



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:21 AM UTC

PDB ID : 3OAY / pdb_00003oay
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

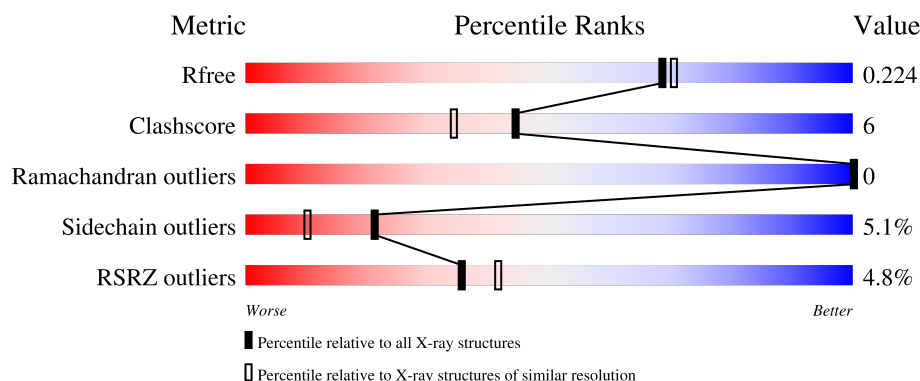
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 of 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	K	213	0% 86% 12% .
1	L	213	4% 86% 13% .
2	H	224	5% 77% 17% ..
2	M	224	8% 78% 17% ..

2 Entry composition [i](#)

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.

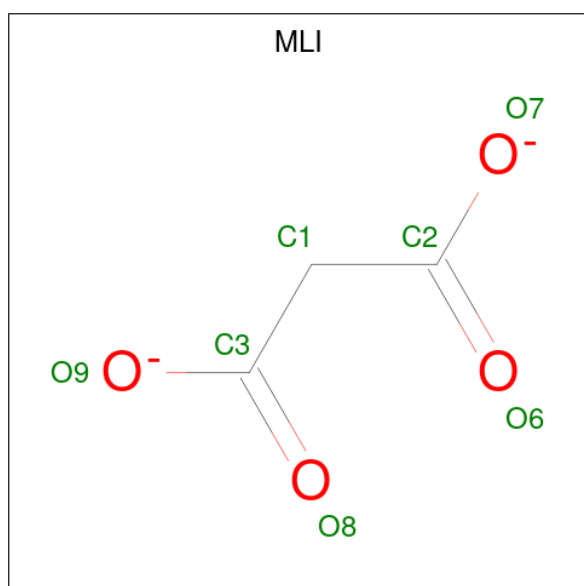
- Molecule 1 is a protein called Fab 2G12, light chain.

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.

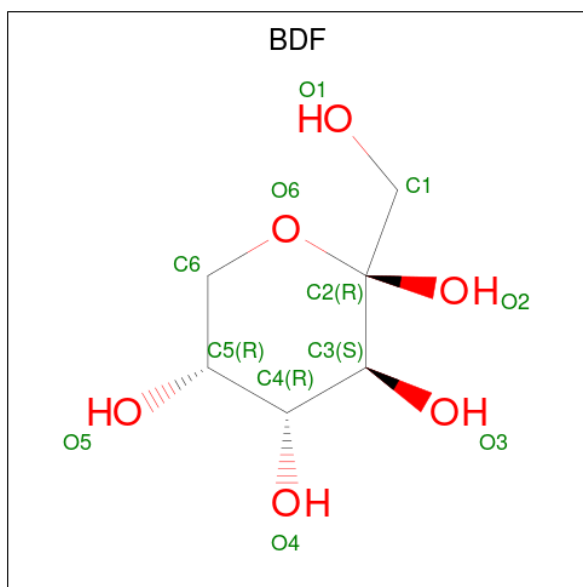
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	218	Total	C	N	O	S	0	6	0
			1664	1055	279	323	7			
2	H	217	Total	C	N	O	S	0	5	0
			1645	1038	279	321	7			

- Molecule 3 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



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

- Molecule 4 is beta-D-fructopyranose (CCD ID: BDF) (formula: $C_6H_{12}O_6$).



