



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:22 PM UTC

PDB ID : 1R6T / pdb_00001r6t
Title : crystal structure of human tryptophanyl-tRNA synthetase
Authors : Yang, X.-L.; Otero, F.J.; Skene, R.J.; McRee, D.E.; Ribas de Pouplana, L.; Schimmel, P.
Deposited on : 2003-10-16
Resolution : 2.10 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

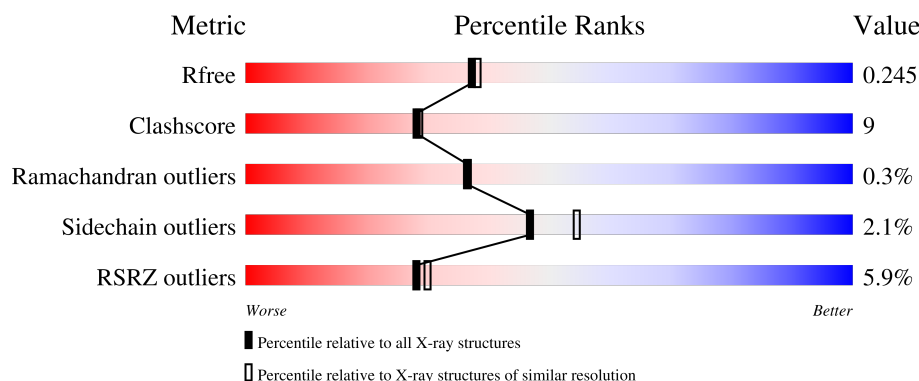
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	477	4% 71% 19% 8%
1	B	477	5% 61% 14% 24%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6778 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 Tryptophanyl-tRNA synthetase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	Se	0	0	0
			3509	2242	592	658	5	12			
1	B	362	Total	C	N	O	S	Se	0	0	0
			2926	1879	497	536	5	9			

There are 50 discrepancies between the modelled and reference sequences:

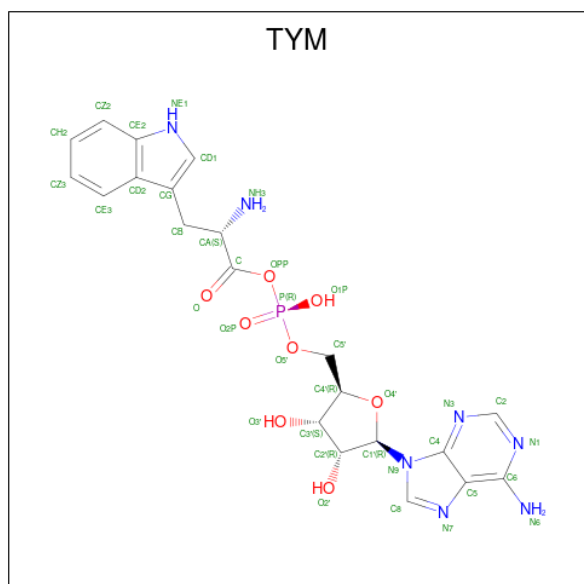
Chain	Residue	Modelled	Actual	Comment	Reference
A	42	MSE	MET	modified residue	UNP P23381
A	48	MSE	MET	modified residue	UNP P23381
A	143	MSE	MET	modified residue	UNP P23381
A	169	MSE	MET	modified residue	UNP P23381
A	195	MSE	MET	modified residue	UNP P23381
A	213	GLY	SER	engineered mutation	UNP P23381
A	214	ASP	TYR	engineered mutation	UNP P23381
A	241	MSE	MET	modified residue	UNP P23381
A	243	MSE	MET	modified residue	UNP P23381
A	319	MSE	MET	modified residue	UNP P23381
A	350	MSE	MET	modified residue	UNP P23381
A	401	MSE	MET	modified residue	UNP P23381
A	425	MSE	MET	modified residue	UNP P23381
A	461	MSE	MET	modified residue	UNP P23381
A	467	ALA	-	cloning artifact	UNP P23381
A	468	ALA	-	cloning artifact	UNP P23381
A	469	ALA	-	cloning artifact	UNP P23381
A	470	LEU	-	cloning artifact	UNP P23381
A	471	GLU	-	cloning artifact	UNP P23381
A	472	HIS	-	expression tag	UNP P23381
A	473	HIS	-	expression tag	UNP P23381
A	474	HIS	-	expression tag	UNP P23381
A	475	HIS	-	expression tag	UNP P23381
A	476	HIS	-	expression tag	UNP P23381
A	477	HIS	-	expression tag	UNP P23381

