



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:06 am GMT

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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

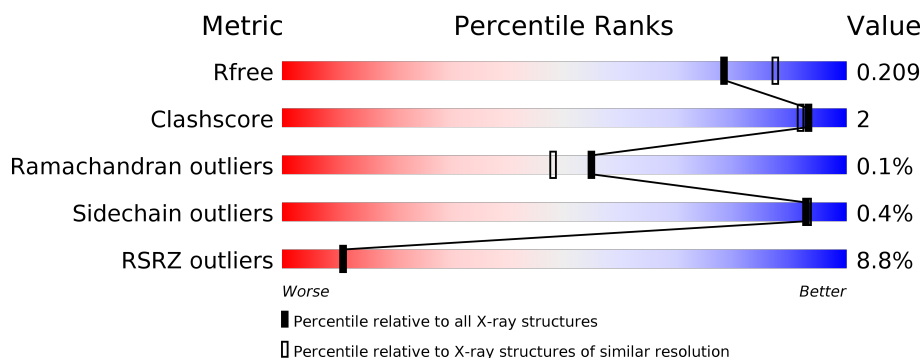
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	100719	2028 (2.08-2.04)
Clashscore	112137	2143 (2.08-2.04)
Ramachandran outliers	110173	2126 (2.08-2.04)
Sidechain outliers	110143	2126 (2.08-2.04)
RSRZ outliers	101464	2035 (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 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 $\leq 5\%$. 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	353	<div> <div>13%</div> <div>91%</div> <div>6%</div> </div>
2	H	234	<div> <div>6%</div> <div>96%</div> <div>•</div> </div>
3	L	214	<div> <div>5%</div> <div>99%</div> <div>•</div> </div>

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	509	-	-	-	X
4	NAG	G	510	-	-	-	X
5	PEG	G	511	-	-	-	X
5	PEG	G	512	-	-	-	X
5	PEG	G	513	-	-	-	X
5	PEG	H	301	-	-	-	X
5	PEG	L	301	-	-	-	X
5	PEG	L	302	-	-	-	X
6	GOL	G	515	-	-	-	X
6	GOL	G	520	-	-	-	X
6	GOL	H	302	-	-	-	X
6	GOL	H	304	-	-	-	X
6	GOL	L	304	-	-	-	X
6	GOL	L	306	-	-	-	X
6	GOL	L	307	-	-	-	X

2 Entry composition

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 N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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		

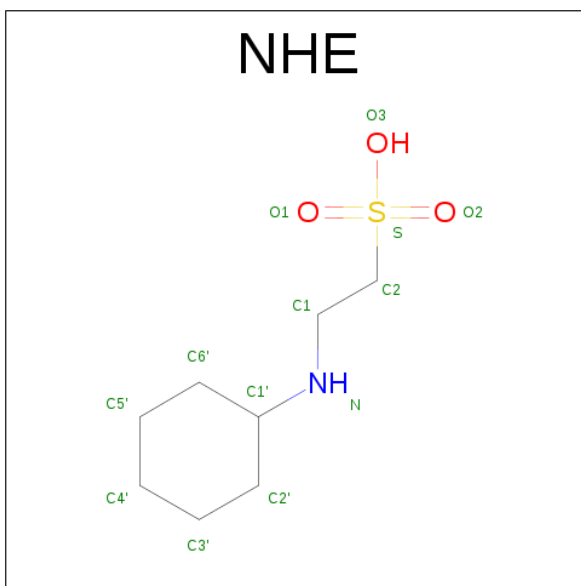
- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

NHE) (formula: C₈H₁₇NO₃S).



