



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 12:48 PM BST

PDB ID : 6H3T
Title : Schmallenberg Virus Glycoprotein Gc Head Domain in Complex with scFv 1C11
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 : 2.84 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 ⓘ 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

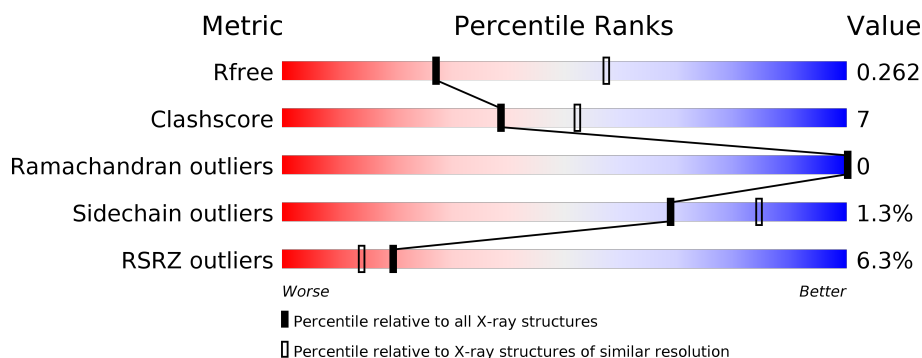
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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.




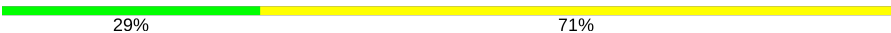


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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	140	<div> <div>4%</div> <div> <div></div> <div>68%</div> <div>16%</div> <div>16%</div> </div> </div>
1	I	140	<div> <div>19%</div> <div> <div></div> <div>67%</div> <div>17%</div> <div>16%</div> </div> </div>
2	L	123	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>18%</div> <div>8%</div> </div> </div>
2	M	123	<div> <div>16%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>8%</div> </div> </div>
3	A	248	<div> <div></div> <div> <div></div> <div>74%</div> <div>19%</div> <div>7%</div> </div> </div>
3	B	248	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	C	7	 29%71%
4	E	7	 29%71%
5	D	3	 100%
5	F	3	 67%33%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7524 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 1C11 VH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	118	Total	C	N	O	S	0	0	0
			923	586	150	181	6			
1	I	118	Total	C	N	O	S	0	0	0
			923	586	150	181	6			

- Molecule 2 is a protein called scFv 1C11 VL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	113	Total	C	N	O	S	0	0	0
			870	554	139	173	4			
2	M	113	Total	C	N	O	S	0	0	0
			870	554	139	173	4			

- Molecule 3 is a protein called Envelopment polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	230	Total	C	N	O	S	0	0	0
			1841	1161	316	350	14			
3	B	232	Total	C	N	O	S	0	0	0
			1855	1169	318	354	14			

There are 20 discrepancies between the modelled and reference sequences:

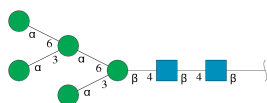
Chain	Residue	Modelled	Actual	Comment	Reference
A	703	GLY	-	expression tag	UNP H2AM12
A	704	GLY	-	expression tag	UNP H2AM12
A	705	TRP	-	expression tag	UNP H2AM12
A	706	SER	-	expression tag	UNP H2AM12
A	707	HIS	-	expression tag	UNP H2AM12
A	708	PRO	-	expression tag	UNP H2AM12
A	709	GLN	-	expression tag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

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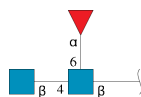
Chain	Residue	Modelled	Actual	Comment	Reference
A	711	GLU	-	expression tag	UNP H2AM12
A	712	LYS	-	expression tag	UNP H2AM12
B	703	GLY	-	expression tag	UNP H2AM12
B	704	GLY	-	expression tag	UNP H2AM12
B	705	TRP	-	expression tag	UNP H2AM12
B	706	SER	-	expression tag	UNP H2AM12
B	707	HIS	-	expression tag	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.



