



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 05:28 pm GMT

PDB ID : 4BWW  
Title : Crystal structure of spin labelled azurin T21R1.  
Authors : Hagelueken, G.  
Deposited on : 2013-07-04  
Resolution : 1.48 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

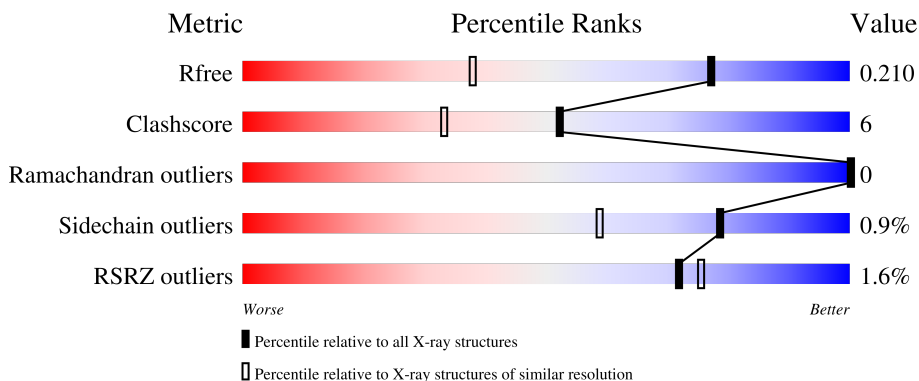
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.48 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	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

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  $\geq 3$ , 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	131	2% 88% 8% . .
1	B	131	2% 90% 8% .
1	C	131	% 87% 10% . .
1	D	131	2% 92% 6% .

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
3	GOL	B	1135	-	-	X	-
3	GOL	B	1137	-	-	X	-
3	GOL	D	1130	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4605 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 AZURIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	128	1012	636	167	195	14	0	5	0
1	B	128	1000	625	166	198	11	0	3	0
1	C	128	1012	635	167	197	13	0	5	0
1	D	128	995	622	166	195	12	0	2	0

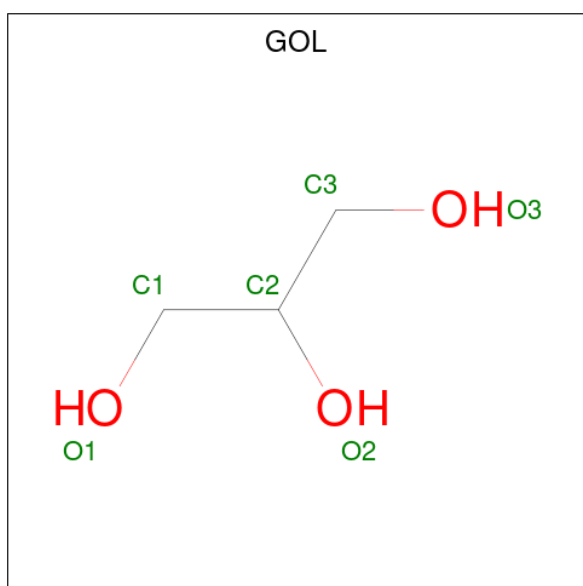
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P00282
A	-1	ALA	-	expression tag	UNP P00282
A	0	MET	-	expression tag	UNP P00282
A	21	R1A	THR	engineered mutation	UNP P00282
B	-2	GLY	-	expression tag	UNP P00282
B	-1	ALA	-	expression tag	UNP P00282
B	0	MET	-	expression tag	UNP P00282
B	21	R1A	THR	engineered mutation	UNP P00282
C	-2	GLY	-	expression tag	UNP P00282
C	-1	ALA	-	expression tag	UNP P00282
C	0	MET	-	expression tag	UNP P00282
C	21	R1A	THR	engineered mutation	UNP P00282
D	-2	GLY	-	expression tag	UNP P00282
D	-1	ALA	-	expression tag	UNP P00282
D	0	MET	-	expression tag	UNP P00282
D	21	R1A	THR	engineered mutation	UNP P00282

