



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 05:27 AM GMT

PDB ID : 4JKP
Title : Restricting HIV-1 Pathways for Escape using Rationally-Designed Anti-HIV-1 Antibodies
Authors : Diskin, R.; Bjorkman, P.J.
Deposited on : 2013-03-11
Resolution : 2.82 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

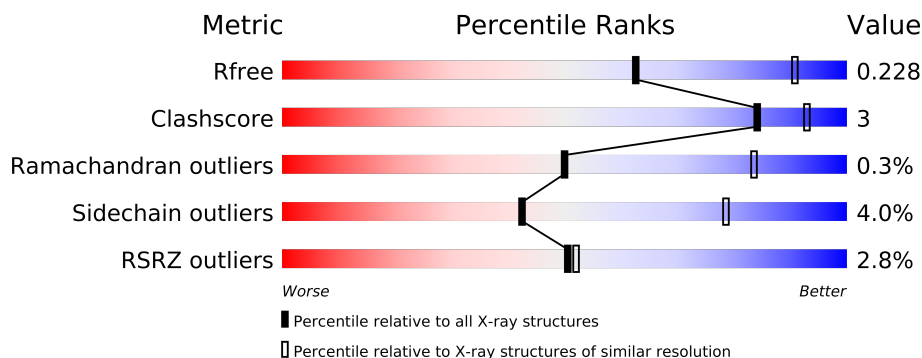
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.82 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}	66092	1963 (2.84-2.80)
Clashscore	79885	2478 (2.84-2.80)
Ramachandran outliers	78287	2429 (2.84-2.80)
Sidechain outliers	78261	2431 (2.84-2.80)
RSRZ outliers	66119	1966 (2.84-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	G	361	
2	H	229	
3	L	210	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6263 atoms, of which 0 are hydrogen and 0 are deuterium.

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 gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	340	Total	C	N	O	S	0	1	0
			2669	1674	463	508	24			

- Molecule 2 is a protein called Heavy chain of antibody 45-46M2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	222	Total	C	N	O	S	0	1	0
			1728	1093	304	321	10			

- Molecule 3 is a protein called Light chain of antibody 45-46M2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	207	Total	C	N	O	S	0	0	0
			1601	1003	273	321	4			

- Molecule 4 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	G	6	Total	C	N	O	0	0
			72	40	2	30		

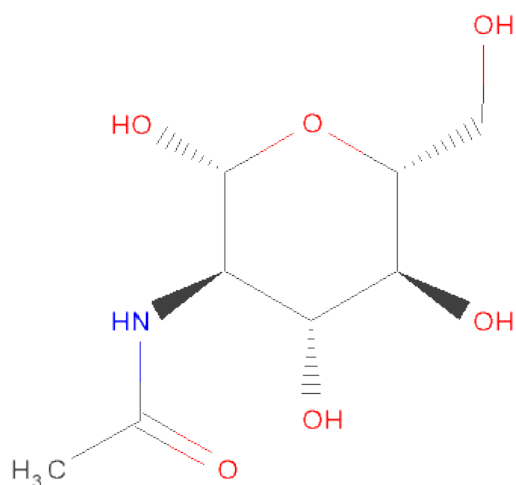
- Molecule 5 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	G	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	G	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	L	1	Total	C	N	O	0	0
			14	8	1	5		

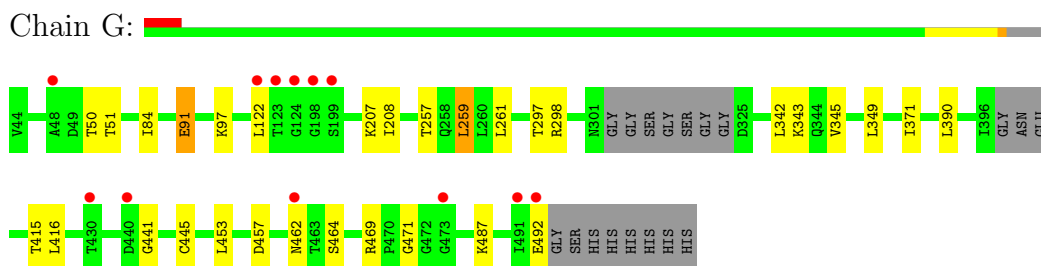
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	7	Total	O	0	0
			7	7		
8	H	13	Total	O	0	0
			13	13		
8	L	3	Total	O	0	0
			3	3		

