



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2020 – 02:47 PM BST

PDB ID : 6VPY  
Title : I33M (I3.2 mutant from CH103 Lineage)  
Authors : Fera, D.; Zhou, J.  
Deposited on : 2020-02-04  
Resolution : 2.36 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.

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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 : 2.14.2  
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) : 2.14.2

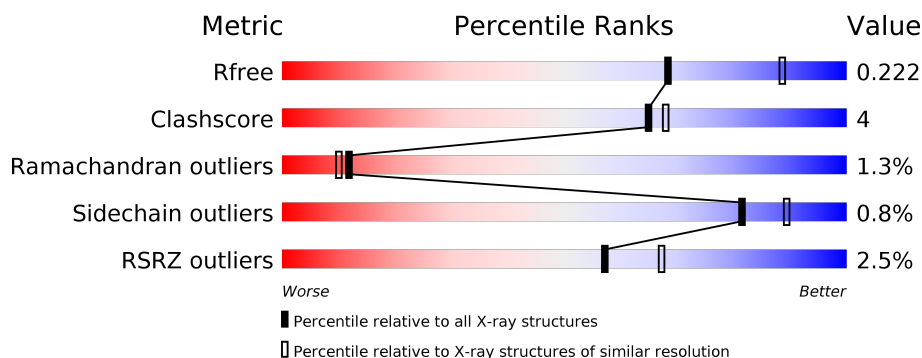
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.36 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	B	213	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div></div> </div> <div></div> </div>
1	L	213	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div></div> </div> <div></div> </div>
2	A	232	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>8%</div> <div>7%</div> <div></div> </div> <div></div> </div>
2	H	232	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>6%</div> <div></div> </div> <div></div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6662 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 I33M light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	208	Total	C	N	O	S	0	0	0
			1543	967	255	315	6			
1	L	209	Total	C	N	O	S	0	0	0
			1554	973	257	318	6			

- Molecule 2 is a protein called I33M heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	216	Total	C	N	O	S	0	0	0
			1616	1024	271	316	5			
2	H	218	Total	C	N	O	S	0	0	0
			1633	1032	275	321	5			

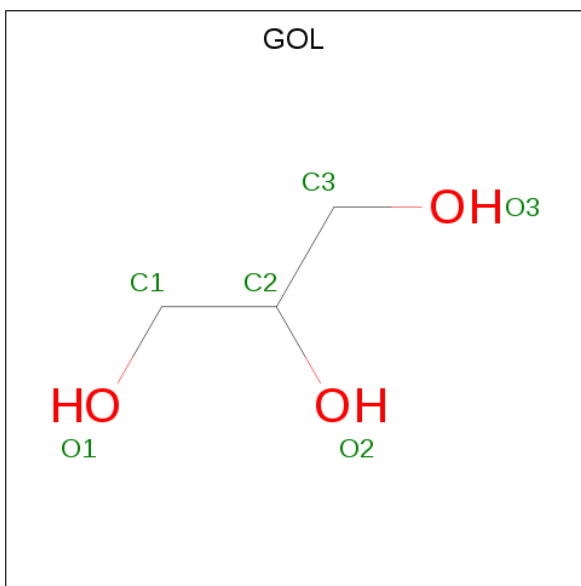
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	ALA	SER	conflict	UNP Q6GMX6
A	210	ARG	LYS	conflict	UNP Q6GMX6
A	219	HIS	-	expression tag	UNP Q6GMX6
A	220	HIS	-	expression tag	UNP Q6GMX6
A	221	HIS	-	expression tag	UNP Q6GMX6
A	222	HIS	-	expression tag	UNP Q6GMX6
A	223	HIS	-	expression tag	UNP Q6GMX6
A	224	HIS	-	expression tag	UNP Q6GMX6
H	112	ALA	SER	conflict	UNP Q6GMX6
H	210	ARG	LYS	conflict	UNP Q6GMX6
H	219	HIS	-	expression tag	UNP Q6GMX6
H	220	HIS	-	expression tag	UNP Q6GMX6
H	221	HIS	-	expression tag	UNP Q6GMX6
H	222	HIS	-	expression tag	UNP Q6GMX6
H	223	HIS	-	expression tag	UNP Q6GMX6
H	224	HIS	-	expression tag	UNP Q6GMX6

