Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:49 PM 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 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

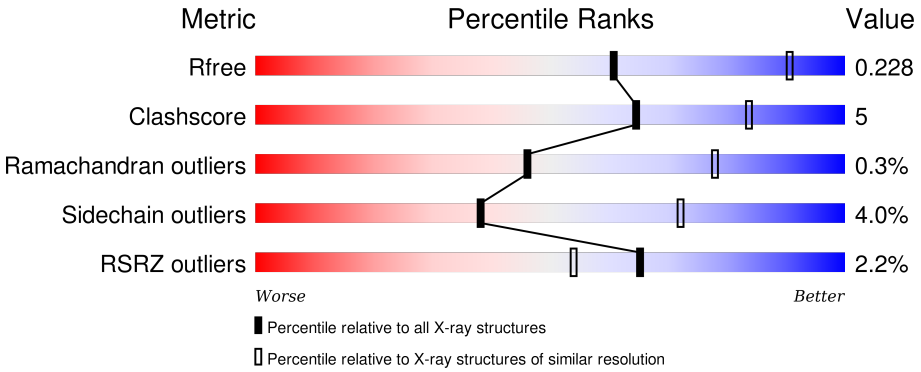
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 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}	91344	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (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. 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	G	361	2% 78% 15% 6%
2	H	229	% 83% 13%
3	L	210	3% 81% 17%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NAG	G	617	-	-	-	X
7	NAG	G	618	-	-	-	X
7	NAG	L	501	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6263 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 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		

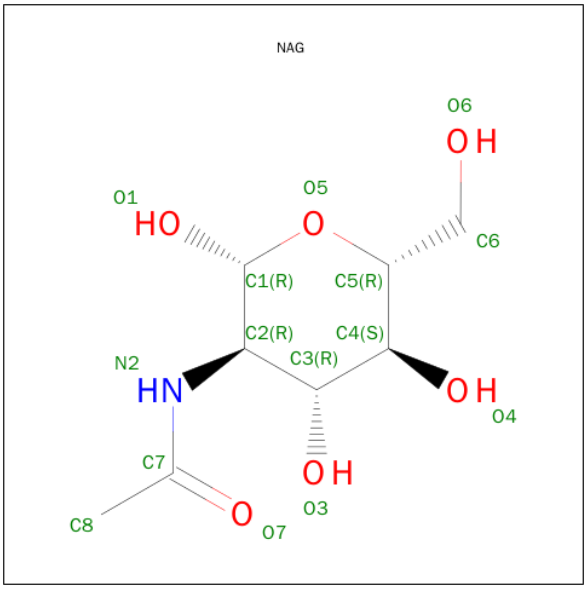
- Molecule 5 is a polymer of unknown type called SUGAR (5-MER).

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 14 8 1 5	0	0
7	G	1	Total C N O 14 8 1 5	0	0
7	G	1	Total C N O 14 8 1 5	0	0
7	G	1	Total C N O 14 8 1 5	0	0
7	L	1	Total C N O 14 8 1 5	0	0

- Molecule 8 is water.

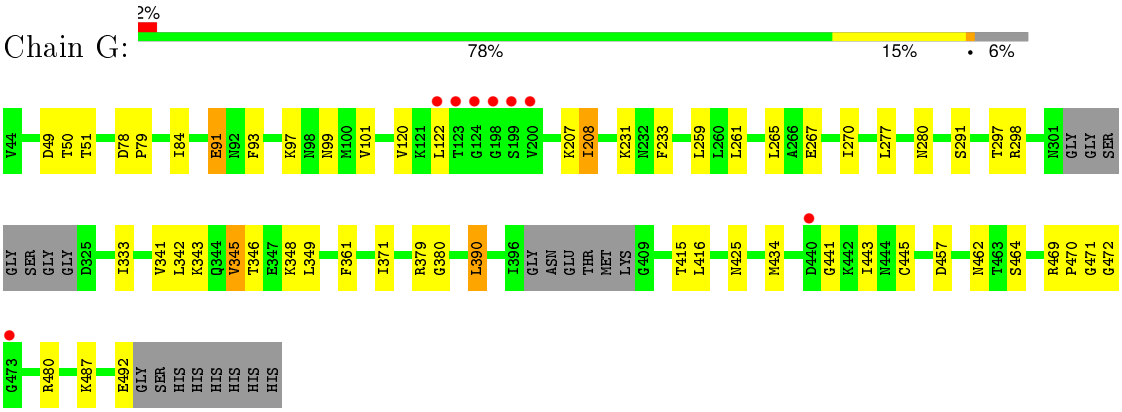
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	G	7	Total O 7 7	0	0
8	H	13	Total O 13 13	0	0
8	L	3	Total O 3 3	0	0

3 Residue-property plots (i)

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.

