



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:43 pm BST

PDB ID : 3N9X  
Title : Crystal structure of Map Kinase from plasmodium berghei, PB000659.00.0  
Authors : Wernimont, A.K.; Hutchinson, A.; Sullivan, H.; MacKenzie, F.; Kozieradzki, I.; Chau, I.; Lew, J.; Senisterra, G.; Artz, J.; Amani, M.; Cossar, D.; Bochkarev, A.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Weigelt, J.; Hui, R.; Hills, T.; Structural Genomics Consortium (SGC)  
Deposited on : 2010-05-31  
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](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	:	2.11
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)	:	2.11

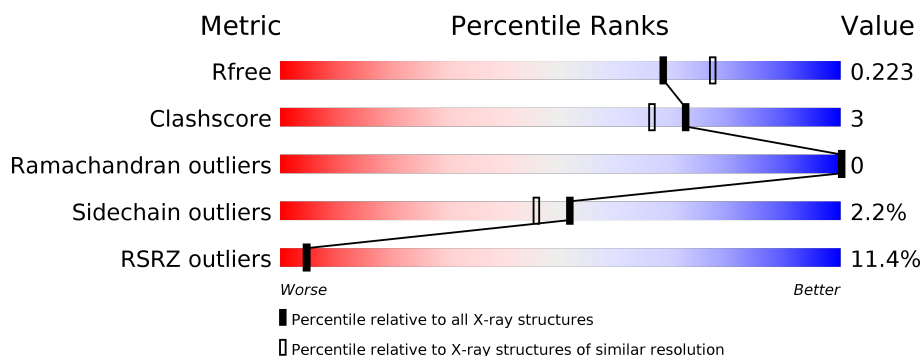
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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  $\geq 3$ , 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	A	432	<div> <div>9%</div> <div>78%</div> <div>7%</div> <div>13%</div> </div>
1	B	432	<div> <div>10%</div> <div>80%</div> <div>6%</div> <div>13%</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
2	GOL	A	435	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6801 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 Phosphotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	12	0
			3167	2050	530	576	11			
1	B	374	Total	C	N	O	S	0	3	0
			3086	2002	516	557	11			

There are 36 discrepancies between the modelled and reference sequences:

