



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:05 PM UTC

PDB ID : 3TY8 / pdb_00003ty8
Title : Crystal Structure of C. Thermocellum PNKP Ligase Domain Apo Form
Authors : Smith, P.; Wang, L.; Shuman, S.
Deposited on : 2011-09-23
Resolution : 2.60 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 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

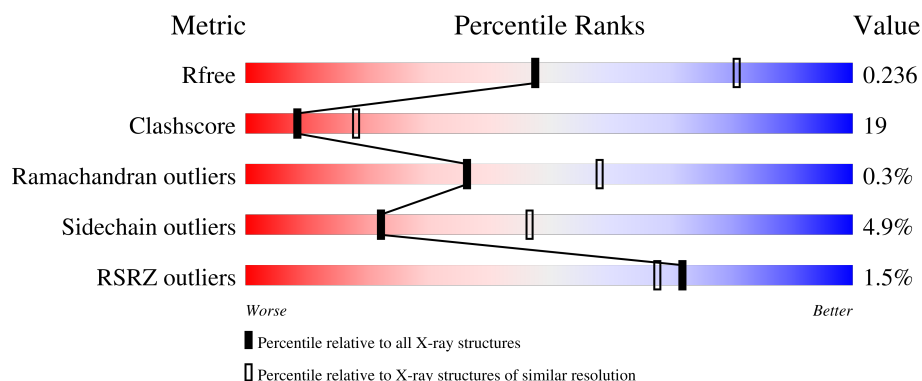
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	413	 65% 24% • 8%
1	B	413	 60% 29% • 8%

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	911	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6236 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 Polynucleotide 2',3'-cyclic phosphate phosphodiesterase / polynucleotide 5'-hydroxyl-kinase / polynucleotide 3'-phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	0	0
			3019	1914	523	559	23			
1	B	379	Total	C	N	O	S	0	5	0
			3064	1943	529	570	22			

There are 42 discrepancies between the modelled and reference sequences:

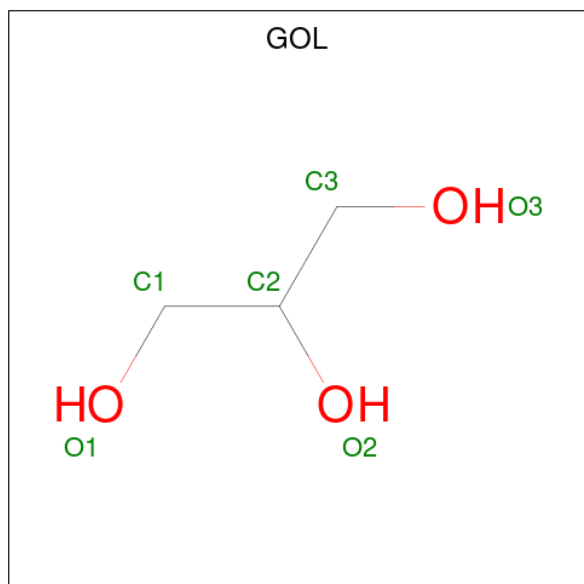
Chain	Residue	Modelled	Actual	Comment	Reference
A	458	MET	-	expression tag	UNP A3DJ38
A	459	GLY	-	expression tag	UNP A3DJ38
A	460	HIS	-	expression tag	UNP A3DJ38
A	461	HIS	-	expression tag	UNP A3DJ38
A	462	HIS	-	expression tag	UNP A3DJ38
A	463	HIS	-	expression tag	UNP A3DJ38
A	464	HIS	-	expression tag	UNP A3DJ38
A	465	HIS	-	expression tag	UNP A3DJ38
A	466	HIS	-	expression tag	UNP A3DJ38
A	467	HIS	-	expression tag	UNP A3DJ38
A	468	HIS	-	expression tag	UNP A3DJ38
A	469	HIS	-	expression tag	UNP A3DJ38
A	470	SER	-	expression tag	UNP A3DJ38
A	471	SER	-	expression tag	UNP A3DJ38
A	472	GLY	-	expression tag	UNP A3DJ38
A	473	HIS	-	expression tag	UNP A3DJ38
A	474	ILE	-	expression tag	UNP A3DJ38
A	475	GLU	-	expression tag	UNP A3DJ38
A	476	GLY	-	expression tag	UNP A3DJ38
A	477	ARG	-	expression tag	UNP A3DJ38
A	478	HIS	-	expression tag	UNP A3DJ38
B	458	MET	-	expression tag	UNP A3DJ38
B	459	GLY	-	expression tag	UNP A3DJ38
B	460	HIS	-	expression tag	UNP A3DJ38

