Full wwPDB X-ray Structure Validation Report (i)

Oct 15, 2023 – 03:49 PM EDT

PDB ID	:	7LVW
Title	:	Structure of RSV F in Complex with VHH Cl184
Authors	:	Hsieh, C.-L.; McLellan, J.S.
Deposited on	:	2021-02-26
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
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 (1)) were used in the production of this report:

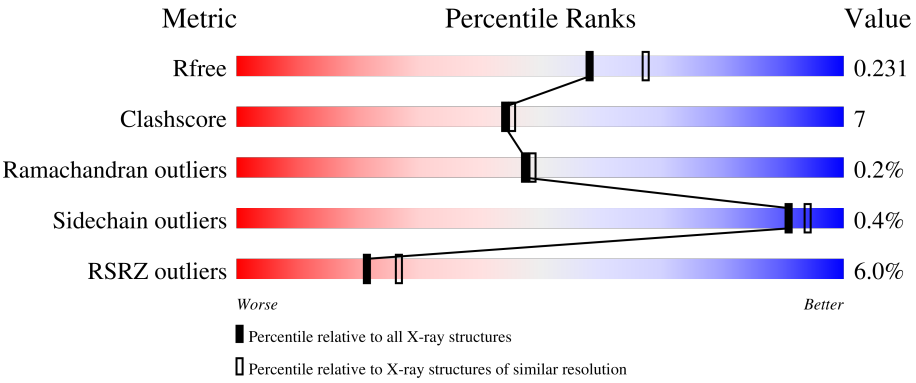
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.



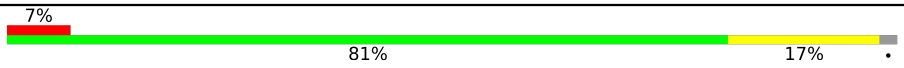
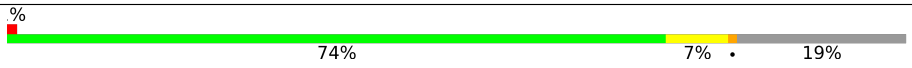
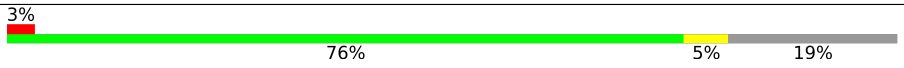
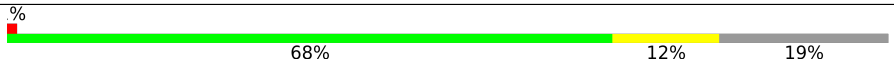
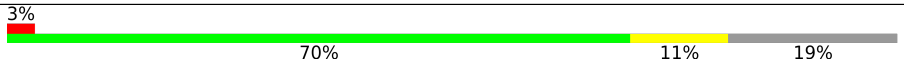
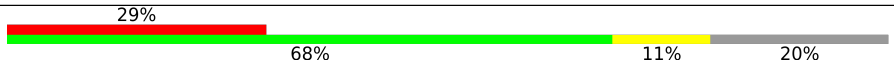
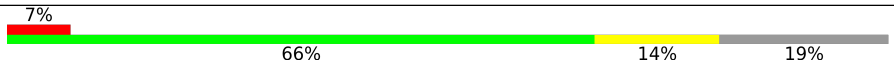
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	500	4% 86% 12%
1	B	500	2% 86% 12%
1	C	500	5% 86% 12%
1	D	500	6% 82% 15%
1	E	500	7% 82% 16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	500	
2	G	152	
2	H	152	
2	I	152	
2	J	152	
2	K	152	
2	L	152	
3	M	3	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 30677 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	0	0
			3783	2398	621	743	21			
1	B	488	Total	C	N	O	S	0	0	0
			3780	2396	621	742	21			
1	C	489	Total	C	N	O	S	0	0	0
			3786	2399	622	744	21			
1	D	489	Total	C	N	O	S	0	0	0
			3786	2399	622	744	21			
1	E	488	Total	C	N	O	S	0	0	0
			3780	2396	621	742	21			
1	F	491	Total	C	N	O	S	0	0	0
			3800	2408	624	747	21			

