



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2025 – 11:23 am BST

PDB ID : 9SFQ / pdb_00009sfq
Title : Structure at 1.9 Å resolution of Thermus thermophilus tyrosyl-tRNA synthetase bound to wild-type tRNA^{Tyr}(GUC).
Authors : Cusack, S.
Deposited on : 2025-08-20
Resolution : 1.89 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 Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

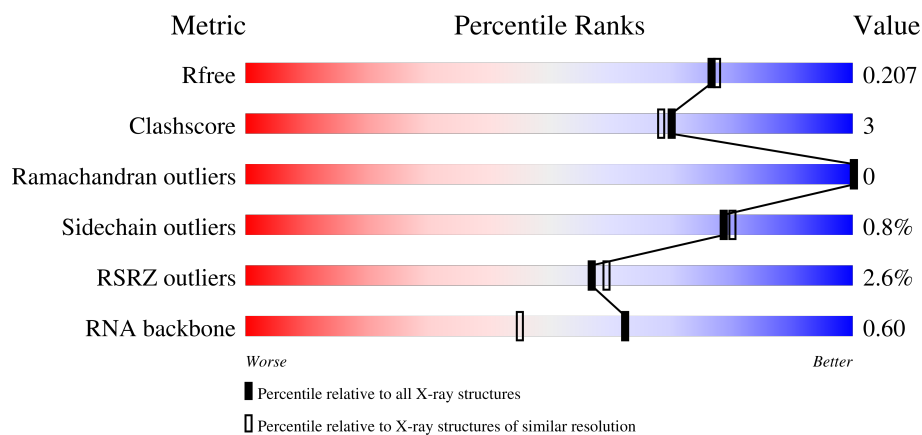
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)
RNA backbone	3690	1046 (2.30-1.50)

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	432	 3% 92% 6%
2	T	86	 2% 74% 23%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PEG	A	507	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10879 atoms, of which 4729 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.

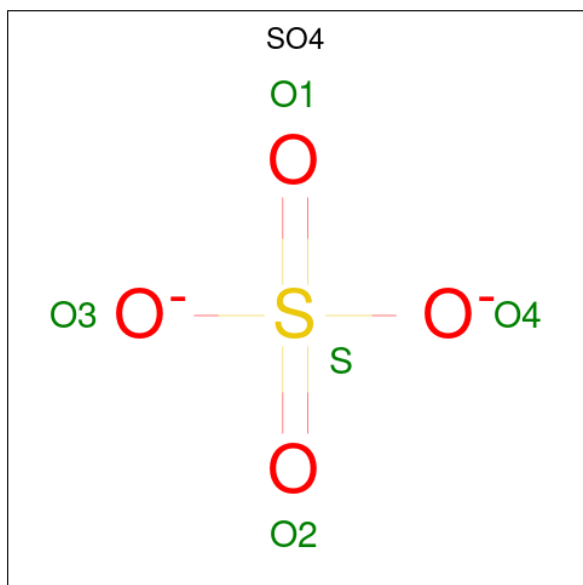
- Molecule 1 is a protein called Tyrosine-tRNA ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	425	7111	2225	3601	633	639	13	0	25	0

- Molecule 2 is a RNA chain called Wild-type, fully modified *Thermus thermophilus* tRNATyr(GUC).

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	T	86	Total	C	H	N	O	P	S	0	4	0
			2858	858	940	341	626	90	3			

