



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 09:24 PM BST

PDB ID : 6H3U
Title : Schmallenberg Virus Glycoprotein Gc Head Domain in Complex with scFv 4B6
Authors : Hellert, J.; Aebischer, A.; Wernike, K.; Haouz, A.; Brocchi, E.; Reiche, S.; Guardado-Calvo, P.; Beer, M.; Rey, F.A.
Deposited on : 2018-07-19
Resolution : 3.17 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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	:	2.13.1
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)	:	2.13.1

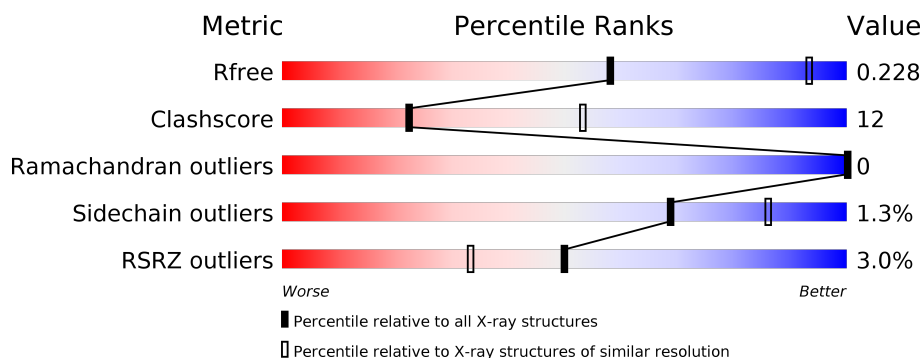
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.17 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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 on 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 $\leq 5\%$. 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	H	142	<div> <div>63%</div> <div>23%</div> <div>15%</div> </div>
1	I	142	<div> <div>58%</div> <div>27%</div> <div>14%</div> </div>
2	L	117	<div> <div>72%</div> <div>25%</div> <div>3%</div> </div>
2	M	117	<div> <div>13%</div> <div>68%</div> <div>23%</div> <div>9%</div> </div>
3	A	248	<div> <div>2%</div> <div>69%</div> <div>29%</div> <div>2%</div> </div>
3	B	248	<div> <div>3%</div> <div>71%</div> <div>27%</div> <div>1%</div> </div>

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Mol	Chain	Length	Quality of chain
4	C	7	<div><div></div><div>14%71%14%</div></div>
4	E	7	<div><div></div><div>14%86%</div></div>
5	D	3	<div><div></div><div>100%</div></div>
5	F	3	<div><div></div><div>33%67%</div></div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7813 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 scFv 4B6 VH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	121	Total	C	N	O	S	0	0	0
			970	620	155	191	4			
1	I	122	Total	C	N	O	S	0	0	0
			976	623	156	193	4			

- Molecule 2 is a protein called scFv 4B6 VL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	113	Total	C	N	O	S	0	0	0
			871	551	140	177	3			
2	M	107	Total	C	N	O	S	0	0	0
			826	522	131	170	3			

- Molecule 3 is a protein called Envelopment polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	246	Total	C	N	O	S	0	0	0
			1969	1244	337	374	14			
3	B	245	Total	C	N	O	S	0	0	0
			1959	1238	335	372	14			

There are 20 discrepancies between the modelled and reference sequences:

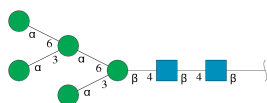
Chain	Residue	Modelled	Actual	Comment	Reference
A	703	GLY	-	expression tag	UNP H2AM12
A	704	GLY	-	expression tag	UNP H2AM12
A	705	TRP	-	expression tag	UNP H2AM12
A	706	SER	-	expression tag	UNP H2AM12
A	707	HIS	-	expression tag	UNP H2AM12
A	708	PRO	-	expression tag	UNP H2AM12
A	709	GLN	-	expression tag	UNP H2AM12
A	710	PHE	-	expression tag	UNP H2AM12

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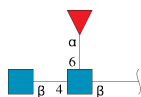
Chain	Residue	Modelled	Actual	Comment	Reference
A	711	GLU	-	expression tag	UNP H2AM12
A	712	LYS	-	expression tag	UNP H2AM12
B	703	GLY	-	expression tag	UNP H2AM12
B	704	GLY	-	expression tag	UNP H2AM12
B	705	TRP	-	expression tag	UNP H2AM12
B	706	SER	-	expression tag	UNP H2AM12
B	707	HIS	-	expression tag	UNP H2AM12
B	708	PRO	-	expression tag	UNP H2AM12
B	709	GLN	-	expression tag	UNP H2AM12
B	710	PHE	-	expression tag	UNP H2AM12
B	711	GLU	-	expression tag	UNP H2AM12
B	712	LYS	-	expression tag	UNP H2AM12