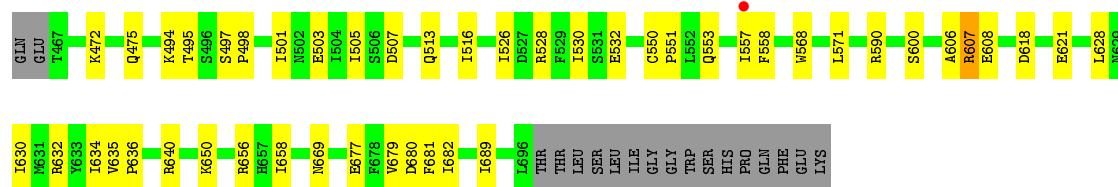
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	E	7	Total	C	N	O	0	0	0
			83	46	2	35			

- 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.



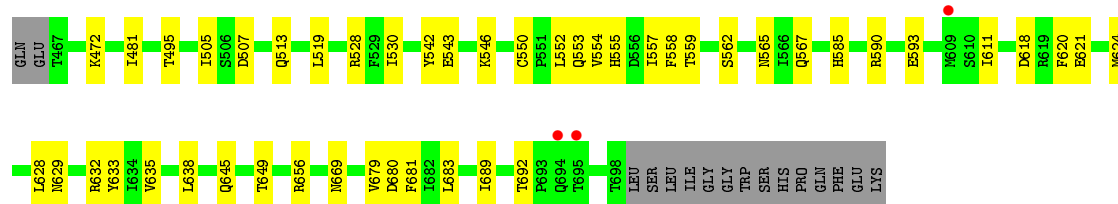
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	D	3	Total	C	N	O	0	0	0
			38	22	2	14			
5	F	3	Total	C	N	O	0	0	0
			38	22	2	14			

Chain A: 



- Molecule 3: Envelopment polypeptide

Chain B: 

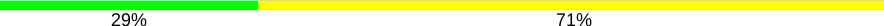


- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 



- 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

Chain E: 



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

Chain D: 



- 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: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	262.79 Å 44.40 Å 93.59 Å 90.00° 91.81° 90.00°	Depositor
Resolution (Å)	46.77 – 2.84 46.77 – 2.84	Depositor EDS
% Data completeness (in resolution range)	63.9 (46.77-2.84) 63.9 (46.77-2.84)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.86 Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.213 , 0.262 0.213 , 0.262	Depositor DCC
R_{free} test set	1684 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å ²)	80.7	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7524	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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	0.29	0/948	0.47	0/1285
1	I	0.28	0/948	0.47	0/1285
2	L	0.31	0/890	0.54	0/1206
2	M	0.26	0/890	0.48	0/1206
3	A	0.32	0/1873	0.47	0/2532
3	B	0.29	0/1887	0.47	0/2552
All	All	0.29	0/7436	0.48	0/10066

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	923	0	878	14	0
1	I	923	0	878	16	0
2	L	870	0	853	13	0
2	M	870	0	853	11	0
3	A	1841	0	1843	29	0
3	B	1855	0	1857	32	0
4	C	83	0	70	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	83	0	70	0	0
5	D	38	0	34	3	0
5	F	38	0	34	1	0
All	All	7524	0	7370	111	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 7.

