Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 06:13 PM EST

PDB ID	:	3TS1
Title	:	STRUCTURE OF TYROSYL-T/RNA SYNTHETASE REFINED AT 2.3 ANGSTROMS RESOLUTION. INTERACTION OF THE ENZYME WITH THE TYROSYL ADENYLATE INTERMEDIATE
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Deposited on	:	1989-06-29
Resolution	:	2.70 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:

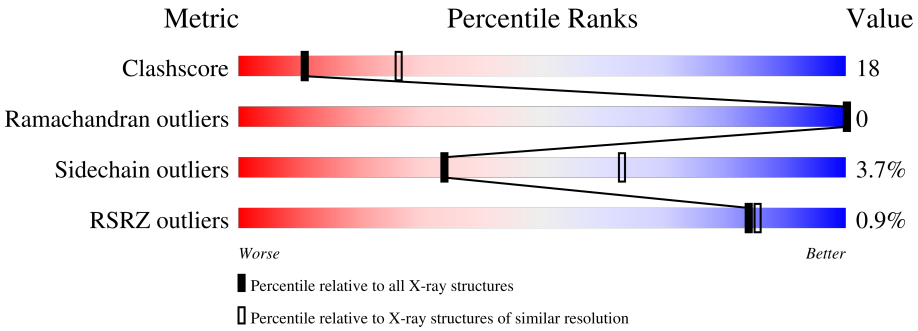
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	419	% 39% 31% 6% 24%

2 Entry composition (i)

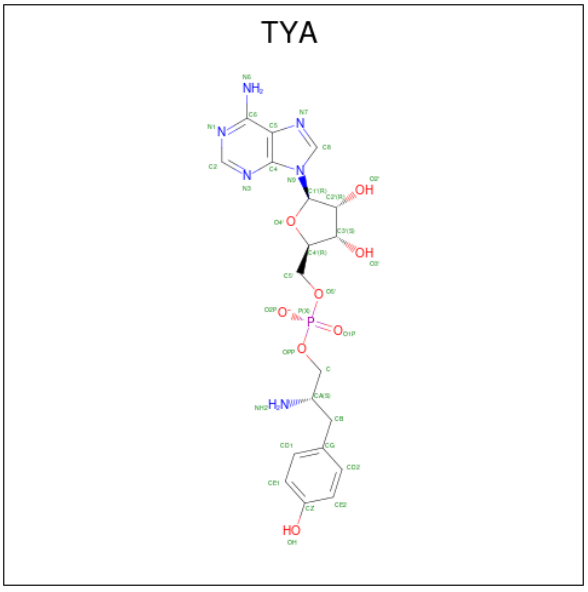
There are 3 unique types of molecules in this entry. The entry contains 2545 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TYROSYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	317	2457	1568	427	455	7	0	0	0

- Molecule 2 is PHOSPHORIC ACID 2-AMINO-3-(4-HYDROXY-PHENYL)-PROPYL ESTER ADENOSIN-5'YL ESTER (three-letter code: TYA) (formula: $C_{19}H_{24}N_6O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	34	19	6	8	1	0	0

- Molecule 3 is water.

