



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 05:27 pm GMT

PDB ID : 4O3W
Title : Crystal structure of the vaccine antigen Transferrin Binding Protein B (TbpB) mutant Tyr-63-Ala from *Actinobacillus suis* H57
Authors : Calmettes, C.; Yu, R.H.; Schryvers, A.B.; Moraes, T.F.
Deposited on : 2013-12-18
Resolution : 2.10 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

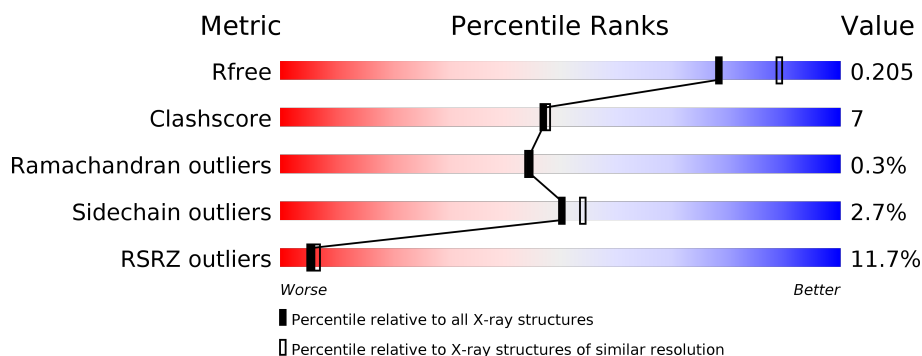
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	572	<div> <div>8%</div> <div>82%</div> <div>12%</div> <div>• 5%</div> </div>
1	B	572	<div> <div>14%</div> <div>79%</div> <div>13%</div> <div>• 6%</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	601	-	-	-	X
2	GOL	B	601	-	-	X	X
3	SO4	B	602	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9062 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.

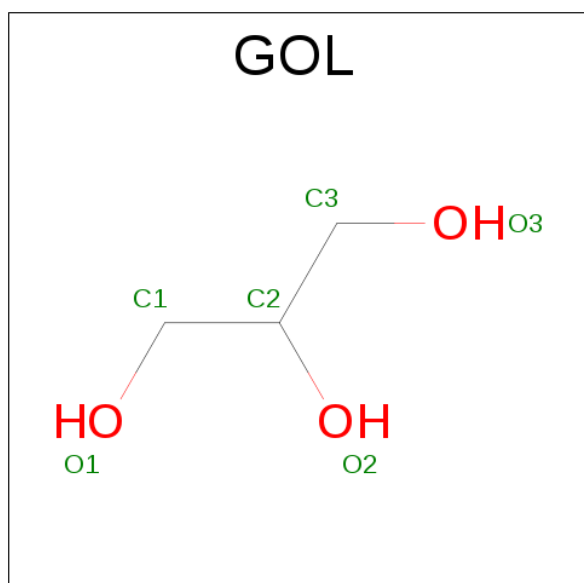
- Molecule 1 is a protein called Transferrin binding protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	546	Total	C	N	O	S	0	2	0
			4259	2663	736	852	8			
1	B	535	Total	C	N	O	S	0	2	0
			4171	2610	720	833	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	GLY	-	EXPRESSION TAG	UNP Q83UA7
A	7	SER	-	EXPRESSION TAG	UNP Q83UA7
A	63	ALA	PHE	ENGINEERED MUTATION	UNP Q83UA7
B	6	GLY	-	EXPRESSION TAG	UNP Q83UA7
B	7	SER	-	EXPRESSION TAG	UNP Q83UA7
B	63	ALA	PHE	ENGINEERED MUTATION	UNP Q83UA7

- 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	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	345	Total	O	0	0
			345	345		
4	B	264	Total	O	0	0
			264	264		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.81Å 74.51Å 106.60Å 90.00° 105.80° 90.00°	Depositor
Resolution (Å)	46.28 – 2.10 46.28 – 2.10	Depositor EDS
% Data completeness (in resolution range)	91.4 (46.28-2.10) 91.4 (46.28-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.190 , 0.205 0.190 , 0.205	Depositor DCC
R_{free} test set	1853 reflections (2.53%)	DCC
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9062	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.04% 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	0.43	0/4342	0.57	1/5839 (0.0%)
1	B	0.41	0/4251	0.57	0/5718
All	All	0.42	0/8593	0.57	1/11557 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ARG	NE-CZ-NH2	5.69	123.15	120.30

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	4259	0	4134	50	0
1	B	4171	0	4053	69	0
2	A	12	0	16	2	0
2	B	6	0	8	7	0
3	B	5	0	0	1	0
4	A	345	0	0	13	0
4	B	264	0	0	4	0
All	All	9062	0	8211	118	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 7.

