21	0.40	0
5	NAG	O	2	5	14,14,15	0.22	0	17,19,21	0.45	0
6	NAG	P	1	2,6	14,14,15	0.67	1 (7%)	17,19,21	0.63	0
6	NAG	P	2	6	14,14,15	0.31	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	BMA	P	3	6	11,11,12	0.55	0	15,15,17	0.92	1 (6%)
6	MAN	P	4	6	11,11,12	0.89	0	15,15,17	1.43	2 (13%)
6	MAN	P	5	6	11,11,12	0.58	0	15,15,17	0.99	1 (6%)
6	MAN	P	6	6	11,11,12	0.60	0	15,15,17	1.02	2 (13%)
5	NAG	Q	1	5,1	14,14,15	0.18	0	17,19,21	0.41	0
5	NAG	Q	2	5	14,14,15	0.23	0	17,19,21	0.46	0
6	NAG	R	1	2,6	14,14,15	0.65	1 (7%)	17,19,21	0.63	0
6	NAG	R	2	6	14,14,15	0.33	0	17,19,21	0.53	0
6	BMA	R	3	6	11,11,12	0.55	0	15,15,17	0.92	0
6	MAN	R	4	6	11,11,12	0.89	0	15,15,17	1.43	2 (13%)
6	MAN	R	5	6	11,11,12	0.57	0	15,15,17	0.99	1 (6%)
6	MAN	R	6	6	11,11,12	0.59	0	15,15,17	1.02	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	M	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
6	NAG	N	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	N	2	6	-	2/6/23/26	0/1/1/1
6	BMA	N	3	6	-	2/2/19/22	0/1/1/1
6	MAN	N	4	6	-	2/2/19/22	0/1/1/1
6	MAN	N	5	6	-	1/2/19/22	0/1/1/1
6	MAN	N	6	6	-	2/2/19/22	0/1/1/1
5	NAG	O	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	O	2	5	-	2/6/23/26	0/1/1/1
6	NAG	P	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	P	2	6	-	2/6/23/26	0/1/1/1
6	BMA	P	3	6	-	2/2/19/22	0/1/1/1
6	MAN	P	4	6	-	2/2/19/22	0/1/1/1
6	MAN	P	5	6	-	1/2/19/22	0/1/1/1
6	MAN	P	6	6	-	2/2/19/22	0/1/1/1
5	NAG	Q	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	2/6/23/26	0/1/1/1
6	NAG	R	1	2,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	R	2	6	-	2/6/23/26	0/1/1/1
6	BMA	R	3	6	-	2/2/19/22	0/1/1/1
6	MAN	R	4	6	-	2/2/19/22	0/1/1/1
6	MAN	R	5	6	-	1/2/19/22	0/1/1/1
6	MAN	R	6	6	-	2/2/19/22	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	-2.34	1.40	1.43
6	N	1	NAG	O5-C1	-2.25	1.40	1.43
6	R	1	NAG	O5-C1	-2.25	1.40	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	P	4	MAN	C1-O5-C5	3.23	116.56	112.19
6	R	4	MAN	C1-O5-C5	3.22	116.55	112.19
6	N	4	MAN	C1-O5-C5	3.21	116.55	112.19
6	P	4	MAN	O2-C2-C3	-3.02	104.08	110.14
6	N	4	MAN	O2-C2-C3	-3.01	104.11	110.14
6	R	4	MAN	O2-C2-C3	-2.99	104.15	110.14
6	N	5	MAN	O2-C2-C3	-2.50	105.14	110.14
6	R	5	MAN	O2-C2-C3	-2.48	105.16	110.14
6	P	5	MAN	O2-C2-C3	-2.48	105.16	110.14
6	P	6	MAN	O2-C2-C3	-2.24	105.64	110.14
6	R	6	MAN	O2-C2-C3	-2.24	105.65	110.14
6	N	6	MAN	O2-C2-C3	-2.24	105.65	110.14
6	R	6	MAN	C1-O5-C5	2.20	115.18	112.19
6	P	6	MAN	C1-O5-C5	2.17	115.13	112.19
6	N	6	MAN	C1-O5-C5	2.16	115.12	112.19
6	P	3	BMA	O2-C2-C3	-2.01	106.12	110.14

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	2	NAG	O5-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
5	Q	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	M	2	NAG	C4-C5-C6-O6
5	O	2	NAG	C4-C5-C6-O6
5	Q	2	NAG	C4-C5-C6-O6
6	P	3	BMA	O5-C5-C6-O6
6	R	3	BMA	O5-C5-C6-O6
6	N	3	BMA	O5-C5-C6-O6
6	P	2	NAG	C4-C5-C6-O6
6	R	2	NAG	C4-C5-C6-O6
6	N	2	NAG	C4-C5-C6-O6
6	P	5	MAN	O5-C5-C6-O6
6	R	5	MAN	O5-C5-C6-O6
6	N	3	BMA	C4-C5-C6-O6
6	P	3	BMA	C4-C5-C6-O6
6	R	3	BMA	C4-C5-C6-O6
6	N	5	MAN	O5-C5-C6-O6
6	R	2	NAG	O5-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6
6	P	2	NAG	O5-C5-C6-O6
5	Q	1	NAG	O5-C5-C6-O6
5	O	1	NAG	O5-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
6	R	4	MAN	C4-C5-C6-O6
6	P	4	MAN	C4-C5-C6-O6
6	N	4	MAN	C4-C5-C6-O6
6	P	6	MAN	C4-C5-C6-O6
6	N	6	MAN	C4-C5-C6-O6
6	R	6	MAN	C4-C5-C6-O6
6	R	4	MAN	O5-C5-C6-O6
6	N	4	MAN	O5-C5-C6-O6
6	P	4	MAN	O5-C5-C6-O6
6	N	6	MAN	O5-C5-C6-O6
6	R	6	MAN	O5-C5-C6-O6
6	P	6	MAN	O5-C5-C6-O6

There are no ring outliers.

21 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	P	4	MAN	3	0
6	R	1	NAG	6	0
6	R	5	MAN	1	0
6	N	3	BMA	4	0

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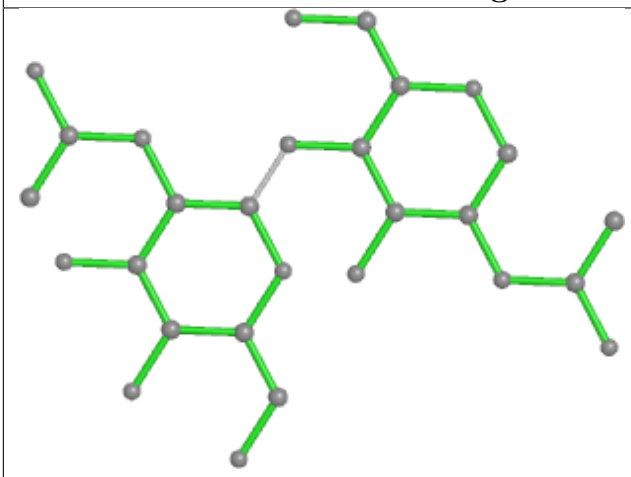
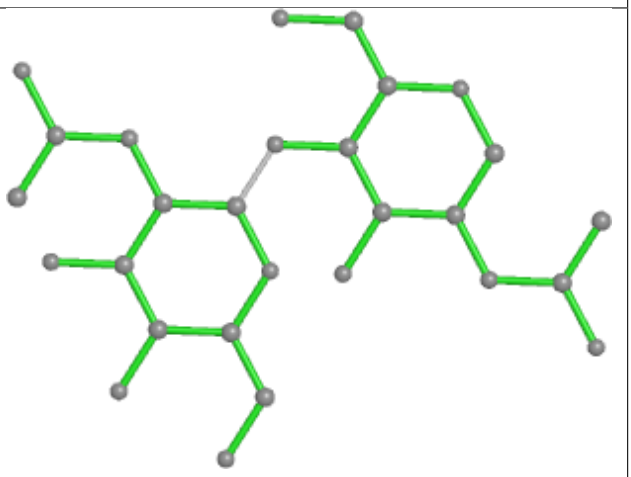
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	N	4	MAN	3	0
5	O	2	NAG	1	0
6	R	4	MAN	3	0
6	P	1	NAG	6	0
6	P	2	NAG	5	0
6	P	3	BMA	4	0
6	R	6	MAN	2	0
5	Q	2	NAG	1	0
6	N	6	MAN	2	0
6	R	3	BMA	4	0
6	R	2	NAG	5	0
6	N	5	MAN	1	0
6	N	1	NAG	6	0
6	P	5	MAN	1	0
6	N	2	NAG	5	0
6	P	6	MAN	2	0
5	M	2	NAG	1	0

