



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:02 PM UTC

PDB ID : 4J6R / pdb_00004j6r
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 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

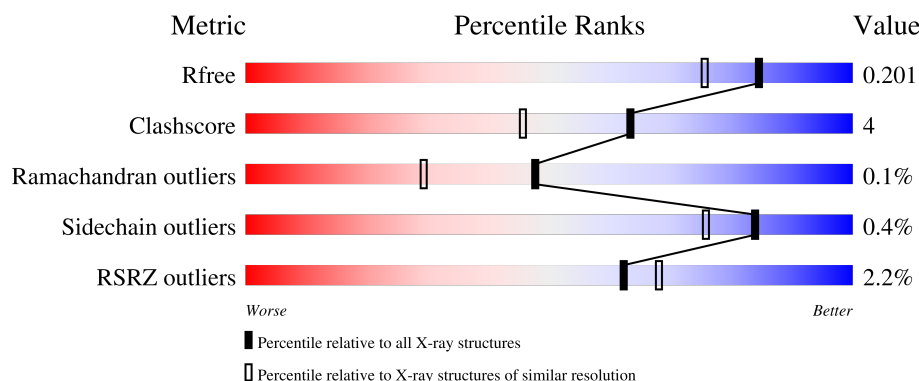
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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}	180053	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	G	359	4% 85% 10% ..
2	H	224	96% ..
3	L	210	96% .

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
9	BU3	L	305	-	-	X	-

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 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 Envelope glycoprotein gp160.

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

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

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

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

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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

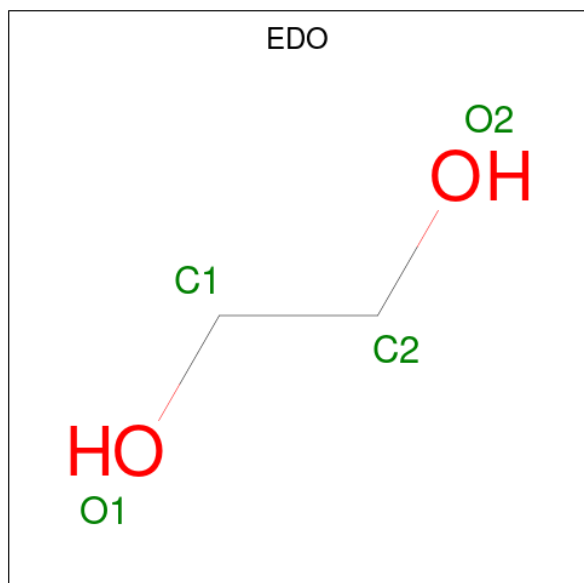


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total C H N O 28 8 14 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C H N O 28 8 14 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C H N O 28 8 14 1 5	0	0
4	G	1	Total C H N O 28 8 14 1 5	0	0
4	G	1	Total C H N O 28 8 14 1 5	0	0
4	G	1	Total C H N 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 (CCD ID: 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 (CCD ID: EDO) (formula: C₂H₆O₂).



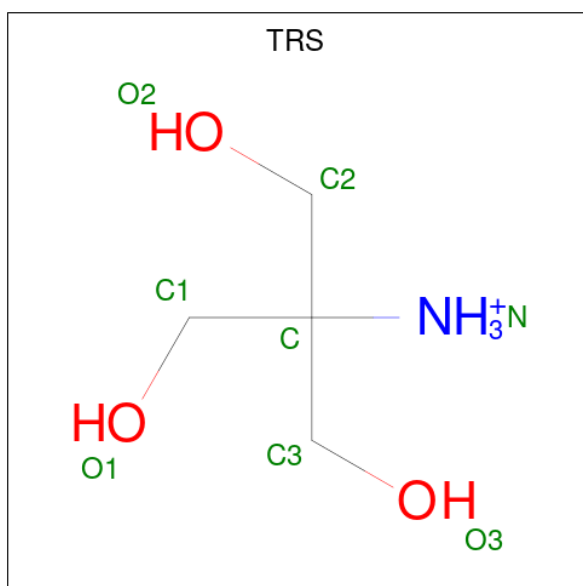
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	G	1	Total	C	H	O	0	0
			10	2	6	2		
6	G	1	Total	C	H	O	0	0
			10	2	6	2		
6	G	1	Total	C	H	O	0	0
			10	2	6	2		
6	G	1	Total	C	H	O	0	0
			10	2	6	2		
6	H	1	Total	C	H	O	0	0
			10	2	6	2		
6	H	1	Total	C	H	O	0	0
			10	2	6	2		
6	H	1	Total	C	H	O	0	0
			10	2	6	2		
6	H	1	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 (CCD ID: MPD) (formula: C₆H₁₄O₂).



