



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2025 – 03:32 pm GMT

PDB ID : 9SDF / pdb_00009sdf
Title : Structure at 1.9 Å resolution of Thermus thermophilus tyrosyl-tRNA synthetase bound to wild-type modified tRNA(Tyr), tyrosine and AMP
Authors : Cusack, S.
Deposited on : 2025-08-13
Resolution : 1.90 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 Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

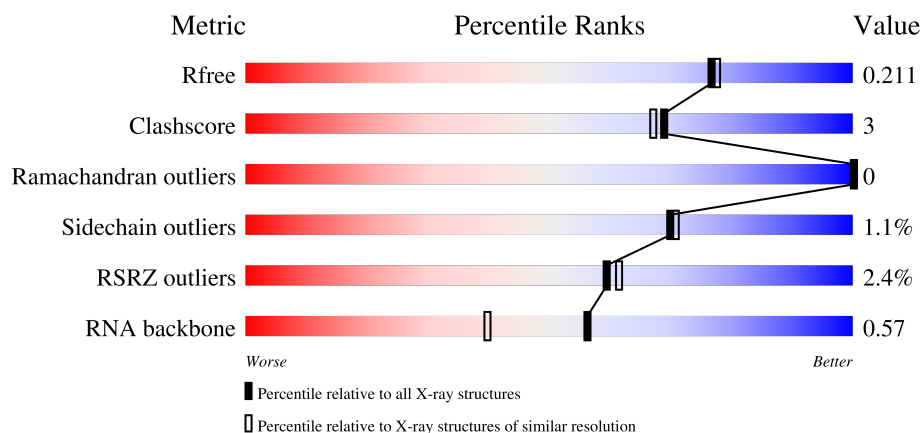
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	<div> <div>3%</div> <div>91%</div> <div>8%</div> </div>
2	T	86	<div> <div>%</div> <div>74%</div> <div>21%</div> <div>5%</div> </div>

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 10714 atoms, of which 4685 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.

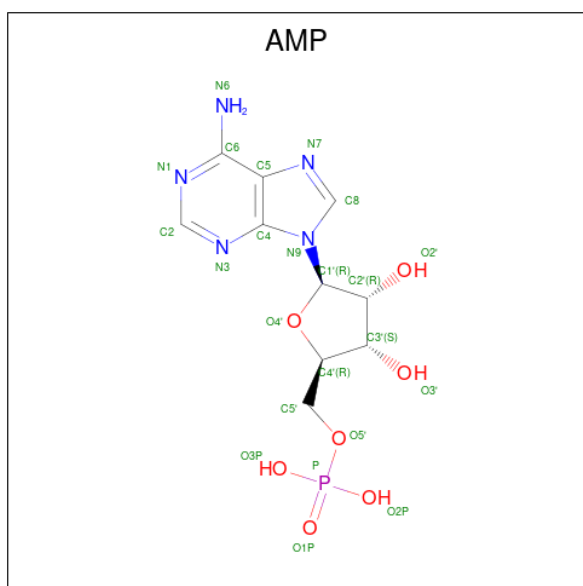
- Molecule 1 is a protein called Tyrosine-tRNA ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	428	Total	C	H	N	O	S	0	28	0
			7159	2238	3626	634	646	15			

- Molecule 2 is a RNA chain called Thermus thermophilus tRNA(Tyr)(GUA) (86-MER).

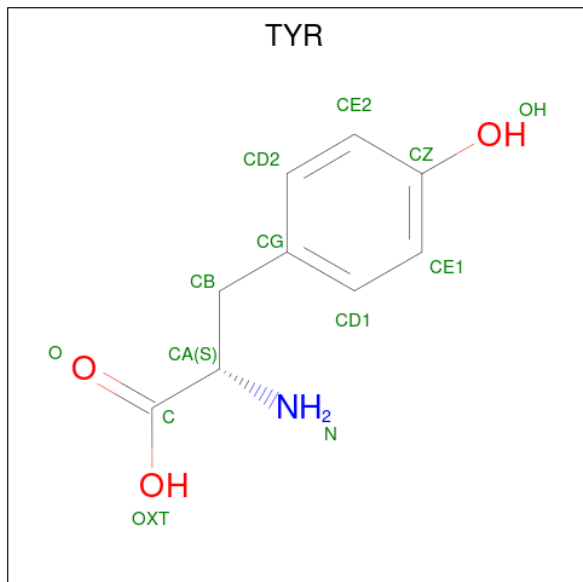
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	T	86	Total	C	H	N	O	P	S	0	1	0
			2709	819	876	324	600	87	3			

