Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 12:17 PM BST

PDB ID	:	3OAY
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	:	2010-08-05
Resolution	:	1.95 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:

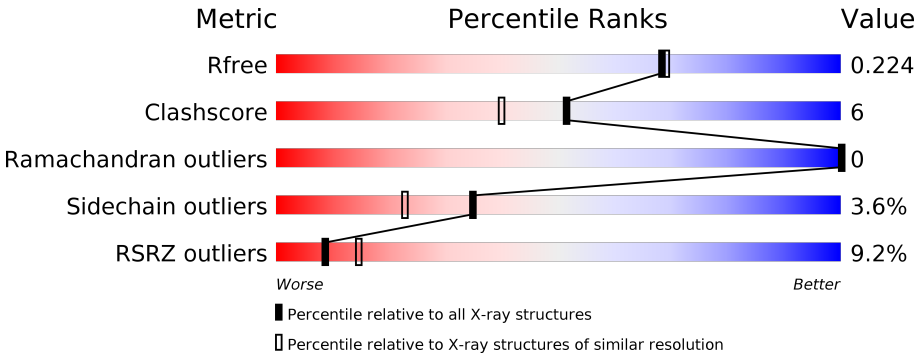
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 <=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	4% 87% 10%
1	L	213	8% 88% 12%
2	H	224	10% 79% 17%
2	M	224	14% 82% 14%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7265 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.

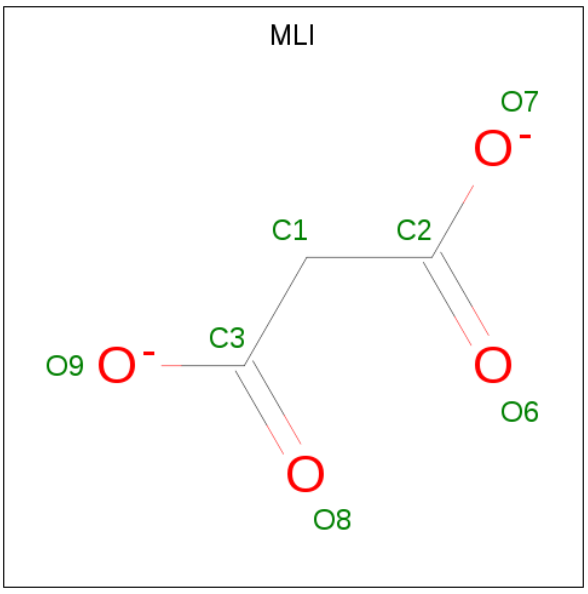
- Molecule 1 is a protein called Fab 2G12, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	K	213	Total	C	N	O	S	0	10	0
			1677	1059	279	334	5			
1	L	213	Total	C	N	O	S	0	8	0
			1669	1054	276	334	5			

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

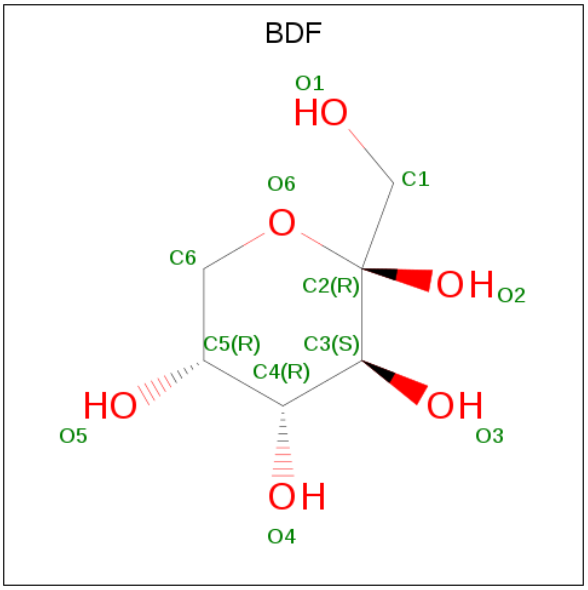
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	218	Total	C	N	O	S	0	6	0
			1664	1055	279	323	7			
2	H	217	Total	C	N	O	S	0	5	0
			1645	1038	279	321	7			

- Molecule 3 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	K	1	Total C O 14 6 8	0	1
3	L	1	Total C O 7 3 4	0	0

- Molecule 4 is beta-D-fructopyranose (three-letter code: BDF) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	1	Total C O 12 6 6	0	0
4	H	1	Total C O 12 6 6	0	0

- Molecule 5 is water.