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

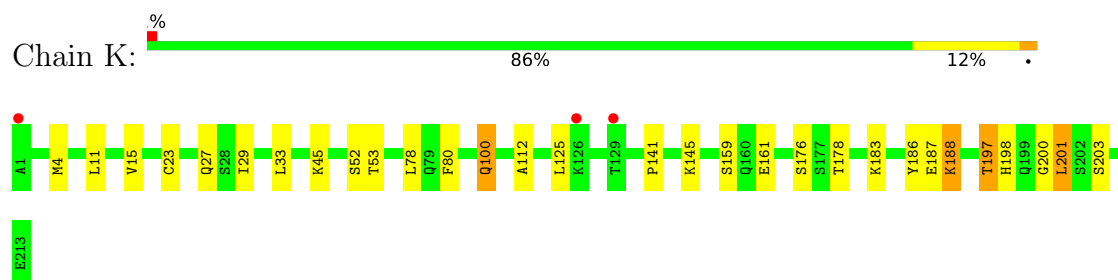
- Molecule 5 is water.

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

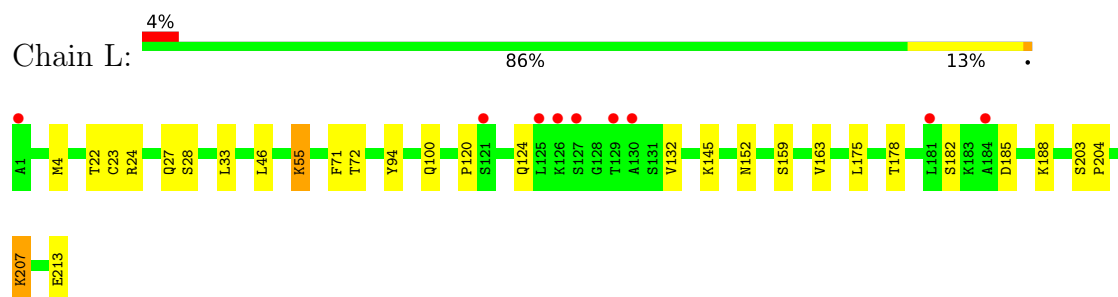
3 Residue-property plots [i](#)

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.

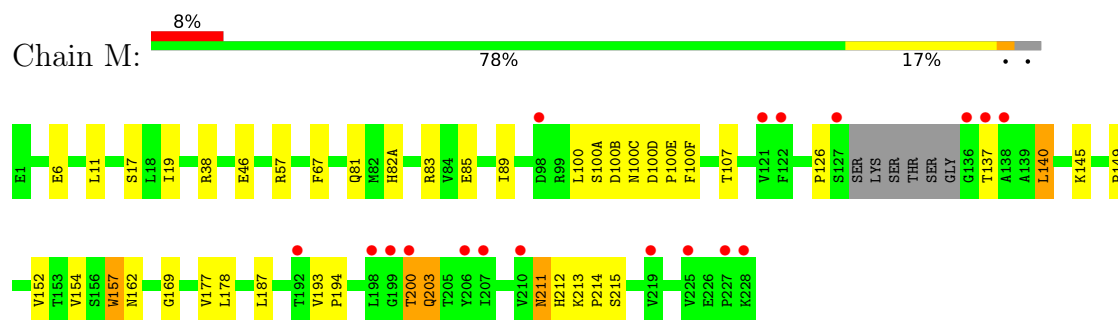
- Molecule 1: Fab 2G12, light chain



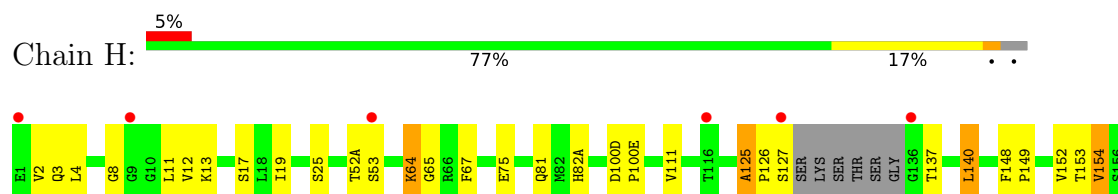
- Molecule 1: Fab 2G12, light chain

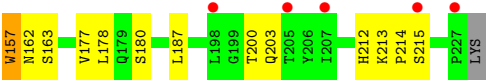


- Molecule 2: Fab 2G12, heavy chain



- Molecule 2: Fab 2G12, heavy chain





4 Data and refinement statistics

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 30.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	89.5 (30.00-1.95) 89.5 (30.00-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.53%)	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)	0.34 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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.*