All (118) 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:81:GLU:HG2	4:B:925:HOH:O	1.59	1.03
1:B:494:GLY:HA2	1:B:495:VAL:HG22	1.49	0.94
1:B:89:ASN:HB2	2:B:601:GOL:H31	1.53	0.88
1:B:88:TRP:H	2:B:601:GOL:H2	1.45	0.82
1:B:81:GLU:CG	4:B:925:HOH:O	2.22	0.82
1:B:87:ILE:HB	2:B:601:GOL:H32	1.60	0.82
1:A:54:LYS:HG2	4:A:888:HOH:O	1.81	0.80
1:A:28:TYR:HB3	1:A:574:GLN:HG2	1.70	0.74
1:B:67:GLY:HA2	1:B:148:VAL:HG11	1.78	0.66
1:B:334:GLU:O	1:B:334:GLU:HG2	1.95	0.66
1:B:490:PHE:CG	1:B:491:ASP:N	2.64	0.66
1:B:334:GLU:O	1:B:335:ASN:ND2	2.29	0.65
1:B:490:PHE:CD1	1:B:491:ASP:N	2.65	0.64
1:B:148:VAL:HA	4:B:955:HOH:O	1.97	0.64
1:B:54:LYS:HZ3	1:B:158:GLY:H	1.45	0.62
1:B:54:LYS:NZ	1:B:158:GLY:H	1.97	0.61
1:A:57:ARG:NE	4:A:964:HOH:O	2.22	0.61
1:B:484:LYS:NZ	1:B:502:ASP:OD1	2.33	0.61
1:A:57:ARG:HB2	4:A:964:HOH:O	2.00	0.61
1:A:69:ARG:HH21	1:A:69:ARG:HG3	1.65	0.61
1:A:323:LYS:NZ	4:A:1031:HOH:O	2.33	0.60
1:B:335:ASN:HD22	1:B:335:ASN:C	2.05	0.60
1:A:349:ILE:HD11	1:A:555:GLN:HG3	1.83	0.59
1:B:471:GLY:HA2	1:B:492:LYS:HG2	1.84	0.59
1:A:232:LYS:NZ	4:A:962:HOH:O	2.36	0.58
1:A:57:ARG:CD	4:A:964:HOH:O	2.50	0.58
1:B:54:LYS:HE2	1:B:157:ASP:OD2	2.05	0.57
1:B:89:ASN:CB	2:B:601:GOL:H31	2.31	0.57
1:B:446:TYR:HB2	1:B:476:PHE:HB2	1.87	0.57
1:A:69:ARG:HH21	1:A:69:ARG:CG	2.17	0.56
1:B:258:TYR:HD1	3:B:602:SO4:O4	1.89	0.56
1:B:460:TRP:HZ2	1:B:491:ASP:HB2	1.70	0.56
1:B:354:PHE:HB2	1:B:559:LYS:HB2	1.89	0.55
1:A:89:ASN:HA	2:A:602:GOL:H31	1.89	0.54
1:A:54:LYS:HE2	4:A:888:HOH:O	2.07	0.54
1:A:561:ASP:OD1	1:A:561:ASP:N	2.39	0.54
1:A:351:LEU:HG	1:A:425:SER:HA	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:THR:HG22	1:A:73:PRO:O	2.09	0.53
1:B:383:LYS:NZ	1:B:463:GLU:HG2	2.25	0.52
1:A:369:ILE:HD13	1:A:374[A]:LYS:HG2	1.91	0.52
1:A:57:ARG:HD3	4:A:964:HOH:O	2.10	0.51
1:B:54:LYS:HD2	1:B:158:GLY:O	2.09	0.51
1:A:337:GLU:HG2	1:A:338:THR:HG23	1.93	0.51
1:A:336:GLY:HA2	1:A:338:THR:N	2.26	0.51
1:A:144:ASN:OD1	1:A:148:VAL:HG13	2.11	0.51
1:B:460:TRP:CZ2	1:B:491:ASP:HB2	2.45	0.51
1:B:560:SER:OG	1:B:561:ASP:N	2.44	0.51
1:A:178:THR:OG1	1:B:334:GLU:OE1	2.21	0.50
1:B:467:ASN:HB3	1:B:471:GLY:HA3	1.94	0.50
1:B:511:ILE:HD11	1:B:539:LYS:HE2	1.94	0.50
1:B:468:ARG:HH12	1:B:574:GLN:HE22	1.59	0.50
1:B:89:ASN:H	2:B:601:GOL:H31	1.77	0.49
1:A:474:THR:HG22	1:A:489:LEU:HG	1.95	0.49
1:B:231:VAL:HG22	1:B:259:ILE:HD13	1.94	0.49
1:A:89:ASN:N	2:A:601:GOL:O2	2.46	0.49
1:B:490:PHE:HZ	1:B:493:GLY:H	1.59	0.49
1:A:456:LYS:O	1:A:562:ASN:ND2	2.46	0.49
1:B:383:LYS:HZ1	1:B:463:GLU:HG2	1.76	0.48
1:B:454:VAL:HB	1:B:460:TRP:HB3	1.96	0.48
1:B:490:PHE:HZ	1:B:493:GLY:N	2.11	0.48
1:B:225:LYS:HD2	1:B:230:GLU:HG2	1.96	0.47
1:A:378:ALA:O	1:A:386:LYS:NZ	2.39	0.47