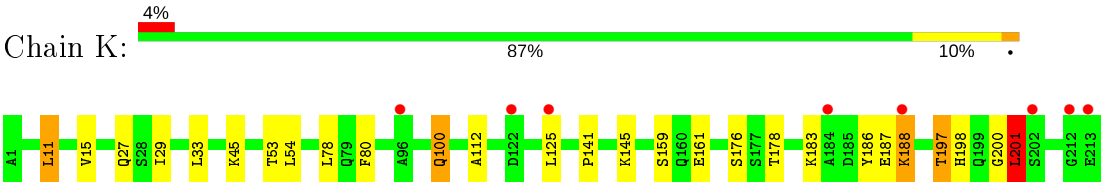
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	K	167	Total O 167 167	0	0
5	M	112	Total O 112 112	0	0
5	H	123	Total O 123 123	0	0
5	L	163	Total O 163 163	0	0

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.

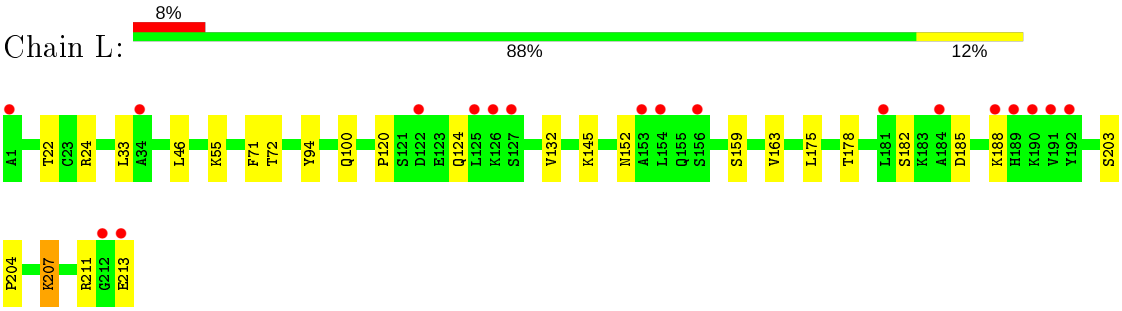
- Molecule 1: Fab 2G12, light chain

Chain K:



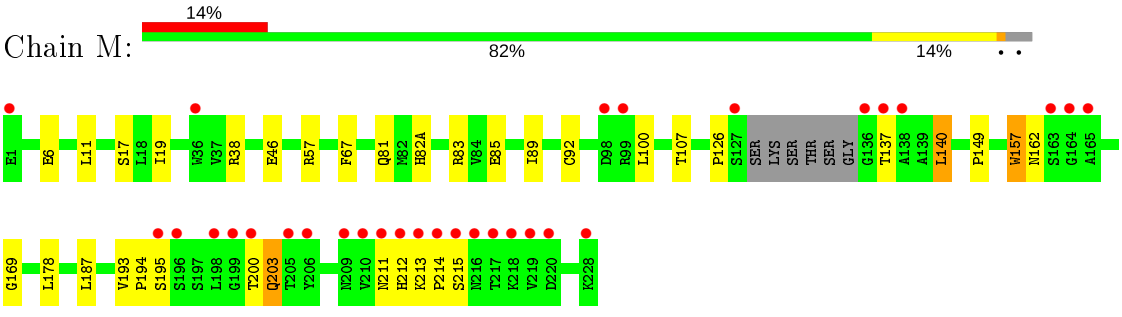
- Molecule 1: Fab 2G12, light chain

Chain L:



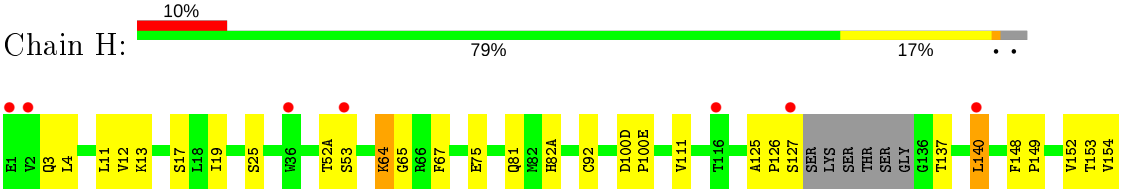
- Molecule 2: Fab 2G12, heavy chain

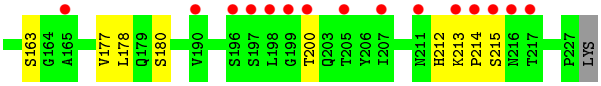
Chain M:



