



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 09:50 AM BST

PDB ID : 4YDI  
Title : Crystal structure of broad and potently neutralizing VRC01-class antibody Z258-VRC27.01, isolated from human donor Z258, in complex with HIV-1 gp120 from clade A strain Q23.17  
Authors : Zhou, T.; Srivatsan, S.; Kwong, P.D.  
Deposited on : 2015-02-22  
Resolution : 3.45 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](mailto: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 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 : 2.13.1  
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) : 2.13.1

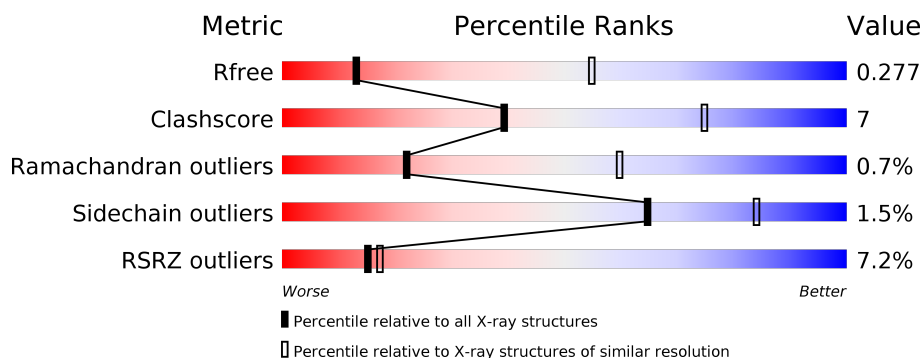
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.45 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	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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  $\geq 3$ , 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	<div> <div>8%</div> <div>78%</div> <div>17%</div> <div>.</div> </div>
2	H	227	<div> <div>7%</div> <div>70%</div> <div>22%</div> <div>8%</div> </div>
3	L	210	<div> <div>5%</div> <div>82%</div> <div>16%</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	509	-	-	-	X
4	NAG	G	511	-	-	-	X
4	NAG	G	512	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6169 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	343	Total	C	N	O	S	0	0	0
			2698	1698	471	509	20			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	124	GLY	-	linker	UNP O55774
G	198	GLY	-	linker	UNP O55774
G	318	GLY	-	linker	UNP O55774
G	319	GLY	-	linker	UNP O55774
G	320	SER	-	linker	UNP O55774
G	321	GLY	-	linker	UNP O55774
G	322	SER	-	linker	UNP O55774
G	323	GLY	-	linker	UNP O55774

- Molecule 2 is a protein called HEAVY CHAIN OF ANTIBODY Z258-VRC27.01.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	209	Total	C	N	O	S	0	0	0
			1643	1050	286	302	5			

- Molecule 3 is a protein called LIGHT CHAIN OF ANTIBODY Z258-VRC27.01.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	208	Total	C	N	O	S	0	0	0
			1603	997	283	318	5			

- 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	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		
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	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	C	O	0	0
			4	2	2		

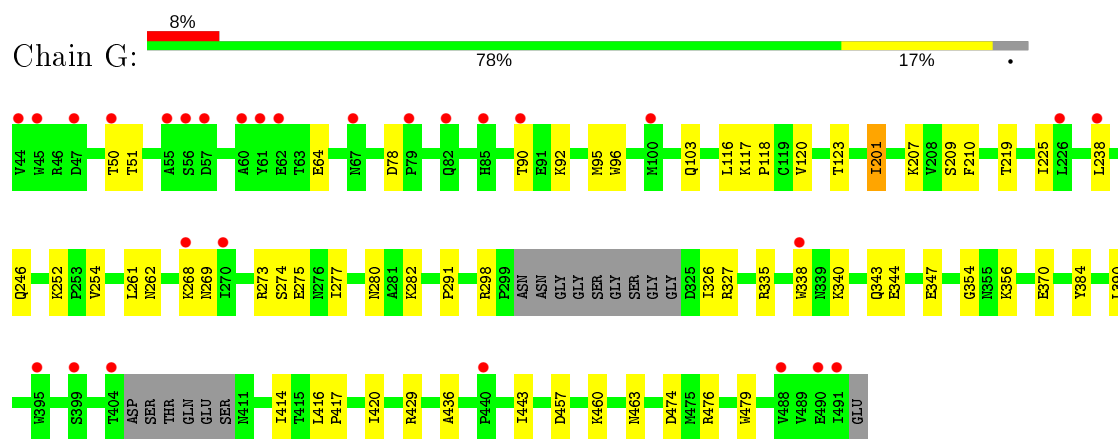
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	9	Total	O	0	0
			9	9		
7	H	8	Total	O	0	0
			8	8		
7	L	2	Total	O	0	0
			2	2		