There are 414 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	GLU	LYS	conflict	UNP W8RJF9
A	67	ILE	ASN	conflict	UNP W8RJF9
A	?	-	ARG	deletion	UNP W8RJF9
A	?	-	ARG	deletion	UNP W8RJF9
A	?	-	GLU	deletion	UNP W8RJF9
A	?	-	LEU	deletion	UNP W8RJF9
A	?	-	PRO	deletion	UNP W8RJF9
A	?	-	ARG	deletion	UNP W8RJF9
A	?	-	PHE	deletion	UNP W8RJF9
A	?	-	MET	deletion	UNP W8RJF9
A	?	-	ASN	deletion	UNP W8RJF9
A	?	-	TYR	deletion	UNP W8RJF9
A	?	-	THR	deletion	UNP W8RJF9
A	?	-	LEU	deletion	UNP W8RJF9
A	?	-	ASN	deletion	UNP W8RJF9
A	?	-	ASN	deletion	UNP W8RJF9
A	?	-	ALA	deletion	UNP W8RJF9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP W8RJF9
A	?	-	LYS	deletion	UNP W8RJF9
A	?	-	THR	deletion	UNP W8RJF9
A	?	-	ASN	deletion	UNP W8RJF9
A	?	-	VAL	deletion	UNP W8RJF9
A	?	-	THR	deletion	UNP W8RJF9
A	?	-	LEU	deletion	UNP W8RJF9
A	?	-	SER	deletion	UNP W8RJF9
A	?	-	LYS	deletion	UNP W8RJF9
A	?	-	LYS	deletion	UNP W8RJF9
A	?	-	ARG	deletion	UNP W8RJF9
A	?	-	LYS	deletion	UNP W8RJF9
A	215	PRO	SER	conflict	UNP W8RJF9
A	514	SER	-	expression tag	UNP W8RJF9
A	515	ALA	-	expression tag	UNP W8RJF9
A	516	ILE	-	expression tag	UNP W8RJF9
A	517	GLY	-	expression tag	UNP W8RJF9
A	518	GLY	-	expression tag	UNP W8RJF9
A	519	TYR	-	expression tag	UNP W8RJF9
A	520	ILE	-	expression tag	UNP W8RJF9
A	521	PRO	-	expression tag	UNP W8RJF9
A	522	GLU	-	expression tag	UNP W8RJF9
A	523	ALA	-	expression tag	UNP W8RJF9
A	524	PRO	-	expression tag	UNP W8RJF9
A	525	ARG	-	expression tag	UNP W8RJF9
A	526	ASP	-	expression tag	UNP W8RJF9
A	527	GLY	-	expression tag	UNP W8RJF9
A	528	GLN	-	expression tag	UNP W8RJF9
A	529	ALA	-	expression tag	UNP W8RJF9
A	530	TYR	-	expression tag	UNP W8RJF9
A	531	VAL	-	expression tag	UNP W8RJF9
A	532	ARG	-	expression tag	UNP W8RJF9
A	533	LYS	-	expression tag	UNP W8RJF9
A	534	ASP	-	expression tag	UNP W8RJF9
A	535	GLY	-	expression tag	UNP W8RJF9
A	536	GLU	-	expression tag	UNP W8RJF9
A	537	TRP	-	expression tag	UNP W8RJF9
A	538	VAL	-	expression tag	UNP W8RJF9
A	539	LEU	-	expression tag	UNP W8RJF9
A	540	LEU	-	expression tag	UNP W8RJF9
A	541	SER	-	expression tag	UNP W8RJF9
A	542	THR	-	expression tag	UNP W8RJF9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	543	PHE	-	expression tag	UNP W8RJF9
A	544	LEU	-	expression tag	UNP W8RJF9
A	545	GLY	-	expression tag	UNP W8RJF9
A	546	SER	-	expression tag	UNP W8RJF9
A	547	LEU	-	expression tag	UNP W8RJF9
A	548	GLU	-	expression tag	UNP W8RJF9
A	549	VAL	-	expression tag	UNP W8RJF9
A	550	LEU	-	expression tag	UNP W8RJF9
A	551	PHE	-	expression tag	UNP W8RJF9
A	552	GLN	-	expression tag	UNP W8RJF9
B	66	GLU	LYS	conflict	UNP W8RJF9
B	67	ILE	ASN	conflict	UNP W8RJF9
B	?	-	ARG	deletion	UNP W8RJF9
B	?	-	ARG	deletion	UNP W8RJF9
B	?	-	GLU	deletion	UNP W8RJF9
B	?	-	LEU	deletion	UNP W8RJF9
B	?	-	PRO	deletion	UNP W8RJF9
B	?	-	ARG	deletion	UNP W8RJF9
B	?	-	PHE	deletion	UNP W8RJF9
B	?	-	MET	deletion	UNP W8RJF9
B	?	-	ASN	deletion	UNP W8RJF9
B	?	-	TYR	deletion	UNP W8RJF9
B	?	-	THR	deletion	UNP W8RJF9
B	?	-	LEU	deletion	UNP W8RJF9
B	?	-	ASN	deletion	UNP W8RJF9
B	?	-	ASN	deletion	UNP W8RJF9
B	?	-	ALA	deletion	UNP W8RJF9
B	?	-	LYS	deletion	UNP W8RJF9
B	?	-	LYS	deletion	UNP W8RJF9
B	?	-	THR	deletion	UNP W8RJF9
B	?	-	ASN	deletion	UNP W8RJF9
B	?	-	VAL	deletion	UNP W8RJF9
B	?	-	THR	deletion	UNP W8RJF9
B	?	-	LEU	deletion	UNP W8RJF9
B	?	-	SER	deletion	UNP W8RJF9
B	?	-	LYS	deletion	UNP W8RJF9
B	?	-	LYS	deletion	UNP W8RJF9
B	?	-	ARG	deletion	UNP W8RJF9
B	?	-	LYS	deletion	UNP W8RJF9
B	215	PRO	SER	conflict	UNP W8RJF9
B	514	SER	-	expression tag	UNP W8RJF9
B	515	ALA	-	expression tag	UNP W8RJF9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	516	ILE	-	expression tag	UNP W8RJF9
B	517	GLY	-	expression tag	UNP W8RJF9
B	518	GLY	-	expression tag	UNP W8RJF9
B	519	TYR	-	expression tag	UNP W8RJF9
B	520	ILE	-	expression tag	UNP W8RJF9
B	521	PRO	-	expression tag	UNP W8RJF9
B	522	GLU	-	expression tag	UNP W8RJF9
B	523	ALA	-	expression tag	UNP W8RJF9
B	524	PRO	-	expression tag	UNP W8RJF9
B	525	ARG	-	expression tag	UNP W8RJF9
B	526	ASP	-	expression tag	UNP W8RJF9
B	527	GLY	-	expression tag	UNP W8RJF9
B	528	GLN	-	expression tag	UNP W8RJF9
B	529	ALA	-	expression tag	UNP W8RJF9
B	530	TYR	-	expression tag	UNP W8RJF9
B	531	VAL	-	expression tag	UNP W8RJF9
B	532	ARG	-	expression tag	UNP W8RJF9
B	533	LYS	-	expression tag	UNP W8RJF9
B	534	ASP	-	expression tag	UNP W8RJF9
B	535	GLY	-	expression tag	UNP W8RJF9
B	536	GLU	-	expression tag	UNP W8RJF9
B	537	TRP	-	expression tag	UNP W8RJF9
B	538	VAL	-	expression tag	UNP W8RJF9
B	539	LEU	-	expression tag	UNP W8RJF9
B	540	LEU	-	expression tag	UNP W8RJF9
B	541	SER	-	expression tag	UNP W8RJF9
B	542	THR	-	expression tag	UNP W8RJF9
B	543	PHE	-	expression tag	UNP W8RJF9
B	544	LEU	-	expression tag	UNP W8RJF9
B	545	GLY	-	expression tag	UNP W8RJF9
B	546	SER	-	expression tag	UNP W8RJF9
B	547	LEU	-	expression tag	UNP W8RJF9
B	548	GLU	-	expression tag	UNP W8RJF9
B	549	VAL	-	expression tag	UNP W8RJF9
B	550	LEU	-	expression tag	UNP W8RJF9
B	551	PHE	-	expression tag	UNP W8RJF9
B	552	GLN	-	expression tag	UNP W8RJF9
C	66	GLU	LYS	conflict	UNP W8RJF9
C	67	ILE	ASN	conflict	UNP W8RJF9
C	?	-	ARG	deletion	UNP W8RJF9
C	?	-	ARG	deletion	UNP W8RJF9
C	?	-	GLU	deletion	UNP W8RJF9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	LEU	deletion	UNP W8RJF9
C	?	-	PRO	deletion	UNP W8RJF9
C	?	-	ARG	deletion	UNP W8RJF9
C	?	-	PHE	deletion	UNP W8RJF9
C	?	-	MET	deletion	UNP W8RJF9
C	?	-	ASN	deletion	UNP W8RJF9
C	?	-	TYR	deletion	UNP W8RJF9
C	?	-	THR	deletion	UNP W8RJF9
C	?	-	LEU	deletion	UNP W8RJF9
C	?	-	ASN	deletion	UNP W8RJF9
C	?	-	ASN	deletion	UNP W8RJF9
C	?	-	ALA	deletion	UNP W8RJF9
C	?	-	LYS	deletion	UNP W8RJF9
C	?	-	LYS	deletion	UNP W8RJF9
C	?	-	THR	deletion	UNP W8RJF9
C	?	-	ASN	deletion	UNP W8RJF9
C	?	-	VAL	deletion	UNP W8RJF9
C	?	-	THR	deletion	UNP W8RJF9
C	?	-	LEU	deletion	UNP W8RJF9
C	?	-	SER	deletion	UNP W8RJF9
C	?	-	LYS	deletion	UNP W8RJF9
C	?	-	LYS	deletion	UNP W8RJF9
C	?	-	ARG	deletion	UNP W8RJF9
C	?	-	LYS	deletion	UNP W8RJF9
C	215	PRO	SER	conflict	UNP W8RJF9
C	514	SER	-	expression tag	UNP W8RJF9
C	515	ALA	-	expression tag	UNP W8RJF9
C	516	ILE	-	expression tag	UNP W8RJF9
C	517	GLY	-	expression tag	UNP W8RJF9
C	518	GLY	-	expression tag	UNP W8RJF9
C	519	TYR	-	expression tag	UNP W8RJF9
C	520	ILE	-	expression tag	UNP W8RJF9
C	521	PRO	-	expression tag	UNP W8RJF9
C	522	GLU	-	expression tag	UNP W8RJF9
C	523	ALA	-	expression tag	UNP W8RJF9
C	524	PRO	-	expression tag	UNP W8RJF9
C	525	ARG	-	expression tag	UNP W8RJF9
C	526	ASP	-	expression tag	UNP W8RJF9
C	527	GLY	-	expression tag	UNP W8RJF9
C	528	GLN	-	expression tag	UNP W8RJF9
C	529	ALA	-	expression tag	UNP W8RJF9
C	530	TYR	-	expression tag	UNP W8RJF9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	531	VAL	-	expression tag	UNP W8RJF9
C	532	ARG	-	expression tag	UNP W8RJF9
C	533	LYS	-	expression tag	UNP W8RJF9
C	534	ASP	-	expression tag	UNP W8RJF9
C	535	GLY	-	expression tag	UNP W8RJF9
C	536	GLU	-	expression tag	UNP W8RJF9
C	537	TRP	-	expression tag	UNP W8RJF9
C	538	VAL	-	expression tag	UNP W8RJF9
C	539	LEU	-	expression tag	UNP W8RJF9
C	540	LEU	-	expression tag	UNP W8RJF9
C	541	SER	-	expression tag	UNP W8RJF9
C	542	THR	-	expression tag	UNP W8RJF9
C	543	PHE	-	expression tag	UNP W8RJF9
C	544	LEU	-	expression tag	UNP W8RJF9
C	545	GLY	-	expression tag	UNP W8RJF9
C	546	SER	-	expression tag	UNP W8RJF9
C	547	LEU	-	expression tag	UNP W8RJF9
C	548	GLU	-	expression tag	UNP W8RJF9
C	549	VAL	-	expression tag	UNP W8RJF9
C	550	LEU	-	expression tag	UNP W8RJF9
C	551	PHE	-	expression tag	UNP W8RJF9
C	552	GLN	-	expression tag	UNP W8RJF9
D	66	GLU	LYS	conflict	UNP W8RJF9
D	67	ILE	ASN	conflict	UNP W8RJF9
D	?	-	ARG	deletion	UNP W8RJF9
D	?	-	ARG	deletion	UNP W8RJF9
D	?	-	GLU	deletion	UNP W8RJF9
D	?	-	LEU	deletion	UNP W8RJF9
D	?	-	PRO	deletion	UNP W8RJF9
D	?	-	ARG	deletion	UNP W8RJF9
D	?	-	PHE	deletion	UNP W8RJF9
D	?	-	MET	deletion	UNP W8RJF9
D	?	-	ASN	deletion	UNP W8RJF9
D	?	-	TYR	deletion	UNP W8RJF9
D	?	-	THR	deletion	UNP W8RJF9
D	?	-	LEU	deletion	UNP W8RJF9
D	?	-	ASN	deletion	UNP W8RJF9
D	?	-	ASN	deletion	UNP W8RJF9
D	?	-	ALA	deletion	UNP W8RJF9
D	?	-	LYS	deletion	UNP W8RJF9
D	?	-	LYS	deletion	UNP W8RJF9
D	?	-	THR	deletion	UNP W8RJF9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ASN	deletion	UNP W8RJF9
D	?	-	VAL	deletion	UNP W8RJF9
D	?	-	THR	deletion	UNP W8RJF9
D	?	-	LEU	deletion	UNP W8RJF9
D	?	-	SER	deletion	UNP W8RJF9
D	?	-	LYS	deletion	UNP W8RJF9
D	?	-	LYS	deletion	UNP W8RJF9
D	?	-	ARG	deletion	UNP W8RJF9
D	?	-	LYS	deletion	UNP W8RJF9
D	215	PRO	SER	conflict	UNP W8RJF9
D	514	SER	-	expression tag	UNP W8RJF9
D	515	ALA	-	expression tag	UNP W8RJF9
D	516	ILE	-	expression tag	UNP W8RJF9
D	517	GLY	-	expression tag	UNP W8RJF9
D	518	GLY	-	expression tag	UNP W8RJF9
D	519	TYR	-	expression tag	UNP W8RJF9
D	520	ILE	-	expression tag	UNP W8RJF9
D	521	PRO	-	expression tag	UNP W8RJF9
D	522	GLU	-	expression tag	UNP W8RJF9
D	523	ALA	-	expression tag	UNP W8RJF9
D	524	PRO	-	expression tag	UNP W8RJF9
D	525	ARG	-	expression tag	UNP W8RJF9
D	526	ASP	-	expression tag	UNP W8RJF9
D	527	GLY	-	expression tag	UNP W8RJF9
D	528	GLN	-	expression tag	UNP W8RJF9
D	529	ALA	-	expression tag	UNP W8RJF9
D	530	TYR	-	expression tag	UNP W8RJF9
D	531	VAL	-	expression tag	UNP W8RJF9
D	532	ARG	-	expression tag	UNP W8RJF9
D	533	LYS	-	expression tag	UNP W8RJF9
D	534	ASP	-	expression tag	UNP W8RJF9
D	535	GLY	-	expression tag	UNP W8RJF9
D	536	GLU	-	expression tag	UNP W8RJF9
D	537	TRP	-	expression tag	UNP W8RJF9
D	538	VAL	-	expression tag	UNP W8RJF9
D	539	LEU	-	expression tag	UNP W8RJF9
D	540	LEU	-	expression tag	UNP W8RJF9
D	541	SER	-	expression tag	UNP W8RJF9
D	542	THR	-	expression tag	UNP W8RJF9
D	543	PHE	-	expression tag	UNP W8RJF9
D	544	LEU	-	expression tag	UNP W8RJF9
D	545	GLY	-	expression tag	UNP W8RJF9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	546	SER	-	expression tag	UNP W8RJF9
D	547	LEU	-	expression tag	UNP W8RJF9
D	548	GLU	-	expression tag	UNP W8RJF9
D	549	VAL	-	expression tag	UNP W8RJF9
D	550	LEU	-	expression tag	UNP W8RJF9
D	551	PHE	-	expression tag	UNP W8RJF9
D	552	GLN	-	expression tag	UNP W8RJF9
E	66	GLU	LYS	conflict	UNP W8RJF9
E	67	ILE	ASN	conflict	UNP W8RJF9
E	?	-	ARG	deletion	UNP W8RJF9
E	?	-	ARG	deletion	UNP W8RJF9
E	?	-	GLU	deletion	UNP W8RJF9
E	?	-	LEU	deletion	UNP W8RJF9
E	?	-	PRO	deletion	UNP W8RJF9
E	?	-	ARG	deletion	UNP W8RJF9
E	?	-	PHE	deletion	UNP W8RJF9
E	?	-	MET	deletion	UNP W8RJF9
E	?	-	ASN	deletion	UNP W8RJF9
E	?	-	TYR	deletion	UNP W8RJF9
E	?	-	THR	deletion	UNP W8RJF9
E	?	-	LEU	deletion	UNP W8RJF9
E	?	-	ASN	deletion	UNP W8RJF9
E	?	-	ASN	deletion	UNP W8RJF9
E	?	-	ALA	deletion	UNP W8RJF9
E	?	-	LYS	deletion	UNP W8RJF9
E	?	-	LYS	deletion	UNP W8RJF9
E	?	-	THR	deletion	UNP W8RJF9
E	?	-	ASN	deletion	UNP W8RJF9
E	?	-	VAL	deletion	UNP W8RJF9
E	?	-	THR	deletion	UNP W8RJF9
E	?	-	LEU	deletion	UNP W8RJF9
E	?	-	SER	deletion	UNP W8RJF9
E	?	-	LYS	deletion	UNP W8RJF9
E	?	-	LYS	deletion	UNP W8RJF9
E	?	-	ARG	deletion	UNP W8RJF9
E	?	-	LYS	deletion	UNP W8RJF9
E	215	PRO	SER	conflict	UNP W8RJF9
E	514	SER	-	expression tag	UNP W8RJF9
E	515	ALA	-	expression tag	UNP W8RJF9
E	516	ILE	-	expression tag	UNP W8RJF9
E	517	GLY	-	expression tag	UNP W8RJF9
E	518	GLY	-	expression tag	UNP W8RJF9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	519	TYR	-	expression tag	UNP W8RJF9
E	520	ILE	-	expression tag	UNP W8RJF9
E	521	PRO	-	expression tag	UNP W8RJF9
E	522	GLU	-	expression tag	UNP W8RJF9
E	523	ALA	-	expression tag	UNP W8RJF9
E	524	PRO	-	expression tag	UNP W8RJF9
E	525	ARG	-	expression tag	UNP W8RJF9
E	526	ASP	-	expression tag	UNP W8RJF9
E	527	GLY	-	expression tag	UNP W8RJF9
E	528	GLN	-	expression tag	UNP W8RJF9
E	529	ALA	-	expression tag	UNP W8RJF9
E	530	TYR	-	expression tag	UNP W8RJF9
E	531	VAL	-	expression tag	UNP W8RJF9
E	532	ARG	-	expression tag	UNP W8RJF9
E	533	LYS	-	expression tag	UNP W8RJF9
E	534	ASP	-	expression tag	UNP W8RJF9
E	535	GLY	-	expression tag	UNP W8RJF9
E	536	GLU	-	expression tag	UNP W8RJF9
E	537	TRP	-	expression tag	UNP W8RJF9
E	538	VAL	-	expression tag	UNP W8RJF9
E	539	LEU	-	expression tag	UNP W8RJF9
E	540	LEU	-	expression tag	UNP W8RJF9
E	541	SER	-	expression tag	UNP W8RJF9
E	542	THR	-	expression tag	UNP W8RJF9
E	543	PHE	-	expression tag	UNP W8RJF9
E	544	LEU	-	expression tag	UNP W8RJF9
E	545	GLY	-	expression tag	UNP W8RJF9
E	546	SER	-	expression tag	UNP W8RJF9
E	547	LEU	-	expression tag	UNP W8RJF9
E	548	GLU	-	expression tag	UNP W8RJF9
E	549	VAL	-	expression tag	UNP W8RJF9
E	550	LEU	-	expression tag	UNP W8RJF9
E	551	PHE	-	expression tag	UNP W8RJF9
E	552	GLN	-	expression tag	UNP W8RJF9
F	66	GLU	LYS	conflict	UNP W8RJF9
F	67	ILE	ASN	conflict	UNP W8RJF9
F	?	-	ARG	deletion	UNP W8RJF9
F	?	-	ARG	deletion	UNP W8RJF9
F	?	-	GLU	deletion	UNP W8RJF9
F	?	-	LEU	deletion	UNP W8RJF9
F	?	-	PRO	deletion	UNP W8RJF9
F	?	-	ARG	deletion	UNP W8RJF9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	PHE	deletion	UNP W8RJF9
F	?	-	MET	deletion	UNP W8RJF9
F	?	-	ASN	deletion	UNP W8RJF9
F	?	-	TYR	deletion	UNP W8RJF9
F	?	-	THR	deletion	UNP W8RJF9
F	?	-	LEU	deletion	UNP W8RJF9
F	?	-	ASN	deletion	UNP W8RJF9
F	?	-	ASN	deletion	UNP W8RJF9
F	?	-	ALA	deletion	UNP W8RJF9
F	?	-	LYS	deletion	UNP W8RJF9
F	?	-	LYS	deletion	UNP W8RJF9
F	?	-	THR	deletion	UNP W8RJF9
F	?	-	ASN	deletion	UNP W8RJF9
F	?	-	VAL	deletion	UNP W8RJF9
F	?	-	THR	deletion	UNP W8RJF9
F	?	-	LEU	deletion	UNP W8RJF9
F	?	-	SER	deletion	UNP W8RJF9
F	?	-	LYS	deletion	UNP W8RJF9
F	?	-	LYS	deletion	UNP W8RJF9
F	?	-	ARG	deletion	UNP W8RJF9
F	?	-	LYS	deletion	UNP W8RJF9
F	215	PRO	SER	conflict	UNP W8RJF9
F	514	SER	-	expression tag	UNP W8RJF9
F	515	ALA	-	expression tag	UNP W8RJF9
F	516	ILE	-	expression tag	UNP W8RJF9
F	517	GLY	-	expression tag	UNP W8RJF9
F	518	GLY	-	expression tag	UNP W8RJF9
F	519	TYR	-	expression tag	UNP W8RJF9
F	520	ILE	-	expression tag	UNP W8RJF9
F	521	PRO	-	expression tag	UNP W8RJF9
F	522	GLU	-	expression tag	UNP W8RJF9
F	523	ALA	-	expression tag	UNP W8RJF9
F	524	PRO	-	expression tag	UNP W8RJF9
F	525	ARG	-	expression tag	UNP W8RJF9
F	526	ASP	-	expression tag	UNP W8RJF9
F	527	GLY	-	expression tag	UNP W8RJF9
F	528	GLN	-	expression tag	UNP W8RJF9
F	529	ALA	-	expression tag	UNP W8RJF9
F	530	TYR	-	expression tag	UNP W8RJF9
F	531	VAL	-	expression tag	UNP W8RJF9
F	532	ARG	-	expression tag	UNP W8RJF9
F	533	LYS	-	expression tag	UNP W8RJF9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	534	ASP	-	expression tag	UNP W8RJF9
F	535	GLY	-	expression tag	UNP W8RJF9
F	536	GLU	-	expression tag	UNP W8RJF9
F	537	TRP	-	expression tag	UNP W8RJF9
F	538	VAL	-	expression tag	UNP W8RJF9
F	539	LEU	-	expression tag	UNP W8RJF9
F	540	LEU	-	expression tag	UNP W8RJF9
F	541	SER	-	expression tag	UNP W8RJF9
F	542	THR	-	expression tag	UNP W8RJF9
F	543	PHE	-	expression tag	UNP W8RJF9
F	544	LEU	-	expression tag	UNP W8RJF9
F	545	GLY	-	expression tag	UNP W8RJF9
F	546	SER	-	expression tag	UNP W8RJF9
F	547	LEU	-	expression tag	UNP W8RJF9
F	548	GLU	-	expression tag	UNP W8RJF9
F	549	VAL	-	expression tag	UNP W8RJF9
F	550	LEU	-	expression tag	UNP W8RJF9
F	551	PHE	-	expression tag	UNP W8RJF9
F	552	GLN	-	expression tag	UNP W8RJF9

