Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2021 – 11:43 PM EDT

PDB ID	:	1R6U
Title	:	Crystal structure of an active fragment of human tryptophanyl-tRNA synthetase with cytokine activity
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	:	2.00 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 following versions of software and data (see references ⓘ) were used in the production of this report:

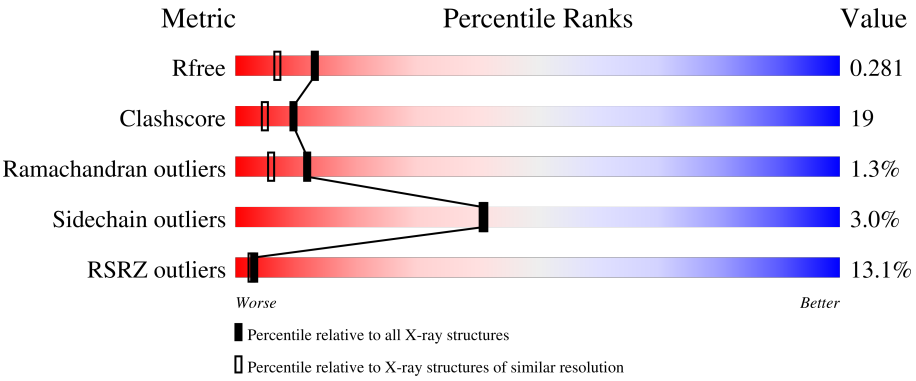
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	437	14% 54% 32% · 11%
1	B	437	8% 53% 29% · 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	601	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6205 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	388	Total	C	N	O	S	Se	0	0	0
			3129	2004	528	582	5	10			
1	B	362	Total	C	N	O	S	Se	0	0	0
			2927	1879	497	537	5	9			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	472	LYS	-	cloning artifact	UNP P23381
A	473	LEU	-	cloning artifact	UNP P23381
A	474	ALA	-	cloning artifact	UNP P23381
A	475	ALA	-	cloning artifact	UNP P23381
A	476	ALA	-	cloning artifact	UNP P23381
A	477	LEU	-	cloning artifact	UNP P23381
A	478	GLU	-	cloning artifact	UNP P23381
A	479	HIS	-	expression tag	UNP P23381
A	480	HIS	-	expression tag	UNP P23381
A	481	HIS	-	expression tag	UNP P23381
A	482	HIS	-	expression tag	UNP P23381
A	483	HIS	-	expression tag	UNP P23381
A	484	HIS	-	expression tag	UNP P23381

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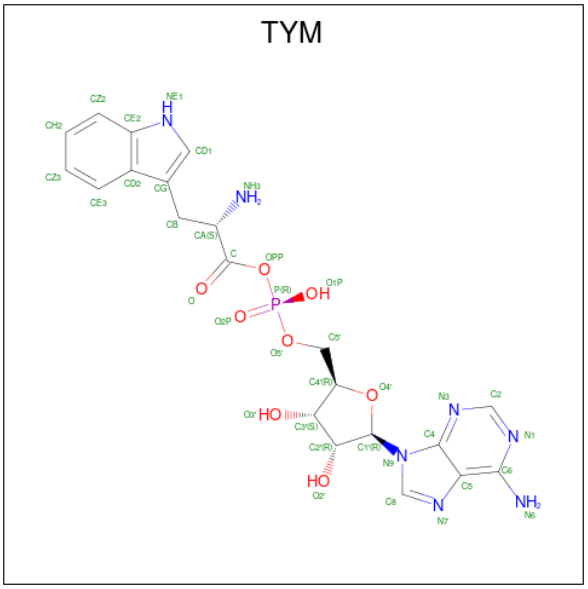
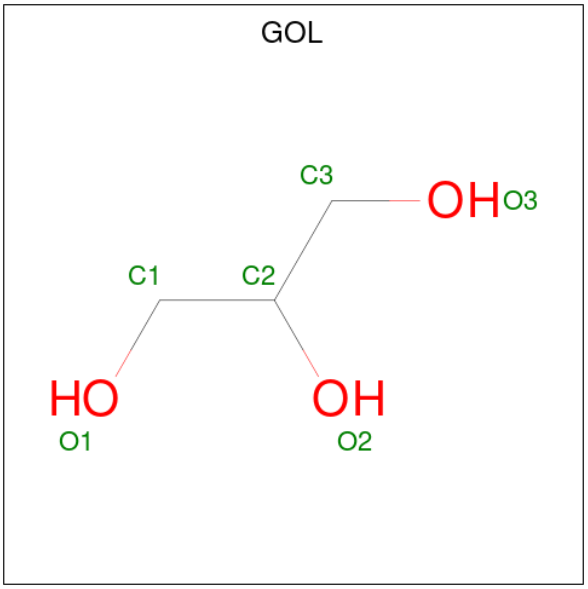
Chain	Residue	Modelled	Actual	Comment	Reference
B	143	MSE	MET	modified residue	UNP P23381