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	E	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

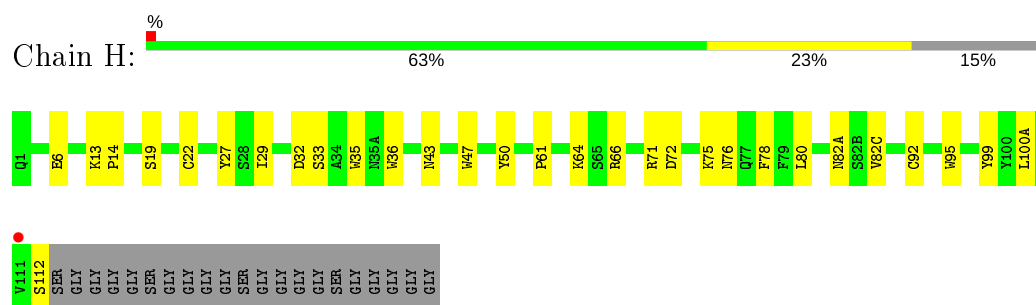


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	D	3	Total	C	N	O	0	0	0
			38	22	2	14			
5	F	3	Total	C	N	O	0	0	0
			38	22	2	14			

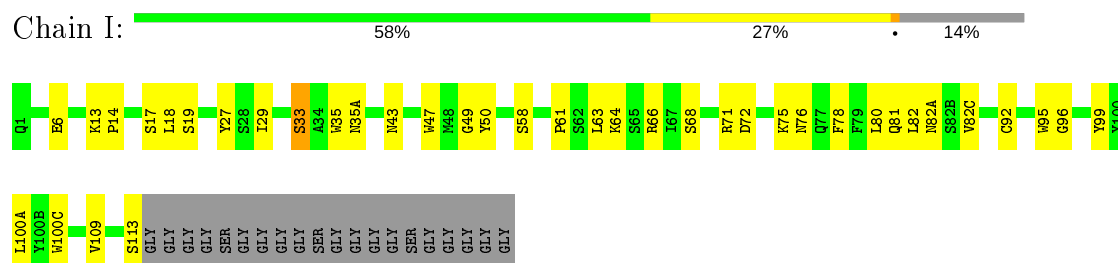
3 Residue-property plots

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.