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



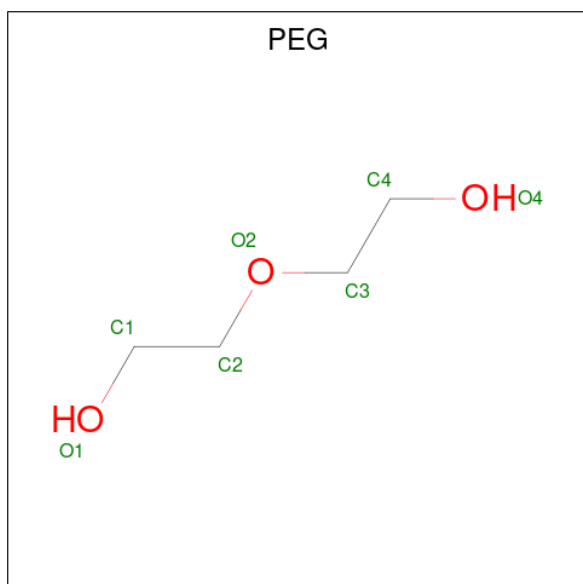
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			35	10	12	5	7	1		

- Molecule 4 is TYROSINE (CCD ID: TYR) (formula: $C_9H_{11}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			21	9	8	1	3		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

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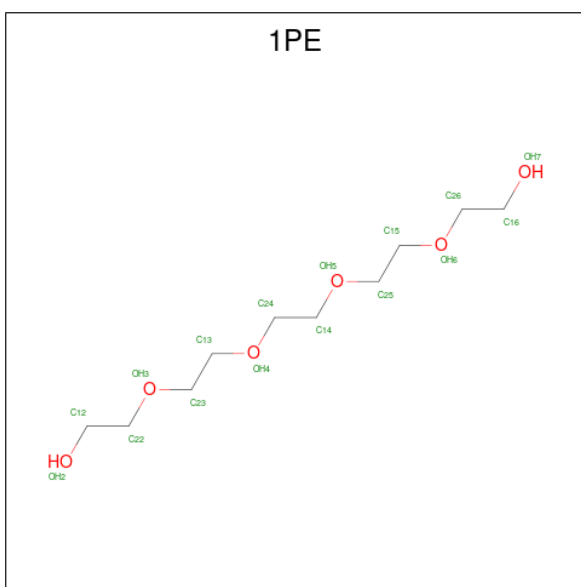
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	T	1	Total	C	H	O	0	0
			17	4	10	3		
5	T	1	Total	C	H	O	0	0
			17	4	10	3		
5	T	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



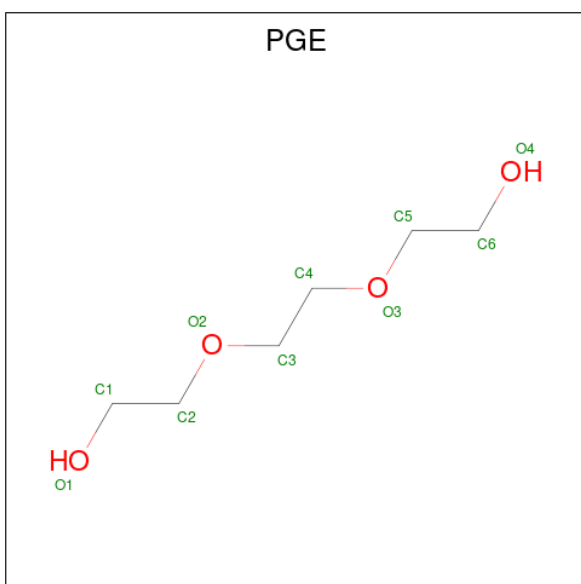
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	T	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			38	10	22	6		
7	A	1	Total	C	H	O	0	0
			38	10	22	6		
7	A	1	Total	C	H	O	0	0
			30	8	17	5		
7	A	1	Total	C	H	O	0	0
			30	8	17	5		
7	T	1	Total	C	H	O	0	0
			38	10	22	6		