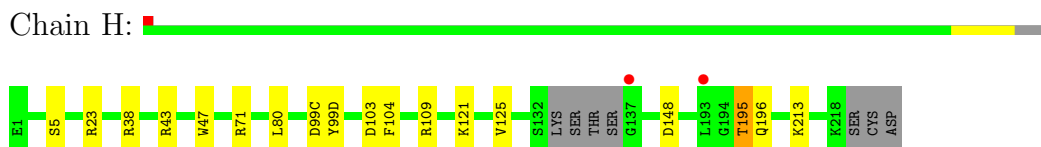
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

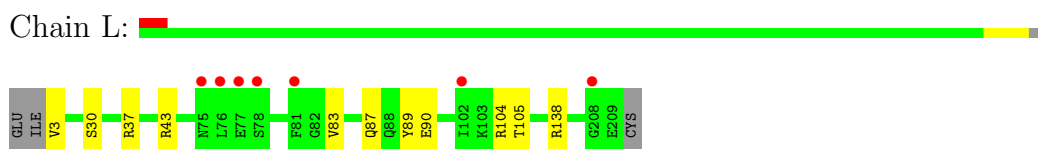
- Molecule 1: gp120



- Molecule 2: Heavy chain of antibody 45-46M2



- Molecule 3: Light chain of antibody 45-46M2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.33Å 70.49Å 232.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.85 – 2.82 34.85 – 2.82	Depositor EDS
% Data completeness (in resolution range)	98.5 (34.85-2.82) 92.6 (34.85-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1334)	Depositor
R, R_{free}	0.193 , 0.231 0.192 , 0.228	Depositor DCC
R_{free} test set	1310 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	66.2	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 39.7	EDS
Estimated twinning fraction	0.033 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 27846 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6263	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, PCA, NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	G	0.32	0/2728	0.51	1/3703 (0.0%)
2	H	0.29	0/1772	0.48	0/2411
3	L	0.31	0/1637	0.53	0/2223
All	All	0.31	0/6137	0.51	1/8337 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	122	LEU	CA-CB-CG	7.32	132.13	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2669	0	0	8	0
2	H	1728	0	6	9	0
3	L	1601	0	0	3	0
4	G	72	0	61	0	0
5	G	61	0	52	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	39	0	34	0	0
7	G	56	0	52	0	0
7	L	14	0	13	0	0
8	G	7	0	0	0	0
8	H	13	0	0	3	0
8	L	3	0	0	0	0
All	All	6263	0	218	19	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (19) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:207:LYS:NZ	5:G:610:MAN:O4	2.09	0.86
1:G:97:LYS:NZ	2:H:99(C):ASP:OD2	2.15	0.80
2:H:103:ASP:OD2	8:H:312:HOH:O	2.03	0.76
2:H:195:THR:OG1	2:H:196:GLN:N	2.30	0.64
3:L:104:ARG:NH1	3:L:105:THR:O	2.31	0.63
2:H:99(C):ASP:OD1	2:H:99(D):TYR:N	2.36	0.59
2:H:47:TRP:N	8:H:309:HOH:O	2.37	0.57
3:L:87:GLN:NE2	3:L:89:TYR:O	2.42	0.53
2:H:125:VAL:O	2:H:213:LYS:NZ	2.43	0.52
1:G:50:THR:OG1	1:G:51:THR:N	2.43	0.51
1:G:91:GLU:OE1	1:G:487:LYS:NZ	2.45	0.49
2:H:121:LYS:NZ	2:H:148:ASP:O	2.47	0.48
1:G:298:ARG:NH2	1:G:441:GLY:O	2.47	0.47
3:L:37:ARG:NH2	3:L:43:ARG:NH1	2.63	0.47
2:H:5:SER:O	2:H:23:ARG:N	2.49	0.45
2:H:109:ARG:N	8:H:303:HOH:O	2.51	0.44
1:G:257:THR:O	1:G:259:LEU:N	2.51	0.43
1:G:457:ASP:OD2	1:G:469:ARG:NH2	2.52	0.42
1:G:453:LEU:O	1:G:471:GLY:N	2.53	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	335/361 (93%)	318 (95%)	17 (5%)	0	100	100
2	H	219/229 (96%)	208 (95%)	10 (5%)	1 (0%)	38	75
3	L	205/210 (98%)	198 (97%)	6 (3%)	1 (0%)	38	75
All	All	759/800 (95%)	724 (95%)	33 (4%)	2 (0%)	50	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	104	PHE
3	L	30	SER

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	G	305/318 (96%)	287 (94%)	18 (6%)	28	62
2	H	189/195 (97%)	184 (97%)	5 (3%)	59	90
3	L	178/181 (98%)	174 (98%)	4 (2%)	64	92
All	All	672/694 (97%)	645 (96%)	27 (4%)	42	78

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	84	ILE
1	G	91	GLU
1	G	208	ILE
1	G	259	LEU
1	G	261	LEU
1	G	297	THR
1	G	342	LEU
1	G	343	LYS
1	G	345	VAL
1	G	349	LEU

