



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:52 PM GMT

PDB ID : 1YSR
Title : Crystal Structure of ATP binding domain of PrrB from Mycobacterium Tuberculosis
Authors : Nowak, E.; Panjikar, S.; Tucker, P.; Mycobacterium Tuberculosis Structural Proteomics Project (XMTB)
Deposited on : 2005-02-09
Resolution : 1.78 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

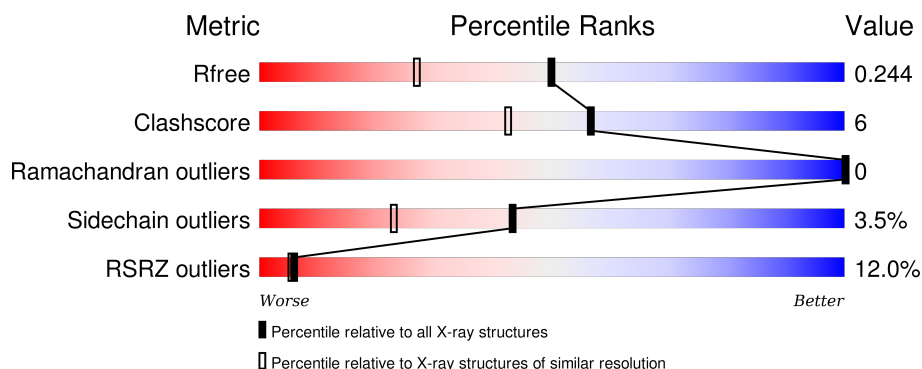
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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}	91344	6655 (1.80-1.76)
Clashscore	102246	7658 (1.80-1.76)
Ramachandran outliers	100387	7570 (1.80-1.76)
Sidechain outliers	100360	7569 (1.80-1.76)
RSRZ outliers	91569	6671 (1.80-1.76)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	150	<div> <div>12%</div> <div>75%</div> <div>15%</div> <div>9%</div> </div>
1	B	150	<div> <div>11%</div> <div>81%</div> <div>9%</div> <div>9%</div> </div>
1	C	150	<div> <div>9%</div> <div>80%</div> <div>10%</div> <div>9%</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
3	GOL	A	2003	-	-	-	X
3	GOL	B	2002	-	-	-	X

2 Entry composition [i](#)

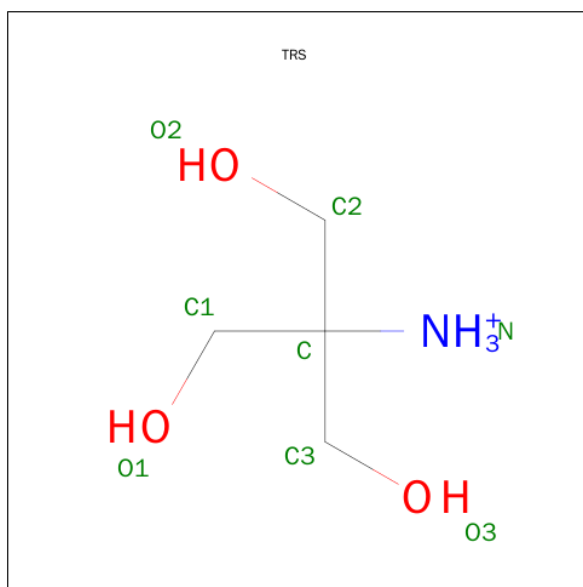
There are 4 unique types of molecules in this entry. The entry contains 3178 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Sensor-type histidine kinase prrB.

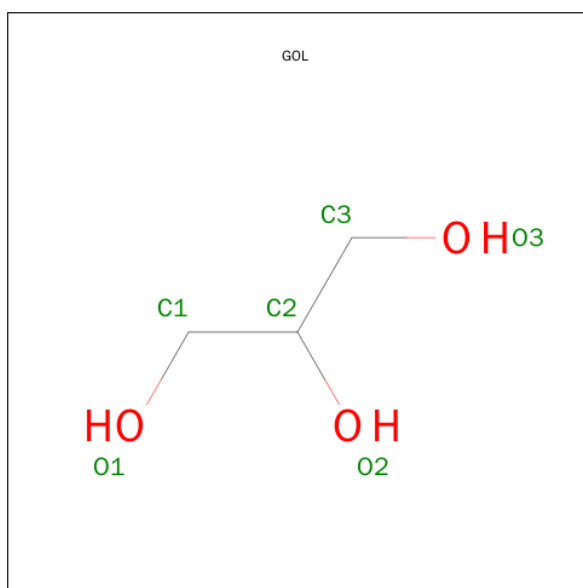
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	137	Total	C	N	O	S	0	1	0
			990	616	179	194	1			
1	B	137	Total	C	N	O	S	13	0	0
			989	616	179	193	1			
1	C	136	Total	C	N	O	S	0	1	0
			990	616	179	193	2			