B	169	MSE	MET	modified residue	UNP P23381
B	195	MSE	MET	modified residue	UNP P23381
B	213	GLY	SER	engineered mutation	UNP P23381
B	214	ASP	TYR	engineered mutation	UNP P23381
B	241	MSE	MET	modified residue	UNP P23381
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	472	LYS	-	cloning artifact	UNP P23381
B	473	LEU	-	cloning artifact	UNP P23381
B	474	ALA	-	cloning artifact	UNP P23381
B	475	ALA	-	cloning artifact	UNP P23381
B	476	ALA	-	cloning artifact	UNP P23381
B	477	LEU	-	cloning artifact	UNP P23381
B	478	GLU	-	cloning artifact	UNP P23381
B	479	HIS	-	expression tag	UNP P23381
B	480	HIS	-	expression tag	UNP P23381
B	481	HIS	-	expression tag	UNP P23381
B	482	HIS	-	expression tag	UNP P23381
B	483	HIS	-	expression tag	UNP P23381
B	484	HIS	-	expression tag	UNP P23381

- Molecule 2 is TRYPTOPHANYL-5'AMP (three-letter code: 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 (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

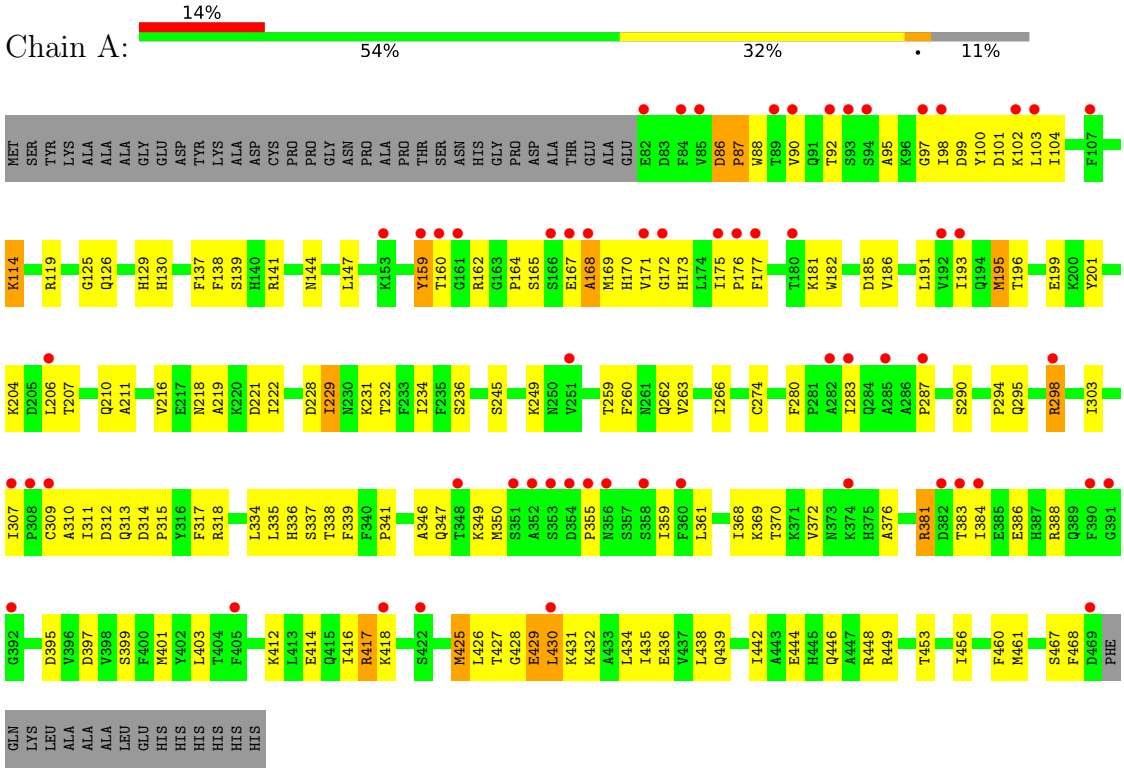
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total	O	0	0
			50	50		
4	B	50	Total	O	0	0
			50	50		

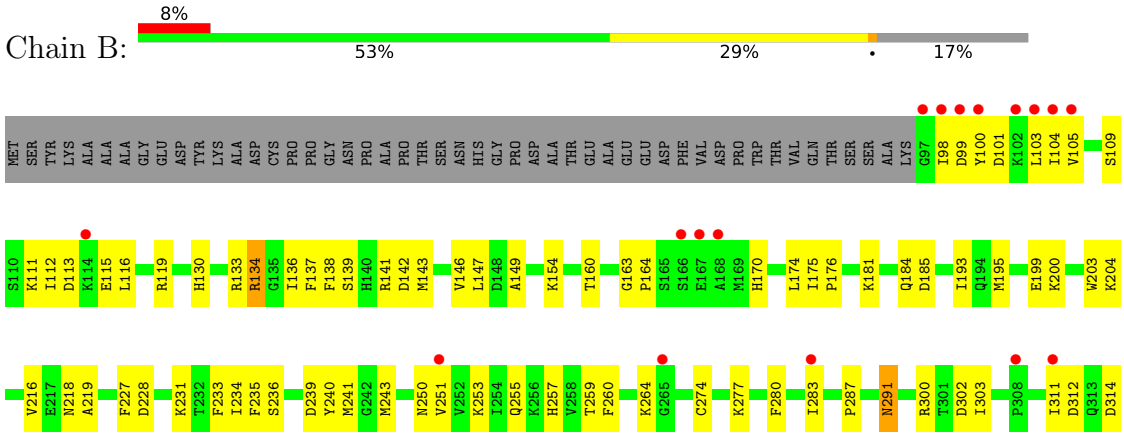
3 Residue-property plots (i)

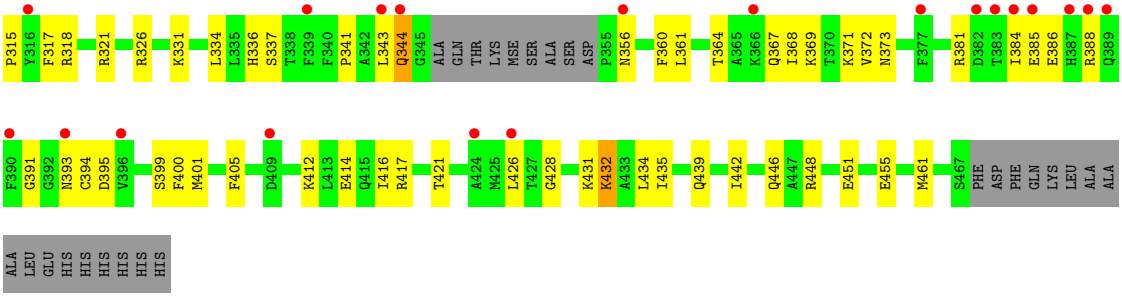
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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




P315 V316 F317 R318 R321 R326 K331 L334 L335 H336 S337 T338 F339 F340 P341 A342 L343 Q344 G345 ALA GLN THR LYS MSE SER ALA SER ASP P355 N356 F360 L361 T364 A365 K366 Q367 I368 K369 T370 K371 V372 N373 F377 R381 D382 T383 I384 E385 E386 H387 R388 Q389
