

Full wwPDB X-ray Structure Validation Report (i)

Jan 17, 2023 – 01:00 AM EST

:	2 Q J V
:	Crystal structure of an iolb-like protein (stm4420) from salmonella ty-
	phimurium lt2 at 1.90 A resolution
:	Joint Center for Structural Genomics (JCSG)
	2007-07-09
:	1.90 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

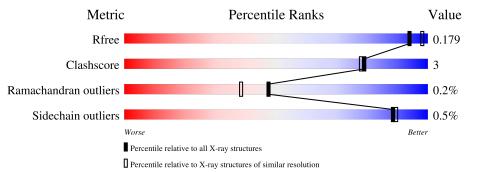
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.90 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 >=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 <=5%

Mol	Chain	Length	Quality of chain					
1	А	270	89%	9%	•			
1	В	270	89%	8%	·			



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5072 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	А	263	Total 2170	C 1375		0		Se 4	0	9	0
1	В	263	Total 2138	C 1357	N 370	O 400	S 7	Se 4	0	6	0

• Molecule 1 is a protein called Uncharacterized IolB-like protein.

Chain	Residue	Modelled	Actual	Comment	Reference
А	0	GLY	-	expression tag	UNP Q8ZK62
А	1	MSE	MET	modified residue	UNP Q8ZK62
А	36	MLY	LYS	modified residue	UNP Q8ZK62
А	62	MLY	LYS	modified residue	UNP Q8ZK62
А	75	MSE	MET	modified residue	UNP Q8ZK62
А	95	MLY	LYS	modified residue	UNP Q8ZK62
А	132	MLY	LYS	modified residue	UNP Q8ZK62
А	161	ALA	GLU	engineered mutation	UNP Q8ZK62
А	163	ALA	ASP	engineered mutation	UNP Q8ZK62
А	171	MLY	LYS	modified residue	UNP Q8ZK62
А	213	MSE	MET	modified residue	UNP Q8ZK62
А	222	MLY	LYS	modified residue	UNP Q8ZK62
А	225	MLY	LYS	modified residue	UNP Q8ZK62
А	244	MSE	MET	modified residue	UNP Q8ZK62
А	250	MLY	LYS	modified residue	UNP Q8ZK62
В	0	GLY	-	expression tag	UNP Q8ZK62
В	1	MSE	MET	modified residue	UNP Q8ZK62
В	36	MLY	LYS	modified residue	UNP Q8ZK62
В	62	MLY	LYS	modified residue	UNP Q8ZK62
В	75	MSE	MET	modified residue	UNP Q8ZK62
В	95	MLY	LYS	modified residue	UNP Q8ZK62
В	132	MLY	LYS	modified residue	UNP Q8ZK62
В	161	ALA	GLU	engineered mutation	UNP Q8ZK62
В	163	ALA	ASP	engineered mutation	UNP Q8ZK62
В	171	MLY	LYS	modified residue	UNP Q8ZK62

There are 30 discrepancies between the modelled and reference sequences:

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Chain	Residue	Modelled	Actual	Comment	Reference				
В	213	MSE	MET	modified residue	UNP Q8ZK62				
В	222	MLY	LYS	modified residue	UNP Q8ZK62				
В	225	MLY	LYS	modified residue	UNP Q8ZK62				
В	244	MSE	MET	modified residue	UNP Q8ZK62				
В	250	MLY	LYS	modified residue	UNP Q8ZK62				

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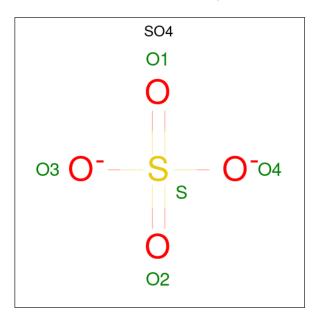
• Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

[Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
	2	А	2	Total Ni 2 2	0	0
	2	В	2	Total Ni 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	4	Total Cl 4 4	0	0
3	В	3	Total Cl 3 3	0	0

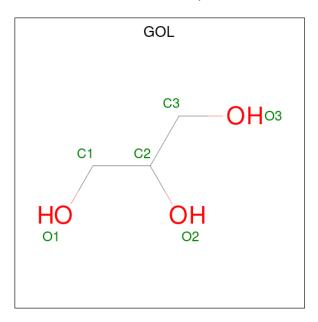
• Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



[Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
	5	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
	5	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 6 is water.