- Molecule 2: Fab 2G12, heavy chain

Chain H:




S163
G164
A165
V177
L178
Q179
S180
V190
S196
S197
L198
G199
T200
Q203
T205
Y206
I207
N211
H212
K213
P214
S215
N216
T217
P227
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.91Å 93.26Å 169.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.95 29.89 – 1.95	Depositor EDS
% Data completeness (in resolution range)	89.5 (30.00-1.95) 89.5 (29.89-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.01 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.182 , 0.223 0.184 , 0.224	Depositor DCC
R_{free} test set	4103 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	36.4	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7265	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.74	0/1743	0.80	4/2365 (0.2%)
1	L	0.85	2/1729 (0.1%)	0.72	1/2348 (0.0%)
2	H	0.74	1/1699 (0.1%)	0.78	0/2316
2	M	0.73	3/1720 (0.2%)	0.79	0/2344
All	All	0.77	6/6891 (0.1%)	0.77	5/9373 (0.1%)

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
2	H	0	3
2	M	0	3
All	All	0	6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	182	SER	CB-OG	14.04	1.60	1.42
2	H	92	CYS	CB-SG	-6.95	1.70	1.82
2	M	195	SER	CB-OG	6.72	1.50	1.42
2	M	92	CYS	CB-SG	-6.37	1.71	1.82
2	M	157	TRP	C-N	6.16	1.48	1.34
1	L	213	GLU	C-O	5.42	1.33	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	78	LEU	CA-CB-CG	5.66	128.32	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	201	LEU	CA-CB-CG	5.27	127.41	115.30
1	L	211	ARG	NE-CZ-NH1	-5.21	117.69	120.30
1	K	11	LEU	CA-CB-CG	5.21	127.28	115.30
1	K	54	LEU	CB-CG-CD1	-5.18	102.20	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	154	VAL	Mainchain
2	H	180	SER	Mainchain
2	H	200	THR	Mainchain
2	M	169	GLY	Mainchain
2	M	200	THR	Mainchain
2	M	203	GLN	Mainchain

5.2 Too-close contacts

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	1677	0	1673	17	0
1	L	1669	0	1656	14	0
2	H	1645	0	1618	24	0
2	M	1664	0	1658	24	0
3	K	14	0	4	1	0
3	L	7	0	2	0	0
4	H	12	0	12	0	0
4	M	12	0	12	0	0
5	H	123	0	0	1	0
5	K	167	0	0	2	0
5	L	163	0	0	1	0
5	M	112	0	0	1	0
All	All	7265	0	6635	74	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 6.