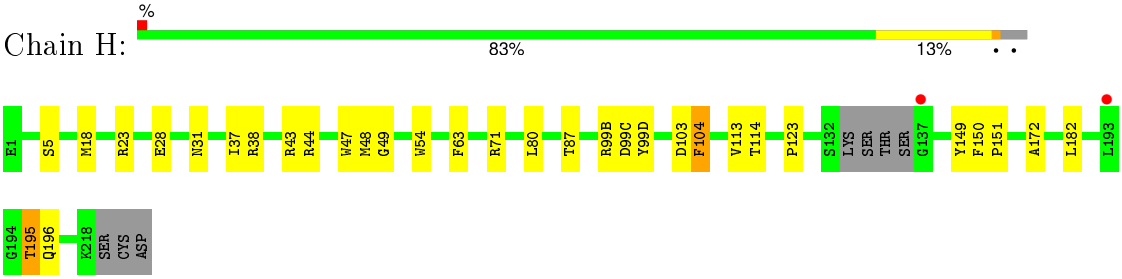
- Molecule 1: gp120

Chain G:



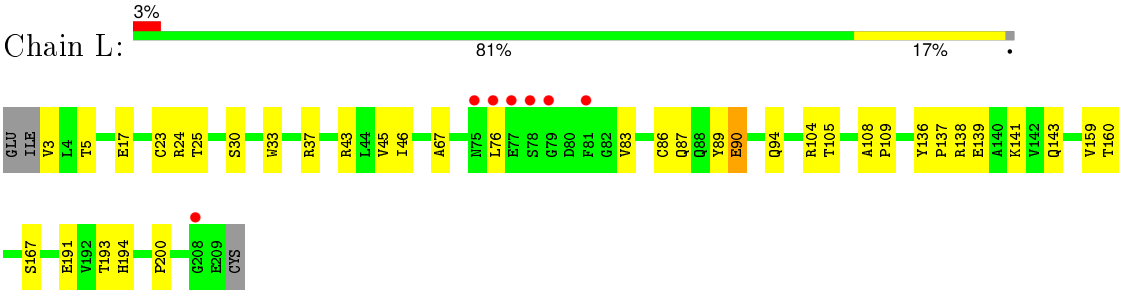
- Molecule 2: Heavy chain of antibody 45-46M2

Chain H:



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

Chain L:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.52 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1334)	Depositor
R, R_{free}	0.193 , 0.231 0.190 , 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)	0.29 , 46.7	EDS
Estimated twinning fraction	0.033 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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(^{o})	Ideal(^{o})
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 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	G	2669	0	2598	26	0
2	H	1728	0	1683	19	0
3	L	1601	0	1538	22	0
4	G	72	0	61	1	0
5	G	61	0	52	1	0
6	G	39	0	34	0	0
7	G	56	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	L	14	0	13	0	0
8	G	7	0	0	0	0
8	H	13	0	0	1	0
8	L	3	0	0	0	0
All	All	6263	0	6031	63	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 5.