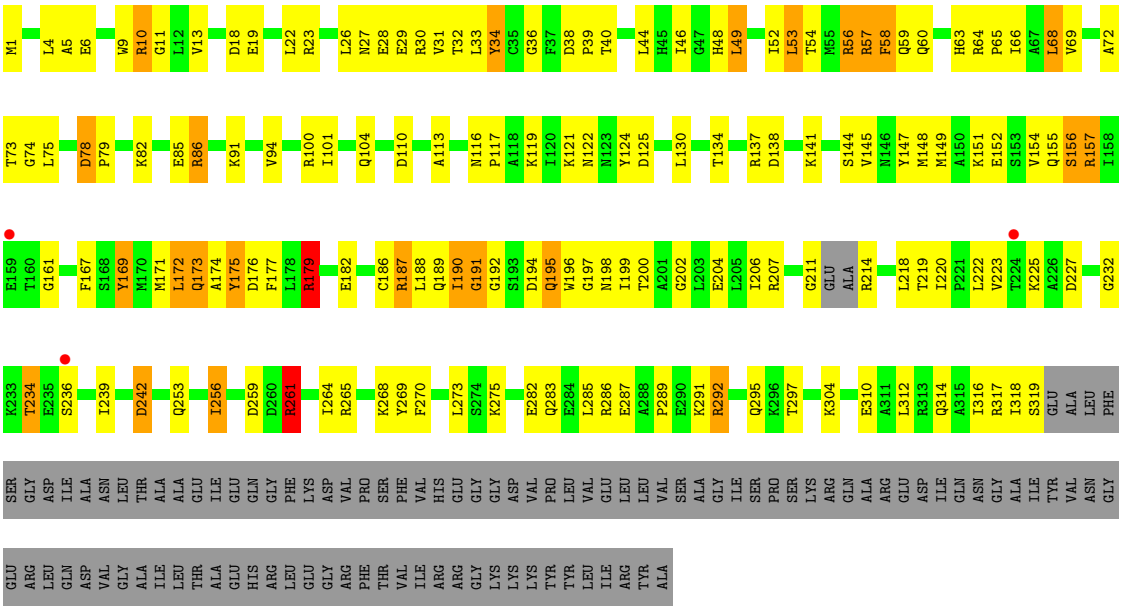
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	54	54	54	0	0

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: TYROSYL-TRNA SYNTHETASE

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	64.63Å 64.63Å 238.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.70 6.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.70) 95.5 (6.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.210 , (Not available) 0.205 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 101.3	EDS
L-test for twinning[1]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.064 for -h,-k,l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	2545	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Theoretical values of $< |L| >$, $< L^2 >$ 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: TYA

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	1.04	2/2505 (0.1%)	2.05	82/3388 (2.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	287	GLU	CB-CG	-6.14	1.40	1.52
1	A	270	PHE	CD1-CE1	-5.16	1.28	1.39