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Chain	Residue	Modelled	Actual	Comment	Reference
B	461	HIS	-	expression tag	UNP A3DJ38
B	462	HIS	-	expression tag	UNP A3DJ38
B	463	HIS	-	expression tag	UNP A3DJ38
B	464	HIS	-	expression tag	UNP A3DJ38
B	465	HIS	-	expression tag	UNP A3DJ38
B	466	HIS	-	expression tag	UNP A3DJ38
B	467	HIS	-	expression tag	UNP A3DJ38
B	468	HIS	-	expression tag	UNP A3DJ38
B	469	HIS	-	expression tag	UNP A3DJ38
B	470	SER	-	expression tag	UNP A3DJ38
B	471	SER	-	expression tag	UNP A3DJ38
B	472	GLY	-	expression tag	UNP A3DJ38
B	473	HIS	-	expression tag	UNP A3DJ38
B	474	ILE	-	expression tag	UNP A3DJ38
B	475	GLU	-	expression tag	UNP A3DJ38
B	476	GLY	-	expression tag	UNP A3DJ38
B	477	ARG	-	expression tag	UNP A3DJ38
B	478	HIS	-	expression tag	UNP A3DJ38

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



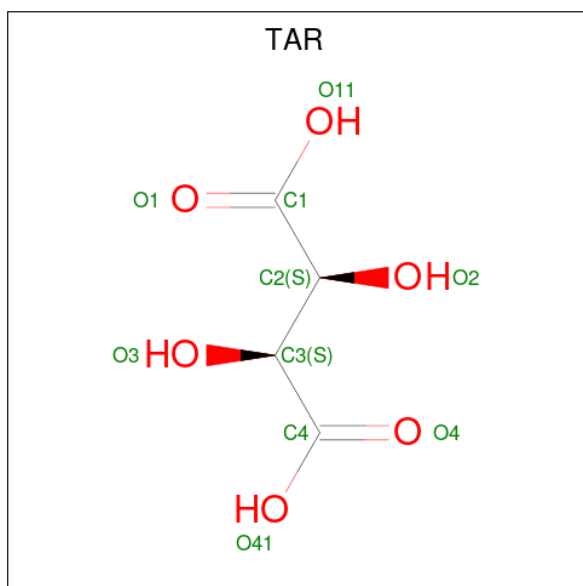
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 3 is D(-)-TARTARIC ACID (CCD ID: TAR) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	4	6		
3	B	1	Total	C	O	0	0
			10	4	6		

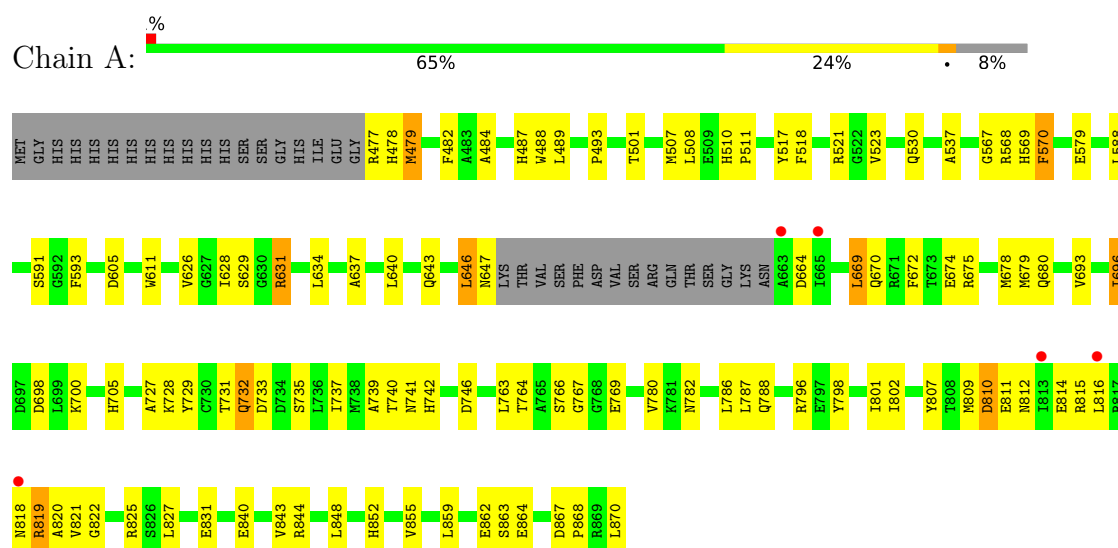
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	73	Total	O	0	0
			73	73		
4	B	42	Total	O	0	0
			42	42		