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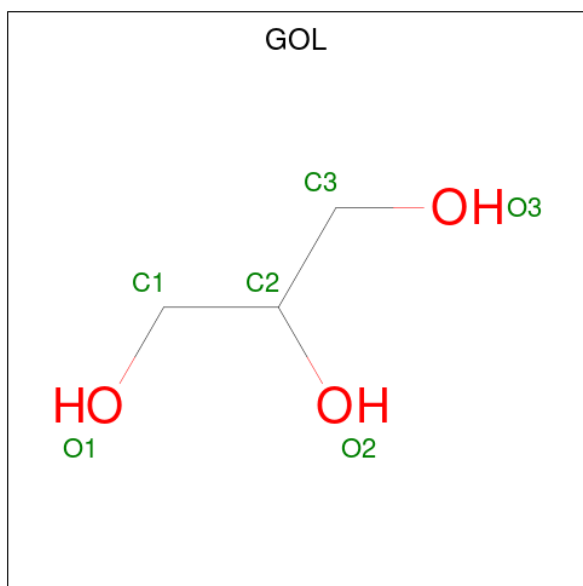
Chain	Residue	Modelled	Actual	Comment	Reference
B	42	MSE	MET	modified residue	UNP P23381
B	48	MSE	MET	modified residue	UNP P23381
B	143	MSE	MET	modified residue	UNP P23381
B	169	MSE	MET	modified residue	UNP P23381
B	195	MSE	MET	modified residue	UNP P23381
B	213	GLY	SER	engineered mutation	UNP P23381
B	214	ASP	TYR	engineered mutation	UNP P23381
B	241	MSE	MET	modified residue	UNP P23381
B	243	MSE	MET	modified residue	UNP P23381
B	319	MSE	MET	modified residue	UNP P23381
B	350	MSE	MET	modified residue	UNP P23381
B	401	MSE	MET	modified residue	UNP P23381
B	425	MSE	MET	modified residue	UNP P23381
B	461	MSE	MET	modified residue	UNP P23381
B	467	ALA	-	cloning artifact	UNP P23381
B	468	ALA	-	cloning artifact	UNP P23381
B	469	ALA	-	cloning artifact	UNP P23381
B	470	LEU	-	cloning artifact	UNP P23381
B	471	GLU	-	cloning artifact	UNP P23381
B	472	HIS	-	expression tag	UNP P23381
B	473	HIS	-	expression tag	UNP P23381
B	474	HIS	-	expression tag	UNP P23381
B	475	HIS	-	expression tag	UNP P23381
B	476	HIS	-	expression tag	UNP P23381
B	477	HIS	-	expression tag	UNP P23381

- Molecule 2 is TRYPTOPHANYL-5'AMP (CCD ID: TYM) (formula: $C_{21}H_{24}N_7O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			37	21	7	8	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

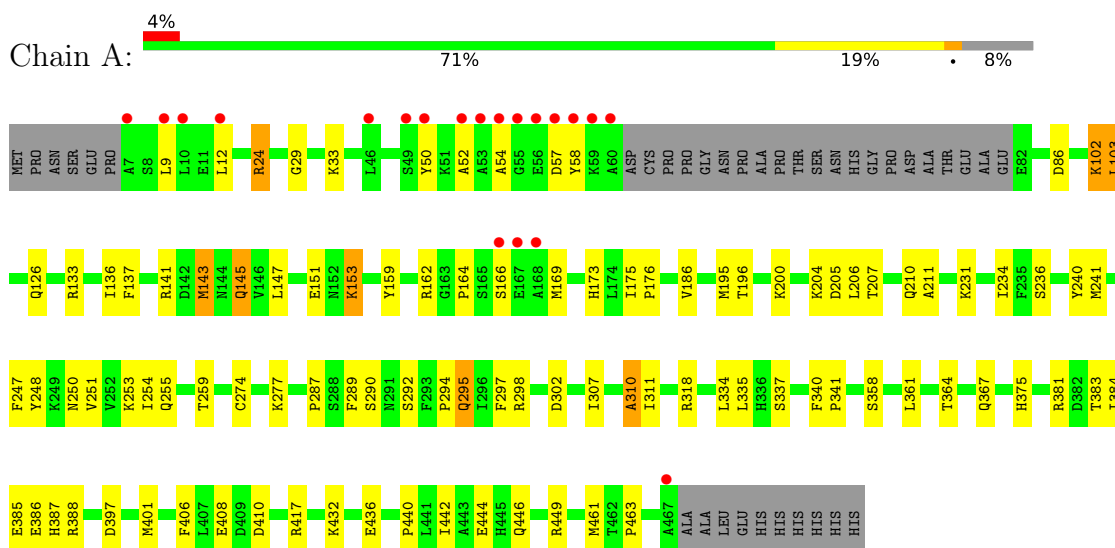
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	195	Total	O	0	0
			195	195		
4	B	99	Total	O	0	0
			99	99		

