wwPDB X-ray Structure Validation Summary Report (i)

Jun 25, 2024 – 07:07 AM EDT

PDB ID	:	5VOB
Title	:	Crystal structure of HCMV Pentamer in complex with neutralizing antibody 8I21
Authors	:	Malito, E.; Chandramouli, S.
Deposited on	:	2017-05-02
Resolution	:	3.02 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/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 (i)) were used in the production of this report:

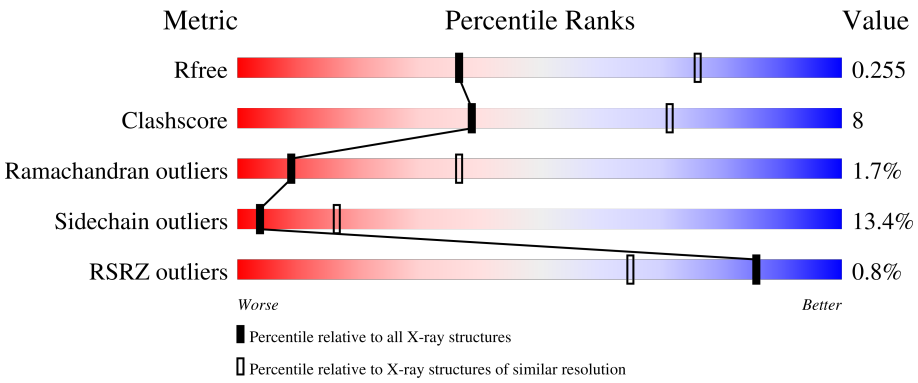
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.02 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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	725	.% 66% 22% • 8%
2	B	278	.% 63% 19% • 15%
3	C	171	2% 56% 20% • 21%
4	D	252	48% 15% • 33%
5	E	129	61% 20% • 16%

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Mol	Chain	Length	Quality of chain
6	H	289	% 62% 13% • 23%
7	L	235	65% 20% 5% 9%
8	F	3	33% 67%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	NAG	B	301	-	-	-	X
9	NAG	D	303	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 14099 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 Envelope glycoprotein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	667	5358	3427	910	996	25	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	716	GLY	-	expression tag	UNP Q6SW67
A	717	SER	-	expression tag	UNP Q6SW67
A	718	GLY	-	expression tag	UNP Q6SW67
A	719	SER	-	expression tag	UNP Q6SW67
A	720	HIS	-	expression tag	UNP Q6SW67
A	721	HIS	-	expression tag	UNP Q6SW67
A	722	HIS	-	expression tag	UNP Q6SW67
A	723	HIS	-	expression tag	UNP Q6SW67
A	724	HIS	-	expression tag	UNP Q6SW67
A	725	HIS	-	expression tag	UNP Q6SW67

- Molecule 2 is a protein called Envelope glycoprotein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	237	1867	1188	326	345	8	0	0	0

- Molecule 3 is a protein called Envelope glycoprotein UL128.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	135	1090	683	197	199	11	0	0	0

- Molecule 4 is a protein called Envelope glycoprotein UL130.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	170	1388	887	243	250	8	0	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	215	GLY	-	expression tag	UNP F5HCP3
D	216	SER	-	expression tag	UNP F5HCP3
D	217	GLU	-	expression tag	UNP F5HCP3
D	218	ASN	-	expression tag	UNP F5HCP3
D	219	LEU	-	expression tag	UNP F5HCP3
D	220	TYR	-	expression tag	UNP F5HCP3
D	221	PHE	-	expression tag	UNP F5HCP3
D	222	GLN	-	expression tag	UNP F5HCP3
D	223	ALA	-	expression tag	UNP F5HCP3
D	224	GLY	-	expression tag	UNP F5HCP3
D	225	TRP	-	expression tag	UNP F5HCP3
D	226	SER	-	expression tag	UNP F5HCP3
D	227	HIS	-	expression tag	UNP F5HCP3
D	228	PRO	-	expression tag	UNP F5HCP3
D	229	GLN	-	expression tag	UNP F5HCP3
D	230	PHE	-	expression tag	UNP F5HCP3
D	231	GLU	-	expression tag	UNP F5HCP3
D	232	LYS	-	expression tag	UNP F5HCP3
D	233	GLY	-	expression tag	UNP F5HCP3
D	234	GLY	-	expression tag	UNP F5HCP3
D	235	GLY	-	expression tag	UNP F5HCP3
D	236	SER	-	expression tag	UNP F5HCP3
D	237	GLY	-	expression tag	UNP F5HCP3
D	238	GLY	-	expression tag	UNP F5HCP3
D	239	GLY	-	expression tag	UNP F5HCP3
D	240	SER	-	expression tag	UNP F5HCP3
D	241	GLY	-	expression tag	UNP F5HCP3
D	242	GLY	-	expression tag	UNP F5HCP3
D	243	GLY	-	expression tag	UNP F5HCP3
D	244	SER	-	expression tag	UNP F5HCP3
D	245	TRP	-	expression tag	UNP F5HCP3
D	246	SER	-	expression tag	UNP F5HCP3
D	247	HIS	-	expression tag	UNP F5HCP3
D	248	PRO	-	expression tag	UNP F5HCP3
D	249	GLN	-	expression tag	UNP F5HCP3
D	250	PHE	-	expression tag	UNP F5HCP3
D	251	GLU	-	expression tag	UNP F5HCP3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	252	LYS	-	expression tag	UNP F5HCP3

