



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 06:26 AM BST

PDB ID : 3OAZ
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 : 1.75 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

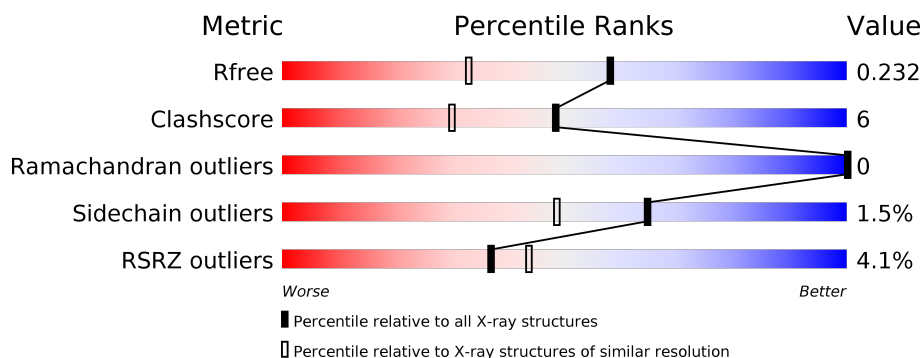
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	223	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>12%</div> </div> </div>
1	M	223	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>• •</div> </div> </div>
2	K	213	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
2	L	213	<div> <div>6%</div> <div> <div></div> <div>88%</div> <div>12%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	H	231	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7891 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.

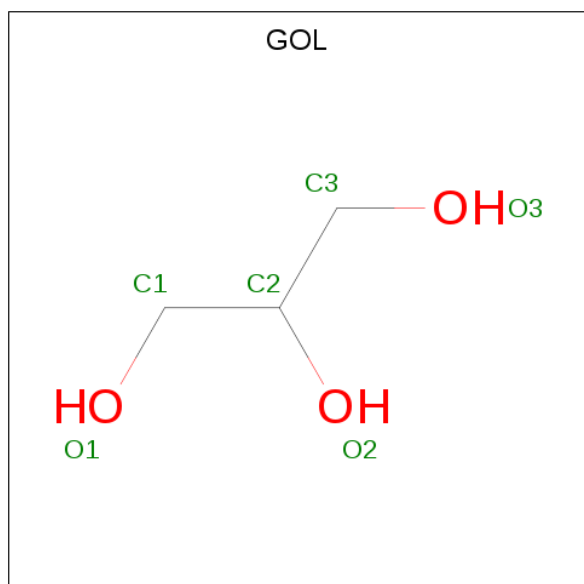
- Molecule 1 is a protein called Fab 2G12, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	223	Total	C	N	O	S	0	20	0
			1746	1111	286	342	7			
1	M	214	Total	C	N	O	S	0	14	0
			1671	1062	277	324	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	213	Total	C	N	O	S	0	7	0
			1659	1050	274	330	5			
2	L	213	Total	C	N	O	S	0	16	0
			1696	1076	274	341	5			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

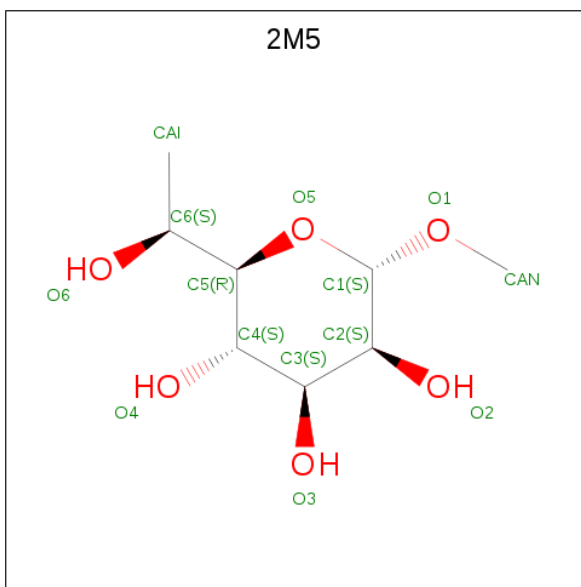


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	K	1	Total C O 6 3 3	0	0
3	K	1	Total C O 6 3 3	0	0
3	K	1	Total C O 6 3 3	0	0
3	L	1	Total C O 6 3 3	0	0
3	M	1	Total C O 6 3 3	0	0
3	M	1	Total C O 6 3 3	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	5	Total Cl 5 5	0	0
4	L	14	Total Cl 14 14	0	0
4	K	6	Total Cl 6 6	0	0
4	M	3	Total Cl 3 3	0	0