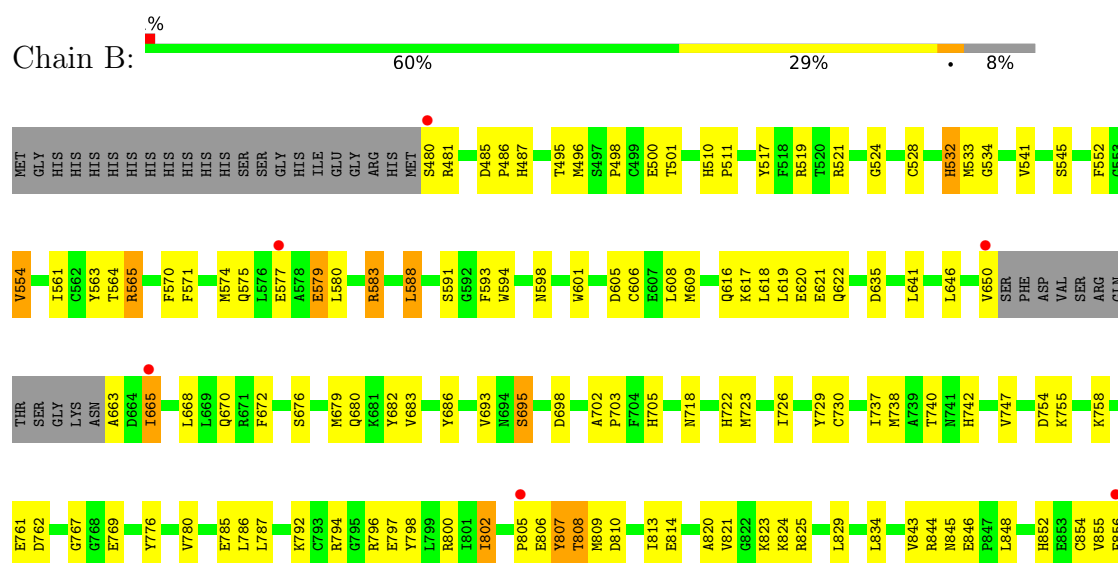
3 Residue-property plots

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: Polynucleotide 2',3'-cyclic phosphate phosphodiesterase / polynucleotide 5'-hydroxyl-kinase / polynucleotide 3'-phosphatase



- Molecule 1: Polynucleotide 2',3'-cyclic phosphate phosphodiesterase / polynucleotide 5'-hydroxyl-kinase / polynucleotide 3'-phosphatase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.14Å 94.16Å 76.03Å 90.00° 95.78° 90.00°	Depositor
Resolution (Å)	37.82 – 2.60 37.82 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.1 (37.82-2.60) 96.0 (37.82-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.195 , 0.241 0.192 , 0.236	Depositor DCC
R_{free} test set	1298 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6236	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, TAR

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	0.38	0/3084	0.78	3/4166 (0.1%)
1	B	0.39	0/3130	0.76	0/4227
All	All	0.38	0/6214	0.77	3/8393 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	810	ASP	N-CA-C	6.06	118.28	108.34
1	A	493	PRO	O-C-N	5.25	123.62	121.15
1	A	802	ILE	N-CA-C	5.13	115.34	110.42

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	A	3019	0	2959	113	0
1	B	3064	0	3008	124	0
2	A	12	0	16	5	0
2	B	6	0	8	0	0
3	A	10	0	4	1	0
3	B	10	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	73	0	0	0	0
4	B	42	0	0	0	0
All	All	6236	0	5999	230	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 19.