All (74) 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:81:GLN:HE21	2:M:82(A):HIS:HE1	1.14	0.89
2:M:212:HIS:HD2	2:M:215:SER:OG	1.60	0.84
2:M:81:GLN:HE21	2:M:82(A):HIS:CE1	1.95	0.83
1:L:46:LEU:HD23	1:L:55:LYS:HD2	1.61	0.81
2:M:81:GLN:NE2	2:M:82(A):HIS:HE1	1.79	0.80
1:K:100[A]:GLN:H	1:K:100[A]:GLN:CD	1.82	0.78
2:H:212:HIS:HD2	2:H:215:SER:OG	1.67	0.77
2:H:3:GLN:HG3	2:H:25:SER:HB2	1.66	0.76
1:K:112:ALA:HB1	1:K:201:LEU:HD13	1.67	0.76
1:K:198:HIS:CD2	1:K:200:GLY:H	2.06	0.74
2:M:11:LEU:HD11	2:H:178:LEU:HD21	1.71	0.70
1:K:183:LYS:O	1:K:187:GLU:HG3	1.94	0.67
1:K:198:HIS:HD2	1:K:200:GLY:H	1.42	0.67
3:K:214[B]:MLI:O6	3:K:214[B]:MLI:O9	2.08	0.67
2:H:13:LYS:HD2	2:H:148:PHE:CE1	2.30	0.66
1:L:120:PRO:HD3	1:L:132:VAL:HG22	1.78	0.64
2:M:11:LEU:HD11	2:H:178:LEU:CD2	2.28	0.64
2:M:126:PRO:HD3	2:M:140:LEU:HB3	1.80	0.63
1:L:22[B]:THR:HG22	1:L:72[B]:THR:HG22	1.83	0.60
2:M:57:ARG:CZ	2:H:75:GLU:HG3	2.32	0.59
1:L:207:LYS:HE2	5:L:291:HOH:O	2.01	0.58
1:K:125:LEU:HD11	1:K:186:TYR:CD2	2.38	0.58
1:K:45[B]:LYS:HE2	5:K:313:HOH:O	2.02	0.57
2:H:17:SER:OG	2:H:82(A):HIS:HD2	1.86	0.57
1:K:15[A]:VAL:HG21	1:K:80:PHE:CZ	2.41	0.55
2:M:187:LEU:HD12	2:M:187:LEU:C	2.27	0.55
2:M:11:LEU:CD1	2:H:178:LEU:HD21	2.36	0.55
5:H:280:HOH:O	1:L:94:TYR:HB3	2.08	0.53
2:M:212:HIS:CD2	2:M:215:SER:OG	2.52	0.51
1:L:33:LEU:HD22	1:L:71:PHE:CG	2.45	0.51
2:H:52(A):THR:O	2:H:53:SER:OG	2.29	0.50
1:L:185:ASP:O	1:L:188:LYS:HG2	2.11	0.50
2:H:81:GLN:OE1	2:H:82(A):HIS:HE1	1.94	0.49
2:H:149:PRO:O	2:H:212:HIS:HE1	1.96	0.48
2:M:6:GLU:HB2	2:M:107[B]:THR:OG1	2.12	0.48
1:L:163[B]:VAL:CG1	1:L:175:LEU:HD12	2.43	0.48
1:K:112:ALA:CB	1:K:201:LEU:HD13	2.40	0.48
1:L:185:ASP:HA	1:L:188:LYS:HD3	1.95	0.48
2:M:17:SER:OG	2:M:82(A):HIS:HD2	1.96	0.48
2:M:149:PRO:O	2:M:212:HIS:HE1	1.95	0.48
1:K:159:SER:HA	1:K:178:THR:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:52(A):THR:C	2:H:53:SER:HG	2.18	0.47
2:M:213:LYS:N	2:M:214:PRO:CD	2.78	0.47
1:K:188:LYS:HB2	1:K:188:LYS:NZ	2.30	0.46
1:K:161:GLU:HG3	5:K:245:HOH:O	2.16	0.46
2:H:4:LEU:N	2:H:4:LEU:HD12	2.31	0.46
1:L:163[B]:VAL:HG12	1:L:175:LEU:HD12	1.97	0.45
1:K:141:PRO:O	1:K:198:HIS:HE1	2.00	0.44
2:M:157:TRP:O	2:M:162:ASN:C	2.56	0.44
2:M:83:ARG:HD3	2:M:85:GLU:OE2	2.18	0.44
2:H:64:LYS:HD3	2:H:65:GLY:N	2.33	0.43
2:M:46[A]:GLU:OE2	5:M:283:HOH:O	2.21	0.43
1:K:27:GLN:O	1:K:29:ILE:HG23	2.18	0.43
2:M:178:LEU:HD21	2:H:11:LEU:HD11	2.00	0.43
1:K:112:ALA:HB1	1:K:201:LEU:CD1	2.45	0.43
2:H:19:ILE:HD12	2:H:81:GLN:HG2	2.00	0.43
1:K:145:LYS:HB3	1:K:197:THR:HG22	1.99	0.42
2:M:19[A]:ILE:HB	2:H:19:ILE:HB	2.00	0.42
2:H:126:PRO:HD3	2:H:140:LEU:HB3	2.02	0.42
2:H:12:VAL:O	2:H:111:VAL:HA	2.20	0.42
1:L:203:SER:HB2	1:L:204:PRO:CD	2.50	0.42
1:L:159:SER:HA	1:L:178:THR:O	2.20	0.42
2:H:100(D):ASP:HB3	2:H:100(E):PRO:HD2	2.03	0.41
1:L:33:LEU:HD22	1:L:71:PHE:CB	2.51	0.41
2:M:193:VAL:HB	2:M:194:PRO:HD2	2.03	0.41
2:H:125:ALA:HA	2:H:126:PRO:HD2	1.69	0.41
2:H:67:PHE:HA	2:H:81:GLN:O	2.21	0.41
2:M:81:GLN:NE2	2:M:82(A):HIS:CE1	2.69	0.41
2:M:67:PHE:HA	2:M:81:GLN:O	2.21	0.41
2:H:213:LYS:N	2:H:214:PRO:CD	2.84	0.41
2:H:212:HIS:CD2	2:H:215:SER:OG	2.58	0.40
2:M:38:ARG:HA	2:M:89:ILE:O	2.20	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	221/213 (104%)	212 (96%)	9 (4%)	0	100	100
1	L	219/213 (103%)	212 (97%)	7 (3%)	0	100	100
2	H	218/224 (97%)	209 (96%)	9 (4%)	0	100	100
2	M	220/224 (98%)	211 (96%)	9 (4%)	0	100	100
All	All	878/874 (100%)	844 (96%)	34 (4%)	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	K	193/183 (106%)	183 (95%)	10 (5%)	23	10
1	L	191/183 (104%)	185 (97%)	6 (3%)	40	28
2	H	187/189 (99%)	179 (96%)	8 (4%)	29	16
2	M	190/189 (100%)	185 (97%)	5 (3%)	46	36
All	All	761/744 (102%)	732 (96%)	29 (4%)	35	21