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



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

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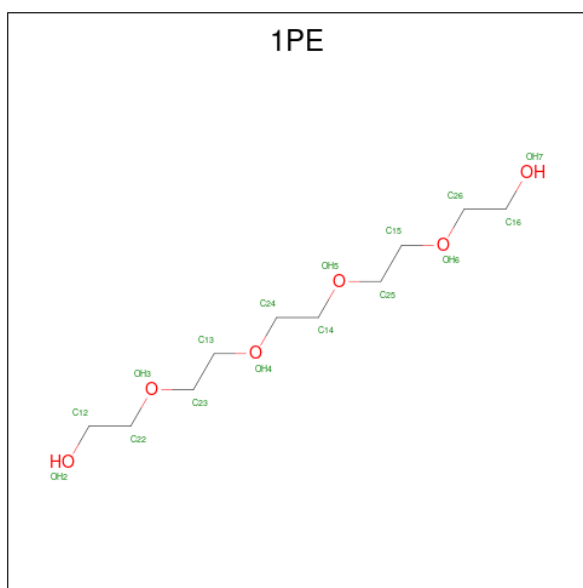
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			17	4	10	3		
4	A	1	Total	C	H	O	0	0
			17	4	10	3		
4	A	1	Total	C	H	O	0	0
			17	4	10	3		
4	A	1	Total	C	H	O	0	0
			17	4	10	3		
4	A	1	Total	C	H	O	0	0
			17	4	10	3		
4	T	1	Total	C	H	O	0	0
			17	4	10	3		
4	T	1	Total	C	H	O	0	0
			17	4	10	3		
4	T	1	Total	C	H	O	0	0
			17	4	10	3		
4	T	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 5 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			38	10	22	6		
5	A	1	Total	C	H	O	0	0
			38	10	22	6		
5	A	1	Total	C	H	O	0	0
			38	10	22	6		
5	T	1	Total	C	H	O	0	0
			38	10	22	6		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	T	2	Total	Mg	0	0
			2	2		

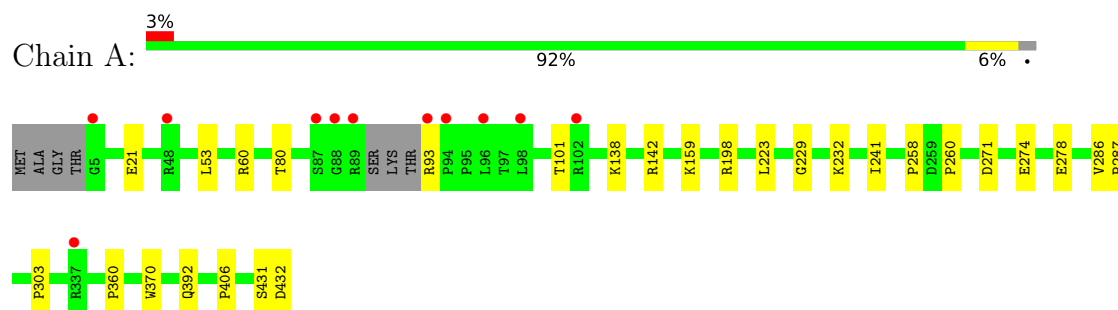
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	357	Total	O	0	0
			357	357		
7	T	214	Total	O	0	0
			214	214		

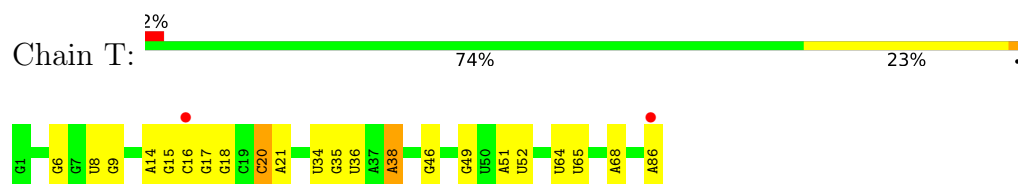
3 Residue-property plots [i](#)

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: Tyrosine-tRNA ligase



- Molecule 2: Wild-type, fully modified *Thermus thermophilus* tRNA^{Tyr}(GUC)



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	124.32Å 67.55Å 111.17Å 90.00° 110.21° 90.00°	Depositor
Resolution (Å)	29.50 – 1.89 29.50 – 1.89	Depositor EDS
% Data completeness (in resolution range)	98.1 (29.50-1.89) 98.1 (29.50-1.89)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419+SVN	Depositor
R, R_{free}	0.173 , 0.209 0.172 , 0.207	Depositor DCC
R_{free} test set	3424 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10879	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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: MIA, OMC, PSU, SO4, 4SU, A1I9V, 1MA, MG, 2MG, PEG, 1PE

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	0.44	0/3677	0.54	0/4964
2	T	0.42	1/1943 (0.1%)	0.54	0/3025
All	All	0.43	1/5620 (0.0%)	0.54	0/7989

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	8	4SU	O3'-P	5.64	1.61	1.56

There are no bond angle outliers.

