



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 04:25 AM BST

PDB ID : 3OB0  
Title : A non-self sugar mimic of the HIV glycan shield shows enhanced antigenicity  
Authors : Doores, K.J.; Fulton, Z.; Hong, V.; Patel, M.K.; Scanlan, C.N.; Wormald, M.R.; Finn, M.G.; Burton, D.R.; Wilson, I.A.; Davis, B.G.  
Deposited on : 2010-08-06  
Resolution : 2.85 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](mailto: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.

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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

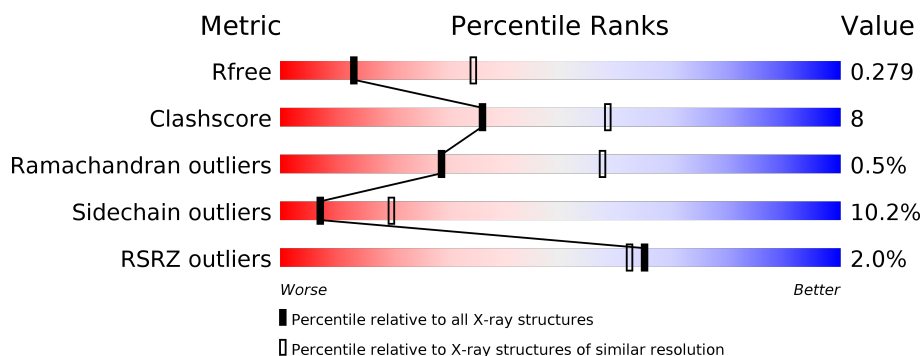
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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  $\geq 3$ , 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	K	213	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>17%</div> <div>.</div> </div> </div>
1	L	213	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>18%</div> </div> </div>
2	H	224	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>..</div> </div> </div>
2	M	224	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>19%</div> <div>6%</div> <div>.</div> </div> </div>
3	A	4	<div> <div></div> <div>100%</div> </div>
3	B	4	<div> <div></div> <div>75%</div> <div>25%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6635 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 Fab 2G12, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	212	Total	C	N	O	S	0	0	0
			1623	1021	273	324	5			
1	K	213	Total	C	N	O	S	0	0	0
			1628	1024	274	325	5			

- Molecule 2 is a protein called Fab 2G12, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	220	Total	C	N	O	S	0	0	0
			1643	1035	281	320	7			
2	M	219	Total	C	N	O	S	0	0	0
			1641	1034	280	320	7			

- Molecule 3 is an oligosaccharide called 7-deoxy-L-glycero- $\alpha$ -D-manno-heptopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-3)- $\alpha$ -D-mannopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	A	4	Total	C	O	0	0	0
			46	25	21			
3	B	4	Total	C	O	0	0	0
			46	25	21			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	2	Total	O	0	0
			2	2		

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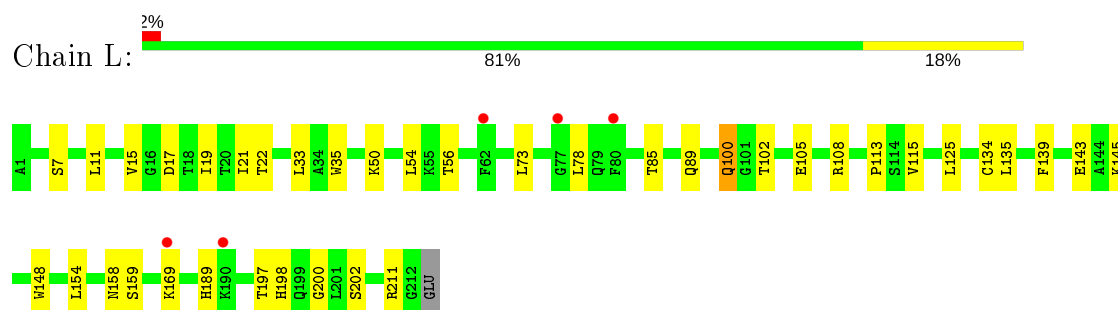
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total 1	O 1	0	0
4	K	3	Total 3	O 3	0	0
4	M	2	Total 2	O 2	0	0

