



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:08 PM GMT

PDB ID : 4J6R
Title : Crystal structure of broadly and potently neutralizing antibody VRC23 in complex with HIV-1 gp120
Authors : Zhou, T.; Moquin, S.; Kwong P.D.
Deposited on : 2013-02-11
Resolution : 1.64 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>

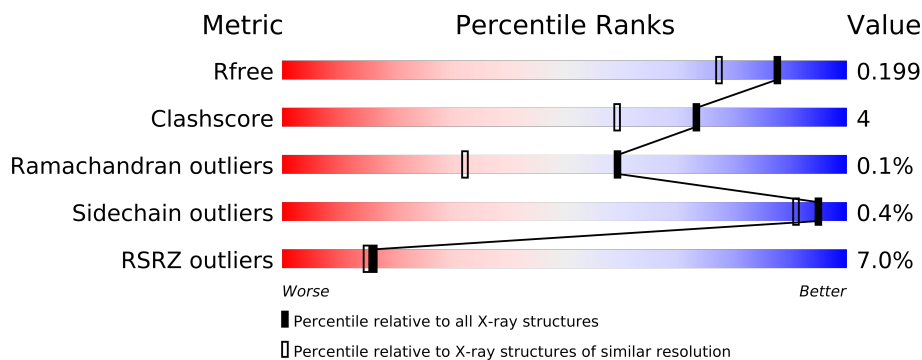
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.64 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	1326 (1.66-1.62)
Clashscore	79885	1525 (1.66-1.62)
Ramachandran outliers	78287	1490 (1.66-1.62)
Sidechain outliers	78261	1490 (1.66-1.62)
RSRZ outliers	66119	1326 (1.66-1.62)

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	359	
2	H	224	
3	L	210	

2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 13345 atoms, of which 6100 are hydrogens 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	G	343	Total	C	H	N	O	S	0	0	0
			5340	1698	2640	471	511	20			

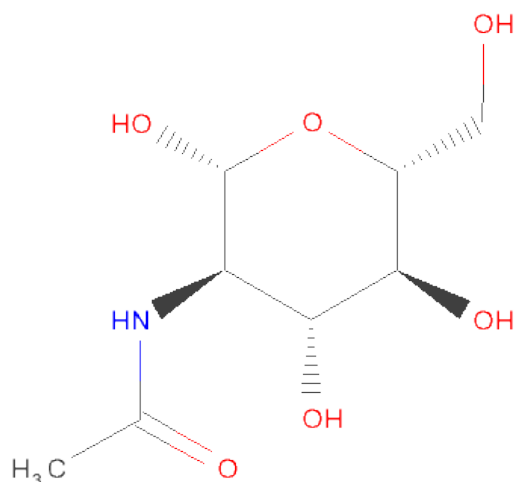
- Molecule 2 is a protein called HEAVY CHAIN OF ANTIBODY VRC23.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	222	Total	C	H	N	O	S	0	0	0
			3385	1088	1675	293	323	6			

- Molecule 3 is a protein called LIGHT CHAIN OF ANTIBODY VRC23.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	L	210	Total	C	H	N	O	S	0	0	0
			3166	1002	1561	274	323	6			

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

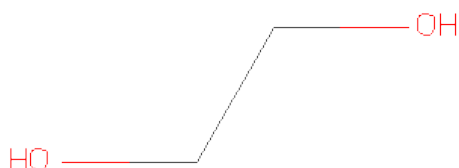


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total C H N O 28 8 14 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C H N O 28 8 14 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C H N O 28 8 14 1 5	0	0
4	G	1	Total C H N O 28 8 14 1 5	0	0
4	G	1	Total C H N O 28 8 14 1 5	0	0
4	G	1	Total C H N O 28 8 14 1 5	0	0
4	G	1	Total C H N O 28 8 14 1 5	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

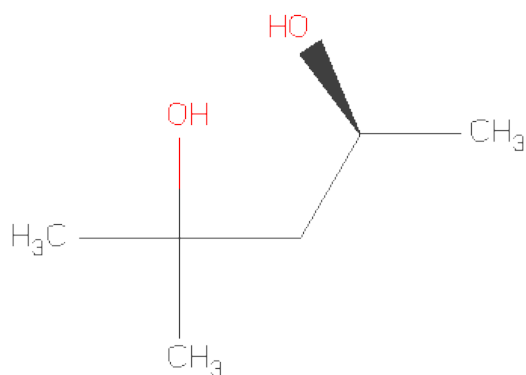
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total Ca 1 1	0	0
5	L	1	Total Ca 1 1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