All (63) 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:G:207:LYS:NZ	5:G:610:MAN:O4	2.09	0.86
2:H:103:ASP:OD2	8:H:312:HOH:O	2.03	0.76
1:G:97:LYS:NZ	2:H:99(C):ASP:OD2	2.15	0.74
1:G:333:ILE:HD12	1:G:390:LEU:HD11	1.72	0.71
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
3:L:37:ARG:HH22	3:L:43:ARG:NH1	1.97	0.62
2:H:99(C):ASP:OD1	2:H:99(D):TYR:N	2.36	0.59
2:H:99(B):ARG:HB2	2:H:99(B):ARG:HH11	1.66	0.59
2:H:123:PRO:HB3	2:H:149:TYR:HB3	1.85	0.58
2:H:44:ARG:HH22	3:L:94:GLN:HE21	1.53	0.56
3:L:104:ARG:HD2	3:L:167:SER:HB2	1.89	0.55
1:G:101:VAL:HG21	1:G:480:ARG:HG2	1.88	0.55
2:H:5:SER:HB2	2:H:23:ARG:HB3	1.89	0.54
1:G:231:LYS:HD2	1:G:267:GLU:HG3	1.89	0.54
1:G:50:THR:OG1	1:G:51:THR:N	2.43	0.51
1:G:265:LEU:HD21	1:G:291:SER:HB3	1.93	0.51
2:H:99(B):ARG:NH1	2:H:99(B):ARG:HB2	2.26	0.50
3:L:193:THR:HG22	3:L:200:PRO:HG3	1.94	0.50
1:G:425:ASN:HB2	2:H:54:TRP:HZ3	1.77	0.49
1:G:93:PHE:HB2	1:G:233:PHE:HZ	1.76	0.49
2:H:172:ALA:HB2	2:H:182:LEU:HD23	1.95	0.48
1:G:91:GLU:OE1	1:G:487:LYS:NZ	2.45	0.48
3:L:143:GLN:HB3	3:L:191:GLU:HB3	1.96	0.48
3:L:87:GLN:NE2	3:L:89:TYR:O	2.42	0.48
3:L:141:LYS:HB3	3:L:193:THR:OG1	2.14	0.47
1:G:298:ARG:NH2	1:G:441:GLY:O	2.47	0.47
1:G:120:VAL:HG22	1:G:434:MET:HB3	1.96	0.47
3:L:5:THR:HA	3:L:94:GLN:HE22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.50	0.46
1:G:277:LEU:HB2	4:G:601:NAG:H82	1.98	0.46
1:G:208:ILE:HG13	1:G:380:GLY:HA3	1.98	0.46
1:G:280:ASN:HD21	3:L:90:GLU:HG2	1.81	0.46
3:L:37:ARG:NH2	3:L:43:ARG:NH1	2.63	0.45
2:H:37:ILE:HD11	2:H:104:PHE:CE2	2.52	0.45
1:G:93:PHE:HB2	1:G:233:PHE:CZ	2.53	0.44
3:L:90:GLU:H	3:L:90:GLU:HG3	1.47	0.44
3:L:33:TRP:CZ3	3:L:86:CYS:HB3	2.52	0.44
3:L:5:THR:OG1	3:L:24:ARG:HB3	2.17	0.44
1:G:270:ILE:HD13	1:G:345:VAL:HG12	1.98	0.44
2:H:172:ALA:HA	2:H:182:LEU:HB3	2.01	0.43
2:H:150:PHE:HA	2:H:151:PRO:HA	1.81	0.43
1:G:346:THR:HG22	1:G:361:PHE:HE2	1.83	0.43
2:H:48:MET:HG2	2:H:63:PHE:CE2	2.53	0.43
3:L:136:TYR:CG	3:L:137:PRO:HA	2.54	0.43
1:G:471:GLY:HA2	1:G:472:GLY:HA3	1.73	0.43
3:L:159:VAL:HG12	3:L:160:THR:O	2.19	0.43
1:G:457:ASP:OD2	1:G:469:ARG:NH2	2.52	0.42
1:G:469:ARG:HA	1:G:470:PRO:HD3	1.89	0.42
3:L:139:GLU:O	3:L:194:HIS:HD2	2.03	0.42
1:G:78:ASP:HA	1:G:79:PRO:HD2	1.89	0.42
1:G:341:VAL:O	1:G:345:VAL:HG13	2.19	0.42
2:H:28:GLU:HB3	2:H:31:ASN:ND2	2.34	0.42
1:G:49:ASP:OD2	1:G:99:ASN:HB2	2.20	0.42
3:L:25:THR:O	3:L:67:ALA:HB1	2.20	0.41
2:H:87:THR:HG23	2:H:114:THR:HA	2.02	0.41
1:G:270:ILE:O	1:G:348:LYS:HE2	2.20	0.41
2:H:18:MET:SD	2:H:113:VAL:HG21	2.60	0.41
3:L:17:GLU:O	3:L:76:LEU:HD13	2.21	0.41
3:L:45:VAL:HG12	3:L:46:ILE:HG13	2.03	0.41
1:G:379:ARG:HG3	1:G:443:ILE:HG23	2.03	0.40
3:L:23:CYS:HB2	3:L:33:TRP:CH2	2.56	0.40
3:L:108:ALA:HA	3:L:109:PRO:HD3	1.89	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	G	335/361 (93%)	318 (95%)	17 (5%)	0	100	100
2	H	219/229 (96%)	208 (95%)	10 (5%)	1 (0%)	34	68
3	L	205/210 (98%)	198 (97%)	6 (3%)	1 (0%)	34	68
All	All	759/800 (95%)	724 (95%)	33 (4%)	2 (0%)	46	78