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	149	MET	CA-CB-CG	24.46	154.88	113.30
1	A	34	TYR	CB-CG-CD1	18.56	132.14	121.00
1	A	261	ARG	NE-CZ-NH1	17.46	129.03	120.30
1	A	179	ARG	NE-CZ-NH1	15.71	128.15	120.30
1	A	292	ARG	NE-CZ-NH1	13.04	126.82	120.30
1	A	173	GLN	CB-CG-CD	11.55	141.63	111.60
1	A	179	ARG	CD-NE-CZ	11.35	139.49	123.60
1	A	261	ARG	CD-NE-CZ	11.19	139.26	123.60
1	A	28	GLU	CA-CB-CG	10.86	137.29	113.40
1	A	34	TYR	CB-CG-CD2	-10.63	114.62	121.00
1	A	57	ARG	NE-CZ-NH1	10.21	125.40	120.30
1	A	86	ARG	NE-CZ-NH1	10.19	125.40	120.30
1	A	191	GLY	C-N-CA	9.81	142.90	122.30
1	A	261	ARG	NE-CZ-NH2	-9.78	115.41	120.30
1	A	157	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	A	64	ARG	NE-CZ-NH1	9.68	125.14	120.30
1	A	10	ARG	NE-CZ-NH2	-9.41	115.59	120.30
1	A	34	TYR	CA-CB-CG	9.14	130.77	113.40
1	A	74	GLY	C-N-CA	8.90	143.95	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	10	ARG	NE-CZ-NH1	8.79	124.69	120.30
1	A	86	ARG	CD-NE-CZ	8.57	135.60	123.60
1	A	13	VAL	CA-CB-CG2	-7.76	99.26	110.90
1	A	169	TYR	CB-CG-CD2	7.55	125.53	121.00
1	A	30	ARG	N-CA-CB	7.53	124.15	110.60
1	A	286	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	A	64	ARG	CD-NE-CZ	7.49	134.08	123.60
1	A	172	LEU	C-N-CA	7.38	140.15	121.70
1	A	187	ARG	C-N-CA	7.37	140.12	121.70
1	A	11	GLY	C-N-CA	7.08	139.41	121.70
1	A	265	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	A	317	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	175	TYR	CB-CG-CD2	-6.86	116.88	121.00
1	A	176	ASP	CB-CG-OD1	6.76	124.39	118.30
1	A	187	ARG	O-C-N	-6.71	111.95	122.70
1	A	40	THR	CA-CB-CG2	6.67	121.74	112.40
1	A	157	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	A	187	ARG	CA-C-N	6.52	131.54	117.20
1	A	270	PHE	CB-CG-CD2	6.52	125.36	120.80
1	A	56	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	A	34	TYR	CG-CD1-CE1	6.45	126.46	121.30
1	A	169	TYR	CB-CG-CD1	-6.43	117.14	121.00
1	A	124	TYR	CB-CG-CD2	-6.32	117.21	121.00
1	A	58	PHE	CB-CG-CD1	6.28	125.19	120.80
1	A	57	ARG	NH1-CZ-NH2	-6.27	112.50	119.40
1	A	195	GLN	CG-CD-OE1	-6.20	109.20	121.60
1	A	173	GLN	CA-CB-CG	6.14	126.92	113.40
1	A	125	ASP	CB-CG-OD1	6.14	123.83	118.30
1	A	182	GLU	CG-CD-OE1	6.05	130.40	118.30
1	A	204	GLU	CG-CD-OE1	5.98	130.26	118.30
1	A	261	ARG	CG-CD-NE	5.94	124.27	111.80
1	A	78	ASP	CB-CG-OD2	-5.93	112.97	118.30
1	A	40	THR	N-CA-CB	5.92	121.56	110.30
1	A	179	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	195	GLN	OE1-CD-NE2	5.87	135.40	121.90
1	A	242	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	53	LEU	CB-CA-C	5.79	121.20	110.20
1	A	147	TYR	CB-CG-CD1	-5.77	117.54	121.00
1	A	189	GLN	N-CA-CB	5.67	120.80	110.60
1	A	124	TYR	CB-CG-CD1	5.65	124.39	121.00
1	A	292	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	A	195	GLN	CA-CB-CG	5.62	125.77	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	78	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	319	SER	CA-C-O	5.59	131.85	120.10
1	A	18	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	145	VAL	CG1-CB-CG2	-5.50	102.10	110.90
1	A	304	LYS	CA-CB-CG	5.46	125.42	113.40
1	A	5	ALA	CB-CA-C	-5.45	101.93	110.10
1	A	19	GLU	CG-CD-OE2	-5.38	107.54	118.30
1	A	74	GLY	O-C-N	-5.34	114.16	122.70
1	A	68	LEU	O-C-N	5.30	131.18	122.70
1	A	200	THR	CA-CB-CG2	-5.30	104.98	112.40
1	A	227	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	49	LEU	CA-CB-CG	5.27	127.41	115.30
1	A	137	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	A	317	ARG	CB-CA-C	5.21	120.82	110.40
1	A	317	ARG	CA-CB-CG	5.20	124.83	113.40
1	A	29	GLU	CA-CB-CG	5.19	124.82	113.40
1	A	223	VAL	CB-CA-C	5.19	121.26	111.40
1	A	222	LEU	CB-CA-C	5.15	119.99	110.20
1	A	86	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	234	THR	CA-CB-CG2	5.02	119.42	112.40
1	A	101	ILE	CA-CB-CG1	-5.00	101.50	111.00

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	2457	0	2380	89	2
2	A	34	0	23	3	0
3	A	54	0	0	4	0
All	All	2545	0	2403	89	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 18.