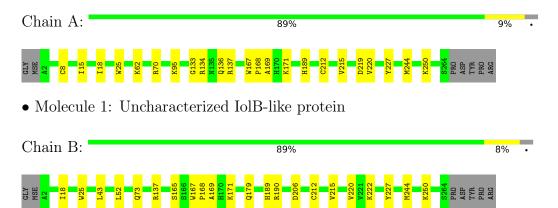
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	366	Total O 366 366	0	0
6	В	355	Total O 355 355	0	0



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. 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. 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: Uncharacterized IolB-like protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants	200.14Å 200.14 Å 200.14 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.51 - 1.90	Depositor
Resolution (A)	29.51 - 1.90	EDS
% Data completeness	99.9(29.51-1.90)	Depositor
(in resolution range)	99.9(29.51-1.90)	EDS
R _{merge}	0.09	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.14 (at 1.91 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0019, PHENIX	Depositor
P. P.	0.160 , 0.181	Depositor
R, R_{free}	0.160 , 0.179	DCC
R_{free} test set	5190 reflections (4.99%)	wwPDB-VP
Wilson B-factor $(Å^2)$	27.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33, 30.3	EDS
L-test for twinning ²	$< L > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.025 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5072	wwPDB-VP
Average B, all atoms $(Å^2)$	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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, MLY, CL, NI, SO4

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	al Chain Bo		nd lengths	Bond angles	
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.82	1/2140~(0.0%)	0.94	4/2918~(0.1%)
1	В	0.82	0/2109	0.92	2/2878~(0.1%)
All	All	0.82	1/4249~(0.0%)	0.93	6/5796~(0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	А	136	GLN	CB-CG	5.07	1.66	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^{o})$
1	А	70[A]	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	А	70[B]	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	В	206	ASP	CB-CG-OD1	5.34	123.11	118.30
1	В	190	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	А	219	ASP	CB-CG-OD1	5.11	122.90	118.30
1	А	134	ARG	NE-CZ-NH1	5.02	122.81	120.30

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	А	2170	0	2071	13	0
1	В	2138	0	2031	13	0
2	А	2	0	0	0	0
2	В	2	0	0	0	0
3	А	4	0	0	1	0
3	В	3	0	0	1	0
4	А	10	0	0	0	0
4	В	10	0	0	0	0
5	А	6	0	8	0	0
5	В	6	0	8	0	0
6	А	366	0	0	5	0
6	В	355	0	0	4	0
All	All	5072	0	4118	24	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 (24) 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:244:MSE:HE2	6:B:428:HOH:O	1.74	0.86
1:A:244:MSE:HE2	6:A:423:HOH:O	1.86	0.74
1:A:8[B]:CYS:SG	6:A:525:HOH:O	2.54	0.64
1:A:212[B]:CYS:HB2	1:B:212[B]:CYS:HB2	1.80	0.63
1:A:62:MLY:HH12	6:A:425:HOH:O	2.01	0.60
1:A:95:MLY:HH22	6:A:572:HOH:O	2.03	0.59
1:B:244:MSE:CE	6:B:428:HOH:O	2.43	0.59
1:B:179[A]:GLN:HG3	6:B:589:HOH:O	2.08	0.52
1:A:137:ARG:NH1	3:A:274:CL:CL	2.81	0.51
1:A:167:TRP:HA	1:A:168:PRO:C	2.32	0.50
1:B:169:ALA:HB1	1:B:227:TYR:HB3	1.92	0.50
1:B:189:HIS:CD2	1:B:215:VAL:HG11	2.47	0.49
1:A:212[B]:CYS:HB2	1:B:212[B]:CYS:CB	2.42	0.49
1:A:189:HIS:CD2	1:A:215:VAL:HG11	2.52	0.45
1:B:18:ILE:HG13	1:B:220:VAL:HG11	1.99	0.45
1:B:167:TRP:HA	1:B:168:PRO:C	2.37	0.44
1:B:250:MLY:HH23	6:B:630:HOH:O	2.16	0.44
1:A:133:GLY:N	6:A:546:HOH:O	2.51	0.43
1:B:43:LEU:CD1	1:B:52:LEU:HD21	2.48	0.43
1:B:137:ARG:HD3	1:B:165:SER:CB	2.49	0.42
1:A:169:ALA:HB1	1:A:227:TYR:HB3	2.01	0.42
1:A:8[A]:CYS:SG	1:A:15:ILE:HD12	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18[A]:ILE:HG13	1:A:220:VAL:HG11	2.03	0.40
1:B:137:ARG:NH1	3:B:273:CL:CL	2.92	0.40

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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	Percer	ntiles
1	А	262/270~(97%)	251 (96%)	11 (4%)	0	100	100
1	В	259/270~(96%)	245~(95%)	12~(5%)	2(1%)	19	9
All	All	521/540~(96%)	496 (95%)	23~(4%)	2~(0%)	47	24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	73[A]	GLN
1	В	73[B]	GLN

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	А	223/218~(102%)	222 (100%)	1 (0%)	91 91
1	В	219/218~(100%)	218 (100%)	1 (0%)	88 89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	442/436 (101%)	440 (100%)	2~(0%)	88 89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	25	TRP
1	В	25	TRP

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. There are no such side chains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

16 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).