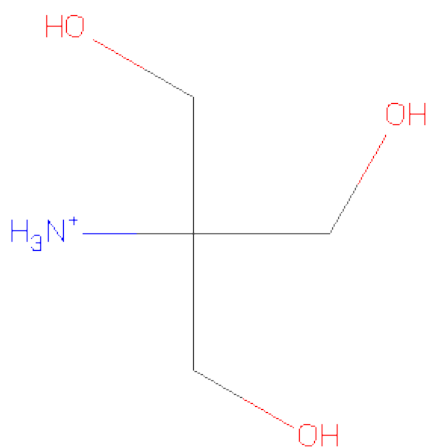
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	G	1	Total	C	H	O	0	0
			10	2	6	2		
6	G	1	Total	C	H	O	0	0
			10	2	6	2		
6	G	1	Total	C	H	O	0	0
			10	2	6	2		
6	G	1	Total	C	H	O	0	0
			10	2	6	2		
6	H	1	Total	C	H	O	0	0
			10	2	6	2		
6	H	1	Total	C	H	O	0	0
			10	2	6	2		
6	H	1	Total	C	H	O	0	0
			10	2	6	2		
6	H	1	Total	C	H	O	0	0
			10	2	6	2		
6	H	1	Total	C	H	O	0	0
			10	2	6	2		
6	H	1	Total	C	H	O	0	0
			10	2	6	2		
6	L	1	Total	C	H	O	0	0
			10	2	6	2		
6	L	1	Total	C	H	O	0	0
			10	2	6	2		
6	L	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



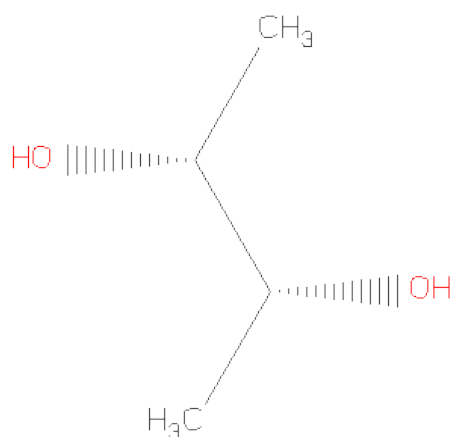
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
7	H	1	22	6	14	2	0	0

- Molecule 8 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
8	H	1	20	4	12	1	3	0	0

- Molecule 9 is (R,R)-2,3-BUTANEDIOL (three-letter code: BU3) (formula: $C_4H_{10}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	L	1	Total	C	H	O	0	0
			16	4	10	2		

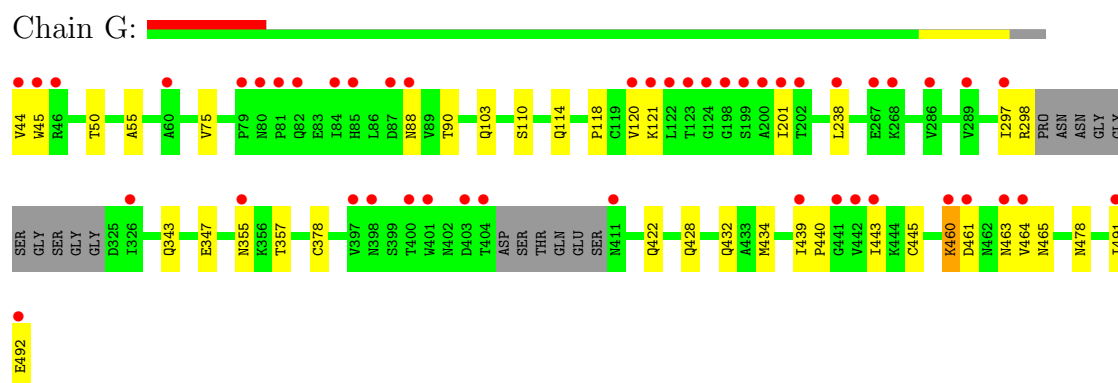
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	G	326	Total	O	0	0
			326	326		
10	H	339	Total	O	0	0
			339	339		
10	L	355	Total	O	0	0
			355	355		

