Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2023 – 02:19 PM EDT

PDB ID	:	4YDK
Title	:	Crystal structure of broadly and potently neutralizing antibody C38-VRC16.01 in complex with HIV-1 clade AE strain 93TH057 gp120
Authors	:	Zhou, T.; Moquin, S.; Zheng, A.; Kwong, P.D.
Deposited on	:	2015-02-22
Resolution	:	2.05 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:

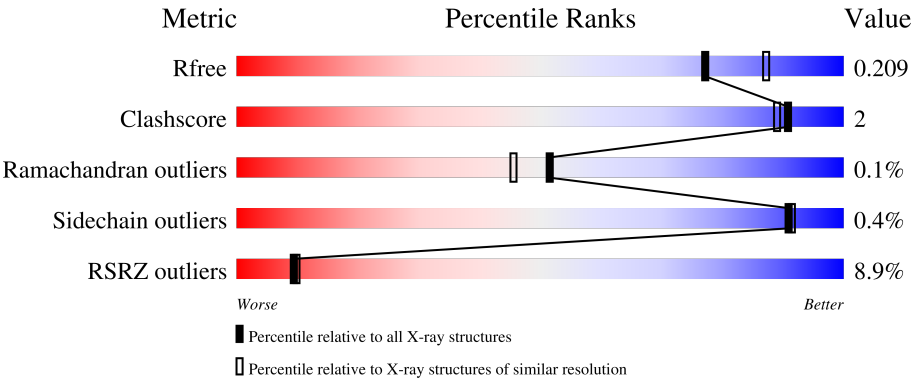
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.05 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}	130704	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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 <=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	353	13% 91% 6% .
2	H	234	6% 96% . .
3	L	214	6% 99% .

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
4	NAG	G	502	-	-	-	X
4	NAG	G	510	-	-	-	X
5	PEG	G	513	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 12823 atoms, of which 6010 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,Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	G	341	Total	C	H	N	O	S	0	0	0
			5207	1676	2539	464	505	23			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	124	GLY	-	linker	UNP Q0ED31
G	198	GLY	-	linker	UNP Q0ED31
G	318	GLY	-	linker	UNP Q0ED31
G	319	GLY	-	linker	UNP Q0ED31
G	320	SER	-	linker	UNP Q0ED31
G	321	GLY	-	linker	UNP Q0ED31
G	322	SER	-	linker	UNP Q0ED31
G	323	GLY	-	linker	UNP Q0ED31

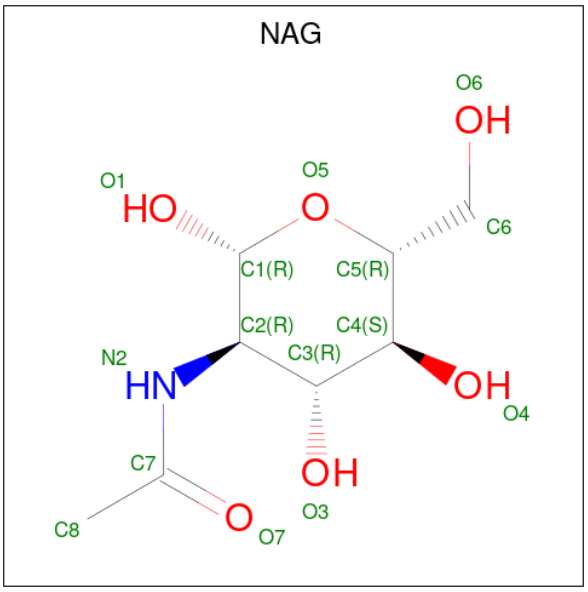
- Molecule 2 is a protein called HEAVY CHAIN OF ANTIBODY C38-VRC16.01.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	230	Total	C	H	N	O	S	0	1	0
			3416	1113	1671	289	336	7			

- Molecule 3 is a protein called LIGHT CHAIN OF ANTIBODY C38-VRC16.01.