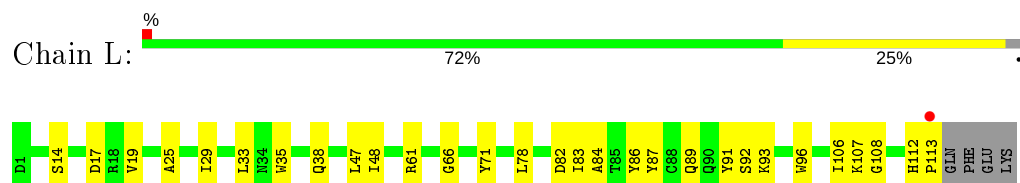
- Molecule 1: scFv 4B6 VH



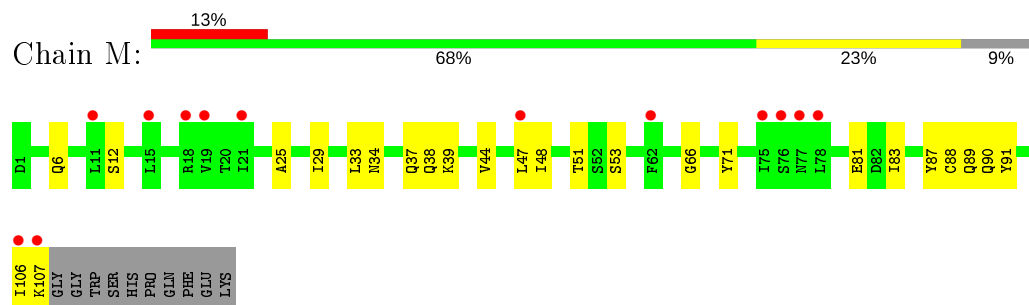
- Molecule 1: scFv 4B6 VH



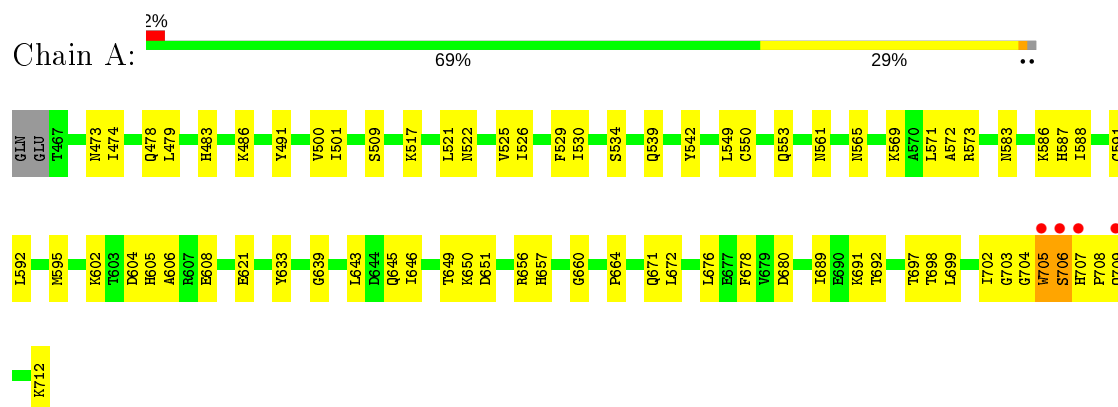
- Molecule 2: scFv 4B6 VL



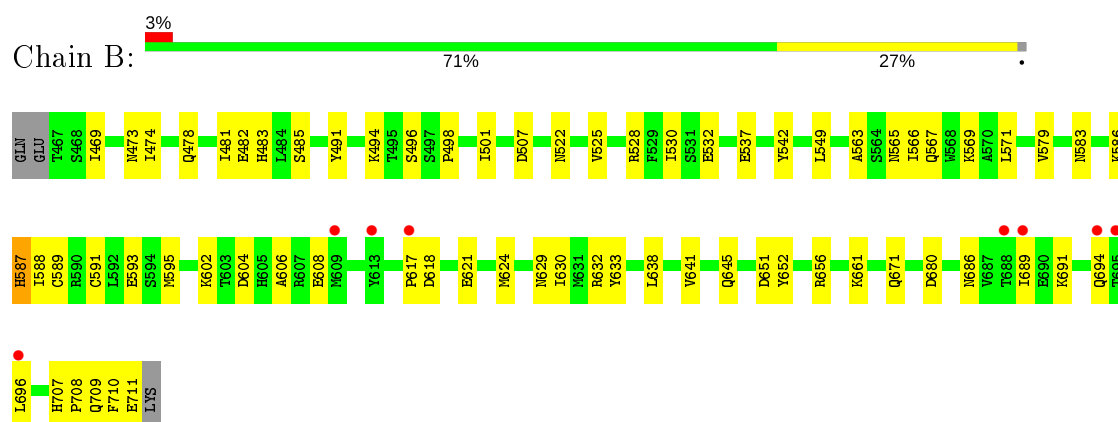
- Molecule 2: scFv 4B6 VL



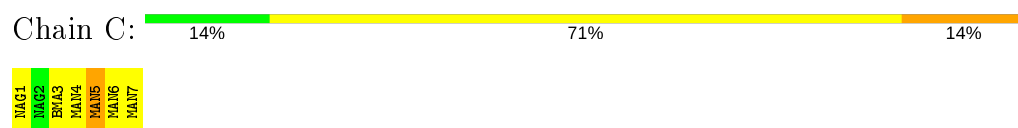
- Molecule 3: Envelopment polypeptide



- Molecule 3: Envelopment polypeptide



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



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



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2
FUC3

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 

MAG1
MAG2
FUC3

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	175.84Å 175.84Å 153.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.55 – 3.17 48.55 – 3.17	Depositor EDS
% Data completeness (in resolution range)	59.0 (48.55-3.17) 59.0 (48.55-3.17)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.200 , 0.228 0.200 , 0.228	Depositor DCC
R_{free} test set	1984 reflections (7.15%)	wwPDB-VP
Wilson B-factor (Å ²)	108.5	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 86.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7813	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: FUC, BMA, NAG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	H	0.27	0/999	0.55	1/1364 (0.1%)
1	I	0.26	0/1005	0.55	0/1372
2	L	0.25	0/894	0.51	0/1216
2	M	0.26	0/845	0.50	0/1148
3	A	0.27	0/2006	0.46	0/2712
3	B	0.27	0/1996	0.45	0/2701
All	All	0.27	0/7745	0.49	1/10513 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	H	32	ASP	C-N-CA	5.08	134.41	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	H	970	0	913	21	0
1	I	976	0	918	32	0
2	L	871	0	831	20	0
2	M	826	0	796	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1969	0	1966	55	0
3	B	1959	0	1953	44	0
4	C	83	0	70	2	0
4	E	83	0	70	1	0
5	D	38	0	34	0	0
5	F	38	0	34	1	0
All	All	7813	0	7585	179	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 12.