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

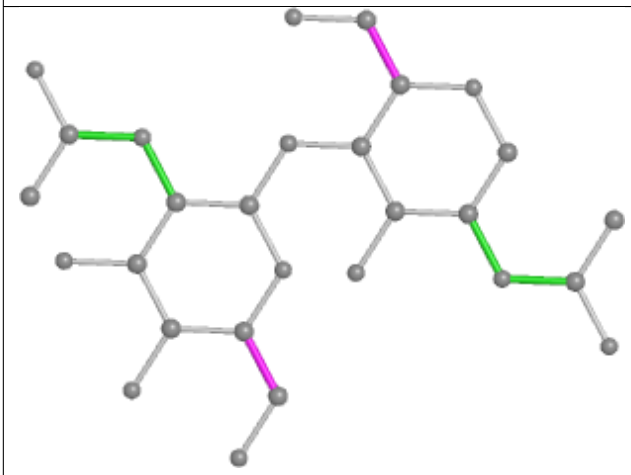
Oligosaccharide Chain M



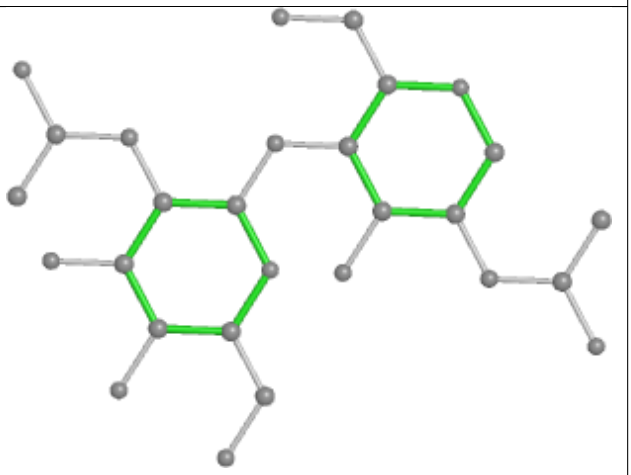
Bond lengths



Bond angles

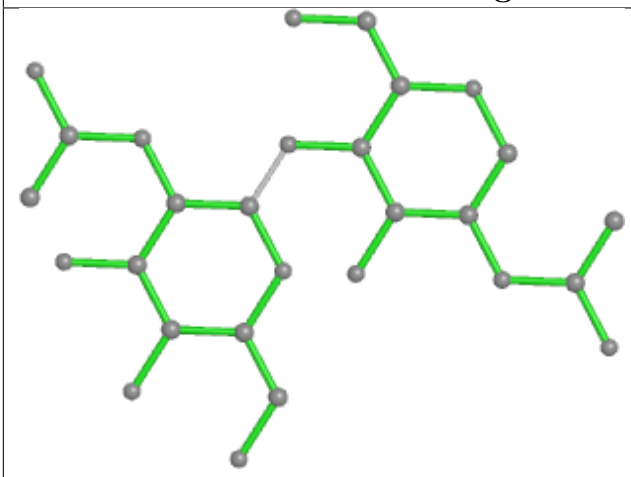


Torsions

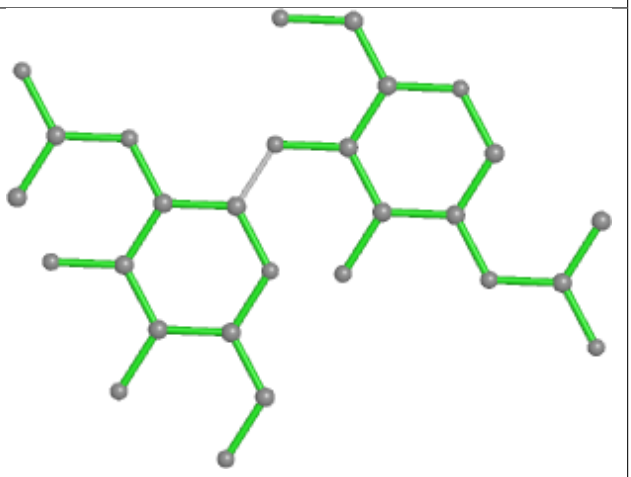


Rings

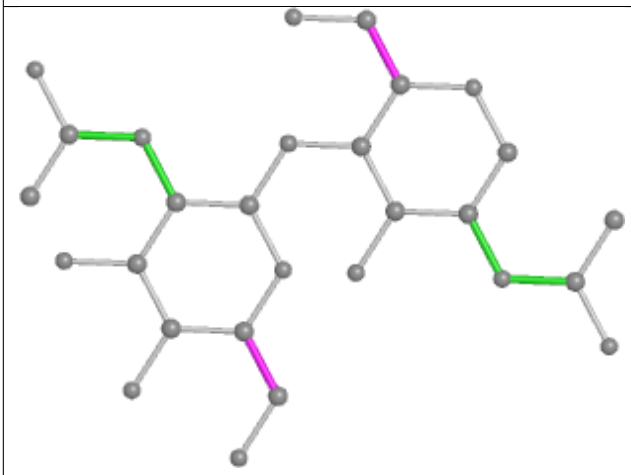
Oligosaccharide Chain O



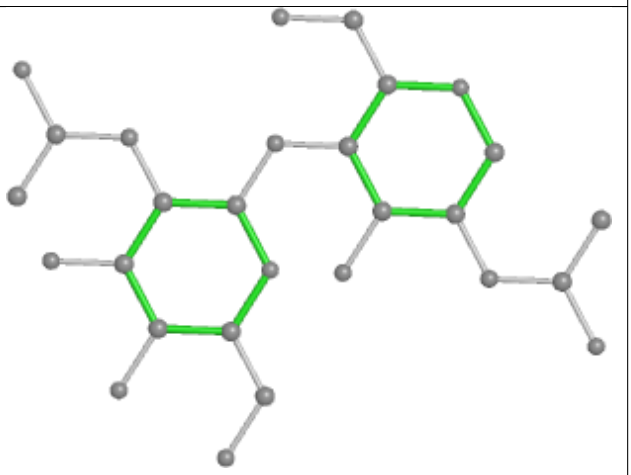
Bond lengths



Bond angles

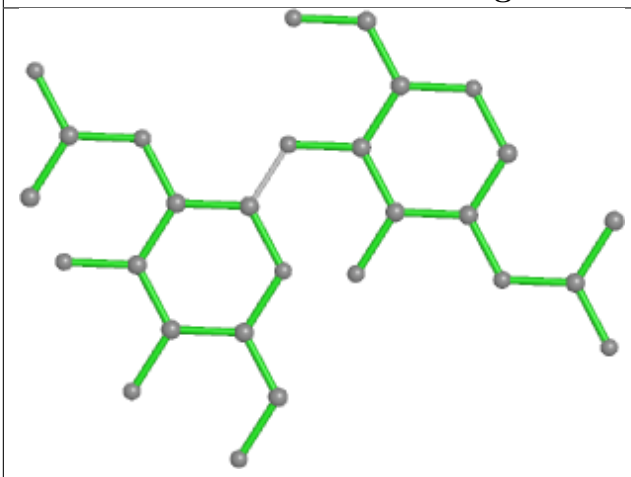


Torsions

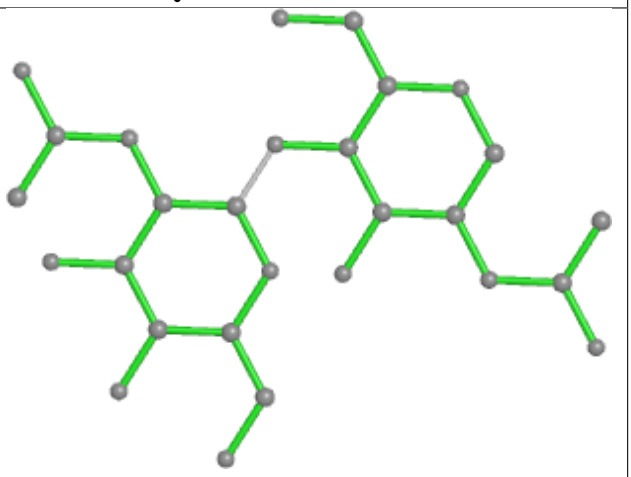


Rings

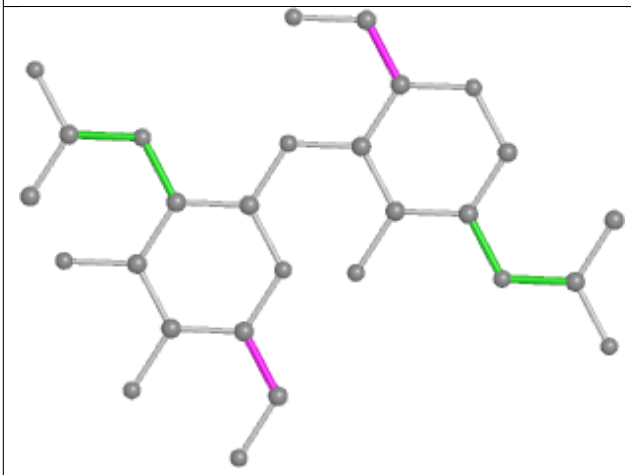
Oligosaccharide Chain Q



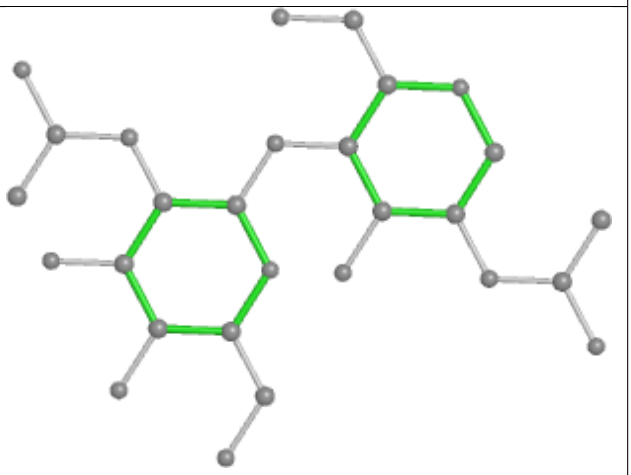
Bond lengths



Bond angles

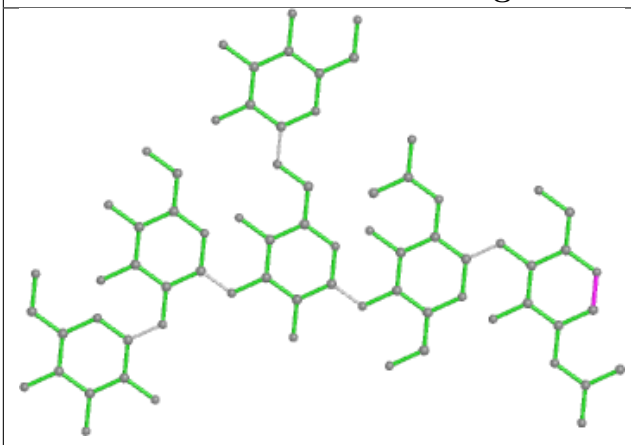


Torsions

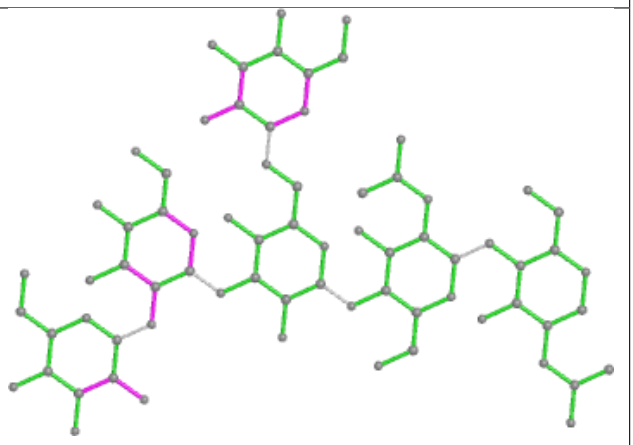


Rings