- Molecule 5 is a protein called Envelope glycoprotein UL131A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	108	893	557	168	166	2	0	0	0

- Molecule 6 is a protein called Fab 8I21 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	H	222	1680	1061	288	324	7	0	0	0

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	228	SER	-	expression tag	UNP S6B291
H	229	SER	-	expression tag	UNP S6B291
H	230	GLY	-	expression tag	UNP S6B291
H	231	LEU	-	expression tag	UNP S6B291
H	232	GLU	-	expression tag	UNP S6B291
H	233	VAL	-	expression tag	UNP S6B291
H	234	LEU	-	expression tag	UNP S6B291
H	235	PHE	-	expression tag	UNP S6B291
H	236	GLN	-	expression tag	UNP S6B291
H	237	GLY	-	expression tag	UNP S6B291
H	238	PRO	-	expression tag	UNP S6B291
H	239	LEU	-	expression tag	UNP S6B291
H	240	GLY	-	expression tag	UNP S6B291
H	241	SER	-	expression tag	UNP S6B291
H	242	ALA	-	expression tag	UNP S6B291
H	243	TRP	-	expression tag	UNP S6B291
H	244	SER	-	expression tag	UNP S6B291
H	245	HIS	-	expression tag	UNP S6B291
H	246	PRO	-	expression tag	UNP S6B291
H	247	GLN	-	expression tag	UNP S6B291
H	248	PHE	-	expression tag	UNP S6B291
H	249	GLU	-	expression tag	UNP S6B291
H	250	LYS	-	expression tag	UNP S6B291
H	251	GLY	-	expression tag	UNP S6B291
H	252	GLY	-	expression tag	UNP S6B291

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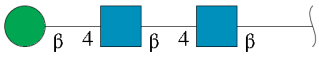
Chain	Residue	Modelled	Actual	Comment	Reference
H	253	GLY	-	expression tag	UNP S6B291
H	254	SER	-	expression tag	UNP S6B291
H	255	GLY	-	expression tag	UNP S6B291
H	256	GLY	-	expression tag	UNP S6B291
H	257	GLY	-	expression tag	UNP S6B291
H	258	SER	-	expression tag	UNP S6B291
H	259	GLY	-	expression tag	UNP S6B291
H	260	GLY	-	expression tag	UNP S6B291
H	261	GLY	-	expression tag	UNP S6B291
H	262	SER	-	expression tag	UNP S6B291
H	263	TRP	-	expression tag	UNP S6B291
H	264	SER	-	expression tag	UNP S6B291
H	265	HIS	-	expression tag	UNP S6B291
H	266	PRO	-	expression tag	UNP S6B291
H	267	GLN	-	expression tag	UNP S6B291
H	268	PHE	-	expression tag	UNP S6B291
H	269	GLU	-	expression tag	UNP S6B291
H	270	LYS	-	expression tag	UNP S6B291

- Molecule 7 is a protein called Fab 8I21 light chain.