- Molecule 8 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			23	6	13	4		

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	T	1	Total	Mg	0	0
			1	1		

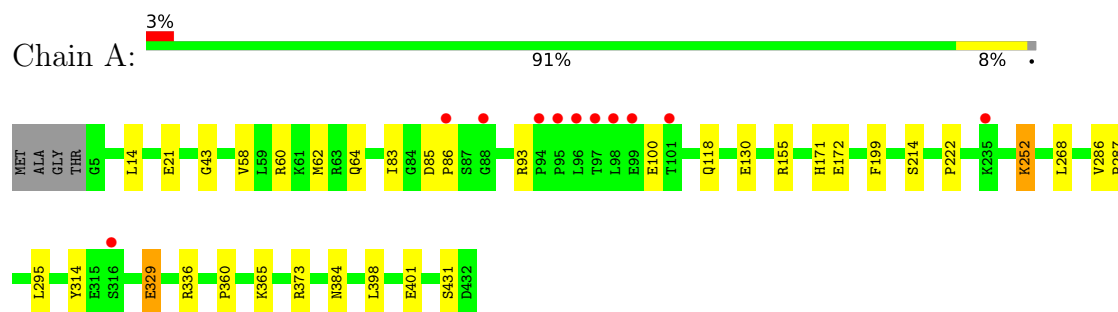
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	286	Total	O	0	0
			286	286		
10	T	211	Total	O	0	0
			211	211		

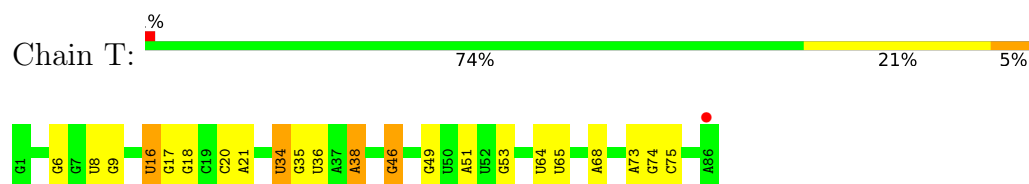
3 Residue-property plots [i](#)

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: Thermus thermophilus tRNA(Tyr)(GUA) (86-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	125.07Å 67.38Å 113.82Å 90.00° 112.25° 90.00°	Depositor
Resolution (Å)	16.74 – 1.90 16.74 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.1 (16.74-1.90) 98.7 (16.74-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.188 , 0.214 0.185 , 0.211	Depositor DCC
R_{free} test set	2761 reflections (3.99%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10714	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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: 1MA, PSU, PGE, MIA, PEG, A1I9V, SO4, OMC, 4SU, 1PE, AMP, 2MG, MG

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	0.20	0/3723	0.42	0/5025
2	T	0.22	0/1847	0.46	0/2874
All	All	0.20	0/5570	0.44	0/7899

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	3533	3626	3481	24	1
2	T	1833	876	929	10	1
3	A	23	12	12	0	0
4	A	13	8	8	1	0
5	A	14	20	20	2	0
5	T	21	30	30	1	0
6	A	5	0	0	0	0
6	T	5	0	0	0	0
7	A	58	78	78	3	0
7	T	16	22	22	0	0
8	A	10	13	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	T	1	0	0	0	0
10	A	286	0	0	4	1
10	T	211	0	0	4	1
All	All	6029	4685	4594	35	2

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 (35) 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:130:GLU:OE1	10:A:601:HOH:O	1.97	0.82
1:A:21:GLU:OE2	10:A:602:HOH:O	2.15	0.63
1:A:214:SER:HB3	7:A:507:1PE:H142	1.81	0.61
2:T:20:OMC:CM2	2:T:20:OMC:O3'	2.48	0.61
7:A:507:1PE:H231	10:A:761:HOH:O	2.04	0.58
1:A:329:GLU:H	1:A:329:GLU:CD	2.13	0.57
2:T:20:OMC:HM21	10:T:212:HOH:O	2.07	0.53
2:T:20:OMC:HM22	10:T:342:HOH:O	2.09	0.52
1:A:83:ILE:HG23	1:A:171:HIS:HD2	1.74	0.52
1:A:365:LYS:HE3	5:A:503:PEG:O4	2.09	0.51
1:A:85:ASP:O	1:A:93:ARG:NE	2.43	0.51
1:A:222:PRO:HG2	1:A:268:LEU:HD21	1.92	0.51
2:T:20:OMC:O3'	2:T:20:OMC:HM23	2.12	0.49
1:A:286:VAL:HB	1:A:287:PRO:HD3	1.96	0.47
1:A:365:LYS:HE3	5:A:503:PEG:H31	1.97	0.47
1:A:398:LEU:O	1:A:401:GLU:HG2	2.16	0.46
2:T:75:C:OP2	10:T:202:HOH:O	2.21	0.46
1:A:43:GLY:HA3	4:A:502:TYR:CE1	2.51	0.45
1:A:252:LYS:NZ	10:A:605:HOH:O	2.37	0.45
1:A:14[B]:LEU:HG	1:A:64[B]:GLN:NE2	2.31	0.44
1:A:86:PRO:HB3	1:A:172:GLU:OE1	2.16	0.44
2:T:20:OMC:HM23	10:T:259:HOH:O	2.17	0.44
1:A:14[B]:LEU:O	1:A:64[B]:GLN:NE2	2.49	0.44
2:T:73:A:H2'	2:T:74:G:C8	2.52	0.44
2:T:46:G:H4'	5:T:102:PEG:H11	2.00	0.43
1:A:118:GLN:HB2	7:A:506:1PE:H162	2.01	0.43
1:A:360:PRO:HA	1:A:431:SER:O	2.18	0.43
1:A:295:LEU:HD21	1:A:314:TYR:HB2	2.01	0.42
2:T:34:U:H2'	2:T:35:G:H2'	2.02	0.42
2:T:38:MIA:H122	2:T:38:MIA:H153	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ARG:HA	1:A:384:ASN:OD1	2.21	0.41
1:A:86:PRO:HB2	1:A:155[A]:ARG:NH2	2.36	0.41
1:A:155[B]:ARG:HG2	1:A:199:PHE:CD2	2.55	0.41
1:A:58:VAL:O	1:A:62[B]:MET:HG2	2.21	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:842:HOH:O	10:T:408:HOH:O[3_455]	2.02	0.18
1:A:336[B]:ARG:HH12	2:T:16:U:O2'[3_455]	1.53	0.07