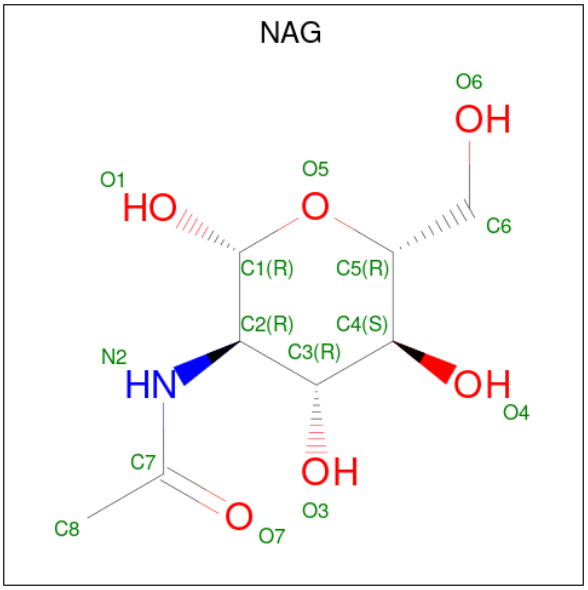
- Molecule 2 is a protein called F-VHH-Cl184.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	123	Total	C	N	O	S	0	0	0
			939	590	163	183	3			
2	I	123	Total	C	N	O	S	0	0	0
			939	590	163	183	3			
2	K	121	Total	C	N	O	S	0	0	0
			927	584	161	179	3			
2	L	123	Total	C	N	O	S	0	0	0
			939	590	163	183	3			
2	J	123	Total	C	N	O	S	0	0	0
			939	590	163	183	3			
2	H	123	Total	C	N	O	S	0	0	0
			939	590	163	183	3			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	M	3	Total C N O 39 22 2 15	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	F	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Cl 2 2	0	0
5	B	1	Total Cl 1 1	0	0
5	E	2	Total Cl 2 2	0	0

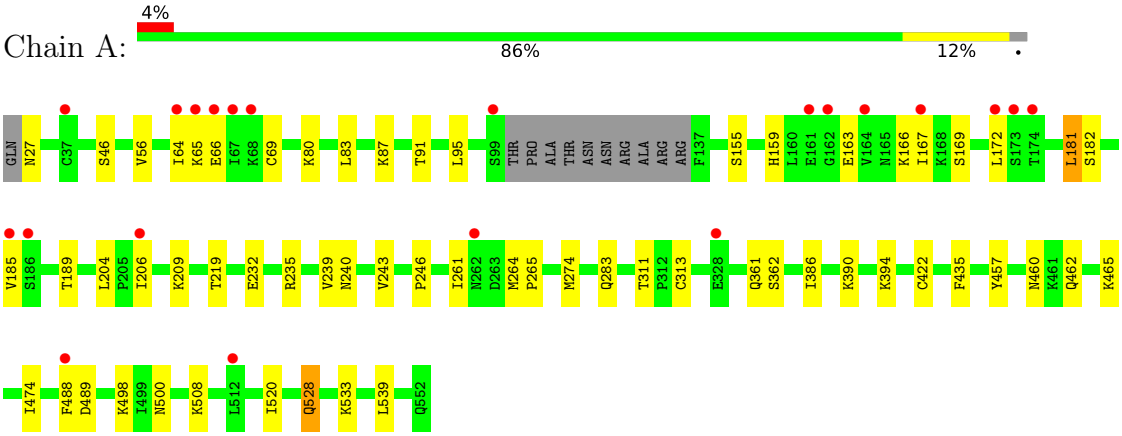
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	332	Total O 332 332	0	0
6	G	98	Total O 98 98	0	0
6	B	369	Total O 369 369	0	0
6	C	294	Total O 294 294	0	0
6	D	346	Total O 346 346	0	0
6	E	274	Total O 274 274	0	0
6	F	268	Total O 268 268	0	0
6	I	86	Total O 86 86	0	0
6	K	16	Total O 16 16	0	0
6	L	27	Total O 27 27	0	0
6	J	54	Total O 54 54	0	0
6	H	90	Total O 90 90	0	0

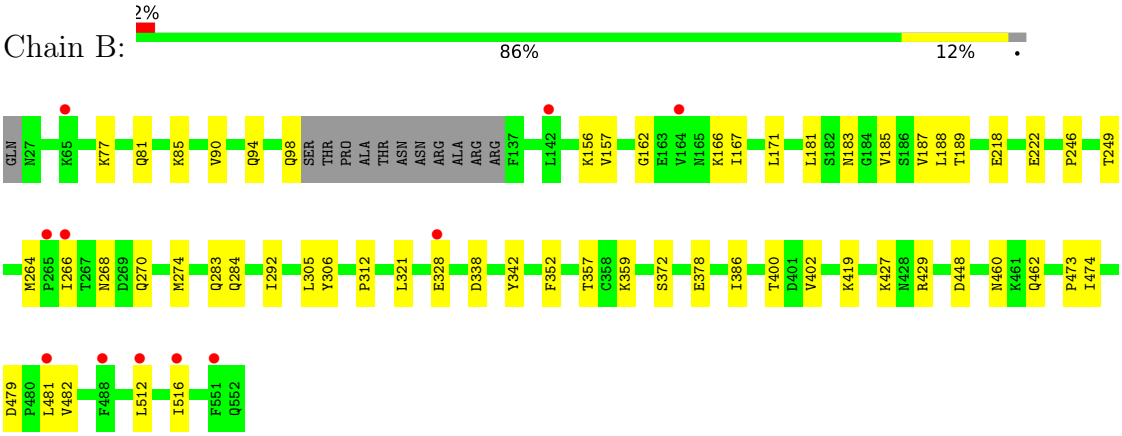
3 Residue-property plots (i)