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	3510	3601	3481	22	0
2	T	1918	940	973	8	0
3	A	15	0	0	0	0
4	A	42	60	60	8	0
4	T	28	40	40	2	0
5	A	48	66	66	2	0
5	T	16	22	22	1	0
6	T	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	357	0	0	4	0
7	T	214	0	0	4	0
All	All	6150	4729	4642	34	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 3.

All (34) 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:60[B]:ARG:HD3	7:A:628:HOH:O	1.99	0.63
1:A:21:GLU:OE1	1:A:198[A]:ARG:NH1	2.34	0.60
1:A:303:PRO:HB2	5:A:509:1PE:H222	1.85	0.59
4:A:507:PEG:H31	7:T:335:HOH:O	2.04	0.57
2:T:20:OMC:CM2	2:T:20:OMC:O3'	2.55	0.53
4:A:507:PEG:H32	2:T:38:MIA:H4'	1.91	0.53
1:A:260:PRO:HG2	4:A:507:PEG:H21	1.91	0.52
1:A:274[A]:GLU:O	1:A:278[A]:GLU:HG2	2.10	0.52
2:T:20:OMC:O3'	2:T:20:OMC:HM22	2.10	0.52
2:T:20:OMC:HM21	7:T:214:HOH:O	2.09	0.51
1:A:229:GLY:O	4:A:507:PEG:H12	2.11	0.50
1:A:21:GLU:CD	1:A:198[A]:ARG:HH12	2.21	0.48
1:A:138:LYS:HE2	1:A:142[B]:ARG:CZ	2.44	0.47
1:A:370:TRP:CE2	5:T:107:1PE:H241	2.50	0.46
4:T:105:PEG:H12	7:T:391:HOH:O	2.17	0.45
1:A:138:LYS:HE2	1:A:142[B]:ARG:NH1	2.32	0.45
1:A:360:PRO:HA	1:A:431:SER:O	2.16	0.45
4:T:105:PEG:H32	7:T:312:HOH:O	2.17	0.45
1:A:60[B]:ARG:HD2	7:A:665:HOH:O	2.16	0.45
1:A:406:PRO:HD3	4:A:511:PEG:H11	1.97	0.45
2:T:34:U:H2'	2:T:35:G:H2'	1.98	0.45
5:A:509:1PE:H221	7:A:878:HOH:O	2.16	0.45
1:A:392:GLN:HG2	4:A:511:PEG:O1	2.17	0.44
1:A:286:VAL:HB	1:A:287:PRO:HD3	1.98	0.44
1:A:223:LEU:HD13	1:A:232:LYS:CE	2.47	0.44
1:A:258:PRO:HB3	4:A:507:PEG:H42	2.01	0.43
2:T:38:MIA:H122	2:T:38:MIA:H153	1.73	0.42
1:A:260:PRO:HD2	4:A:507:PEG:H42	2.00	0.42
1:A:60[B]:ARG:NH2	1:A:271:ASP:CG	2.79	0.41
1:A:80:THR:HG23	7:A:696:HOH:O	2.21	0.41
1:A:53:LEU:HD12	1:A:241:ILE:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:14:A:H2'	2:T:15[B]:G:O4'	2.21	0.41
2:T:16[A]:C:C3'	2:T:17[A]:G:H5'	2.51	0.40

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	445/432 (103%)	442 (99%)	3 (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	382/363 (105%)	378 (99%)	4 (1%)	73	74

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93[A]	ARG
1	A	93[B]	ARG
1	A	101	THR
1	A	432	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	T	79/86 (91%)	8 (10%)	0

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	T	9	G
2	T	18	G
2	T	21	A
2	T	46	G
2	T	49	G
2	T	51	A
2	T	52	U
2	T	86	A