### 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





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.74Å 172.25Å 91.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.04 – 3.45 46.04 – 3.45	Depositor EDS
% Data completeness (in resolution range)	87.3 (46.04-3.45) 79.4 (46.04-3.45)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.94 (at 3.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.222 , 0.276 0.223 , 0.277	Depositor DCC
$R_{free}$ test set	677 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.3	Xtriage
Anisotropy	1.050	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 77.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6169	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SO4, EDO, 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	0.29	0/2757	0.53	1/3746 (0.0%)
2	H	0.26	0/1690	0.45	0/2300
3	L	0.27	0/1637	0.45	0/2220
All	All	0.28	0/6084	0.49	1/8266 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	201	ILE	CG1-CB-CG2	-5.08	100.21	111.40

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	2698	0	2630	42	0
2	H	1643	0	1607	32	0
3	L	1603	0	1550	20	0
4	G	168	0	156	3	0
4	L	14	0	13	0	0
5	G	5	0	0	1	0
5	H	15	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	4	0	6	0	0
7	G	9	0	0	0	0
7	H	8	0	0	1	0
7	L	2	0	0	0	0
All	All	6169	0	5962	89	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 7.

All (89) 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)
3:L:145:LYS:HB3	3:L:147:GLN:HE22	1.47	0.79
1:G:327:ARG:NH2	5:G:513:SO4:O1	2.23	0.69
3:L:189:HIS:O	3:L:211:ARG:NH1	2.26	0.69
1:G:50:THR:O	1:G:103:GLN:NE2	2.27	0.68
1:G:474:ASP:OD2	1:G:476:ARG:NH2	2.26	0.68
1:G:78:ASP:OD2	1:G:246:GLN:NE2	2.28	0.67
3:L:186:TYR:O	3:L:211:ARG:NH1	2.29	0.66
2:H:66:ARG:NH2	2:H:86:ASP:OD2	2.28	0.65
3:L:113:PRO:HD2	3:L:201:LEU:HD11	1.79	0.64
2:H:123:PRO:HD3	2:H:209:LYS:NZ	2.12	0.64
2:H:87:THR:HG23	2:H:110:VAL:HA	1.79	0.64
2:H:101:ASP:HB3	2:H:102:PRO:HD3	1.82	0.62
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.82	0.61
2:H:123:PRO:HB3	2:H:211:VAL:HG12	1.81	0.61
1:G:90:THR:HG22	1:G:238:LEU:HD22	1.82	0.60
2:H:11:VAL:HG22	2:H:110:VAL:HB	1.84	0.59
2:H:69:LEU:HD21	2:H:80:LEU:HD12	1.84	0.59
1:G:252:LYS:HE2	1:G:262:ASN:HB3	1.85	0.58
1:G:92:LYS:HE2	1:G:238:LEU:HG	1.85	0.58
1:G:123:THR:HG21	1:G:429:ARG:HE	1.69	0.58
3:L:128:GLY:HA2	3:L:183:LYS:HD3	1.85	0.58
1:G:219:THR:HG23	1:G:225:ILE:HG13	1.85	0.58
2:H:40:ALA:HB3	2:H:43:ARG:HB3	1.85	0.57
3:L:39:LYS:HB2	3:L:42:ARG:HD2	1.87	0.56
2:H:151:THR:OG1	2:H:199:ASN:OD1	2.22	0.55
3:L:145:LYS:HB2	3:L:197:THR:HB	1.88	0.55
2:H:34:LEU:HB2	7:H:405:HOH:O	2.07	0.55
2:H:82:LEU:HD22	2:H:82(C):LEU:HD23	1.88	0.55
1:G:298:ARG:HH21	1:G:326:ILE:HB	1.70	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:61:ARG:NH2	3:L:82:ASP:OD2	2.41	0.54
1:G:274:SER:HB3	1:G:277:ILE:HG13	1.89	0.54