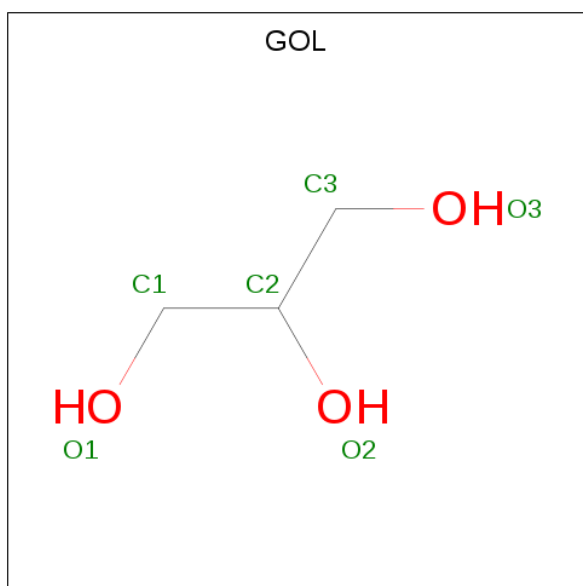
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q4Z5A3
A	2	HIS	-	EXPRESSION TAG	UNP Q4Z5A3
A	3	HIS	-	EXPRESSION TAG	UNP Q4Z5A3
A	4	HIS	-	EXPRESSION TAG	UNP Q4Z5A3
A	5	HIS	-	EXPRESSION TAG	UNP Q4Z5A3
A	6	HIS	-	EXPRESSION TAG	UNP Q4Z5A3
A	7	HIS	-	EXPRESSION TAG	UNP Q4Z5A3
A	8	SER	-	EXPRESSION TAG	UNP Q4Z5A3
A	9	SER	-	EXPRESSION TAG	UNP Q4Z5A3
A	10	GLY	-	EXPRESSION TAG	UNP Q4Z5A3
A	11	ARG	-	EXPRESSION TAG	UNP Q4Z5A3
A	12	GLU	-	EXPRESSION TAG	UNP Q4Z5A3
A	13	ASN	-	EXPRESSION TAG	UNP Q4Z5A3
A	14	LEU	-	EXPRESSION TAG	UNP Q4Z5A3
A	15	TYR	-	EXPRESSION TAG	UNP Q4Z5A3
A	16	PHE	-	EXPRESSION TAG	UNP Q4Z5A3
A	17	GLN	-	EXPRESSION TAG	UNP Q4Z5A3
A	18	GLY	-	EXPRESSION TAG	UNP Q4Z5A3
B	1	MET	-	EXPRESSION TAG	UNP Q4Z5A3
B	2	HIS	-	EXPRESSION TAG	UNP Q4Z5A3
B	3	HIS	-	EXPRESSION TAG	UNP Q4Z5A3
B	4	HIS	-	EXPRESSION TAG	UNP Q4Z5A3
B	5	HIS	-	EXPRESSION TAG	UNP Q4Z5A3
B	6	HIS	-	EXPRESSION TAG	UNP Q4Z5A3
B	7	HIS	-	EXPRESSION TAG	UNP Q4Z5A3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	8	SER	-	EXPRESSION TAG	UNP Q4Z5A3
B	9	SER	-	EXPRESSION TAG	UNP Q4Z5A3
B	10	GLY	-	EXPRESSION TAG	UNP Q4Z5A3
B	11	ARG	-	EXPRESSION TAG	UNP Q4Z5A3
B	12	GLU	-	EXPRESSION TAG	UNP Q4Z5A3
B	13	ASN	-	EXPRESSION TAG	UNP Q4Z5A3
B	14	LEU	-	EXPRESSION TAG	UNP Q4Z5A3
B	15	TYR	-	EXPRESSION TAG	UNP Q4Z5A3
B	16	PHE	-	EXPRESSION TAG	UNP Q4Z5A3
B	17	GLN	-	EXPRESSION TAG	UNP Q4Z5A3
B	18	GLY	-	EXPRESSION TAG	UNP Q4Z5A3

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		

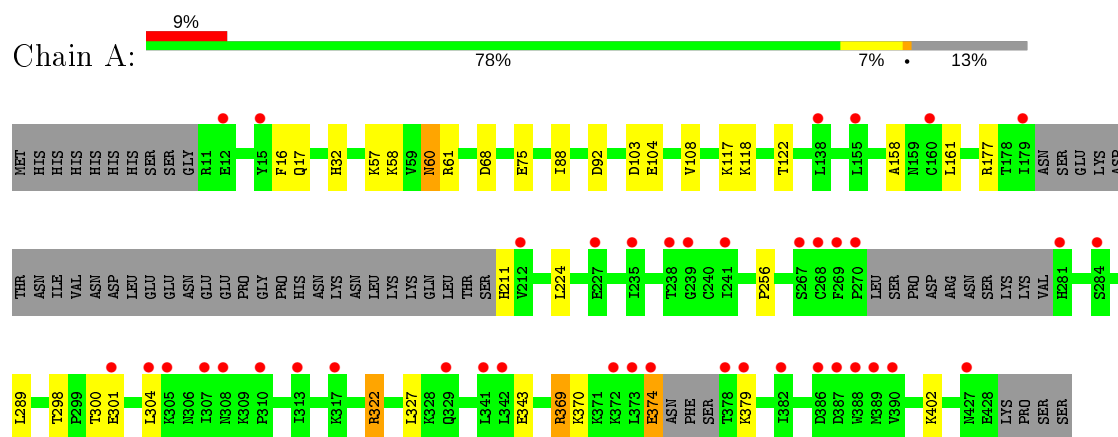
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	237	Total	O	0	0
			237	237		
3	B	269	Total	O	0	0
			269	269		