- Molecule 5 is methyl 7-deoxy-L-glycero-alpha-D-manno-heptopyranoside (three-letter code: 2M5) (formula: C₈H₁₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	O	0	0
			14	8	6		
5	M	1	Total	C	O	0	0
			14	8	6		

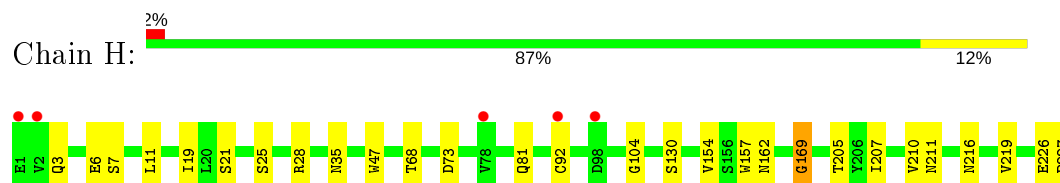
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	282	Total	O	0	0
			282	282		
6	K	264	Total	O	0	0
			264	264		
6	L	227	Total	O	0	0
			227	227		
6	M	230	Total	O	0	0
			230	230		

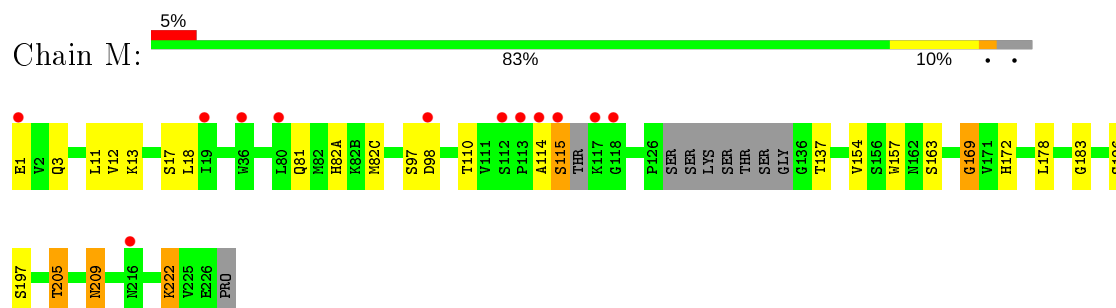
3 Residue-property plots [i](#)

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.