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	11	LEU
1	K	33	LEU
1	K	53	THR
1	K	100[A]	GLN
1	K	100[B]	GLN
1	K	176[A]	SER
1	K	176[B]	SER
1	K	188	LYS
1	K	197	THR
1	K	201	LEU

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Mol	Chain	Res	Type
2	M	100	LEU
2	M	137	THR
2	M	140	LEU
2	M	203	GLN
2	M	211	ASN
2	H	64	LYS
2	H	127	SER
2	H	137	THR
2	H	140	LEU
2	H	152	VAL
2	H	153	THR
2	H	163	SER
2	H	177	VAL
1	L	24	ARG
1	L	100[A]	GLN
1	L	100[B]	GLN
1	L	145	LYS
1	L	152	ASN
1	L	207	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	89	GLN
1	K	152	ASN
1	K	198	HIS
1	K	210	ASN
2	M	81	GLN
2	M	82(A)	HIS
2	M	212	HIS
2	H	82(A)	HIS
2	H	212	HIS
1	L	89	GLN
1	L	152	ASN
1	L	210	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	BDF	M	229	-	12,12,12	1.66	2 (16%)	18,18,18	2.31	8 (44%)
4	BDF	H	229	-	12,12,12	1.77	1 (8%)	18,18,18	1.46	5 (27%)
3	MLI	L	214	-	0,6,6	0.00	-	0,7,7	0.00	-
3	MLI	K	214[A]	-	0,6,6	0.00	-	0,7,7	0.00	-
3	MLI	K	214[B]	-	0,6,6	0.00	-	0,7,7	0.00	-