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	454/432 (105%)	447 (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	388/363 (107%)	383 (99%)	5 (1%)	65	65

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60[A]	ARG
1	A	60[B]	ARG
1	A	100	GLU
1	A	252	LYS
1	A	329	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	409	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	T	63/86 (73%)	10 (15%)	0

All (10) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	T	9	G
2	T	16	U
2	T	17	G
2	T	18	G
2	T	21	A
2	T	34	U
2	T	46	G
2	T	49	G
2	T	51	A
2	T	53	G

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	PSU	T	36	2	18,21,22	1.14	1 (5%)	22,30,33	1.79	3 (13%)
2	2MG	T	6	2	18,26,27	1.32	4 (22%)	16,38,41	1.07	1 (6%)
2	A1I9V	T	64	2	18,22,23	5.21	1 (5%)	23,32,35	0.91	2 (8%)
2	PSU	T	65	2	18,21,22	1.08	1 (5%)	22,30,33	1.72	4 (18%)
2	4SU	T	8	2	18,21,22	0.46	0	26,30,33	1.17	3 (11%)
2	1MA	T	68	2	16,25,26	0.91	2 (12%)	18,37,40	1.16	2 (11%)
2	OMC	T	20	2	19,22,23	0.62	0	26,31,34	0.73	0
2	MIA	T	38	2	24,31,32	2.28	4 (16%)	26,44,47	2.93	9 (34%)

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	PSU	T	36	2	-	3/7/25/26	0/2/2/2
2	2MG	T	6	2	-	2/5/27/28	0/3/3/3
2	A1I9V	T	64	2	-	0/7/25/26	0/2/2/2
2	PSU	T	65	2	-	1/7/25/26	0/2/2/2
2	4SU	T	8	2	-	0/7/25/26	0/2/2/2
2	1MA	T	68	2	-	1/3/25/26	0/3/3/3
2	OMC	T	20	2	-	1/9/27/28	0/2/2/2
2	MIA	T	38	2	-	1/11/33/34	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	64	A1I9V	C2-S2	-22.04	1.32	1.67
2	T	38	MIA	C13-C14	7.21	1.53	1.32
2	T	38	MIA	C2-S10	-6.91	1.69	1.75
2	T	36	PSU	C6-C5	3.80	1.39	1.35
2	T	65	PSU	C6-C5	3.61	1.39	1.35
2	T	6	2MG	C8-N7	-3.04	1.29	1.35
2	T	38	MIA	C5-C4	2.44	1.47	1.40
2	T	38	MIA	C6-N1	2.42	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	6	2MG	C5-C6	-2.33	1.42	1.47
2	T	6	2MG	CM2-N2	-2.29	1.41	1.45
2	T	68	1MA	C5-C4	-2.19	1.37	1.43
2	T	68	1MA	C8-N7	-2.17	1.31	1.35
2	T	6	2MG	C5-C4	-2.04	1.37	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	38	MIA	C11-S10-C2	8.27	108.44	102.27
2	T	38	MIA	C12-C13-C14	-8.03	111.51	127.14
2	T	36	PSU	C4-N3-C2	-4.85	119.35	126.34
2	T	36	PSU	N1-C2-N3	4.63	120.38	115.13
2	T	65	PSU	N1-C2-N3	4.52	120.26	115.13
2	T	65	PSU	C4-N3-C2	-4.36	120.05	126.34
2	T	8	4SU	C4-N3-C2	-4.16	123.30	127.34
2	T	38	MIA	C2-N3-C4	4.05	120.91	115.32
2	T	38	MIA	C16-C14-C13	-3.95	111.24	122.65
2	T	38	MIA	C5-C6-N1	-3.92	117.56	120.81
2	T	38	MIA	C15-C14-C13	-3.91	111.36	122.65
2	T	38	MIA	C2-N1-C6	2.76	122.12	117.19
2	T	68	1MA	C5-C6-N1	-2.69	109.88	113.90
2	T	8	4SU	C5-C4-N3	2.56	117.06	114.69
2	T	68	1MA	N1-C6-N6	2.53	126.20	119.77
2	T	38	MIA	N3-C2-N1	-2.42	122.54	126.98
2	T	65	PSU	O2-C2-N1	-2.36	120.19	122.79
2	T	36	PSU	O2-C2-N1	-2.36	120.19	122.79
2	T	65	PSU	C6-N1-C2	-2.34	120.30	122.68
2	T	64	A1I9V	C5M-C5-C4	2.29	121.28	118.77
2	T	6	2MG	O6-C6-C5	2.25	128.76	124.37
2	T	8	4SU	N3-C2-N1	2.21	117.82	114.89
2	T	38	MIA	C4-C5-N7	-2.16	107.15	109.40
2	T	64	A1I9V	C5M-C5-C6	-2.13	120.00	122.85