All (89) 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:292:ARG:HH11	1:A:295:GLN:HG2	1.29	0.95
1:A:1:MET:N	1:A:27:ASN:HD21	1.68	0.91
1:A:234:THR:HG22	1:A:236:SER:H	1.38	0.88
1:A:292:ARG:NH1	1:A:295:GLN:HG2	1.90	0.85
1:A:72:ALA:O	1:A:75:LEU:HB2	1.82	0.79
1:A:253:GLN:HA	1:A:256:ILE:HG22	1.67	0.77
1:A:1:MET:H1	1:A:27:ASN:HD21	1.33	0.73
1:A:152:GLU:O	1:A:156:SER:HB3	1.88	0.73
1:A:31:VAL:H	1:A:63:HIS:HD2	1.36	0.73
1:A:314:GLN:O	1:A:318:ILE:HG13	1.89	0.72
1:A:110:ASP:OD2	1:A:113:ALA:HB2	1.93	0.69
1:A:196:TRP:HE3	1:A:219:THR:HG23	1.58	0.69
1:A:44:LEU:HD13	1:A:52:ILE:HD11	1.74	0.68
1:A:78:ASP:HB2	1:A:169:TYR:CZ	2.32	0.65
1:A:191:GLY:O	1:A:219:THR:HA	1.96	0.65
1:A:82:LYS:CG	1:A:86:ARG:HH21	2.10	0.65
1:A:134:THR:O	1:A:138:ASP:HB2	1.97	0.65
1:A:54:THR:HG21	1:A:220:ILE:HD11	1.81	0.63
1:A:73:THR:HB	1:A:169:TYR:CE1	2.34	0.62
1:A:82:LYS:HG2	1:A:86:ARG:HH21	1.64	0.62
1:A:78:ASP:HB2	1:A:169:TYR:CE2	2.35	0.61
1:A:9:TRP:CZ2	1:A:275:LYS:HG3	2.36	0.61
1:A:1:MET:H1	1:A:27:ASN:ND2	1.99	0.60
1:A:36:GLY:HA3	2:A:420:TYA:CD1	2.30	0.60
1:A:273:LEU:HD11	1:A:297:THR:HG21	1.84	0.59
1:A:75:LEU:HD21	1:A:91:LYS:HA	1.85	0.59
1:A:48:HIS:O	1:A:52:ILE:HG13	2.03	0.59
1:A:173:GLN:HG2	1:A:198:ASN:HB3	1.86	0.58
1:A:310:GLU:O	1:A:314:GLN:HG3	2.03	0.57
1:A:86:ARG:HG2	3:A:431:HOH:O	2.05	0.56
1:A:171:MET:O	1:A:174:ALA:HB3	2.05	0.56
1:A:82:LYS:HD3	1:A:86:ARG:HH21	1.71	0.56
1:A:196:TRP:HE3	1:A:219:THR:CG2	2.17	0.55
1:A:6:GLU:O	1:A:10:ARG:HG3	2.06	0.55
1:A:234:THR:HG22	1:A:236:SER:N	2.18	0.55
1:A:1:MET:H3	1:A:27:ASN:HD21	1.51	0.53
1:A:190:ILE:HA	1:A:218:LEU:O	2.09	0.53
1:A:259:ASP:OD1	1:A:261:ARG:HD3	2.09	0.53
1:A:144:SER:O	1:A:148:MET:HG3	2.09	0.53
1:A:264:ILE:O	1:A:268:LYS:HG3	2.10	0.52
1:A:33:LEU:HA	1:A:188:LEU:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:LEU:O	1:A:316:ILE:HG13	2.09	0.52
1:A:285:LEU:O	1:A:289:PRO:HB3	2.10	0.52
1:A:291:LYS:O	1:A:292:ARG:HB2	2.10	0.51
1:A:154:VAL:O	1:A:155:GLN:C	2.51	0.49
1:A:38:ASP:OD2	2:A:420:TYA:HD2	2.12	0.49
1:A:44:LEU:HB2	1:A:104:GLN:OE1	2.12	0.49
1:A:82:LYS:HD3	1:A:86:ARG:HE	1.78	0.49
1:A:82:LYS:CD	1:A:86:ARG:HH21	2.26	0.48
1:A:59:GLN:HA	1:A:63:HIS:O	2.14	0.48
1:A:57:ARG:NH2	1:A:269:TYR:O	2.47	0.48
1:A:46:ILE:HG23	1:A:239:ILE:O	2.14	0.47
1:A:196:TRP:HB2	1:A:219:THR:HG21	1.95	0.47
1:A:202:GLY:O	1:A:206:ILE:HG13	2.15	0.47
1:A:69:VAL:O	1:A:122:ASN:HA	2.16	0.46
1:A:100:ARG:NH2	1:A:242:ASP:OD1	2.48	0.46
1:A:26:LEU:HD11	1:A:58:PHE:HE1	1.81	0.46
1:A:116:ASN:N	1:A:117:PRO:HD3	2.31	0.46
1:A:196:TRP:CE3	1:A:219:THR:HG23	2.45	0.45
1:A:207:ARG:O	1:A:211:GLY:N	2.50	0.44
1:A:256:ILE:O	1:A:292:ARG:NH1	2.50	0.44
1:A:1:MET:N	1:A:23:ARG:HG3	2.32	0.44
1:A:59:GLN:HG3	1:A:65:PRO:HD3	1.97	0.44
1:A:94:VAL:HG12	3:A:451:HOH:O	2.17	0.44
1:A:154:VAL:HG11	1:A:167:PHE:HE1	1.83	0.44
1:A:78:ASP:HA	1:A:79:PRO:HD2	1.79	0.44
1:A:56:ARG:O	1:A:60:GLN:HG3	2.16	0.44
1:A:22:LEU:HD12	1:A:22:LEU:O	2.17	0.43
1:A:116:ASN:N	1:A:117:PRO:CD	2.80	0.43
1:A:232:GLY:N	3:A:464:HOH:O	2.50	0.43
1:A:151:LYS:HE3	1:A:197:GLY:O	2.18	0.43
1:A:4:LEU:HD23	1:A:23:ARG:HB2	2.01	0.42
1:A:32:THR:HB	1:A:186:CYS:HA	2.01	0.42
1:A:225:LYS:HE2	1:A:225:LYS:HB3	1.89	0.42
1:A:49:LEU:HD22	1:A:53:LEU:HG	2.02	0.42
1:A:157:ARG:O	1:A:161:GLY:N	2.41	0.42
1:A:194:ASP:N	1:A:194:ASP:OD2	2.53	0.42
1:A:197:GLY:HA3	3:A:471:HOH:O	2.19	0.42
1:A:49:LEU:HD22	1:A:53:LEU:CD1	2.50	0.42
1:A:119:LYS:HD2	1:A:121:LYS:HE3	2.02	0.41
1:A:38:ASP:HA	1:A:39:PRO:HD3	1.84	0.41
1:A:141:LYS:HD2	1:A:141:LYS:HA	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LEU:O	1:A:175:TYR:HB3	2.20	0.41
1:A:34:TYR:HA	1:A:66:ILE:O	2.21	0.41
1:A:49:LEU:HD22	1:A:53:LEU:HD11	2.02	0.41
1:A:154:VAL:HG11	1:A:167:PHE:CE1	2.56	0.41
1:A:187:ARG:HD3	1:A:214:ARG:O	2.21	0.40
1:A:192:GLY:HA3	2:A:420:TYA:O2'	2.21	0.40
1:A:195:GLN:O	1:A:199:ILE:HG13	2.21	0.40