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

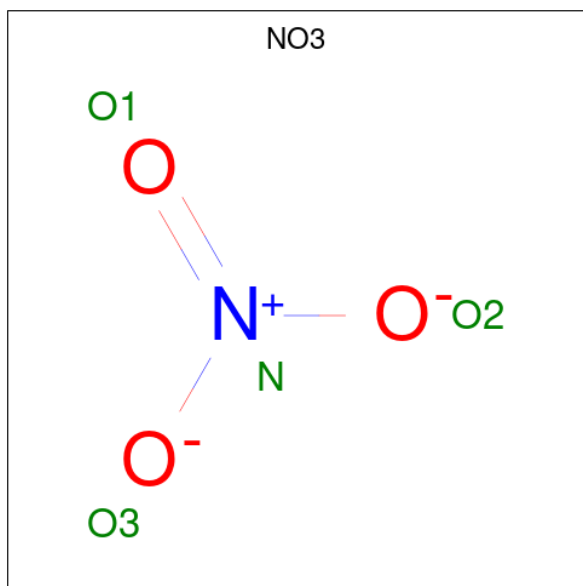
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cu 1 1	0	0
2	B	1	Total Cu 1 1	0	0
2	C	1	Total Cu 1 1	0	0
2	D	1	Total Cu 1 1	0	0

- Molecule 3 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
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	N	O	0	0
			4	1	3		
4	B	1	Total	N	O	0	0
			4	1	3		
4	B	1	Total	N	O	0	0
			4	1	3		
4	C	1	Total	N	O	0	0
			4	1	3		
4	D	1	Total	N	O	0	0
			4	1	3		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

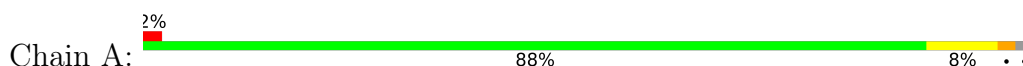
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	155	Total	O	0	0
			155	155		
6	B	118	Total	O	0	0
			118	118		
6	C	122	Total	O	0	0
			122	122		
6	D	94	Total	O	0	0
			94	94		

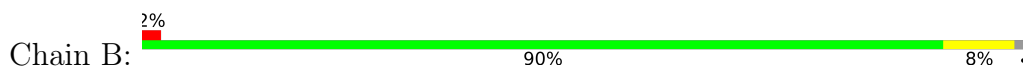
### 3 Residue-property plots [i](#)

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.

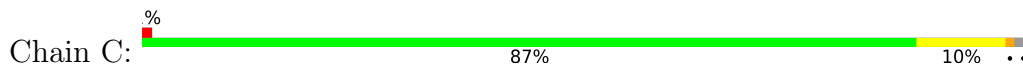
- Molecule 1: AZURIN



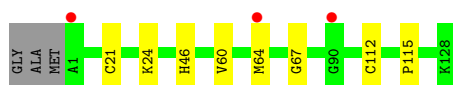
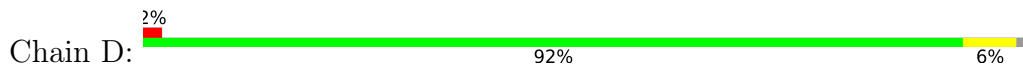
- Molecule 1: AZURIN



- Molecule 1: AZURIN



- Molecule 1: AZURIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	36.95Å 53.66Å 73.21Å 74.40° 89.33° 83.41°	Depositor
Resolution (Å)	48.12 – 1.48 51.34 – 1.48	Depositor EDS
% Data completeness (in resolution range)	91.8 (48.12-1.48) 91.8 (51.34-1.48)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 1.48Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.179 , 0.210 0.180 , 0.210	Depositor DCC
$R_{free}$ test set	2000 reflections (2.43%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.3	Xtrriage
Anisotropy	0.411	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 46.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4605	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.19% 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: NO3, CU, SO4, R1A, 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	0.46	0/1025	0.63	0/1375
1	B	0.42	0/1007	0.61	0/1355
1	C	0.41	0/1025	0.59	0/1376
1	D	0.45	0/999	0.60	0/1343
All	All	0.44	0/4056	0.61	0/5449

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	A	1012	0	1011	11	0
1	B	1000	0	982	16	0
1	C	1012	0	1006	11	0
1	D	995	0	978	7	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	32	14	0
3	C	12	0	16	1	0
3	D	6	0	8	6	0
4	A	4	0	0	0	0
4	B	8	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
5	B	10	0	0	1	0
5	C	5	0	0	1	0
5	D	10	0	0	0	0
6	A	155	0	0	1	0
6	B	118	0	0	2	0
6	C	122	0	0	1	1
6	D	94	0	0	1	1
All	All	4605	0	4041	45	1

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 6.