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

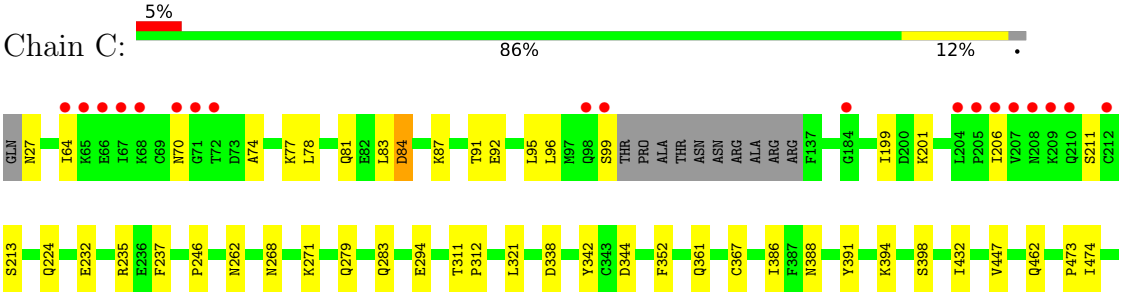
• Molecule 1: Fusion glycoprotein F0

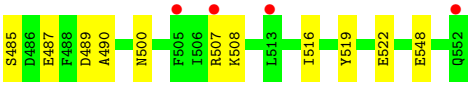


• Molecule 1: Fusion glycoprotein F0

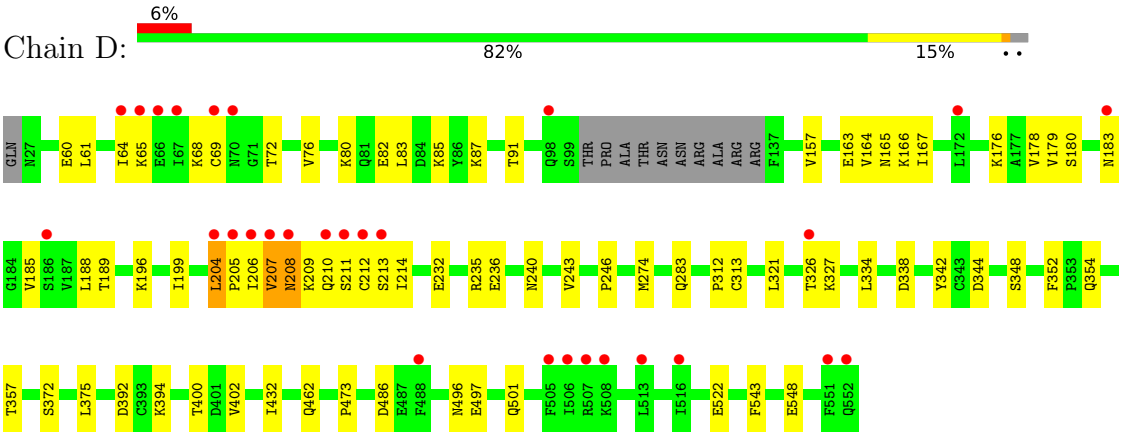


• Molecule 1: Fusion glycoprotein F0

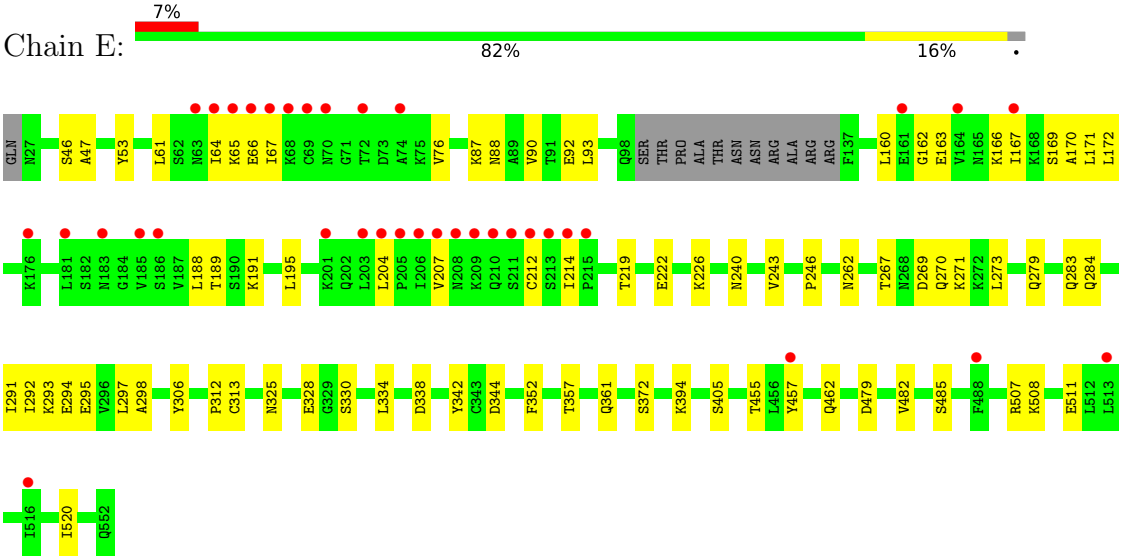




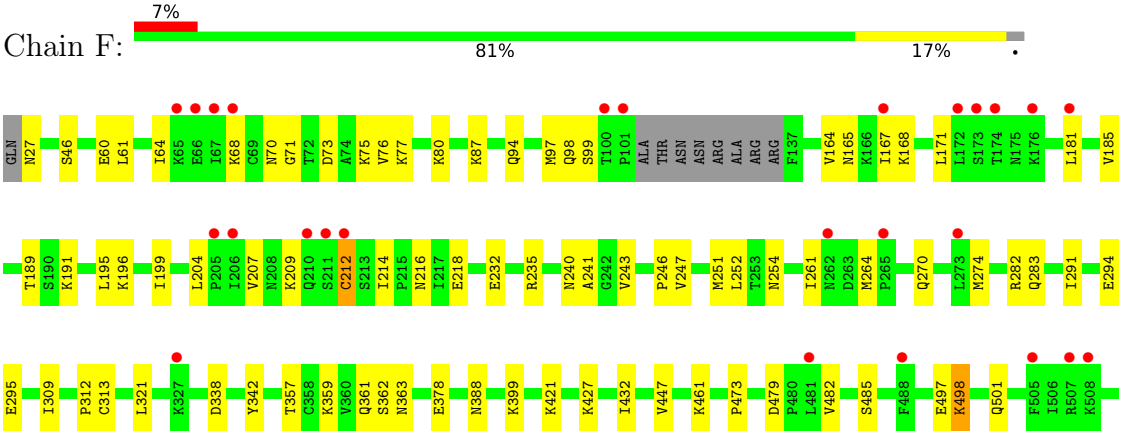
• Molecule 1: Fusion glycoprotein F0

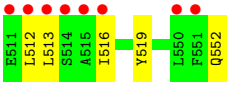


• Molecule 1: Fusion glycoprotein F0



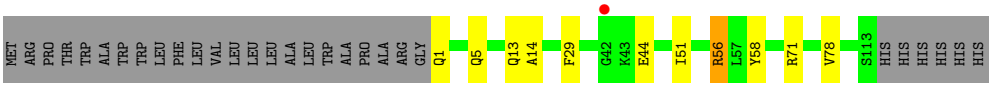
• Molecule 1: Fusion glycoprotein F0





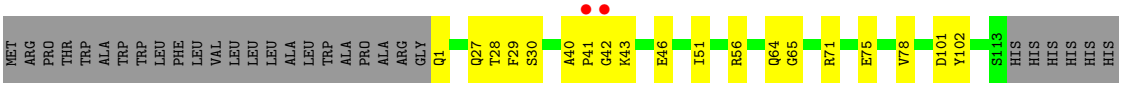
• Molecule 2: F-VHH-Cl184

Chain G:



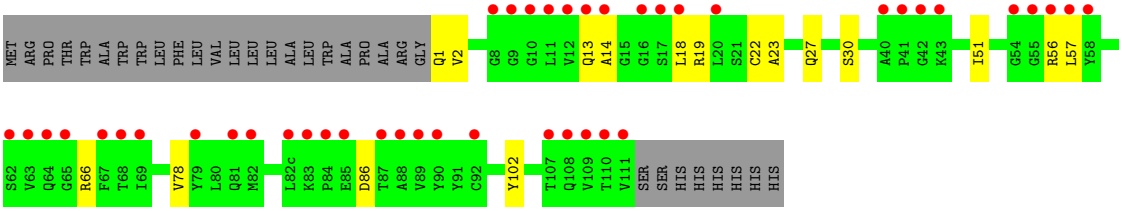
• Molecule 2: F-VHH-Cl184

Chain I:



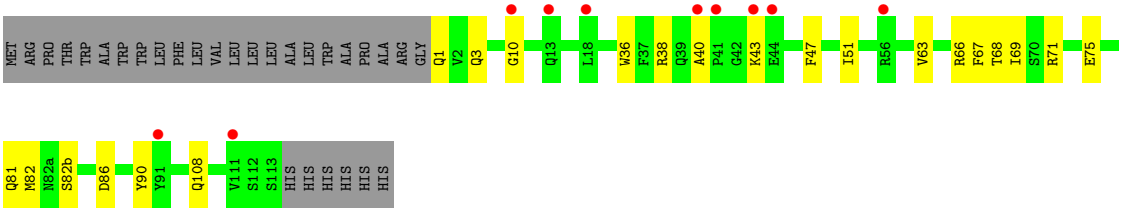
• Molecule 2: F-VHH-Cl184

Chain K:



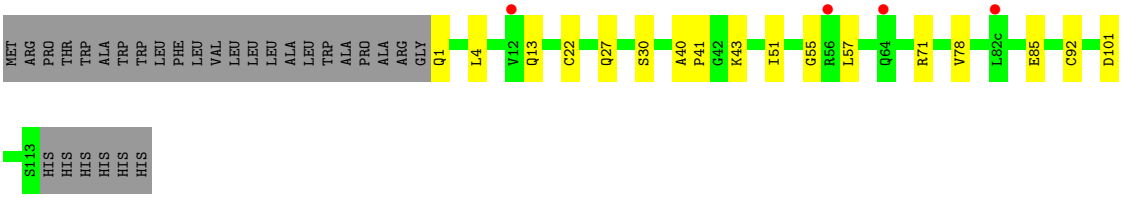
• Molecule 2: F-VHH-Cl184

Chain L:



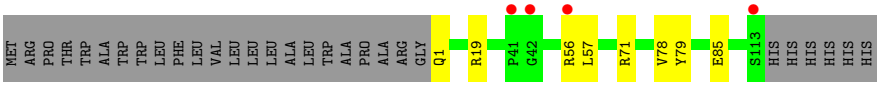
• Molecule 2: F-VHH-Cl184

Chain J:



• Molecule 2: F-VHH-Cl184

Chain H:



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

Chain M:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	104.49Å 200.56Å 134.66Å 90.00° 105.87° 90.00°	Depositor
Resolution (Å)	50.25 – 2.10 50.25 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.3 (50.25-2.10) 97.3 (50.25-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.201 , 0.230 0.202 , 0.231	Depositor DCC
R_{free} test set	15057 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	33.5	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	30677	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.39	0/3841	0.58	1/5206 (0.0%)
1	B	0.35	0/3838	0.56	1/5202 (0.0%)
1	C	0.36	1/3844 (0.0%)	0.54	1/5210 (0.0%)
1	D	0.37	1/3844 (0.0%)	0.59	1/5210 (0.0%)
1	E	0.35	0/3838	0.56	1/5202 (0.0%)
1	F	0.36	1/3859 (0.0%)	0.59	4/5232 (0.1%)
2	G	0.33	0/960	0.53	0/1302
2	H	0.34	0/960	0.57	0/1302
2	I	0.33	0/960	0.56	0/1302
2	J	0.37	0/960	0.60	0/1302
2	K	0.29	0/948	0.55	0/1286
2	L	0.30	0/960	0.52	0/1302
All	All	0.36	3/28812 (0.0%)	0.57	9/39058 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	498	LYS	CE-NZ	8.29	1.69	1.49
1	D	207	VAL	CB-CG2	-5.54	1.41	1.52
1	C	548	GLU	CD-OE2	5.16	1.31	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	498	LYS	CD-CE-NZ	-8.92	91.18	111.70
1	F	498	LYS	CA-CB-CG	8.48	132.06	113.40
1	F	513	LEU	CA-CB-CG	7.06	131.54	115.30
1	E	334	LEU	CA-CB-CG	6.00	129.10	115.30
1	F	212	CYS	CA-CB-SG	-5.70	103.74	114.00
1	B	188	LEU	CB-CG-CD2	-5.68	101.35	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	528	GLN	CA-CB-CG	5.60	125.72	113.40
1	D	334	LEU	CA-CB-CG	5.36	127.62	115.30
1	C	84	ASP	CB-CG-OD2	-5.09	113.72	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3783	0	3826	38	0
1	B	3780	0	3826	45	0
1	C	3786	0	3831	40	0
1	D	3786	0	3829	74	0
1	E	3780	0	3826	50	0
1	F	3800	0	3844	64	0
2	G	939	0	891	10	0
2	H	939	0	891	7	0
2	I	939	0	891	16	0
2	J	939	0	891	11	0
2	K	927	0	881	14	0
2	L	939	0	891	13	0
3	M	39	0	34	4	1
4	A	14	0	13	0	0
4	D	14	0	13	0	0
4	F	14	0	13	0	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
5	E	2	0	0	0	0
6	A	332	0	0	9	5
6	B	369	0	0	14	3
6	C	294	0	0	10	0
6	D	346	0	0	19	0
6	E	274	0	0	9	1
6	F	268	0	0	12	1
6	G	98	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	90	0	0	1	1
6	I	86	0	0	7	0
6	J	54	0	0	2	0
6	K	16	0	0	2	0
6	L	27	0	0	1	0
All	All	30677	0	28391	365	6

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 7.