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0

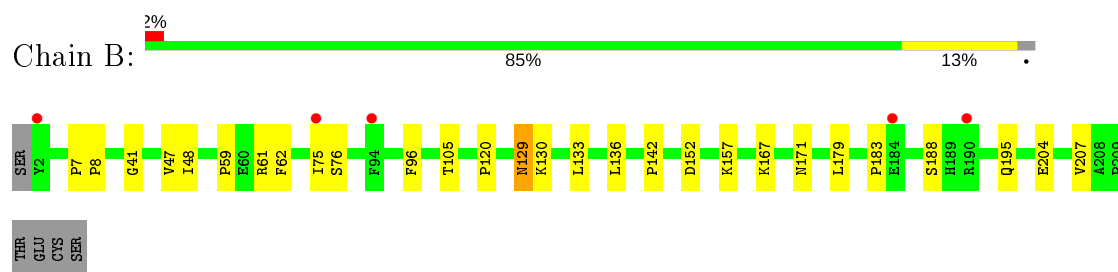
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	70	Total O 70 70	0	0
5	A	76	Total O 76 76	0	0
5	H	81	Total O 81 81	0	0
5	L	76	Total O 76 76	0	0

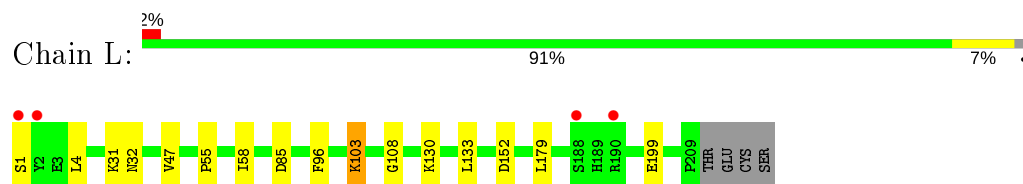
### 3 Residue-property plots [i](#)

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.

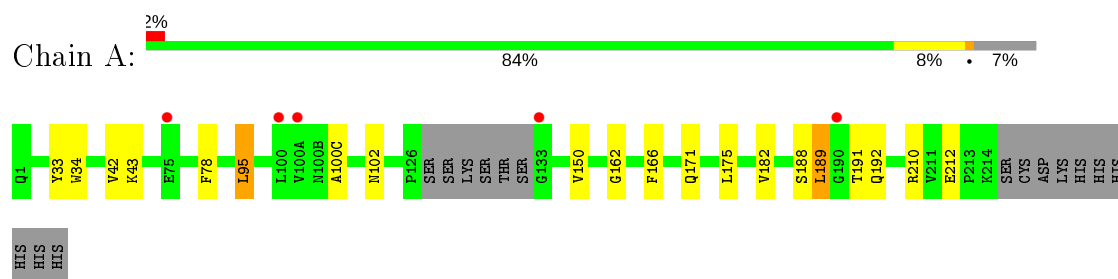
- Molecule 1: I33M light chain



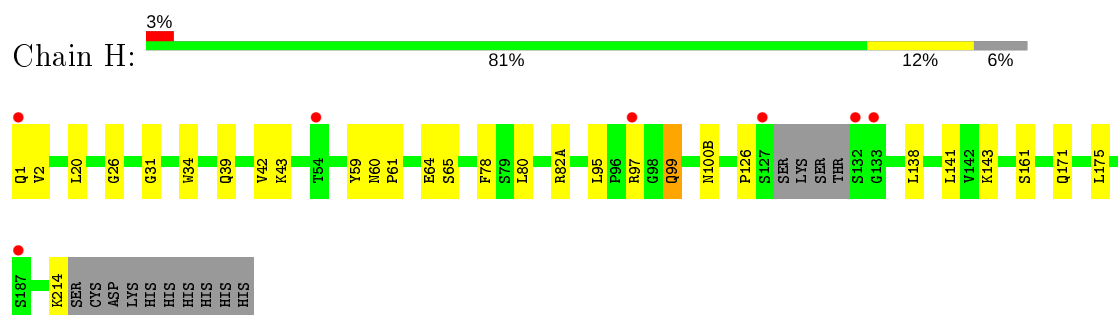
- Molecule 1: I33M light chain



- Molecule 2: I33M heavy chain



- Molecule 2: I33M heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.60Å 131.60Å 104.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.65 – 2.36 47.65 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.65-2.36) 99.1 (47.65-2.35)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, $R_{free}$	0.185 , 0.223 0.189 , 0.222	Depositor DCC
$R_{free}$ test set	2014 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.9	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 52.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.063 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6662	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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: GOL, CL