All (45) 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:64:MET:HB2	3:B:1137:GOL:H31	1.54	0.89
1:C:64:MET:HG3	1:C:115:PRO:HG3	1.64	0.78
1:A:64[B]:MET:HE1	1:A:116:GLY:H	1.52	0.73
1:A:42:ASN:HB2	3:D:1130:GOL:H31	1.77	0.67
3:B:1135:GOL:H2	1:C:68:LEU:HD23	1.77	0.66
1:A:68:LEU:HD23	3:D:1130:GOL:H2	1.77	0.65
1:B:69:ASP:HB2	3:B:1135:GOL:H12	1.81	0.62
1:C:21:R1A:HE3	1:C:128:LYS:HD3	1.80	0.62
1:B:64:MET:HB2	3:B:1137:GOL:H12	1.81	0.61
1:B:64:MET:CB	3:B:1137:GOL:H31	2.27	0.61
1:B:115:PRO:HA	3:B:1137:GOL:H32	1.83	0.61
1:A:68:LEU:CD2	3:D:1130:GOL:H2	2.32	0.60
1:C:81:ILE:HG23	1:C:101:LYS:HE2	1.90	0.54
1:B:104[B]:GLU:OE2	6:B:2100:HOH:O	2.17	0.53
1:C:27:LYS:HD3	1:C:28[A]:GLN:HG3	1.91	0.52
1:C:38:ASN:ND2	3:C:1131:GOL:O2	2.41	0.52
1:D:67:GLY:HA3	3:D:1130:GOL:H32	1.92	0.52
1:A:109[B]:MET:SD	6:A:2147:HOH:O	2.59	0.51
1:B:64:MET:HB2	3:B:1137:GOL:C3	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104[A]:GLU:OE2	6:B:2099:HOH:O	2.18	0.51
1:B:64:MET:HB2	3:B:1137:GOL:C1	2.40	0.50
1:A:64[B]:MET:CE	1:A:116:GLY:H	2.20	0.50
1:A:42:ASN:HD22	3:D:1130:GOL:H11	1.77	0.49
1:D:60:VAL:O	1:D:64[A]:MET:HG3	2.14	0.48
1:B:1:ALA:N	5:B:1133:SO4:O2	2.50	0.45
1:D:67:GLY:HA3	3:D:1130:GOL:H11	1.99	0.45
1:C:92:LYS:HE2	1:C:92:LYS:HB2	1.71	0.44
1:B:60:VAL:HG12	3:B:1137:GOL:H11	1.99	0.44
1:A:122:LYS:HE3	1:B:72:TYR:OH	2.17	0.43
3:B:1135:GOL:H2	1:C:68:LEU:CD2	2.46	0.43
1:C:21:R1A:SD	1:C:128:LYS:HB3	2.58	0.43
1:D:24:LYS:NZ	6:D:2031:HOH:O	2.37	0.43
1:D:64[A]:MET:SD	1:D:115:PRO:HA	2.58	0.43
1:D:60:VAL:HG12	1:D:64[A]:MET:HE2	2.00	0.42
1:A:46:HIS:CE1	1:A:121:MET:SD	3.12	0.42
1:B:64:MET:CA	3:B:1137:GOL:H31	2.50	0.42
1:B:67:GLY:HA3	3:B:1135:GOL:H32	2.03	0.41
1:A:49:VAL:O	1:A:110:PHE:HA	2.21	0.41
5:C:1132:SO4:O3	6:C:2097:HOH:O	2.22	0.41
1:B:83:HIS:HE2	3:B:1131:GOL:H31	1.86	0.41
1:C:27:LYS:CD	1:C:28[A]:GLN:HG3	2.51	0.41
1:C:85[B]:LYS:HG3	1:C:93:ASP:OD2	2.21	0.41
1:B:67:GLY:HA3	3:B:1135:GOL:H11	2.03	0.40
1:A:128:LYS:O	1:A:128:LYS:HG3	2.21	0.40
1:D:46:HIS:HA	1:D:112:CYS:SG	2.61	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:2024:HOH:O	6:D:2078:HOH:O[1_565]	2.16	0.04