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)
1:A:179:ARG:NH1	1:A:282:GLU:OE1[4_565]	2.06	0.14
1:A:85:GLU:OE1	1:A:141:LYS:NZ[4_555]	2.12	0.08

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	313/419 (75%)	297 (95%)	16 (5%)	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	243/349 (70%)	234 (96%)	9 (4%)	34 63

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	LEU
1	A	130	LEU
1	A	156	SER
1	A	177	PHE
1	A	179	ARG
1	A	190	ILE
1	A	256	ILE
1	A	261	ARG
1	A	283	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	27	ASN
1	A	60	GLN
1	A	63	HIS
1	A	155	GLN
1	A	195	GLN
1	A	283	GLN
1	A	314	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	TYA	A	420	-	34,37,37	1.21	2 (5%)	37,54,54	1.53	6 (16%)

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	TYA	A	420	-	-	8/16/36/36	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	420	TYA	CB-CG	-4.20	1.41	1.51
2	A	420	TYA	C2'-C1'	-2.74	1.49	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	420	TYA	O4'-C1'-C2'	4.41	113.38	106.93
2	A	420	TYA	O2P-P-O1P	-3.81	93.38	112.24
2	A	420	TYA	C5-C6-N6	3.34	125.42	120.35
2	A	420	TYA	OPP-P-O1P	2.60	119.22	109.07
2	A	420	TYA	C1'-N9-C4	-2.56	122.14	126.64
2	A	420	TYA	O4'-C4'-C5'	-2.18	102.19	109.37