1:B:501:VAL:HG12	1:B:514:ALA:HB2	1.98	0.46
1:B:91:ASN:ND2	1:B:94:GLU:HB2	2.31	0.46
1:A:31:GLU:HG3	1:A:33:THR:HG23	1.98	0.46
1:A:561:ASP:HA	1:A:562:ASN:HA	1.37	0.46
1:B:456:LYS:HB2	1:B:523:LEU:HD21	1.97	0.46
1:A:173:LYS:HD3	1:A:341:GLU:HB2	1.97	0.45
1:B:516:THR:HG22	1:B:517:SER:H	1.81	0.45
1:B:87:ILE:HG22	2:B:601:GOL:H11	1.97	0.45
1:A:148:VAL:HA	4:A:1029:HOH:O	2.17	0.45
1:B:227:GLY:HA3	4:B:962:HOH:O	2.17	0.45
1:A:418:LYS:HA	1:A:419:GLN:HA	1.59	0.45
1:B:488:LYS:HB3	1:B:497:PRO:HB3	1.98	0.45
1:A:413:TRP:CD1	1:A:421:VAL:HG13	2.52	0.45
1:B:29:GLN:O	1:B:574:GLN:HG3	2.17	0.45
1:A:492:LYS:HE3	1:A:492:LYS:HB2	1.67	0.45
1:A:67:GLY:HA2	1:A:148:VAL:HG21	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ARG:HD2	1:A:156:ILE:O	2.17	0.44
1:A:232:LYS:NZ	4:A:1032:HOH:O	2.41	0.44
1:B:540:VAL:HB	1:B:556:PHE:HB3	1.99	0.44
1:B:269:LYS:HD2	1:B:289:GLU:HG3	2.00	0.44
1:A:226:LEU:O	1:A:261:ARG:HA	2.18	0.44
1:B:456:LYS:HG2	1:B:563:GLY:HA2	1.99	0.44
1:B:460:TRP:HZ2	1:B:491:ASP:CG	2.21	0.43
1:B:49:LEU:HD23	1:B:49:LEU:HA	1.81	0.43
1:A:510:PHE:CZ	1:A:542:GLY:HA3	2.53	0.43
1:B:498:VAL:HG23	1:B:499:PHE:HD1	1.83	0.43
1:A:535:PHE:CD1	1:A:538:ILE:HD11	2.53	0.43
1:A:400:CYS:HA	1:A:401:CYS:HA	1.84	0.43
1:B:456:LYS:NZ	1:B:533:ALA:HA	2.33	0.43
1:A:102:ASN:ND2	4:A:875:HOH:O	2.36	0.43
1:B:90:GLU:H	1:B:90:GLU:HG2	1.54	0.43
1:A:441:GLY:HA2	1:A:442:GLY:HA2	1.82	0.42
1:B:460:TRP:HZ2	1:B:491:ASP:CB	2.30	0.42
1:A:38:LYS:HB2	1:A:38:LYS:HE2	1.84	0.42
1:B:348:LYS:HB2	1:B:359:LEU:HD21	2.01	0.42
1:B:521:PHE:O	1:B:532:ASN:HB2	2.20	0.42
1:B:225:LYS:HZ2	1:B:228:ASP:HA	1.85	0.42
1:A:148:VAL:HA	1:A:149:PRO:HD3	1.89	0.41
1:B:127:TYR:O	1:B:165:THR:HG22	2.19	0.41
1:B:438:MET:HA	1:B:439:PRO:HD3	1.87	0.41
1:B:450:TRP:CE3	1:B:489:LEU:HD23	2.55	0.41
1:B:488:LYS:HG2	1:B:497:PRO:HG3	2.02	0.41
1:B:400:CYS:HA	1:B:401:CYS:HA	1.87	0.41
1:B:456:LYS:HB2	1:B:523:LEU:HD11	2.02	0.41
1:A:446:TYR:HB2	1:A:476:PHE:HB2	2.03	0.41
1:A:398:VAL:O	1:A:410:GLY:HA3	2.21	0.41
1:B:490:PHE:CZ	1:B:492:LYS:N	2.89	0.41
1:A:248:LYS:HE2	4:A:980:HOH:O	2.20	0.41
1:A:57:ARG:NH2	4:A:805:HOH:O	2.50	0.40
1:B:170:GLU:HG2	1:B:342:ARG:HG3	2.03	0.40
1:A:509:GLY:HA2	1:A:543:GLY:HA2	2.03	0.40
1:B:335:ASN:ND2	1:B:335:ASN:C	2.73	0.40
1:A:520:GLY:HA3	1:A:534:VAL:HG22	2.04	0.40
1:A:54:LYS:HG3	1:A:159:TYR:CE1	2.57	0.40
1:B:450:TRP:HB2	1:B:568:VAL:O	2.21	0.40
1:B:89:ASN:H	2:B:601:GOL:C3	2.34	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	544/572 (95%)	521 (96%)	22 (4%)	1 (0%)	51	52
1	B	531/572 (93%)	502 (94%)	27 (5%)	2 (0%)	38	35
All	All	1075/1144 (94%)	1023 (95%)	49 (5%)	3 (0%)	44	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	495	VAL
1	A	202	GLY
1	B	202	GLY