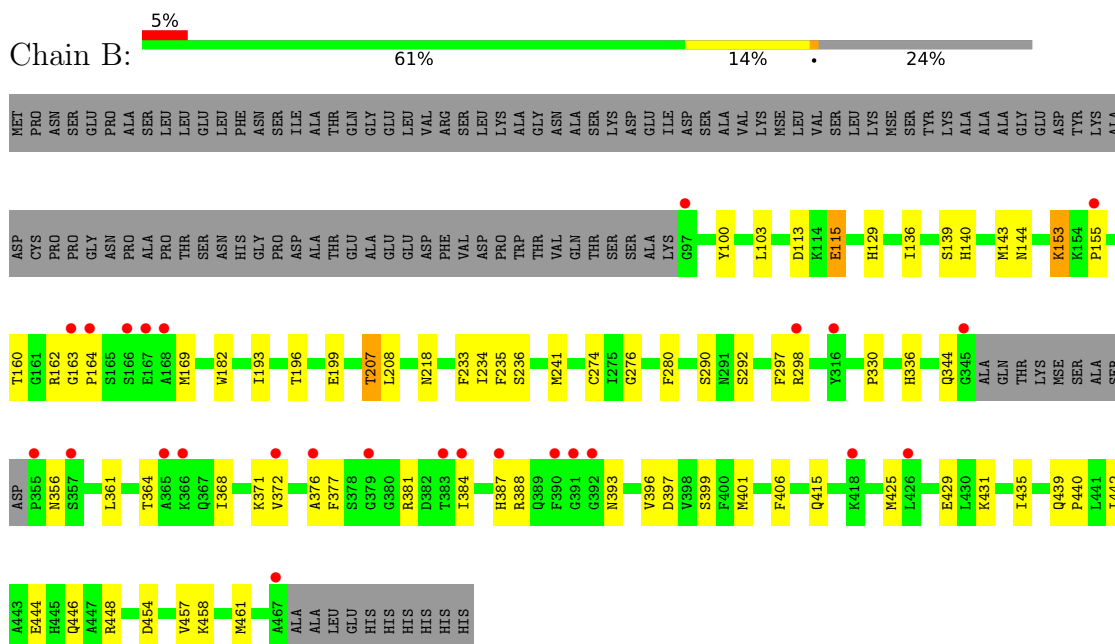
3 Residue-property plots [i](#)

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: Tryptophanyl-tRNA synthetase



• Molecule 1: Tryptophanyl-tRNA synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	152.15Å 95.71Å 98.51Å 90.00° 91.62° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.10) 87.2 (20.00-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.80 (at 2.09Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.208 , 0.239 0.217 , 0.245	Depositor DCC
R_{free} test set	7631 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6778	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: TYM, GOL

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	0.39	0/3574	0.90	13/4800 (0.3%)
1	B	0.37	0/2987	0.84	5/4013 (0.1%)
All	All	0.38	0/6561	0.87	18/8813 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	ILE	N-CA-C	-8.05	103.01	110.82
1	A	318	ARG	N-CA-C	-7.65	103.02	111.36
1	A	307	ILE	N-CA-C	7.27	115.38	107.60
1	A	310	ALA	N-CA-C	-7.01	100.10	110.48
1	A	358	SER	N-CA-C	6.50	120.21	110.14
1	A	406	PHE	N-CA-C	6.41	122.06	113.72
1	A	292	SER	N-CA-C	-6.39	104.96	112.89
1	B	290	SER	N-CA-C	6.29	118.94	111.33
1	B	136	ILE	N-CA-C	-5.72	105.15	110.53
1	A	408	GLU	N-CA-C	5.70	118.43	111.82
1	B	292	SER	N-CA-C	-5.55	106.00	112.89
1	A	290	SER	N-CA-C	5.38	117.84	111.33
1	A	340	PHE	N-CA-C	-5.35	99.76	109.44
1	A	375	HIS	N-CA-C	5.32	120.42	113.88
1	B	207	THR	N-CA-C	-5.23	103.78	110.53
1	A	341	PRO	N-CA-C	5.17	119.17	111.41
1	A	196	THR	N-CA-C	5.12	117.52	109.39
1	B	406	PHE	N-CA-C	5.11	120.52	113.97

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	3509	0	3475	67	0
1	B	2926	0	2893	52	0
2	A	37	0	23	1	0
3	A	6	0	7	0	0
3	B	6	0	7	1	0
4	A	195	0	0	2	0
4	B	99	0	0	3	0
All	All	6778	0	6405	115	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 9.