F390 G391 G392 N393 C394 D395 V396 S399 F400 M401 F405 D409 K412 L413 E414 Q415 I416 R417 T421 A424 M425 L426 T427 G428 K431 K432 A433 L434 I435 Q439 I442 Q446 A447 R448 E451 E455 M461 S467 PHE ASP PHE GLN LYS LEU ALA ALA
ALA LEU GLU HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	134.66Å 96.46Å 97.13Å 90.00° 129.90° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 29.88 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.00) 96.6 (29.88-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.254 , 0.297 0.242 , 0.281	Depositor DCC
R_{free} test set	6233 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	37.7	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 52.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6205	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] 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: 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	0.38	0/3195	0.62	1/4297 (0.0%)
1	B	0.36	0/2988	0.58	0/4014
All	All	0.37	0/6183	0.60	1/8311 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	430	LEU	N-CA-C	-8.34	88.49	111.00

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	3129	0	3075	131	0
1	B	2927	0	2893	108	0
2	A	37	0	23	3	0
3	A	12	0	14	2	0
4	A	50	0	0	4	0
4	B	50	0	0	3	0
All	All	6205	0	6005	236	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (236) 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:429:GLU:HB3	1:A:432:LYS:HB2	1.18	1.12
1:A:95:ALA:HA	1:A:347:GLN:NE2	1.88	0.89
1:A:416:ILE:HA	1:A:425:MSE:HE1	1.56	0.86
1:B:250:ASN:HD21	1:B:291:ASN:ND2	1.74	0.86
1:B:143:MSE:HE3	1:B:146:VAL:HB	1.57	0.84
1:A:245:SER:O	1:A:249:LYS:HE2	1.81	0.80
1:B:250:ASN:HD21	1:B:291:ASN:HD21	1.32	0.77