All (2) Ramachandran outliers are listed below:

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

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	G	305/318 (96%)	287 (94%)	18 (6%)	24	55
2	H	189/195 (97%)	184 (97%)	5 (3%)	54	85
3	L	178/181 (98%)	174 (98%)	4 (2%)	60	88
All	All	672/694 (97%)	645 (96%)	27 (4%)	38	72

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

Mol	Chain	Res	Type
1	G	84	ILE

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Mol	Chain	Res	Type
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
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. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	354	ASN
3	L	194	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	7,8,9	1.56	1 (14%)	9,10,12	2.10	4 (44%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	PCA	CD-N	4.00	1.47	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1	PCA	CA-N-CD	-3.13	103.33	113.81
2	H	1	PCA	CB-CA-C	-3.08	108.55	112.76
2	H	1	PCA	OE-CD-CG	-2.46	121.31	126.81
2	H	1	PCA	CB-CA-N	2.54	110.61	103.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

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	14,14,15	0.51	0	15,19,21	0.97	1 (6%)
4	NAG	G	602	4	14,14,15	0.55	0	15,19,21	0.98	1 (6%)
4	BMA	G	603	4	11,11,12	2.26	3 (27%)	14,15,17	1.10	2 (14%)
4	MAN	G	604	4	11,11,12	0.61	0	14,15,17	1.44	1 (7%)
4	MAN	G	605	4	11,11,12	0.60	0	14,15,17	0.59	0
4	MAN	G	606	4	11,11,12	0.57	0	14,15,17	0.63	0
5	NAG	G	607	1,5	14,14,15	0.53	0	15,19,21	1.16	2 (13%)
5	NAG	G	608	5	14,14,15	0.62	0	15,19,21	0.53	0
5	BMA	G	609	5	11,11,12	2.19	3 (27%)	14,15,17	1.27	2 (14%)
5	MAN	G	610	5	11,11,12	0.56	0	14,15,17	0.76	1 (7%)
5	MAN	G	611	5	11,11,12	0.67	0	14,15,17	0.80	0
6	NAG	G	612	1,6	14,14,15	0.44	0	15,19,21	0.90	1 (6%)
6	NAG	G	613	6	14,14,15	0.56	0	15,19,21	0.73	0
6	BMA	G	614	6	11,11,12	2.17	3 (27%)	14,15,17	1.42	1 (7%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	603	BMA	C4-C3	-5.10	1.39	1.52
6	G	614	BMA	C4-C3	-4.86	1.39	1.52
5	G	609	BMA	C4-C3	-4.80	1.39	1.52
4	G	603	BMA	C2-C3	-4.25	1.46	1.52
5	G	609	BMA	C2-C3	-4.03	1.47	1.52
6	G	614	BMA	C2-C3	-4.01	1.47	1.52
5	G	609	BMA	O5-C1	-2.89	1.38	1.43
6	G	614	BMA	O5-C1	-2.52	1.39	1.43
4	G	603	BMA	O5-C1	-2.47	1.39	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	614	BMA	O3-C3-C2	-3.26	104.11	110.00
5	G	609	BMA	O4-C4-C3	-2.49	104.72	110.34
5	G	609	BMA	C1-C2-C3	-2.38	106.73	109.54
5	G	607	NAG	C6-C5-C4	-2.14	107.73	113.02
5	G	610	MAN	O5-C1-C2	-2.10	107.46	110.86
4	G	603	BMA	O4-C4-C3	-2.01	105.81	110.34
4	G	603	BMA	C1-O5-C5	2.15	114.98	112.25
4	G	601	NAG	C1-O5-C5	2.38	115.26	112.25
6	G	612	NAG	C1-O5-C5	2.45	115.36	112.25
5	G	607	NAG	C1-O5-C5	2.86	115.88	112.25
4	G	602	NAG	C3-C4-C5	2.97	115.38	110.20
4	G	604	MAN	C1-C2-C3	4.70	115.10	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	601	NAG	1	0
5	G	610	MAN	1	0