There are no chirality outliers.

All (9) 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	6	2MG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	T	36	PSU	O4'-C1'-C5-C4
2	T	36	PSU	O4'-C1'-C5-C6
2	T	65	PSU	O4'-C1'-C5-C6
2	T	6	2MG	C3'-C4'-C5'-O5'
2	T	68	1MA	C4'-C5'-O5'-P

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	20	OMC	5	0
2	T	38	MIA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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	$\# Z > 2$
7	1PE	A	507	-	12,12,15	0.32	0	11,11,14	0.32	0
7	1PE	T	106	-	15,15,15	0.31	0	14,14,14	0.24	0
7	1PE	A	506	-	15,15,15	0.31	0	14,14,14	0.25	0
5	PEG	A	508	-	6,6,6	0.27	0	5,5,5	0.21	0
6	SO4	A	504	-	4,4,4	0.63	0	6,6,6	0.19	0
5	PEG	T	103	-	6,6,6	0.25	0	5,5,5	0.42	0
5	PEG	T	104	-	6,6,6	0.24	0	5,5,5	0.30	0
8	PGE	A	509	-	9,9,9	0.29	0	8,8,8	0.29	0
5	PEG	T	102	-	6,6,6	0.26	0	5,5,5	0.42	0
6	SO4	T	105	-	4,4,4	0.62	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AMP	A	501	-	22,25,25	0.76	0	25,38,38	1.31	2 (8%)
7	1PE	A	505	-	15,15,15	0.27	0	14,14,14	0.31	0
7	1PE	A	510	-	12,12,15	0.30	0	11,11,14	0.28	0
5	PEG	A	503	-	6,6,6	0.24	0	5,5,5	0.25	0
4	TYR	A	502	-	12,13,13	0.71	1 (8%)	16,17,17	0.93	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
7	1PE	A	507	-	-	3/10/10/13	-
7	1PE	T	106	-	-	6/13/13/13	-
7	1PE	A	506	-	-	2/13/13/13	-
5	PEG	A	508	-	-	2/4/4/4	-
8	PGE	A	509	-	-	4/7/7/7	-
5	PEG	T	103	-	-	3/4/4/4	-
5	PEG	T	104	-	-	0/4/4/4	-
5	PEG	T	102	-	-	2/4/4/4	-
7	1PE	A	510	-	-	5/10/10/13	-
3	AMP	A	501	-	-	0/6/26/26	0/3/3/3
7	1PE	A	505	-	-	8/13/13/13	-
5	PEG	A	503	-	-	0/4/4/4	-
4	TYR	A	502	-	-	4/8/8/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	TYR	OXT-C	-2.16	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	AMP	N3-C2-N1	-3.93	122.54	128.68
4	A	502	TYR	OXT-C-O	-2.31	118.84	124.09
4	A	502	TYR	OXT-C-CA	2.26	121.09	113.38
3	A	501	AMP	N6-C6-N1	2.25	123.24	118.57

There are no chirality outliers.