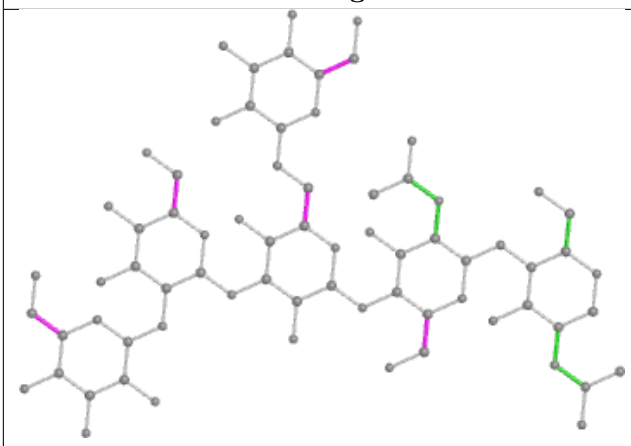
Oligosaccharide Chain N



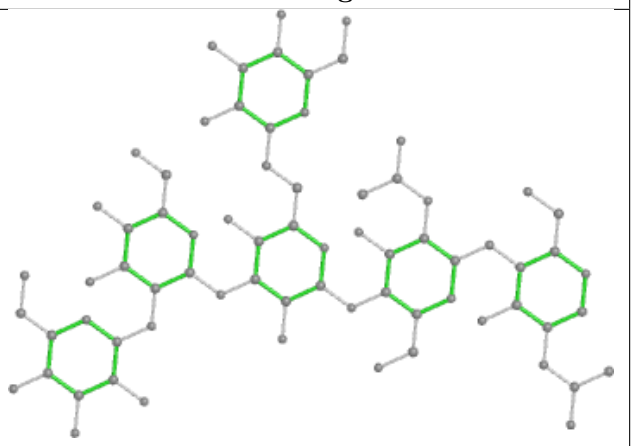
Bond lengths



Bond angles

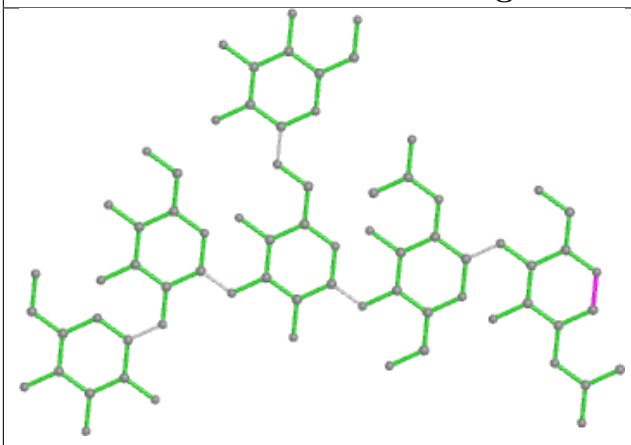


Torsions

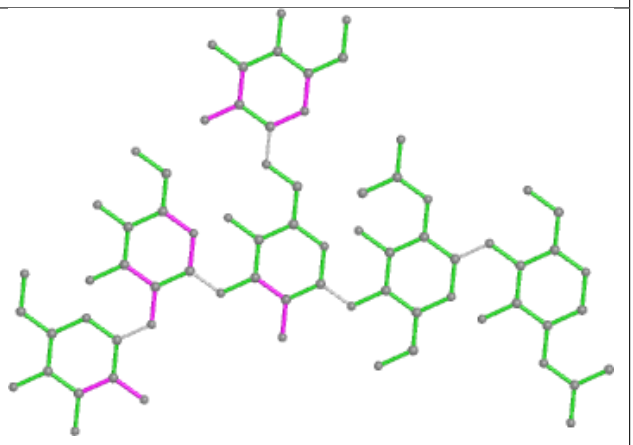


Rings

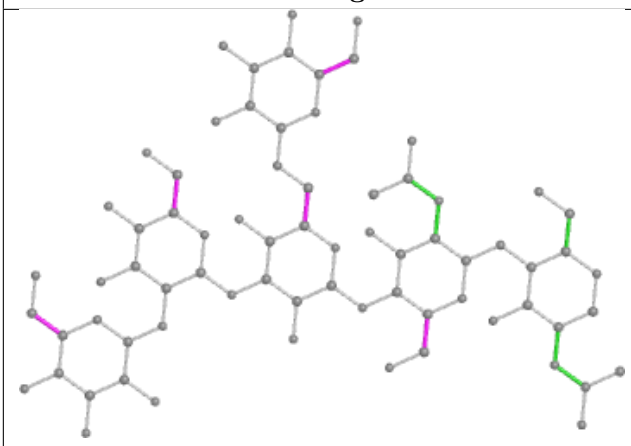
Oligosaccharide Chain P



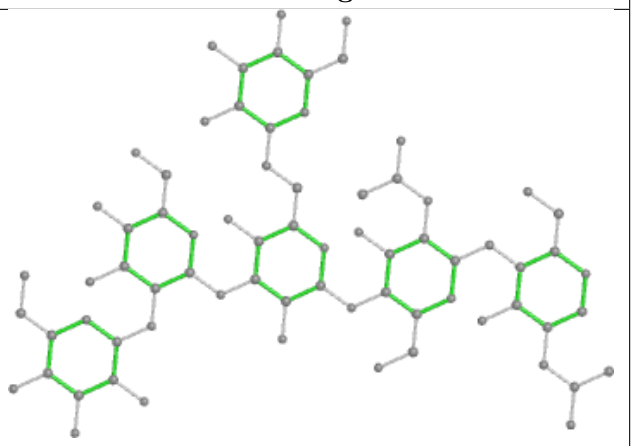
Bond lengths



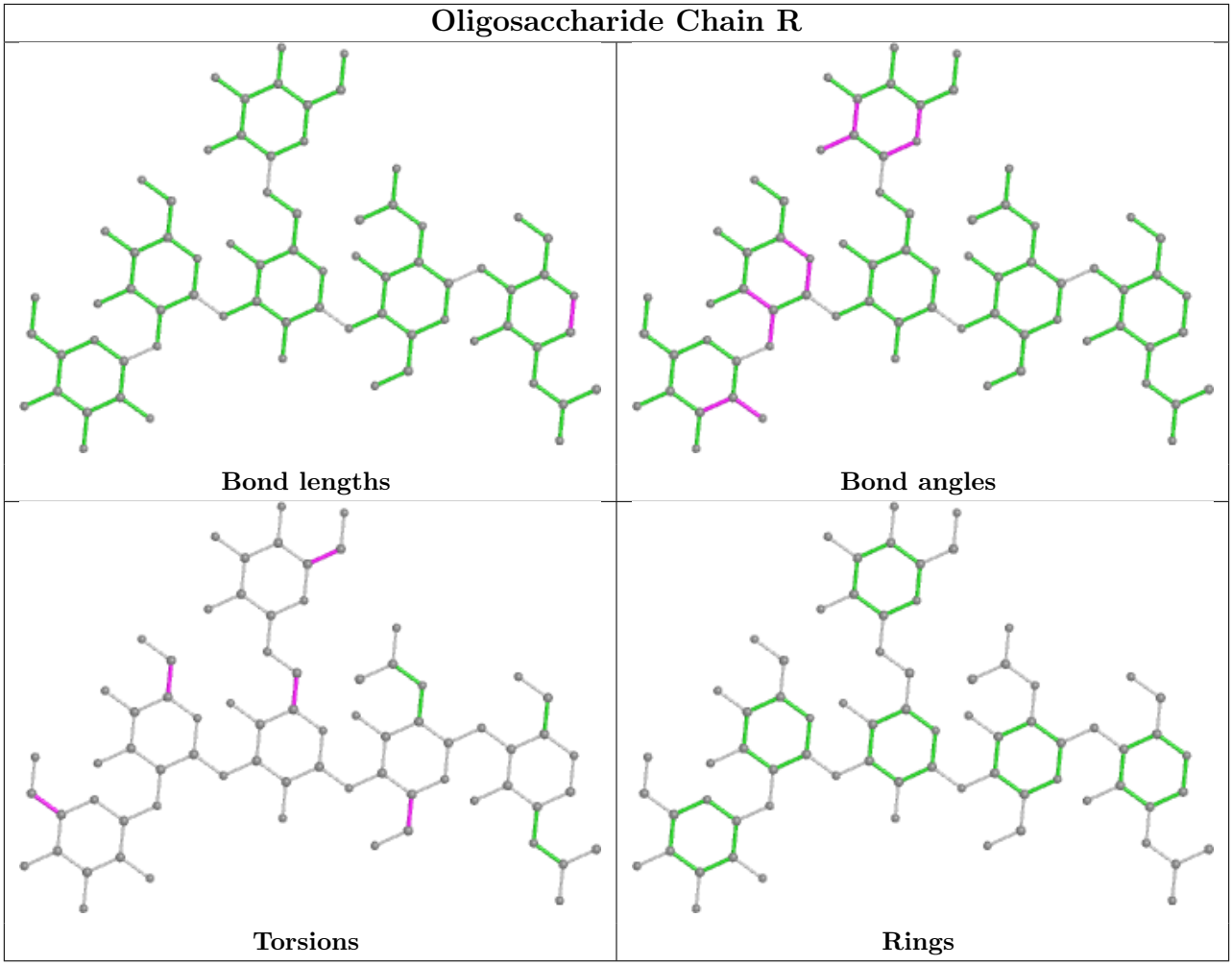
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

6 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	B	403	1	14,14,15	0.25	0	17,19,21	0.40	0
7	NAG	C	403	1	14,14,15	0.24	0	17,19,21	0.40	0
7	NAG	B	404	1	14,14,15	0.31	0	17,19,21	0.99	2 (11%)
7	NAG	C	404	1	14,14,15	0.30	0	17,19,21	1.01	2 (11%)