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	420	TYA	C-OPP-P-O1P
2	A	420	TYA	C-OPP-P-O2P
2	A	420	TYA	C-OPP-P-O5'
2	A	420	TYA	O4'-C4'-C5'-O5'
2	A	420	TYA	NH2-CA-CB-CG
2	A	420	TYA	C5'-O5'-P-OPP
2	A	420	TYA	C-CA-CB-CG
2	A	420	TYA	C3'-C4'-C5'-O5'

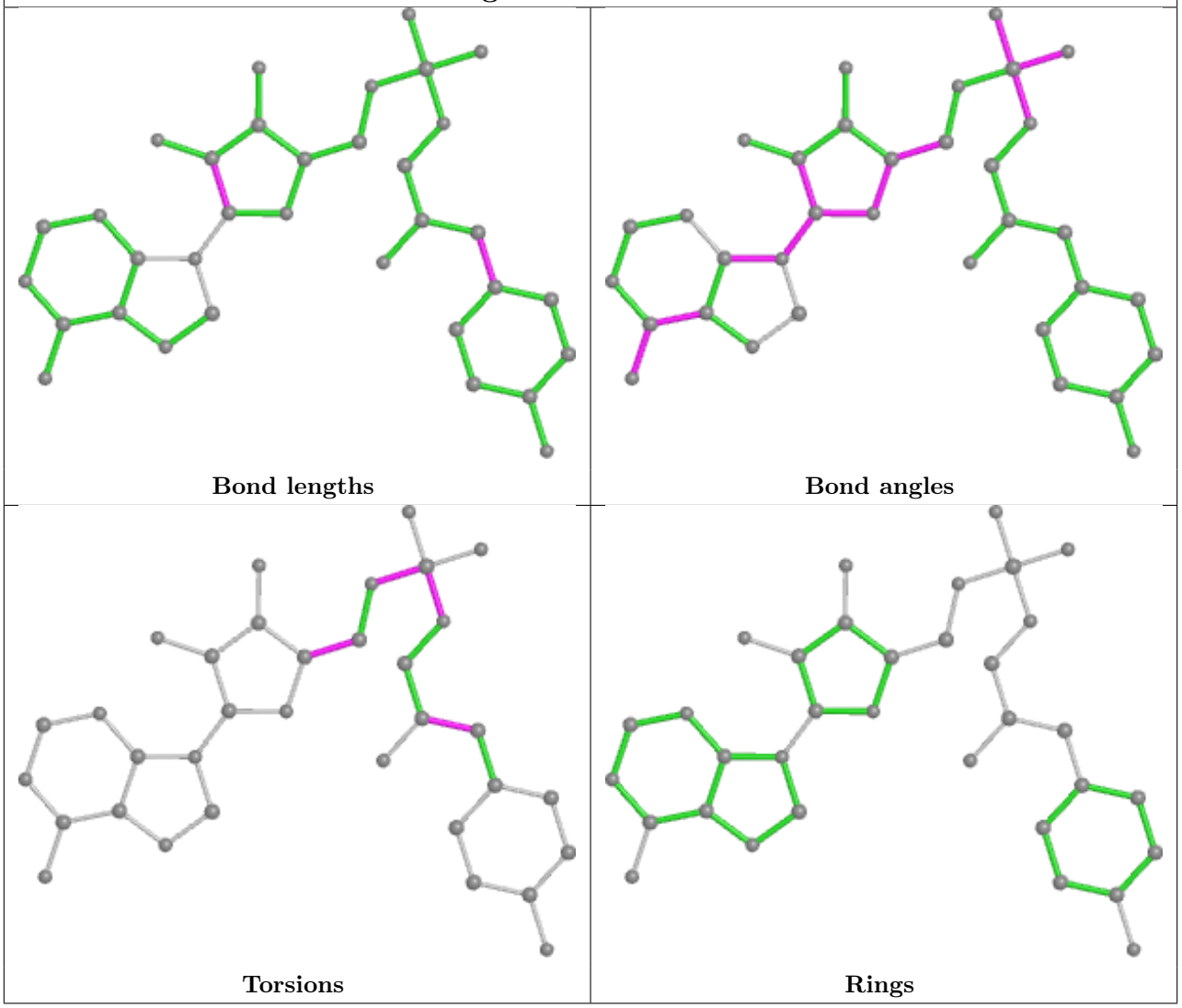
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	420	TYA	3	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 then 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.