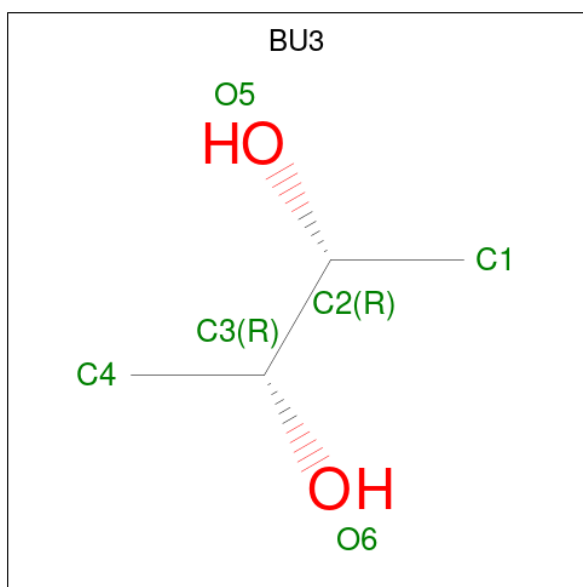
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	H	1	Total	C	H	O	0	0
			22	6	14	2		

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



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

- Molecule 9 is (R,R)-2,3-BUTANEDIOL (CCD ID: 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		

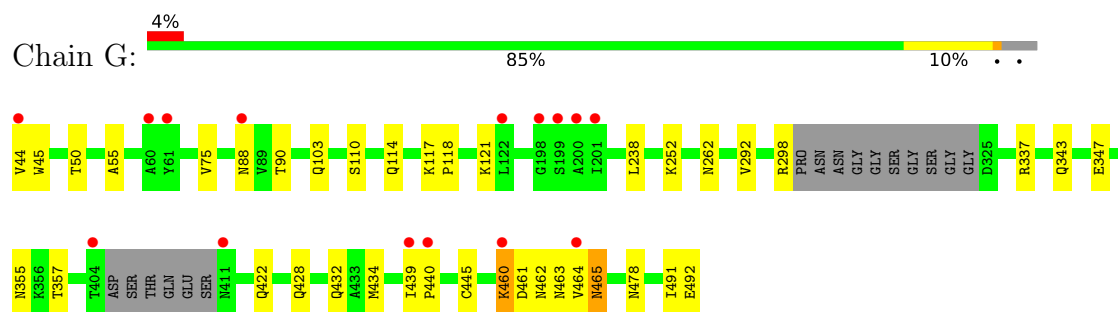
- Molecule 10 is water.

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		

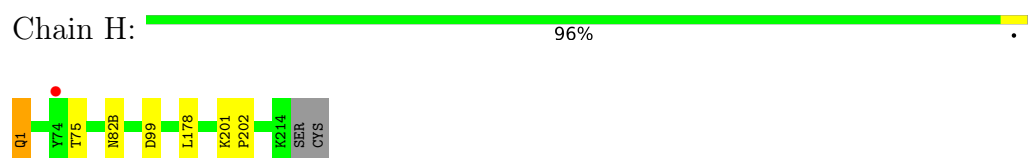
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

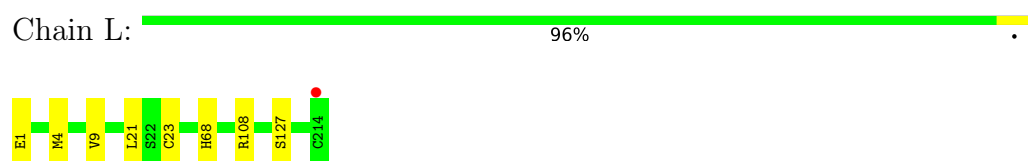
- Molecule 1: Envelope glycoprotein gp160



- 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) 94.8 (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 0.166 , 0.201	Depositor DCC
R_{free} test set	5396 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

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: PCA, BU3, EDO, CA, TRS, MPD, NAG