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: BDF, MLI

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	0.82	0/1743	0.95	4/2365 (0.2%)
1	L	0.89	2/1729 (0.1%)	0.93	0/2348
2	H	0.86	1/1699 (0.1%)	0.99	4/2316 (0.2%)
2	M	0.89	2/1720 (0.1%)	1.04	6/2344 (0.3%)
All	All	0.87	5/6891 (0.1%)	0.98	14/9373 (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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	157	TRP	C-N	11.45	1.48	1.33
1	L	182	SER	CB-OG	9.17	1.60	1.42
2	H	157	TRP	C-N	8.75	1.44	1.33
2	M	154	VAL	C-N	5.24	1.40	1.33
1	L	213	GLU	C-O	5.05	1.33	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	157	TRP	CA-C-N	-6.80	112.87	122.46
2	M	157	TRP	C-N-CA	-6.80	112.87	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	125	ALA	CA-C-N	6.73	126.77	119.90
2	H	125	ALA	C-N-CA	6.73	126.77	119.90
2	H	8	GLY	N-CA-C	-6.42	101.92	112.83
2	M	152	VAL	N-CA-C	-5.95	99.59	108.46
2	M	145	LYS	N-CA-C	5.89	118.65	109.52
1	K	203	SER	CA-C-N	-5.29	114.33	119.78
1	K	203	SER	C-N-CA	-5.29	114.33	119.78
1	K	52	SER	CA-C-N	-5.24	114.80	122.19
1	K	52	SER	C-N-CA	-5.24	114.80	122.19
2	M	200	THR	CA-C-N	-5.12	115.77	122.99
2	M	200	THR	C-N-CA	-5.12	115.77	122.99
2	H	154	VAL	O-C-N	-5.12	118.06	123.03

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 [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	1677	0	1673	18	0
1	L	1669	0	1656	16	0
2	H	1645	0	1618	25	0
2	M	1664	0	1658	26	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	80	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 (80) 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:K:100[A]:GLN:H	1:K:100[A]:GLN:CD	1.82	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
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:187:LEU:C	2:M:187:LEU:HD12	2.27	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
1:L:4:MET:HE3	1:L:23:CYS:SG	2.47	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
1:K:4:MET:HE3	1:K:23:CYS:SG	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:M:157:TRP:O	2:M:162:ASN:C	2.56	0.49
2:M:6:GLU:HB2	2:M:107[B]:THR:OG1	2.12	0.48
2:H:149:PRO:O	2:H:212:HIS:HE1	1.96	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
2:H:52(A):THR:O	2:H:53:SER:OG	2.29	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:HD12	2:H:4:LEU:N	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:83:ARG:HD3	2:M:85:GLU:OE2	2.18	0.44
2:M:46[A]:GLU:OE2	5:M:283:HOH:O	2.21	0.43
2:H:64:LYS:HD3	2:H:65:GLY:N	2.33	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
1:L:27:GLN:O	1:L:28:SER:C	2.60	0.43
2:H:19:ILE:HD12	2:H:81:GLN:HG2	2.00	0.43
2:M:187:LEU:C	2:M:187:LEU:CD1	2.92	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:M:81:GLN:NE2	2:M:82(A):HIS:CE1	2.69	0.41
2:H:67:PHE:HA	2:H:81:GLN:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:67:PHE:HA	2:M:81:GLN:O	2.21	0.41
2:H:157:TRP:O	2:H:162:ASN:C	2.63	0.41
2:H:187:LEU:C	2:H:187:LEU:HD12	2.46	0.41
2:H:213:LYS:N	2:H:214:PRO:CD	2.84	0.41
2:M:38:ARG:HA	2:M:89:ILE:O	2.20	0.40
2:H:212:HIS:CD2	2:H:215:SER:OG	2.58	0.40
2:M:211:ASN:ND2	2:M:211:ASN:C	2.79	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%)	182 (94%)	11 (6%)	18	8
1	L	191/183 (104%)	184 (96%)	7 (4%)	30	20
2	H	187/189 (99%)	177 (95%)	10 (5%)	20	9
2	M	190/189 (100%)	178 (94%)	12 (6%)	16	6
All	All	761/744 (102%)	721 (95%)	40 (5%)	21	9

All (40) 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	78	LEU
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
2	M	100	LEU
2	M	100(A)	SER
2	M	100(B)	ASP
2	M	100(C)	ASN
2	M	100(D)	ASP
2	M	100(E)	PRO
2	M	100(F)	PHE
2	M	137	THR
2	M	140	LEU
2	M	177	VAL
2	M	203	GLN
2	M	211	ASN
2	H	2	VAL
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
2	H	203	GLN