## 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	130/131 (99%)	127 (98%)	3 (2%)	0	100	100
1	B	128/131 (98%)	127 (99%)	1 (1%)	0	100	100
1	C	130/131 (99%)	127 (98%)	3 (2%)	0	100	100
1	D	127/131 (97%)	124 (98%)	3 (2%)	0	100	100
All	All	515/524 (98%)	505 (98%)	10 (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	114/110 (104%)	110 (96%)	4 (4%)	36	8
1	B	112/110 (102%)	112 (100%)	0	100	100
1	C	114/110 (104%)	113 (99%)	1 (1%)	78	59
1	D	111/110 (101%)	111 (100%)	0	100	100
All	All	451/440 (102%)	446 (99%)	5 (1%)	78	50

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64[A]	MET
1	A	64[B]	MET
1	A	104	GLU
1	A	122	LYS
1	C	104	GLU

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

Mol	Chain	Res	Type
1	A	42	ASN
1	C	38	ASN
1	D	38	ASN
1	D	57	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](#)

4 non-standard protein/DNA/RNA residues 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
1	R1A	A	21	1	15,18,19	2.86	5 (33%)	15,27,29	4.67	6 (40%)
1	R1A	C	21	1	15,18,19	2.96	5 (33%)	15,27,29	4.67	6 (40%)
1	R1A	D	21	1	15,18,19	2.89	5 (33%)	15,27,29	4.84	6 (40%)
1	R1A	B	21	1	15,18,19	2.89	5 (33%)	15,27,29	4.52	6 (40%)

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
1	R1A	A	21	1	-	0/5/32/34	0/1/1/1
1	R1A	C	21	1	-	0/5/32/34	0/1/1/1
1	R1A	D	21	1	-	1/5/32/34	0/1/1/1
1	R1A	B	21	1	-	1/5/32/34	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	21	R1A	C4-C3	-9.91	1.22	1.32
1	A	21	R1A	C4-C3	-9.60	1.23	1.32
1	B	21	R1A	C4-C3	-9.58	1.23	1.32
1	D	21	R1A	C4-C3	-9.52	1.23	1.32
1	C	21	R1A	C5-C4	-3.21	1.45	1.50
1	D	21	R1A	C5-C4	-2.94	1.45	1.50
1	B	21	R1A	C5-C4	-2.82	1.46	1.50
1	D	21	R1A	CE-SD	-2.66	1.78	1.81
1	B	21	R1A	CE-SD	-2.65	1.78	1.81
1	A	21	R1A	C5-C4	-2.60	1.46	1.50
1	A	21	R1A	CE-SD	-2.43	1.78	1.81
1	C	21	R1A	CE-SD	-2.41	1.78	1.81
1	D	21	R1A	C2-N1	2.31	1.53	1.47
1	C	21	R1A	C2-N1	2.29	1.53	1.47
1	B	21	R1A	C5-N1	2.19	1.53	1.47
1	B	21	R1A	C2-N1	2.18	1.53	1.47
1	D	21	R1A	C5-N1	2.16	1.53	1.47
1	A	21	R1A	C2-N1	2.15	1.53	1.47
1	A	21	R1A	C5-N1	2.05	1.52	1.47
1	C	21	R1A	C5-N1	2.02	1.52	1.47