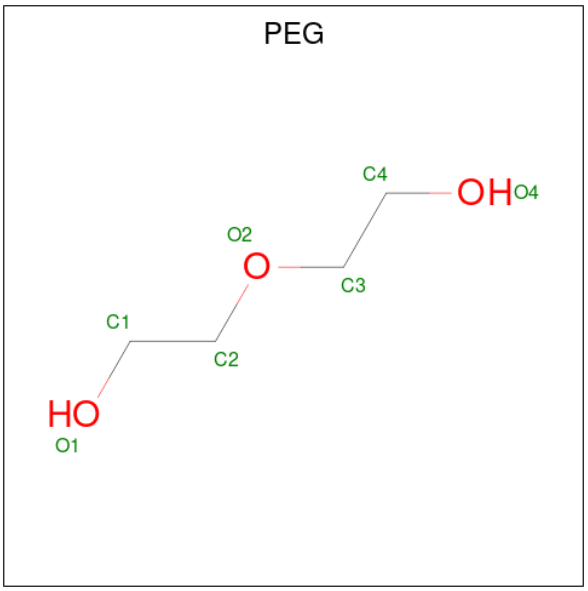
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	L	214	Total	C	H	N	O	S	0	0	0
			3253	1035	1595	288	329	6			

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



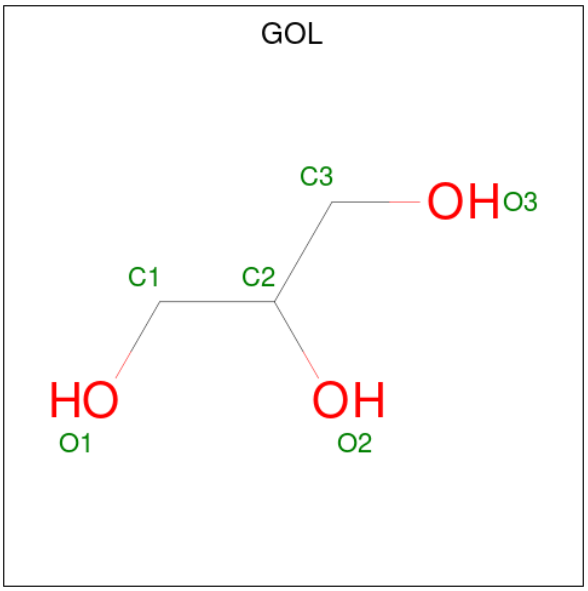
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C H N O 28 8 14 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	G	1	Total	C	H	O	0	0
			17	4	10	3		
5	G	1	Total	C	H	O	0	0
			17	4	10	3		
5	G	1	Total	C	H	O	0	0
			17	4	10	3		
5	G	1	Total	C	H	O	0	0
			17	4	10	3		
5	H	1	Total	C	H	O	0	0
			17	4	10	3		
5	L	1	Total	C	H	O	0	0
			17	4	10	3		
5	L	1	Total	C	H	O	0	0
			17	4	10	3		

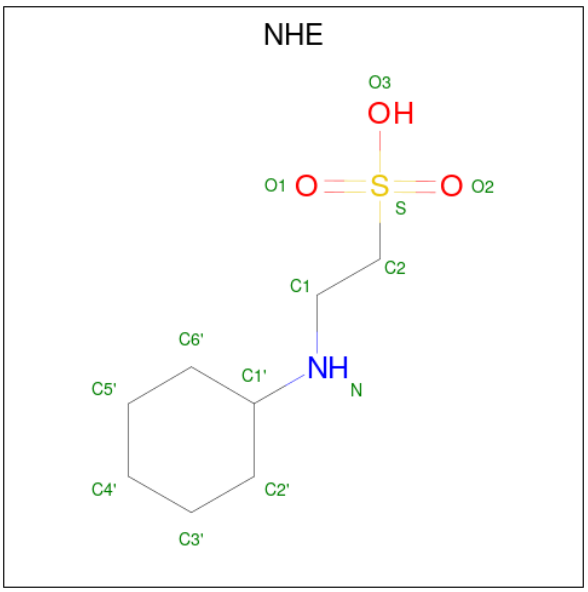
- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total C H O 14 3 8 3	0	0
6	G	1	Total C H O 14 3 8 3	0	0
6	G	1	Total C H O 14 3 8 3	0	0
6	G	1	Total C H O 14 3 8 3	0	0
6	G	1	Total C H O 14 3 8 3	0	0
6	H	1	Total C H O 14 3 8 3	0	0
6	H	1	Total C H O 14 3 8 3	0	0
6	H	1	Total C H O 14 3 8 3	0	0
6	L	1	Total C H O 14 3 8 3	0	0
6	L	1	Total C H O 14 3 8 3	0	0
6	L	1	Total C H O 14 3 8 3	0	0
6	L	1	Total C H O 14 3 8 3	0	0
6	L	1	Total C H O 14 3 8 3	0	0