The worst 5 of 230 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:A:810:ASP:HA	1:A:812:ASN:H	1.08	1.17
1:A:489:LEU:HD21	1:A:855:VAL:HG11	1.24	1.11
1:B:533[B]:MET:HE3	1:B:769:GLU:HB2	1.36	1.06
1:A:489:LEU:CD2	1:A:855:VAL:HG11	1.87	1.04
1:A:477:ARG:HA	1:A:859:LEU:HD13	1.39	1.03

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	375/413 (91%)	361 (96%)	13 (4%)	1 (0%)	36	58
1	B	380/413 (92%)	364 (96%)	15 (4%)	1 (0%)	36	58
All	All	755/826 (91%)	725 (96%)	28 (4%)	2 (0%)	36	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	808	THR
1	A	732	GLN

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	322/361 (89%)	310 (96%)	12 (4%)	30	57
1	B	329/361 (91%)	308 (94%)	21 (6%)	16	35
All	All	651/722 (90%)	618 (95%)	33 (5%)	22	45

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	762	ASP
1	B	786	LEU
1	B	843	VAL
1	B	500	GLU
1	A	864	GLU

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

Mol	Chain	Res	Type
1	A	532	HIS
1	A	643	GLN
1	A	788	GLN
1	A	845	ASN
1	B	719	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
3	TAR	B	901	-	9,9,9	1.52	0	12,12,12	1.15	2 (16%)
2	GOL	B	903	-	5,5,5	0.41	0	5,5,5	0.21	0
2	GOL	A	910	-	5,5,5	0.34	0	5,5,5	0.30	0
3	TAR	A	912	-	9,9,9	1.61	2 (22%)	12,12,12	1.28	2 (16%)
2	GOL	A	911	-	5,5,5	0.37	0	5,5,5	0.33	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
3	TAR	B	901	-	-	8/12/12/12	-
2	GOL	B	903	-	-	4/4/4/4	-
2	GOL	A	910	-	-	2/4/4/4	-
3	TAR	A	912	-	-	8/12/12/12	-
2	GOL	A	911	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	912	TAR	C3-C4	-2.08	1.49	1.52
3	A	912	TAR	O3-C3	-2.07	1.38	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	912	TAR	O11-C1-C2	2.49	120.23	113.31
3	B	901	TAR	O11-C1-C2	2.31	119.74	113.31
3	B	901	TAR	O41-C4-C3	2.30	119.70	113.31
3	A	912	TAR	O41-C4-C3	2.28	119.64	113.31

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	910	GOL	O1-C1-C2-C3
2	A	911	GOL	O1-C1-C2-O2
2	A	911	GOL	O1-C1-C2-C3
2	B	903	GOL	C1-C2-C3-O3
3	A	912	TAR	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	912	TAR	1	0
2	A	911	GOL	5	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	379/413 (91%)	-0.29	5 (1%) 75 71	27, 48, 108, 142	0
1	B	379/413 (91%)	-0.06	6 (1%) 70 66	25, 60, 107, 162	5 (1%)
All	All	758/826 (91%)	-0.18	11 (1%) 72 68	25, 53, 108, 162	5 (0%)

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	813	ILE	5.5
1	A	816	LEU	4.0
1	B	805	PRO	2.9
1	B	650	VAL	2.8
1	B	665	ILE	2.8

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($\text{\AA}^2$)	Q<0.9
3	TAR	A	912	10/10	0.59	0.11	80,82,85,85	0
2	GOL	A	911	6/6	0.67	0.20	58,60,62,62	0
3	TAR	B	901	10/10	0.74	0.11	80,82,84,84	0
2	GOL	A	910	6/6	0.76	0.13	71,72,72,72	0
2	GOL	B	903	6/6	0.78	0.22	70,74,74,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.