All (365) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:498:LYS:CE	1:F:498:LYS:NZ	1.69	1.49
1:D:208:ASN:HD22	1:D:212:CYS:HA	1.29	0.97
1:E:511:GLU:OE1	6:E:701:HOH:O	1.83	0.97
1:C:268:ASN:ND2	6:C:601:HOH:O	1.97	0.97
1:D:166:LYS:NZ	1:D:180:SER:O	2.00	0.95
2:J:41:PRO:O	6:J:201:HOH:O	1.85	0.94
1:F:498:LYS:NZ	1:F:498:LYS:CD	2.30	0.93
1:C:27:ASN:ND2	6:C:602:HOH:O	2.02	0.92
1:A:69:CYS:SG	6:A:941:HOH:O	2.30	0.90
1:E:405:SER:HB3	1:E:457:TYR:CE2	2.09	0.88
1:F:185:VAL:O	6:F:701:HOH:O	1.93	0.85
1:A:27:ASN:ND2	6:A:705:HOH:O	2.10	0.84
1:F:359:LYS:NZ	6:F:704:HOH:O	2.09	0.84
1:C:64:ILE:HD11	1:C:199:ILE:HG21	1.58	0.84
1:D:208:ASN:HB2	1:D:213:SER:H	1.42	0.83
1:A:508:LYS:NZ	6:A:704:HOH:O	2.10	0.83
1:E:270:GLN:NE2	6:E:703:HOH:O	2.12	0.82
1:B:460:ASN:HB3	1:B:462:GLN:HE22	1.45	0.82
1:F:64:ILE:HD13	1:F:204:LEU:HD11	1.59	0.82
1:D:392:ASP:OD2	6:D:701:HOH:O	1.96	0.81
1:A:265:PRO:O	6:A:702:HOH:O	1.98	0.81
2:J:85:GLU:OE1	2:J:85:GLU:N	2.11	0.81
1:B:222:GLU:OE2	6:B:701:HOH:O	1.98	0.80
1:F:165:ASN:ND2	6:F:705:HOH:O	2.14	0.80
1:F:261:ILE:HG12	1:F:274:MET:HE1	1.64	0.79
1:D:213:SER:N	6:D:705:HOH:O	2.15	0.79
1:B:460:ASN:HB3	1:B:462:GLN:NE2	1.98	0.78
1:D:68:LYS:NZ	6:D:703:HOH:O	2.16	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:ASN:ND2	1:D:212:CYS:HA	1.99	0.77
1:B:246:PRO:HB3	1:B:283:GLN:HA	1.65	0.77
1:F:246:PRO:HB3	1:F:283:GLN:HA	1.65	0.77
1:F:357:THR:OG1	6:F:702:HOH:O	2.02	0.77
1:D:210:GLN:NE2	6:D:703:HOH:O	2.09	0.76
2:I:28:THR:HG23	2:I:30:SER:H	1.50	0.76
1:A:64:ILE:HD13	1:A:204:LEU:HD11	1.66	0.76
2:I:56:ARG:O	6:I:201:HOH:O	2.03	0.76
2:H:1:GLN:NE2	6:H:201:HOH:O	2.08	0.76
1:B:157:VAL:HG21	1:B:183:ASN:HD22	1.51	0.75
1:B:268:ASN:ND2	6:B:705:HOH:O	2.18	0.75
1:D:246:PRO:HB3	1:D:283:GLN:HA	1.68	0.74
1:A:533:LYS:NZ	6:A:701:HOH:O	1.97	0.74
2:G:5:GLN:NE2	6:G:201:HOH:O	2.02	0.73
2:G:56:ARG:HH12	2:G:58:TYR:HB2	1.54	0.73
3:M:1:NAG:O3	3:M:2:NAG:N2	2.22	0.73
1:D:64:ILE:HD13	1:D:199:ILE:HG21	1.69	0.73
1:C:211:SER:OG	6:C:604:HOH:O	2.06	0.72
1:E:246:PRO:HB3	1:E:283:GLN:HA	1.72	0.72
1:A:390:LYS:NZ	6:A:707:HOH:O	2.22	0.71
2:L:40:ALA:HB3	2:L:43:LYS:HD2	1.71	0.71
1:B:429:ARG:NH2	6:B:704:HOH:O	2.16	0.71
1:D:212:CYS:SG	6:D:709:HOH:O	2.49	0.71
1:D:204:LEU:HA	1:D:207:VAL:HG22	1.73	0.70
1:C:294:GLU:OE1	6:C:605:HOH:O	2.10	0.70
1:F:252:LEU:O	1:F:282:ARG:NH2	2.18	0.69
1:F:77:LYS:HA	1:F:80:LYS:HE3	1.74	0.69
1:D:327:LYS:N	6:D:706:HOH:O	2.15	0.69
1:B:284:GLN:OE1	1:B:306:TYR:OH	2.05	0.69
1:C:500:ASN:ND2	6:C:610:HOH:O	2.26	0.68
1:D:207:VAL:HG12	1:D:208:ASN:OD1	1.93	0.68
1:B:427:LYS:HG3	1:B:448:ASP:OD2	1.92	0.68
1:D:274:MET:SD	6:D:944:HOH:O	2.52	0.68
2:I:46:GLU:OE2	6:I:202:HOH:O	2.10	0.68
1:E:361:GLN:NE2	1:F:99:SER:HB3	2.08	0.68
1:A:246:PRO:HB3	1:A:283:GLN:HA	1.75	0.68
1:C:246:PRO:HB3	1:C:283:GLN:HA	1.75	0.68
1:E:462:GLN:OE1	6:E:702:HOH:O	2.11	0.67
1:D:208:ASN:HD22	1:D:212:CYS:CA	2.06	0.66
1:D:209:LYS:HE3	1:D:211:SER:HB2	1.77	0.66
1:F:97:MET:HG3	1:F:291:ILE:HA	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:GLU:OE1	6:D:704:HOH:O	2.12	0.66
2:G:44:GLU:OE1	6:G:202:HOH:O	2.14	0.65
1:A:498:LYS:NZ	1:D:486:ASP:OD1	2.28	0.65
1:C:516:ILE:HD11	1:F:516:ILE:HD12	1.76	0.65
2:I:56:ARG:HB2	6:I:234:HOH:O	1.97	0.65
1:B:157:VAL:HG21	1:B:183:ASN:ND2	2.12	0.65
2:J:4:LEU:HD23	2:J:92:CYS:SG	2.37	0.65
2:H:1:GLN:OE1	2:H:1:GLN:N	2.16	0.64
2:G:56:ARG:O	6:G:203:HOH:O	2.15	0.64
2:I:1:GLN:OE1	2:I:1:GLN:N	2.22	0.64
1:F:321:LEU:HD11	1:F:473:PRO:HB3	1.79	0.64
2:J:101:ASP:OD1	6:J:202:HOH:O	2.15	0.63
1:C:489:ASP:OD2	6:C:606:HOH:O	2.15	0.63
1:B:357:THR:OG1	6:B:703:HOH:O	2.16	0.62
1:D:208:ASN:ND2	1:D:212:CYS:SG	2.72	0.62
1:F:270:GLN:HG2	1:F:309:ILE:HD12	1.79	0.62
1:D:208:ASN:HB2	1:D:213:SER:N	2.14	0.62
1:D:501:GLN:NE2	6:D:708:HOH:O	2.31	0.62
2:G:1:GLN:N	2:G:1:GLN:OE1	2.31	0.62
1:C:312:PRO:HG2	1:C:344:ASP:OD2	1.99	0.62
1:B:270:GLN:O	1:B:274:MET:HG3	1.99	0.62
1:B:427:LYS:HE3	1:B:448:ASP:OD1	2.00	0.62
1:B:266:ILE:HB	1:B:270:GLN:HE21	1.65	0.62
1:C:462:GLN:NE2	6:C:603:HOH:O	2.04	0.61
2:G:56:ARG:NH1	2:G:58:TYR:HB2	2.14	0.61
1:C:99:SER:HB3	1:F:361:GLN:HE22	1.65	0.61
1:B:462:GLN:NE2	6:B:719:HOH:O	2.33	0.61
1:D:64:ILE:HD12	1:D:83:LEU:HD11	1.83	0.61
1:A:65:LYS:HG3	1:A:66:GLU:H	1.65	0.60
1:F:27:ASN:N	6:F:712:HOH:O	2.34	0.60
1:E:455:THR:CG2	1:E:457:TYR:HE1	2.14	0.60
1:E:267:THR:HG22	1:E:269:ASP:H	1.66	0.60
1:B:427:LYS:H	1:B:427:LYS:HD2	1.66	0.60
1:E:325:ASN:HB2	6:E:726:HOH:O	2.01	0.60
1:A:239:VAL:HG13	1:D:246:PRO:HG2	1.84	0.59
1:C:84:ASP:HA	1:C:87:LYS:HD2	1.85	0.59
1:E:169:SER:O	1:E:172:LEU:HD22	2.03	0.59
1:C:70:ASN:OD1	6:C:607:HOH:O	2.16	0.59
1:A:163:GLU:OE1	1:A:181:LEU:HB3	2.02	0.59
1:B:167:ILE:HG23	1:B:189:THR:HG21	1.85	0.58
1:D:82:GLU:OE1	6:D:707:HOH:O	2.16	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:THR:HG22	2:G:1:GLN:HE22	1.68	0.58
1:E:170:ALA:HB2	6:E:725:HOH:O	2.03	0.58
1:E:312:PRO:HG2	1:E:344:ASP:OD2	2.03	0.58
1:B:77:LYS:O	1:B:81:GLN:HG3	2.04	0.58
1:E:479:ASP:OD2	6:E:704:HOH:O	2.17	0.57
1:E:171:LEU:HD13	1:E:191:LYS:HG3	1.85	0.57
1:D:232:GLU:OE1	1:D:235:ARG:NH1	2.38	0.57
1:E:65:LYS:HA	1:E:87:LYS:HE3	1.85	0.57
1:F:71:GLY:HA3	1:F:212:CYS:HB3	1.86	0.57
1:D:501:GLN:NE2	6:D:722:HOH:O	2.36	0.57
1:E:167:ILE:HG23	1:E:189:THR:HG21	1.87	0.57
1:F:261:ILE:HA	1:F:264:MET:HG3	1.87	0.56
2:I:1:GLN:N	6:I:203:HOH:O	2.15	0.56
2:J:13:GLN:OE1	2:J:13:GLN:N	2.39	0.56
1:B:321:LEU:HD11	1:B:473:PRO:HB3	1.88	0.56
1:B:479:ASP:OD1	1:B:481:LEU:HG	2.05	0.56
1:C:432:ILE:HD11	1:C:447:VAL:HG22	1.88	0.56
1:E:284:GLN:OE1	1:E:306:TYR:OH	2.09	0.56
1:D:354:GLN:O	1:D:357:THR:HG22	2.07	0.55
1:F:427:LYS:NZ	6:F:714:HOH:O	2.39	0.55
3:M:1:NAG:HO3	3:M:2:NAG:HN2	1.51	0.55
1:F:73:ASP:HB3	1:F:76:VAL:HG22	1.88	0.55
1:D:204:LEU:CA	1:D:207:VAL:HG22	2.36	0.55
1:F:362:SER:OG	1:F:363:ASN:N	2.39	0.55
1:D:209:LYS:N	6:D:705:HOH:O	2.36	0.54
1:D:167:ILE:HD12	1:D:189:THR:HG21	1.88	0.54
1:F:68:LYS:H	1:F:68:LYS:HD3	1.71	0.54
1:A:163:GLU:O	1:A:167:ILE:HD12	2.07	0.54
1:B:481:LEU:HD12	1:B:482:VAL:HG13	1.89	0.54
1:F:312:PRO:HG2	2:K:1:GLN:H1	1.73	0.54
2:J:40:ALA:HB3	2:J:43:LYS:HD3	1.89	0.54
1:D:176:LYS:NZ	6:D:725:HOH:O	2.40	0.54
1:E:293:LYS:HG2	1:E:294:GLU:HG3	1.89	0.54
1:B:419:LYS:HD2	6:B:1050:HOH:O	2.08	0.54
1:C:232:GLU:OE2	1:C:235:ARG:NH1	2.41	0.53
1:D:208:ASN:OD1	1:D:208:ASN:N	2.41	0.53
1:F:75:LYS:HB3	1:F:214:ILE:HD11	1.91	0.53
1:B:156:LYS:NZ	6:B:717:HOH:O	2.32	0.53
1:D:69:CYS:HB2	1:D:80:LYS:NZ	2.23	0.53
1:D:432:ILE:HD12	1:F:421:LYS:HD3	1.91	0.53
1:E:53:TYR:OH	1:E:188:LEU:HD13	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:497:GLU:O	1:F:501:GLN:HG3	2.08	0.53
2:K:51:ILE:HD13	2:K:57:LEU:HG	1.90	0.53
1:B:328:GLU:OE2	6:B:706:HOH:O	2.18	0.53
1:D:501:GLN:OE1	6:D:708:HOH:O	2.18	0.53
2:L:47:PHE:N	6:L:201:HOH:O	2.20	0.53
2:I:42:GLY:C	2:I:43:LYS:HD3	2.29	0.52
1:E:291:ILE:HG12	1:E:298:ALA:HB3	1.91	0.52
1:F:181:LEU:HG	6:F:701:HOH:O	2.09	0.52
1:F:432:ILE:HD11	1:F:447:VAL:HG22	1.92	0.52
1:A:56:VAL:HB	1:A:189:THR:HG22	1.92	0.52
2:K:1:GLN:H2	2:K:27:GLN:NE2	2.06	0.52
1:A:386:ILE:HG21	1:A:474:ILE:HD13	1.92	0.52
1:E:361:GLN:HE21	1:F:99:SER:HB3	1.73	0.52
1:C:206:ILE:HG23	1:C:213:SER:HB2	1.91	0.52
1:C:224:GLN:NE2	6:C:618:HOH:O	2.43	0.52
1:C:77:LYS:O	1:C:81:GLN:HG3	2.10	0.52
1:D:501:GLN:CD	6:D:708:HOH:O	2.48	0.52
1:E:455:THR:CG2	1:E:457:TYR:CE1	2.93	0.52
1:E:67:ILE:HD11	1:E:207:VAL:HG11	1.92	0.51
1:A:169:SER:O	1:A:172:LEU:HD22	2.10	0.51
1:A:460:ASN:HB3	1:A:462:GLN:OE1	2.09	0.51
2:J:51:ILE:HG23	2:J:71:ARG:HD3	1.92	0.51
1:F:61:LEU:O	1:F:295:GLU:HB2	2.11	0.51
2:G:51:ILE:HG23	2:G:71:ARG:HD3	1.91	0.51
1:C:83:LEU:HG	1:C:87:LYS:NZ	2.25	0.51
1:D:207:VAL:C	1:D:208:ASN:OD1	2.48	0.51
1:D:207:VAL:O	1:D:208:ASN:C	2.48	0.50
1:F:378:GLU:OE2	2:K:30:SER:OG	2.29	0.50
2:I:27:GLN:HB3	6:I:209:HOH:O	2.12	0.50
1:E:162:GLY:O	1:E:166:LYS:HG3	2.12	0.50
1:F:171:LEU:HD11	1:F:189:THR:HG22	1.92	0.50
1:B:85:LYS:NZ	6:B:718:HOH:O	2.32	0.50
1:C:91:THR:O	1:C:95:LEU:HD23	2.12	0.50
1:F:195:LEU:O	1:F:199:ILE:HG13	2.11	0.50
1:C:338:ASP:HB2	1:C:342:TYR:OH	2.12	0.49