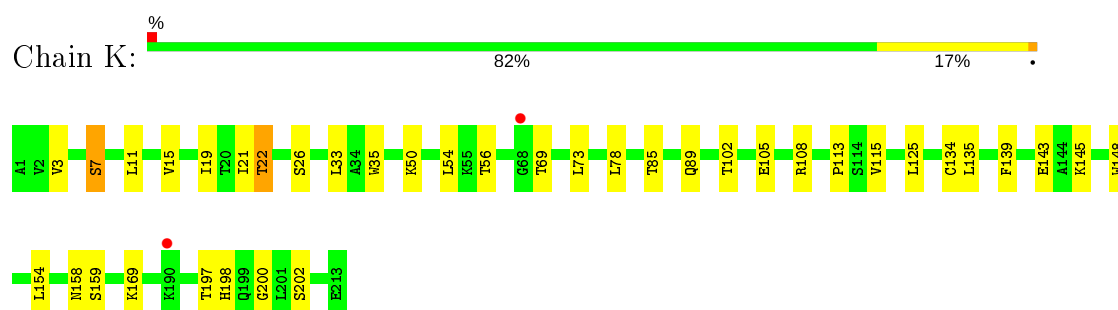
### 3 Residue-property plots [i](#)

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.

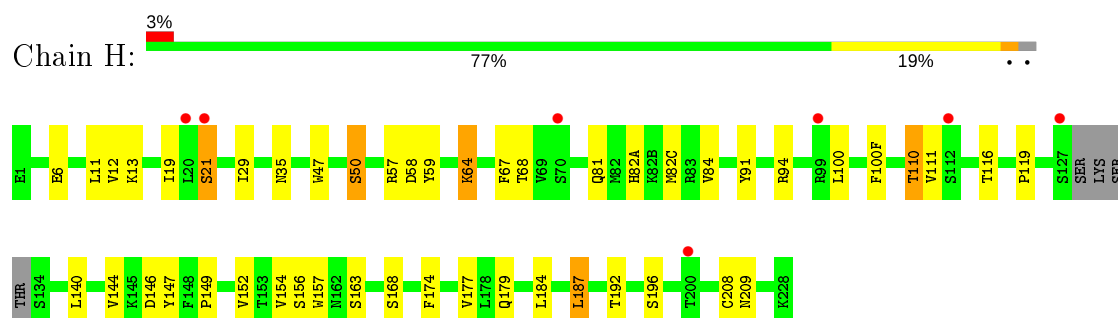
- Molecule 1: Fab 2G12, light chain



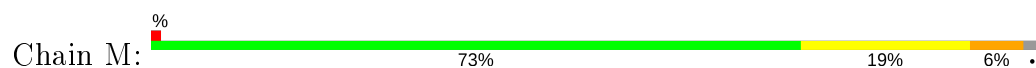
- Molecule 1: Fab 2G12, light chain

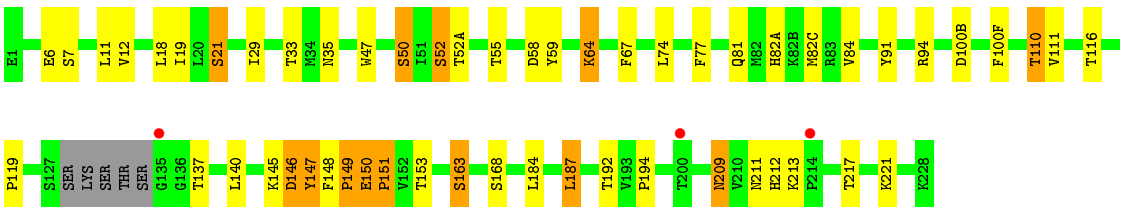


- Molecule 2: Fab 2G12, heavy chain



- Molecule 2: Fab 2G12, heavy chain

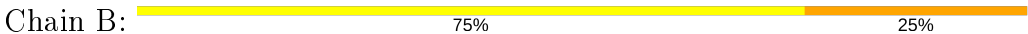




- Molecule 3: 7-deoxy-L-glycero-alpha-D-manno-heptopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose



- Molecule 3: 7-deoxy-L-glycero-alpha-D-manno-heptopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.74Å 131.16Å 169.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.85 29.96 – 2.85	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.85) 88.4 (29.96-2.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.28 (at 2.85Å)	Xtriage
Refinement program	REFMAC, BUSTER 2.8.0	Depositor
R, $R_{free}$	0.232 , 0.280 0.236 , 0.279	Depositor DCC
$R_{free}$ test set	1045 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.8	Xtriage
Anisotropy	0.826	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 45.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6635	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: YYH, 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	K	0.43	0/1664	0.68	0/2260
1	L	0.42	0/1659	0.68	0/2253
2	H	0.48	0/1681	0.75	0/2289
2	M	0.50	0/1679	0.74	0/2286
All	All	0.46	0/6683	0.71	0/9088