7	NAG	A	404	1	14,14,15	0.31	0	17,19,21	1.00	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	A	403	1	14,14,15	0.24	0	17,19,21	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	403	1	-	2/6/23/26	0/1/1/1
7	NAG	C	403	1	-	2/6/23/26	0/1/1/1
7	NAG	B	404	1	-	0/6/23/26	0/1/1/1
7	NAG	C	404	1	-	0/6/23/26	0/1/1/1
7	NAG	A	404	1	-	0/6/23/26	0/1/1/1
7	NAG	A	403	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	404	NAG	C1-O5-C5	2.54	115.64	112.19
7	A	404	NAG	C1-O5-C5	2.54	115.63	112.19
7	B	404	NAG	C1-O5-C5	2.46	115.53	112.19
7	C	404	NAG	O5-C1-C2	-2.09	107.98	111.29
7	A	404	NAG	O5-C1-C2	-2.08	108.01	111.29
7	B	404	NAG	O5-C1-C2	-2.08	108.01	111.29

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	403	NAG	O5-C5-C6-O6
7	C	403	NAG	O5-C5-C6-O6
7	A	403	NAG	O5-C5-C6-O6
7	A	403	NAG	C4-C5-C6-O6
7	B	403	NAG	C4-C5-C6-O6
7	C	403	NAG	C4-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.