- Molecule 7 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code:

NHE) (formula: $C_8H_{17}NO_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	G	1	Total	C	H	N	O	S	0	0
			30	8	17	1	3	1		

- Molecule 8 is water.

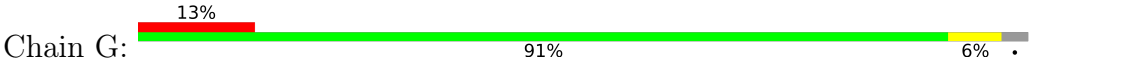
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	144	Total	O	0	0
			144	144		
8	H	150	Total	O	0	0
			150	150		
8	L	168	Total	O	0	0
			168	168		

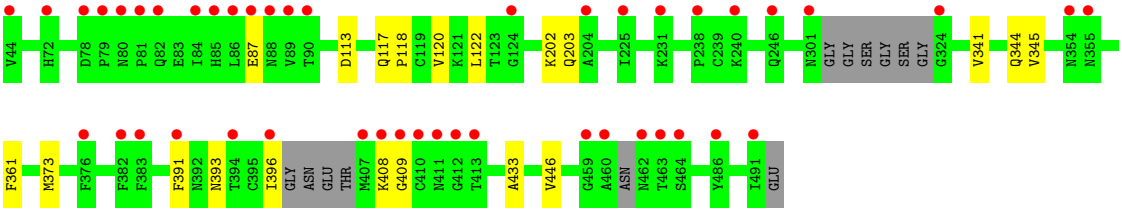
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Envelope glycoprotein gp160,Envelope glycoprotein gp160

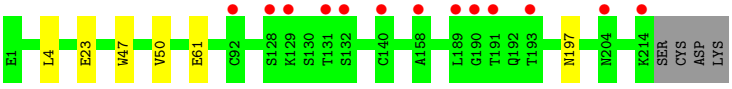
Chain G:





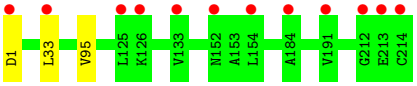
• Molecule 2: HEAVY CHAIN OF ANTIBODY C38-VRC16.01

Chain H:



• Molecule 3: LIGHT CHAIN OF ANTIBODY C38-VRC16.01

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	125.84Å 109.69Å 100.06Å 90.00° 126.26° 90.00°	Depositor
Resolution (Å)	24.25 – 2.05 24.25 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.5 (24.25-2.05) 93.3 (24.25-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 2.06Å)	Xtriage
Refinement program	PHENIX dev_1702	Depositor
R, R_{free}	0.166 , 0.206 0.170 , 0.209	Depositor DCC
R_{free} test set	3411 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	32.7	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 55.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12823	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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, 0.333 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: NHE, NAG, GOL, PEG

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	0.22	0/2723	0.41	0/3693
2	H	0.24	0/1796	0.42	0/2443
3	L	0.24	0/1697	0.42	0/2304
All	All	0.23	0/6216	0.42	0/8440

There are no bond length outliers.

There are no bond angle outliers.