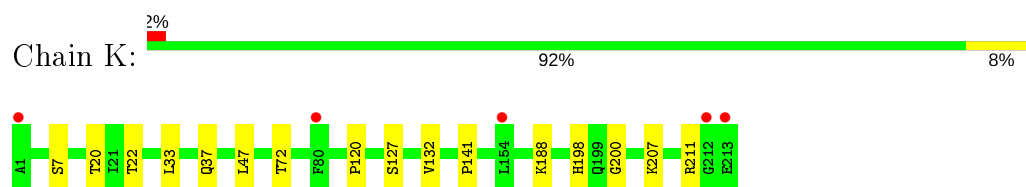
- Molecule 1: Fab 2G12, heavy chain



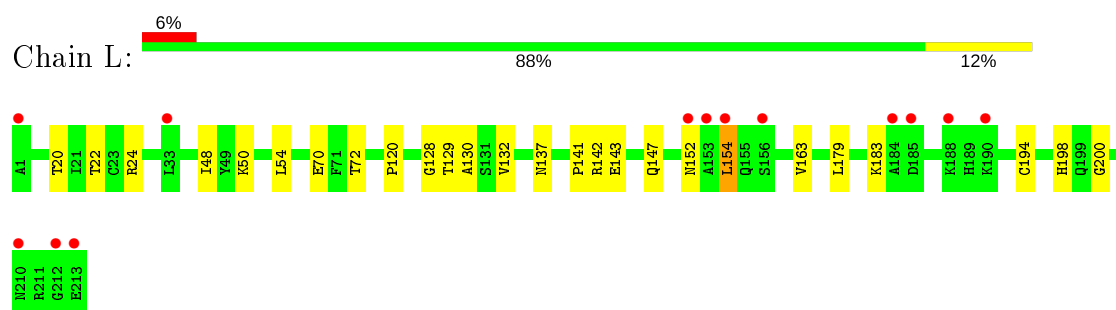
- Molecule 1: Fab 2G12, heavy chain



- Molecule 2: Fab 2G12, light chain



- Molecule 2: Fab 2G12, light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.62Å 72.09Å 84.07Å 90.00° 95.78° 90.00°	Depositor
Resolution (Å)	29.65 – 1.75 29.65 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.65-1.75) 98.2 (29.65-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.176 , 0.217 0.191 , 0.232	Depositor DCC
R_{free} test set	4297 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	20.2	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7891	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL, 2M5

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	0.85	5/1845 (0.3%)	0.75	0/2518
1	M	0.79	4/1746 (0.2%)	0.77	1/2377 (0.0%)
2	K	0.63	0/1716	0.64	0/2332
2	L	0.67	1/1780 (0.1%)	0.68	0/2421
All	All	0.74	10/7087 (0.1%)	0.71	1/9648 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1
1	M	0	3
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	157	TRP	C-N	10.60	1.58	1.34
1	H	130	SER	C-N	10.53	1.58	1.34
1	M	222	LYS	C-N	9.39	1.55	1.34
1	H	169	GLY	C-N	9.30	1.55	1.34
1	H	157	TRP	C-N	7.79	1.51	1.34
1	H	92	CYS	CB-SG	-7.41	1.69	1.82
1	M	169	GLY	C-N	6.40	1.48	1.34
1	M	154	VAL	C-N	6.26	1.48	1.34
2	L	194	CYS	CB-SG	-5.85	1.72	1.81
1	H	154	VAL	C-N	5.61	1.47	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	169	GLY	O-C-N	-8.46	109.17	122.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	169	GLY	Mainchain
1	M	169	GLY	Mainchain
1	M	205[A]	THR	Mainchain
1	M	205[B]	THR	Mainchain

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	1746	0	1781	20	0
1	M	1671	0	1678	25	0
2	K	1659	0	1646	18	0
2	L	1696	0	1704	23	0
3	H	24	0	29	5	0
3	K	18	0	24	5	0
3	L	6	0	8	3	0
3	M	12	0	14	2	0
4	H	5	0	0	1	0
4	K	6	0	0	1	0
4	L	14	0	0	1	0
4	M	3	0	0	0	0
5	H	14	0	16	0	0
5	M	14	0	16	0	0
6	H	282	0	0	2	0
6	K	264	0	0	4	1
6	L	227	0	0	0	0
6	M	230	0	0	4	1
All	All	7891	0	6916	83	1

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 6.

