



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 09:31 pm BST

PDB ID : 3FXU
Title : Crystal structure of TsaR in complex with its effector p-toluenesulfonate
Authors : Monferrer, D.; Tralau, T.; Kertesz, M.A.; Kikhney, A.; Svergun, D.; Uson, I.
Deposited on : 2009-01-21
Resolution : 1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

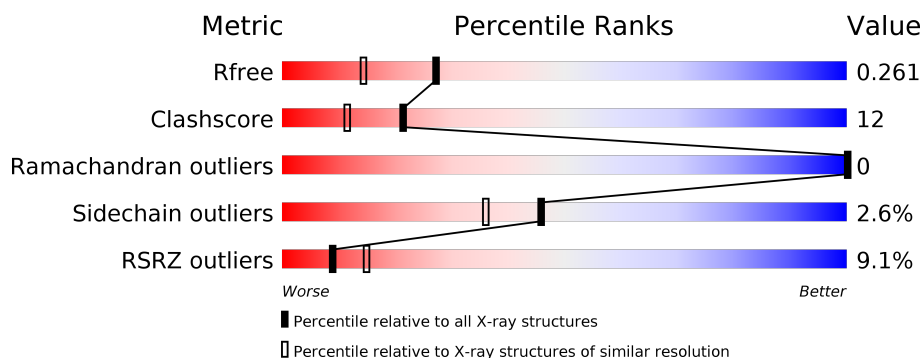
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 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	305	<div> <div>9%</div> <div>83%</div> <div>13%</div> <div>••</div> </div>
1	B	305	<div> <div>8%</div> <div>79%</div> <div>8%</div> <div>• 12%</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	TSU	A	1003	-	-	X	-
2	TSU	A	1006	-	-	X	-
2	TSU	B	1007	-	-	X	-
2	TSU	B	1010	-	-	-	X
2	TSU	B	1011	-	-	X	-
4	GOL	A	3002	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4748 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.

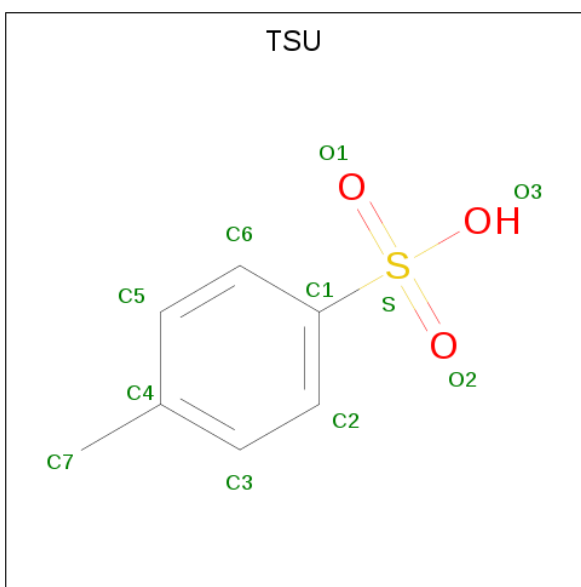
- Molecule 1 is a protein called LysR type regulator of tsaMBCD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	2	0
			2300	1466	414	410	10			
1	B	267	Total	C	N	O	S	0	2	0
			2085	1331	374	371	9			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	LEU	-	SEE REMARK 999	UNP P94678
A	300	HIS	-	EXPRESSION TAG	UNP P94678
A	301	HIS	-	EXPRESSION TAG	UNP P94678
A	302	HIS	-	EXPRESSION TAG	UNP P94678
A	303	HIS	-	EXPRESSION TAG	UNP P94678
A	304	HIS	-	EXPRESSION TAG	UNP P94678
A	305	HIS	-	EXPRESSION TAG	UNP P94678
B	2	LEU	-	SEE REMARK 999	UNP P94678
B	300	HIS	-	EXPRESSION TAG	UNP P94678
B	301	HIS	-	EXPRESSION TAG	UNP P94678
B	302	HIS	-	EXPRESSION TAG	UNP P94678
B	303	HIS	-	EXPRESSION TAG	UNP P94678
B	304	HIS	-	EXPRESSION TAG	UNP P94678
B	305	HIS	-	EXPRESSION TAG	UNP P94678