All (115) 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:24:ARG:HH11	1:A:24:ARG:HB3	1.31	0.94
1:A:24:ARG:HB3	1:A:24:ARG:NH1	1.86	0.89
1:B:393:ASN:HD22	1:B:396:VAL:HG22	1.38	0.88
1:A:102:LYS:HA	1:A:102:LYS:HE2	1.58	0.84
1:B:164:PRO:HB2	4:B:1293:HOH:O	1.87	0.73
1:A:254:ILE:HD11	1:A:289:PHE:HE2	1.55	0.71
1:A:432:LYS:O	1:A:436:GLU:HG3	1.90	0.71
1:A:169:MSE:HE2	1:A:173:HIS:HB3	1.73	0.71
1:B:113:ASP:OD1	1:B:115:GLU:HG2	1.93	0.69
1:B:393:ASN:ND2	1:B:396:VAL:HG22	2.06	0.69
1:B:139:SER:HB3	1:B:336:HIS:HB2	1.74	0.68
1:A:295:GLN:HG3	1:A:463:PRO:HB2	1.75	0.67
1:A:364:THR:OG1	1:A:367:GLN:HG3	1.95	0.67
1:B:140:HIS:HD2	1:B:143:MSE:H	1.43	0.66
1:B:140:HIS:CD2	1:B:143:MSE:H	2.15	0.64
1:A:175:ILE:HB	1:A:176:PRO:HD3	1.79	0.63
1:A:440:PRO:O	1:A:444:GLU:HG3	1.98	0.63
1:B:100:TYR:HA	1:B:103:LEU:HD23	1.81	0.62
1:A:9:LEU:HD11	1:A:54:ALA:HB2	1.80	0.60
1:A:254:ILE:HD11	1:A:289:PHE:CE2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LYS:HE3	1:A:205:ASP:O	2.01	0.59
1:A:274:CYS:SG	1:A:277:LYS:HG3	2.43	0.58
1:B:199:GLU:HB2	1:B:280:PHE:CZ	2.39	0.58
1:A:381:ARG:H	1:A:387:HIS:HD2	1.52	0.58
1:B:381:ARG:H	1:B:387:HIS:HD2	1.51	0.58
1:B:144:ASN:HB2	4:B:1005:HOH:O	2.04	0.57
1:A:145:GLN:HE21	1:A:145:GLN:H	1.52	0.56
1:A:207:THR:OG1	1:A:210:GLN:HG3	2.05	0.56
1:B:162:ARG:HG2	1:B:162:ARG:HH11	1.70	0.56
1:A:50:TYR:HD2	1:A:57:ASP:O	1.90	0.55
1:A:310:ALA:HB3	2:A:501:TYM:O2'	2.06	0.55
1:A:255:GLN:NE2	4:A:1296:HOH:O	2.41	0.53
1:B:164:PRO:HA	1:B:218:ASN:OD1	2.09	0.53
1:A:147:LEU:O	1:A:151:GLU:HG3	2.10	0.52
1:B:431:LYS:O	1:B:435:ILE:HG13	2.10	0.52
1:A:442:ILE:O	1:A:446:GLN:HG3	2.10	0.52
1:A:234:ILE:O	1:A:461:MSE:HA	2.10	0.52
1:B:169:MSE:HE2	1:B:361:LEU:CD1	2.40	0.52
1:A:383:THR:OG1	1:A:386:GLU:HG3	2.09	0.52
1:B:435:ILE:O	1:B:439:GLN:HG3	2.10	0.52
1:B:115:GLU:H	1:B:115:GLU:CD	2.18	0.51
1:A:145:GLN:HE21	1:A:145:GLN:N	2.08	0.51
1:A:259:THR:HA	1:B:274:CYS:HA	1.93	0.51
1:A:169:MSE:HE2	1:A:173:HIS:CB	2.40	0.50
1:B:381:ARG:H	1:B:387:HIS:CD2	2.29	0.50
1:B:234:ILE:O	1:B:461:MSE:HA	2.11	0.50
1:A:137:PHE:CZ	1:A:337:SER:HB3	2.48	0.49
1:B:160:THR:O	1:B:193:ILE:HA	2.12	0.49
1:B:454:ASP:HA	1:B:457:VAL:HG12	1.94	0.49
1:A:294:PRO:HG2	1:A:295:GLN:NE2	2.28	0.49
1:B:444:GLU:HB3	1:B:448:ARG:HH12	1.76	0.49
1:B:162:ARG:HD3	1:B:163:GLY:N	2.28	0.48
1:B:364:THR:O	1:B:368:ILE:HG13	2.13	0.48
1:A:417:ARG:HG2	1:A:417:ARG:HH11	1.78	0.48
1:A:240:TYR:OH	1:A:295:GLN:NE2	2.47	0.48
1:A:29:GLY:O	1:A:204:LYS:HE3	2.14	0.47
1:B:113:ASP:CG	1:B:115:GLU:HG2	2.40	0.46