All (83) 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:H:211:ASN:OD1	4:H:235:CL:CL	2.07	1.09
1:M:137[A]:THR:HG22	6:M:266:HOH:O	1.51	1.08
2:K:211:ARG:NH1	3:K:214:GOL:H11	1.70	1.06
2:K:211:ARG:HH11	3:K:214:GOL:H11	1.20	1.03
1:H:73:ASP:H	3:H:228:GOL:H31	1.26	1.00
3:K:214:GOL:H12	6:K:1112:HOH:O	1.62	0.97
1:M:163[A]:SER:H	1:M:209:ASN:HD21	1.23	0.87
2:L:132[A]:VAL:CG2	2:L:179:LEU:HB3	2.05	0.86
1:H:68[B]:THR:HG23	1:H:81:GLN:HB2	1.57	0.85
1:M:163[B]:SER:H	1:M:209:ASN:HD21	1.23	0.83
2:K:20[A]:THR:HG23	2:K:72:THR:CG2	2.07	0.83
2:L:20[A]:THR:HG23	2:L:72[A]:THR:HG23	1.63	0.80
2:L:198:HIS:HD2	2:L:200:GLY:H	1.27	0.80
2:L:198:HIS:CD2	2:L:200:GLY:H	2.00	0.80
2:K:127:SER:HA	3:L:214:GOL:H32	1.64	0.78
6:H:868:HOH:O	4:K:222:CL:CL	2.37	0.77
2:L:132[A]:VAL:HG22	2:L:179:LEU:HB3	1.68	0.75
2:K:20[A]:THR:HG23	2:K:72:THR:HG23	1.68	0.74
1:M:12[A]:VAL:HG11	1:M:82(C)[A]:MET:HE3	1.69	0.74
2:L:142:ARG:O	4:L:225:CL:CL	2.43	0.73
2:L:120:PRO:HD3	2:L:132[A]:VAL:HG12	1.70	0.72
1:M:12[A]:VAL:HG11	1:M:82(C)[A]:MET:CE	2.21	0.70
2:L:24:ARG:NH1	2:L:70:GLU:OE1	2.21	0.69
2:K:198:HIS:CD2	2:K:200:GLY:H	2.09	0.69
2:L:22[B]:THR:HG22	2:L:72[B]:THR:HG22	1.74	0.69
1:M:11:LEU:HD23	1:M:110:THR:HB	1.75	0.67
2:L:147:GLN:HE22	2:L:154:LEU:HD13	1.63	0.64
1:H:73:ASP:N	3:H:228:GOL:H31	2.07	0.64
2:K:20[A]:THR:CG2	2:K:72:THR:HG23	2.27	0.63
1:H:11[B]:LEU:HD11	1:M:178:LEU:HD11	1.81	0.62
1:M:1:GLU:HG3	1:M:3[B]:GLN:HE21	1.65	0.62
1:H:11[B]:LEU:HG	1:M:178:LEU:HD21	1.82	0.61
1:H:210:VAL:HB	1:H:219[B]:VAL:HG13	1.83	0.61
1:H:7[A]:SER:OG	1:H:21[A]:SER:OG	2.19	0.60
1:H:226:GLU:HB2	1:H:227:PRO:HA	1.83	0.60
2:K:207:LYS:HE3	6:K:436:HOH:O	2.01	0.60
1:M:205[B]:THR:HG23	1:M:222:LYS:HE3	1.82	0.60
2:L:20[A]:THR:HG23	2:L:72[A]:THR:CG2	2.31	0.60
1:M:1:GLU:HG3	1:M:3[B]:GLN:NE2	2.16	0.59
1:M:137[A]:THR:HG23	6:M:264:HOH:O	2.02	0.59
2:L:147:GLN:HE22	2:L:154:LEU:CD1	2.16	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:11[B]:LEU:CD1	1:M:183:GLY:HA2	2.35	0.57
3:M:228:GOL:O1	6:M:538:HOH:O	2.13	0.57
2:L:132[A]:VAL:HG23	2:L:179:LEU:HB3	1.87	0.56
2:K:198:HIS:HD2	2:K:200:GLY:H	1.51	0.56
1:H:28:ARG:HG2	3:H:231:GOL:H2	1.87	0.55
2:K:20[A]:THR:CG2	2:K:72:THR:CG2	2.83	0.55
2:L:24:ARG:HD3	2:L:70:GLU:OE1	2.08	0.54
1:H:28:ARG:CD	3:H:231:GOL:H2	2.38	0.53
1:H:162:ASN:ND2	1:H:207:ILE:H	2.07	0.53
2:L:137:ASN:HD21	1:M:172:HIS:HD2	1.58	0.52
1:H:11[B]:LEU:HD11	1:M:183:GLY:HA2	1.92	0.52
2:L:142:ARG:HD2	2:L:163[A]:VAL:HG11	1.92	0.51
1:M:81:GLN:OE1	1:M:82(A):HIS:HE1	1.93	0.51
2:K:207:LYS:CE	6:K:436:HOH:O	2.58	0.50
2:L:128:GLY:O	3:L:214:GOL:H31	2.10	0.50
1:H:35:ASN:HD22	1:H:47:TRP:HE1	1.59	0.50
2:L:137:ASN:HD21	1:M:172:HIS:CD2	2.30	0.50
1:H:3:GLN:HB2	1:H:25[B]:SER:OG	2.11	0.49
1:M:17:SER:OG	1:M:82(A):HIS:HD2	1.96	0.49
2:K:188:LYS:HB3	3:K:216:GOL:H2	1.93	0.49
1:H:205[A]:THR:HG23	6:H:279:HOH:O	2.13	0.48
2:L:141:PRO:O	2:L:198:HIS:HE1	1.96	0.48
2:K:7:SER:HG	2:K:22[B]:THR:HG1	1.60	0.48
1:M:196:SER:HA	3:M:228:GOL:O2	2.14	0.48
1:M:18:LEU:HB2	1:M:82(C)[A]:MET:HE1	1.96	0.48
1:H:19:ILE:HD12	1:H:81:GLN:HG2	1.97	0.47
1:M:12[A]:VAL:HG11	1:M:82(C)[A]:MET:HE1	1.97	0.47
1:M:163[A]:SER:H	1:M:209:ASN:ND2	2.03	0.46
1:M:163[B]:SER:H	1:M:209:ASN:ND2	2.03	0.46
2:K:120:PRO:HD3	2:K:132:VAL:HG22	1.99	0.45
2:K:37:GLN:HB2	2:K:47[B]:LEU:HD11	1.98	0.44
2:L:183:LYS:HB3	3:L:214:GOL:H11	2.00	0.44
2:K:141:PRO:O	2:K:198:HIS:HE1	2.01	0.44
1:H:28:ARG:CG	3:H:231:GOL:H2	2.48	0.43
2:K:207:LYS:HD2	6:K:436:HOH:O	2.18	0.43
2:L:48:ILE:HG12	2:L:54[A]:LEU:HD12	2.00	0.43
1:H:6:GLU:OE1	1:H:104:GLY:HA3	2.19	0.43
2:L:20[A]:THR:CG2	2:L:72[A]:THR:HG23	2.41	0.42
2:L:129:THR:HG22	2:L:130:ALA:N	2.34	0.42
1:M:114:ALA:HA	1:M:115:SER:HA	1.80	0.41
2:K:207:LYS:HD3	3:K:215:GOL:H2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:197:SER:HB3	6:M:726:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:1103:HOH:O	6:M:1147:HOH:O[2_645]	2.02	0.18