- Molecule 2 is PARA-TOLUENE SULFONATE (three-letter code: TSU) (formula: C₇H₈O₃S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			11	7	3	1		
2	A	1	Total	C	O	S	0	0
			11	7	3	1		
2	A	1	Total	C	O	S	0	0
			11	7	3	1		
2	A	1	Total	C	O	S	0	0
			11	7	3	1		
2	A	1	Total	C	O	S	0	0
			11	7	3	1		
2	B	1	Total	C	O	S	0	0
			11	7	3	1		
2	B	1	Total	C	O	S	0	0
			11	7	3	1		
2	B	1	Total	C	O	S	0	0
			11	7	3	1		
2	B	1	Total	C	O	S	0	0
			11	7	3	1		

- Molecule 3 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			5	3	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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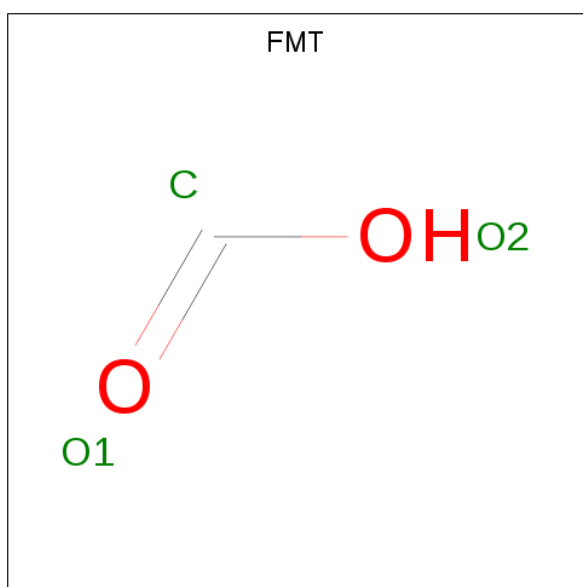
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Cl	0	0
			2	2		
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



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

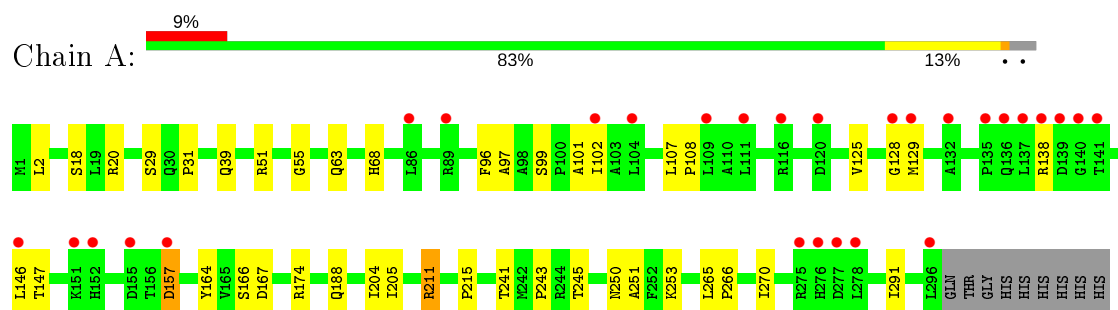
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	100	Total	O	0	0
			100	100		
7	B	107	Total	O	0	0
			107	107		

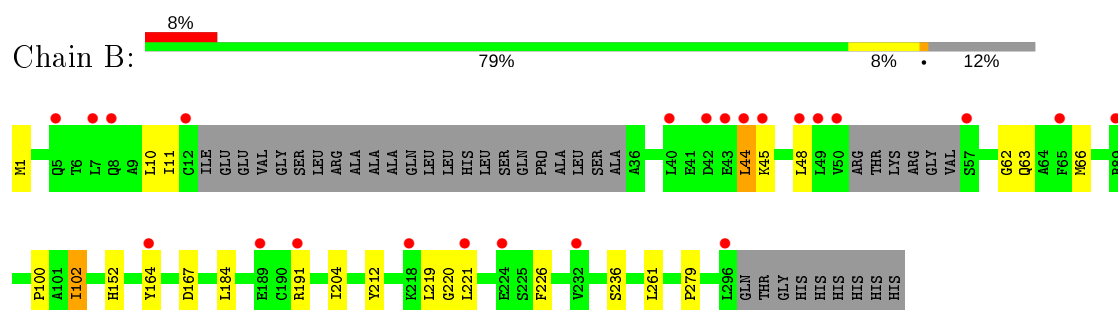
3 Residue-property plots [i](#)