1:B:397:ASP:O	1:B:401:MSE:HG3	2.15	0.46
1:A:164:PRO:O	1:A:200:LYS:HE3	2.15	0.46
1:A:103:LEU:HD13	1:A:311:ILE:HD13	1.97	0.46
1:A:133:ARG:NH1	1:A:410:ASP:OD2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LYS:HE3	1:B:208:LEU:HD22	1.97	0.46
1:B:440:PRO:O	1:B:444:GLU:HG3	2.16	0.46
1:A:52:ALA:C	1:A:54:ALA:H	2.23	0.46
1:A:86:ASP:OD2	1:A:86:ASP:C	2.59	0.46
1:B:162:ARG:HG2	1:B:162:ARG:NH1	2.31	0.46
1:B:356:ASN:HD22	1:B:371:LYS:HE2	1.80	0.46
1:A:397:ASP:O	1:A:401:MSE:HG3	2.15	0.45
1:B:393:ASN:HD22	1:B:396:VAL:CG2	2.18	0.45
1:A:102:LYS:HA	1:A:102:LYS:CE	2.38	0.45
1:B:344:GLN:HA	1:B:377:PHE:HB2	1.98	0.45
1:A:126:GLN:HG3	1:A:186:VAL:HG12	1.99	0.45
1:A:297:PHE:O	1:A:298:ARG:HB2	2.16	0.45
1:B:442:ILE:O	1:B:446:GLN:HG3	2.16	0.45
1:A:231:LYS:NZ	1:A:231:LYS:HB2	2.32	0.45
1:A:302:ASP:OD2	1:A:302:ASP:N	2.50	0.45
1:B:297:PHE:O	1:B:298:ARG:HB2	2.18	0.44
1:A:52:ALA:C	1:A:54:ALA:N	2.75	0.44
1:A:143:MSE:CG	1:A:335:LEU:HD21	2.48	0.44
1:A:141:ARG:HD2	1:A:334:LEU:HD13	2.00	0.44
1:B:425:MSE:HG3	1:B:429:GLU:CD	2.42	0.44
1:B:444:GLU:HB3	1:B:448:ARG:NH1	2.32	0.44
1:B:381:ARG:HB2	1:B:387:HIS:HB2	1.99	0.43
1:B:384:ILE:O	1:B:388:ARG:HG2	2.18	0.43
1:B:129:HIS:HB2	1:B:182:TRP:CD2	2.52	0.43
1:A:251:VAL:O	1:A:255:GLN:HG3	2.19	0.43
1:A:294:PRO:HA	1:A:298:ARG:O	2.18	0.43
1:A:417:ARG:HG2	1:A:417:ARG:NH1	2.33	0.43
1:B:330:PRO:HD2	4:B:1214:HOH:O	2.19	0.43
1:A:206:LEU:HD13	1:A:211:ALA:HB2	2.01	0.43
1:B:207:THR:HA	3:B:601:GOL:H12	2.01	0.43
1:A:449:ARG:HD2	4:A:1297:HOH:O	2.18	0.43
1:A:384:ILE:O	1:A:388:ARG:HG2	2.19	0.43
1:A:173:HIS:O	1:A:176:PRO:HD2	2.19	0.42
1:A:241:MSE:SE	1:A:247:PHE:HD2	2.52	0.42
1:A:164:PRO:HG3	1:A:195:MSE:HE3	2.01	0.42
1:B:233:PHE:CZ	1:B:235:PHE:HB3	2.55	0.42
1:A:231:LYS:HB2	1:A:231:LYS:HZ2	1.85	0.42
1:B:153:LYS:HZ3	1:B:153:LYS:HA	1.85	0.42
1:B:397:ASP:OD2	1:B:399:SER:HB2	2.20	0.42
1:A:162:ARG:O	1:A:164:PRO:HD3	2.20	0.41
1:A:250:ASN:O	1:A:254:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:GLN:HG3	1:A:463:PRO:CB	2.46	0.41
1:B:153:LYS:O	1:B:155:PRO:HD3	2.21	0.41
1:B:457:VAL:HG13	1:B:458:LYS:N	2.34	0.41
1:B:196:THR:HB	1:B:199:GLU:HB3	2.02	0.41
1:A:248:TYR:CG	1:B:241:MSE:HG2	2.56	0.41
1:A:169:MSE:CE	1:A:173:HIS:HB3	2.48	0.41
1:A:153:LYS:HE2	1:A:153:LYS:N	2.36	0.40
1:B:372:VAL:O	1:B:376:ALA:HB3	2.21	0.40
1:A:159:TYR:CZ	1:A:287:PRO:HB2	2.57	0.40
1:A:164:PRO:O	1:A:200:LYS:HG3	2.21	0.40
1:A:255:GLN:HB3	1:B:276:GLY:CA	2.52	0.40
1:B:153:LYS:C	1:B:155:PRO:HD3	2.47	0.40
1:A:175:ILE:HD12	1:A:175:ILE:N	2.37	0.40