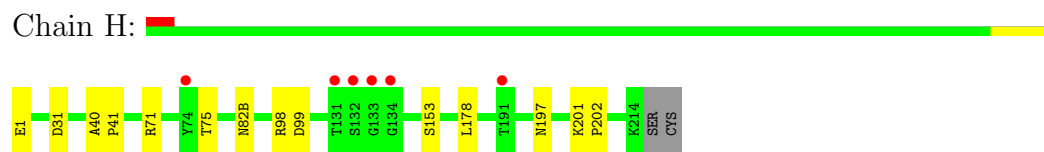
3 Residue-property plots

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: Envelope glycoprotein gp160



- Molecule 2: HEAVY CHAIN OF ANTIBODY VRC23



- Molecule 3: LIGHT CHAIN OF ANTIBODY VRC23



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.04Å 68.69Å 214.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.17 – 1.64 23.17 – 1.64	Depositor EDS
% Data completeness (in resolution range)	94.6 (23.17-1.64) 94.6 (23.17-1.64)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 1.63Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1069)	Depositor
R, R_{free}	0.164 , 0.198 0.165 , 0.199	Depositor DCC
R_{free} test set	5397 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 53.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 107955 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13345	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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: MPD, NAG, BU3, CA, EDO, TRS, PCA

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	0.28	0/2758	0.49	0/3746
2	H	0.34	0/1751	0.54	0/2389
3	L	0.37	0/1639	0.53	0/2225
All	All	0.33	0/6148	0.52	0/8360

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	428	GLN	Peptide

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	2700	2640	0	29	0
2	H	1710	1675	0	10	0
3	L	1605	1561	0	7	0
4	G	126	98	26	1	0
5	G	1	0	0	0	0
5	L	1	0	0	0	0
6	G	16	24	0	0	0
6	H	32	48	0	1	0
6	L	12	18	0	0	0
7	H	8	14	0	4	0
8	H	8	12	0	0	0
9	L	6	10	0	3	0
10	G	326	0	0	12	1
10	H	339	0	0	4	3
10	L	355	0	0	4	3
All	All	7245	6100	26	52	4

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 4.

All (52) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:461:ASP:OD1	10:G:902:HOH:O	1.77	1.02
1:G:460:LYS:O	10:G:793:HOH:O	1.92	0.88
1:G:88:ASN:ND2	10:G:739:HOH:O	2.11	0.82
1:G:461:ASP:OD1	10:G:903:HOH:O	1.99	0.80
1:G:460:LYS:HD2	10:H:435:HOH:O	1.81	0.78
3:L:127:SER:OG	10:L:624:HOH:O	2.08	0.71
1:G:445:CYS:SG	10:G:874:HOH:O	2.48	0.71
1:G:465:ASN:OD1	10:G:924:HOH:O	2.10	0.69
2:H:82(B):ASN:ND2	10:H:684:HOH:O	2.25	0.69
3:L:108:ARG:HB2	9:L:305:BU3:H2	1.79	0.63
1:G:50:THR:O	1:G:103:GLN:NE2	2.30	0.63
9:L:305:BU3:H13	10:L:537:HOH:O	2.00	0.60
10:G:883:HOH:O	3:L:1:GLU:HG3	2.02	0.59
9:L:305:BU3:C1	10:L:537:HOH:O	2.52	0.57
1:G:298:ARG:HD2	1:G:298:ARG:C	2.25	0.57
1:G:44:VAL:HG12	1:G:45:TRP:CE3	2.40	0.56
1:G:355:ASN:ND2	10:G:817:HOH:O	2.38	0.56
1:G:491:ILE:O	10:G:836:HOH:O	2.18	0.55
7:H:301:MPD:H53	7:H:301:MPD:C1	2.36	0.55
7:H:301:MPD:H53	7:H:301:MPD:H11	1.91	0.51
1:G:463:ASN:O	1:G:464:VAL:HB	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:H:301:MPD:HM1	7:H:301:MPD:O4	2.11	0.50
2:H:75:THR:O	7:H:301:MPD:CM	2.60	0.50
1:G:439:ILE:HG23	1:G:440:PRO:HD2	1.94	0.49
2:H:201:LYS:N	2:H:202:PRO:CD	2.76	0.49
2:H:1:PCA:N	10:H:689:HOH:O	2.46	0.47
1:G:90:THR:HG22	1:G:238:LEU:HD22	1.95	0.47
1:G:44:VAL:CG1	1:G:45:TRP:CE3	2.99	0.46
1:G:118:PRO:HG2	1:G:121:LYS:HG2	1.99	0.45
1:G:343:GLN:O	1:G:347:GLU:HG2	2.17	0.45
2:H:99:ASP:OD2	10:H:669:HOH:O	2.21	0.44
1:G:491:ILE:O	1:G:492:GLU:C	2.56	0.44
1:G:463:ASN:O	1:G:464:VAL:CB	2.65	0.44
1:G:422:GLN:O	1:G:434:MET:HA	2.18	0.44
3:L:4:MET:HE3	3:L:23:CYS:SG	2.59	0.43
4:G:505:NAG:O4	10:G:881:HOH:O	2.20	0.43
3:L:198:HIS:HD1	3:L:200:GLY:H	1.67	0.42
1:G:357:THR:HB	1:G:465:ASN:HB3	2.00	0.42
2:H:153:SER:HG	2:H:197:ASN:HB2	1.84	0.42
1:G:297:ILE:HA	1:G:443:ILE:O	2.19	0.42
1:G:55:ALA:HA	1:G:75:VAL:O	2.20	0.42
1:G:110:SER:O	1:G:114:GLN:HG2	2.19	0.41
1:G:120:VAL:HA	1:G:201:ILE:O	2.20	0.41
3:L:21:LEU:HD12	3:L:21:LEU:N	2.35	0.41
2:H:178:LEU:HD12	2:H:178:LEU:C	2.39	0.41
1:G:478:ASN:OD1	10:G:784:HOH:O	2.21	0.41
1:G:44:VAL:HG12	1:G:45:TRP:N	2.35	0.41
2:H:40:ALA:HB1	2:H:41:PRO:HD2	2.02	0.41
3:L:9:VAL:HG12	10:L:691:HOH:O	2.20	0.41
2:H:202:PRO:HG3	6:H:305:EDO:H12	2.03	0.41
2:H:31:ASP:O	2:H:98:ARG:HG3	2.21	0.40
1:G:378:CYS:HB2	10:G:874:HOH:O	2.22	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:H:402:HOH:O	10:L:610:HOH:O[4_545]	1.76	0.44
10:L:605:HOH:O	10:L:611:HOH:O[4_435]	1.88	0.32
10:G:882:HOH:O	10:H:728:HOH:O[3_555]	1.93	0.27
10:H:593:HOH:O	10:L:681:HOH:O[4_545]	2.12	0.08