All (39) torsion outliers are listed below:

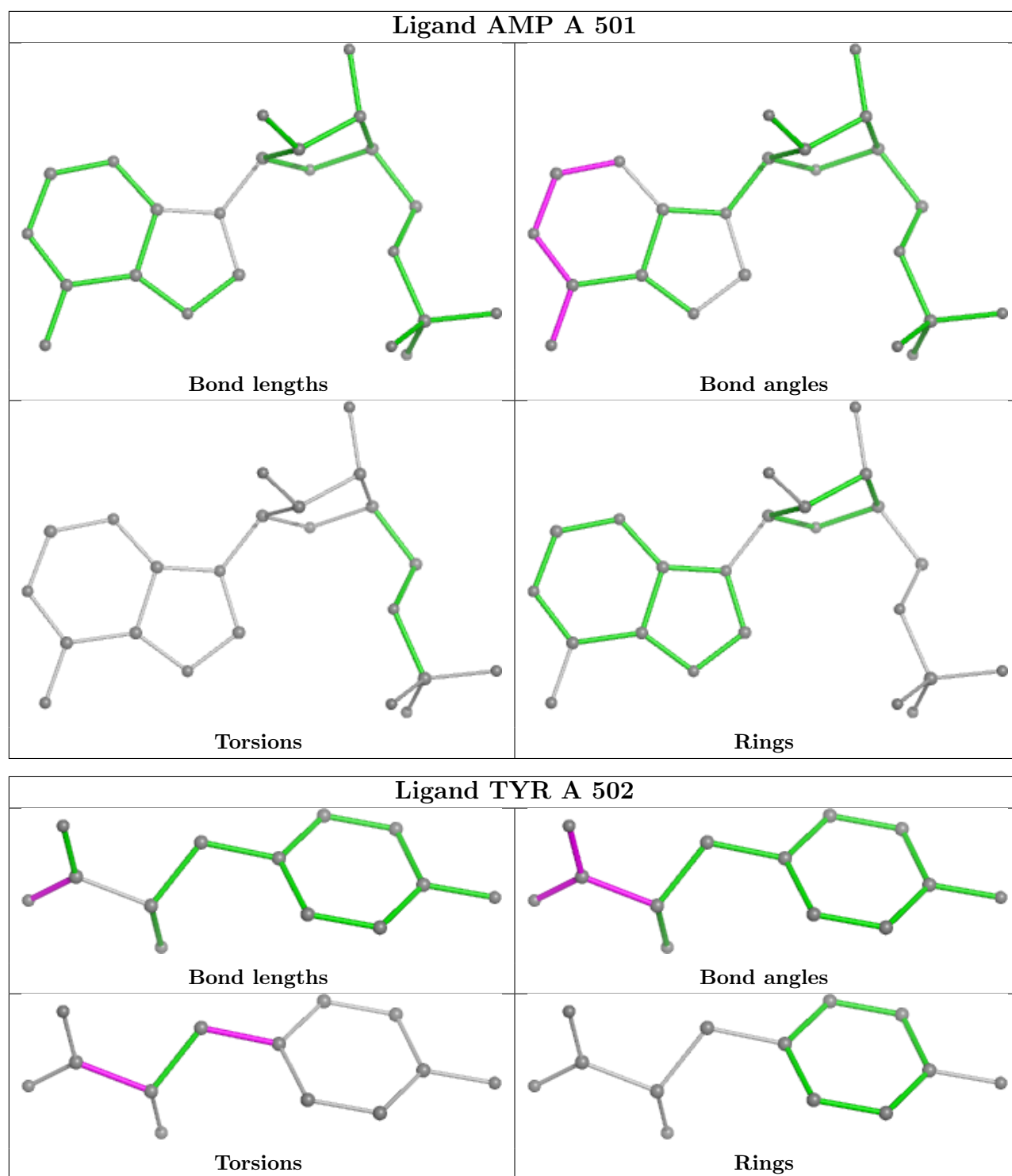
Mol	Chain	Res	Type	Atoms
7	T	106	1PE	OH7-C16-C26-OH6
7	A	505	1PE	OH5-C14-C24-OH4
7	T	106	1PE	OH6-C15-C25-OH5
5	T	102	PEG	O1-C1-C2-O2
8	A	509	PGE	O1-C1-C2-O2
7	A	505	1PE	OH4-C13-C23-OH3
7	A	505	1PE	OH2-C12-C22-OH3
7	T	106	1PE	OH2-C12-C22-OH3
7	A	507	1PE	OH4-C13-C23-OH3
5	T	103	PEG	O1-C1-C2-O2
8	A	509	PGE	O2-C3-C4-O3
7	A	510	1PE	OH4-C13-C23-OH3
7	A	510	1PE	OH2-C12-C22-OH3
8	A	509	PGE	C4-C3-O2-C2
7	A	505	1PE	C16-C26-OH6-C15
7	A	506	1PE	C16-C26-OH6-C15
7	A	510	1PE	C14-C24-OH4-C13
7	A	505	1PE	C23-C13-OH4-C24
5	A	508	PEG	C4-C3-O2-C2
7	A	506	1PE	OH4-C13-C23-OH3
7	T	106	1PE	C25-C15-OH6-C26
5	A	508	PEG	C1-C2-O2-C3
4	A	502	TYR	CA-CB-CG-CD1
7	A	505	1PE	C24-C14-OH5-C25
7	A	507	1PE	C14-C24-OH4-C13
4	A	502	TYR	CA-CB-CG-CD2
4	A	502	TYR	O-C-CA-CB
4	A	502	TYR	OXT-C-CA-CB
7	T	106	1PE	C15-C25-OH5-C14
8	A	509	PGE	C6-C5-O3-C4
5	T	102	PEG	C1-C2-O2-C3
7	A	505	1PE	C14-C24-OH4-C13
7	A	510	1PE	C13-C23-OH3-C22
7	T	106	1PE	OH4-C13-C23-OH3
7	A	505	1PE	OH6-C15-C25-OH5
7	A	507	1PE	C13-C23-OH3-C22
5	T	103	PEG	C4-C3-O2-C2
7	A	510	1PE	C23-C13-OH4-C24
5	T	103	PEG	C1-C2-O2-C3