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



- Molecule 1: LysR type regulator of tsaMBCD



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	135.22Å 52.11Å 109.28Å 90.00° 111.51° 90.00°	Depositor
Resolution (Å)	19.75 – 1.95 19.75 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.75-1.95) 99.9 (19.75-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.5.0046	Depositor
R, R_{free}	0.223 , 0.258 0.225 , 0.261	Depositor DCC
R_{free} test set	2644 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 58.6	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	0.93	EDS
Total number of atoms	4748	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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, FMT, TSU, IMD, CL

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	0.50	0/2359	0.61	0/3212
1	B	0.52	0/2143	0.64	0/2917
All	All	0.51	0/4502	0.62	0/6129

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

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	2300	0	2347	64	0
1	B	2085	0	2110	45	0
2	A	66	0	47	28	0
2	B	55	0	40	34	0
3	A	5	0	5	2	0
4	A	18	0	24	7	0
4	B	6	0	8	0	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
6	B	3	0	1	0	0
7	A	100	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	107	0	0	2	0
All	All	4748	0	4582	110	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 12.

The worst 5 of 110 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:164[B]:TYR:CE2	2:B:1007:TSU:H73	1.15	1.60
1:B:164[B]:TYR:CZ	2:B:1007:TSU:C7	1.82	1.57
1:A:166:SER:HB2	2:A:1006:TSU:C3	1.43	1.47
1:B:164[B]:TYR:CE2	2:B:1007:TSU:C7	1.97	1.37
1:B:164[B]:TYR:CZ	2:B:1007:TSU:C4	2.08	1.36

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	Percentiles	
1	A	296/305 (97%)	292 (99%)	4 (1%)	0	100	100
1	B	263/305 (86%)	261 (99%)	2 (1%)	0	100	100
All	All	559/610 (92%)	553 (99%)	6 (1%)	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	242/248 (98%)	236 (98%)	6 (2%)	47	38
1	B	220/248 (89%)	214 (97%)	6 (3%)	44	34
All	All	462/496 (93%)	450 (97%)	12 (3%)	46	36

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	ARG
1	B	10	LEU
1	B	102	ILE
1	A	174	ARG
1	B	45	LYS

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

Mol	Chain	Res	Type
1	A	188	GLN
1	B	207	ASN

5.3.3 RNA [i](#)

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](#)

Of 20 ligands modelled in this entry, 3 are monoatomic - leaving 17 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	GOL	A	3003	-	5,5,5	0.36	0	5,5,5	0.09	0
2	TSU	B	1005	-	11,11,11	2.45	1 (9%)	16,16,16	0.79	0
2	TSU	B	1009	-	11,11,11	2.47	1 (9%)	16,16,16	0.77	0
2	TSU	A	1002	-	11,11,11	2.44	1 (9%)	16,16,16	0.94	1 (6%)
2	TSU	A	1006	-	11,11,11	3.02	2 (18%)	16,16,16	1.74	2 (12%)
2	TSU	B	1010	-	11,11,11	2.49	1 (9%)	16,16,16	0.96	1 (6%)
2	TSU	A	1008	-	11,11,11	2.47	1 (9%)	16,16,16	0.97	1 (6%)
6	FMT	B	4001	-	0,2,2	0.00	-	0,1,1	0.00	-
4	GOL	A	3001	-	5,5,5	0.69	0	5,5,5	0.56	0
2	TSU	B	1007	-	11,11,11	2.34	1 (9%)	16,16,16	0.86	0
2	TSU	A	1003	-	11,11,11	2.46	1 (9%)	16,16,16	0.85	0
4	GOL	A	3002	-	5,5,5	0.35	0	5,5,5	0.61	0
2	TSU	B	1011	-	11,11,11	2.56	1 (9%)	16,16,16	0.70	0
3	IMD	A	2001	-	3,5,5	0.38	0	4,5,5	0.56	0
2	TSU	A	1004	-	11,11,11	2.59	1 (9%)	16,16,16	0.82	0
4	GOL	B	3004	-	5,5,5	0.41	0	5,5,5	0.19	0
2	TSU	A	1001	-	11,11,11	2.19	1 (9%)	16,16,16	1.17	2 (12%)