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	337/359 (94%)	327 (97%)	10 (3%)	0	100	100
2	H	220/224 (98%)	217 (99%)	3 (1%)	0	100	100
3	L	208/210 (99%)	201 (97%)	6 (3%)	1 (0%)	38	13
All	All	765/793 (96%)	745 (97%)	19 (2%)	1 (0%)	59	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	68	HIS

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	303/314 (96%)	301 (99%)	2 (1%)	91	80
2	H	187/189 (99%)	186 (100%)	1 (0%)	94	87
3	L	181/181 (100%)	181 (100%)	0	100	100
All	All	671/684 (98%)	668 (100%)	3 (0%)	95	91

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	432	GLN
1	G	460	LYS
2	H	71	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
1	G	287	GLN
1	G	425	ASN
2	H	64	GLN
2	H	192	GLN
3	L	90	GLN

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	6.59	2 (25%)	8,10,12	5.37	4 (50%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	PCA	O-C	17.52	1.23	1.11
2	H	1	PCA	CD-N	5.84	1.46	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	PCA	CA-N-CD	-14.33	103.17	114.37
2	H	1	PCA	OE-CD-CG	-3.22	121.64	126.70
2	H	1	PCA	CB-CA-N	2.35	110.49	103.72
2	H	1	PCA	C-CA-N	-2.10	110.24	110.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 29 ligands modelled in this entry, 2 are monoatomic - leaving 27 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	G	501	1	12,14,15	0.71	1 (8%)	15,19,21	1.07	1 (6%)
4	NAG	G	502	1	12,14,15	0.64	0	15,19,21	0.85	1 (6%)
4	NAG	G	503	1	12,14,15	0.55	0	15,19,21	1.01	1 (6%)
4	NAG	G	504	1	12,14,15	0.61	0	15,19,21	0.78	0
4	NAG	G	505	1	12,14,15	0.62	0	15,19,21	0.76	1 (6%)
4	NAG	G	506	1	12,14,15	0.61	0	15,19,21	0.89	0
4	NAG	G	507	1	12,14,15	0.66	1 (8%)	15,19,21	0.87	1 (6%)
4	NAG	G	508	1	12,14,15	0.67	1 (8%)	15,19,21	0.93	1 (6%)
4	NAG	G	509	1	12,14,15	0.58	0	15,19,21	1.21	1 (6%)
6	EDO	G	511	-	3,3,3	0.51	0	2,2,2	0.69	0
6	EDO	G	512	-	3,3,3	0.53	0	2,2,2	0.32	0
6	EDO	G	513	-	3,3,3	0.58	0	2,2,2	0.21	0
6	EDO	G	514	-	3,3,3	0.55	0	2,2,2	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MPD	H	301	-	7,7,7	0.28	0	10,10,10	0.39	0
6	EDO	H	302	-	3,3,3	0.51	0	2,2,2	0.48	0
6	EDO	H	303	-	3,3,3	0.51	0	2,2,2	0.42	0
6	EDO	H	304	-	3,3,3	0.58	0	2,2,2	0.26	0
6	EDO	H	305	-	3,3,3	0.61	0	2,2,2	0.05	0
6	EDO	H	306	-	3,3,3	0.59	0	2,2,2	0.41	0
6	EDO	H	307	-	3,3,3	0.53	0	2,2,2	0.39	0
6	EDO	H	308	-	3,3,3	0.52	0	2,2,2	0.45	0
6	EDO	H	309	-	3,3,3	0.52	0	2,2,2	0.43	0
8	TRS	H	310	-	7,7,7	1.02	1 (14%)	9,9,9	0.94	0
6	EDO	L	302	-	3,3,3	0.53	0	2,2,2	0.29	0
6	EDO	L	303	-	3,3,3	0.55	0	2,2,2	0.56	0
6	EDO	L	304	-	3,3,3	0.55	0	2,2,2	0.37	0
9	BU3	L	305	-	5,5,5	1.42	1 (20%)	6,6,6	0.34	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	NAG	G	501	1	-	0/6/23/26	0/1/1/1
4	NAG	G	502	1	-	0/6/23/26	0/1/1/1