All (111) 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:656:ARG:NH1	3:B:680:ASP:OD1	1.97	0.97
2:L:39:LYS:NZ	2:L:81:GLU:O	2.19	0.74
3:B:472:LYS:NZ	3:B:507:ASP:OD1	2.21	0.73
3:A:472:LYS:NZ	3:A:507:ASP:OD1	2.21	0.73
3:A:505:ILE:O	3:A:513:GLN:NE2	2.22	0.71
2:L:92:TYR:OH	3:A:590:ARG:NH2	2.23	0.71
2:L:83:LEU:HD12	2:L:104:LEU:O	1.92	0.69
1:H:53:TYR:O	5:D:3:FUC:O3	2.11	0.68
1:I:33:ASN:HA	1:I:52(A):PRO:HD3	1.76	0.66
2:M:92:TYR:OH	3:B:590:ARG:NH2	2.30	0.65
3:A:568:TRP:HE1	3:A:630:ILE:HG22	1.62	0.64
3:A:656:ARG:NH1	3:A:680:ASP:OD1	2.31	0.64
3:B:543:GLU:HG3	3:B:638:LEU:HB2	1.79	0.63
1:I:52(A):PRO:O	1:I:73:LYS:NZ	2.31	0.63
3:B:620:PHE:O	3:B:624:MET:HB2	2.00	0.61
2:L:83:LEU:CD1	2:L:105:GLU:HA	2.31	0.61
2:M:93:SER:HA	3:B:585:HIS:HB3	1.83	0.60
1:I:68:THR:HB	1:I:81:HIS:HB3	1.85	0.58
1:I:54:ASN:ND2	3:B:611:ILE:O	2.37	0.57
1:I:17:SER:HA	1:I:82:LEU:O	2.06	0.56
3:B:505:ILE:O	3:B:513:GLN:NE2	2.39	0.55
1:H:59:TYR:HE1	1:H:69:LEU:HG	1.72	0.55
3:A:590:ARG:HA	3:A:590:ARG:HH11	1.72	0.54
5:D:2:NAG:H3	5:D:2:NAG:H83	1.90	0.54
2:M:42:GLN:HG2	2:M:43:SER:H	1.72	0.53
3:B:495:THR:HG22	3:B:555:HIS:CG	2.44	0.53
3:A:621:GLU:OE1	3:A:650:LYS:NZ	2.35	0.53
3:B:590:ARG:NH1	3:B:593:GLU:OE1	2.41	0.53
3:B:530:ILE:HD13	3:B:543:GLU:HG2	1.91	0.52
3:B:481:ILE:HD11	3:B:645:GLN:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:33:ASN:HA	1:H:52(A):PRO:HD3	1.89	0.52
3:B:618:ASP:OD1	3:B:618:ASP:N	2.42	0.52
1:I:38:LYS:HB2	1:I:48:ILE:HD11	1.92	0.51
2:L:19:VAL:HG12	2:L:75:ILE:HB	1.91	0.51
1:I:53:TYR:O	5:F:3:FUC:O3	2.21	0.51
3:B:557:ILE:HG23	3:B:558:PHE:CD1	2.46	0.51
3:A:494:LYS:HE3	3:A:497:SER:HB2	1.94	0.50
3:A:600:SER:O	3:A:677:GLU:HG2	2.12	0.50
3:A:557:ILE:HG23	3:A:558:PHE:CD1	2.47	0.49
1:I:83:THR:OG1	1:I:84:SER:N	2.45	0.49
3:B:628:LEU:O	3:B:632:ARG:HB2	2.12	0.49
3:A:607:ARG:NH2	3:A:608:GLU:HG2	2.27	0.49
3:A:550:CYS:HB3	3:A:553:GLN:HG3	1.94	0.48
3:B:550:CYS:HB3	3:B:553:GLN:HG3	1.95	0.48
3:B:546:LYS:HE2	3:B:554:VAL:HG22	1.95	0.48
3:A:606:ALA:HA	3:A:681:PHE:CE1	2.48	0.48
1:I:94:ARG:NH2	1:I:101:ASP:OD2	2.29	0.48
1:H:38:LYS:HB2	1:H:48:ILE:HD11	1.94	0.48
1:I:20:VAL:O	1:I:79:PHE:HA	2.14	0.48
3:A:568:TRP:NE1	3:A:630:ILE:HG22	2.27	0.47
1:H:50:TYR:CE1	1:H:58:SER:HB3	2.50	0.47
3:A:618:ASP:N	3:A:618:ASP:OD1	2.48	0.47
1:I:32:TYR:CE2	1:I:96:TYR:HB2	2.50	0.47
2:L:63:THR:O	2:L:73:LEU:HD12	2.15	0.47
2:M:34:ALA:HB2	2:M:91:TYR:HE2	1.80	0.47
3:B:621:GLU:OE2	3:B:689:ILE:HD11	2.16	0.46
1:H:59:TYR:HB2	1:H:64:LYS:HG2	1.96	0.46
3:A:526:ILE:O	3:A:530:ILE:HG13	2.16	0.46
1:H:52(A):PRO:O	1:H:73:LYS:HE2	2.15	0.46
2:L:32:TYR:HD2	2:L:91:TYR:HD1	1.64	0.46
3:A:501:ILE:HD11	3:A:516:ILE:HG22	1.97	0.46
1:I:52:ASP:HB3	1:I:54:ASN:HB2	1.98	0.45
2:L:83:LEU:HD13	2:L:105:GLU:HA	1.97	0.45
3:B:567:GLN:OE1	3:B:633:TYR:OH	2.34	0.45