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	B	0.38	0/1582	0.55	0/2165
1	L	0.39	0/1593	0.52	0/2178
2	A	0.40	0/1657	0.58	0/2267
2	H	0.38	0/1674	0.58	0/2288
All	All	0.39	0/6506	0.56	0/8898

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	B	1543	0	1477	15	0
1	L	1554	0	1499	10	0
2	A	1616	0	1571	10	0
2	H	1633	0	1589	21	0
3	B	1	0	0	0	0
4	L	12	0	16	1	0
5	A	76	0	0	0	0
5	B	70	0	0	1	0
5	H	81	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	76	0	0	2	0
All	All	6662	0	6152	51	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 4.

All (51) 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:B:157:LYS:HG2	2:H:64:GLU:OE2	1.82	0.79
2:H:99:GLN:OE1	2:H:100(B):ASN:ND2	2.13	0.74
1:L:199:GLU:O	5:L:401:HOH:O	2.15	0.65
2:H:39:GLN:NE2	5:H:302:HOH:O	2.29	0.62
2:H:171:GLN:HG2	2:H:175:LEU:O	1.99	0.62
1:L:55:PRO:HB2	1:L:58:ILE:HD13	1.81	0.61
2:A:171:GLN:HG2	2:A:175:LEU:O	2.02	0.60
2:H:1:GLN:OE1	2:H:1:GLN:N	2.35	0.60
1:L:108:GLY:HA3	4:L:302:GOL:H2	1.85	0.59
1:B:129:ASN:O	1:B:183:PRO:HG3	2.03	0.58
2:H:1:GLN:HG2	2:H:2:VAL:H	1.69	0.57
1:B:105:THR:HG21	1:B:142:PRO:HB3	1.87	0.56
1:L:47:VAL:HA	1:L:58:ILE:HG12	1.91	0.53
1:B:47:VAL:O	1:B:48:ILE:HG13	2.10	0.52
2:A:210:ARG:HH11	2:A:212:GLU:CD	2.13	0.52
2:A:42:VAL:HG13	2:A:43:LYS:HG2	1.92	0.52
2:H:126:PRO:HB3	2:H:138:LEU:HB3	1.91	0.51
1:B:120:PRO:HA	1:B:133:LEU:HD23	1.91	0.51
2:A:95:LEU:HD21	2:A:100(C):ALA:HB1	1.94	0.50
1:B:61:ARG:HB2	1:B:75:ILE:O	2.11	0.50
2:A:33:TYR:HB2	2:A:95:LEU:HB3	1.92	0.50
2:H:65:SER:O	2:H:82(A):ARG:NH1	2.44	0.50
1:B:133:LEU:HD12	1:B:179:LEU:HD23	1.95	0.49
1:L:1:SER:HB2	1:L:31:LYS:NZ	2.28	0.49
1:L:133:LEU:HD12	1:L:179:LEU:HD23	1.96	0.48
2:H:95:LEU:HD11	1:L:96:PHE:CZ	2.50	0.47
1:B:167:LYS:NZ	1:B:171:ASN:OD1	2.48	0.47
2:H:141:LEU:HG	2:H:143:LYS:HG3	1.96	0.47
1:B:195:GLN:HG2	1:B:204:GLU:HG3	1.96	0.47
1:B:96:PHE:HZ	2:A:95:LEU:HD11	1.80	0.46
2:H:61:PRO:HA	2:H:64:GLU:HB2	1.97	0.45
2:H:34:TRP:HB3	2:H:78:PHE:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:34:TRP:HB3	2:H:78:PHE:CE1	2.52	0.44
2:H:42:VAL:HG12	5:H:359:HOH:O	2.16	0.44
2:H:59:TYR:HB2	2:H:64:GLU:HG3	1.99	0.43
1:L:85:ASP:OD1	1:L:103:LYS:NZ	2.51	0.43
2:H:42:VAL:HG13	2:H:43:LYS:HG2	2.01	0.42
1:B:41:GLY:O	5:B:401:HOH:O	2.21	0.42
2:H:31:GLY:C	2:H:97:ARG:HG3	2.40	0.42
2:A:34:TRP:HB3	2:A:78:PHE:CE1	2.55	0.41
1:B:59:PRO:HG2	1:B:62:PHE:CE1	2.56	0.41
1:B:136:LEU:HB3	2:A:166:PHE:CZ	2.56	0.41
2:A:189:LEU:C	2:A:191:THR:H	2.24	0.41
2:H:20:LEU:HD12	2:H:80:LEU:HD23	2.02	0.41
1:B:7:PRO:HA	1:B:8:PRO:HD3	1.96	0.41
1:B:120:PRO:HD3	1:B:207:VAL:HG11	2.03	0.40
2:H:60:ASN:HA	2:H:61:PRO:HD2	1.88	0.40
1:L:130:LYS:HD2	5:L:411:HOH:O	2.20	0.40
2:A:162:GLY:O	2:A:182:VAL:HA	2.22	0.40
2:H:1:GLN:O	2:H:26:GLY:HA3	2.21	0.40
2:H:100(B):ASN:OD1	1:L:32:ASN:ND2	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	206/213 (97%)	196 (95%)	6 (3%)	4 (2%)	8	6
1	L	207/213 (97%)	199 (96%)	6 (3%)	2 (1%)	15	15
2	A	212/232 (91%)	205 (97%)	3 (1%)	4 (2%)	8	6
2	H	214/232 (92%)	210 (98%)	3 (1%)	1 (0%)	29	32
All	All	839/890 (94%)	810 (96%)	18 (2%)	11 (1%)	12	10