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	BDF	M	229	-	-	0/3/23/23	0/1/1/1
4	BDF	H	229	-	-	0/3/23/23	0/1/1/1
3	MLI	L	214	-	-	0/0/4/4	-
3	MLI	K	214[A]	-	-	0/0/4/4	-
3	MLI	K	214[B]	-	-	0/0/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	229	BDF	C2-C3	5.04	1.58	1.53
4	M	229	BDF	C2-C3	4.47	1.57	1.53
4	M	229	BDF	C5-C4	2.33	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	229	BDF	O6-C2-C1	4.89	111.63	105.58
4	M	229	BDF	O2-C2-O6	-3.70	104.67	110.69
4	M	229	BDF	C5-C4-C3	-3.68	106.36	110.48
4	M	229	BDF	O6-C6-C5	-3.18	106.34	111.11
4	M	229	BDF	O3-C3-C2	3.14	114.93	109.95
4	M	229	BDF	O2-C2-C3	2.91	112.50	107.79
4	H	229	BDF	O2-C2-C1	-2.85	106.69	111.12
4	M	229	BDF	C6-O6-C2	-2.64	111.10	114.09
4	H	229	BDF	O3-C3-C2	2.54	113.98	109.95
4	M	229	BDF	O2-C2-C1	-2.47	107.28	111.12
4	H	229	BDF	C6-O6-C2	2.39	116.79	114.09
4	H	229	BDF	O3-C3-C4	-2.25	105.03	110.03
4	H	229	BDF	O1-C1-C2	-2.10	107.41	111.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	214[B]	MLI	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, 95^{th} 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	K	213/213 (100%)	-0.01	8 (3%) 40 50	28, 39, 73, 90	0
1	L	213/213 (100%)	0.19	18 (8%) 10 17	29, 40, 89, 107	0
2	H	217/224 (96%)	0.48	22 (10%) 7 11	27, 44, 84, 110	0
2	M	218/224 (97%)	0.69	31 (14%) 2 4	29, 46, 101, 134	0
All	All	861/874 (98%)	0.34	79 (9%) 9 14	27, 41, 89, 134	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	198	LEU	8.1
2	M	199	GLY	7.0
2	M	200	THR	6.3
2	M	219	VAL	6.3
2	H	199	GLY	5.6
2	M	198	LEU	5.4
2	M	228	LYS	5.2
1	L	184	ALA	5.1
2	H	165	ALA	4.9
2	M	165	ALA	4.8
2	M	218	LYS	4.8
1	K	212	GLY	4.7
1	L	154	LEU	4.5
2	H	216	ASN	4.5
2	H	200	THR	4.3
2	M	217	THR	4.3
1	L	125	LEU	4.0
1	L	188	LYS	4.0
1	L	126	LYS	3.9
2	M	136	GLY	3.9
1	K	213	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
2	M	196	SER	3.6
2	M	215	SER	3.6
1	L	153	ALA	3.5
2	M	98	ASP	3.4
2	M	164	GLY	3.2
1	L	156	SER	3.2
1	K	188	LYS	3.2
2	M	206	TYR	3.2
2	M	214	PRO	3.1
2	M	1	GLU	3.1
2	H	217	THR	3.1
2	M	99	ARG	3.1
2	H	213	LYS	3.0
1	L	122	ASP	3.0
1	L	1	ALA	2.9
1	L	127[A]	SER	2.9
2	H	215	SER	2.9
2	H	127	SER	2.8
2	H	196	SER	2.8
2	M	210	VAL	2.8
2	M	205	THR	2.7
2	H	1	GLU	2.8
1	K	125	LEU	2.7
2	H	116	THR	2.7
2	H	214	PRO	2.7
2	M	195	SER	2.7
2	M	211	ASN	2.6
2	M	213	LYS	2.6
1	K	184	ALA	2.6
2	H	2	VAL	2.6
1	L	181	LEU	2.5
2	M	163	SER	2.5
2	M	127	SER	2.5
2	M	220	ASP	2.4
1	L	192	TYR	2.4
1	L	190	LYS	2.4
1	L	34	ALA	2.4
2	H	207	ILE	2.3
1	L	212	GLY	2.3
1	L	191	VAL	2.3
2	H	53	SER	2.3
2	H	211	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
2	M	209	ASN	2.2
2	M	138	ALA	2.2
2	M	36	TRP	2.2
1	L	189	HIS	2.2
2	H	197	SER	2.2
1	K	96	ALA	2.2
2	M	137	THR	2.1
1	K	122	ASP	2.1
2	H	190	VAL	2.1
2	H	140	LEU	2.1
1	K	202	SER	2.1
2	H	36	TRP	2.1
1	L	213	GLU	2.1
2	M	212	HIS	2.1
2	H	205	THR	2.0
2	M	216	ASN	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, 95^{th} 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
3	MLI	K	214[A]	7/7	0.94	0.12	32,33,39,39	7
3	MLI	K	214[B]	7/7	0.94	0.12	28,33,39,44	7
3	MLI	L	214	7/7	0.97	0.12	41,45,51,53	0
4	BDF	H	229	12/12	0.98	0.13	29,33,33,34	0
4	BDF	M	229	12/12	0.98	0.06	32,36,40,44	0

6.5 Other polymers (i)

There are no such residues in this entry.