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	1	3		
2	B	1	Total	C	N	O	0	0
			8	4	1	3		
2	C	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

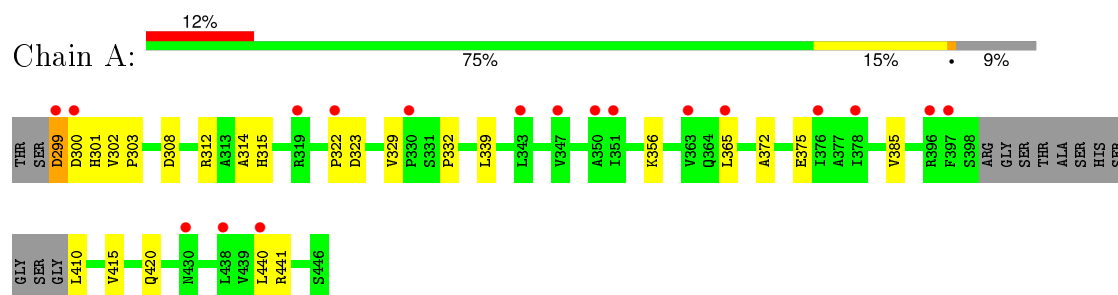
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	61	Total	O	0	0
			61	61		
4	B	53	Total	O	0	0
			53	53		
4	C	53	Total	O	0	0
			53	53		

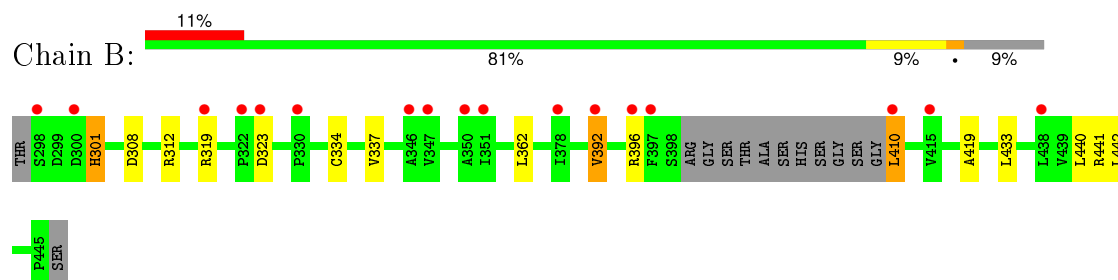
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

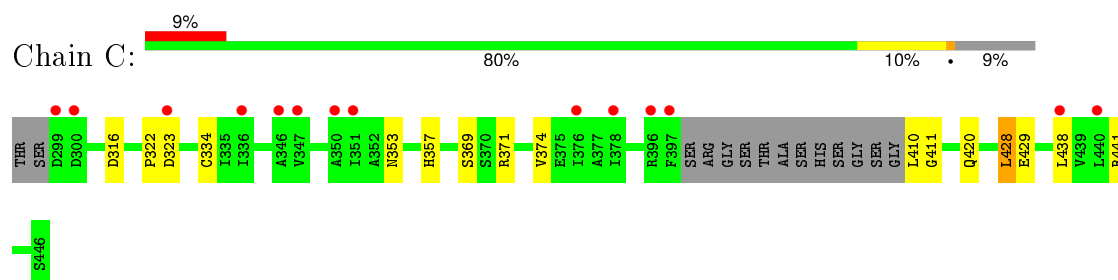
• Molecule 1: Sensor-type histidine kinase prrB



• Molecule 1: Sensor-type histidine kinase prrB



• Molecule 1: Sensor-type histidine kinase prrB



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	61.05Å 61.05Å 208.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.98 – 1.78 19.98 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.98-1.78) 99.2 (19.98-1.78)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.200 , 0.246 0.199 , 0.244	Depositor DCC
R_{free} test set	2088 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.5	EDS
Estimated twinning fraction	0.067 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 41403 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3178	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, TRS

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	0.87	0/1004	0.88	0/1369
1	B	0.83	0/1003	0.86	3/1369 (0.2%)
1	C	0.95	0/1004	0.97	3/1369 (0.2%)
All	All	0.89	0/3011	0.90	6/4107 (0.1%)