1:H:3:GLN:HB3	1:H:25:SER:OG	2.17	0.45
3:A:498:PRO:HB3	3:A:551:PRO:CD	2.46	0.45
3:A:634:ILE:HG22	3:A:635:VAL:HG13	1.99	0.44
3:B:528:ARG:HA	3:B:528:ARG:HD2	1.80	0.44
3:B:590:ARG:HD3	3:B:590:ARG:HA	1.79	0.44
3:B:565:ASN:HD21	3:B:669:ASN:HD21	1.65	0.44
3:A:475:GLN:HA	3:A:475:GLN:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:42:GLN:HG2	2:L:43:SER:H	1.83	0.44
3:B:565:ASN:HD21	3:B:669:ASN:ND2	2.16	0.44
3:B:559:THR:HB	3:B:562:SER:OG	2.18	0.44
1:I:32:TYR:CD2	1:I:96:TYR:HB2	2.52	0.44
2:M:27(B):LEU:HD12	2:M:71:PHE:CE2	2.52	0.44
2:M:63:THR:O	2:M:73:LEU:HD12	2.18	0.44
1:H:47:TRP:CE3	2:L:96:PRO:HD2	2.52	0.44
1:H:47:TRP:CZ3	1:H:49:GLY:HA2	2.53	0.44
2:L:21:MET:HG2	2:L:102:THR:HG21	1.99	0.43
2:L:7:ALA:HB2	2:L:22:SER:HB2	2.00	0.43
3:A:628:LEU:O	3:A:632:ARG:HB2	2.18	0.43
2:M:19:VAL:HG12	2:M:75:ILE:HB	2.00	0.43
3:B:519:LEU:HD11	3:B:542:TYR:OH	2.19	0.42
3:A:505:ILE:HD12	3:A:513:GLN:HA	2.01	0.42
3:B:635:VAL:O	3:B:635:VAL:HG23	2.19	0.42
3:A:632:ARG:HG3	3:A:640:ARG:HG3	2.01	0.42
1:I:30:THR:HB	1:I:53:TYR:HD2	1.84	0.42
2:M:12:ALA:HA	2:M:105:GLU:HB2	2.00	0.42
3:B:543:GLU:OE1	3:B:546:LYS:HD3	2.19	0.42
1:I:51:ILE:HB	1:I:57:THR:HG22	2.02	0.42
5:D:1:NAG:H61	5:D:2:NAG:O5	2.19	0.42
1:H:51:ILE:HD11	1:H:71:VAL:HG22	2.02	0.41
3:A:498:PRO:HB3	3:A:551:PRO:HD2	2.02	0.41
3:A:590:ARG:HA	3:A:590:ARG:HD3	1.68	0.41
1:H:94:ARG:NH2	1:H:101:ASP:OD2	2.37	0.41
2:M:21:MET:HG2	2:M:102:THR:HG21	2.02	0.41
3:B:649:THR:HA	3:B:692:THR:OG1	2.19	0.41
2:L:27(B):LEU:HD12	2:L:71:PHE:CE2	2.56	0.41
2:M:27(B):LEU:HD12	2:M:71:PHE:HE2	1.84	0.41
3:A:528:ARG:O	3:A:532:GLU:HG2	2.21	0.41
1:H:81:HIS:HE1	1:H:82(A):ASN:HB3	1.85	0.41
3:B:552:LEU:H	3:B:552:LEU:HD23	1.85	0.41
2:M:13:VAL:HG11	2:M:19:VAL:HG23	2.02	0.41
3:B:543:GLU:HG3	3:B:638:LEU:CB	2.47	0.41
1:H:93:ALA:HB1	1:H:100(C):MET:HB3	2.01	0.41
3:A:607:ARG:NH2	3:A:608:GLU:CG	2.84	0.41
3:A:636:PRO:HB3	3:A:640:ARG:HH12	1.85	0.41
3:A:679:VAL:HA	3:A:682:ILE:HG22	2.02	0.40
3:B:679:VAL:O	3:B:683:LEU:HG	2.21	0.40
1:I:56:LEU:HD12	3:B:611:ILE:HA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	116/140 (83%)	113 (97%)	3 (3%)	0	100	100
1	I	116/140 (83%)	111 (96%)	5 (4%)	0	100	100
2	L	111/123 (90%)	104 (94%)	7 (6%)	0	100	100
2	M	111/123 (90%)	104 (94%)	7 (6%)	0	100	100
3	A	228/248 (92%)	224 (98%)	4 (2%)	0	100	100
3	B	230/248 (93%)	226 (98%)	4 (2%)	0	100	100
All	All	912/1022 (89%)	882 (97%)	30 (3%)	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	101/106 (95%)	101 (100%)	0	100	100
1	I	101/106 (95%)	101 (100%)	0	100	100
2	L	97/105 (92%)	96 (99%)	1 (1%)	76	88
2	M	97/105 (92%)	96 (99%)	1 (1%)	76	88
3	A	215/231 (93%)	208 (97%)	7 (3%)	38	63
3	B	217/231 (94%)	215 (99%)	2 (1%)	78	89
All	All	828/884 (94%)	817 (99%)	11 (1%)	69	84