The worst 5 of 179 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:494:LYS:NZ	3:B:496:SER:O	2.08	0.84
3:B:567:GLN:HB3	3:B:633:TYR:HD2	1.43	0.82
3:B:583:ASN:HB3	3:B:586:LYS:HE2	1.66	0.77
3:A:649:THR:HG23	3:A:651:ASP:H	1.49	0.76
2:M:39:LYS:NZ	2:M:81:GLU:O	2.16	0.76

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	H	119/142 (84%)	112 (94%)	7 (6%)	0	100	100
1	I	120/142 (84%)	112 (93%)	8 (7%)	0	100	100
2	L	111/117 (95%)	107 (96%)	4 (4%)	0	100	100
2	M	105/117 (90%)	102 (97%)	3 (3%)	0	100	100
3	A	244/248 (98%)	237 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	243/248 (98%)	235 (97%)	8 (3%)	0	100	100
All	All	942/1014 (93%)	905 (96%)	37 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	H	108/112 (96%)	106 (98%)	2 (2%)	57	80
1	I	109/112 (97%)	107 (98%)	2 (2%)	59	81
2	L	98/102 (96%)	98 (100%)	0	100	100
2	M	94/102 (92%)	94 (100%)	0	100	100
3	A	229/231 (99%)	225 (98%)	4 (2%)	60	82
3	B	228/231 (99%)	225 (99%)	3 (1%)	69	86
All	All	866/890 (97%)	855 (99%)	11 (1%)	69	86

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	705	TRP
3	A	706	SER
3	B	671	GLN
3	A	698	THR
3	B	588	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	561	ASN
3	A	671	GLN
3	A	707	HIS

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Mol	Chain	Res	Type
3	B	587	HIS

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 ⓘ

20 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$
4	NAG	C	1	3,4	14,14,15	0.28	0	17,19,21	0.41	0
4	NAG	C	2	4	14,14,15	0.20	0	17,19,21	0.45	0
4	BMA	C	3	4	11,11,12	0.79	0	15,15,17	0.99	1 (6%)
4	MAN	C	4	4	11,11,12	0.65	0	15,15,17	1.02	2 (13%)
4	MAN	C	5	4	11,11,12	0.70	0	15,15,17	0.96	2 (13%)
4	MAN	C	6	4	11,11,12	0.95	1 (9%)	15,15,17	1.26	2 (13%)
4	MAN	C	7	4	11,11,12	0.98	1 (9%)	15,15,17	0.98	2 (13%)
5	NAG	D	1	3,5	14,14,15	0.59	1 (7%)	17,19,21	0.61	0
5	NAG	D	2	5	14,14,15	0.28	0	17,19,21	0.60	1 (5%)
5	FUC	D	3	5	10,10,11	0.99	1 (10%)	14,14,16	1.10	1 (7%)
4	NAG	E	1	3,4	14,14,15	0.24	0	17,19,21	0.40	0
4	NAG	E	2	4	14,14,15	0.21	0	17,19,21	0.49	0
4	BMA	E	3	4	11,11,12	0.90	0	15,15,17	1.08	1 (6%)
4	MAN	E	4	4	11,11,12	0.84	1 (9%)	15,15,17	1.22	2 (13%)
4	MAN	E	5	4	11,11,12	1.04	0	15,15,17	1.00	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	E	6	4	11,11,12	1.17	1 (9%)	15,15,17	1.61	4 (26%)
4	MAN	E	7	4	11,11,12	0.93	1 (9%)	15,15,17	0.98	2 (13%)
5	NAG	F	1	3,5	14,14,15	0.31	0	17,19,21	0.45	0
5	NAG	F	2	5	14,14,15	0.30	0	17,19,21	0.39	0
5	FUC	F	3	5	10,10,11	1.14	1 (10%)	14,14,16	1.40	2 (14%)