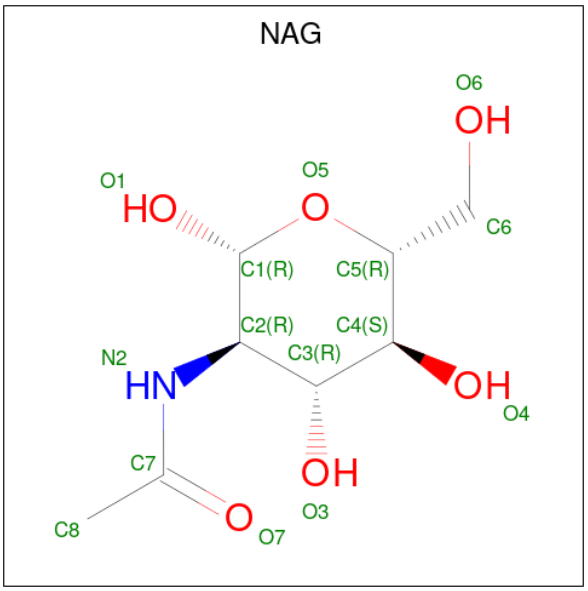
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	L	214	1644	1031	279	329	5	0	0	0

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



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

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



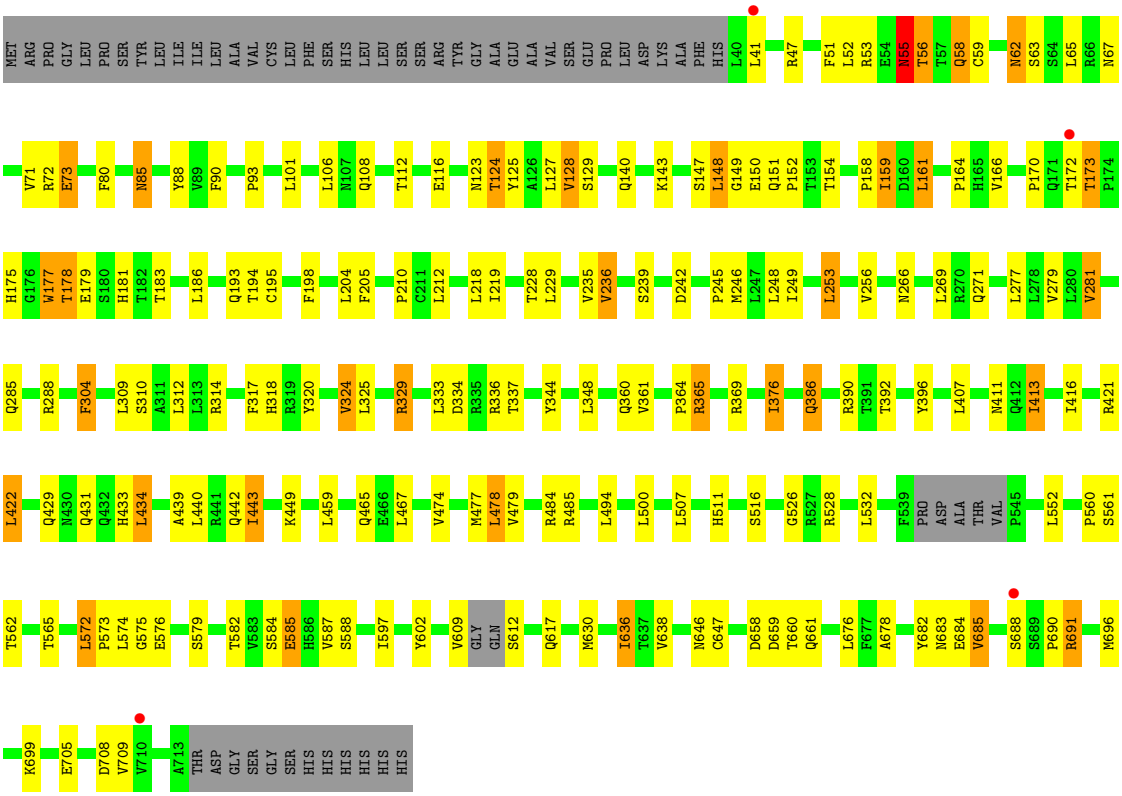
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	A	1	14	8	1	5	0	0
			Total	C	N	O		
9	A	1	14	8	1	5	0	0
			Total	C	N	O		
9	A	1	14	8	1	5	0	0
			Total	C	N	O		
9	A	1	14	8	1	5	0	0
			Total	C	N	O		
9	A	1	14	8	1	5	0	0
			Total	C	N	O		
9	A	1	14	8	1	5	0	0
			Total	C	N	O		
9	B	1	14	8	1	5	0	0
			Total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