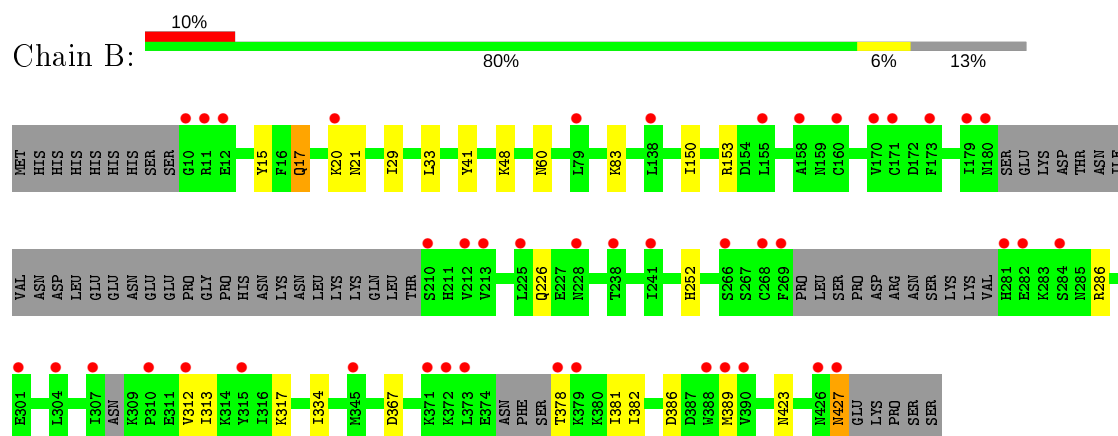
### 3 Residue-property plots [i](#)

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: Phosphotransferase



#### • Molecule 1: Phosphotransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.31Å 120.73Å 96.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.17 – 2.05 32.17 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (32.17-2.05) 99.9 (32.17-2.05)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 2.05Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.191 , 0.229 0.187 , 0.223	Depositor DCC
$R_{free}$ test set	4141 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.9	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6801	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5236e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	A	0.44	0/3235	0.54	0/4379
1	B	0.46	0/3152	0.54	0/4266
All	All	0.45	0/6387	0.54	0/8645

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	A	3167	0	3165	27	0
1	B	3086	0	3100	17	0
2	A	18	0	24	6	0
2	B	24	0	32	4	0
3	A	237	0	0	0	0
3	B	269	0	0	2	0
All	All	6801	0	6321	43	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 3.