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

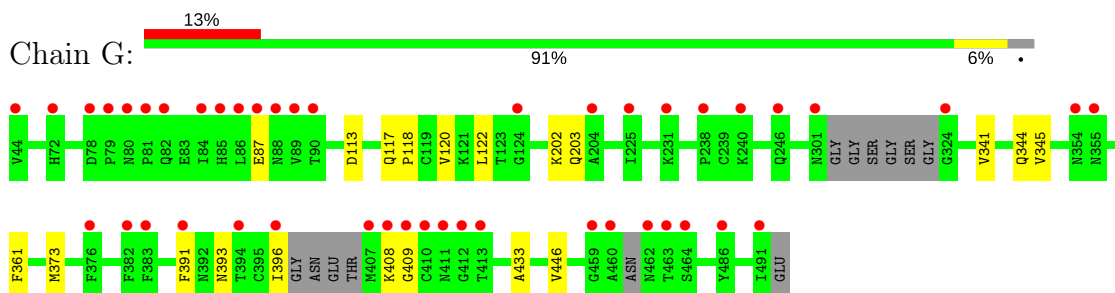
- Molecule 8 is water.

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		

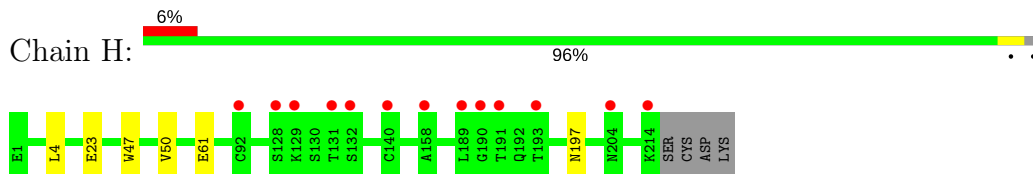
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

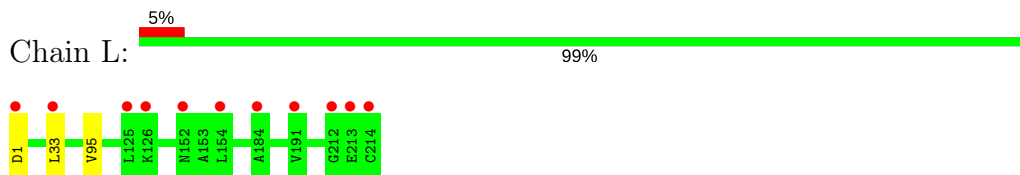
- Molecule 1: Envelope glycoprotein gp160,Envelope glycoprotein gp160



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



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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.06Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.166 , 0.206 0.178 , 0.209	Depositor DCC
R_{free} test set	3411 reflections (5.62%)	DCC
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 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.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NHE, GOL, PEG, 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	0.22	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 [i](#)

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

Continued on next page...

Continued from previous page...

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%)	44	35
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%)	55	48

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%)	80	79
3	L	188/188 (100%)	187 (100%)	1 (0%)	91	91
All	All	683/693 (99%)	680 (100%)	3 (0%)	93	93