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	0.34	0/2758	0.66	1/3746 (0.0%)
2	H	0.39	0/1751	0.65	0/2389
3	L	0.41	0/1639	0.64	0/2225
All	All	0.38	0/6148	0.65	1/8360 (0.0%)

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.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	465	ASN	N-CA-C	6.06	118.40	109.24

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	428	GLN	Peptide

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	2700	2640	2632	29	0
2	H	1710	1675	1672	7	0
3	L	1605	1561	1557	6	0
4	G	126	98	117	1	0
5	G	1	0	0	0	0
5	L	1	0	0	0	0
6	G	16	24	24	0	0
6	H	32	48	48	1	0
6	L	12	18	18	0	0
7	H	8	14	14	4	0
8	H	8	12	12	0	0
9	L	6	10	10	4	0
10	G	326	0	0	11	1
10	H	339	0	0	5	3
10	L	355	0	0	5	3
All	All	7245	6100	6104	49	4

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 4.

All (49) 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: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	1.80	0.79
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	1.74	0.68
1:G:50:THR:O	1:G:103:GLN:NE2	2.30	0.63
1:G:298:ARG:HD2	1:G:298:ARG:C	2.27	0.60
10:G:883:HOH:O	3:L:1:GLU:HG3	2.03	0.59
1:G:44:VAL:HG12	1:G:45:TRP:CE3	2.38	0.58
7:H:301:MPD:HM1	10:H:505:HOH:O	2.04	0.58
9:L:305:BU3:C1	10:L:537:HOH:O	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:463:ASN:O	1:G:464:VAL:HB	2.10	0.51
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
1:G:491:ILE:O	1:G:492:GLU:C	2.56	0.49
1:G:90:THR:HG22	1:G:238:LEU:HD22	1.94	0.48
4:G:505:NAG:O4	10:G:881:HOH:O	2.20	0.48
2:H:1:PCA:N	10:H:689:HOH:O	2.46	0.47
9:L:305:BU3:H13	10:L:537:HOH:O	2.14	0.47
9:L:305:BU3:H11	10:L:537:HOH:O	2.12	0.47
2:H:178:LEU:C	2:H:178:LEU:HD12	2.39	0.46
1:G:343:GLN:O	1:G:347:GLU:HG2	2.15	0.46
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
7:H:301:MPD:H11	7:H:301:MPD:H53	1.98	0.44
2:H:99:ASP:OD2	10:H:669:HOH:O	2.21	0.44
1:G:357:THR:HB	1:G:465:ASN:HB3	1.98	0.44
3:L:4:MET:HE3	3:L:23:CYS:SG	2.58	0.44
1:G:463:ASN:O	1:G:464:VAL:CB	2.65	0.44
1:G:117:LYS:HA	1:G:118:PRO:HD3	1.91	0.43
1:G:422:GLN:O	1:G:434:MET:HA	2.19	0.43
3:L:9:VAL:HG12	10:L:691:HOH:O	2.19	0.42
2:H:202:PRO:HG3	6:H:305:EDO:H11	2.02	0.41
3:L:21:LEU:HD12	3:L:21:LEU:N	2.35	0.41
1:G:478:ASN:OD1	10:G:784:HOH:O	2.21	0.41
1:G:55:ALA:HA	1:G:75:VAL:O	2.21	0.41
1:G:44:VAL:HG12	1:G:45:TRP:N	2.36	0.41
1:G:292:VAL:HG22	1:G:337:ARG:HG2	2.03	0.41
1:G:110:SER:O	1:G:114:GLN:HG2	2.21	0.40
7:H:301:MPD:H11	7:H:301:MPD:C5	2.51	0.40
1:G:252:LYS:CE	1:G:262:ASN:HB3	2.51	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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	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%)	24	9
All	All	765/793 (96%)	745 (97%)	19 (2%)	1 (0%)	48	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	68	HIS

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	303/314 (96%)	300 (99%)	3 (1%)	68	49
2	H	187/189 (99%)	187 (100%)	0	100	100
3	L	181/181 (100%)	181 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	671/684 (98%)	668 (100%)	3 (0%)	84	76

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

Mol	Chain	Res	Type
1	G	432	GLN
1	G	460	LYS
1	G	462	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	99	ASN
1	G	290	GLN
1	G	377	ASN
1	G	425	ASN
2	H	39	GLN
3	L	37	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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	7,8,9	2.25	2 (28%)	9,10,12	2.40	5 (55%)