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	2668	2539	2607	13	0
2	H	1745	1671	1684	5	0
3	L	1658	1595	1588	3	0
4	G	140	14	130	6	0
5	G	28	40	40	1	0
5	H	7	10	10	0	0
5	L	14	20	20	0	0
6	G	30	40	40	1	0
6	H	18	24	24	0	0
6	L	30	40	40	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	13	17	16	0	0
8	G	144	0	0	2	0
8	H	150	0	0	1	0
8	L	168	0	0	1	0
All	All	6813	6010	6199	21	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 2.

All (21) 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:393:ASN:HA	1:G:396:ILE:HD13	1.50	0.91
1:G:408:LYS:HD3	1:G:409:GLY:N	2.01	0.76
1:G:113:ASP:O	1:G:117:GLN:NE2	2.24	0.70
2:H:23:GLU:OE2	8:H:548:HOH:O	2.14	0.63
1:G:361:PHE:HB3	1:G:391:PHE:HB3	1.88	0.55
4:G:503:NAG:O4	8:G:688:HOH:O	2.19	0.53
1:G:446:VAL:HG11	4:G:506:NAG:H82	1.92	0.52
1:G:203:GLN:O	6:G:515:GOL:O3	2.28	0.51
1:G:120:VAL:HG12	1:G:122:LEU:CD1	2.41	0.49
1:G:373:MET:CE	4:G:508:NAG:H82	2.41	0.49
1:G:341:VAL:O	1:G:345:VAL:HG23	2.12	0.48
1:G:344:GLN:OE1	4:G:505:NAG:H3	2.13	0.47
1:G:408:LYS:HD2	4:G:509:NAG:O6	2.14	0.47
2:H:47:TRP:CZ3	3:L:95:VAL:HG13	2.51	0.46
2:H:61:GLU:OE1	2:H:61:GLU:N	2.49	0.45
3:L:1:ASP:N	8:L:497:HOH:O	2.47	0.44
1:G:202:LYS:NZ	8:G:604:HOH:O	2.42	0.44
2:H:47:TRP:CH2	2:H:50[B]:VAL:HG22	2.54	0.43
2:H:47:TRP:CE3	3:L:95:VAL:HG13	2.55	0.42
1:G:118:PRO:HB3	1:G:433:ALA:HB1	2.02	0.41
4:G:510:NAG:H82	5:G:512:PEG:C1	2.50	0.41

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	333/353 (94%)	318 (96%)	14 (4%)	1 (0%)	41 32
2	H	229/234 (98%)	224 (98%)	5 (2%)	0	100 100
3	L	212/214 (99%)	206 (97%)	6 (3%)	0	100 100
All	All	774/801 (97%)	748 (97%)	25 (3%)	1 (0%)	51 45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	87	GLU

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	304/311 (98%)	304 (100%)	0	100 100
2	H	191/194 (98%)	189 (99%)	2 (1%)	76 75
3	L	188/188 (100%)	187 (100%)	1 (0%)	88 89
All	All	683/693 (99%)	680 (100%)	3 (0%)	91 91

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

Mol	Chain	Res	Type
2	H	4	LEU
2	H	197	ASN

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Mol	Chain	Res	Type
3	L	33	LEU

Sometimes 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 molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