1:C:519:TYR:CZ	1:F:519:TYR:HB2	2.47	0.49
1:F:185:VAL:N	6:F:716:HOH:O	2.44	0.49
1:C:321:LEU:HD11	1:C:473:PRO:HB3	1.95	0.49
1:F:388:ASN:OD1	1:F:388:ASN:C	2.50	0.49
2:I:28:THR:OG1	2:I:75:GLU:O	2.30	0.49
1:A:500:ASN:ND2	6:A:706:HOH:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:216:ASN:HB3	1:F:218:GLU:OE1	2.12	0.49
2:I:65:GLY:N	6:I:206:HOH:O	2.33	0.49
1:D:76:VAL:HG23	1:D:214:ILE:H	1.78	0.49
1:D:64:ILE:CD1	1:D:83:LEU:HD11	2.42	0.49
1:E:226:LYS:HA	1:E:226:LYS:HD3	1.61	0.49
1:A:155:SER:O	1:A:159:HIS:HD2	1.96	0.48
1:F:164:VAL:O	1:F:168:LYS:HG3	2.13	0.48
2:L:67:PHE:CD2	2:L:82:MET:HA	2.47	0.48
1:D:312:PRO:HG2	1:D:344:ASP:OD2	2.13	0.48
2:K:18:LEU:HD23	2:K:19:ARG:N	2.27	0.48
2:I:101:ASP:HB2	2:I:102:TYR:CE2	2.48	0.48
2:K:23:ALA:O	6:K:201:HOH:O	2.20	0.48
1:C:92:GLU:HG2	1:F:254:ASN:ND2	2.29	0.48
1:F:68:LYS:HD3	1:F:68:LYS:N	2.29	0.48
2:L:66:ARG:NH1	2:L:86:ASP:OD2	2.46	0.48
1:A:232:GLU:OE2	1:A:235:ARG:NH1	2.47	0.48
1:E:455:THR:HG22	1:E:457:TYR:CE1	2.49	0.48
2:K:1:GLN:N	2:K:27:GLN:NE2	2.61	0.47
1:A:69:CYS:O	1:A:80:LYS:NZ	2.26	0.47
1:B:218:GLU:OE2	6:B:707:HOH:O	2.20	0.47
1:D:183:ASN:HB3	1:D:185:VAL:HG12	1.95	0.47
1:D:326:THR:OG1	6:D:706:HOH:O	2.20	0.47
1:A:394:LYS:NZ	1:A:489:ASP:OD1	2.32	0.47
1:B:181:LEU:HD12	1:B:185:VAL:HG13	1.96	0.47
1:B:312:PRO:HG2	2:J:1:GLN:H1	1.78	0.47
1:D:543:PHE:HB3	1:D:548:GLU:OE2	2.14	0.47
1:E:219:THR:HA	1:E:222:GLU:HG2	1.96	0.47
1:F:60:GLU:OE2	1:F:196:LYS:HE2	2.15	0.47
2:L:71:ARG:NH1	2:L:75:GLU:OE2	2.42	0.47
1:D:68:LYS:O	6:D:709:HOH:O	2.20	0.47
1:D:176:LYS:HD2	1:D:188:LEU:HD11	1.96	0.47
1:E:65:LYS:HG3	1:E:66:GLU:HG2	1.96	0.47
1:E:508:LYS:NZ	6:E:713:HOH:O	2.43	0.47
1:F:232:GLU:OE2	1:F:235:ARG:NH2	2.44	0.47
2:K:13:GLN:HG3	2:K:14:ALA:N	2.30	0.46
2:K:66:ARG:NH1	2:K:86:ASP:OD1	2.48	0.46
1:A:465:LYS:NZ	6:A:727:HOH:O	2.48	0.46
2:L:36:TRP:HD1	2:L:69:ILE:HD12	1.81	0.46
1:A:181:LEU:HD12	1:A:185:VAL:HB	1.96	0.46
1:C:507:ARG:HH21	1:C:508:LYS:HG3	1.79	0.46
1:E:338:ASP:HB2	1:E:342:TYR:OH	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:461:LYS:HD2	1:F:461:LYS:HA	1.74	0.46
1:D:167:ILE:HD13	1:D:179:VAL:HG11	1.97	0.46
1:E:262:ASN:HA	1:E:271:LYS:HD3	1.98	0.46
1:F:498:LYS:NZ	1:F:498:LYS:HD3	2.22	0.46
2:I:41:PRO:O	2:I:43:LYS:NZ	2.47	0.46
2:L:38:ARG:NH1	2:L:90:TYR:OH	2.49	0.46
1:A:361:GLN:O	1:A:362:SER:OG	2.31	0.46
1:C:394:LYS:HD3	6:C:606:HOH:O	2.16	0.45
2:K:56:ARG:HA	2:K:56:ARG:HD3	1.54	0.45
1:B:264:MET:CE	1:B:305:LEU:HD23	2.46	0.45
1:A:209:LYS:HA	6:A:941:HOH:O	2.16	0.45
1:B:162:GLY:O	1:B:166:LYS:HG3	2.16	0.45
1:B:352:PHE:CE2	1:B:372:SER:HB3	2.52	0.45
1:D:432:ILE:HD12	1:F:421:LYS:CD	2.46	0.45
1:D:208:ASN:HA	1:D:214:ILE:HA	1.99	0.45
1:A:528:GLN:HG3	1:A:539:LEU:HD22	1.98	0.45
1:B:187:VAL:HA	6:B:909:HOH:O	2.16	0.45
1:E:46:SER:HB3	1:E:313:CYS:SG	2.57	0.45
1:E:90:VAL:HG13	1:E:292:ILE:HD11	1.99	0.45
1:A:166:LYS:N	1:A:166:LYS:HD3	2.32	0.45
1:B:90:VAL:HG13	1:B:292:ILE:HD11	1.98	0.45
1:C:74:ALA:O	1:C:78:LEU:HG	2.16	0.45
1:C:386:ILE:HG21	1:C:474:ILE:HD13	1.98	0.45
1:D:61:LEU:C	1:D:196:LYS:HB2	2.37	0.45
1:D:65:LYS:HD3	1:D:65:LYS:HA	1.67	0.45
1:D:76:VAL:HG22	1:D:214:ILE:HG23	1.99	0.44
1:D:338:ASP:HB2	1:D:342:TYR:OH	2.16	0.44
1:D:394:LYS:NZ	6:D:702:HOH:O	2.02	0.44
1:E:214:ILE:HG13	6:E:709:HOH:O	2.17	0.44
1:E:357:THR:OG1	6:E:705:HOH:O	2.20	0.44
1:E:507:ARG:O	1:E:511:GLU:HG3	2.17	0.44
1:F:338:ASP:HB2	1:F:342:TYR:OH	2.17	0.44
1:C:262:ASN:HA	1:C:271:LYS:HD3	1.99	0.44
1:D:157:VAL:O	1:D:163:GLU:HG3	2.16	0.44
2:H:19:ARG:NH2	2:H:79:TYR:CE1	2.83	0.44
1:A:240:ASN:HB3	1:A:243:VAL:O	2.18	0.44
1:A:520:ILE:HD11	1:D:522:GLU:HA	1.99	0.44
1:E:76:VAL:HG11	1:E:212:CYS:HB3	2.00	0.44
1:B:400:THR:HG22	1:B:402:VAL:HG13	1.99	0.44
1:E:279:GLN:HG3	1:F:241:ALA:HA	1.99	0.44
1:F:479:ASP:HB3	1:F:482:VAL:HG12	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:LEU:O	1:B:516:ILE:HG12	2.18	0.44
1:D:321:LEU:HD11	1:D:473:PRO:HB3	2.00	0.44
1:C:311:THR:HG22	2:L:1:GLN:HE22	1.81	0.44
1:D:240:ASN:HB3	1:D:243:VAL:O	2.17	0.44
2:L:10:GLY:N	2:L:108:GLN:O	2.51	0.44
2:I:51:ILE:HG23	2:I:71:ARG:HD3	1.99	0.43
1:A:261:ILE:HA	1:A:264:MET:SD	2.58	0.43
2:L:68:THR:OG1	2:L:81:GLN:HB3	2.17	0.43
1:C:398:SER:HA	1:C:485:SER:O	2.19	0.43
1:F:94:GLN:O	1:F:98:GLN:HG3	2.18	0.43
2:G:13:GLN:HG3	2:G:14:ALA:N	2.33	0.43
1:F:270:GLN:NE2	6:F:708:HOH:O	2.28	0.43
1:E:61:LEU:O	1:E:295:GLU:HB3	2.18	0.43
2:I:29:PHE:CE2	2:I:78:VAL:HG23	2.53	0.43
1:F:191:LYS:NZ	6:F:723:HOH:O	2.50	0.43
1:B:218:GLU:O	1:B:222:GLU:HG3	2.18	0.43
1:C:487:GLU:HB3	1:C:490:ALA:HB2	2.00	0.43
1:E:93:LEU:HD13	1:E:297:LEU:HD13	2.00	0.43
1:B:94:GLN:O	1:B:98:GLN:HG3	2.19	0.43
1:C:388:ASN:ND2	1:C:391:TYR:H	2.17	0.43
1:D:178:VAL:HG22	1:D:188:LEU:HD13	2.01	0.43
1:D:204:LEU:O	1:D:207:VAL:CG2	2.66	0.43
1:B:171:LEU:HD11	1:B:189:THR:HG22	2.01	0.43
1:F:204:LEU:O	1:F:207:VAL:HG22	2.19	0.43
2:I:64:GLN:HA	6:I:206:HOH:O	2.18	0.43
1:C:279:GLN:NE2	1:C:361:GLN:OE1	2.52	0.43
1:D:208:ASN:CB	1:D:213:SER:H	2.24	0.43
1:F:399:LYS:HG3	1:F:485:SER:HB3	2.00	0.43
1:C:64:ILE:HD11	1:C:199:ILE:CG2	2.41	0.42
1:F:46:SER:HB3	1:F:313:CYS:SG	2.59	0.42
2:K:102:TYR:HA	6:K:210:HOH:O	2.19	0.42
1:D:85:LYS:NZ	6:D:707:HOH:O	2.51	0.42
2:H:19:ARG:NH2	2:H:79:TYR:CD1	2.87	0.42
1:E:64:ILE:HG21	1:E:204:LEU:HD11	2.00	0.42
2:L:51:ILE:HG23	2:L:71:ARG:HD3	2.01	0.42
1:D:496:ASN:HB3	3:M:1:NAG:H81	2.01	0.42
1:E:88:ASN:O	1:E:92:GLU:HB2	2.18	0.42
2:K:1:GLN:OE1	2:K:27:GLN:NE2	2.52	0.42
1:A:206:ILE:HD11	1:A:219:THR:HG21	2.02	0.42
1:C:96:LEU:HD13	1:C:237:PHE:HB3	2.01	0.42
1:D:497:GLU:OE1	3:M:1:NAG:H83	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:ASN:ND2	6:F:727:HOH:O	2.53	0.42
2:L:1:GLN:O	2:L:3:GLN:NE2	2.52	0.42
2:J:55:GLY:O	2:J:57:LEU:HD12	2.20	0.42
1:B:338:ASP:HB2	1:B:342:TYR:OH	2.20	0.42
1:A:261:ILE:HD13	1:A:274:MET:HB3	2.01	0.42
1:D:313:CYS:HA	1:D:342:TYR:O	2.20	0.42
1:E:394:LYS:HE3	1:E:394:LYS:HB3	1.82	0.42
1:F:247:VAL:HG13	1:F:251:MET:HB2	2.02	0.41
1:B:249:THR:OG1	6:B:709:HOH:O	2.21	0.41
1:B:378:GLU:OE2	2:J:30:SER:OG	2.32	0.41
1:F:164:VAL:HG12	6:F:705:HOH:O	2.20	0.41
1:F:270:GLN:HG2	1:F:309:ILE:CD1	2.48	0.41
1:F:512:LEU:O	1:F:516:ILE:HG12	2.20	0.41
1:B:264:MET:N	6:B:708:HOH:O	2.53	0.41
1:B:264:MET:O	6:B:708:HOH:O	2.21	0.41
1:D:208:ASN:H	1:D:214:ILE:HG22	1.85	0.41
1:D:348:SER:HB2	1:D:375:LEU:O	2.20	0.41
1:D:400:THR:HG22	1:D:402:VAL:HG13	2.02	0.41
1:F:164:VAL:HA	1:F:167:ILE:HG12	2.02	0.41
2:K:22:CYS:HB3	2:K:78:VAL:HG13	2.01	0.41
2:H:71:ARG:HD2	2:H:78:VAL:HG22	2.02	0.41
1:E:352:PHE:CE2	1:E:372:SER:HB3	2.56	0.41
1:A:83:LEU:HG	1:A:87:LYS:HE2	2.02	0.41
1:B:386:ILE:HG21	1:B:474:ILE:HD13	2.02	0.41
1:C:352:PHE:CE2	1:C:367:CYS:HB3	2.55	0.41
1:C:388:ASN:HD21	1:C:391:TYR:H	1.69	0.41
1:D:352:PHE:CE2	1:D:372:SER:HB3	2.56	0.41
1:B:359:LYS:HB3	1:B:359:LYS:HE3	1.73	0.41
1:D:69:CYS:HB2	1:D:80:LYS:HZ2	1.85	0.41
1:D:87:LYS:O	1:D:91:THR:HG23	2.21	0.41
1:E:482:VAL:HG12	1:E:482:VAL:O	2.21	0.41
2:L:63:VAL:HB	2:L:67:PHE:CD1	2.55	0.41
1:D:60:GLU:HG2	1:D:196:LYS:HB3	2.02	0.41
1:E:240:ASN:HB3	1:E:243:VAL:O	2.21	0.41
2:I:40:ALA:HB1	2:I:41:PRO:HD2	2.03	0.41
2:J:22:CYS:HB3	2:J:78:VAL:HG13	2.03	0.41
2:H:56:ARG:HE	2:H:57:LEU:H	1.67	0.41
1:A:91:THR:O	1:A:95:LEU:HD13	2.21	0.41
1:D:164:VAL:HG13	1:D:165:ASN:N	2.35	0.41
1:E:160:LEU:HB2	1:E:163:GLU:HG3	2.03	0.41
1:E:195:LEU:HD23	1:E:195:LEU:HA	1.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:2:VAL:HB	2:K:27:GLN:HG3	2.02	0.40
1:C:522:GLU:HA	1:E:520:ILE:HD11	2.03	0.40
1:E:47:ALA:HB1	1:E:273:LEU:HD21	2.04	0.40
1:F:294:GLU:O	1:F:295:GLU:HG2	2.21	0.40
1:A:46:SER:HB3	1:A:313:CYS:SG	2.61	0.40
2:G:29:PHE:CE2	2:G:78:VAL:HG23	2.57	0.40
1:F:240:ASN:HB3	1:F:243:VAL:O	2.21	0.40
1:A:422:CYS:HB2	1:A:435:PHE:HB2	2.04	0.40
2:H:85:GLU:CD	2:H:85:GLU:H	2.25	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:964:HOH:O	6:E:900:HOH:O[1_556]	1.70	0.50
6:A:932:HOH:O	6:B:866:HOH:O[1_655]	1.86	0.34
6:A:824:HOH:O	6:B:978:HOH:O[1_655]	1.99	0.21
6:A:729:HOH:O	6:H:237:HOH:O[1_556]	2.02	0.18
6:A:783:HOH:O	6:F:865:HOH:O[1_456]	2.12	0.08
3:M:3:BMA:O3	6:B:1061:HOH:O[1_455]	2.12	0.08