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues 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	1MA	T	68	2	16,25,26	0.94	2 (12%)	18,37,40	0.99	1 (5%)
2	OMC	T	20	2	19,22,23	0.66	0	26,31,34	0.97	1 (3%)
2	PSU	T	36	2	18,21,22	0.93	1 (5%)	22,30,33	1.70	3 (13%)
2	PSU	T	65	2	18,21,22	1.11	1 (5%)	22,30,33	1.41	3 (13%)
2	A1I9V	T	64	2	18,22,23	4.97	1 (5%)	23,32,35	0.84	1 (4%)
2	4SU	T	8	2	18,21,22	0.45	0	26,30,33	1.12	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MIA	T	38	2	24,31,32	2.28	4 (16%)	26,44,47	2.43	8 (30%)
2	2MG	T	6	2	18,26,27	1.37	3 (16%)	16,38,41	1.01	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
2	1MA	T	68	2	-	1/3/25/26	0/3/3/3
2	OMC	T	20	2	-	3/9/27/28	0/2/2/2
2	PSU	T	36	2	-	3/7/25/26	0/2/2/2
2	PSU	T	65	2	-	0/7/25/26	0/2/2/2
2	A1I9V	T	64	2	-	0/7/25/26	0/2/2/2
2	4SU	T	8	2	-	0/7/25/26	0/2/2/2
2	MIA	T	38	2	-	1/11/33/34	0/3/3/3
2	2MG	T	6	2	-	0/5/27/28	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	64	A1I9V	C2-S2	-20.98	1.34	1.67
2	T	38	MIA	C13-C14	7.29	1.53	1.32
2	T	38	MIA	C2-S10	-6.72	1.70	1.75
2	T	65	PSU	C6-C5	3.80	1.39	1.35
2	T	6	2MG	C8-N7	-3.07	1.29	1.35
2	T	36	PSU	C6-C5	2.69	1.38	1.35
2	T	6	2MG	C5-C4	-2.63	1.36	1.43
2	T	38	MIA	C6-N1	2.60	1.36	1.32
2	T	68	1MA	C5-C4	-2.41	1.36	1.43
2	T	38	MIA	C5-C4	2.30	1.47	1.40
2	T	68	1MA	C8-N7	-2.21	1.31	1.35
2	T	6	2MG	C5-C6	-2.20	1.42	1.47

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	38	MIA	C12-C13-C14	-7.30	112.93	127.14
2	T	36	PSU	C4-N3-C2	-4.41	119.98	126.34
2	T	36	PSU	N1-C2-N3	4.40	120.11	115.13
2	T	38	MIA	C15-C14-C13	-4.34	110.10	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	38	MIA	C5-C6-N1	-4.15	117.37	120.81
2	T	8	4SU	C4-N3-C2	-3.99	123.46	127.34
2	T	65	PSU	N1-C2-N3	3.69	119.31	115.13
2	T	38	MIA	C11-S10-C2	3.69	105.02	102.27
2	T	38	MIA	C16-C14-C13	-3.42	112.78	122.65
2	T	65	PSU	C4-N3-C2	-3.40	121.44	126.34
2	T	38	MIA	C2-N3-C4	3.36	119.95	115.32
2	T	38	MIA	C4-C5-N7	-3.15	106.12	109.40
2	T	20	OMC	CM2-O2'-C2'	2.58	121.30	114.52
2	T	6	2MG	O6-C6-C5	2.50	129.26	124.37
2	T	64	A1I9V	C5M-C5-C4	2.38	121.39	118.77
2	T	38	MIA	C2-N1-C6	2.35	121.39	117.19
2	T	8	4SU	N3-C2-N1	2.27	117.90	114.89
2	T	6	2MG	C5-C6-N1	-2.10	110.25	113.95
2	T	8	4SU	C5-C4-N3	2.08	116.62	114.69
2	T	36	PSU	C6-C5-C4	2.06	119.64	118.20
2	T	68	1MA	N1-C6-N6	2.03	124.94	119.77
2	T	65	PSU	C6-N1-C2	-2.03	120.61	122.68

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	20	OMC	C3'-C2'-O2'-CM2
2	T	36	PSU	C2'-C1'-C5-C4
2	T	38	MIA	C12-C13-C14-C15
2	T	20	OMC	O4'-C4'-C5'-O5'
2	T	20	OMC	C3'-C4'-C5'-O5'
2	T	36	PSU	O4'-C1'-C5-C4
2	T	36	PSU	O4'-C1'-C5-C6
2	T	68	1MA	C4'-C5'-O5'-P