All (43) 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:423:ASN:HD21	2:B:436:GOL:H2	1.46	0.79
1:A:17:GLN:HB2	2:A:435:GOL:H11	1.66	0.75
1:A:369:ARG:NH1	1:A:374:GLU:OE2	2.22	0.72
1:B:382:ILE:HG21	1:B:427:ASN:HB2	1.71	0.72
1:B:29:ILE:HD11	1:B:48:LYS:HD2	1.71	0.71
1:A:374:GLU:O	1:A:374:GLU:HG2	1.90	0.71
1:B:386:ASP:H	1:B:389[B]:MET:HE3	1.55	0.70
1:A:16:PHE:N	2:A:435:GOL:H31	2.09	0.68
1:A:301[B]:GLU:H	1:A:301[B]:GLU:CD	2.02	0.63
1:B:423:ASN:ND2	2:B:436:GOL:H2	2.14	0.62
1:A:17:GLN:HB2	2:A:435:GOL:C1	2.29	0.61
1:A:17:GLN:OE1	1:A:32:HIS:HB2	2.03	0.59
1:A:374:GLU:O	1:A:374:GLU:CG	2.52	0.57
1:A:58:LYS:HE2	1:A:60[A]:ASN:HD21	1.69	0.56
1:B:386:ASP:H	1:B:389[B]:MET:CE	2.16	0.56
1:A:301[B]:GLU:N	1:A:301[B]:GLU:CD	2.60	0.54
1:A:17:GLN:H	2:A:435:GOL:H11	1.73	0.53
1:A:300:THR:O	1:A:304:LEU:HD12	2.09	0.52
1:A:57:LYS:NZ	1:A:75:GLU:OE2	2.44	0.51
1:A:298:THR:HG23	1:A:322:ARG:HD3	1.93	0.50
1:B:313:ILE:O	1:B:317:LYS:HG2	2.11	0.50
1:A:88:ILE:HG13	1:A:161:LEU:HD22	1.92	0.50
1:A:17:GLN:CB	2:A:435:GOL:H11	2.40	0.47
1:A:16:PHE:H	2:A:435:GOL:H31	1.79	0.46
1:A:117:LYS:HD2	1:A:158:ALA:HB2	1.97	0.46
1:A:68:ASP:OD2	1:A:211:HIS:NE2	2.47	0.46
1:B:17:GLN:HG3	1:B:33:LEU:HB3	1.98	0.46
1:B:153:ARG:NH2	2:B:435:GOL:O3	2.49	0.45
1:A:224:LEU:HD21	1:A:289:LEU:HD11	1.99	0.45
1:B:60:ASN:HB2	3:B:581:HOH:O	2.17	0.45
1:B:367:ASP:HB2	3:B:563:HOH:O	2.17	0.45
1:A:92:ASP:HB3	1:A:108:VAL:HB	1.99	0.44
1:B:423:ASN:HD21	2:B:436:GOL:C2	2.24	0.43
1:A:61[B]:ARG:HA	1:A:103:ASP:OD2	2.19	0.43
1:A:60[A]:ASN:HA	1:A:60[A]:ASN:HD22	1.62	0.41
1:A:327:LEU:HD12	1:A:343:GLU:HG3	2.01	0.41
1:B:252:HIS:CE1	1:B:334:ILE:HG12	2.55	0.41
1:A:118:LYS:O	1:A:122:THR:HG23	2.21	0.41
1:A:58:LYS:HE2	1:A:60[A]:ASN:ND2	2.35	0.41
1:A:256:PRO:HB2	1:B:41:TYR:OH	2.21	0.40
1:B:150:ILE:HD11	1:B:381:ILE:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:GLN:HE22	1:B:312:VAL:HG21	1.87	0.40
1:B:15:TYR:CG	1:B:20:LYS:HE3	2.57	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	A	378/432 (88%)	370 (98%)	8 (2%)	0	100	100
1	B	367/432 (85%)	359 (98%)	8 (2%)	0	100	100
All	All	745/864 (86%)	729 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	A	355/411 (86%)	345 (97%)	10 (3%)	43	37
1	B	346/411 (84%)	339 (98%)	7 (2%)	55	50
All	All	701/822 (85%)	684 (98%)	17 (2%)	52	42

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60[A]	ASN
1	A	60[B]	ASN
1	A	104	GLU
1	A	177	ARG
1	A	322	ARG
1	A	369	ARG
1	A	370	LYS
1	A	374	GLU
1	A	379	LYS
1	A	402	LYS
1	B	17	GLN
1	B	21[A]	ASN
1	B	21[B]	ASN
1	B	83	LYS
1	B	286	ARG
1	B	378	THR
1	B	427	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	426	ASN
1	B	423	ASN
1	B	427	ASN