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L	33	LEU

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

5.3.3 RNA ⓘ

There are no RNA 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 carbohydrates 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	501	1	14,14,15	0.24	0	15,19,21	0.40	0
4	NAG	G	502	1	14,14,15	0.26	0	15,19,21	0.44	0
4	NAG	G	503	1	14,14,15	0.24	0	15,19,21	0.55	0
4	NAG	G	504	1	14,14,15	0.26	0	15,19,21	0.51	0
4	NAG	G	505	1	14,14,15	0.28	0	15,19,21	0.53	0
4	NAG	G	506	1	14,14,15	0.24	0	15,19,21	0.48	0
4	NAG	G	507	1	14,14,15	0.20	0	15,19,21	0.49	0
4	NAG	G	508	1	14,14,15	0.26	0	15,19,21	0.49	0
4	NAG	G	509	1	14,14,15	0.22	0	15,19,21	0.46	0
4	NAG	G	510	1	14,14,15	0.20	0	15,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PEG	G	511	-	6,6,6	0.55	0	5,5,5	0.29	0
5	PEG	G	512	-	6,6,6	0.55	0	5,5,5	0.28	0
5	PEG	G	513	-	6,6,6	0.55	0	5,5,5	0.32	0
5	PEG	G	514	-	6,6,6	0.56	0	5,5,5	0.31	0
6	GOL	G	515	-	5,5,5	0.36	0	5,5,5	0.26	0
7	NHE	G	516	-	13,13,13	0.90	0	15,17,17	2.39	4 (26%)
6	GOL	G	517	-	5,5,5	0.34	0	5,5,5	0.24	0
6	GOL	G	518	-	5,5,5	0.34	0	5,5,5	0.23	0
6	GOL	G	519	-	5,5,5	0.35	0	5,5,5	0.18	0
6	GOL	G	520	-	5,5,5	0.35	0	5,5,5	0.25	0
5	PEG	H	301	-	6,6,6	0.59	0	5,5,5	0.36	0
6	GOL	H	302	-	5,5,5	0.36	0	5,5,5	0.20	0
6	GOL	H	303	-	5,5,5	0.33	0	5,5,5	0.27	0
6	GOL	H	304	-	5,5,5	0.36	0	5,5,5	0.19	0
5	PEG	L	301	-	6,6,6	0.55	0	5,5,5	0.38	0
5	PEG	L	302	-	6,6,6	0.53	0	5,5,5	0.40	0
6	GOL	L	303	-	5,5,5	0.35	0	5,5,5	0.18	0
6	GOL	L	304	-	5,5,5	0.35	0	5,5,5	0.23	0
6	GOL	L	305	-	5,5,5	0.35	0	5,5,5	0.18	0
6	GOL	L	306	-	5,5,5	0.35	0	5,5,5	0.12	0
6	GOL	L	307	-	5,5,5	0.36	0	5,5,5	0.17	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
4	NAG	G	510	1	-	0/6/23/26	0/1/1/1
5	PEG	G	511	-	-	0/4/4/4	0/0/0/0
5	PEG	G	512	-	-	0/4/4/4	0/0/0/0
5	PEG	G	513	-	-	0/4/4/4	0/0/0/0
5	PEG	G	514	-	-	0/4/4/4	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	G	515	-	-	0/4/4/4	0/0/0/0
7	NHE	G	516	-	-	0/7/15/15	0/1/1/1
6	GOL	G	517	-	-	0/4/4/4	0/0/0/0
6	GOL	G	518	-	-	0/4/4/4	0/0/0/0
6	GOL	G	519	-	-	0/4/4/4	0/0/0/0
6	GOL	G	520	-	-	0/4/4/4	0/0/0/0
5	PEG	H	301	-	-	0/4/4/4	0/0/0/0
6	GOL	H	302	-	-	0/4/4/4	0/0/0/0
6	GOL	H	303	-	-	0/4/4/4	0/0/0/0
6	GOL	H	304	-	-	0/4/4/4	0/0/0/0
5	PEG	L	301	-	-	0/4/4/4	0/0/0/0
5	PEG	L	302	-	-	0/4/4/4	0/0/0/0
6	GOL	L	303	-	-	0/4/4/4	0/0/0/0
6	GOL	L	304	-	-	0/4/4/4	0/0/0/0
6	GOL	L	305	-	-	0/4/4/4	0/0/0/0
6	GOL	L	306	-	-	0/4/4/4	0/0/0/0
6	GOL	L	307	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	516	NHE	O2-S-O1	-3.52	101.66	113.86
7	G	516	NHE	O3-S-C2	3.18	109.96	106.06
7	G	516	NHE	O1-S-C2	4.54	110.69	106.79
7	G	516	NHE	O2-S-C2	6.13	112.05	106.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	503	NAG	1	0
4	G	505	NAG	1	0
4	G	506	NAG	1	0
4	G	508	NAG	1	0
4	G	509	NAG	1	0
4	G	510	NAG	1	0
5	G	512	PEG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	515	GOL	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, 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	341/353 (96%)	0.51	45 (13%) 4 3	26, 57, 97, 131	0
2	H	230/234 (98%)	0.07	13 (5%) 24 25	22, 41, 80, 104	0
3	L	214/214 (100%)	0.15	11 (5%) 29 29	23, 38, 84, 116	0
All	All	785/801 (98%)	0.28	69 (8%) 11 11	22, 48, 91, 131	0