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	21	R1A	C7-C5-C4	9.38	122.51	112.78
1	C	21	R1A	C7-C5-C4	9.25	122.38	112.78
1	B	21	R1A	C7-C5-C4	9.16	122.28	112.78
1	A	21	R1A	C7-C5-C4	9.10	122.22	112.78
1	A	21	R1A	C6-C5-C7	-8.85	98.46	110.99
1	D	21	R1A	C6-C5-C7	-8.77	98.58	110.99
1	D	21	R1A	C6-C5-C4	8.39	121.49	112.78
1	B	21	R1A	C6-C5-C7	-8.22	99.36	110.99
1	C	21	R1A	C6-C5-C7	-8.20	99.38	110.99
1	C	21	R1A	C6-C5-C4	8.01	121.09	112.78
1	A	21	R1A	C6-C5-C4	7.98	121.06	112.78
1	C	21	R1A	C5-C4-C3	7.45	119.48	113.64
1	B	21	R1A	C5-C4-C3	7.01	119.13	113.64
1	A	21	R1A	C5-C4-C3	6.90	119.05	113.64
1	D	21	R1A	C5-C4-C3	6.86	119.02	113.64
1	B	21	R1A	C6-C5-C4	6.86	119.90	112.78
1	D	21	R1A	C8-C2-C9	-6.67	99.60	112.26
1	B	21	R1A	C8-C2-C9	-6.58	99.78	112.26
1	A	21	R1A	C8-C2-C9	-6.40	100.12	112.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	21	R1A	C8-C2-C9	-5.63	101.58	112.26
1	D	21	R1A	CE-SD-SG	-4.13	99.07	103.67
1	C	21	R1A	CE-SD-SG	3.95	108.07	103.67
1	B	21	R1A	CE-SD-SG	-2.61	100.76	103.67
1	A	21	R1A	CE-SD-SG	2.38	106.32	103.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	21	R1A	CA-CB-SG-SD
1	D	21	R1A	CA-CB-SG-SD

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	21	R1A	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 4 are monoatomic - leaving 18 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	NO3	B	1130	-	1,3,3	3.53	1 (100%)	0,3,3	-	-
4	NO3	B	1136	-	1,3,3	3.35	1 (100%)	0,3,3	-	-
4	NO3	D	1131	-	1,3,3	3.19	1 (100%)	0,3,3	-	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NO3	C	1133	-	1,3,3	3.43	1 (100%)	0,3,3	-	-
5	SO4	C	1132	-	4,4,4	0.16	0	6,6,6	0.11	0
5	SO4	D	1133	-	4,4,4	0.14	0	6,6,6	0.08	0
3	GOL	B	1135	-	5,5,5	0.39	0	5,5,5	0.55	0
3	GOL	B	1131	-	5,5,5	0.40	0	5,5,5	0.26	0
3	GOL	D	1130	-	5,5,5	0.43	0	5,5,5	0.86	0
3	GOL	C	1130	-	5,5,5	0.36	0	5,5,5	0.27	0
3	GOL	B	1132	-	5,5,5	0.34	0	5,5,5	0.30	0
5	SO4	B	1134	-	4,4,4	0.14	0	6,6,6	0.12	0
5	SO4	B	1133	-	4,4,4	0.13	0	6,6,6	0.14	0
5	SO4	D	1132	-	4,4,4	0.14	0	6,6,6	0.10	0
3	GOL	B	1137	-	5,5,5	0.55	0	5,5,5	0.50	0
3	GOL	A	1130	-	5,5,5	0.33	0	5,5,5	0.42	0
4	NO3	A	1131	-	1,3,3	3.50	1 (100%)	0,3,3	-	-
3	GOL	C	1131	-	5,5,5	0.47	0	5,5,5	0.63	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
3	GOL	B	1135	-	-	0/4/4/4	-
3	GOL	B	1131	-	-	4/4/4/4	-
3	GOL	D	1130	-	-	2/4/4/4	-
3	GOL	C	1130	-	-	4/4/4/4	-
3	GOL	B	1132	-	-	0/4/4/4	-
3	GOL	B	1137	-	-	2/4/4/4	-
3	GOL	A	1130	-	-	0/4/4/4	-
3	GOL	C	1131	-	-	2/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1130	NO3	O1-N	3.53	1.40	1.24
4	A	1131	NO3	O1-N	3.50	1.40	1.24
4	C	1133	NO3	O1-N	3.43	1.39	1.24
4	B	1136	NO3	O1-N	3.35	1.39	1.24
4	D	1131	NO3	O1-N	3.19	1.38	1.24