1:G:298:ARG:HD3	1:G:443:ILE:HD12	1.90	0.54
3:L:158:ASN:O	3:L:179:LEU:HD12	2.09	0.53
2:H:123:PRO:HD3	2:H:209:LYS:HZ3	1.74	0.53
1:G:457:ASP:HA	2:H:58:ASN:HD21	1.73	0.52
2:H:100(C):TRP:CD1	3:L:91:ILE:HG22	2.44	0.52
1:G:338:TRP:CE2	1:G:390:LEU:HG	2.46	0.51
4:G:504:NAG:N2	3:L:32:ASP:OD2	2.44	0.51
3:L:198:HIS:HB3	3:L:201:LEU:HD12	1.93	0.50
1:G:254:VAL:HG21	1:G:262:ASN:HB2	1.94	0.50
1:G:335:ARG:CZ	1:G:414:ILE:HG12	2.42	0.50
1:G:96:TRP:CG	1:G:275:GLU:HG3	2.46	0.49
3:L:35:TRP:CZ3	3:L:88:CYS:HB3	2.47	0.49
1:G:92:LYS:HG2	1:G:238:LEU:HD23	1.93	0.49
1:G:201:ILE:HG23	1:G:201:ILE:HD12	1.58	0.48
2:H:96:ARG:CD	2:H:101:ASP:HB2	2.44	0.48
1:G:95:MET:SD	1:G:273:ARG:HD3	2.54	0.48
2:H:50:TRP:CZ3	2:H:52:LYS:HG3	2.49	0.47
1:G:340:LYS:O	1:G:344:GLU:HG2	2.15	0.47
1:G:123:THR:HG21	1:G:429:ARG:HH21	1.79	0.47
1:G:268:LYS:HE3	1:G:269:ASN:ND2	2.30	0.47
3:L:198:HIS:HB3	3:L:201:LEU:CD1	2.44	0.47
1:G:298:ARG:HD2	1:G:420:ILE:HD12	1.97	0.47
1:G:51:THR:HA	1:G:103:GLN:HE22	1.80	0.46
1:G:280:ASN:OD1	2:H:50:TRP:NE1	2.44	0.46
2:H:12:ARG:HH21	2:H:16:SER:HB2	1.81	0.46
2:H:123:PRO:HD3	2:H:209:LYS:HZ1	1.80	0.46
1:G:120:VAL:HA	1:G:201:ILE:O	2.16	0.45
2:H:24:THR:HG21	2:H:29:PHE:HD1	1.82	0.44
1:G:254:VAL:HG11	1:G:261:LEU:HB2	1.98	0.44
3:L:105:ASP:OD2	3:L:106:ILE:N	2.49	0.44
1:G:64:GLU:HA	1:G:209:SER:HB3	1.99	0.44
1:G:343:GLN:O	1:G:347:GLU:HG3	2.18	0.44
3:L:104:LEU:HD12	3:L:104:LEU:HA	1.84	0.44
3:L:33:LEU:HD12	3:L:89:GLN:O	2.17	0.44
1:G:116:LEU:HD11	1:G:210:PHE:CE1	2.53	0.43
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.53	0.43
1:G:207:LYS:HE2	1:G:436:ALA:HB3	1.99	0.43
2:H:50:TRP:CH2	2:H:52:LYS:HE3	2.53	0.43
1:G:354:GLY:O	1:G:356:LYS:N	2.51	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:100(D):ARG:HD3	3:L:49:HIS:CD2	2.54	0.43
2:H:170:LEU:HG	2:H:176:TYR:CE1	2.54	0.42
2:H:210:LYS:NZ	2:H:212:GLU:OE1	2.52	0.42
2:H:59:TYR:CZ	2:H:68:THR:HA	2.54	0.42
2:H:97:LEU:HD22	2:H:100(B):SER:HB3	2.02	0.42
2:H:18:VAL:HG12	2:H:82(C):LEU:HD21	2.01	0.42
1:G:282:LYS:NZ	2:H:100(A):SER:H	2.18	0.42
3:L:48:ILE:HD13	3:L:73:PHE:HE2	1.84	0.41
1:G:291:PRO:CG	4:G:509:NAG:H82	2.50	0.41
1:G:338:TRP:CZ2	1:G:390:LEU:HG	2.55	0.41
1:G:298:ARG:NE	1:G:326:ILE:O	2.44	0.41
1:G:117:LYS:HA	1:G:118:PRO:HD3	1.83	0.41
1:G:370:GLU:HG3	1:G:384:TYR:CE2	2.56	0.41
1:G:416:LEU:HA	1:G:417:PRO:HD3	1.91	0.41
1:G:476:ARG:HA	1:G:479:TRP:CD1	2.56	0.41
1:G:291:PRO:HG2	4:G:509:NAG:H82	2.04	0.40
3:L:196:VAL:HB	3:L:205:VAL:HG23	2.03	0.40
2:H:33:ILE:HG13	2:H:52:LYS:HG2	2.03	0.40
2:H:44:SER:OG	2:H:45:PHE:N	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	337/359 (94%)	327 (97%)	9 (3%)	1 (0%)	41	75
2	H	205/227 (90%)	188 (92%)	15 (7%)	2 (1%)	15	52
3	L	206/210 (98%)	190 (92%)	14 (7%)	2 (1%)	15	52
All	All	748/796 (94%)	705 (94%)	38 (5%)	5 (1%)	22	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	463	ASN
3	L	27	GLN
3	L	91	ILE
2	H	41	PRO
2	H	51	ILE