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	CD-N	4.97	1.46	1.34
2	H	1	PCA	CA-N	3.13	1.50	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	PCA	CB-CA-C	-4.17	106.94	112.66
2	H	1	PCA	CA-N-CD	-3.04	103.17	113.58
2	H	1	PCA	OE-CD-CG	-2.85	121.64	126.72
2	H	1	PCA	CB-CA-N	2.63	110.49	103.24
2	H	1	PCA	CG-CD-N	2.49	114.47	108.39

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
2	H	1	PCA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
6	EDO	G	511	-	3,3,3	0.40	0	2,2,2	0.66	0
4	NAG	G	506	1	14,14,15	0.47	0	17,19,21	1.02	1 (5%)
4	NAG	G	505	1	14,14,15	0.45	0	17,19,21	0.74	0
6	EDO	H	309	-	3,3,3	0.41	0	2,2,2	0.42	0
6	EDO	H	302	-	3,3,3	0.41	0	2,2,2	0.48	0
4	NAG	G	503	1	14,14,15	0.49	0	17,19,21	0.88	1 (5%)
6	EDO	L	302	-	3,3,3	0.42	0	2,2,2	0.30	0
7	MPD	H	301	-	7,7,7	0.31	0	9,10,10	0.47	0
9	BU3	L	305	-	4,5,5	1.25	0	6,6,6	0.42	0
8	TRS	H	310	-	7,7,7	0.34	0	9,9,9	0.59	0
6	EDO	H	303	-	3,3,3	0.39	0	2,2,2	0.42	0
6	EDO	H	305	-	3,3,3	0.48	0	2,2,2	0.06	0
6	EDO	G	513	-	3,3,3	0.46	0	2,2,2	0.22	0
4	NAG	G	501	1	14,14,15	0.55	0	17,19,21	0.85	0
6	EDO	L	304	-	3,3,3	0.44	0	2,2,2	0.38	0
4	NAG	G	509	1	14,14,15	0.44	0	17,19,21	1.06	1 (5%)
6	EDO	H	304	-	3,3,3	0.47	0	2,2,2	0.28	0
6	EDO	H	308	-	3,3,3	0.40	0	2,2,2	0.45	0
6	EDO	G	514	-	3,3,3	0.44	0	2,2,2	0.34	0
6	EDO	L	303	-	3,3,3	0.44	0	2,2,2	0.55	0
4	NAG	G	508	1	14,14,15	0.56	0	17,19,21	0.74	0
6	EDO	G	512	-	3,3,3	0.43	0	2,2,2	0.33	0
4	NAG	G	504	1	14,14,15	0.48	0	17,19,21	0.72	0
6	EDO	H	307	-	3,3,3	0.42	0	2,2,2	0.39	0
6	EDO	H	306	-	3,3,3	0.50	0	2,2,2	0.41	0
4	NAG	G	507	1	14,14,15	0.52	0	17,19,21	0.69	0
4	NAG	G	502	1	14,14,15	0.48	0	17,19,21	0.60	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
6	EDO	G	511	-	-	0/1/1/1	-
4	NAG	G	506	1	-	0/6/23/26	0/1/1/1
4	NAG	G	505	1	-	0/6/23/26	0/1/1/1
6	EDO	H	309	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	H	302	-	-	0/1/1/1	-
4	NAG	G	503	1	-	0/6/23/26	0/1/1/1
6	EDO	L	302	-	-	0/1/1/1	-
7	MPD	H	301	-	-	2/5/5/5	-
9	BU3	L	305	-	-	0/4/4/4	-
8	TRS	H	310	-	-	4/9/9/9	-
6	EDO	H	303	-	-	0/1/1/1	-
6	EDO	H	305	-	-	0/1/1/1	-
6	EDO	G	513	-	-	0/1/1/1	-
4	NAG	G	501	1	-	0/6/23/26	0/1/1/1
6	EDO	L	304	-	-	1/1/1/1	-
4	NAG	G	509	1	-	0/6/23/26	0/1/1/1
6	EDO	H	304	-	-	0/1/1/1	-
6	EDO	H	308	-	-	0/1/1/1	-
6	EDO	G	514	-	-	0/1/1/1	-
6	EDO	L	303	-	-	1/1/1/1	-
4	NAG	G	508	1	-	0/6/23/26	0/1/1/1
6	EDO	G	512	-	-	0/1/1/1	-
4	NAG	G	504	1	-	0/6/23/26	0/1/1/1
6	EDO	H	307	-	-	0/1/1/1	-
6	EDO	H	306	-	-	0/1/1/1	-
4	NAG	G	507	1	-	0/6/23/26	0/1/1/1
4	NAG	G	502	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	509	NAG	O5-C1-C2	-2.43	107.53	111.29
4	G	506	NAG	C1-O5-C5	2.20	115.13	112.19
4	G	503	NAG	C1-O5-C5	2.08	114.98	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	304	EDO	O1-C1-C2-O2
8	H	310	TRS	N-C-C2-O2
8	H	310	TRS	C1-C-C2-O2
8	H	310	TRS	C3-C-C2-O2
8	H	310	TRS	C3-C-C1-O1