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	453/471 (96%)	436 (96%)	17 (4%)	38	38
1	B	444/471 (94%)	437 (98%)	7 (2%)	68	74
All	All	897/942 (95%)	873 (97%)	24 (3%)	50	54

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ARG
1	A	85	MET
1	A	92	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	196	SER
1	A	290	LYS
1	A	335	ASN
1	A	337	GLU
1	A	353	GLN
1	A	369	ILE
1	A	394	THR
1	A	401	CYS
1	A	455	SER
1	A	458	THR
1	A	468	ARG
1	A	516	THR
1	A	523	LEU
1	A	574	GLN
1	B	85	MET
1	B	335	ASN
1	B	401	CYS
1	B	450	TRP
1	B	492	LYS
1	B	516	THR
1	B	555	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	ASN
1	A	381	ASN
1	A	414	GLN
1	A	529	GLN
1	A	557	HIS
1	B	29	GLN
1	B	229	ASN
1	B	262	ASN
1	B	335	ASN
1	B	391	ASN
1	B	574	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	601	-	5,5,5	0.46	0	5,5,5	0.25	0
2	GOL	A	602	-	5,5,5	0.29	0	5,5,5	0.25	0
2	GOL	B	601	-	5,5,5	0.40	0	5,5,5	0.87	0
3	SO4	B	602	-	4,4,4	0.24	0	6,6,6	0.26	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	601	-	-	0/4/4/4	0/0/0/0
2	GOL	A	602	-	-	0/4/4/4	0/0/0/0
2	GOL	B	601	-	-	0/4/4/4	0/0/0/0
3	SO4	B	602	-	-	0/0/0/0	0/0/0/0