### 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%)	302 (100%)	1 (0%)	92	98
2	H	182/195 (93%)	178 (98%)	4 (2%)	52	77
3	L	180/183 (98%)	175 (97%)	5 (3%)	43	72
All	All	665/692 (96%)	655 (98%)	10 (2%)	65	84

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	460	LYS
2	H	38	ARG
2	H	71	ARG
2	H	82	LEU
2	H	189	LEU
3	L	50	HIS
3	L	54	ARG
3	L	58	VAL
3	L	69	THR
3	L	205	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	L	147	GLN

### 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 ⓘ

18 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	$\# Z  > 2$
6	EDO	H	303	-	3,3,3	0.46	0	2,2,2	0.32	0
4	NAG	L	301	3	14,14,15	0.25	0	17,19,21	0.45	0
4	NAG	G	501	1	14,14,15	0.26	0	17,19,21	0.38	0
5	SO4	G	513	-	4,4,4	0.17	0	6,6,6	0.11	0
4	NAG	G	508	1	14,14,15	0.21	0	17,19,21	0.43	0
5	SO4	H	304	-	4,4,4	0.14	0	6,6,6	0.07	0
4	NAG	G	502	1	14,14,15	0.25	0	17,19,21	0.53	0
5	SO4	H	301	-	4,4,4	0.13	0	6,6,6	0.06	0
4	NAG	G	504	1	14,14,15	0.38	0	17,19,21	0.46	0
4	NAG	G	505	1	14,14,15	0.18	0	17,19,21	0.56	0
4	NAG	G	510	1	14,14,15	0.28	0	17,19,21	0.38	0
4	NAG	G	503	1	14,14,15	0.26	0	17,19,21	0.60	1 (5%)
5	SO4	H	302	-	4,4,4	0.13	0	6,6,6	0.05	0
4	NAG	G	511	1	14,14,15	0.35	0	17,19,21	0.47	0
4	NAG	G	507	1	14,14,15	0.34	0	17,19,21	0.54	0
4	NAG	G	512	1	14,14,15	0.26	0	17,19,21	0.46	0
4	NAG	G	509	1	14,14,15	0.43	0	17,19,21	0.57	0
4	NAG	G	506	1	14,14,15	0.33	0	17,19,21	0.36	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	H	303	-	-	0/1/1/1	-
4	NAG	L	301	3	-	0/6/23/26	0/1/1/1
4	NAG	G	501	1	-	0/6/23/26	0/1/1/1
4	NAG	G	508	1	-	1/6/23/26	0/1/1/1
4	NAG	G	505	1	-	2/6/23/26	0/1/1/1
4	NAG	G	502	1	-	2/6/23/26	0/1/1/1
4	NAG	G	504	1	-	4/6/23/26	0/1/1/1
4	NAG	G	510	1	-	4/6/23/26	0/1/1/1
4	NAG	G	503	1	-	2/6/23/26	0/1/1/1
4	NAG	G	511	1	-	4/6/23/26	0/1/1/1
4	NAG	G	507	1	-	2/6/23/26	0/1/1/1
4	NAG	G	512	1	-	2/6/23/26	0/1/1/1
4	NAG	G	509	1	-	2/6/23/26	0/1/1/1
4	NAG	G	506	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	503	NAG	C1-O5-C5	2.09	115.02	112.19