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	20	OMC	3	0
2	T	38	MIA	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 2 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	PEG	A	505	-	6,6,6	0.23	0	5,5,5	0.66	0
5	1PE	A	509	-	15,15,15	0.29	0	14,14,14	0.32	0
4	PEG	A	506	-	6,6,6	0.28	0	5,5,5	0.11	0
5	1PE	T	107	-	15,15,15	0.29	0	14,14,14	0.37	0
3	SO4	A	502	-	4,4,4	0.77	0	6,6,6	0.43	0
4	PEG	T	106	-	6,6,6	0.27	0	5,5,5	0.41	0
5	1PE	A	508	-	15,15,15	0.41	0	14,14,14	0.80	0
3	SO4	A	501	-	4,4,4	0.64	0	6,6,6	0.28	0
4	PEG	T	103	-	6,6,6	0.23	0	5,5,5	0.36	0
4	PEG	A	511	-	6,6,6	0.26	0	5,5,5	0.21	0
4	PEG	T	105	-	6,6,6	0.35	0	5,5,5	0.53	0
4	PEG	A	504	-	6,6,6	0.23	0	5,5,5	0.20	0
4	PEG	A	512	-	6,6,6	0.29	0	5,5,5	0.27	0
5	1PE	A	510	-	15,15,15	0.35	0	14,14,14	0.53	0
3	SO4	A	503	-	4,4,4	0.68	0	6,6,6	0.21	0
4	PEG	A	507	-	6,6,6	0.28	0	5,5,5	0.47	0
4	PEG	T	104	-	6,6,6	0.23	0	5,5,5	1.20	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
4	PEG	A	505	-	-	3/4/4/4	-
5	1PE	A	509	-	-	6/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	A	506	-	-	0/4/4/4	-
5	1PE	T	107	-	-	4/13/13/13	-
4	PEG	T	106	-	-	2/4/4/4	-
5	1PE	A	508	-	-	6/13/13/13	-
4	PEG	T	103	-	-	2/4/4/4	-
4	PEG	A	511	-	-	4/4/4/4	-
4	PEG	T	105	-	-	2/4/4/4	-
5	1PE	A	510	-	-	6/13/13/13	-
4	PEG	A	512	-	-	3/4/4/4	-
4	PEG	A	504	-	-	4/4/4/4	-
4	PEG	A	507	-	-	2/4/4/4	-
4	PEG	T	104	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	508	1PE	C14-C24-OH4-C13
5	A	510	1PE	OH5-C14-C24-OH4
4	T	104	PEG	C4-C3-O2-C2
4	A	505	PEG	O2-C3-C4-O4
4	A	507	PEG	O1-C1-C2-O2
5	A	510	1PE	OH6-C15-C25-OH5
5	T	107	1PE	OH6-C15-C25-OH5
5	A	508	1PE	OH6-C15-C25-OH5
4	T	103	PEG	O2-C3-C4-O4
4	T	106	PEG	O1-C1-C2-O2
4	T	106	PEG	O2-C3-C4-O4
5	A	509	1PE	OH7-C16-C26-OH6
5	A	510	1PE	OH4-C13-C23-OH3
5	T	107	1PE	OH5-C14-C24-OH4
4	A	507	PEG	O2-C3-C4-O4
4	A	505	PEG	O1-C1-C2-O2
4	A	512	PEG	O1-C1-C2-O2
5	A	508	1PE	OH4-C13-C23-OH3
4	T	104	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
4	A	504	PEG	O1-C1-C2-O2
4	T	104	PEG	O1-C1-C2-O2
5	A	509	1PE	OH2-C12-C22-OH3
4	A	511	PEG	O2-C3-C4-O4
5	T	107	1PE	OH7-C16-C26-OH6
5	A	510	1PE	C15-C25-OH5-C14
5	A	509	1PE	C14-C24-OH4-C13
4	T	105	PEG	C1-C2-O2-C3
5	A	508	1PE	C13-C23-OH3-C22
4	A	511	PEG	C4-C3-O2-C2
4	T	104	PEG	C1-C2-O2-C3
4	A	505	PEG	C1-C2-O2-C3
5	A	508	1PE	C23-C13-OH4-C24
5	A	509	1PE	C24-C14-OH5-C25
4	A	512	PEG	C4-C3-O2-C2
4	A	511	PEG	C1-C2-O2-C3
5	A	509	1PE	OH6-C15-C25-OH5
4	A	504	PEG	C1-C2-O2-C3
4	T	103	PEG	C1-C2-O2-C3
5	A	510	1PE	C14-C24-OH4-C13
5	T	107	1PE	C12-C22-OH3-C23
4	A	511	PEG	O1-C1-C2-O2
5	A	510	1PE	C23-C13-OH4-C24
5	A	509	1PE	C25-C15-OH6-C26
4	A	504	PEG	O2-C3-C4-O4
4	T	105	PEG	O2-C3-C4-O4
4	A	512	PEG	O2-C3-C4-O4
4	A	504	PEG	C4-C3-O2-C2
5	A	508	1PE	C25-C15-OH6-C26