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	B	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	392	VAL	CA-C-O	-6.46	106.53	120.10
1	C	428	LEU	CB-CG-CD1	5.91	121.04	111.00
1	C	428	LEU	CA-CB-CG	5.78	128.59	115.30
1	B	392	VAL	N-CA-C	-5.59	95.90	111.00
1	C	316	ASP	CB-CG-OD1	5.24	123.02	118.30
1	B	392	VAL	CB-CA-C	5.12	121.13	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	323	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	B	392	VAL	Mainchain

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	990	0	995	17	0
1	B	989	0	996	13	0
1	C	990	0	995	9	0
2	A	8	0	12	0	0
2	B	8	0	12	0	0
2	C	8	0	12	0	0
3	A	6	0	8	1	0
3	B	6	0	8	1	0
3	C	6	0	8	1	0
4	A	61	0	0	2	0
4	B	53	0	0	1	0
4	C	53	0	0	2	0
All	All	3178	0	3046	37	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 6.

All (37) 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:362:LEU:HD12	1:B:433:LEU:HD13	1.42	0.98
1:C:441:ARG:HB3	3:C:2001:GOL:H11	1.54	0.89
1:B:362:LEU:CD1	1:B:433:LEU:HD13	2.15	0.76
1:C:353:ASN:HD21	1:C:411:GLY:H	1.37	0.73
1:C:334[A]:CYS:SG	4:C:24:HOH:O	2.50	0.69
1:B:301:HIS:HB3	1:B:337:VAL:HG12	1.77	0.67
1:B:334:CYS:SG	4:B:39:HOH:O	2.54	0.66
1:A:301:HIS:CD2	1:A:339:LEU:HD21	2.30	0.66
1:A:322:PRO:O	1:A:323:ASP:HB2	1.97	0.63
1:B:419:ALA:HB2	1:B:440:LEU:HD21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ASP:OD2	1:A:312:ARG:NH1	2.35	0.60
1:B:301:HIS:HB3	1:B:337:VAL:CG1	2.32	0.60
1:C:353:ASN:ND2	1:C:411:GLY:H	1.98	0.59
1:A:375:GLU:OE1	1:A:441:ARG:NH1	2.36	0.59
1:B:308:ASP:O	1:B:312:ARG:HG2	2.01	0.59
1:B:441:ARG:HB3	3:B:2002:GOL:H2	1.86	0.57
1:A:315:HIS:HE1	4:A:128:HOH:O	1.90	0.55
1:A:301:HIS:CD2	1:A:339:LEU:CD2	2.90	0.54
1:B:396:ARG:HD2	1:B:410:LEU:O	2.08	0.54
1:A:299:ASP:HB3	1:A:301:HIS:H	1.74	0.53
1:A:315:HIS:CE1	4:A:128:HOH:O	2.63	0.51
1:B:396:ARG:NH1	1:B:410:LEU:O	2.44	0.50
1:B:419:ALA:HB2	1:B:440:LEU:CD2	2.40	0.49
1:C:322:PRO:O	1:C:323:ASP:HB2	2.13	0.49
1:A:301:HIS:HD2	1:A:339:LEU:HD21	1.78	0.48
1:B:440:LEU:HD22	1:B:442:LEU:HD21	1.95	0.48
1:A:356:LYS:HG2	1:C:371:ARG:HH21	1.81	0.46
1:A:332:PRO:HB3	1:B:319:ARG:NH1	2.32	0.45
1:A:322:PRO:O	1:A:323:ASP:CB	2.62	0.45
1:C:357:HIS:CE1	1:C:410:LEU:HD22	2.51	0.45
1:C:334[A]:CYS:SG	1:C:374:VAL:HB	2.57	0.44
1:A:415:VAL:CG1	1:A:440:LEU:HD21	2.47	0.44
1:C:323:ASP:HA	4:C:129:HOH:O	2.19	0.43
1:A:314:ALA:HB2	1:A:365:LEU:HD12	2.02	0.42
1:A:372:ALA:HB1	3:A:2003:GOL:O2	2.19	0.42
1:A:385:VAL:HG22	1:A:410:LEU:HD21	2.03	0.41
1:A:302:VAL:HB	1:A:303:PRO:CD	2.51	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	A	133/150 (89%)	131 (98%)	2 (2%)	0	100	100
1	B	133/150 (89%)	131 (98%)	2 (2%)	0	100	100
1	C	133/150 (89%)	130 (98%)	3 (2%)	0	100	100
All	All	399/450 (89%)	392 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	105/114 (92%)	101 (96%)	4 (4%)	40	20
1	B	105/114 (92%)	103 (98%)	2 (2%)	65	49
1	C	105/114 (92%)	100 (95%)	5 (5%)	31	12
All	All	315/342 (92%)	304 (96%)	11 (4%)	43	23

