



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:20 AM UTC

PDB ID : 4GWO / pdb_00004gwo
Title : Crystal structure of ligand binding domain of LysR family member, CysB in complex with sulfate from Salmonella typhimurium LT2
Authors : Mittal, M.; Singh, A.K.; Kumaran, S.
Deposited on : 2012-09-03
Resolution : 2.39 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

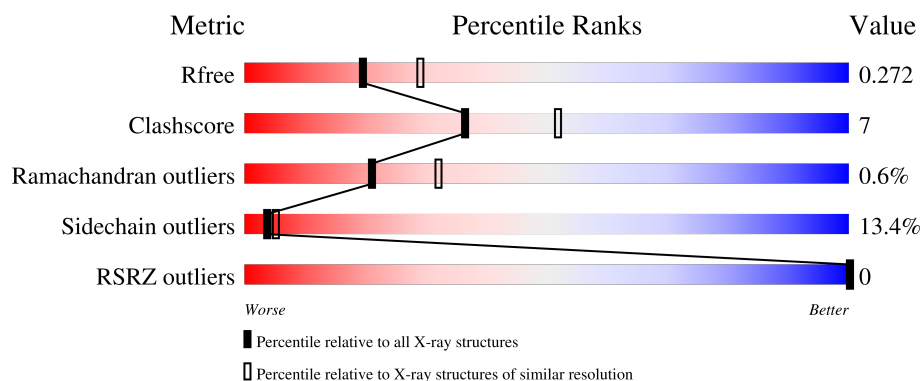
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 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 $\leq 5\%$. 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	330	 53% 17% • 28%
1	B	330	 51% 18% •• 28%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3760 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 HTH-type transcriptional regulator CysB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1852	1187	312	347	6			
1	B	239	Total	C	N	O	S	0	0	0
			1875	1200	322	347	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP P06614
A	-4	HIS	-	expression tag	UNP P06614
A	-3	HIS	-	expression tag	UNP P06614
A	-2	HIS	-	expression tag	UNP P06614
A	-1	HIS	-	expression tag	UNP P06614
A	0	HIS	-	expression tag	UNP P06614
B	-5	HIS	-	expression tag	UNP P06614
B	-4	HIS	-	expression tag	UNP P06614
B	-3	HIS	-	expression tag	UNP P06614
B	-2	HIS	-	expression tag	UNP P06614
B	-1	HIS	-	expression tag	UNP P06614
B	0	HIS	-	expression tag	UNP P06614

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

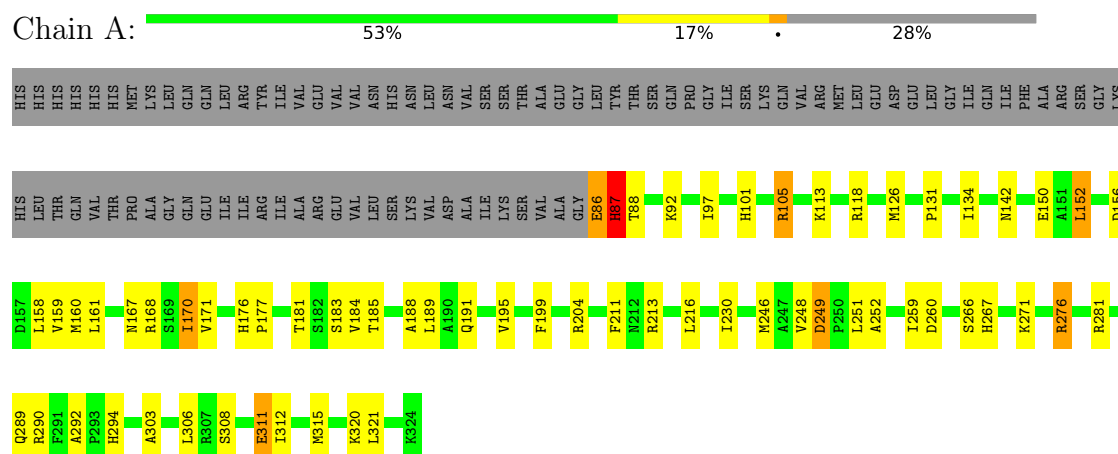
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total 6	O 6	0	0
4	B	11	Total 11	O 11	0	0