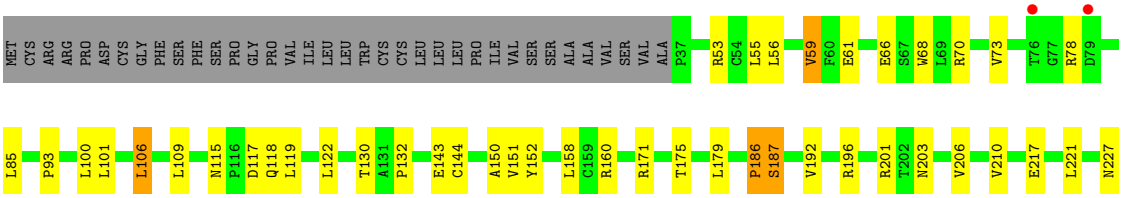
- Molecule 1: Envelope glycoprotein H

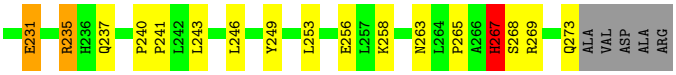
Chain A:



- Molecule 2: Envelope glycoprotein L

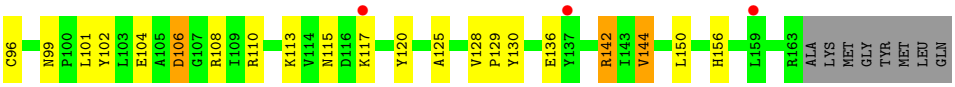
Chain B:





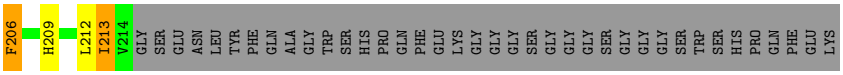
• Molecule 3: Envelope glycoprotein UL128

Chain C:



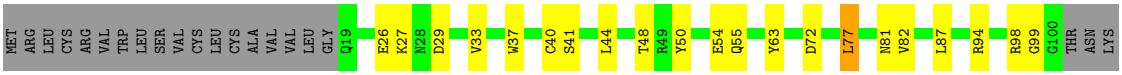
• Molecule 4: Envelope glycoprotein UL130

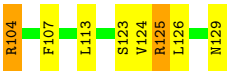
Chain D:



• Molecule 5: Envelope glycoprotein UL131A

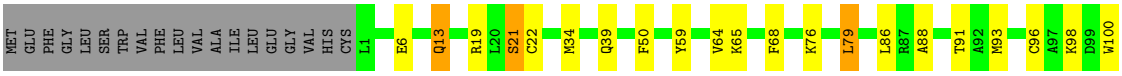
Chain E:

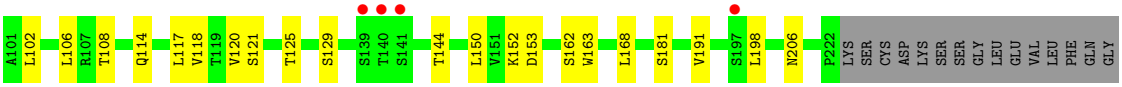


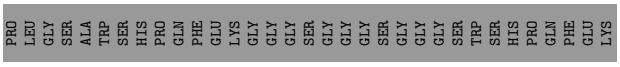


• Molecule 6: Fab 8I21 heavy chain

Chain H:







• Molecule 7: Fab 8I21 light chain

Chain L:

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

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	124.16Å 145.42Å 173.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.35 – 3.02 49.35 – 3.02	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.35-3.02) 99.5 (49.35-3.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.28	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.190 , 0.237 0.208 , 0.255	Depositor DCC
R_{free} test set	3167 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	88.5	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 60.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14099	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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 (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.50	0/5484	0.75	1/7473 (0.0%)
2	B	0.51	0/1913	0.72	0/2612
3	C	0.50	0/1112	0.75	0/1503
4	D	0.54	1/1427 (0.1%)	0.79	1/1939 (0.1%)
5	E	0.45	0/912	0.65	0/1233
6	H	0.45	0/1724	0.70	0/2348
7	L	0.48	0/1683	0.72	0/2289
All	All	0.49	1/14255 (0.0%)	0.73	2/19397 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	118	ASN	CG-ND2	-6.20	1.17	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	136	ASN	C-N-CA	6.31	137.47	121.70
1	A	179	GLU	C-N-CA	5.09	134.42	121.70