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	503	NAG	O5-C5-C6-O6
4	G	506	NAG	O5-C5-C6-O6
4	G	511	NAG	O5-C5-C6-O6
4	G	502	NAG	O5-C5-C6-O6
4	G	510	NAG	O5-C5-C6-O6
4	G	506	NAG	C4-C5-C6-O6
4	G	507	NAG	O5-C5-C6-O6
4	G	503	NAG	C4-C5-C6-O6
4	G	511	NAG	C4-C5-C6-O6
4	G	502	NAG	C4-C5-C6-O6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	G	504	NAG	C8-C7-N2-C2
4	G	504	NAG	O7-C7-N2-C2
4	G	510	NAG	C8-C7-N2-C2
4	G	510	NAG	O7-C7-N2-C2
4	G	510	NAG	C4-C5-C6-O6
4	G	512	NAG	O5-C5-C6-O6
4	G	507	NAG	C4-C5-C6-O6
4	G	504	NAG	O5-C5-C6-O6
4	G	512	NAG	C4-C5-C6-O6
4	G	509	NAG	O5-C5-C6-O6
4	G	511	NAG	C1-C2-N2-C7
4	G	504	NAG	C4-C5-C6-O6
4	G	509	NAG	C1-C2-N2-C7
4	G	505	NAG	C4-C5-C6-O6
4	G	508	NAG	O5-C5-C6-O6
4	G	505	NAG	O5-C5-C6-O6
4	G	511	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	513	SO4	1	0
4	G	504	NAG	1	0
4	G	509	NAG	2	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	G	343/359 (95%)	0.60	28 (8%)	11 14	49, 106, 177, 218	0
2	H	209/227 (92%)	0.60	17 (8%)	12 14	47, 98, 166, 193	0
3	L	208/210 (99%)	0.47	10 (4%)	30 30	65, 113, 170, 200	0
All	All	760/796 (95%)	0.56	55 (7%)	15 17	47, 107, 173, 218	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	209	PHE	4.5
2	H	212	GLU	4.4
1	G	490	GLU	3.9
3	L	131	SER	3.9
1	G	44	VAL	3.7
1	G	55	ALA	3.6
2	H	161	SER	3.6
2	H	194	TYR	3.6
2	H	213	PRO	3.4
2	H	191	THR	3.4
2	H	142	VAL	3.2
1	G	404	THR	3.1
3	L	192	TYR	3.1
1	G	79	PRO	3.1
1	G	57	ASP	2.9
3	L	210	ASN	2.9
1	G	56	SER	2.9
2	H	121	VAL	2.8
1	G	491	ILE	2.8
1	G	45	TRP	2.8
2	H	192	GLN	2.8
2	H	211	VAL	2.8
2	H	159	LEU	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	H	193	THR	2.7
1	G	50	THR	2.7
1	G	440	PRO	2.6
1	G	90	THR	2.6
2	H	140	CYS	2.6
2	H	124	LEU	2.6
1	G	226	LEU	2.6
1	G	270	ILE	2.5
2	H	202	PRO	2.4
2	H	138	LEU	2.4
3	L	153	ALA	2.4
3	L	150	VAL	2.3
3	L	33	LEU	2.3
2	H	184	VAL	2.3
3	L	132	VAL	2.3
1	G	67	ASN	2.3
1	G	100	MET	2.2
1	G	399	SER	2.2
1	G	62	GLU	2.2
3	L	120	PRO	2.2
3	L	29	ILE	2.2
1	G	61	TYR	2.2
1	G	85	HIS	2.1
1	G	395	TRP	2.1
1	G	47	ASP	2.1
1	G	238	LEU	2.1
1	G	82	GLN	2.1
1	G	338	TRP	2.1
1	G	60	ALA	2.0
2	H	152	VAL	2.0
1	G	488	VAL	2.0
1	G	268	LYS	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NAG	G	510	14/15	0.57	0.28	137,150,166,172	0
4	NAG	G	509	14/15	0.58	0.80	191,207,219,221	0
5	SO4	H	302	5/5	0.65	0.38	161,165,165,166	0
4	NAG	G	505	14/15	0.68	0.34	120,128,133,134	0
4	NAG	G	512	14/15	0.68	0.47	164,178,184,190	0
5	SO4	H	304	5/5	0.68	0.21	158,158,159,160	0
4	NAG	G	502	14/15	0.70	0.34	164,184,207,208	0
4	NAG	G	511	14/15	0.74	0.52	154,163,170,170	0
5	SO4	H	301	5/5	0.75	0.33	132,134,138,143	0
4	NAG	L	301	14/15	0.79	0.21	116,123,129,133	0
4	NAG	G	501	14/15	0.82	0.29	124,131,144,148	0
4	NAG	G	506	14/15	0.83	0.27	101,111,118,119	0
4	NAG	G	508	14/15	0.85	0.27	93,110,122,126	0
4	NAG	G	504	14/15	0.85	0.25	133,143,147,150	0
6	EDO	H	303	4/4	0.89	0.74	73,75,78,78	0
4	NAG	G	507	14/15	0.92	0.25	86,96,110,113	0
4	NAG	G	503	14/15	0.92	0.18	87,112,121,122	0
5	SO4	G	513	5/5	0.98	0.13	59,75,81,90	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.