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	K	1628	0	1590	11	0
1	L	1623	0	1588	12	0
2	H	1643	0	1613	27	0
2	M	1641	0	1612	58	0
3	A	46	0	29	0	0
3	B	46	0	29	1	0
4	H	1	0	0	0	0
4	K	3	0	0	0	0
4	L	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	2	0	0	0	0
All	All	6635	0	6461	104	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.

All (104) 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)
2:M:148:PHE:CE2	2:M:149:PRO:HB3	1.56	1.40
2:M:148:PHE:CD2	2:M:149:PRO:HB3	1.69	1.25
2:M:148:PHE:CZ	2:M:149:PRO:HB3	1.75	1.21
2:M:147:TYR:HD2	2:M:148:PHE:N	1.45	1.12
2:M:148:PHE:CZ	2:M:149:PRO:CB	2.40	1.05
2:M:148:PHE:CG	2:M:149:PRO:HB3	1.96	1.01
2:M:147:TYR:CD2	2:M:148:PHE:N	2.29	0.99
2:M:148:PHE:CE2	2:M:149:PRO:CB	2.45	0.98
2:M:148:PHE:CE1	2:M:149:PRO:CB	2.48	0.96
2:M:148:PHE:CE1	2:M:149:PRO:HB3	2.02	0.93
2:M:147:TYR:CD2	2:M:147:TYR:C	2.44	0.92
2:M:148:PHE:O	2:M:212:HIS:NE2	2.05	0.88
2:M:148:PHE:CD1	2:M:149:PRO:HB3	2.11	0.86
2:M:150:GLU:HA	2:M:150:GLU:OE1	1.75	0.83
2:M:148:PHE:CD2	2:M:149:PRO:CB	2.59	0.83
2:M:148:PHE:CD1	2:M:149:PRO:CB	2.61	0.83
2:M:148:PHE:CD1	2:M:149:PRO:HA	2.17	0.80
2:M:149:PRO:O	2:M:150:GLU:O	2.01	0.78
2:M:148:PHE:CG	2:M:149:PRO:CB	2.66	0.78
2:M:148:PHE:CZ	2:M:149:PRO:HB2	2.24	0.72
2:M:148:PHE:CD1	2:M:149:PRO:CA	2.72	0.72
2:M:148:PHE:CE1	2:M:149:PRO:HB2	2.24	0.71
2:M:148:PHE:CG	2:M:149:PRO:CA	2.73	0.71
2:M:149:PRO:O	2:M:150:GLU:C	2.28	0.70
2:M:147:TYR:HD2	2:M:148:PHE:CA	2.05	0.68
1:L:198:HIS:CD2	1:L:200:GLY:H	2.13	0.67
2:M:148:PHE:C	2:M:212:HIS:HE2	1.98	0.67
1:K:198:HIS:CD2	1:K:200:GLY:H	2.13	0.67
2:M:149:PRO:O	2:M:149:PRO:HG2	1.96	0.66
2:H:12:VAL:HG21	2:H:82(C):MET:HE3	1.78	0.65
2:M:148:PHE:O	2:M:212:HIS:CE1	2.52	0.62
2:M:147:TYR:O	2:M:148:PHE:HB2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:119:PRO:HA	2:M:147:TYR:HB3	1.84	0.59
2:M:149:PRO:O	2:M:149:PRO:CG	2.51	0.59
1:L:19:ILE:HG12	1:L:78:LEU:HD11	1.87	0.57
2:H:116:THR:HG22	2:H:149:PRO:HD3	1.87	0.57
2:H:21:SER:HB3	2:M:19:ILE:HG12	1.86	0.56
1:K:19:ILE:HG12	1:K:78:LEU:HD11	1.88	0.56
2:M:145:LYS:O	2:M:147:TYR:HB3	2.05	0.55
2:M:148:PHE:CG	2:M:149:PRO:HA	2.39	0.55
2:M:11:LEU:HD12	2:M:110:THR:HB	1.89	0.54
2:H:163:SER:H	2:H:209:ASN:HD21	1.56	0.54
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.89	0.54
2:H:11:LEU:HD12	2:H:110:THR:HB	1.90	0.53
2:H:67:PHE:HA	2:H:81:GLN:O	2.08	0.53
1:L:189:HIS:O	1:L:211:ARG:HD3	2.08	0.52
2:M:150:GLU:CA	2:M:150:GLU:OE1	2.50	0.52
2:M:33:THR:HG23	2:M:52:SER:HA	1.91	0.52
2:M:67:PHE:HA	2:M:81:GLN:O	2.09	0.51
2:H:81:GLN:HE21	2:H:82(A):HIS:HE1	1.58	0.51
2:H:59:TYR:HB2	2:H:64:LYS:HG3	1.94	0.50
2:M:81:GLN:HE21	2:M:82(A):HIS:HE1	1.59	0.50