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	5358	0	5306	104	0
2	B	1867	0	1858	34	0
3	C	1090	0	1075	17	0
4	D	1388	0	1359	29	0
5	E	893	0	851	12	0
6	H	1680	0	1636	15	0
7	L	1644	0	1588	28	0
8	F	39	0	34	1	0
9	A	84	0	78	0	0
9	B	14	0	13	0	0
9	D	42	0	39	0	0
All	All	14099	0	13837	210	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 210 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:A:159:ILE:CD1	1:A:159:ILE:CG1	1.77	1.58
7:L:94:TRP:HB3	7:L:95:PRO:HD3	1.26	1.16
7:L:13:VAL:HG11	7:L:78:LEU:HD13	1.35	1.06
7:L:94:TRP:HB3	7:L:95:PRO:CD	1.93	0.93
2:B:144:CYS:HB3	3:C:144:VAL:HG11	1.63	0.78

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 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	661/725 (91%)	604 (91%)	41 (6%)	16 (2%)	6 28
2	B	235/278 (84%)	214 (91%)	18 (8%)	3 (1%)	12 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	133/171 (78%)	109 (82%)	20 (15%)	4 (3%)	4	22
4	D	168/252 (67%)	160 (95%)	7 (4%)	1 (1%)	25	62
5	E	104/129 (81%)	99 (95%)	4 (4%)	1 (1%)	15	50
6	H	220/289 (76%)	200 (91%)	19 (9%)	1 (0%)	29	66
7	L	212/235 (90%)	199 (94%)	9 (4%)	4 (2%)	8	34
All	All	1733/2079 (83%)	1585 (92%)	118 (7%)	30 (2%)	9	37

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	THR
1	A	170	PRO
1	A	178	THR
3	C	30	CYS
6	H	153	ASP

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	607/655 (93%)	530 (87%)	77 (13%)	4	18
2	B	204/238 (86%)	177 (87%)	27 (13%)	4	17
3	C	122/154 (79%)	105 (86%)	17 (14%)	3	15
4	D	156/222 (70%)	136 (87%)	20 (13%)	4	18
5	E	95/114 (83%)	80 (84%)	15 (16%)	2	12
6	H	188/239 (79%)	169 (90%)	19 (10%)	7	27
7	L	183/202 (91%)	150 (82%)	33 (18%)	1	8
All	All	1555/1824 (85%)	1347 (87%)	208 (13%)	4	16

5 of 208 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	115	ASN
5	E	33	VAL
7	L	169	SER
3	C	150	LEU
4	D	157	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	617	GLN
7	L	27	GLN
2	B	273	GLN
6	H	13	GLN
2	B	203	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	$\#\|Z\| > 2$
8	NAG	F	1	5,8	14,14,15	0.43	0	17,19,21	1.37	2 (11%)
8	NAG	F	2	8	14,14,15	0.43	0	17,19,21	1.52	3 (17%)
8	BMA	F	3	8	11,11,12	0.44	0	15,15,17	0.68	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
8	NAG	F	1	5,8	-	0/6/23/26	0/1/1/1
8	NAG	F	2	8	-	0/6/23/26	0/1/1/1
8	BMA	F	3	8	-	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})
8	F	1	NAG	C1-O5-C5	4.54	118.34	112.19
8	F	2	NAG	O5-C1-C2	-4.34	104.43	111.29
8	F	2	NAG	C1-C2-N2	3.27	116.08	110.49
8	F	1	NAG	O5-C1-C2	-2.86	106.77	111.29
8	F	2	NAG	C1-O5-C5	2.54	115.64	112.19

There are no chirality outliers.

There are no torsion outliers.