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	241/223 (108%)	235 (98%)	6 (2%)	0	100	100
1	M	222/223 (100%)	216 (97%)	6 (3%)	0	100	100
2	K	218/213 (102%)	213 (98%)	5 (2%)	0	100	100
2	L	227/213 (107%)	224 (99%)	3 (1%)	0	100	100
All	All	908/872 (104%)	888 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	H	208/188 (111%)	206 (99%)	2 (1%)	76	63
1	M	194/188 (103%)	189 (97%)	5 (3%)	46	23
2	K	189/183 (103%)	188 (100%)	1 (0%)	88	83
2	L	199/183 (109%)	195 (98%)	4 (2%)	55	34
All	All	790/742 (106%)	778 (98%)	12 (2%)	65	49

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	216[A]	ASN
1	H	216[B]	ASN
2	K	33	LEU
2	L	50	LYS
2	L	143	GLU
2	L	152	ASN
2	L	154	LEU
1	M	13	LYS
1	M	97	SER
1	M	98	ASP
1	M	115	SER
1	M	209	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	35	ASN
1	H	162	ASN
2	K	79	GLN
2	K	137	ASN
2	K	147	GLN
2	K	160	GLN
2	K	198	HIS
2	L	89	GLN
2	L	137	ASN
2	L	147	GLN
2	L	152	ASN
2	L	160	GLN
2	L	198	HIS
2	L	210	ASN
1	M	82(A)	HIS

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Mol	Chain	Res	Type
1	M	100(C)	ASN
1	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 40 ligands modelled in this entry, 28 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	M	228	-	5,5,5	1.14	0	5,5,5	2.23	2 (40%)
5	2M5	M	232	-	14,14,14	1.22	1 (7%)	20,20,20	0.76	1 (5%)
3	GOL	M	229	-	5,5,5	0.96	0	5,5,5	1.60	1 (20%)
3	GOL	K	214	-	5,5,5	0.56	0	5,5,5	0.48	0
3	GOL	H	231	-	5,5,5	1.56	2 (40%)	5,5,5	2.83	2 (40%)
5	2M5	H	237	-	14,14,14	1.75	2 (14%)	20,20,20	1.48	3 (15%)
3	GOL	L	214	-	5,5,5	0.51	0	5,5,5	0.54	0
3	GOL	H	228	-	5,5,5	0.31	0	5,5,5	0.80	0
3	GOL	K	215	-	5,5,5	0.92	1 (20%)	5,5,5	0.33	0
3	GOL	K	216	-	5,5,5	0.55	0	5,5,5	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	H	230	-	5,5,5	0.66	0	5,5,5	0.91	0
3	GOL	H	229	-	5,5,5	1.09	0	5,5,5	1.75	1 (20%)