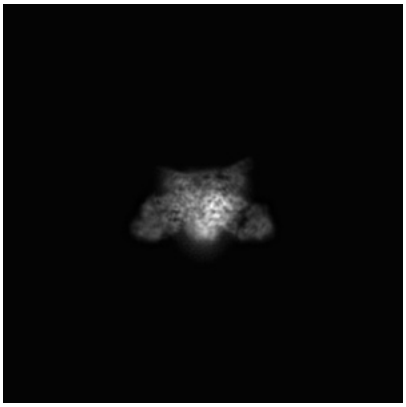
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8935. These allow visual inspection of the internal detail of the map and identification of artifacts.

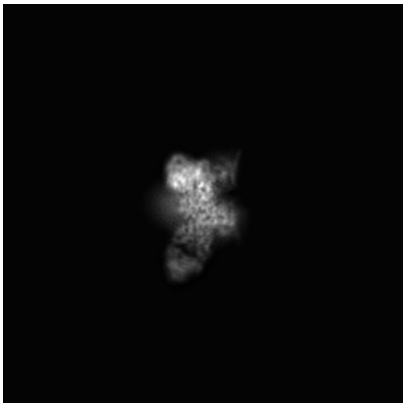
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

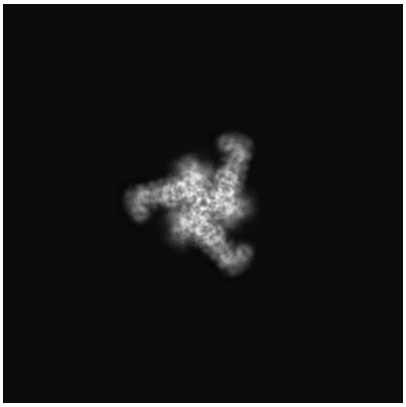
6.1.1 Primary map



X



Y

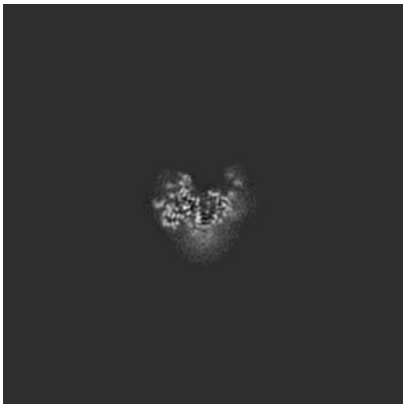


Z

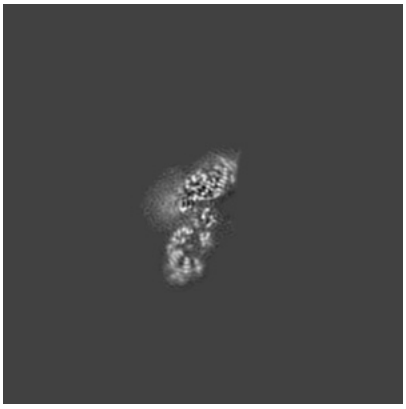
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 200



Y Index: 200

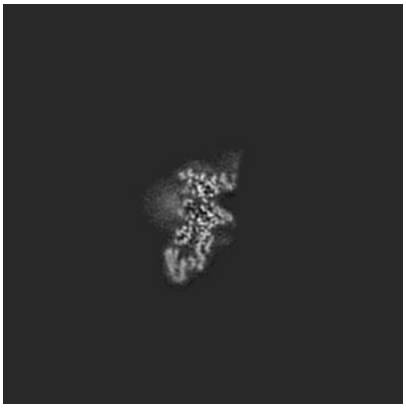
Z Index: 200

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

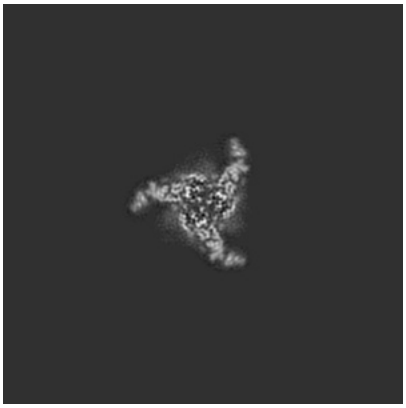
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 225



Y Index: 209

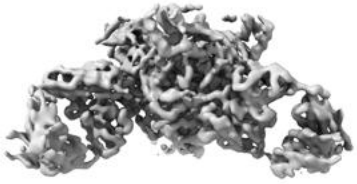


Z Index: 195

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

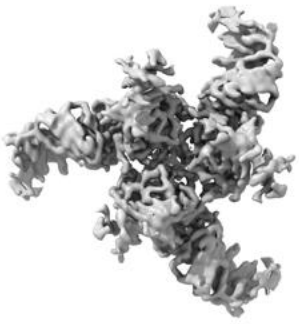
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0455. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

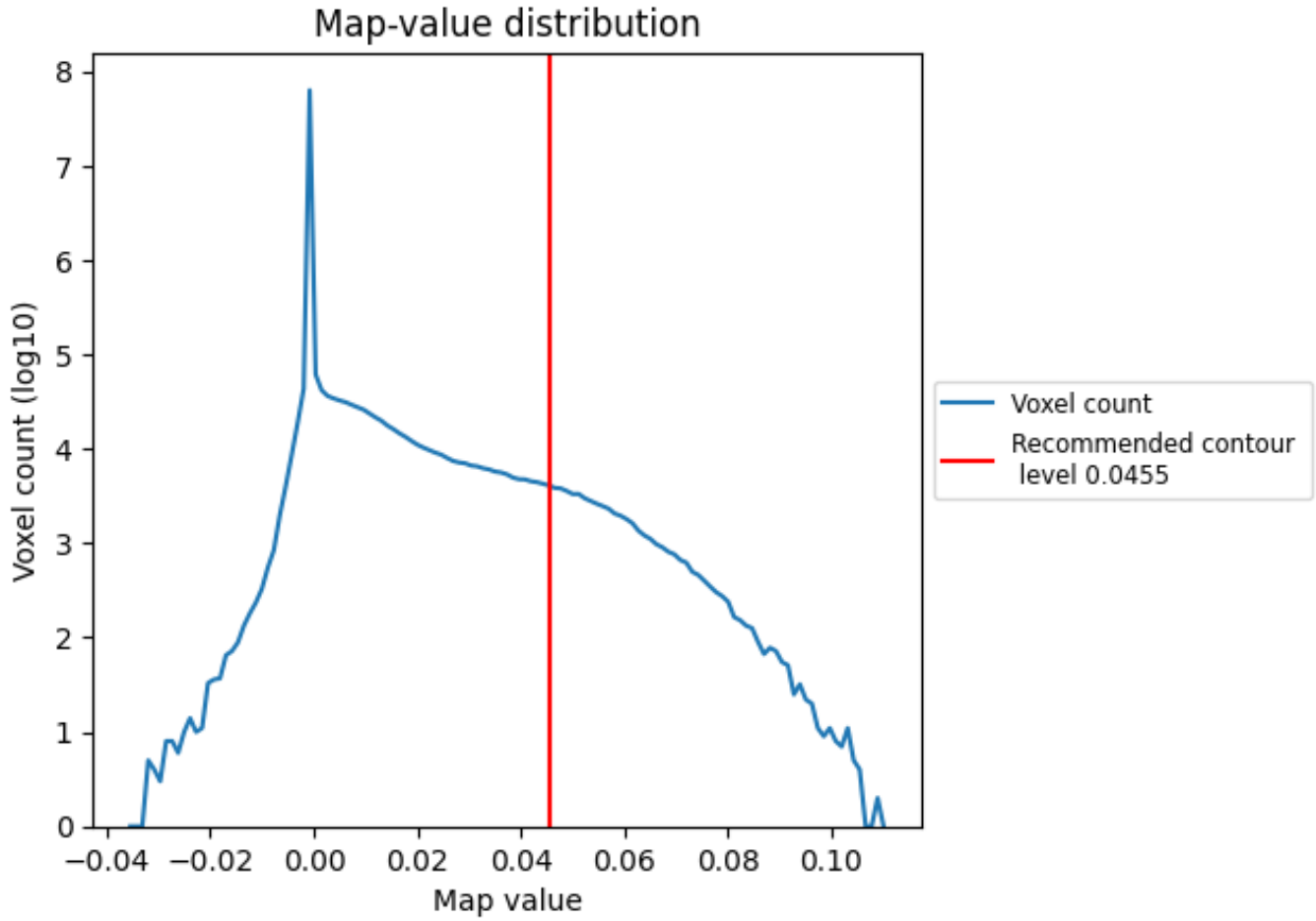
6.5 Mask visualisation (i)