31 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	G	505	1	14,14,15	0.28	0	17,19,21	0.49	0
5	PEG	L	301	-	6,6,6	0.54	0	5,5,5	0.38	0
4	NAG	G	507	1	14,14,15	0.21	0	17,19,21	0.45	0
4	NAG	G	501	1	14,14,15	0.25	0	17,19,21	0.33	0
6	GOL	L	304	-	5,5,5	0.36	0	5,5,5	0.24	0
4	NAG	G	508	1	14,14,15	0.26	0	17,19,21	0.45	0
5	PEG	G	514	-	6,6,6	0.54	0	5,5,5	0.30	0
7	NHE	G	516	-	13,13,13	0.93	0	16,17,17	1.82	4 (25%)
4	NAG	G	506	1	14,14,15	0.25	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	G	504	1	14,14,15	0.26	0	17,19,21	0.48	0
4	NAG	G	510	1	14,14,15	0.20	0	17,19,21	0.36	0
5	PEG	H	301	-	6,6,6	0.57	0	5,5,5	0.35	0
6	GOL	L	305	-	5,5,5	0.37	0	5,5,5	0.19	0
6	GOL	G	517	-	5,5,5	0.36	0	5,5,5	0.26	0
4	NAG	G	503	1	14,14,15	0.24	0	17,19,21	0.50	0
5	PEG	G	512	-	6,6,6	0.54	0	5,5,5	0.26	0
6	GOL	G	520	-	5,5,5	0.37	0	5,5,5	0.26	0
6	GOL	G	515	-	5,5,5	0.38	0	5,5,5	0.27	0
6	GOL	H	303	-	5,5,5	0.35	0	5,5,5	0.28	0
4	NAG	G	502	1	14,14,15	0.27	0	17,19,21	0.38	0
6	GOL	L	303	-	5,5,5	0.38	0	5,5,5	0.18	0
6	GOL	L	306	-	5,5,5	0.38	0	5,5,5	0.11	0
5	PEG	L	302	-	6,6,6	0.51	0	5,5,5	0.39	0
4	NAG	G	509	1	14,14,15	0.23	0	17,19,21	0.41	0
6	GOL	L	307	-	5,5,5	0.38	0	5,5,5	0.18	0
6	GOL	H	304	-	5,5,5	0.37	0	5,5,5	0.21	0
6	GOL	H	302	-	5,5,5	0.38	0	5,5,5	0.20	0
5	PEG	G	513	-	6,6,6	0.53	0	5,5,5	0.32	0
6	GOL	G	518	-	5,5,5	0.36	0	5,5,5	0.23	0
5	PEG	G	511	-	6,6,6	0.53	0	5,5,5	0.28	0
6	GOL	G	519	-	5,5,5	0.37	0	5,5,5	0.18	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	505	1	-	0/6/23/26	0/1/1/1
5	PEG	L	301	-	-	1/4/4/4	-
4	NAG	G	507	1	-	4/6/23/26	0/1/1/1
4	NAG	G	501	1	-	0/6/23/26	0/1/1/1
6	GOL	L	304	-	-	2/4/4/4	-
4	NAG	G	508	1	-	0/6/23/26	0/1/1/1
5	PEG	G	514	-	-	1/4/4/4	-
7	NHE	G	516	-	-	0/7/15/15	0/1/1/1
4	NAG	G	506	1	-	2/6/23/26	0/1/1/1
4	NAG	G	504	1	-	0/6/23/26	0/1/1/1
4	NAG	G	510	1	-	0/6/23/26	0/1/1/1
5	PEG	H	301	-	-	4/4/4/4	-
6	GOL	L	305	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	G	517	-	-	0/4/4/4	-
4	NAG	G	503	1	-	0/6/23/26	0/1/1/1
5	PEG	G	512	-	-	1/4/4/4	-
6	GOL	G	520	-	-	0/4/4/4	-
6	GOL	G	515	-	-	2/4/4/4	-
6	GOL	H	303	-	-	1/4/4/4	-
4	NAG	G	502	1	-	4/6/23/26	0/1/1/1
6	GOL	L	303	-	-	2/4/4/4	-
6	GOL	L	306	-	-	0/4/4/4	-
5	PEG	L	302	-	-	2/4/4/4	-
4	NAG	G	509	1	-	4/6/23/26	0/1/1/1
6	GOL	L	307	-	-	2/4/4/4	-
6	GOL	H	304	-	-	2/4/4/4	-
6	GOL	H	302	-	-	0/4/4/4	-
5	PEG	G	513	-	-	2/4/4/4	-
6	GOL	G	518	-	-	2/4/4/4	-
5	PEG	G	511	-	-	2/4/4/4	-
6	GOL	G	519	-	-	0/4/4/4	-