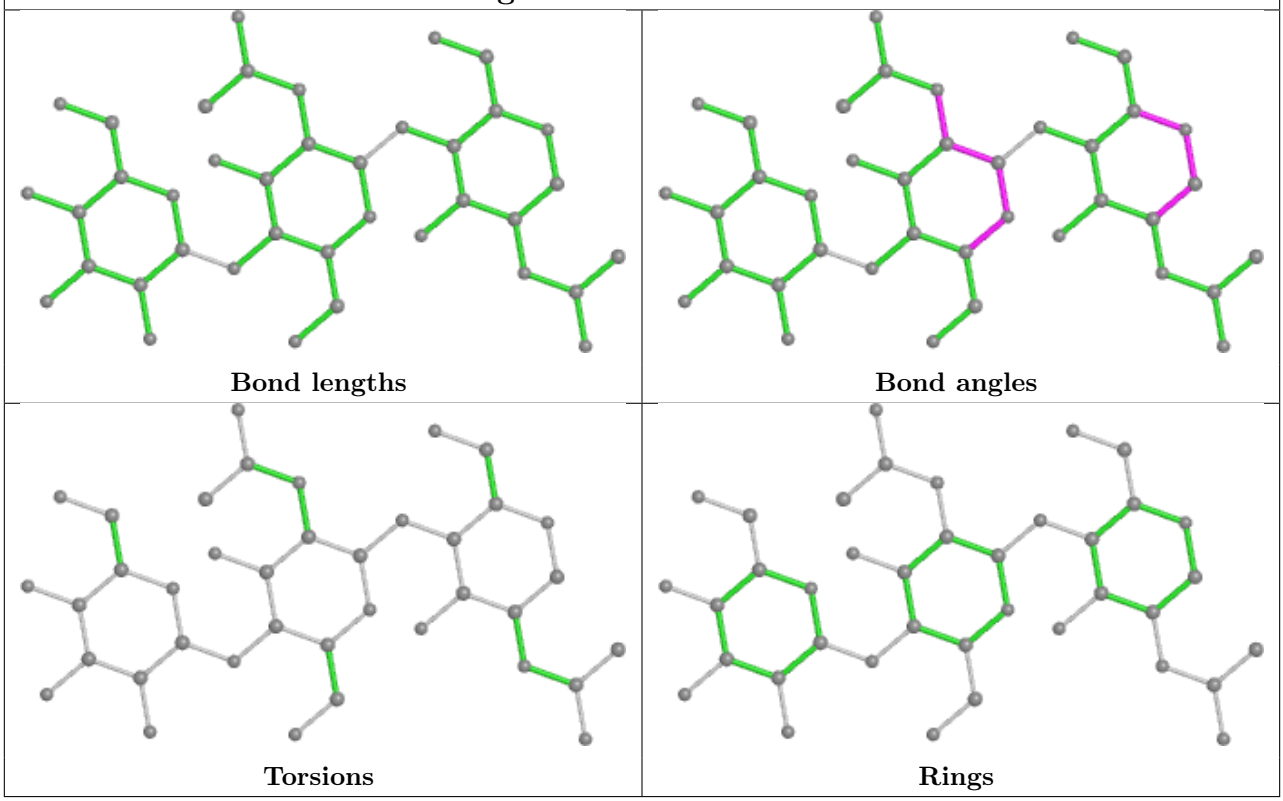
There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	2	NAG	1	0
8	F	1	NAG	1	0

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

Oligosaccharide Chain F



5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	NAG	A	804	1	14,14,15	0.29	0	17,19,21	0.72	1 (5%)
9	NAG	A	802	1	14,14,15	0.35	0	17,19,21	0.47	0
9	NAG	A	805	1	14,14,15	0.36	0	17,19,21	2.19	3 (17%)
9	NAG	A	801	1	14,14,15	0.28	0	17,19,21	2.28	2 (11%)
9	NAG	B	301	2	14,14,15	0.44	0	17,19,21	1.80	2 (11%)
9	NAG	D	301	4	14,14,15	0.31	0	17,19,21	0.75	0
9	NAG	D	303	4	14,14,15	0.31	0	17,19,21	0.74	1 (5%)
9	NAG	A	806	1	14,14,15	0.33	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	NAG	A	803	1	14,14,15	0.34	0	17,19,21	0.61	0
9	NAG	D	302	4	14,14,15	0.33	0	17,19,21	0.57	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	A	804	1	-	0/6/23/26	0/1/1/1
9	NAG	A	802	1	-	0/6/23/26	0/1/1/1
9	NAG	A	805	1	-	1/6/23/26	0/1/1/1
9	NAG	A	801	1	-	0/6/23/26	0/1/1/1
9	NAG	B	301	2	-	0/6/23/26	0/1/1/1
9	NAG	D	301	4	-	0/6/23/26	0/1/1/1
9	NAG	D	303	4	-	0/6/23/26	0/1/1/1
9	NAG	A	806	1	-	1/6/23/26	0/1/1/1
9	NAG	A	803	1	-	1/6/23/26	0/1/1/1
9	NAG	D	302	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	801	NAG	C1-O5-C5	8.01	123.04	112.19
9	A	805	NAG	C1-O5-C5	6.53	121.04	112.19
9	B	301	NAG	C1-O5-C5	6.27	120.69	112.19
9	A	805	NAG	O5-C1-C2	5.49	119.96	111.29
9	A	801	NAG	O5-C1-C2	4.32	118.12	111.29