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	$\#\|Z\|>2$
7	NAG	G	615	1	14,14,15	0.53	0	15,19,21	1.20	1 (6%)
7	NAG	G	616	1	14,14,15	0.48	0	15,19,21	0.60	0
7	NAG	G	617	1	14,14,15	0.53	0	15,19,21	0.70	0
7	NAG	G	618	1	14,14,15	0.45	0	15,19,21	1.50	2 (13%)
7	NAG	L	501	3	14,14,15	0.66	0	15,19,21	0.68	1 (6%)

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	618	NAG	C3-C2-N2	-2.89	103.64	110.56
7	L	501	NAG	C1-O5-C5	2.27	115.13	112.25
7	G	615	NAG	C1-O5-C5	3.37	116.53	112.25
7	G	618	NAG	C1-O5-C5	3.95	117.26	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	G	340/361 (94%)	-0.11	8 (2%)	62	50	39, 67, 125, 174	0
2	H	221/229 (96%)	-0.21	2 (0%)	85	79	42, 69, 98, 142	0
3	L	207/210 (98%)	-0.01	7 (3%)	49	37	56, 89, 121, 147	0
All	All	768/800 (96%)	-0.11	17 (2%)	65	54	39, 73, 119, 174	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	124	GLY	7.7
2	H	137	GLY	5.4
1	G	123	THR	4.2
1	G	198	GLY	4.0
3	L	81	PHE	3.9
3	L	76	LEU	3.9
1	G	199	SER	3.8
3	L	78	SER	3.7
2	H	193	LEU	3.4
3	L	208	GLY	3.1
3	L	79	GLY	3.1
1	G	122	LEU	2.3
3	L	77	GLU	2.2
1	G	440	ASP	2.2
3	L	75	ASN	2.1
1	G	473	GLY	2.1
1	G	200	VAL	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, 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	LLDF	B-factors(Å^2)	Q<0.9
2	PCA	H	1	8/9	0.91	0.30	-	74,83,88,90	0

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	G	601	14/15	0.86	0.22	0.24	79,99,112,122	0
5	NAG	G	608	14/15	0.94	0.16	0.08	75,79,85,101	0
5	NAG	G	607	14/15	0.96	0.15	-0.46	46,59,68,71	0
6	NAG	G	612	14/15	0.93	0.13	-1.07	68,81,87,95	0
6	NAG	G	613	14/15	0.87	0.23	-	104,112,118,125	0
4	MAN	G	605	11/12	0.68	0.35	-	144,150,151,153	0
4	BMA	G	603	11/12	0.77	0.15	-	155,162,165,169	0
5	BMA	G	609	11/12	0.77	0.12	-	113,118,127,127	0
4	MAN	G	606	11/12	0.68	0.27	-	163,172,173,175	0
5	MAN	G	610	11/12	0.66	0.24	-	116,128,130,130	0
4	MAN	G	604	11/12	0.79	0.18	-	147,150,153,154	0
5	MAN	G	611	11/12	0.75	0.23	-	121,126,127,129	0
6	BMA	G	614	11/12	0.71	0.22	-	121,129,131,132	0
4	NAG	G	602	14/15	0.73	0.36	-	138,146,153,158	0

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. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
7	NAG	L	501	14/15	0.79	0.25	3.16	119,128,133,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	NAG	G	617	14/15	0.87	0.31	2.67	91,105,112,116	0
7	NAG	G	618	14/15	0.88	0.27	2.48	89,107,113,113	0
7	NAG	G	616	14/15	0.92	0.18	-0.12	69,79,85,90	0
7	NAG	G	615	14/15	0.92	0.17	-0.17	74,94,97,97	0

6.5 Other polymers (i)

There are no such residues in this entry.