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	516	NHE	O2-S-C2	4.27	112.05	106.92
7	G	516	NHE	O2-S-O1	-3.55	101.66	113.95
7	G	516	NHE	O1-S-C2	3.13	110.69	106.92
7	G	516	NHE	O3-S-C2	2.59	109.96	105.77

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	515	GOL	O1-C1-C2-C3
6	H	304	GOL	O1-C1-C2-C3
4	G	509	NAG	O5-C5-C6-O6
4	G	507	NAG	C8-C7-N2-C2
4	G	507	NAG	O7-C7-N2-C2
4	G	509	NAG	C8-C7-N2-C2
4	G	509	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	G	509	NAG	C4-C5-C6-O6
4	G	507	NAG	C4-C5-C6-O6
4	G	506	NAG	O5-C5-C6-O6
5	G	511	PEG	O1-C1-C2-O2
5	G	514	PEG	O2-C3-C4-O4
5	H	301	PEG	O1-C1-C2-O2
5	L	301	PEG	O1-C1-C2-O2
4	G	506	NAG	C4-C5-C6-O6
5	H	301	PEG	O2-C3-C4-O4
4	G	507	NAG	O5-C5-C6-O6
6	L	303	GOL	C1-C2-C3-O3
6	L	304	GOL	O1-C1-C2-C3
6	L	307	GOL	O1-C1-C2-C3
5	G	511	PEG	O2-C3-C4-O4
5	L	302	PEG	O2-C3-C4-O4
4	G	502	NAG	O5-C5-C6-O6
6	G	515	GOL	O1-C1-C2-O2
4	G	502	NAG	C1-C2-N2-C7
5	G	512	PEG	O2-C3-C4-O4
6	H	304	GOL	O1-C1-C2-O2
6	L	304	GOL	O1-C1-C2-O2
5	L	302	PEG	C1-C2-O2-C3
5	G	513	PEG	O2-C3-C4-O4
5	H	301	PEG	C1-C2-O2-C3
5	G	513	PEG	C1-C2-O2-C3
5	H	301	PEG	C4-C3-O2-C2
6	H	303	GOL	O1-C1-C2-C3
6	L	303	GOL	O2-C2-C3-O3
6	G	518	GOL	O1-C1-C2-C3
4	G	502	NAG	C4-C5-C6-O6
6	G	518	GOL	O1-C1-C2-O2
6	L	307	GOL	O1-C1-C2-O2
4	G	502	NAG	C3-C2-N2-C7

There are no ring outliers.