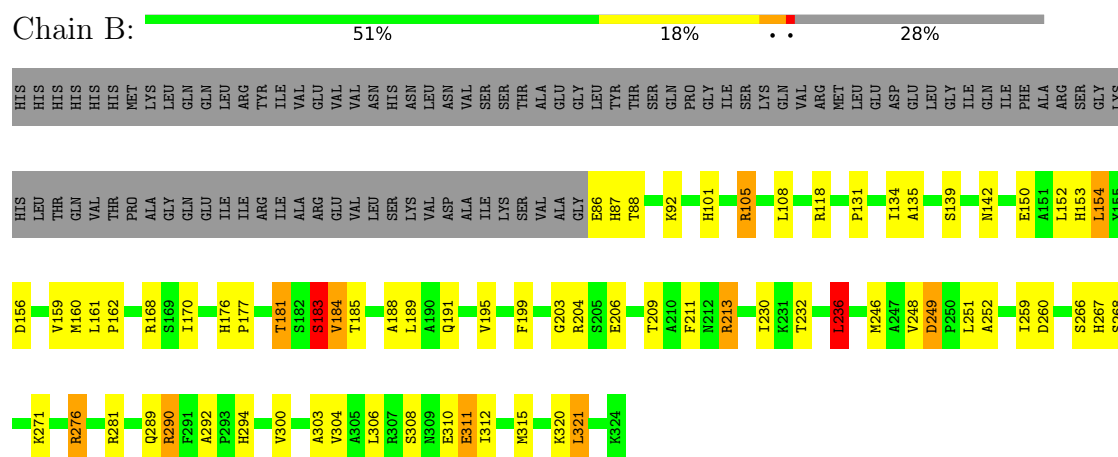
3 Residue-property plots

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: HTH-type transcriptional regulator CysB



- Molecule 1: HTH-type transcriptional regulator CysB



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.92Å 105.30Å 47.75Å 90.00° 103.26° 90.00°	Depositor
Resolution (Å)	26.32 – 2.39 26.32 – 2.39	Depositor EDS
% Data completeness (in resolution range)	90.8 (26.32-2.39) 87.1 (26.32-2.39)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.34 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.198 , 0.268 0.203 , 0.272	Depositor DCC
R_{free} test set	823 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.735	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.114 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3760	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.65	1/1900 (0.1%)	1.00	7/2597 (0.3%)
1	B	0.65	1/1923 (0.1%)	1.03	10/2622 (0.4%)
All	All	0.65	2/3823 (0.1%)	1.01	17/5219 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	142	ASN	CG-ND2	-6.51	1.19	1.33
1	A	142	ASN	CG-ND2	-6.38	1.19	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	VAL	CB-CA-C	-8.95	101.20	111.59
1	B	184	VAL	N-CA-C	8.29	118.22	106.53
1	B	290	ARG	NE-CZ-NH1	-7.78	113.72	121.50
1	B	290	ARG	NE-CZ-NH2	7.53	125.98	119.20
1	A	184	VAL	N-CA-CB	-6.48	104.31	112.15
1	A	290	ARG	NE-CZ-NH2	-6.46	113.38	119.20
1	B	183	SER	CA-C-N	-6.13	115.51	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	183	SER	C-N-CA	-6.13	115.51	122.93
1	A	290	ARG	CD-NE-CZ	6.03	132.84	124.40
1	B	236	LEU	CA-CB-CG	5.57	135.78	116.30
1	A	216	LEU	N-CA-C	5.53	117.43	110.24
1	B	290	ARG	CD-NE-CZ	5.47	132.06	124.40
1	A	290	ARG	NE-CZ-NH1	5.43	126.93	121.50
1	A	87	HIS	N-CA-C	5.25	121.98	110.80
1	B	108	LEU	CA-C-N	-5.16	113.33	119.05
1	B	108	LEU	C-N-CA	-5.16	113.33	119.05
1	A	88	THR	N-CA-C	5.02	117.09	108.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	86	GLU	Peptide
1	B	183	SER	Peptide

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	1852	0	1795	22	1
1	B	1875	0	1847	32	1
2	A	6	0	8	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	6	0	0	0	0
4	B	11	0	0	0	0
All	All	3760	0	3650	53	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 7.