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

7 Map analysis

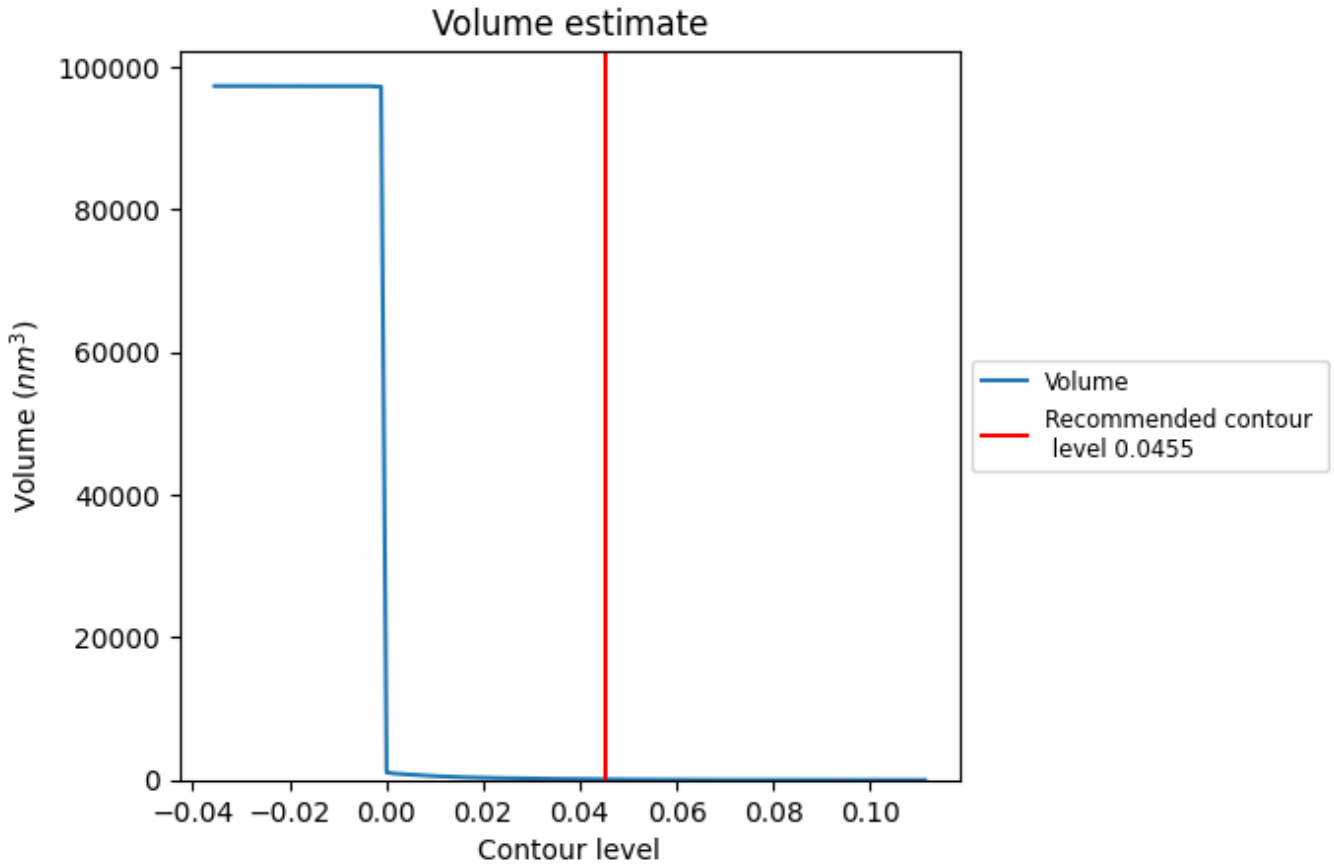
This section contains the results of statistical analysis of the map.

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.