### 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

7 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	$\# Z  > 2$
2	GOL	B	436	-	5,5,5	0.41	0	5,5,5	0.23	0
2	GOL	A	434	-	5,5,5	0.33	0	5,5,5	0.29	0
2	GOL	A	433	-	5,5,5	0.52	0	5,5,5	0.83	0
2	GOL	B	434	-	5,5,5	0.33	0	5,5,5	0.38	0
2	GOL	B	433	-	5,5,5	0.39	0	5,5,5	0.30	0
2	GOL	A	435	-	5,5,5	0.28	0	5,5,5	0.63	0
2	GOL	B	435	-	5,5,5	0.33	0	5,5,5	0.46	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
2	GOL	B	436	-	-	2/4/4/4	-
2	GOL	A	434	-	-	0/4/4/4	-
2	GOL	A	433	-	-	4/4/4/4	-
2	GOL	B	434	-	-	0/4/4/4	-
2	GOL	B	433	-	-	0/4/4/4	-
2	GOL	A	435	-	-	2/4/4/4	-
2	GOL	B	435	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	433	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	A	435	GOL	O1-C1-C2-C3
2	A	433	GOL	O2-C2-C3-O3
2	B	436	GOL	C1-C2-C3-O3
2	A	433	GOL	C1-C2-C3-O3
2	B	435	GOL	O1-C1-C2-C3
2	B	435	GOL	C1-C2-C3-O3
2	A	433	GOL	O1-C1-C2-O2
2	A	435	GOL	O1-C1-C2-O2
2	B	435	GOL	O2-C2-C3-O3
2	B	436	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	436	GOL	3	0
2	A	435	GOL	6	0
2	B	435	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	A	374/432 (86%)	0.53	41 (10%)	5 5	29, 41, 70, 77	8 (2%)
1	B	374/432 (86%)	0.54	44 (11%)	4 4	28, 40, 68, 75	8 (2%)
All	All	748/864 (86%)	0.54	85 (11%)	5 5	28, 41, 69, 77	16 (2%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	373	LEU	7.4
1	A	304	LEU	6.8
1	A	270	PRO	6.4
1	B	388	TRP	5.9
1	A	307	ILE	5.7
1	B	427	ASN	5.5
1	A	388	TRP	5.4
1	B	10	GLY	5.4
1	B	210	SER	5.2
1	A	269	PHE	5.1
1	A	372	LYS	4.8
1	B	213	VAL	4.7
1	B	180	ASN	4.6
1	B	179	ILE	4.6
1	B	281	HIS	4.6
1	A	308	ASN	4.5
1	B	312	VAL	4.3
1	B	225	LEU	4.3
1	B	378	THR	4.3
1	B	315	TYR	4.3
1	B	268	CYS	4.1
1	B	304	LEU	4.0
1	A	212	VAL	3.9
1	B	212	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	228	ASN	3.7
1	A	305	LYS	3.5
1	A	427	ASN	3.4
1	A	310	PRO	3.3
1	A	301[A]	GLU	3.3
1	B	379	LYS	3.3
1	B	310	PRO	3.3
1	B	373	LEU	3.3
1	A	268	CYS	3.2
1	A	179	ILE	3.1
1	B	426	ASN	3.1
1	A	378	THR	3.0
1	A	387	ASP	3.0
1	B	269	PHE	2.9
1	A	329	GLN	2.8
1	B	307	ILE	2.8
1	A	379	LYS	2.8
1	A	341	LEU	2.8
1	B	170	VAL	2.8
1	A	15	TYR	2.8
1	B	301	GLU	2.8
1	A	284	SER	2.7
1	A	267	SER	2.7
1	A	389[A]	MET	2.7
1	B	372	LYS	2.7
1	A	241	ILE	2.6
1	B	12	GLU	2.6
1	B	389[A]	MET	2.6
1	B	20	LYS	2.5
1	A	138	LEU	2.5
1	A	374	GLU	2.5
1	B	138	LEU	2.4
1	B	160	CYS	2.4
1	B	171	CYS	2.4
1	B	11	ARG	2.4
1	B	79	LEU	2.3
1	A	317	LYS	2.3
1	B	155	LEU	2.3
1	A	382	ILE	2.3
1	A	342	LEU	2.3
1	A	155[A]	LEU	2.2
1	B	173	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	281	HIS	2.2
1	A	390	VAL	2.2
1	A	160	CYS	2.2
1	B	266[A]	SER	2.2
1	B	390	VAL	2.2
1	B	158	ALA	2.1
1	B	238	THR	2.1
1	B	282	GLU	2.1
1	A	235	ILE	2.1
1	A	313	ILE	2.1
1	B	284	SER	2.1
1	A	238	THR	2.1
1	B	345	MET	2.0
1	A	227	GLU	2.0
1	A	12	GLU	2.0
1	B	241	ILE	2.0
1	A	239	GLY	2.0
1	A	386	ASP	2.0
1	B	371	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 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. 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
2	GOL	A	435	6/6	0.77	0.26	51,52,53,55	0
2	GOL	B	435	6/6	0.77	0.18	65,65,66,66	0
2	GOL	B	436	6/6	0.80	0.36	29,30,31,33	6
2	GOL	A	433	6/6	0.94	0.25	33,38,39,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	B	433	6/6	0.94	0.18	37,39,40,42	0
2	GOL	B	434	6/6	0.95	0.26	31,33,35,39	0
2	GOL	A	434	6/6	0.95	0.15	38,40,42,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.