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	11	LEU
3	A	495	THR
3	A	503	GLU
3	A	571	LEU
3	A	607	ARG
3	A	658	ILE
3	A	669	ASN
3	A	689	ILE
2	M	91	TYR
3	B	629	ASN
3	B	681	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	565	ASN

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	0.35	0	17,19,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	2	4	14,14,15	0.33	0	17,19,21	0.41	0
4	BMA	C	3	4	11,11,12	1.31	2 (18%)	15,15,17	1.67	2 (13%)
4	MAN	C	4	4	11,11,12	1.02	1 (9%)	15,15,17	0.93	1 (6%)
4	MAN	C	5	4	11,11,12	0.86	1 (9%)	15,15,17	0.90	1 (6%)
4	MAN	C	6	4	11,11,12	1.34	3 (27%)	15,15,17	1.90	3 (20%)
4	MAN	C	7	4	11,11,12	0.67	0	15,15,17	1.02	2 (13%)
5	NAG	D	1	3,5	14,14,15	0.92	1 (7%)	17,19,21	1.57	2 (11%)
5	NAG	D	2	5	14,14,15	0.87	1 (7%)	17,19,21	1.38	2 (11%)
5	FUC	D	3	5	10,10,11	1.06	0	14,14,16	1.67	5 (35%)
4	NAG	E	1	3,4	14,14,15	0.30	0	17,19,21	0.38	0
4	NAG	E	2	4	14,14,15	0.18	0	17,19,21	0.38	0
4	BMA	E	3	4	11,11,12	1.08	1 (9%)	15,15,17	1.53	3 (20%)
4	MAN	E	4	4	11,11,12	0.84	0	15,15,17	0.84	1 (6%)
4	MAN	E	5	4	11,11,12	0.79	0	15,15,17	0.91	1 (6%)
4	MAN	E	6	4	11,11,12	1.41	2 (18%)	15,15,17	1.93	3 (20%)
4	MAN	E	7	4	11,11,12	0.66	0	15,15,17	0.99	2 (13%)
5	NAG	F	1	3,5	14,14,15	0.79	1 (7%)	17,19,21	1.48	2 (11%)
5	NAG	F	2	5	14,14,15	0.91	1 (7%)	17,19,21	1.02	1 (5%)
5	FUC	F	3	5	10,10,11	1.35	2 (20%)	14,14,16	1.62	3 (21%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
4	MAN	E	5	4	-	0/2/19/22	0/1/1/1
4	MAN	E	6	4	-	0/2/19/22	0/1/1/1
4	MAN	E	7	4	-	1/2/19/22	0/1/1/1
5	NAG	F	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	FUC	F	3	5	-	-	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1	NAG	O5-C1	3.03	1.48	1.43
4	E	6	MAN	C2-C3	2.99	1.56	1.52
4	C	4	MAN	O5-C1	-2.92	1.39	1.43
5	F	2	NAG	C1-C2	2.75	1.56	1.52
4	C	3	BMA	C2-C3	2.73	1.56	1.52
5	F	3	FUC	C2-C3	2.67	1.56	1.52
5	D	2	NAG	C1-C2	2.60	1.56	1.52
4	C	6	MAN	C2-C3	2.47	1.56	1.52
5	F	1	NAG	O5-C1	2.45	1.47	1.43
4	C	3	BMA	O3-C3	2.36	1.48	1.43
4	C	6	MAN	C1-C2	2.29	1.57	1.52
4	E	3	BMA	C2-C3	2.27	1.55	1.52
4	C	6	MAN	C4-C3	2.18	1.57	1.52
4	C	5	MAN	O5-C1	-2.17	1.40	1.43
4	E	6	MAN	C4-C3	2.11	1.57	1.52
5	F	3	FUC	O5-C5	2.08	1.48	1.43