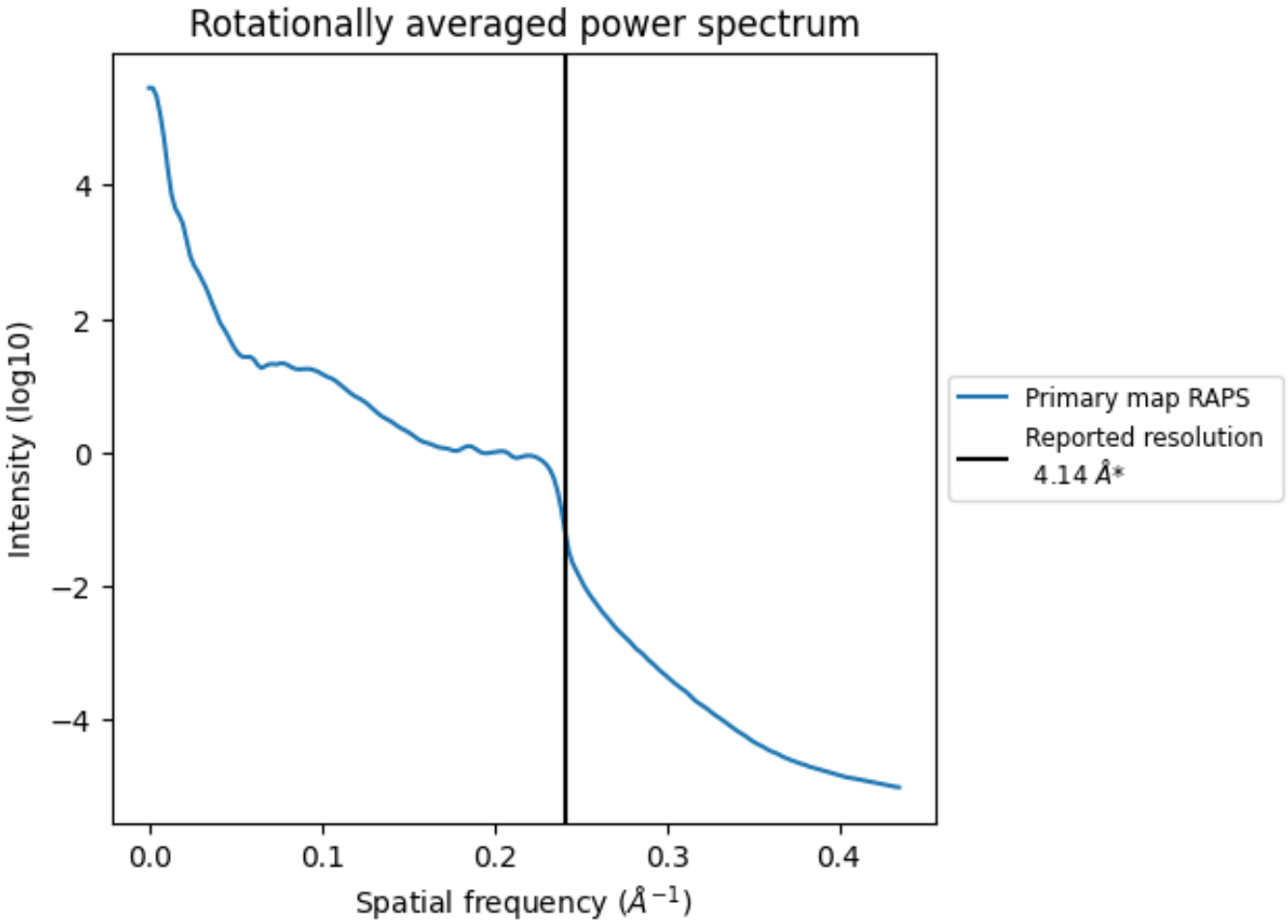
7.2 Volume estimate



The volume at the recommended contour level is 83 nm^3; this corresponds to an approximate mass of 75 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)

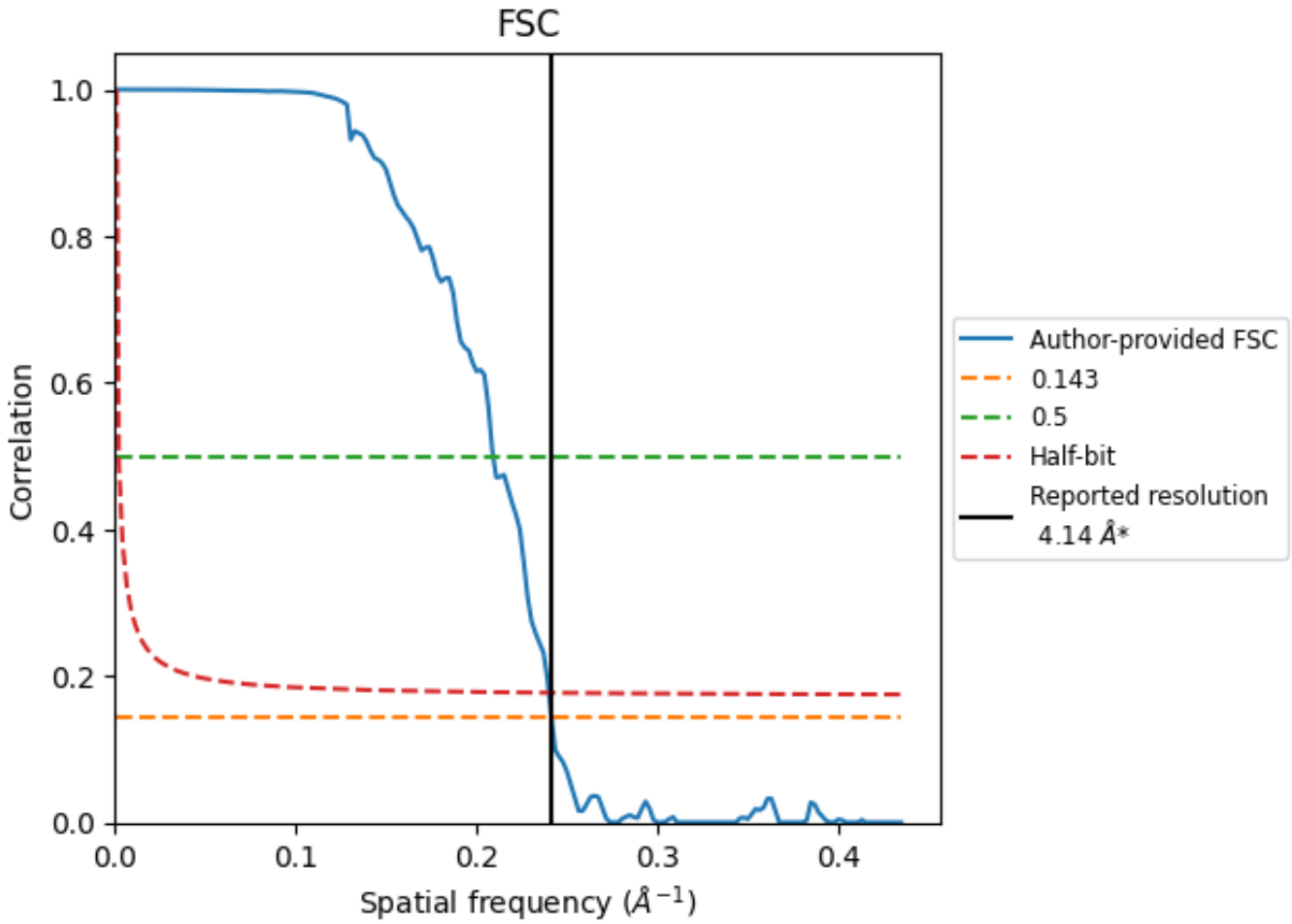


*Reported resolution corresponds to spatial frequency of 0.242 $Å^{-1}$

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 0.242 Å^{-1}

8.2 Resolution estimates (i)

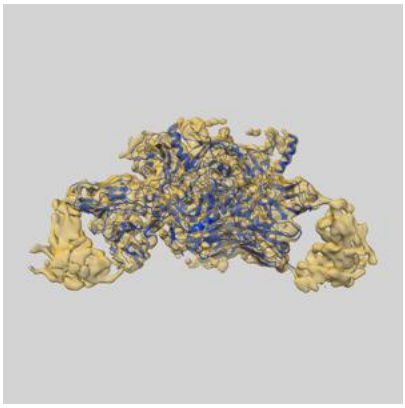
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.14	-	-
Author-provided FSC curve	4.14	4.78	4.17
Unmasked-calculated*	-	-	-

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

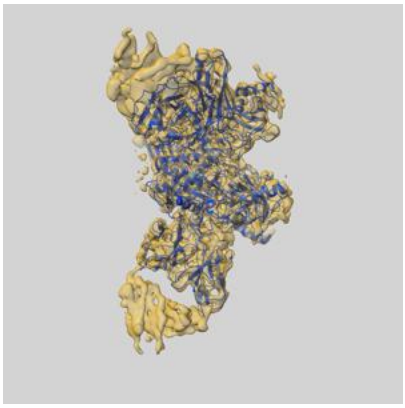
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8935 and PDB model 6DZL. Per-residue inclusion information can be found in section 3 on page 13.