2:M:59:TYR:HB2	2:M:64:LYS:HG3	1.93	0.49
1:L:35:TRP:CE2	1:L:73:LEU:HB2	2.49	0.48
2:H:94:ARG:O	2:H:100(F):PHE:HA	2.13	0.48
1:K:35:TRP:CE2	1:K:73:LEU:HB2	2.49	0.48
1:L:113:PRO:HB3	1:L:139:PHE:HB3	1.96	0.47
2:H:174:PHE:O	2:H:187:LEU:HD12	2.14	0.47
2:M:147:TYR:CD2	2:M:148:PHE:CA	2.93	0.47
2:H:179:GLN:HG2	2:H:184:LEU:O	2.15	0.47
2:M:18:LEU:HB3	2:M:82(C):MET:HE1	1.97	0.47
2:H:154:VAL:HA	2:H:209:ASN:O	2.16	0.46
1:K:113:PRO:HB3	1:K:139:PHE:HB3	1.97	0.46
2:M:137:THR:HA	2:M:194:PRO:HA	1.97	0.46
1:L:100:GLN:H	1:L:100:GLN:HE21	1.62	0.46
2:M:116:THR:HG22	2:M:149:PRO:HD3	1.96	0.46
1:K:21:ILE:HG12	1:K:102:THR:HG21	1.98	0.46
2:M:35:ASN:ND2	2:M:50:SER:HB2	2.31	0.46
2:M:212:HIS:HB3	2:M:217:THR:HB	1.97	0.46
2:M:47:TRP:HZ2	2:M:50:SER:HB3	1.81	0.46
2:H:47:TRP:HZ2	2:H:50:SER:HB3	1.81	0.45
1:L:21:ILE:HG12	1:L:102:THR:HG21	1.98	0.45
2:H:68:THR:HG21	2:M:77:PHE:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:146:ASP:HB3	2:H:184:LEU:HD13	2.00	0.44
2:H:157:TRP:CH2	2:H:208:CYS:HB3	2.53	0.43
2:H:146:ASP:HA	2:H:184:LEU:HB3	2.00	0.43
2:M:94:ARG:O	2:M:100(F):PHE:HA	2.17	0.43
2:H:19:ILE:HD12	2:H:81:GLN:HG2	2.00	0.43
2:H:57:ARG:NH2	2:M:74:LEU:HB2	2.33	0.43
2:M:146:ASP:HB3	2:M:184:LEU:HD23	2.01	0.43
2:M:100(B):ASP:OD1	3:B:1:MAN:H2	2.19	0.42
2:H:35:ASN:ND2	2:H:50:SER:HB2	2.32	0.42
2:M:163:SER:H	2:M:209:ASN:HD21	1.66	0.42
2:H:19:ILE:HG13	2:M:21:SER:HB3	2.01	0.42
1:L:134:CYS:HB2	1:L:148:TRP:CZ2	2.55	0.42
1:K:7:SER:HB3	1:K:22:THR:HG22	2.01	0.42
2:M:150:GLU:HA	2:M:151:PRO:HA	1.80	0.42
2:M:6:GLU:OE1	2:M:91:TYR:HA	2.20	0.42
2:H:84:VAL:HA	2:H:111:VAL:HB	2.01	0.42
2:M:147:TYR:HE1	2:M:187:LEU:HD23	1.85	0.41
1:K:3:VAL:HB	1:K:26:SER:HB3	2.02	0.41
2:M:84:VAL:HA	2:M:111:VAL:HB	2.01	0.41
2:H:12:VAL:HG11	2:H:82(C):MET:HE1	2.03	0.41
2:H:163:SER:H	2:H:209:ASN:ND2	2.17	0.41
2:H:6:GLU:OE1	2:H:91:TYR:HA	2.20	0.41
1:K:115:VAL:HA	1:K:135:LEU:O	2.20	0.41
1:L:145:LYS:HB3	1:L:197:THR:HB	2.01	0.41
1:L:85:THR:HA	1:L:102:THR:O	2.21	0.41
1:K:85:THR:HA	1:K:102:THR:O	2.21	0.41
1:L:115:VAL:HA	1:L:135:LEU:O	2.21	0.41
1:K:134:CYS:HB2	1:K:148:TRP:CZ2	2.56	0.40
1:L:17:ASP:HB2	1:L:78:LEU:HD12	2.01	0.40
2:H:144:VAL:HG11	2:H:152:VAL:HG11	2.03	0.40
1:K:145:LYS:HB3	1:K:197:THR:HB	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	K	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
1	L	210/213 (99%)	199 (95%)	11 (5%)	0	100	100
2	H	216/224 (96%)	202 (94%)	14 (6%)	0	100	100
2	M	215/224 (96%)	198 (92%)	13 (6%)	4 (2%)	8	24
All	All	852/874 (98%)	797 (94%)	51 (6%)	4 (0%)	29	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	149	PRO
2	M	150	GLU
2	M	151	PRO
2	M	146	ASP