1:B:241:MSE:HE1	1:B:283:ILE:HD12	1.68	0.75
1:A:206:LEU:HB2	1:A:210:GLN:HE21	1.52	0.75
1:A:432:LYS:O	1:A:436:GLU:HG3	1.86	0.75
1:A:312:ASP:HB3	1:A:339:PHE:CZ	2.23	0.74
1:B:174:LEU:HD21	1:B:361:LEU:HD21	1.69	0.73
1:B:253:LYS:O	1:B:257:HIS:HD2	1.71	0.73
1:B:141:ARG:HD3	1:B:321:ARG:NH1	2.03	0.72
1:A:95:ALA:HA	1:A:347:GLN:HE22	1.54	0.71
1:A:312:ASP:HB3	1:A:339:PHE:HZ	1.54	0.71
1:B:428:GLY:O	1:B:432:LYS:HG2	1.91	0.71
1:B:141:ARG:HD2	1:B:334:LEU:HD12	1.73	0.70
1:B:373:ASN:HA	1:B:431:LYS:HD3	1.71	0.70
1:A:137:PHE:CZ	1:A:337:SER:HB3	2.27	0.69
1:B:104:ILE:HG21	4:B:1080:HOH:O	1.92	0.69
1:B:175:ILE:HB	1:B:176:PRO:HD3	1.74	0.69
1:B:448:ARG:O	1:B:451:GLU:HG2	1.93	0.69
1:A:169:MSE:HE3	1:A:221:ASP:HB2	1.74	0.68
1:A:141:ARG:HG3	1:A:141:ARG:HH11	1.59	0.67
1:A:309:CYS:SG	4:A:1087:HOH:O	2.52	0.67
1:B:251:VAL:O	1:B:255:GLN:HG3	1.95	0.66
1:A:90:VAL:HG23	1:A:349:LYS:HE3	1.78	0.65
1:A:181:LYS:HE2	1:A:185:ASP:OD2	1.96	0.64
1:A:229:ILE:HG12	1:A:460:PHE:CE1	2.32	0.64
1:B:112:ILE:HG23	1:B:116:LEU:HD23	1.80	0.64
1:A:310:ALA:HB3	1:A:312:ASP:OD1	1.99	0.63
1:B:300:ARG:HG2	1:B:300:ARG:HH11	1.62	0.63
1:B:104:ILE:HD11	1:B:111:LYS:N	2.14	0.62
1:A:429:GLU:HB3	1:A:432:LYS:CB	2.11	0.62
1:B:104:ILE:HD13	1:B:139:SER:HB3	1.82	0.62
1:B:321:ARG:O	1:B:331:LYS:HE3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:HIS:CD2	4:A:1087:HOH:O	2.53	0.61
1:B:104:ILE:HD12	1:B:109:SER:OG	2.00	0.61
1:B:356:ASN:HA	1:B:371:LYS:HE2	1.82	0.61
1:B:369:LYS:HA	1:B:435:ILE:HD13	1.83	0.61
1:A:429:GLU:C	1:A:432:LYS:H	2.04	0.61
1:A:144:ASN:HB2	4:A:1034:HOH:O	2.01	0.61
1:A:418:LYS:HB2	1:A:418:LYS:NZ	2.15	0.61
1:B:112:ILE:HB	1:B:138:PHE:O	2.02	0.60