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Mol	Chain	Res	Type
1	L	24	ARG
1	L	55	LYS
1	L	100[A]	GLN
1	L	100[B]	GLN
1	L	145	LYS
1	L	152	ASN
1	L	207	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	89	GLN
1	K	147	GLN
1	K	152	ASN
1	K	189	HIS
1	K	198	HIS
1	K	210	ASN
2	M	81	GLN
2	M	82(A)	HIS
2	M	212	HIS
2	H	35	ASN
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	H	229	-	12,12,12	1.59	1 (8%)	18,18,18	1.38	3 (16%)
3	MLI	L	214	-	6,6,6	1.26	1 (16%)	7,7,7	1.16	0
3	MLI	K	214[B]	-	6,6,6	1.05	0	7,7,7	1.88	2 (28%)
4	BDF	M	229	-	12,12,12	1.49	2 (16%)	18,18,18	2.01	8 (44%)
3	MLI	K	214[A]	-	6,6,6	1.44	1 (16%)	7,7,7	0.93	0

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	229	BDF	C2-C3	4.39	1.58	1.53
4	M	229	BDF	C2-C3	3.90	1.57	1.53
3	K	214[A]	MLI	O6-C2	2.26	1.29	1.22
4	M	229	BDF	C5-C4	2.26	1.55	1.52
3	L	214	MLI	O7-C2	-2.02	1.24	1.30

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	M	229	BDF	O6-C2-C1	4.48	111.63	105.41
4	M	229	BDF	O3-C3-C2	3.24	114.93	109.89
4	M	229	BDF	O2-C2-O6	-2.99	104.67	110.39
4	M	229	BDF	O6-C6-C5	-2.96	106.34	111.06
3	K	214[B]	MLI	O6-C2-C1	-2.84	114.03	122.11
4	H	229	BDF	O2-C2-C1	-2.67	106.69	111.35
3	K	214[B]	MLI	O8-C3-C1	-2.65	114.56	122.11
4	H	229	BDF	O3-C3-C2	2.63	113.98	109.89
4	M	229	BDF	O2-C2-C3	2.55	112.50	107.93
4	M	229	BDF	O2-C2-C1	-2.34	107.28	111.35
4	M	229	BDF	C5-C4-C3	-2.25	106.36	110.49
4	H	229	BDF	O3-C3-C4	-2.21	105.03	110.00
4	M	229	BDF	C6-O6-C2	-2.14	111.10	114.09

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, 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	K	213/213 (100%)	-0.07	3 (1%) 73 79	21, 39, 73, 90	10 (4%)
1	L	213/213 (100%)	0.15	9 (4%) 40 47	22, 40, 89, 107	8 (3%)
2	H	217/224 (96%)	0.23	11 (5%) 33 39	21, 43, 84, 110	5 (2%)
2	M	218/224 (97%)	0.39	18 (8%) 17 20	20, 46, 101, 134	6 (2%)
All	All	861/874 (98%)	0.18	41 (4%) 35 41	20, 41, 88, 134	29 (3%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	53	SER	4.0
1	L	125	LEU	3.9
2	H	198	LEU	3.9
1	L	184	ALA	3.9
2	M	225	VAL	3.8
1	L	127[A]	SER	3.6
2	M	206	TYR	3.6
2	M	137	THR	3.5
1	L	129[A]	THR	3.4
2	M	198	LEU	3.3
2	M	228	LYS	3.2
2	M	138	ALA	3.2
2	M	199	GLY	3.1
2	M	127	SER	3.0
2	H	215	SER	2.7
1	L	130	ALA	2.7
2	H	227	PRO	2.7
1	L	1	ALA	2.7
2	M	122	PHE	2.7
2	H	1	GLU	2.7
2	M	200	THR	2.6

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Mol	Chain	Res	Type	RSRZ
2	M	207	ILE	2.6
2	H	9	GLY	2.6
1	K	1	ALA	2.4
1	K	129	THR	2.4
2	H	207	ILE	2.4
1	K	126	LYS	2.3
1	L	121	SER	2.3
2	M	136	GLY	2.2
2	H	136	GLY	2.2
2	M	98	ASP	2.2
1	L	126	LYS	2.2
2	H	205	THR	2.2
2	M	227	PRO	2.2
2	M	192	THR	2.1
2	H	116	THR	2.1
1	L	181	LEU	2.1
2	M	210	VAL	2.0
2	M	219	VAL	2.0
2	H	127	SER	2.0
2	M	121[A]	VAL	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 oligosaccharides 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(Å ²)	Q<0.9
3	MLI	K	214[A]	7/7	0.90	0.11	32,33,39,39	7
3	MLI	K	214[B]	7/7	0.90	0.11	28,33,39,44	7
3	MLI	L	214	7/7	0.95	0.06	41,45,51,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BDF	M	229	12/12	0.95	0.07	32,36,40,44	0
4	BDF	H	229	12/12	0.97	0.05	29,33,33,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.