There are no symmetry-related clashes.

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	436/477 (91%)	423 (97%)	11 (2%)	2 (0%)	24	22
1	B	358/477 (75%)	346 (97%)	12 (3%)	0	100	100
All	All	794/954 (83%)	769 (97%)	23 (3%)	2 (0%)	36	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	TYR
1	A	166	SER

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	382/400 (96%)	371 (97%)	11 (3%)	37	42
1	B	319/400 (80%)	315 (99%)	4 (1%)	61	69
All	All	701/800 (88%)	686 (98%)	15 (2%)	47	54

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	24	ARG
1	A	102	LYS
1	A	103	LEU
1	A	143	MSE
1	A	145	GLN
1	A	153	LYS
1	A	236	SER
1	A	295	GLN
1	A	361	LEU
1	A	385	GLU
1	B	115	GLU
1	B	153	LYS
1	B	236	SER
1	B	415	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	145	GLN
1	A	152	ASN
1	A	230	ASN
1	A	295	GLN
1	A	387	HIS
1	A	389	GLN

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Mol	Chain	Res	Type
1	B	126	GLN
1	B	140	HIS
1	B	152	ASN
1	B	184	GLN
1	B	255	GLN
1	B	261	ASN
1	B	284	GLN
1	B	304	GLN
1	B	336	HIS
1	B	344	GLN
1	B	356	ASN
1	B	387	HIS
1	B	393	ASN
1	B	445	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	GOL	A	602	-	5,5,5	0.24	0	5,5,5	1.94	3 (60%)
3	GOL	B	601	-	5,5,5	0.35	0	5,5,5	1.94	3 (60%)
2	TYM	A	501	-	40,41,41	0.92	3 (7%)	58,61,61	0.59	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	GOL	A	602	-	-	2/4/4/4	-
3	GOL	B	601	-	-	2/4/4/4	-
2	TYM	A	501	-	-	1/21/39/39	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	TYM	CE3-CD2	2.61	1.43	1.39
2	A	501	TYM	CH2-CZ3	2.31	1.43	1.38
2	A	501	TYM	CZ2-CE2	2.06	1.43	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	GOL	C3-C2-C1	2.60	121.33	111.80
3	A	602	GOL	O2-C2-C1	2.56	119.78	109.18
3	A	602	GOL	C3-C2-C1	2.47	120.86	111.80
3	B	601	GOL	O2-C2-C1	2.47	119.41	109.18
3	A	602	GOL	O2-C2-C3	2.46	119.36	109.18
3	B	601	GOL	O2-C2-C3	2.43	119.26	109.18

There are no chirality outliers.

All (5) torsion outliers are listed below:

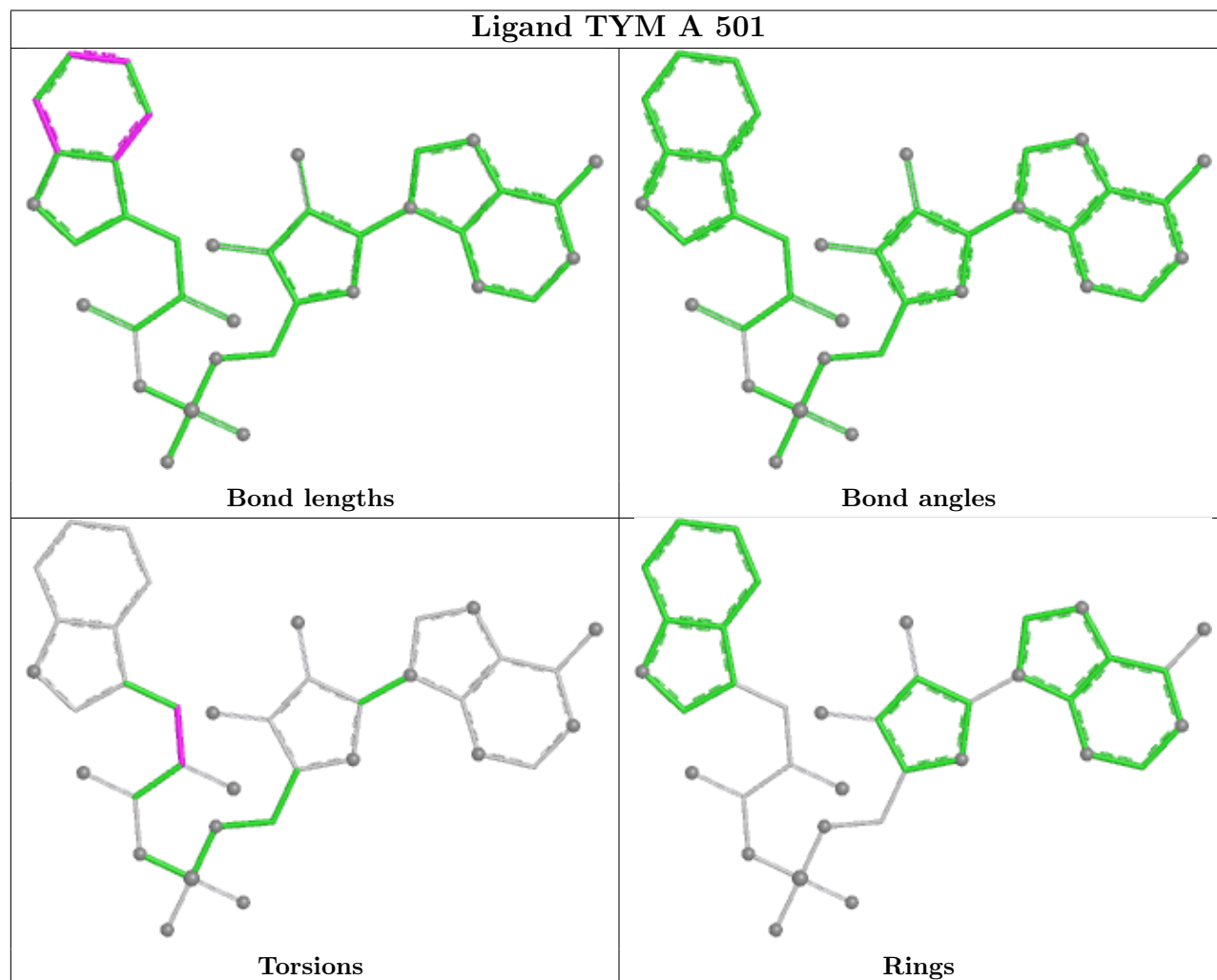
Mol	Chain	Res	Type	Atoms
3	A	602	GOL	C1-C2-C3-O3
3	B	601	GOL	O1-C1-C2-C3
3	B	601	GOL	C1-C2-C3-O3
3	A	602	GOL	O1-C1-C2-O2
2	A	501	TYM	NH3-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	GOL	1	0
2	A	501	TYM	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

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	428/477 (89%)	0.05	20 (4%) 36 38	22, 35, 62, 96	5 (1%)
1	B	353/477 (74%)	0.38	26 (7%) 20 22	22, 37, 72, 92	6 (1%)
All	All	781/954 (81%)	0.20	46 (5%) 28 30	22, 36, 70, 96	11 (1%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	167	GLU	15.5
1	B	168	ALA	13.8
1	B	166	SER	10.9
1	A	167	GLU	4.6
1	A	467	ALA	4.6
1	A	7	ALA	4.2
1	B	384	ILE	4.1
1	A	12	LEU	3.9
1	B	391	GLY	3.8
1	B	390	PHE	3.8
1	A	52	ALA	3.7
1	A	60	ALA	3.7
1	B	467	ALA	3.6
1	B	345	GLY	3.6
1	B	355	PRO	3.6
1	B	163	GLY	3.5
1	A	56	GLU	3.2
1	A	168	ALA	2.9
1	B	392	GLY	2.9
1	A	58	TYR	2.8
1	B	387	HIS	2.7
1	B	316	TYR	2.7
1	A	10	LEU	2.7
1	A	46	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	418	LYS	2.7
1	A	55	GLY	2.7
1	B	164	PRO	2.6
1	B	383	THR	2.4
1	A	9	LEU	2.4
1	A	59	LYS	2.4
1	B	365	ALA	2.3
1	B	379	GLY	2.3
1	A	166	SER	2.3
1	B	155	PRO	2.3
1	B	298	ARG	2.2
1	A	53	ALA	2.2
1	A	54	ALA	2.2
1	B	357	SER	2.2
1	B	376	ALA	2.2
1	A	50	TYR	2.2
1	B	97	GLY	2.1
1	A	57	ASP	2.1
1	A	49	SER	2.1
1	B	426	LEU	2.0
1	B	366	LYS	2.0
1	B	372	VAL	2.0