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	509	1PE	2	0
5	T	107	1PE	1	0
4	A	511	PEG	2	0
4	T	105	PEG	2	0
4	A	507	PEG	6	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	425/432 (98%)	-0.30	11 (2%) 57 59	7, 24, 55, 82	13 (3%)
2	T	78/86 (90%)	-0.11	2 (2%) 57 59	10, 36, 55, 91	4 (5%)
All	All	503/518 (97%)	-0.27	13 (2%) 57 59	7, 27, 55, 91	17 (3%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	93[A]	ARG	5.6
2	T	16[A]	C	4.4
1	A	94	PRO	4.1
2	T	86	A	3.6
1	A	89	ARG	3.5
1	A	98	LEU	3.3
1	A	102[A]	ARG	2.8
1	A	88	GLY	2.7
1	A	48	ARG	2.7
1	A	5	GLY	2.5
1	A	96	LEU	2.3
1	A	337	ARG	2.1
1	A	87	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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	OMC	T	20	21/22	0.90	0.12	35,45,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	A1I9V	T	64	21/22	0.92	0.11	32,39,47,48	0
2	PSU	T	65	20/21	0.92	0.10	34,43,52,63	0
2	2MG	T	6	24/25	0.94	0.08	20,26,32,34	0
2	MIA	T	38	29/30	0.95	0.10	22,29,39,50	0
2	1MA	T	68	23/24	0.96	0.08	29,34,42,42	0
2	4SU	T	8	20/21	0.98	0.06	23,28,32,33	0
2	PSU	T	36	20/21	0.98	0.05	18,23,31,32	0

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(\AA^2)	Q<0.9
4	PEG	T	105	7/7	0.64	0.23	34,47,67,67	0
4	PEG	A	512	7/7	0.73	0.16	46,56,64,64	0
3	SO4	A	503	5/5	0.77	0.14	49,56,76,78	0
4	PEG	A	511	7/7	0.78	0.14	43,52,61,64	0
4	PEG	T	106	7/7	0.80	0.16	35,47,58,58	0
5	1PE	A	508	16/16	0.80	0.14	32,43,56,60	0
4	PEG	A	504	7/7	0.83	0.14	44,54,65,73	0
4	PEG	A	506	7/7	0.85	0.13	33,42,59,61	0
3	SO4	A	502	5/5	0.86	0.13	38,39,57,73	0
4	PEG	T	103	7/7	0.87	0.12	41,50,60,60	0
3	SO4	A	501	5/5	0.87	0.12	33,53,69,69	0
5	1PE	A	509	16/16	0.87	0.13	34,46,56,56	0
4	PEG	A	507	7/7	0.88	0.10	32,40,47,47	0
5	1PE	T	107	16/16	0.89	0.10	46,55,69,73	0
5	1PE	A	510	16/16	0.90	0.12	25,50,75,76	0
4	PEG	T	104	7/7	0.90	0.11	25,31,43,44	0
4	PEG	A	505	7/7	0.93	0.08	20,28,38,38	0
6	MG	T	102	1/1	0.96	0.18	30,30,30,30	0
6	MG	T	101	1/1	0.99	0.06	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.