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Mol	Chain	Res	Type
1	G	371	ILE
1	G	390	LEU
1	G	415	THR
1	G	416	LEU
1	G	445	CYS
1	G	462	ASN
1	G	464	SER
1	G	492	GLU
2	H	38	ARG
2	H	43	ARG
2	H	71	ARG
2	H	80	LEU
2	H	195	THR
3	L	3	VAL
3	L	83	VAL
3	L	90	GLU
3	L	138	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
2	PCA	H	1	2	8,8,9	6.71	3 (37%)	8,10,12	5.29	3 (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
2	PCA	H	1	2	-	0/0/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	PCA	O-C	17.86	1.23	1.11
2	H	1	PCA	CD-N	5.93	1.47	1.34
2	H	1	PCA	CA-C	2.48	1.52	1.48

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	PCA	CA-N-CD	-14.12	103.33	114.37
2	H	1	PCA	OE-CD-CG	-3.44	121.31	126.70
2	H	1	PCA	CB-CA-N	2.39	110.61	103.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

14 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	G	601	1,4	12,14,15	0.69	1 (8%)	15,19,21	0.94	0
4	NAG	G	602	4	12,14,15	0.58	0	15,19,21	1.49	3 (20%)
4	BMA	G	603	4	10,11,12	1.91	2 (20%)	11,15,17	1.37	3 (27%)
4	MAN	G	604	4	10,11,12	0.83	1 (10%)	11,15,17	1.39	2 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	G	605	4	10,11,12	0.79	0	11,15,17	0.93	1 (9%)
4	MAN	G	606	4	10,11,12	0.83	1 (10%)	11,15,17	0.66	0
5	NAG	G	607	1,5	12,14,15	0.70	0	15,19,21	1.26	3 (20%)
5	NAG	G	608	5	12,14,15	0.80	1 (8%)	15,19,21	0.72	0
5	BMA	G	609	5	10,11,12	1.79	2 (20%)	11,15,17	1.54	2 (18%)
5	MAN	G	610	5	10,11,12	0.74	0	11,15,17	0.57	0
5	MAN	G	611	5	10,11,12	0.79	0	11,15,17	0.99	1 (9%)
6	NAG	G	612	1,6	12,14,15	0.64	0	15,19,21	0.76	0
6	NAG	G	613	6	12,14,15	0.70	1 (8%)	15,19,21	0.87	1 (6%)
6	BMA	G	614	6	10,11,12	1.84	2 (20%)	11,15,17	1.81	3 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	602	4	-	0/6/23/26	0/1/1/1
4	BMA	G	603	4	-	0/2/19/22	0/1/1/1
4	MAN	G	604	4	-	0/2/19/22	0/1/1/1
4	MAN	G	605	4	-	0/2/19/22	0/1/1/1
4	MAN	G	606	4	-	0/2/19/22	0/1/1/1
5	NAG	G	607	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	608	5	-	0/6/23/26	0/1/1/1
5	BMA	G	609	5	-	0/2/19/22	0/1/1/1
5	MAN	G	610	5	-	0/2/19/22	0/1/1/1
5	MAN	G	611	5	-	0/2/19/22	0/1/1/1
6	NAG	G	612	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	613	6	-	0/6/23/26	0/1/1/1
6	BMA	G	614	6	-	0/2/19/22	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	603	BMA	C4-C3	-5.03	1.39	1.52
6	G	614	BMA	C4-C3	-4.80	1.39	1.52
5	G	609	BMA	C4-C3	-4.74	1.39	1.52
4	G	603	BMA	C3-C2	-2.80	1.46	1.52
5	G	609	BMA	C3-C2	-2.66	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	614	BMA	C3-C2	-2.65	1.47	1.52
5	G	608	NAG	O5-C5	-2.33	1.41	1.45
4	G	606	MAN	O5-C5	-2.08	1.41	1.45
6	G	613	NAG	O5-C5	-2.06	1.41	1.45
4	G	604	MAN	O5-C5	-2.04	1.41	1.45
4	G	601	NAG	O5-C5	-2.04	1.41	1.45