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
4	GOL	A	3003	-	-	2/4/4/4	-
2	TSU	B	1005	-	-	0/6/6/6	0/1/1/1
2	TSU	B	1009	-	-	0/6/6/6	0/1/1/1
2	TSU	A	1002	-	-	0/6/6/6	0/1/1/1
2	TSU	A	1006	-	-	0/6/6/6	0/1/1/1
2	TSU	B	1010	-	-	0/6/6/6	0/1/1/1
2	TSU	A	1008	-	-	0/6/6/6	0/1/1/1
4	GOL	A	3001	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TSU	B	1007	-	-	0/6/6/6	0/1/1/1
2	TSU	A	1003	-	-	0/6/6/6	0/1/1/1
4	GOL	A	3002	-	-	4/4/4/4	-
2	TSU	B	1011	-	-	0/6/6/6	0/1/1/1
3	IMD	A	2001	-	-	-	0/1/1/1
2	TSU	A	1004	-	-	0/6/6/6	0/1/1/1
4	GOL	B	3004	-	-	2/4/4/4	-
2	TSU	A	1001	-	-	0/6/6/6	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1006	TSU	C1-S	-9.38	1.57	1.77
2	A	1004	TSU	C1-S	-8.44	1.59	1.77
2	B	1011	TSU	C1-S	-8.32	1.59	1.77
2	B	1010	TSU	C1-S	-8.10	1.60	1.77
2	A	1008	TSU	C1-S	-8.02	1.60	1.77

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1006	TSU	C6-C1-S	4.25	125.57	119.79
2	A	1006	TSU	C2-C1-S	-4.11	114.21	119.79
2	B	1010	TSU	O1-S-C1	2.43	112.23	106.65
2	A	1001	TSU	O2-S-C1	2.32	111.97	106.65
2	A	1002	TSU	O2-S-C1	2.27	111.86	106.65

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3002	GOL	O1-C1-C2-C3
4	A	3002	GOL	C1-C2-C3-O3
4	A	3001	GOL	O1-C1-C2-C3
4	A	3001	GOL	C1-C2-C3-O3
4	B	3004	GOL	C1-C2-C3-O3

There are no ring outliers.

10 monomers are involved in 71 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1005	TSU	2	0
2	A	1006	TSU	24	0
2	B	1010	TSU	3	0
4	A	3001	GOL	3	0
2	B	1007	TSU	21	0
2	A	1003	TSU	4	0
4	A	3002	GOL	4	0
2	B	1011	TSU	8	0
3	A	2001	IMD	2	0
2	A	1004	TSU	2	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	296/305 (97%)	0.51	28 (9%) 8 13	9, 18, 32, 40	7 (2%)
1	B	267/305 (87%)	0.36	23 (8%) 10 16	5, 17, 37, 46	6 (2%)
All	All	563/610 (92%)	0.44	51 (9%) 9 15	5, 18, 36, 46	13 (2%)

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	50	VAL	5.6
1	A	157	ASP	5.5
1	A	278	LEU	4.9
1	A	152	HIS	4.7
1	A	276	HIS	4.7

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. 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(\AA^2)	Q<0.9
3	IMD	A	2001	5/5	0.53	0.22	46,46,47,48	0
4	GOL	A	3001	6/6	0.60	0.24	31,34,35,36	0
2	TSU	A	1006	11/11	0.70	0.34	21,24,28,30	11
4	GOL	A	3003	6/6	0.74	0.14	45,47,47,49	0
5	CL	B	5003	1/1	0.76	0.09	62,62,62,62	0
2	TSU	B	1010	11/11	0.77	0.41	52,53,55,56	7
2	TSU	A	1008	11/11	0.77	0.28	29,31,33,34	11
4	GOL	B	3004	6/6	0.77	0.18	55,56,57,57	0
2	TSU	B	1007	11/11	0.82	0.30	29,31,32,32	11
2	TSU	B	1011	11/11	0.83	0.26	39,41,41,41	11
2	TSU	A	1002	11/11	0.85	0.15	40,41,41,42	4
2	TSU	A	1004	11/11	0.87	0.36	28,28,29,30	11
5	CL	A	5002	1/1	0.87	0.10	60,60,60,60	0
4	GOL	A	3002	6/6	0.88	0.15	32,33,35,35	0
5	CL	B	5001	1/1	0.90	0.10	46,46,46,46	0
6	FMT	B	4001	3/3	0.91	0.10	43,43,44,44	0
2	TSU	B	1009	11/11	0.94	0.15	31,32,34,34	0
2	TSU	A	1001	11/11	0.94	0.12	27,29,33,35	0
2	TSU	B	1005	11/11	0.95	0.12	42,45,47,48	0
2	TSU	A	1003	11/11	0.96	0.15	40,44,45,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.