### 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	K	182/183 (100%)	163 (90%)	19 (10%)	7	19
1	L	182/183 (100%)	163 (90%)	19 (10%)	7	19
2	H	184/189 (97%)	169 (92%)	15 (8%)	11	29
2	M	184/189 (97%)	162 (88%)	22 (12%)	5	13
All	All	732/744 (98%)	657 (90%)	75 (10%)	7	20

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	SER
1	L	11	LEU
1	L	15	VAL
1	L	22	THR

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Mol	Chain	Res	Type
1	L	33	LEU
1	L	50	LYS
1	L	54	LEU
1	L	56	THR
1	L	89	GLN
1	L	100	GLN
1	L	105	GLU
1	L	108	ARG
1	L	125	LEU
1	L	143	GLU
1	L	154	LEU
1	L	158	ASN
1	L	159	SER
1	L	169	LYS
1	L	202	SER
2	H	13	LYS
2	H	21	SER
2	H	29	ILE
2	H	50	SER
2	H	58	ASP
2	H	64	LYS
2	H	100	LEU
2	H	110	THR
2	H	140	LEU
2	H	156	SER
2	H	168	SER
2	H	177	VAL
2	H	187	LEU
2	H	192	THR
2	H	196	SER
1	K	7	SER
1	K	11	LEU
1	K	15	VAL
1	K	22	THR
1	K	33	LEU
1	K	50	LYS
1	K	54	LEU
1	K	56	THR
1	K	69	THR
1	K	89	GLN
1	K	105	GLU
1	K	108	ARG

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Mol	Chain	Res	Type
1	K	125	LEU
1	K	143	GLU
1	K	154	LEU
1	K	158	ASN
1	K	159	SER
1	K	169	LYS
1	K	202	SER
2	M	7	SER
2	M	12	VAL
2	M	21	SER
2	M	29	ILE
2	M	50	SER
2	M	52	SER
2	M	52(A)	THR
2	M	55	THR
2	M	58	ASP
2	M	64	LYS
2	M	110	THR
2	M	140	LEU
2	M	147	TYR
2	M	153	THR
2	M	163	SER
2	M	168	SER
2	M	187	LEU
2	M	192	THR
2	M	209	ASN
2	M	211	ASN
2	M	213	LYS
2	M	221	LYS

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

Mol	Chain	Res	Type
1	L	38	GLN
1	L	87	HIS
1	L	89	GLN
1	L	100	GLN
1	L	138	ASN
1	L	198	HIS
2	H	35	ASN
2	H	81	GLN
2	H	82(A)	HIS

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Mol	Chain	Res	Type
2	H	162	ASN
2	H	209	ASN
1	K	38	GLN
1	K	87	HIS
1	K	89	GLN
1	K	138	ASN
1	K	198	HIS
2	M	35	ASN
2	M	81	GLN
2	M	82(A)	HIS
2	M	209	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 ⓘ