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 X-ray entries followed by that with respect to entries of similar resolution.

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	485/500 (97%)	467 (96%)	18 (4%)	0	100	100
1	B	484/500 (97%)	469 (97%)	15 (3%)	0	100	100
1	C	485/500 (97%)	467 (96%)	18 (4%)	0	100	100
1	D	485/500 (97%)	460 (95%)	21 (4%)	4 (1%)	19	15
1	E	484/500 (97%)	466 (96%)	18 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	487/500 (97%)	468 (96%)	18 (4%)	1 (0%)	47 49
2	G	121/152 (80%)	119 (98%)	2 (2%)	0	100 100
2	H	121/152 (80%)	121 (100%)	0	0	100 100
2	I	121/152 (80%)	120 (99%)	1 (1%)	0	100 100
2	J	121/152 (80%)	118 (98%)	3 (2%)	0	100 100
2	K	119/152 (78%)	114 (96%)	5 (4%)	0	100 100
2	L	121/152 (80%)	119 (98%)	1 (1%)	1 (1%)	19 15
All	All	3634/3912 (93%)	3508 (96%)	120 (3%)	6 (0%)	47 49

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	72	THR
1	F	209	LYS
2	L	82(b)	SER
1	D	204	LEU
1	D	206	ILE
1	D	205	PRO

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 X-ray entries followed by that with respect to entries of similar resolution.

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	441/451 (98%)	437 (99%)	4 (1%)	78 84
1	B	441/451 (98%)	441 (100%)	0	100 100
1	C	442/451 (98%)	441 (100%)	1 (0%)	93 96
1	D	442/451 (98%)	440 (100%)	2 (0%)	88 92
1	E	441/451 (98%)	438 (99%)	3 (1%)	84 88
1	F	444/451 (98%)	442 (100%)	2 (0%)	88 92
2	G	93/117 (80%)	92 (99%)	1 (1%)	73 79
2	H	93/117 (80%)	93 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	I	93/117 (80%)	93 (100%)	0	100 100
2	J	93/117 (80%)	92 (99%)	1 (1%)	73 79
2	K	91/117 (78%)	91 (100%)	0	100 100
2	L	93/117 (80%)	93 (100%)	0	100 100
All	All	3207/3408 (94%)	3193 (100%)	14 (0%)	91 94

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	LEU
1	A	182	SER
1	A	457	TYR
1	A	488	PHE
2	G	56	ARG
1	C	201	LYS
1	D	208	ASN
1	D	462	GLN
1	E	328	GLU
1	E	330	SER
1	E	485	SER
1	F	87	LYS
1	F	552	GLN
2	J	27	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	159	HIS
1	A	501	GLN
1	B	268	ASN
1	B	270	GLN
1	B	462	GLN
1	C	388	ASN
1	D	361	GLN
1	E	361	GLN
1	F	27	ASN
1	F	165	ASN
1	F	197	ASN
1	F	254	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	283	GLN
1	F	361	GLN
1	F	501	GLN
2	I	27	GLN
2	K	27	GLN
2	L	3	GLN
2	H	27	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

3 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	$\#\|Z\| > 2$
3	NAG	M	1	3,1	14,14,15	0.41	0	17,19,21	0.65	0
3	NAG	M	2	3	14,14,15	0.78	0	17,19,21	0.94	1 (5%)
3	BMA	M	3	3	11,11,12	0.74	0	15,15,17	2.16	4 (26%)

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
3	NAG	M	1	3,1	-	1/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	M	2	3	-	3/6/23/26	0/1/1/1
3	BMA	M	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	3	BMA	O5-C1-C2	4.98	118.46	110.77
3	M	3	BMA	C1-O5-C5	4.42	118.19	112.19
3	M	3	BMA	C1-C2-C3	3.57	114.05	109.67
3	M	3	BMA	O2-C2-C3	-2.76	104.60	110.14
3	M	2	NAG	O4-C4-C3	-2.17	105.34	110.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

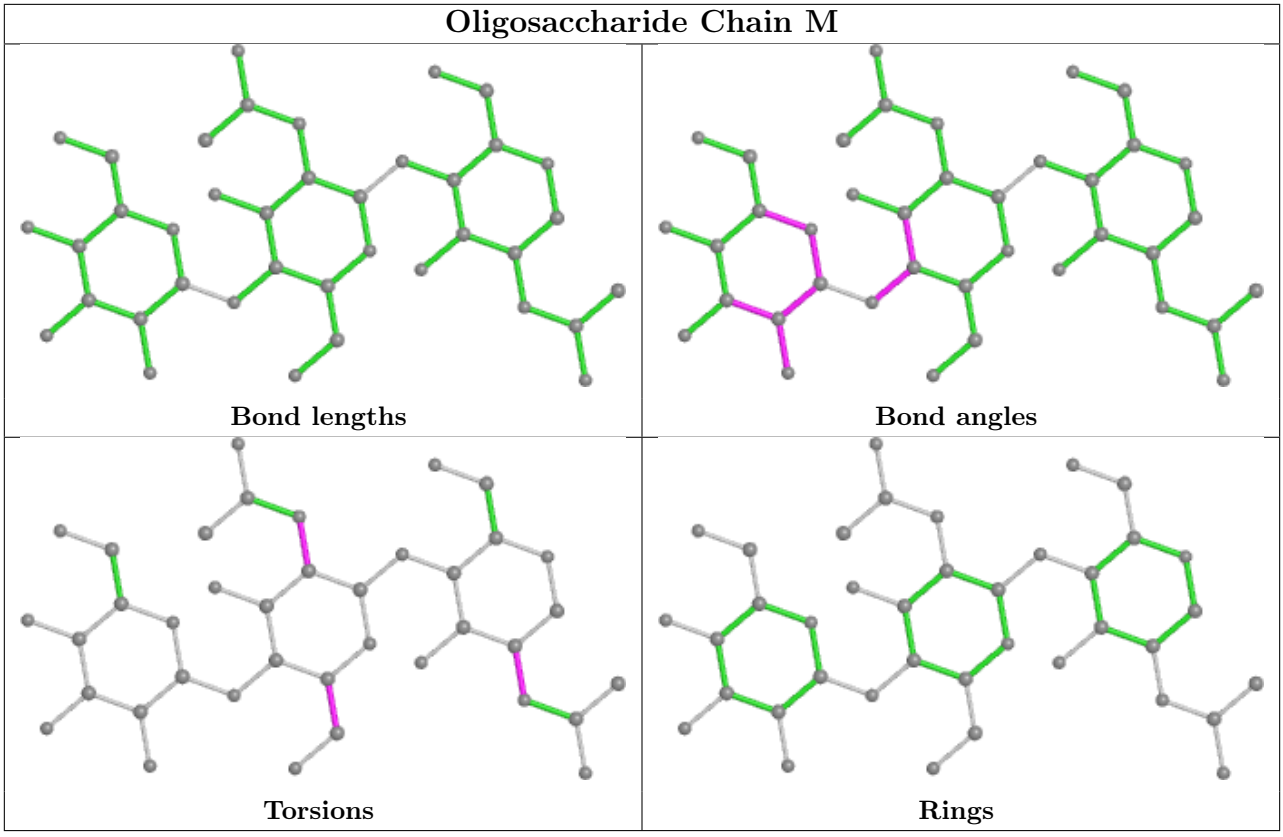
Mol	Chain	Res	Type	Atoms
3	M	2	NAG	O5-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
3	M	2	NAG	C1-C2-N2-C7
3	M	1	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	2	NAG	2	0
3	M	3	BMA	0	1
3	M	1	NAG	4	0

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



5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	F	601	1	14,14,15	0.82	1 (7%)	17,19,21	0.74	0
4	NAG	A	601	1	14,14,15	0.32	0	17,19,21	0.56	0
4	NAG	D	601	1	14,14,15	0.33	0	17,19,21	1.09	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	601	1	-	3/6/23/26	0/1/1/1
4	NAG	A	601	1	-	2/6/23/26	0/1/1/1
4	NAG	D	601	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	601	NAG	C1-C2	2.75	1.56	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	601	NAG	C2-N2-C7	2.56	126.54	122.90