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	6	MAN	C1-C2-C3	4.77	115.53	109.67
4	C	6	MAN	C1-C2-C3	4.71	115.45	109.67
4	C	3	BMA	O3-C3-C2	4.60	118.81	109.99
5	D	1	NAG	O4-C4-C5	4.40	120.22	109.30
5	D	2	NAG	C2-N2-C7	3.94	128.52	122.90
4	E	3	BMA	O3-C3-C2	3.93	117.52	109.99
5	F	1	NAG	C1-O5-C5	3.85	117.41	112.19
4	C	6	MAN	C2-C3-C4	3.76	117.41	110.89
4	E	6	MAN	C2-C3-C4	3.75	117.39	110.89
5	D	1	NAG	C1-O5-C5	3.66	117.15	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	2	NAG	C1-O5-C5	3.48	116.91	112.19
5	F	1	NAG	O4-C4-C5	3.42	117.80	109.30
5	F	3	FUC	C1-C2-C3	3.18	113.58	109.67
5	D	3	FUC	C1-C2-C3	3.08	113.45	109.67
5	D	2	NAG	C1-O5-C5	2.99	116.24	112.19
5	D	3	FUC	C1-O5-C5	2.98	119.52	112.78
5	F	3	FUC	O5-C5-C4	2.93	114.78	109.52
4	C	4	MAN	O2-C2-C3	-2.81	104.51	110.14
5	D	3	FUC	O5-C5-C4	2.74	114.44	109.52
5	F	3	FUC	C1-O5-C5	2.65	118.79	112.78
4	C	7	MAN	O2-C2-C3	-2.52	105.09	110.14
4	C	3	BMA	C3-C4-C5	-2.51	105.77	110.24
4	E	6	MAN	O2-C2-C3	-2.48	105.18	110.14
4	E	3	BMA	C3-C4-C5	-2.39	105.98	110.24
4	C	6	MAN	O2-C2-C3	-2.38	105.38	110.14
4	C	7	MAN	C1-O5-C5	2.36	115.39	112.19
4	E	7	MAN	C1-O5-C5	2.26	115.25	112.19
4	E	7	MAN	O2-C2-C3	-2.24	105.64	110.14
4	E	5	MAN	O2-C2-C3	-2.20	105.72	110.14
5	D	3	FUC	C2-C3-C4	2.20	114.70	110.89
4	E	4	MAN	O2-C2-C3	-2.16	105.81	110.14
5	D	3	FUC	C3-C4-C5	2.10	113.04	109.77
4	E	3	BMA	C1-C2-C3	-2.07	107.12	109.67
4	C	5	MAN	O2-C2-C3	-2.01	106.12	110.14

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	1	NAG	C4-C5-C6-O6
4	C	1	NAG	O5-C5-C6-O6
4	C	1	NAG	C4-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6
5	D	1	NAG	O5-C5-C6-O6
4	C	1	NAG	C8-C7-N2-C2
4	C	1	NAG	O7-C7-N2-C2
5	D	2	NAG	C8-C7-N2-C2
5	D	2	NAG	O7-C7-N2-C2
5	D	1	NAG	C4-C5-C6-O6
5	D	2	NAG	C4-C5-C6-O6
5	D	2	NAG	O5-C5-C6-O6
4	C	7	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	E	7	MAN	O5-C5-C6-O6
4	C	2	NAG	C4-C5-C6-O6
4	C	2	NAG	O5-C5-C6-O6
5	D	2	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	3	FUC	1	0
5	D	2	NAG	2	0
5	D	1	NAG	1	0
5	D	3	FUC	1	0