8 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	505	NAG	1	0
4	G	508	NAG	1	0
4	G	506	NAG	1	0
4	G	510	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	503	NAG	1	0
5	G	512	PEG	1	0
6	G	515	GOL	1	0
4	G	509	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	341/353 (96%)	0.51	45 (13%)	3	2	26, 57, 97, 131	0
2	H	230/234 (98%)	0.07	13 (5%)	23	24	22, 41, 80, 104	0
3	L	214/214 (100%)	0.15	12 (5%)	24	25	23, 38, 84, 116	0
All	All	785/801 (98%)	0.28	70 (8%)	9	10	22, 48, 91, 131	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	407	MET	8.6
3	L	214	CYS	6.4
1	G	324	GLY	5.7
1	G	462	ASN	5.5
3	L	212	GLY	5.3
2	H	128	SER	4.9
1	G	84	ILE	4.9
2	H	190	GLY	4.9
1	G	301	ASN	4.8
1	G	355	ASN	4.6
1	G	409	GLY	4.6
1	G	44	VAL	4.5
1	G	80	ASN	4.4
2	H	92	CYS	4.1
1	G	87	GLU	4.0
1	G	408	LYS	3.9
1	G	411	ASN	3.8
1	G	82	GLN	3.7
1	G	240	LYS	3.7
1	G	88	ASN	3.7
1	G	86	LEU	3.7
1	G	85	HIS	3.6
1	G	463	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	410	CYS	3.5
1	G	79	PRO	3.5
3	L	1	ASP	3.4
3	L	126	LYS	3.4
1	G	246	GLN	3.4
2	H	204	ASN	3.3
1	G	231	LYS	3.3
2	H	214	LYS	3.3
1	G	464	SER	3.3
1	G	81	PRO	3.3
1	G	89	VAL	3.2
1	G	90	THR	3.2
3	L	213	GLU	3.1
2	H	191	THR	3.1
1	G	376	PHE	3.1
2	H	140	CYS	3.1
1	G	238	PRO	3.0
1	G	394	THR	3.0
3	L	154	LEU	3.0
1	G	383	PHE	3.0
1	G	486	TYR	2.9
2	H	129	LYS	2.9
3	L	191	VAL	2.9
1	G	391	PHE	2.9
2	H	158	ALA	2.8
2	H	193	THR	2.8
1	G	124	GLY	2.8
1	G	396	ILE	2.6
1	G	354	ASN	2.5
1	G	491	ILE	2.5
3	L	184	ALA	2.5
3	L	33	LEU	2.4
1	G	225	ILE	2.4
1	G	382	PHE	2.3
1	G	412	GLY	2.2
1	G	460	ALA	2.2
2	H	132	SER	2.2
1	G	204	ALA	2.2
2	H	189	LEU	2.2
1	G	78	ASP	2.1
1	G	459	GLY	2.1
3	L	152	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
2	H	131	THR	2.0
3	L	133	VAL	2.0
1	G	72	HIS	2.0
1	G	413	THR	2.0
3	L	125	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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, 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	B-factors(Å^2)	Q<0.9
5	PEG	G	513	7/7	0.50	0.40	97,116,133,133	0
5	PEG	G	512	7/7	0.54	0.26	95,114,125,125	0
5	PEG	G	511	7/7	0.56	0.24	77,106,126,126	0
6	GOL	G	520	6/6	0.61	0.26	70,86,103,103	0
4	NAG	G	502	14/15	0.64	0.64	99,131,158,160	0
5	PEG	H	301	7/7	0.64	0.34	61,94,123,123	0
5	PEG	L	302	7/7	0.64	0.30	65,84,101,115	0
4	NAG	G	510	14/15	0.64	0.52	107,130,138,142	0
6	GOL	G	518	6/6	0.66	0.24	95,114,135,135	0
5	PEG	G	514	7/7	0.74	0.26	88,106,124,124	0
6	GOL	G	515	6/6	0.75	0.25	81,102,117,124	0
6	GOL	L	304	6/6	0.76	0.21	79,106,125,133	0
4	NAG	G	507	14/15	0.81	0.30	93,101,104,106	0
5	PEG	L	301	7/7	0.82	0.20	42,91,119,119	0
4	NAG	G	509	14/15	0.82	0.43	92,106,116,121	0
4	NAG	G	505	14/15	0.84	0.17	62,78,83,84	0
4	NAG	G	506	14/15	0.85	0.20	47,68,79,82	0
4	NAG	G	501	14/15	0.86	0.24	75,88,96,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	H	302	6/6	0.87	0.19	57,71,82,96	0
4	NAG	G	503	14/15	0.88	0.11	38,45,54,56	0
6	GOL	G	519	6/6	0.89	0.15	79,99,119,119	0
4	NAG	G	504	14/15	0.90	0.21	54,63,75,82	0
6	GOL	H	304	6/6	0.91	0.26	86,104,110,115	0
4	NAG	G	508	14/15	0.92	0.22	56,72,102,112	0
6	GOL	G	517	6/6	0.92	0.16	56,67,71,79	0
6	GOL	L	306	6/6	0.92	0.15	29,71,77,89	0
6	GOL	L	305	6/6	0.93	0.16	44,58,73,83	0
6	GOL	L	303	6/6	0.93	0.14	31,63,83,84	0
6	GOL	H	303	6/6	0.96	0.12	29,72,94,101	0
6	GOL	L	307	6/6	0.97	0.22	45,58,70,78	0
7	NHE	G	516	13/13	0.98	0.09	34,54,72,74	0

6.5 Other polymers (i)

There are no such residues in this entry.