1:A:438:LEU:O	1:A:442:ILE:HG12	2.01	0.60
1:A:444:GLU:HB3	1:A:448:ARG:HH12	1.65	0.60
1:A:442:ILE:O	1:A:446:GLN:HG3	2.01	0.60
1:B:384:ILE:HG23	1:B:385:GLU:OE2	2.02	0.60
1:B:113:ASP:OD1	1:B:115:GLU:HB3	2.02	0.59
1:B:234:ILE:O	1:B:461:MSE:HA	2.02	0.59
1:A:201:TYR:HA	1:A:206:LEU:HD11	1.84	0.59
1:B:181:LYS:HD3	1:B:185:ASP:OD2	2.02	0.59
1:A:171:VAL:HG23	1:A:359:ILE:O	2.02	0.59
1:B:119:ARG:HD3	1:B:147:LEU:HD13	1.86	0.58
1:B:101:ASP:O	1:B:104:ILE:HG22	2.03	0.58
1:A:137:PHE:CE1	1:A:337:SER:HB3	2.38	0.58
1:A:431:LYS:O	1:A:435:ILE:HG13	2.04	0.57
1:A:206:LEU:CB	1:A:210:GLN:HE21	2.18	0.56
1:A:100:TYR:O	1:A:101:ASP:HB3	2.06	0.56
1:A:368:ILE:O	1:A:372:VAL:HG23	2.05	0.56
1:A:199:GLU:HB2	1:A:280:PHE:CZ	2.40	0.56
1:A:229:ILE:HD13	1:A:229:ILE:O	2.05	0.56
1:A:416:ILE:HG23	1:A:425:MSE:SE	2.55	0.55
1:A:274:CYS:HA	1:B:259:THR:HA	1.87	0.55
1:A:427:THR:O	1:A:428:GLY:C	2.44	0.55
1:A:141:ARG:HG3	1:A:141:ARG:NH1	2.22	0.55
1:A:169:MSE:HA	1:A:173:HIS:ND1	2.21	0.55
1:B:137:PHE:CE1	1:B:337:SER:HB3	2.42	0.55
1:A:234:ILE:O	1:A:461:MSE:HA	2.06	0.55
1:B:442:ILE:O	1:B:446:GLN:HG3	2.07	0.55
1:B:139:SER:OG	1:B:311:ILE:HD13	2.07	0.54
1:B:104:ILE:HG12	1:B:111:LYS:HB2	1.89	0.54
1:B:203:TRP:CD1	1:B:277:LYS:HE2	2.43	0.54
1:A:100:TYR:C	1:A:102:LYS:H	2.11	0.53
1:A:453:THR:O	1:A:456:ILE:HB	2.09	0.53
1:A:164:PRO:HG3	1:A:195:MSE:HG3	1.89	0.53
1:B:98:ILE:HG21	1:B:100:TYR:HE2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ILE:HD12	1:B:405:PHE:CE1	2.44	0.53
1:A:307:ILE:HB	1:A:334:LEU:HD23	1.90	0.53
1:B:318:ARG:HG2	1:B:318:ARG:HH11	1.73	0.53
1:B:199:GLU:HB2	1:B:280:PHE:CZ	2.44	0.53
1:B:98:ILE:HG21	1:B:100:TYR:CE2	2.43	0.53