All (53) 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:181:THR:HB	1:B:183:SER:HA	1.50	0.92
1:A:185:THR:HG23	1:A:188:ALA:H	1.45	0.82
1:B:185:THR:HG23	1:B:188:ALA:H	1.43	0.81
1:B:86:GLU:O	1:B:88:THR:N	2.16	0.78
1:B:183:SER:HB3	1:B:259:ILE:HG21	1.72	0.71
1:A:170:ILE:HG12	1:A:259:ILE:HB	1.76	0.67
1:B:303:ALA:HA	1:B:315:MET:HE1	1.76	0.67
1:A:306:LEU:HD13	1:A:311:GLU:HB3	1.75	0.66
1:B:152:LEU:HD13	1:B:160:MET:HE1	1.78	0.65
1:B:199:PHE:HA	1:B:204:ARG:HG2	1.81	0.63
1:B:306:LEU:HD13	1:B:311:GLU:HB3	1.80	0.63
1:A:303:ALA:HA	1:A:315:MET:HE1	1.81	0.62
1:A:199:PHE:HA	1:A:204:ARG:HG2	1.81	0.62
1:B:170:ILE:HG12	1:B:259:ILE:HB	1.81	0.62
1:B:249:ASP:OD2	1:B:252:ALA:N	2.30	0.57
1:A:308:SER:O	1:A:312:ILE:HG13	2.05	0.56
1:B:195:VAL:HG12	1:B:230:ILE:HG23	1.90	0.53
1:A:195:VAL:HG12	1:A:230:ILE:HG23	1.91	0.53
1:B:308:SER:O	1:B:312:ILE:HG13	2.09	0.52
1:A:131:PRO:HG2	1:A:150:GLU:HB2	1.91	0.52
1:B:92:LYS:O	1:B:281:ARG:NH2	2.44	0.51
1:B:131:PRO:HG2	1:B:150:GLU:HB2	1.93	0.51
1:B:152:LEU:HB3	1:B:160:MET:CE	2.42	0.50
1:B:276:ARG:NH2	1:B:306:LEU:O	2.45	0.50
1:A:249:ASP:OD2	1:A:252:ALA:N	2.36	0.50
1:A:92:LYS:O	1:A:281:ARG:NH2	2.45	0.49
1:A:276:ARG:NH2	1:A:306:LEU:O	2.46	0.49
1:A:189:LEU:HD23	1:A:211:PHE:HZ	1.79	0.46
1:B:189:LEU:HD23	1:B:211:PHE:HZ	1.80	0.46
1:B:135:ALA:HB2	1:B:152:LEU:HD23	1.98	0.46
1:A:266:SER:HA	2:A:401:GOL:H32	1.99	0.45
1:A:101:HIS:CE1	1:A:105:ARG:HG3	2.52	0.45
1:B:101:HIS:CE1	1:B:105:ARG:HG3	2.51	0.45
1:B:232:THR:O	1:B:236:LEU:HD23	2.17	0.44
1:A:176:HIS:CG	1:A:177:PRO:HD2	2.53	0.44
1:B:300:VAL:O	1:B:304:VAL:HG23	2.18	0.44
1:B:176:HIS:CG	1:B:177:PRO:HD2	2.53	0.44
1:B:183:SER:HB3	1:B:259:ILE:CG2	2.46	0.43
1:A:167:ASN:OD1	1:A:168:ARG:N	2.42	0.43
1:B:153:HIS:CD2	1:B:154:LEU:HD13	2.53	0.43
1:A:292:ALA:HB1	1:A:294:HIS:CE1	2.54	0.42
1:B:292:ALA:HB1	1:B:294:HIS:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ILE:O	1:A:126:MET:HA	2.18	0.42
1:B:303:ALA:CA	1:B:315:MET:HE1	2.45	0.42
1:B:168:ARG:NH2	1:B:266:SER:O	2.52	0.41
1:B:162:PRO:HB2	1:B:321:LEU:HD21	2.02	0.41
1:A:86:GLU:O	1:A:87:HIS:HB3	2.20	0.41
1:B:150:GLU:OE2	1:B:203:GLY:N	2.52	0.41
1:A:113:LYS:HB2	1:B:236:LEU:HD13	2.02	0.41
1:B:206:GLU:OE2	1:B:268:SER:OG	2.31	0.41
1:A:101:HIS:O	1:A:105:ARG:HB2	2.20	0.41
1:A:152:LEU:HD23	1:A:160:MET:HE1	2.01	0.40
1:B:209:THR:O	1:B:213:ARG:HG3	2.21	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)
1:A:281:ARG:NH1	1:B:310:GLU:OE1[2_555]	2.09	0.11