Ligand TYA A 420



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	317/419 (75%)	-0.99	3 (0%)	84	85	2, 14, 41, 57	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	236	SER	3.6
1	A	224	THR	2.2
1	A	159	GLU	2.2

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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.

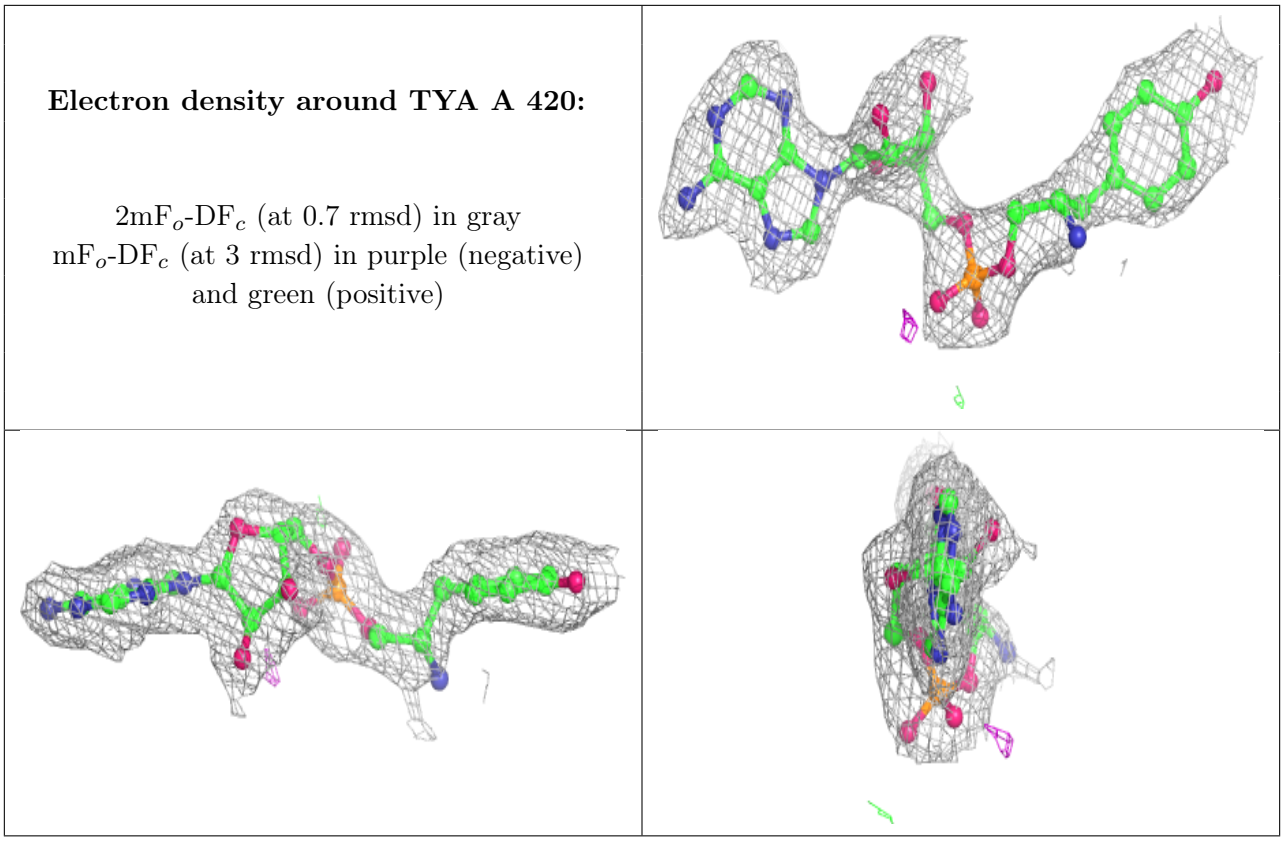
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TYA	A	420	34/34	0.98	0.10	10,23,29,33	0

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 TYA A 420:

$2mF_o$-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.