5.6 Ligand geometry [i](#)

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 ⓘ

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, 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	118/140 (84%)	0.34	5 (4%) 36 28	42, 81, 122, 146	0
1	I	118/140 (84%)	1.24	27 (22%) 0 0	74, 120, 168, 210	0
2	L	113/123 (91%)	0.01	2 (1%) 68 63	33, 59, 88, 109	0
2	M	113/123 (91%)	0.79	20 (17%) 1 1	81, 117, 168, 233	0
3	A	230/248 (92%)	0.07	1 (0%) 92 91	35, 75, 125, 193	0
3	B	232/248 (93%)	0.14	3 (1%) 77 74	38, 77, 121, 172	0
All	All	924/1022 (90%)	0.36	58 (6%) 20 14	33, 84, 145, 233	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	18	VAL	8.0
1	I	111	VAL	7.0
2	M	106	ILE	6.2
1	I	109	VAL	5.9
1	I	90	TYR	5.7
2	M	63	THR	4.8
2	M	8	ALA	4.6
3	B	694	GLN	4.6
1	I	87	SER	4.5
1	I	42	GLY	4.4
1	H	82	LEU	4.1
1	I	47	TRP	4.0
1	I	108	SER	3.6
3	B	695	THR	3.5
2	M	14	SER	3.5
1	I	86	ASP	3.2
1	I	82	LEU	3.2
1	I	41	HIS	3.1
1	I	43	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	I	44	SER	3.1
2	M	27(A)	SER	3.0
1	I	29	PHE	3.0
2	M	104	LEU	3.0
2	M	36	TYR	2.9
2	M	83	LEU	2.9
1	I	12	VAL	2.9
2	M	85	VAL	2.9
1	H	11	LEU	2.7
1	I	20	VAL	2.7
1	I	11	LEU	2.7
2	M	87	TYR	2.7
3	B	609	MET	2.6
2	M	86	TYR	2.6
1	H	12	VAL	2.5
2	M	62	PHE	2.5
3	A	557	ILE	2.5
2	M	75	ILE	2.4
1	I	37	VAL	2.4
2	M	6	GLN	2.4
1	H	43	LYS	2.4
1	I	82(B)	SER	2.4
1	I	46	GLU	2.4
1	I	75	SER	2.3
1	H	105	GLN	2.3
1	I	17	SER	2.3
1	I	104	GLY	2.2
2	M	70	ASP	2.2
1	I	38	LYS	2.2
2	M	98	PHE	2.2
2	M	103	LYS	2.2
2	M	34	ALA	2.1
2	L	104	LEU	2.1
1	I	79	PHE	2.1
2	M	11	LEU	2.1
1	I	19	LYS	2.1
2	L	7	ALA	2.0
1	I	59	TYR	2.0
2	M	10	SER	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, 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
5	FUC	F	3	10/11	0.67	0.32	139,147,153,155	0
4	MAN	C	7	11/12	0.73	0.14	129,133,139,142	0
4	MAN	E	6	11/12	0.73	0.29	154,161,167,170	0
5	NAG	F	2	14/15	0.75	0.37	141,164,174,174	0
5	NAG	F	1	14/15	0.78	0.16	99,110,138,142	0
4	BMA	E	3	11/12	0.78	0.12	132,142,147,149	0
5	FUC	D	3	10/11	0.79	0.24	121,127,133,135	0
5	NAG	D	2	14/15	0.80	0.20	127,145,151,158	0
4	MAN	E	7	11/12	0.83	0.15	143,148,155,157	0
4	BMA	C	3	11/12	0.84	0.18	95,105,124,129	0
4	NAG	E	2	14/15	0.86	0.18	107,117,123,135	0
5	NAG	D	1	14/15	0.86	0.15	97,108,121,127	0
4	MAN	C	6	11/12	0.89	0.20	101,112,131,133	0
4	MAN	E	4	11/12	0.91	0.09	118,130,149,151	0
4	MAN	C	4	11/12	0.91	0.13	87,99,110,111	0
4	MAN	C	5	11/12	0.92	0.20	73,81,87,90	0
4	NAG	C	1	14/15	0.93	0.17	80,93,113,114	0
4	NAG	C	2	14/15	0.94	0.18	73,87,113,113	0
4	MAN	E	5	11/12	0.94	0.14	85,96,111,111	0
4	NAG	E	1	14/15	0.96	0.14	68,75,94,99	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.