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Mol	Chain	Res	Type	Atoms
6	L	303	EDO	O1-C1-C2-O2
7	H	301	MPD	O2-C2-C3-C4
7	H	301	MPD	C1-C2-C3-C4

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	505	NAG	1	0
7	H	301	MPD	4	0
9	L	305	BU3	4	0
6	H	305	EDO	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.18	15 (4%) 39 43	23, 43, 83, 113	0
2	H	221/224 (98%)	-0.48	1 (0%) 87 90	18, 26, 46, 74	0
3	L	210/210 (100%)	-0.42	1 (0%) 87 90	18, 26, 46, 87	0
All	All	774/793 (97%)	-0.17	17 (2%) 62 68	18, 31, 72, 113	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	460	LYS	3.3
2	H	74	TYR	2.7
1	G	198	GLY	2.7
1	G	44	VAL	2.5
1	G	439	ILE	2.5
1	G	404	THR	2.4
1	G	122	LEU	2.4
1	G	199	SER	2.2
1	G	411	ASN	2.2
1	G	200	ALA	2.2
1	G	440	PRO	2.1
1	G	60	ALA	2.1
1	G	464	VAL	2.1
3	L	214	CYS	2.1
1	G	88	ASN	2.1
1	G	61	TYR	2.1
1	G	201	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	PCA	H	1	8/9	0.95	0.07	30,44,55,55	0

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
4	NAG	G	509	14/15	0.49	0.16	72,95,113,121	0
7	MPD	H	301	8/8	0.64	0.15	62,79,86,89	0
4	NAG	G	502	14/15	0.71	0.13	64,74,82,87	0
4	NAG	G	508	14/15	0.73	0.10	54,69,81,90	0
6	EDO	L	304	4/4	0.78	0.14	57,68,74,75	0
6	EDO	H	309	4/4	0.80	0.12	55,67,69,76	0
9	BU3	L	305	6/6	0.80	0.17	35,64,69,69	0
8	TRS	H	310	8/8	0.82	0.12	30,40,49,54	0
6	EDO	H	308	4/4	0.83	0.13	26,54,65,68	0
6	EDO	H	304	4/4	0.83	0.13	50,61,62,68	0
4	NAG	G	506	14/15	0.85	0.10	42,52,76,87	0
4	NAG	G	507	14/15	0.86	0.10	35,50,59,62	0
6	EDO	G	514	4/4	0.86	0.14	66,79,82,82	0
4	NAG	G	505	14/15	0.86	0.09	38,56,69,69	0
4	NAG	G	501	14/15	0.87	0.10	42,53,73,82	0
6	EDO	H	305	4/4	0.90	0.17	30,38,45,47	0
4	NAG	G	504	14/15	0.90	0.09	25,38,48,53	0
6	EDO	G	511	4/4	0.90	0.10	32,39,46,53	0
6	EDO	L	303	4/4	0.90	0.11	38,48,58,63	0
6	EDO	L	302	4/4	0.91	0.08	35,42,50,50	0
6	EDO	H	307	4/4	0.92	0.10	29,35,48,48	0
6	EDO	G	512	4/4	0.92	0.10	36,58,75,81	0
6	EDO	H	303	4/4	0.92	0.10	27,34,42,42	0
4	NAG	G	503	14/15	0.93	0.07	24,36,57,71	0
6	EDO	H	302	4/4	0.93	0.11	32,38,54,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	G	513	4/4	0.94	0.11	28,40,43,50	0
6	EDO	H	306	4/4	0.96	0.09	21,25,26,32	0
5	CA	L	301	1/1	0.96	0.14	61,61,61,61	0
5	CA	G	510	1/1	0.97	0.06	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.