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	299	ASP
1	A	300	ASP
1	A	329	VAL
1	A	420	GLN
1	B	301	HIS
1	B	410	LEU
1	C	369	SER
1	C	420	GLN
1	C	428	LEU
1	C	429	GLU
1	C	438	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	HIS
1	B	301	HIS
1	B	315	HIS
1	B	420	GLN
1	C	353	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 ⓘ

6 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	TRS	A	1001	-	7,7,7	0.71	0	9,9,9	1.54	2 (22%)
3	GOL	A	2003	-	5,5,5	0.49	0	5,5,5	0.63	0
2	TRS	B	1002	-	7,7,7	0.95	0	9,9,9	2.00	1 (11%)
3	GOL	B	2002	-	5,5,5	0.40	0	5,5,5	1.09	0
2	TRS	C	1003	-	7,7,7	0.78	0	9,9,9	1.96	2 (22%)
3	GOL	C	2001	-	5,5,5	0.48	0	5,5,5	1.21	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	TRS	A	1001	-	-	0/9/9/9	0/0/0/0
3	GOL	A	2003	-	-	0/4/4/4	0/0/0/0
2	TRS	B	1002	-	-	0/9/9/9	0/0/0/0
3	GOL	B	2002	-	-	0/4/4/4	0/0/0/0
2	TRS	C	1003	-	-	0/9/9/9	0/0/0/0
3	GOL	C	2001	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1002	TRS	O3-C3-C	-5.33	100.40	111.18
2	C	1003	TRS	O1-C1-C	-3.79	103.52	111.18
2	A	1001	TRS	O2-C2-C	-2.97	105.18	111.18
2	A	1001	TRS	C2-C-N	-2.20	104.08	108.09
2	C	1003	TRS	O3-C3-C	3.71	118.69	111.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2003	GOL	1	0
3	B	2002	GOL	1	0
3	C	2001	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, 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	137/150 (91%)	0.50	18 (13%) 5 4	25, 35, 51, 64	0
1	B	137/150 (91%)	0.68	17 (12%) 5 5	29, 39, 56, 63	3 (2%)
1	C	136/150 (90%)	0.44	14 (10%) 9 8	26, 35, 48, 60	0
All	All	410/450 (91%)	0.54	49 (11%) 6 5	25, 36, 52, 64	3 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	351	ILE	5.4
1	B	350	ALA	4.9
1	B	392	VAL	4.5
1	A	347	VAL	4.5
1	B	323	ASP	4.5
1	C	378	ILE	4.1
1	C	347	VAL	4.1
1	B	347	VAL	3.9
1	C	397	PHE	3.8
1	C	299	ASP	3.8
1	B	322	PRO	3.7
1	C	438	LEU	3.5
1	B	319	ARG	3.4
1	A	299	ASP	3.3
1	B	397	PHE	3.3
1	B	330	PRO	3.2
1	A	351	ILE	3.2
1	B	378	ILE	3.2
1	A	440	LEU	3.1
1	A	438	LEU	3.1
1	A	350	ALA	3.1
1	A	300	ASP	3.0
1	A	397	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	396	ARG	2.9
1	A	363	VAL	2.9
1	B	396	ARG	2.9
1	C	351	ILE	2.8
1	A	376	ILE	2.8
1	A	330	PRO	2.8
1	C	336	ILE	2.6
1	A	430	ASN	2.6
1	B	410	LEU	2.6
1	C	346	ALA	2.6
1	C	440	LEU	2.5
1	A	319	ARG	2.4
1	C	323	ASP	2.4
1	A	343	LEU	2.4
1	C	350	ALA	2.3
1	A	378	ILE	2.3
1	B	300	ASP	2.3
1	C	300	ASP	2.2
1	B	298	SER	2.2
1	C	376	ILE	2.2
1	B	415	VAL	2.2
1	B	438	LEU	2.1
1	A	396	ARG	2.1
1	B	346	ALA	2.1
1	A	365	LEU	2.1
1	A	322	PRO	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	GOL	B	2002	6/6	0.88	0.20	6.70	42,43,52,55	0
3	GOL	A	2003	6/6	0.64	0.19	3.31	47,55,58,73	0
3	GOL	C	2001	6/6	0.90	0.14	1.93	44,54,56,58	0
2	TRS	B	1002	8/8	0.85	0.13	1.15	34,36,38,41	0
2	TRS	A	1001	8/8	0.93	0.10	-0.36	36,42,43,43	0
2	TRS	C	1003	8/8	0.94	0.09	-0.71	38,39,40,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.