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	76	SER
1	B	130	LYS
2	A	102	ASN
2	A	189	LEU
2	A	188	SER
1	L	4	LEU
1	L	152	ASP
1	B	129	ASN
2	A	192	GLN
2	H	99	GLN
1	B	152	ASP

### 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	B	173/182 (95%)	172 (99%)	1 (1%)	86	93
1	L	176/182 (97%)	175 (99%)	1 (1%)	86	93
2	A	182/200 (91%)	180 (99%)	2 (1%)	73	84
2	H	185/200 (92%)	183 (99%)	2 (1%)	73	84
All	All	716/764 (94%)	710 (99%)	6 (1%)	81	89

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	188	SER
2	A	95	LEU
2	A	150	VAL
2	H	161	SER
2	H	214	LYS
1	L	103	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	32	ASN
1	L	79	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	GOL	L	302	-	5,5,5	0.32	0	5,5,5	0.47	0
4	GOL	L	301	-	5,5,5	0.28	0	5,5,5	0.32	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	GOL	L	302	-	-	2/4/4/4	-
4	GOL	L	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	301	GOL	O1-C1-C2-C3
4	L	302	GOL	O1-C1-C2-C3
4	L	301	GOL	O1-C1-C2-O2
4	L	302	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	302	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, 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	B	208/213 (97%)	0.19	5 (2%) 59 68	33, 51, 86, 100	0
1	L	209/213 (98%)	0.13	4 (1%) 66 76	36, 49, 72, 107	0
2	A	216/232 (93%)	0.14	5 (2%) 60 70	33, 48, 75, 102	0
2	H	218/232 (93%)	0.24	7 (3%) 47 59	33, 49, 86, 129	0
All	All	851/890 (95%)	0.17	21 (2%) 57 67	33, 49, 80, 129	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	190	ARG	4.2
1	L	2	TYR	3.4
1	L	1	SER	3.4
2	H	132	SER	3.0
2	H	1	GLN	3.0
1	B	2	TYR	2.8
1	B	94	PHE	2.8
2	A	133	GLY	2.7
1	L	188	SER	2.6
2	H	133	GLY	2.6
2	A	190	GLY	2.6
2	A	100(A)	VAL	2.3
2	A	100	LEU	2.2
2	A	75	GLU	2.2
2	H	187	SER	2.2
2	H	97	ARG	2.2
1	L	190	ARG	2.1
1	B	75	ILE	2.1
2	H	127	SER	2.1
2	H	54	THR	2.0
1	B	184	GLU	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( $\text{\AA}^2$ )	Q<0.9
4	GOL	L	302	6/6	0.66	0.30	20,20,20,20	0
4	GOL	L	301	6/6	0.69	0.27	20,20,20,20	0
3	CL	B	301	1/1	0.98	0.47	49,49,49,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.