4	NAG	G	503	1	-	0/6/23/26	0/1/1/1
4	NAG	G	504	1	-	0/6/23/26	0/1/1/1
4	NAG	G	505	1	-	0/6/23/26	0/1/1/1
4	NAG	G	506	1	-	0/6/23/26	0/1/1/1
4	NAG	G	507	1	-	0/6/23/26	0/1/1/1
4	NAG	G	508	1	-	0/6/23/26	0/1/1/1
4	NAG	G	509	1	-	0/6/23/26	0/1/1/1
6	EDO	G	511	-	-	0/1/1/1	0/0/0/0
6	EDO	G	512	-	-	0/1/1/1	0/0/0/0
6	EDO	G	513	-	-	0/1/1/1	0/0/0/0
6	EDO	G	514	-	-	0/1/1/1	0/0/0/0
7	MPD	H	301	-	-	0/5/5/5	0/0/0/0
6	EDO	H	302	-	-	0/1/1/1	0/0/0/0
6	EDO	H	303	-	-	0/1/1/1	0/0/0/0
6	EDO	H	304	-	-	0/1/1/1	0/0/0/0
6	EDO	H	305	-	-	0/1/1/1	0/0/0/0
6	EDO	H	306	-	-	0/1/1/1	0/0/0/0
6	EDO	H	307	-	-	0/1/1/1	0/0/0/0
6	EDO	H	308	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	H	309	-	-	0/1/1/1	0/0/0/0
8	TRS	H	310	-	-	0/9/9/9	0/0/0/0
6	EDO	L	302	-	-	0/1/1/1	0/0/0/0
6	EDO	L	303	-	-	0/1/1/1	0/0/0/0
6	EDO	L	304	-	-	0/1/1/1	0/0/0/0
9	BU3	L	305	-	-	0/4/4/4	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	310	TRS	C-N	-2.65	1.46	1.50
9	L	305	BU3	O6-C3	-2.15	1.38	1.43
4	G	501	NAG	O5-C5	-2.06	1.41	1.45
4	G	508	NAG	O5-C5	-2.01	1.41	1.45
4	G	507	NAG	O5-C5	-2.01	1.41	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	509	NAG	O5-C5-C6	3.57	110.73	106.98
4	G	501	NAG	O5-C5-C6	2.73	109.85	106.98
4	G	507	NAG	O5-C5-C6	2.68	109.79	106.98
4	G	503	NAG	O5-C5-C6	2.67	109.78	106.98
4	G	502	NAG	O5-C5-C6	2.58	109.69	106.98
4	G	508	NAG	O5-C5-C6	2.31	109.40	106.98
4	G	505	NAG	O5-C5-C6	2.22	109.31	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	343/359 (95%)	0.68	47 (13%) 4 3	22, 39, 78, 105	0
2	H	222/224 (99%)	-0.07	6 (2%) 52 53	17, 24, 41, 60	0
3	L	210/210 (100%)	-0.10	2 (0%) 79 83	17, 24, 40, 80	0
All	All	775/793 (97%)	0.26	55 (7%) 16 14	17, 29, 65, 105	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	198	GLY	9.2
1	G	44	VAL	9.0
1	G	404	THR	8.4
1	G	84	ILE	7.9
1	G	491	ILE	7.6
1	G	442	VAL	7.4
1	G	201	ILE	6.1
1	G	464	VAL	6.0
1	G	200	ALA	6.0
1	G	199	SER	5.8
1	G	123	THR	5.6
2	H	132	SER	5.1
1	G	124	GLY	5.1
3	L	214	CYS	5.0
2	H	133	GLY	4.9
1	G	492	GLU	4.9
1	G	397	VAL	4.8
1	G	82	GLN	4.5
2	H	74	TYR	4.4
1	G	88	ASN	4.3
1	G	297	ILE	4.3
1	G	461	ASP	4.2
1	G	439	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	G	122	LEU	4.0
1	G	238	LEU	4.0
2	H	191	THR	4.0
1	G	460	LYS	3.8
1	G	411	ASN	3.8
1	G	401	TRP	3.7
1	G	268	LYS	3.6
1	G	81	PRO	3.6
1	G	289	VAL	3.5
1	G	441	GLY	3.3
1	G	326	ILE	3.1
1	G	60	ALA	3.0
2	H	131	THR	3.0
1	G	121	LYS	3.0
1	G	45	TRP	2.8
1	G	398	ASN	2.8
1	G	79	PRO	2.8
3	L	9	VAL	2.8
1	G	267	GLU	2.8
1	G	120	VAL	2.7
1	G	286	VAL	2.7
1	G	80	ASN	2.6
1	G	355	ASN	2.6
1	G	46	ARG	2.5
1	G	85	HIS	2.4
2	H	134	GLY	2.4
1	G	87	ASP	2.4
1	G	403	ASP	2.4
1	G	202	THR	2.4
1	G	400	THR	2.3
1	G	463	ASN	2.3
1	G	443	ILE	2.3