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	602	NAG	O5-C5-C4	3.73	115.39	110.65
4	G	604	MAN	O5-C5-C6	3.52	110.68	106.98
6	G	614	BMA	O3-C3-C2	-3.18	104.11	109.94
6	G	614	BMA	O5-C5-C6	3.15	110.29	106.98
5	G	609	BMA	O5-C5-C4	2.98	114.43	110.65
4	G	602	NAG	C3-C4-C5	2.90	115.38	110.20
4	G	602	NAG	O5-C5-C6	2.85	109.98	106.98
5	G	607	NAG	C3-C2-N2	-2.85	107.42	111.76
5	G	611	MAN	O5-C5-C6	2.80	109.92	106.98
4	G	604	MAN	O5-C5-C4	-2.51	107.47	110.65
5	G	609	BMA	O4-C4-C3	-2.51	104.72	110.35
5	G	607	NAG	O5-C5-C6	2.48	109.58	106.98
4	G	603	BMA	O5-C5-C6	2.30	109.39	106.98
4	G	605	MAN	O5-C5-C6	2.27	109.36	106.98
5	G	607	NAG	C6-C5-C4	-2.18	107.73	113.00
4	G	603	BMA	O5-C5-C4	2.11	113.34	110.65
6	G	613	NAG	C3-C2-N2	-2.03	108.66	111.76
4	G	603	BMA	O4-C4-C3	-2.03	105.81	110.35
6	G	614	BMA	C4-C3-C2	2.01	113.20	110.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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$
7	NAG	G	615	1	12,14,15	0.56	0	15,19,21	0.85	0
7	NAG	G	616	1	12,14,15	0.63	0	15,19,21	0.77	0
7	NAG	G	617	1	12,14,15	0.67	1 (8%)	15,19,21	0.63	0
7	NAG	G	618	1	12,14,15	0.71	0	15,19,21	1.71	2 (13%)
7	NAG	L	501	3	12,14,15	0.39	0	15,19,21	0.61	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
7	NAG	G	615	1	-	0/6/23/26	0/1/1/1
7	NAG	G	616	1	-	0/6/23/26	0/1/1/1
7	NAG	G	617	1	-	0/6/23/26	0/1/1/1
7	NAG	G	618	1	-	0/6/23/26	0/1/1/1
7	NAG	L	501	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	617	NAG	O5-C5	-2.05	1.41	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	618	NAG	C3-C2-N2	-5.33	103.64	111.76
7	G	618	NAG	O5-C5-C6	2.55	109.66	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	G	340/361 (94%)	-0.07	13 (3%) 38 39	39, 67, 125, 174	0
2	H	222/229 (96%)	-0.19	2 (0%) 81 81	42, 69, 98, 142	0
3	L	207/210 (98%)	-0.00	7 (3%) 43 44	56, 89, 121, 147	0
All	All	769/800 (96%)	-0.09	22 (2%) 50 51	39, 73, 119, 174	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	124	GLY	6.7
2	H	137	GLY	5.2
3	L	76	LEU	4.6
2	H	193	LEU	4.0
1	G	123	THR	3.9
3	L	81	PHE	3.8
1	G	198	GLY	3.6
1	G	473	GLY	3.2
3	L	208	GLY	3.1
1	G	122	LEU	2.9
1	G	199	SER	2.8
1	G	430	THR	2.6
1	G	492	GLU	2.5
3	L	78	SER	2.4
1	G	491	ILE	2.4
3	L	75	ASN	2.3
1	G	48	ALA	2.2
1	G	440	ASP	2.2
1	G	409	GLY	2.2
3	L	102	ILE	2.2
3	L	77	GLU	2.1
1	G	462	ASN	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	PCA	H	1	8/9	0.30	-	74,83,88,90	0

6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MAN	G	605	11/12	0.32	-	144,150,151,153	0
4	BMA	G	603	11/12	0.14	-	155,162,165,169	0
4	MAN	G	604	11/12	0.16	-	147,150,153,154	0
6	BMA	G	614	11/12	0.23	-	121,129,131,132	0
6	NAG	G	613	14/15	0.22	-	104,112,118,125	0
4	NAG	G	601	14/15	0.21	-	79,99,112,122	0
5	NAG	G	608	14/15	0.15	-	75,79,85,101	0
5	BMA	G	609	11/12	0.12	-	113,118,127,127	0
4	MAN	G	606	11/12	0.23	-	163,172,173,175	0
5	MAN	G	610	11/12	0.26	-	116,128,130,130	0
5	NAG	G	607	14/15	0.14	-	46,59,68,71	0
5	MAN	G	611	11/12	0.28	-	121,126,127,129	0
6	NAG	G	612	14/15	0.10	-	68,81,87,95	0
4	NAG	G	602	14/15	0.33	-	138,146,153,158	0

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	NAG	G	618	14/15	0.34	-	89,107,113,113	0
7	NAG	G	616	14/15	0.20	-	69,79,85,90	0
7	NAG	G	617	14/15	0.33	-	91,105,112,116	0
7	NAG	L	501	14/15	0.25	-	119,128,133,134	0
7	NAG	G	615	14/15	0.15	-	74,94,97,97	0

6.5 Other polymers ⓘ

There are no such residues in this entry.