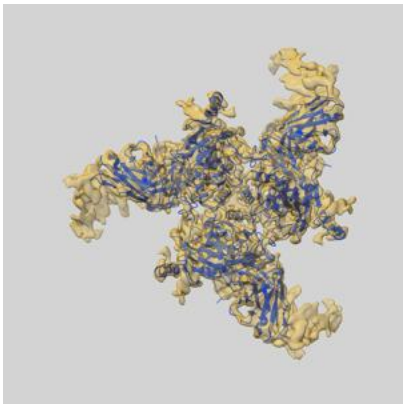
9.1 Map-model overlay



X



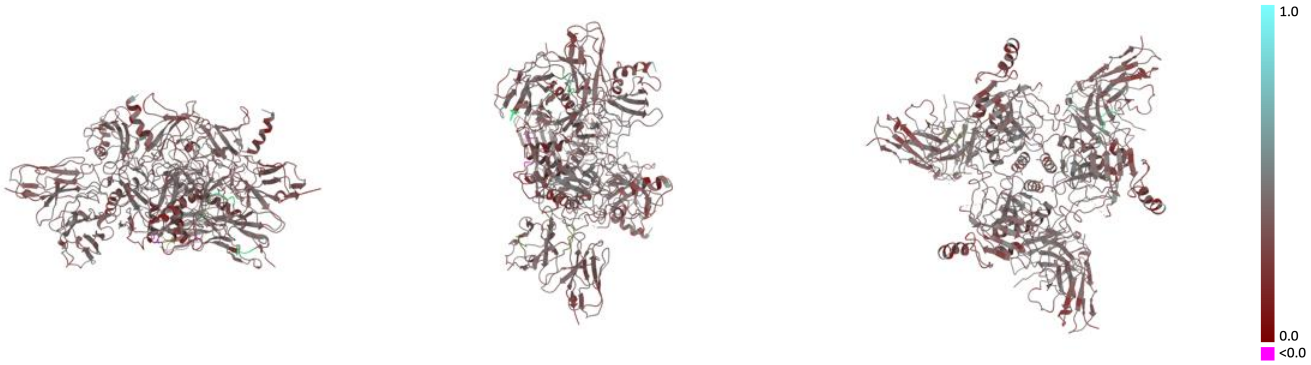
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0455 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.

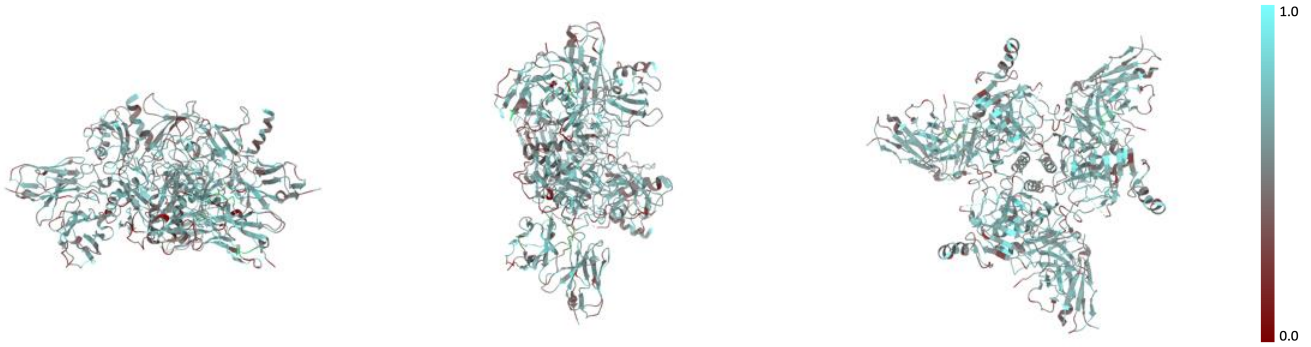
9.2 Q-score mapped to coordinate model (i)



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.

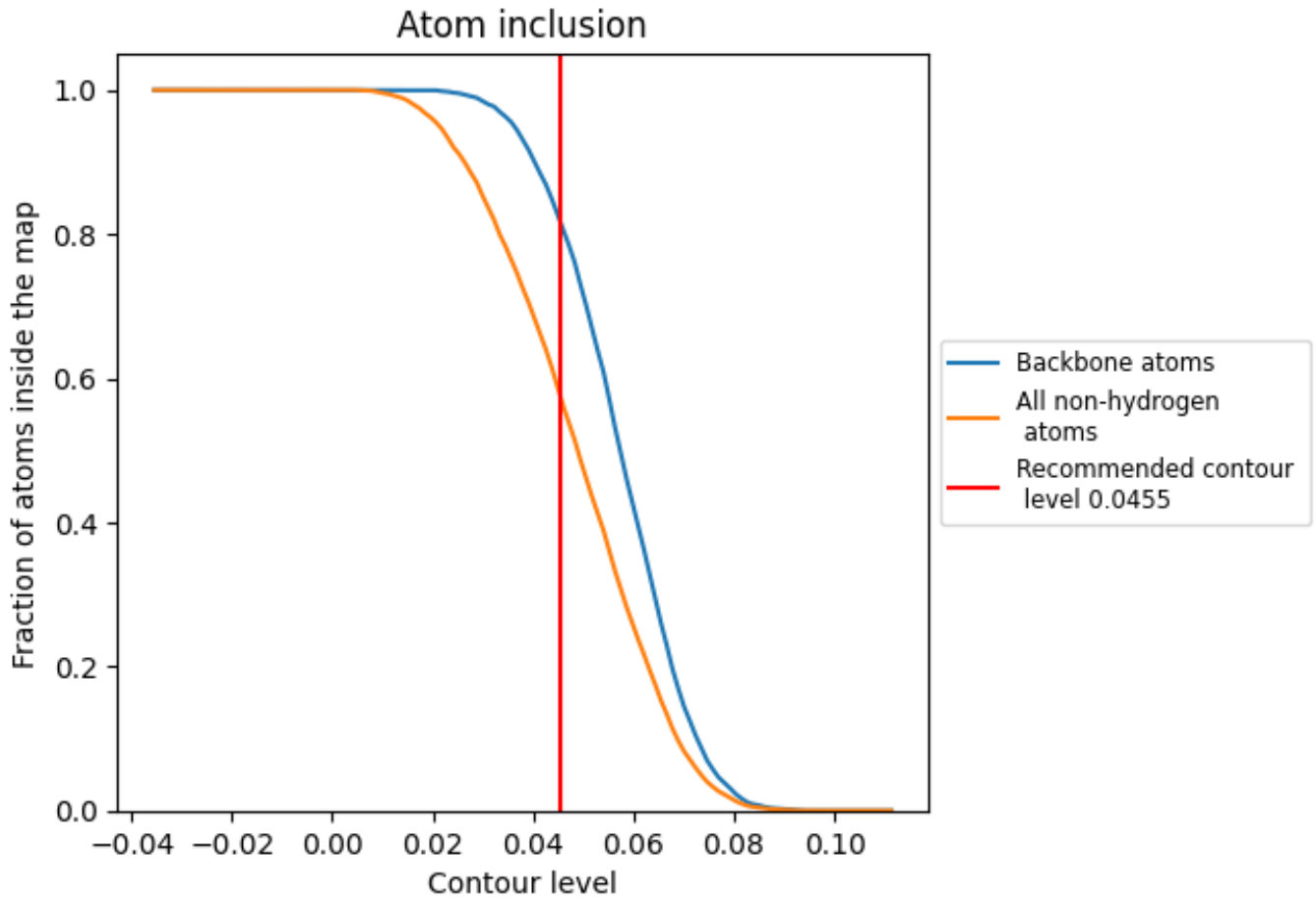
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0455).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 57% 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 (0.0455) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5737	0.3670
A	0.5486	0.3670
B	0.5510	0.3660
C	0.5492	0.3650
D	0.5825	0.3500
E	0.5940	0.3520
F	0.5825	0.3470
G	0.6088	0.3880
H	0.6077	0.3880
I	0.6166	0.3850
J	0.5911	0.3570
K	0.5949	0.3600
L	0.5911	0.3590
M	0.1786	0.3240
N	0.5000	0.3920
O	0.1429	0.3140
P	0.5000	0.3820
Q	0.1429	0.3270
R	0.4861	0.3790