8 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	MAN	A	1	3	12,12,12	1.08	1 (8%)	17,17,17	2.91	8 (47%)
3	MAN	A	2	3	11,11,12	1.15	1 (9%)	15,15,17	2.69	6 (40%)
3	MAN	A	3	3	11,11,12	1.03	0	15,15,17	2.43	4 (26%)
3	YYH	A	4	3	12,12,13	0.90	1 (8%)	16,17,19	2.70	8 (50%)
3	MAN	B	1	3	12,12,12	1.43	2 (16%)	17,17,17	2.58	9 (52%)
3	MAN	B	2	3	11,11,12	1.42	3 (27%)	15,15,17	2.14	8 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MAN	B	3	3	11,11,12	1.35	2 (18%)	15,15,17	2.43	4 (26%)
3	YYH	B	4	3	12,12,13	2.13	2 (16%)	16,17,19	2.62	6 (37%)

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	MAN	A	1	3	-	2/2/22/22	0/1/1/1
3	MAN	A	2	3	-	0/2/19/22	0/1/1/1
3	MAN	A	3	3	-	0/2/19/22	0/1/1/1
3	YYH	A	4	3	-	4/4/21/24	0/1/1/1
3	MAN	B	1	3	-	2/2/22/22	0/1/1/1
3	MAN	B	2	3	-	2/2/19/22	0/1/1/1
3	MAN	B	3	3	-	0/2/19/22	0/1/1/1
3	YYH	B	4	3	-	3/4/21/24	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	4	YYH	O5-C1	5.51	1.52	1.43
3	B	4	YYH	O5-C5	4.39	1.48	1.43
3	B	2	MAN	C2-C3	3.02	1.57	1.52
3	B	1	MAN	O1-C1	2.80	1.48	1.39
3	B	3	MAN	O4-C4	2.68	1.49	1.43
3	B	1	MAN	C4-C5	2.28	1.57	1.53
3	B	3	MAN	C2-C3	-2.21	1.49	1.52
3	A	2	MAN	C4-C5	2.15	1.57	1.53
3	B	2	MAN	C1-C2	2.13	1.57	1.52
3	B	2	MAN	O2-C2	2.09	1.47	1.43
3	A	4	YYH	O5-C5	2.08	1.45	1.43
3	A	1	MAN	O1-C1	2.01	1.46	1.39

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	4	YYH	C6M-C6-C5	-7.58	103.14	112.02
3	A	4	YYH	C6M-C6-C5	-7.32	103.44	112.02
3	A	3	MAN	C1-O5-C5	6.74	121.32	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3	MAN	C1-O5-C5	6.46	120.94	112.19
3	B	1	MAN	O3-C3-C4	-5.58	97.45	110.35
3	A	2	MAN	C1-C2-C3	5.57	116.52	109.67
3	A	1	MAN	O3-C3-C4	-5.31	98.07	110.35
3	B	1	MAN	O5-C5-C4	4.82	118.44	109.69
3	A	2	MAN	O5-C1-C2	-4.79	103.38	110.77
3	A	1	MAN	O5-C1-C2	4.75	118.76	110.28
3	A	2	MAN	O2-C2-C3	-4.70	100.71	110.14
3	A	1	MAN	C3-C4-C5	4.41	118.11	110.24
3	A	1	MAN	O5-C5-C4	4.30	117.50	109.69
3	B	4	YYH	C1-O5-C5	4.11	118.22	111.48
3	B	3	MAN	O2-C2-C3	-4.00	102.13	110.14
3	B	2	MAN	O5-C1-C2	-3.91	104.73	110.77
3	B	1	MAN	C3-C4-C5	3.79	117.01	110.24
3	B	4	YYH	O5-C1-C2	-3.55	105.28	110.77
3	A	1	MAN	O5-C5-C6	3.54	115.23	106.44
3	A	3	MAN	C1-C2-C3	-3.47	105.40	109.67
3	A	3	MAN	O5-C5-C4	3.30	118.86	110.83
3	A	4	YYH	O5-C1-C2	-3.20	105.83	110.77
3	A	1	MAN	C1-O5-C5	3.17	119.64	113.66
3	A	2	MAN	O5-C5-C6	-3.15	102.26	107.20
3	B	3	MAN	O5-C5-C4	3.15	118.49	110.83
3	A	2	MAN	O2-C2-C1	-3.02	102.97	109.15
3	B	1	MAN	C1-C2-C3	3.00	116.54	110.31
3	B	2	MAN	O3-C3-C4	-2.98	103.46	110.35
3	A	1	MAN	C1-C2-C3	2.97	116.48	110.31
3	A	3	MAN	O5-C1-C2	2.94	115.30	110.77
3	A	4	YYH	O3-C3-C2	2.90	115.55	109.99
3	A	4	YYH	C1-O5-C5	2.90	116.23	111.48
3	A	1	MAN	C4-C3-C2	2.80	115.70	110.82
3	A	4	YYH	O6-C6-C5	2.78	114.16	108.72
3	B	1	MAN	C1-O5-C5	2.69	118.74	113.66
3	B	4	YYH	O5-C5-C4	2.69	115.45	110.73
3	B	2	MAN	C2-C3-C4	2.53	115.27	110.89
3	B	1	MAN	O1-C1-O5	2.51	117.92	110.38
3	A	4	YYH	C2-C3-C4	2.49	115.21	110.89
3	B	2	MAN	C1-C2-C3	2.47	112.70	109.67
3	B	1	MAN	C4-C3-C2	2.47	115.14	110.82
3	B	3	MAN	O2-C2-C1	2.42	114.10	109.15
3	B	2	MAN	O2-C2-C3	-2.37	105.39	110.14
3	A	2	MAN	O4-C4-C5	2.31	115.03	109.30
3	B	2	MAN	O5-C5-C4	2.23	116.25	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4	YYH	O4-C4-C3	-2.17	105.34	110.35
3	B	1	MAN	O1-C1-C2	2.14	115.05	109.03
3	B	4	YYH	O6-C6-C6M	-2.11	103.50	109.74
3	B	2	MAN	C3-C4-C5	2.10	113.98	110.24
3	B	2	MAN	O4-C4-C5	-2.05	104.21	109.30
3	A	4	YYH	O5-C5-C4	2.05	114.33	110.73
3	B	4	YYH	O6-C6-C5	2.03	112.69	108.72
3	B	1	MAN	O3-C3-C2	2.00	114.98	110.35