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	C	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	4/6/23/26	0/1/1/1
4	BMA	C	3	4	-	2/2/19/22	0/1/1/1
4	MAN	C	4	4	-	0/2/19/22	0/1/1/1
4	MAN	C	5	4	-	2/2/19/22	0/1/1/1
4	MAN	C	6	4	-	2/2/19/22	0/1/1/1
4	MAN	C	7	4	-	1/2/19/22	1/1/1/1
5	NAG	D	1	3,5	-	1/6/23/26	0/1/1/1
5	NAG	D	2	5	-	1/6/23/26	0/1/1/1
5	FUC	D	3	5	-	-	0/1/1/1
4	NAG	E	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	2/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
4	MAN	E	5	4	-	2/2/19/22	0/1/1/1
4	MAN	E	6	4	-	2/2/19/22	0/1/1/1
4	MAN	E	7	4	-	1/2/19/22	1/1/1/1
5	NAG	F	1	3,5	-	4/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1
5	FUC	F	3	5	-	-	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	6	MAN	C1-C2	3.40	1.60	1.52
5	F	3	FUC	C1-C2	3.02	1.59	1.52
4	C	6	MAN	C1-C2	2.61	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	3	FUC	C1-C2	2.52	1.57	1.52
4	E	4	MAN	C1-C2	2.49	1.57	1.52

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	6	MAN	C1-O5-C5	3.38	116.78	112.19
4	E	6	MAN	C1-C2-C3	3.35	113.78	109.67
5	F	3	FUC	C1-C2-C3	3.29	113.71	109.67
4	E	4	MAN	C1-O5-C5	3.16	116.48	112.19
4	E	3	BMA	C1-C2-C3	2.81	113.12	109.67

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	3	BMA	O5-C5-C6-O6
4	C	2	NAG	O5-C5-C6-O6
4	E	5	MAN	O5-C5-C6-O6
4	C	3	BMA	O5-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	7	MAN	C1-C2-C3-C4-C5-O5
4	C	7	MAN	C1-C2-C3-C4-C5-O5

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	5	MAN	1	0
4	E	1	NAG	1	0
4	C	1	NAG	1	0
5	F	1	NAG	1	0

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	H	121/142 (85%)	0.05	1 (0%) 86 78	69, 105, 145, 167	0
1	I	122/142 (85%)	-0.07	0 100 100	84, 113, 158, 170	0
2	L	113/117 (96%)	-0.01	1 (0%) 84 75	62, 94, 139, 199	0
2	M	107/117 (91%)	0.57	15 (14%) 2 1	104, 144, 189, 209	0
3	A	246/248 (99%)	-0.01	4 (1%) 72 59	58, 99, 140, 178	0
3	B	245/248 (98%)	0.15	8 (3%) 46 29	62, 109, 171, 213	0
All	All	954/1014 (94%)	0.10	29 (3%) 50 33	58, 107, 165, 213	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	695	THR	8.7
3	A	707	HIS	5.2
3	A	705	TRP	4.6
2	M	106	ILE	4.1
3	B	613	TYR	4.0

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, 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(\AA^2)	Q<0.9
5	NAG	F	1	14/15	0.72	0.35	191,219,229,236	0
4	MAN	E	6	11/12	0.75	0.32	156,176,189,194	0
4	MAN	E	7	11/12	0.77	0.18	178,187,207,210	0
5	FUC	D	3	10/11	0.80	0.54	159,200,206,207	0
5	NAG	F	2	14/15	0.80	0.43	198,236,240,240	0
4	MAN	C	7	11/12	0.81	0.14	150,175,184,188	0
5	FUC	F	3	10/11	0.88	0.43	193,220,230,239	0
4	MAN	C	5	11/12	0.88	0.22	103,132,152,161	0
4	MAN	C	6	11/12	0.88	0.12	118,147,160,166	0
5	NAG	D	1	14/15	0.89	0.33	161,181,205,207	0
5	NAG	D	2	14/15	0.90	0.50	188,216,225,226	0
4	BMA	C	3	11/12	0.92	0.20	136,146,165,176	0
4	BMA	E	3	11/12	0.93	0.23	151,158,177,180	0
4	MAN	C	4	11/12	0.93	0.15	111,126,146,146	0
4	NAG	E	2	14/15	0.94	0.22	93,125,149,156	0
4	NAG	C	2	14/15	0.94	0.21	97,123,137,139	0
4	MAN	E	5	11/12	0.94	0.24	92,138,151,152	0
4	MAN	E	4	11/12	0.95	0.26	122,147,170,171	0
4	NAG	E	1	14/15	0.96	0.16	97,106,121,124	0
4	NAG	C	1	14/15	0.98	0.13	94,112,123,133	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.