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	507	1PE	2	0
7	A	506	1PE	1	0
5	T	102	PEG	1	0
5	A	503	PEG	2	0
4	A	502	TYR	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	428/432 (99%)	-0.24	11 (2%) 57 59	7, 25, 52, 75	14 (3%)
2	T	78/86 (90%)	-0.14	1 (1%) 74 76	10, 35, 59, 71	1 (1%)
All	All	506/518 (97%)	-0.23	12 (2%) 59 61	7, 28, 53, 75	15 (2%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	LEU	4.1
1	A	95	PRO	3.7
1	A	86	PRO	3.6
1	A	97	THR	3.5
1	A	88	GLY	3.0
1	A	96	LEU	2.9
1	A	235	LYS	2.5
1	A	94	PRO	2.4
1	A	316	SER	2.3
1	A	101	THR	2.3
2	T	86	A	2.2
1	A	99	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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	0.86	0.12	32,40,49,49	0
2	2MG	T	6	24/25	0.93	0.08	20,26,37,39	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	0.93	0.09	28,34,37,40	0
2	PSU	T	65	20/21	0.93	0.09	30,34,41,43	0
2	1MA	T	68	23/24	0.95	0.07	25,29,36,37	0
2	MIA	T	38	29/30	0.96	0.09	20,29,43,45	0
2	PSU	T	36	20/21	0.96	0.06	21,24,26,27	0
2	4SU	T	8	20/21	0.97	0.08	23,25,29,33	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