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(\AA^2)	Q<0.9
2	PCA	H	1	8/9	0.16	-	30,44,55,55	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

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
4	NAG	G	504	14/15	0.13	-	25,38,48,53	0
6	EDO	H	302	4/4	0.20	-	32,38,54,65	0
4	NAG	G	505	14/15	0.25	-	38,56,69,69	0
6	EDO	G	511	4/4	0.10	-	32,39,46,53	0
4	NAG	G	501	14/15	0.15	-	42,53,73,82	0
6	EDO	G	512	4/4	0.11	-	36,58,75,81	0
6	EDO	H	305	4/4	0.22	-	30,38,45,47	0
4	NAG	G	503	14/15	0.10	-	24,36,57,71	0
7	MPD	H	301	8/8	0.39	-	62,79,86,89	0
5	CA	G	510	1/1	0.05	-	39,39,39,39	0
6	EDO	L	302	4/4	0.08	-	35,42,50,50	0
4	NAG	G	506	14/15	0.27	-	42,52,76,87	0
6	EDO	L	303	4/4	0.12	-	38,48,58,63	0
8	TRS	H	310	8/8	0.16	-	30,40,49,54	0
6	EDO	H	308	4/4	0.22	-	26,54,65,68	0
6	EDO	H	306	4/4	0.07	-	21,25,26,32	0
6	EDO	G	514	4/4	0.09	-	66,79,82,82	0
6	EDO	H	307	4/4	0.13	-	29,35,48,48	0
6	EDO	H	304	4/4	0.25	-	50,61,62,68	0
6	EDO	G	513	4/4	0.10	-	28,40,43,50	0
5	CA	L	301	1/1	0.11	-	61,61,61,61	0
9	BU3	L	305	6/6	0.20	-	35,64,69,69	0
6	EDO	L	304	4/4	0.26	-	57,68,74,75	0
4	NAG	G	502	14/15	0.37	-	64,74,82,87	0
6	EDO	H	303	4/4	0.11	-	27,34,42,42	0
6	EDO	H	309	4/4	0.15	-	55,67,69,76	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	G	509	14/15	0.51	-	72,95,113,121	0
4	NAG	G	507	14/15	0.14	-	35,50,59,62	0
4	NAG	G	508	14/15	0.33	-	54,69,81,90	0

6.5 Other polymers

There are no such residues in this entry.