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4	YYH	C4-C5-C6-O6
3	A	4	YYH	C4-C5-C6-C6M
3	A	4	YYH	O5-C5-C6-O6
3	B	4	YYH	C4-C5-C6-O6
3	B	4	YYH	C4-C5-C6-C6M
3	B	4	YYH	O5-C5-C6-O6
3	A	1	MAN	O5-C5-C6-O6
3	B	2	MAN	O5-C5-C6-O6
3	B	2	MAN	C4-C5-C6-O6
3	B	1	MAN	O5-C5-C6-O6
3	A	1	MAN	C4-C5-C6-O6
3	A	4	YYH	O5-C5-C6-C6M
3	B	1	MAN	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1	MAN	1	0

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	K	213/213 (100%)	0.04	2 (0%) 84 84	55, 75, 95, 106	0
1	L	212/213 (99%)	0.02	5 (2%) 59 56	58, 75, 99, 111	0
2	H	220/224 (98%)	0.28	7 (3%) 47 42	52, 76, 101, 130	0
2	M	219/224 (97%)	0.25	3 (1%) 75 74	57, 76, 122, 218	0
All	All	864/874 (98%)	0.15	17 (1%) 65 62	52, 76, 106, 218	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	127	SER	4.0
2	M	135	GLY	4.0
1	L	80	PHE	2.9
1	K	68	GLY	2.9
2	H	200	THR	2.9
2	H	99	ARG	2.7
2	H	70	SER	2.7
2	M	200	THR	2.3
1	L	62	PHE	2.3
2	H	21	SER	2.3
1	L	169	LYS	2.3
1	L	77	GLY	2.3
2	M	214	PRO	2.2
1	L	190	LYS	2.2
2	H	20	LEU	2.2
2	H	112	SER	2.1
1	K	190	LYS	2.0

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

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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	MAN	B	3	11/12	0.93	0.17	61,62,68,71	0
3	MAN	A	1	12/12	0.94	0.15	75,78,80,81	0
3	YYH	B	4	12/13	0.94	0.16	60,69,72,74	0
3	YYH	A	4	12/13	0.95	0.15	63,70,72,72	0
3	MAN	A	3	11/12	0.95	0.19	70,74,78,79	0
3	MAN	B	1	12/12	0.95	0.22	68,72,74,77	0
3	MAN	A	2	11/12	0.95	0.14	78,81,82,83	0
3	MAN	B	2	11/12	0.96	0.16	68,71,73,74	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.