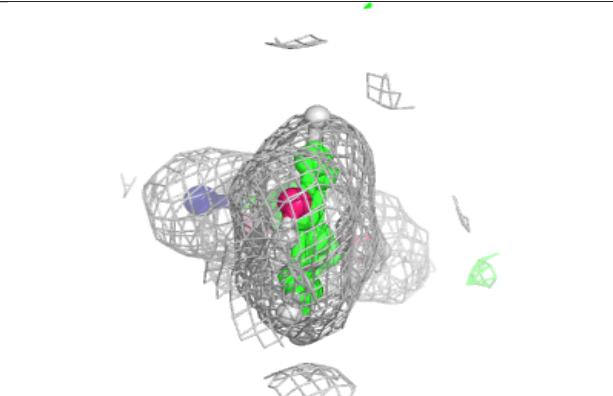
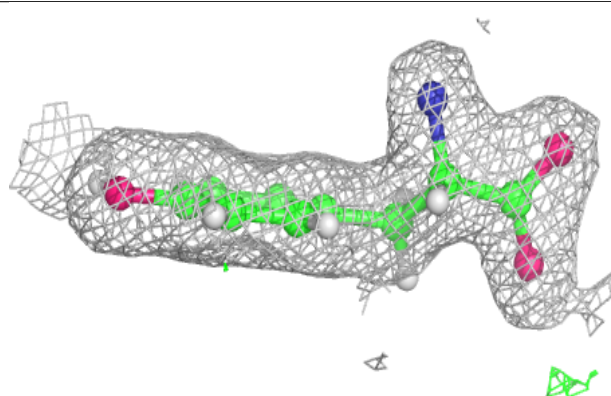
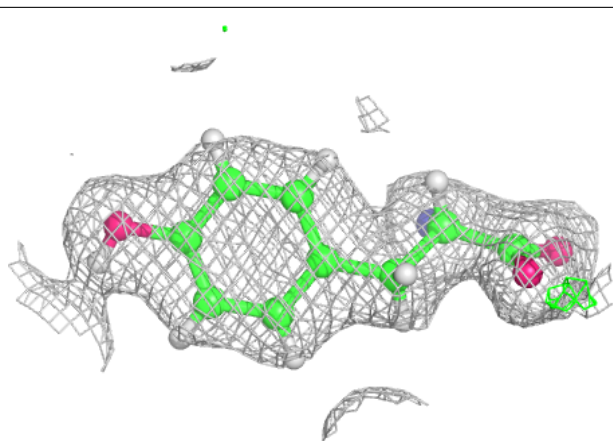
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	1PE	A	506	16/16	0.74	0.13	35,44,55,55	0
5	PEG	A	503	7/7	0.80	0.10	43,52,62,67	0
7	1PE	A	505	16/16	0.82	0.10	34,44,54,58	0
6	SO4	A	504	5/5	0.85	0.16	39,48,54,68	0
6	SO4	T	105	5/5	0.85	0.14	43,53,62,66	0
8	PGE	A	509	10/10	0.85	0.11	25,37,47,47	0
7	1PE	A	510	13/16	0.86	0.11	28,46,59,64	0
5	PEG	A	508	7/7	0.86	0.09	36,43,49,53	0
7	1PE	T	106	16/16	0.87	0.11	45,57,69,71	0
5	PEG	T	103	7/7	0.87	0.14	34,42,49,55	0
7	1PE	A	507	13/16	0.88	0.10	23,40,48,50	0
5	PEG	T	102	7/7	0.90	0.09	39,47,48,52	0
5	PEG	T	104	7/7	0.92	0.08	22,29,39,47	0
4	TYR	A	502	13/13	0.97	0.05	13,18,23,23	0
3	AMP	A	501	23/23	0.97	0.05	13,16,24,25	0
9	MG	T	101	1/1	0.99	0.03	23,23,23,23	0

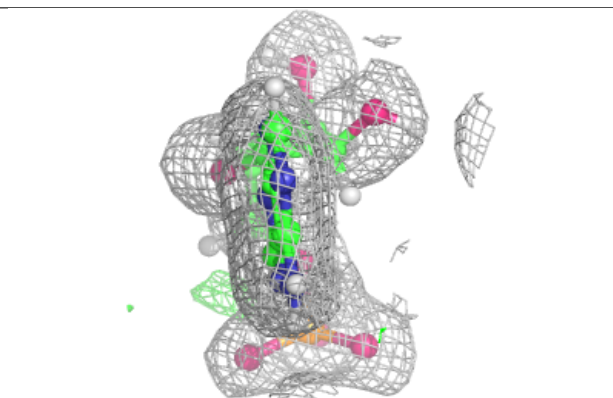
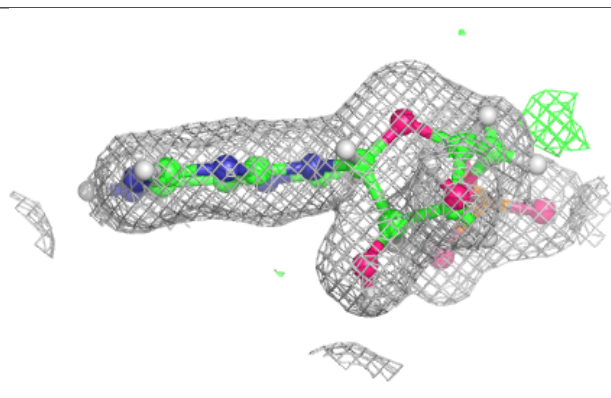
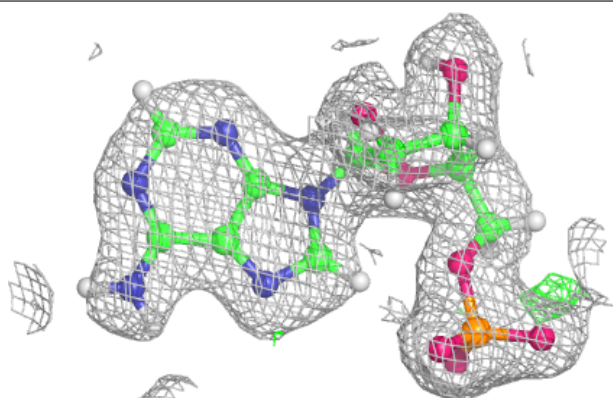
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around TYR A 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around AMP A 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.