All (69) 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
2	H	190	GLY	4.9
1	G	84	ILE	4.8
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	3.9
1	G	408	LYS	3.9
1	G	82	GLN	3.7
1	G	411	ASN	3.7
1	G	86	LEU	3.7
1	G	240	LYS	3.7
1	G	88	ASN	3.7
1	G	85	HIS	3.6
1	G	410	CYS	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	463	THR	3.5
1	G	79	PRO	3.5
3	L	126	LYS	3.4
3	L	1	ASP	3.4
1	G	246	GLN	3.4
2	H	204	ASN	3.3
1	G	81	PRO	3.3
2	H	214	LYS	3.3
1	G	231	LYS	3.3
1	G	464	SER	3.3
1	G	89	VAL	3.2
1	G	90	THR	3.2
3	L	213	GLU	3.2
2	H	191	THR	3.2
1	G	376	PHE	3.1
2	H	140	CYS	3.1
1	G	394	THR	3.0
1	G	238	PRO	3.0
3	L	154	LEU	3.0
1	G	383	PHE	3.0
1	G	486	TYR	3.0
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
3	L	184	ALA	2.5
1	G	225	ILE	2.5
3	L	33	LEU	2.4
1	G	491	ILE	2.4
1	G	460	ALA	2.3
1	G	382	PHE	2.3
2	H	132	SER	2.3
1	G	412	GLY	2.2
1	G	204	ALA	2.2
2	H	189	LEU	2.2
1	G	459	GLY	2.1
1	G	78	ASP	2.1
3	L	125	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	72	HIS	2.0
2	H	131	THR	2.0
3	L	152	ASN	2.0
1	G	413	THR	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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NAG	G	510	14/15	0.64	0.53	12.74	107,130,138,142	0
5	PEG	G	513	7/7	0.50	0.41	11.69	97,116,133,133	0
5	PEG	L	302	7/7	0.64	0.30	6.89	65,84,101,115	0
6	GOL	H	304	6/6	0.91	0.25	5.18	86,104,110,115	0
5	PEG	H	301	7/7	0.65	0.34	4.73	61,94,123,123	0
5	PEG	G	512	7/7	0.53	0.27	4.50	95,114,125,125	0
6	GOL	L	306	6/6	0.92	0.15	4.49	29,71,77,89	0
6	GOL	L	307	6/6	0.97	0.22	4.16	45,58,70,78	0
4	NAG	G	502	14/15	0.64	0.64	4.11	99,131,158,160	0
6	GOL	G	520	6/6	0.61	0.26	3.41	70,86,103,103	0
6	GOL	H	302	6/6	0.87	0.19	2.95	57,71,82,96	0
5	PEG	L	301	7/7	0.82	0.20	2.72	42,91,119,119	0
6	GOL	L	304	6/6	0.76	0.21	2.42	79,106,125,133	0
6	GOL	G	515	6/6	0.75	0.25	2.41	81,102,117,124	0
5	PEG	G	511	7/7	0.56	0.23	2.35	77,106,126,126	0
4	NAG	G	507	14/15	0.81	0.30	2.00	93,101,104,106	0
6	GOL	G	517	6/6	0.92	0.16	1.89	56,67,71,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	G	509	14/15	0.82	0.43	1.66	92,106,116,121	0
4	NAG	G	501	14/15	0.86	0.24	1.42	75,88,96,98	0
4	NAG	G	506	14/15	0.85	0.20	1.21	47,68,79,82	0
6	GOL	G	519	6/6	0.89	0.14	1.06	79,99,119,119	0
6	GOL	L	303	6/6	0.93	0.14	1.05	31,63,83,84	0
5	PEG	G	514	7/7	0.75	0.26	0.84	88,106,124,124	0
6	GOL	G	518	6/6	0.67	0.24	0.84	95,114,135,135	0
6	GOL	L	305	6/6	0.93	0.16	0.43	44,58,73,83	0
6	GOL	H	303	6/6	0.96	0.12	0.10	29,72,94,101	0
4	NAG	G	505	14/15	0.84	0.17	-0.18	62,78,83,84	0
4	NAG	G	503	14/15	0.89	0.11	-0.39	38,45,54,56	0
7	NHE	G	516	13/13	0.98	0.09	-0.86	34,54,72,74	0
4	NAG	G	504	14/15	0.90	0.21	-	54,63,75,82	0
4	NAG	G	508	14/15	0.92	0.22	-	56,72,102,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.