Mal	Trune	Chain	Dec	Link	B	ond leng	gths	В	ond ang	gles
Mol	Type	Chain	Res		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
1	MLY	А	222	1	9,10,11	1.01	0	$6,\!11,\!13$	0.53	0
1	MLY	А	250	1	9,10,11	1.17	1 (11%)	$6,\!11,\!13$	0.68	0
1	MLY	А	171	1	$9,\!10,\!11$	0.84	0	$6,\!11,\!13$	0.95	1 (16%)
1	MLY	А	62	1	9,10,11	0.88	0	$6,\!11,\!13$	0.98	0
1	MLY	В	222	1	9,10,11	1.11	1 (11%)	$6,\!11,\!13$	0.64	0
1	MLY	В	62	1	9,10,11	0.91	0	6,11,13	0.27	0
1	MLY	В	225	1	$9,\!10,\!11$	1.03	0	$6,\!11,\!13$	0.85	0
1	MLY	А	225	1	$9,\!10,\!11$	1.06	0	$6,\!11,\!13$	0.60	0
1	MLY	В	36	1	9,10,11	0.85	0	$6,\!11,\!13$	0.30	0
1	MLY	В	250	1	9,10,11	0.94	0	$6,\!11,\!13$	0.40	0
1	MLY	А	132	1	5,6,11	0.96	0	$2,\!6,\!13$	0.16	0
1	MLY	В	132	1	4,5,11	0.69	0	$1,\!5,\!13$	0.29	0



Mol	Type	Chain	Res	Link	Bond lengths				Bond angles		
IVI01	туре	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
1	MLY	А	36	1	9,10,11	0.95	0	6,11,13	0.33	0	
1	MLY	В	95	1	9,10,11	0.69	0	6,11,13	0.34	0	
1	MLY	А	95	1	9,10,11	0.94	0	6,11,13	0.56	0	
1	MLY	В	171	1	9,10,11	0.82	0	6,11,13	0.89	1 (16%)	

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	MLY	А	222	1	-	0/8/9/11	-
1	MLY	А	250	1	-	2/8/9/11	-
1	MLY	А	171	1	-	0/8/9/11	-
1	MLY	А	62	1	-	1/8/9/11	-
1	MLY	В	222	1	-	0/8/9/11	-
1	MLY	В	62	1	-	0/8/9/11	-
1	MLY	В	225	1	-	1/8/9/11	-
1	MLY	А	225	1	-	1/8/9/11	-
1	MLY	В	36	1	-	0/8/9/11	-
1	MLY	В	250	1	-	1/8/9/11	-
1	MLY	А	132	1	-	1/4/5/11	-
1	MLY	В	132	1	-	1/3/4/11	-
1	MLY	А	36	1	-	0/8/9/11	-
1	MLY	В	95	1	-	0/8/9/11	-
1	MLY	А	95	1	-	0/8/9/11	-
1	MLY	В	171	1	-	0/8/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
1	В	222	MLY	CH2-NZ	2.18	1.52	1.46
1	А	250	MLY	CE-NZ	2.07	1.53	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	В	171	MLY	CD-CE-NZ	2.10	119.46	113.79
1	А	171	MLY	CD-CE-NZ	2.06	119.37	113.79

There are no chirality outliers.



Mol	Chain	Res	Type	Atoms
1	А	132	MLY	O-C-CA-CB
1	В	250	MLY	C-CA-CB-CG
1	В	225	MLY	CD-CE-NZ-CH1
1	А	225	MLY	CD-CE-NZ-CH1
1	А	250	MLY	C-CA-CB-CG
1	А	62	MLY	CD-CE-NZ-CH1
1	В	132	MLY	N-CA-CB-CG
1	А	250	MLY	CE-CD-CG-CB

All (8) torsion outliers are listed below:

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	А	62	MLY	1	0
1	В	250	MLY	1	0
1	А	95	MLY	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 11 are monoatomic - leaving 6 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	Trune	Chain	Res	Link	B	ond leng	gths	Bond angles		
	Type	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
4	SO4	А	277	-	4,4,4	0.21	0	$6,\!6,\!6$	0.70	0
5	GOL	В	277	-	$5,\!5,\!5$	0.51	0	$5,\!5,\!5$	0.85	0
5	GOL	А	278	-	$5,\!5,\!5$	0.33	0	$5,\!5,\!5$	0.76	0
4	SO4	В	275	-	4,4,4	0.23	0	$6,\!6,\!6$	0.71	0
4	SO4	А	276	-	4,4,4	0.25	0	$6,\!6,\!6$	0.68	0
4	SO4	В	276	-	4,4,4	0.19	0	$6,\!6,\!6$	0.58	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
5	GOL	А	278	-	-	2/4/4/4	-
5	GOL	В	277	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	А	278	GOL	O1-C1-C2-C3
5	А	278	GOL	O1-C1-C2-O2
5	В	277	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