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.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	GOL	1	0
2	A	602	GOL	1	0
2	B	601	GOL	7	0
3	B	602	SO4	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	546/572 (95%)	0.44	48 (8%) 11 14	13, 38, 81, 125	0
1	B	535/572 (93%)	0.71	79 (14%) 3 4	18, 46, 109, 134	0
All	All	1081/1144 (94%)	0.57	127 (11%) 5 6	13, 42, 94, 134	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	490	PHE	8.5
1	A	563	GLY	7.2
1	A	523	LEU	6.2
1	B	471	GLY	6.1
1	B	461	ILE	5.8
1	B	563	GLY	5.7
1	B	519	SER	5.6
1	B	516	THR	5.5
1	A	419	GLN	5.2
1	A	561	ASP	5.1
1	B	562	ASN	5.1
1	B	564	SER	5.1
1	B	538	ILE	5.0
1	B	535	PHE	4.7
1	B	458	THR	4.7
1	B	495	VAL	4.6
1	A	456	LYS	4.6
1	B	501	VAL	4.5
1	B	533	ALA	4.4
1	B	534	VAL	4.3
1	B	521	PHE	4.3
1	B	440	ALA	4.3
1	B	453	LEU	4.2
1	B	485	VAL	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	523	LEU	4.2
1	B	457	GLY	4.2
1	A	421	VAL	4.0
1	B	560	SER	4.0
1	B	462	ALA	3.9
1	B	496	ASN	3.8
1	A	146	ASN	3.7
1	A	227	GLY	3.7
1	B	517	SER	3.7
1	B	460	TRP	3.7
1	A	530	HIS	3.6
1	B	146	ASN	3.6
1	B	497	PRO	3.5
1	A	489	LEU	3.5
1	B	450	TRP	3.5
1	B	145	LYS	3.4
1	B	565	VAL	3.4
1	A	27	SER	3.3
1	B	392	GLY	3.3
1	B	500	THR	3.3
1	A	145	LYS	3.2
1	B	489	LEU	3.2
1	B	456	LYS	3.2
1	B	518	ASP	3.2
1	A	493	GLY	3.2
1	B	441	GLY	3.1
1	A	517	SER	3.1
1	A	560	SER	3.1
1	B	261	ARG	3.1
1	A	529	GLN	3.1
1	B	540	VAL	3.1
1	B	228	ASP	3.1
1	B	502	ASP	3.1
1	B	443	ASN	3.1
1	B	420	GLN	3.0
1	A	226	LEU	3.0
1	B	227	GLY	3.0
1	B	498	VAL	2.9
1	A	392	GLY	2.9
1	A	335	ASN	2.9
1	B	494	GLY	2.8
1	A	34	LYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	354	PHE	2.8
1	A	518	ASP	2.8
1	B	515	LYS	2.8
1	B	561	ASP	2.8
1	B	520	GLY	2.7
1	B	393	LYS	2.7
1	A	562	ASN	2.7
1	B	532	ASN	2.7
1	B	511	ILE	2.7
1	B	144	ASN	2.7
1	A	521	PHE	2.6
1	B	480	PHE	2.6
1	B	493	GLY	2.6
1	B	473	ARG	2.6
1	B	34	LYS	2.6
1	A	420	GLN	2.6
1	B	499	PHE	2.6
1	B	463	GLU	2.6
1	A	336	GLY	2.6
1	B	491	ASP	2.5
1	B	537	ASP	2.5
1	A	454	VAL	2.5
1	B	335	ASN	2.5
1	A	352	THR	2.5
1	A	452	ALA	2.5
1	A	440	ALA	2.4
1	A	490	PHE	2.4
1	A	418	LYS	2.4
1	B	421	VAL	2.4
1	B	505	ILE	2.4
1	B	475	GLU	2.3
1	B	446	TYR	2.3
1	A	470	SER	2.3
1	B	226	LEU	2.3
1	A	351	LEU	2.2
1	A	380	VAL	2.2
1	A	497	PRO	2.2
1	A	453	LEU	2.2
1	B	478	VAL	2.2
1	B	482	ASP	2.2
1	A	540	VAL	2.1
1	B	262	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	33	THR	2.1
1	B	455	SER	2.1
1	B	558	HIS	2.1
1	A	460	TRP	2.1
1	A	498	VAL	2.1
1	B	570	GLY	2.1
1	A	519	SER	2.1
1	A	535	PHE	2.1
1	A	415	LYS	2.1
1	B	350	ASP	2.1
1	A	459	ASN	2.1
1	A	495	VAL	2.1
1	A	558	HIS	2.1
1	A	417	GLY	2.1
1	B	258	TYR	2.0
1	B	472	TYR	2.0
1	B	536	SER	2.0
1	B	148	VAL	2.0
1	A	261	ARG	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(Å ²)	Q<0.9
2	GOL	A	601	6/6	0.84	0.26	5.89	38,47,50,50	0
2	GOL	B	601	6/6	0.84	0.24	5.15	45,46,59,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SO4	B	602	5/5	0.72	0.32	3.58	94,96,129,180	0
2	GOL	A	602	6/6	0.85	0.28	-	57,60,63,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.