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	237/330 (72%)	226 (95%)	10 (4%)	1 (0%)	30	43
1	B	237/330 (72%)	227 (96%)	8 (3%)	2 (1%)	16	25
All	All	474/660 (72%)	453 (96%)	18 (4%)	3 (1%)	21	32

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	87	HIS
1	B	183	SER

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Mol	Chain	Res	Type
1	A	87	HIS

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	A	195/281 (69%)	169 (87%)	26 (13%)	4	5
1	B	200/281 (71%)	173 (86%)	27 (14%)	4	5
All	All	395/562 (70%)	342 (87%)	53 (13%)	4	5

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ARG
1	A	118	ARG
1	A	134	ILE
1	A	152	LEU
1	A	156	ASP
1	A	158	LEU
1	A	159	VAL
1	A	161	LEU
1	A	170	ILE
1	A	171	VAL
1	A	181	THR
1	A	183	SER
1	A	191	GLN
1	A	213	ARG
1	A	246	MET
1	A	248	VAL
1	A	249	ASP
1	A	251	LEU
1	A	260	ASP
1	A	267	HIS
1	A	271	LYS
1	A	276	ARG

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Mol	Chain	Res	Type
1	A	289	GLN
1	A	311	GLU
1	A	320	LYS
1	A	321	LEU
1	B	105	ARG
1	B	118	ARG
1	B	134	ILE
1	B	139	SER
1	B	154	LEU
1	B	156	ASP
1	B	159	VAL
1	B	161	LEU
1	B	181	THR
1	B	183	SER
1	B	184	VAL
1	B	191	GLN
1	B	213	ARG
1	B	236	LEU
1	B	246	MET
1	B	248	VAL
1	B	249	ASP
1	B	251	LEU
1	B	260	ASP
1	B	267	HIS
1	B	271	LYS
1	B	276	ARG
1	B	289	GLN
1	B	290	ARG
1	B	311	GLU
1	B	320	LYS
1	B	321	LEU

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

Mol	Chain	Res	Type
1	A	289	GLN
1	B	153	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	A	401	-	5,5,5	0.32	0	5,5,5	0.36	0
3	SO4	B	401	-	4,4,4	0.41	0	6,6,6	0.53	0
3	SO4	A	402	-	4,4,4	0.33	0	6,6,6	0.24	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	A	401	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	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, 95th 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 ²)	Q<0.9
1	A	239/330 (72%)	-1.23	0 100 100	32, 44, 65, 79	0
1	B	239/330 (72%)	-1.16	0 100 100	32, 49, 77, 95	0
All	All	478/660 (72%)	-1.20	0 100 100	32, 47, 75, 95	0

There are no RSRZ outliers to report.

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 oligosaccharides 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, 95th 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 ²)	Q<0.9
2	GOL	A	401	6/6	0.97	0.06	54,55,56,57	0
3	SO4	A	402	5/5	1.00	0.05	34,35,38,39	0
3	SO4	B	401	5/5	1.00	0.04	32,32,35,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.