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	GOL	M	228	-	-	2/4/4/4	-
5	2M5	M	232	-	-	0/6/26/26	0/1/1/1
3	GOL	M	229	-	-	0/4/4/4	-
3	GOL	K	214	-	-	0/4/4/4	-
3	GOL	H	231	-	-	2/4/4/4	-
5	2M5	H	237	-	-	0/6/26/26	0/1/1/1
3	GOL	L	214	-	-	2/4/4/4	-
3	GOL	H	228	-	-	0/4/4/4	-
3	GOL	K	215	-	-	2/4/4/4	-
3	GOL	K	216	-	-	2/4/4/4	-
3	GOL	H	230	-	-	4/4/4/4	-
3	GOL	H	229	-	-	2/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	237	2M5	O5-C5	4.55	1.51	1.44
5	M	232	2M5	O1-C1	3.77	1.46	1.40
5	H	237	2M5	O1-C1	3.39	1.46	1.40
3	H	231	GOL	O2-C2	-2.54	1.35	1.43
3	H	231	GOL	O1-C1	-2.15	1.33	1.42
3	K	215	GOL	O2-C2	-2.04	1.37	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	237	2M5	CAN-O1-C1	-5.00	105.55	113.27
3	H	231	GOL	O1-C1-C2	-4.68	87.75	110.20
3	H	231	GOL	O2-C2-C1	-4.05	91.29	109.12
3	M	228	GOL	C3-C2-C1	3.83	126.59	111.70
3	H	229	GOL	C3-C2-C1	3.31	124.58	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	229	GOL	O3-C3-C2	-2.84	96.58	110.20
3	M	228	GOL	O2-C2-C3	2.34	119.44	109.12
5	H	237	2M5	O1-C1-C2	2.20	110.73	108.15
5	H	237	2M5	O5-C5-C4	2.17	110.91	107.87
5	M	232	2M5	C1-O5-C5	2.10	116.44	113.06

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	230	GOL	O1-C1-C2-C3
3	H	230	GOL	C1-C2-C3-O3
3	K	215	GOL	O1-C1-C2-C3
3	K	216	GOL	C1-C2-C3-O3
3	H	231	GOL	O1-C1-C2-O2
3	H	231	GOL	O1-C1-C2-C3
3	K	215	GOL	O1-C1-C2-O2
3	H	229	GOL	C1-C2-C3-O3
3	H	230	GOL	O1-C1-C2-O2
3	H	230	GOL	O2-C2-C3-O3
3	M	228	GOL	O1-C1-C2-O2
3	M	228	GOL	O2-C2-C3-O3
3	H	229	GOL	O1-C1-C2-O2
3	K	216	GOL	O2-C2-C3-O3
3	L	214	GOL	O2-C2-C3-O3
3	L	214	GOL	C1-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	228	GOL	2	0
3	K	214	GOL	3	0
3	H	231	GOL	3	0
3	L	214	GOL	3	0
3	H	228	GOL	2	0
3	K	215	GOL	1	0
3	K	216	GOL	1	0