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.

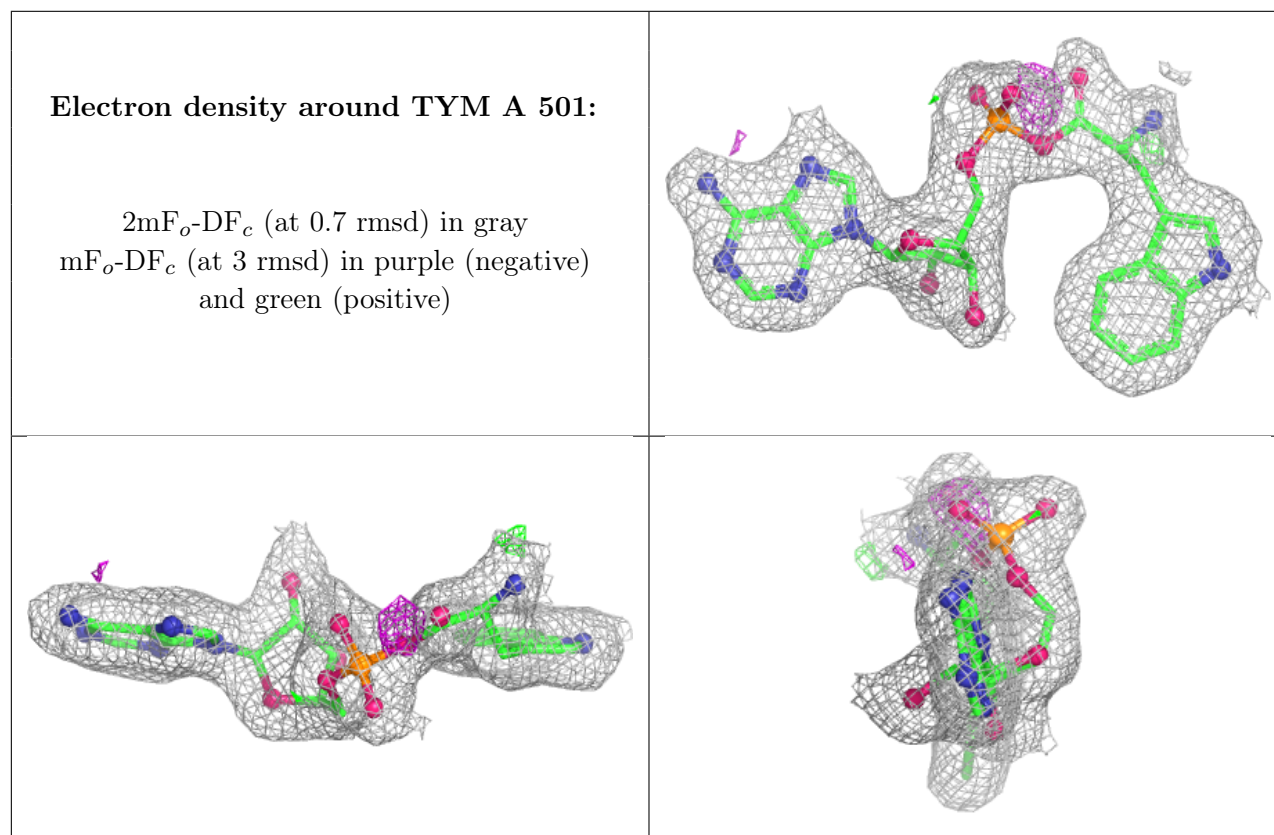
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	A	602	6/6	0.84	0.20	55,56,58,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	601	6/6	0.84	0.17	56,59,60,61	0
2	TYM	A	501	37/37	0.96	0.06	21,25,32,33	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.