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	601	NAG	C1-C2-N2-C7
4	F	601	NAG	C4-C5-C6-O6
4	A	601	NAG	C3-C2-N2-C7
4	D	601	NAG	C3-C2-N2-C7
4	A	601	NAG	C1-C2-N2-C7
4	F	601	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	489/500 (97%)	0.39	21 (4%)	35	41	18, 36, 60, 67	0
1	B	488/500 (97%)	0.06	11 (2%)	60	65	22, 35, 50, 54	0
1	C	489/500 (97%)	0.18	23 (4%)	31	37	27, 41, 67, 77	0
1	D	489/500 (97%)	0.36	29 (5%)	22	27	21, 39, 60, 76	0
1	E	488/500 (97%)	0.51	36 (7%)	14	18	21, 42, 80, 100	0
1	F	491/500 (98%)	0.44	34 (6%)	16	21	28, 44, 72, 94	0
2	G	123/152 (80%)	-0.21	1 (0%)	86	88	22, 36, 47, 53	0
2	H	123/152 (80%)	-0.10	4 (3%)	46	53	25, 39, 54, 66	0
2	I	123/152 (80%)	-0.11	2 (1%)	72	75	25, 40, 58, 68	0
2	J	123/152 (80%)	0.16	4 (3%)	46	53	25, 48, 71, 82	0
2	K	121/152 (79%)	1.54	44 (36%)	0	0	39, 74, 109, 127	0
2	L	123/152 (80%)	0.58	10 (8%)	12	15	35, 63, 98, 121	0
All	All	3670/3912 (93%)	0.32	219 (5%)	21	27	18, 41, 74, 127	0

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	206	ILE	7.6
2	K	11	LEU	7.6
2	K	18	LEU	6.7
1	E	64	ILE	6.5
1	E	67	ILE	6.0
1	E	210	GLN	5.8
1	E	65	LYS	5.8
1	E	212	CYS	5.6
2	K	82(c)	LEU	5.5
1	F	68	LYS	5.2
1	D	70	ASN	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	65	LYS	5.0
1	C	505	PHE	5.0
2	K	84	PRO	4.9
2	K	17	SER	4.9
1	A	172	LEU	4.9
1	A	65	LYS	4.9
2	K	67	PHE	4.8
1	C	204	LEU	4.7
1	C	209	LYS	4.5
2	K	111	VAL	4.5
2	I	41	PRO	4.5
1	F	65	LYS	4.5
2	K	82	MET	4.3
1	D	66	GLU	4.3
1	A	185	VAL	4.2
1	D	206	ILE	4.2
2	L	41	PRO	4.2
1	D	208	ASN	4.2
2	K	107	THR	4.2
1	B	65	LYS	4.1
1	D	213	SER	4.1
1	D	205	PRO	4.1
1	F	512	LEU	4.0
2	K	41	PRO	4.0
1	E	207	VAL	4.0
2	K	109	VAL	4.0
1	E	211	SER	4.0
2	L	13	GLN	4.0
1	A	64	ILE	4.0
1	C	64	ILE	4.0
1	D	69	CYS	4.0
1	E	161	GLU	3.9
1	F	516	ILE	3.9
2	K	40	ALA	3.8
1	F	551	PHE	3.8
1	D	326	THR	3.8
1	F	211	SER	3.8
2	L	40	ALA	3.8
1	E	167	ILE	3.7
1	A	66	GLU	3.7
1	D	204	LEU	3.7
1	C	206	ILE	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	212	CYS	3.7
1	E	185	VAL	3.6
1	D	211	SER	3.6
1	C	70	ASN	3.6
1	C	184	GLY	3.6
1	C	513	LEU	3.6
1	A	488	PHE	3.6
1	D	505	PHE	3.5
1	C	208	ASN	3.5
1	C	210	GLN	3.5
1	E	204	LEU	3.4
1	E	213	SER	3.4
1	F	513	LEU	3.4
2	K	12	VAL	3.4
2	K	85	GLU	3.4
1	B	488	PHE	3.3
1	F	262	ASN	3.3
2	J	56	ARG	3.3
1	F	101	PRO	3.3
2	K	10	GLY	3.3
1	D	506	ILE	3.3
1	D	65	LYS	3.3
1	D	183	ASN	3.3
2	K	42	GLY	3.3
1	D	516	ILE	3.3
1	D	207	VAL	3.3
1	E	516	ILE	3.2
1	A	68	LYS	3.2
1	C	66	GLU	3.2
2	K	13	GLN	3.2
2	K	110	THR	3.2
2	K	57	LEU	3.2
1	E	181	LEU	3.2
2	K	68	THR	3.2
1	E	69	CYS	3.1
1	F	265	PRO	3.1
1	F	515	ALA	3.1
1	E	209	LYS	3.1
1	C	68	LYS	3.1
1	C	67	ILE	3.1
1	F	507	ARG	3.1
1	B	481	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	K	88	ALA	3.0
1	E	201	LYS	3.0
1	E	72	THR	3.0
1	F	210	GLN	3.0
1	C	212	CYS	3.0
1	F	172	LEU	3.0
1	E	205	PRO	3.0
2	K	81	GLN	3.0
2	L	18	LEU	3.0
1	E	70	ASN	3.0
2	H	42	GLY	3.0
1	B	516	ILE	2.9
1	A	328	GLU	2.9
2	L	10	GLY	2.9
1	F	206	ILE	2.9
2	K	9	GLY	2.9
1	E	186	SER	2.9
1	F	212	CYS	2.9
2	K	63	VAL	2.9
1	A	161	GLU	2.9
1	A	164	VAL	2.9
2	J	12	VAL	2.8
1	A	67	ILE	2.8
1	F	181	LEU	2.8
1	F	273	LEU	2.8
1	F	100	THR	2.8
2	K	90	TYR	2.8
1	C	98	GLN	2.8
1	C	207	VAL	2.8
1	D	507	ARG	2.8
1	E	66	GLU	2.8
1	A	99	SER	2.8
1	F	514	SER	2.8
1	C	205	PRO	2.7
1	D	551	PHE	2.7
1	E	68	LYS	2.7
1	D	172	LEU	2.7
1	D	513	LEU	2.7
2	K	20	LEU	2.7
2	K	64	GLN	2.7
1	E	208	ASN	2.7
1	A	206	ILE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	56	ARG	2.7
1	F	173	SER	2.6
1	F	511	GLU	2.6
1	A	186	SER	2.6
1	C	72	THR	2.6
1	C	71	GLY	2.5
1	F	505	PHE	2.5
1	D	186	SER	2.5
2	K	8	GLY	2.5
2	K	54	GLY	2.5
1	F	488	PHE	2.5
1	B	512	LEU	2.5
2	I	42	GLY	2.5
2	J	82(c)	LEU	2.5
1	A	167	ILE	2.5
1	F	167	ILE	2.5
1	F	174	THR	2.4
2	K	65	GLY	2.4
2	K	58	TYR	2.4
2	G	42	GLY	2.4
2	K	55	GLY	2.4
2	K	79	TYR	2.4
1	E	74	ALA	2.4
1	E	214	ILE	2.4
1	F	67	ILE	2.4
2	L	44	GLU	2.4
1	A	162	GLY	2.4
1	B	551	PHE	2.3
1	B	328	GLU	2.3
1	F	481	LEU	2.3
2	K	83	LYS	2.3
2	K	43	LYS	2.3
1	E	164	VAL	2.3
1	B	265	PRO	2.3
1	F	205	PRO	2.3
1	D	210	GLN	2.3
1	B	164	VAL	2.3
1	C	552	GLN	2.3
2	K	69	ILE	2.3
1	D	508	LYS	2.2
1	F	176	LYS	2.2
2	H	113	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	111	VAL	2.2
2	L	91	TYR	2.2
1	F	508	LYS	2.2
1	D	488	PHE	2.2
1	D	98	GLN	2.2
2	L	43	LYS	2.2
1	D	64	ILE	2.2
1	A	262	ASN	2.2
1	D	552	GLN	2.1
1	A	512	LEU	2.1
1	E	488	PHE	2.1
1	A	173	SER	2.1
2	J	64	GLN	2.1
2	H	56	ARG	2.1
1	B	266	ILE	2.1
2	K	14	ALA	2.1
2	H	41	PRO	2.1
1	E	63	ASN	2.1
1	F	327	LYS	2.1
2	K	108	GLN	2.1
2	K	16	GLY	2.1
2	K	89	VAL	2.1
1	C	99	SER	2.1
2	K	62	SER	2.1
2	K	56	ARG	2.1
1	E	203	LEU	2.1
1	F	66	GLU	2.1
1	E	176	LYS	2.1
1	D	67	ILE	2.1
1	E	183	ASN	2.1
1	A	174	THR	2.1
2	K	87	THR	2.1
1	B	142	LEU	2.0
1	C	507	ARG	2.0
1	E	215	PRO	2.0
1	E	513	LEU	2.0
1	E	457	TYR	2.0
2	K	92	CYS	2.0
1	F	550	LEU	2.0
1	A	37	CYS	2.0

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

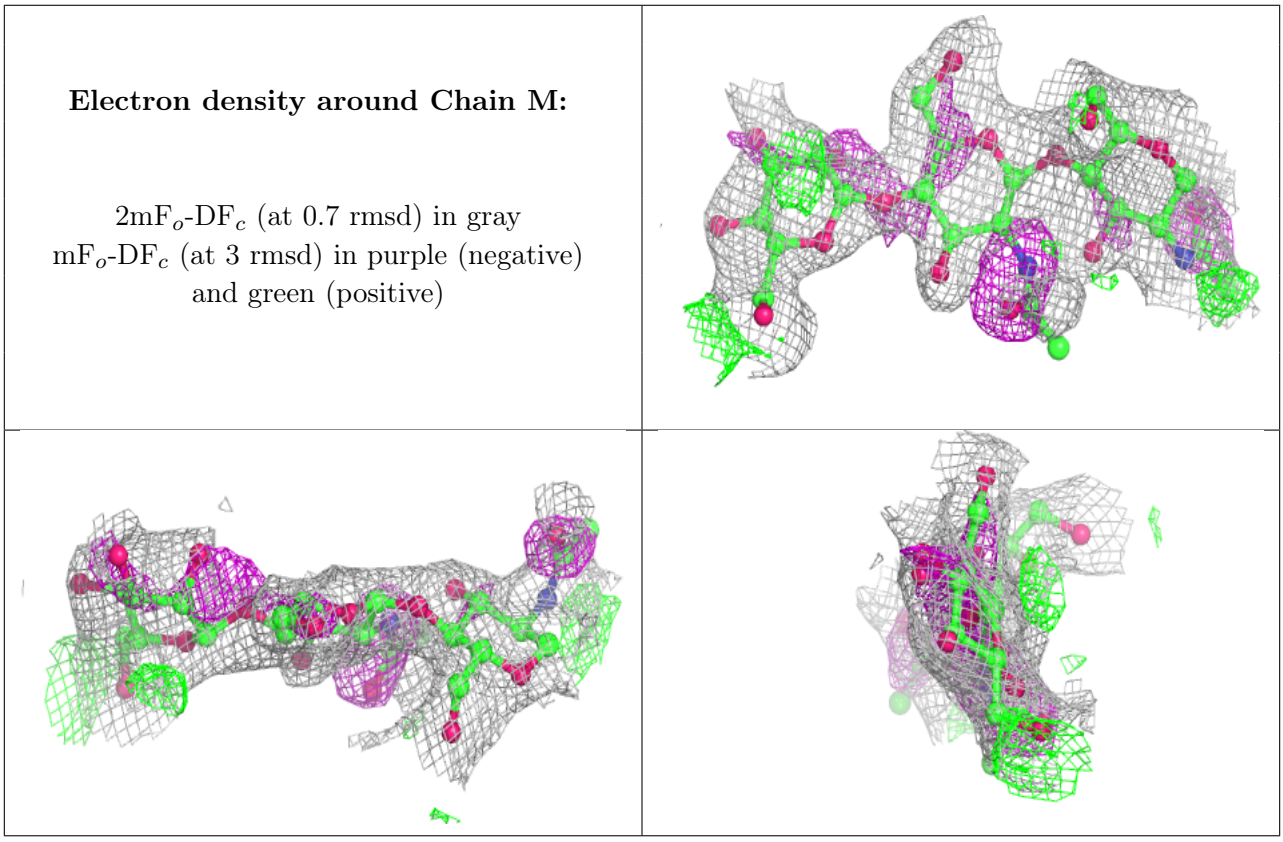
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	M	2	14/15	0.66	0.32	54,55,58,59	0
3	NAG	M	1	14/15	0.79	0.23	53,54,55,55	0
3	BMA	M	3	11/12	0.80	0.21	51,53,55,55	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	F	601	14/15	0.75	0.36	57,59,61,61	0
4	NAG	A	601	14/15	0.76	0.34	67,69,70,71	0
4	NAG	D	601	14/15	0.86	0.25	51,53,56,56	0
5	CL	A	603	1/1	0.99	0.12	24,24,24,24	0
5	CL	E	601	1/1	0.99	0.10	28,28,28,28	0
5	CL	E	602	1/1	0.99	0.18	39,39,39,39	0
5	CL	A	602	1/1	1.00	0.12	28,28,28,28	0
5	CL	B	601	1/1	1.00	0.16	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.