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1131	GOL	C1-C2-C3-O3
3	C	1130	GOL	C1-C2-C3-O3
3	C	1131	GOL	C1-C2-C3-O3
3	D	1130	GOL	O1-C1-C2-O2
3	D	1130	GOL	O1-C1-C2-C3
3	B	1131	GOL	O1-C1-C2-O2
3	B	1131	GOL	O1-C1-C2-C3
3	B	1137	GOL	C1-C2-C3-O3
3	C	1130	GOL	O1-C1-C2-C3
3	B	1131	GOL	O2-C2-C3-O3
3	C	1130	GOL	O2-C2-C3-O3
3	C	1131	GOL	O2-C2-C3-O3
3	C	1130	GOL	O1-C1-C2-O2
3	B	1137	GOL	O2-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1132	SO4	1	0
3	B	1135	GOL	5	0
3	B	1131	GOL	1	0
3	D	1130	GOL	6	0
5	B	1133	SO4	1	0
3	B	1137	GOL	8	0
3	C	1131	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	127/131 (96%)	-0.17	2 (1%) 72 75	11, 16, 32, 53	0
1	B	127/131 (96%)	-0.13	2 (1%) 72 75	13, 21, 34, 54	0
1	C	127/131 (96%)	-0.13	1 (0%) 86 88	14, 20, 40, 53	0
1	D	127/131 (96%)	-0.06	3 (2%) 59 63	14, 22, 38, 55	0
All	All	508/524 (96%)	-0.12	8 (1%) 72 75	11, 20, 37, 55	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	ALA	5.6
1	B	1	ALA	4.9
1	C	1	ALA	4.3
1	D	90	GLY	3.1
1	A	1	ALA	3.0
1	D	64[A]	MET	2.5
1	B	38	ASN	2.1
1	A	104	GLU	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	R1A	A	21	18/19	0.96	0.12	18,37,43,47	0
1	R1A	C	21	18/19	0.96	0.12	17,37,40,44	0
1	R1A	B	21	18/19	0.97	0.08	12,25,27,28	0
1	R1A	D	21	18/19	0.97	0.08	12,26,30,31	0

### 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
3	GOL	C	1131	6/6	0.61	0.27	36,40,41,43	0
3	GOL	B	1135	6/6	0.72	0.27	37,40,41,43	0
3	GOL	B	1131	6/6	0.77	0.16	39,41,42,42	0
3	GOL	D	1130	6/6	0.79	0.26	34,35,36,37	0
3	GOL	B	1137	6/6	0.83	0.23	21,25,27,29	0
3	GOL	C	1130	6/6	0.83	0.11	48,49,49,49	0
3	GOL	A	1130	6/6	0.85	0.13	29,33,35,35	0
4	NO3	C	1133	4/4	0.86	0.25	37,39,42,43	0
3	GOL	B	1132	6/6	0.87	0.19	24,32,34,34	0
5	SO4	B	1134	5/5	0.87	0.18	40,42,43,44	5
4	NO3	B	1136	4/4	0.90	0.20	38,40,42,44	0
5	SO4	B	1133	5/5	0.91	0.27	68,68,69,69	0
4	NO3	B	1130	4/4	0.93	0.15	34,34,34,38	0
4	NO3	D	1131	4/4	0.93	0.13	29,30,30,34	0
4	NO3	A	1131	4/4	0.94	0.14	41,42,42,44	0
5	SO4	D	1132	5/5	0.94	0.36	57,59,59,59	0
5	SO4	C	1132	5/5	0.95	0.25	59,59,59,59	0
5	SO4	D	1133	5/5	0.95	0.34	55,56,57,57	0
2	CU	A	1129	1/1	0.99	0.10	13,13,13,13	0
2	CU	B	1129	1/1	0.99	0.08	16,16,16,16	0
2	CU	C	1129	1/1	0.99	0.08	15,15,15,15	0
2	CU	D	1129	1/1	1.00	0.08	16,16,16,16	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.