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	223/223 (100%)	0.19	5 (2%) 62 69	13, 21, 30, 45	0
1	M	214/223 (95%)	0.39	12 (5%) 24 30	13, 23, 38, 52	0
2	K	213/213 (100%)	0.16	5 (2%) 60 67	12, 21, 33, 43	0
2	L	213/213 (100%)	0.31	13 (6%) 21 26	13, 20, 50, 59	0
All	All	863/872 (98%)	0.26	35 (4%) 37 44	12, 21, 38, 59	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	216	ASN	4.8
2	L	154	LEU	4.5
2	L	212	GLY	4.0
1	M	114	ALA	3.9
1	M	118	GLY	3.9
1	M	1	GLU	3.4
1	H	1	GLU	3.4
2	L	188	LYS	3.3
1	M	113	PRO	3.2
2	K	212	GLY	3.2
1	M	98	ASP	3.0
2	L	153	ALA	3.0
2	L	152	ASN	3.0
2	L	156	SER	2.9
2	K	154	LEU	2.8
1	M	117	LYS	2.8
1	H	98[A]	ASP	2.7
2	K	1	ALA	2.6
1	H	78	VAL	2.6
1	H	2[A]	VAL	2.6
2	L	184	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	L	213	GLU	2.4
2	L	190	LYS	2.3
1	M	36	TRP	2.3
1	M	19[A]	ILE	2.2
1	H	92	CYS	2.2
2	L	185	ASP	2.1
2	L	210	ASN	2.1
1	M	115	SER	2.1
2	L	1	ALA	2.0
2	K	213	GLU	2.0
1	M	112[A]	SER	2.0
1	M	80	LEU	2.0
2	K	80	PHE	2.0
2	L	33	LEU	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](#)

There are no monosaccharides in this entry.

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(\AA^2)	Q<0.9
3	GOL	K	215	6/6	0.77	0.29	29,35,37,39	0
3	GOL	H	230	6/6	0.78	0.34	15,30,38,39	0
3	GOL	L	214	6/6	0.80	0.24	42,43,47,49	0
3	GOL	H	228	6/6	0.83	0.21	39,42,43,43	0
3	GOL	K	216	6/6	0.85	0.22	33,37,38,42	0
3	GOL	M	229	6/6	0.86	0.28	20,34,40,40	0
3	GOL	H	229	6/6	0.89	0.23	3,25,29,29	0
3	GOL	M	228	6/6	0.90	0.25	3,22,31,32	0
4	CL	H	236	1/1	0.93	0.10	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	K	214	6/6	0.93	0.13	32,33,34,34	0
3	GOL	H	231	6/6	0.93	0.22	18,23,32,37	0
4	CL	K	220	1/1	0.94	0.12	24,24,24,24	0
5	2M5	M	232	14/14	0.95	0.09	23,26,29,29	0
4	CL	L	226	1/1	0.96	0.13	29,29,29,29	0
4	CL	L	219	1/1	0.96	0.17	24,24,24,24	0
4	CL	M	233	1/1	0.97	0.08	23,23,23,23	0
4	CL	L	222	1/1	0.97	0.09	23,23,23,23	0
4	CL	H	234	1/1	0.97	0.14	30,30,30,30	0
4	CL	L	227	1/1	0.97	0.10	28,28,28,28	0
4	CL	L	224	1/1	0.97	0.14	25,25,25,25	0
4	CL	H	235	1/1	0.97	0.05	30,30,30,30	0
4	CL	L	228	1/1	0.97	0.09	25,25,25,25	0
4	CL	L	217	1/1	0.98	0.12	26,26,26,26	0
4	CL	L	223	1/1	0.98	0.12	27,27,27,27	0
4	CL	L	221	1/1	0.98	0.12	23,23,23,23	0
5	2M5	H	237	14/14	0.98	0.06	17,18,20,20	0
4	CL	M	231	1/1	0.98	0.16	21,21,21,21	0
4	CL	M	230	1/1	0.99	0.24	9,9,9,9	0
4	CL	K	223	1/1	0.99	0.09	28,28,28,28	0
4	CL	L	218	1/1	0.99	0.13	19,19,19,19	0
4	CL	K	219	1/1	0.99	0.14	17,17,17,17	0
4	CL	H	233	1/1	0.99	0.12	18,18,18,18	0
4	CL	L	220	1/1	0.99	0.10	23,23,23,23	0
4	CL	L	225	1/1	0.99	0.09	24,24,24,24	0
4	CL	L	215	1/1	0.99	0.26	9,9,9,9	0
4	CL	L	216	1/1	0.99	0.20	12,12,12,12	0
4	CL	K	218	1/1	0.99	0.20	17,17,17,17	0
4	CL	H	232	1/1	0.99	0.16	15,15,15,15	0
4	CL	K	217	1/1	1.00	0.31	2,2,2,2	0
4	CL	K	222	1/1	1.00	0.12	23,23,23,23	0

6.5 Other polymers

There are no such residues in this entry.