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	806	NAG	O5-C5-C6-O6
9	A	805	NAG	C3-C2-N2-C7
9	A	803	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 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	667/725 (92%)	-0.18	4 (0%)	89	72	63, 91, 123, 150	0
2	B	237/278 (85%)	-0.20	2 (0%)	86	65	65, 93, 138, 151	0
3	C	135/171 (78%)	0.08	3 (2%)	62	32	63, 97, 132, 149	2 (1%)
4	D	170/252 (67%)	-0.25	1 (0%)	89	72	55, 73, 106, 138	0
5	E	108/129 (83%)	-0.01	0	100	100	58, 91, 130, 137	0
6	H	222/289 (76%)	-0.16	4 (1%)	68	39	58, 91, 133, 163	0
7	L	214/235 (91%)	-0.15	0	100	100	54, 92, 136, 157	0
All	All	1753/2079 (84%)	-0.15	14 (0%)	86	65	54, 90, 132, 163	2 (0%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	H	139	SER	5.5
4	D	133	SER	4.2
3	C	137	TYR	3.8
1	A	688	SER	3.7
6	H	141	SER	3.2

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)

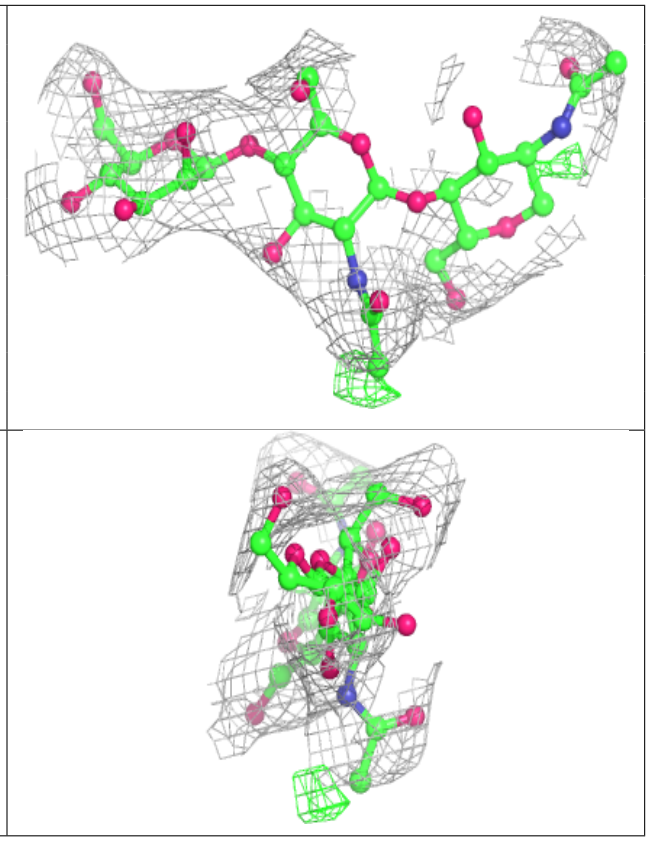
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	BMA	F	3	11/12	0.70	0.26	149,152,153,154	0
8	NAG	F	2	14/15	0.89	0.19	131,137,143,148	0
8	NAG	F	1	14/15	0.89	0.13	113,116,127,130	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.

Electron density around Chain F:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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, 95th 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
9	NAG	A	806	14/15	0.72	0.37	174,177,178,178	0
9	NAG	B	301	14/15	0.73	0.71	182,185,186,186	0
9	NAG	D	303	14/15	0.78	0.46	135,138,141,141	0
9	NAG	A	802	14/15	0.84	0.20	146,151,152,153	0
9	NAG	A	803	14/15	0.84	0.27	149,151,154,154	0
9	NAG	A	805	14/15	0.84	0.18	161,165,168,169	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	NAG	D	302	14/15	0.88	0.16	112,114,116,117	0
9	NAG	A	801	14/15	0.92	0.14	104,116,118,119	0
9	NAG	D	301	14/15	0.93	0.21	76,82,91,94	0
9	NAG	A	804	14/15	0.94	0.15	90,94,97,100	0

6.5 Other polymers (i)

There are no such residues in this entry.