1:B:130:HIS:O	1:B:134:ARG:HB2	2.08	0.53
1:A:429:GLU:C	1:A:431:LYS:N	2.53	0.53
1:A:260:PHE:O	1:A:263:VAL:HG12	2.09	0.52
1:A:294:PRO:HA	1:A:298:ARG:O	2.08	0.52
1:B:141:ARG:HD3	1:B:321:ARG:HH11	1.71	0.52
1:B:317:PHE:O	1:B:321:ARG:HG3	2.10	0.52
1:B:364:THR:O	1:B:368:ILE:HG13	2.09	0.52
1:A:162:ARG:HG3	1:A:162:ARG:HH11	1.74	0.52
1:B:432:LYS:HE3	1:B:432:LYS:HA	1.90	0.52
1:A:98:ILE:HD12	1:A:98:ILE:N	2.25	0.52
1:B:241:MSE:CE	1:B:283:ILE:HD12	2.38	0.52
1:A:99:ASP:OD1	1:A:102:LYS:HD2	2.10	0.52
1:A:453:THR:OG1	1:A:456:ILE:HG12	2.10	0.52
1:A:159:TYR:CZ	1:A:287:PRO:HB2	2.45	0.51
1:B:204:LYS:HE3	4:B:1078:HOH:O	2.08	0.51
1:B:341:PRO:HG3	1:B:401:MSE:HE2	1.92	0.51
1:B:368:ILE:CD1	1:B:442:ILE:HD12	2.40	0.51
1:B:112:ILE:HG12	1:B:116:LEU:HD23	1.91	0.51
1:B:341:PRO:HG2	1:B:401:MSE:HB3	1.91	0.51
1:B:233:PHE:CZ	1:B:235:PHE:HB3	2.45	0.51
1:A:129:HIS:CD2	3:A:602:GOL:H31	2.45	0.50
1:A:141:ARG:HG3	1:A:334:LEU:HD12	1.93	0.50
1:A:173:HIS:O	1:A:176:PRO:HD2	2.12	0.50
1:B:326:ARG:HH11	1:B:326:ARG:HG3	1.76	0.50
1:A:412:LYS:O	1:A:416:ILE:HG13	2.11	0.50
1:A:429:GLU:OE1	1:A:432:LYS:HG3	2.12	0.50
1:A:444:GLU:HB3	1:A:448:ARG:NH1	2.26	0.50
1:A:172:GLY:O	1:A:175:ILE:HG12	2.12	0.49
1:A:177:PHE:CE1	1:A:222:ILE:HD12	2.47	0.49
1:A:372:VAL:HG12	1:A:431:LYS:HB3	1.94	0.49
1:A:103:LEU:HD23	1:A:311:ILE:HD13	1.93	0.49
1:A:206:LEU:CD1	1:A:211:ALA:HB2	2.42	0.49
1:A:283:ILE:N	1:A:283:ILE:HD12	2.27	0.49
1:A:383:THR:HG22	1:A:386:GLU:OE1	2.12	0.49
1:B:143:MSE:HE3	1:B:146:VAL:CB	2.36	0.49
1:B:228:ASP:CB	1:B:231:LYS:HE2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:LYS:HG2	1:A:468:PHE:CE1	2.47	0.49
1:A:86:ASP:OD2	1:A:88:TRP:HE3	1.96	0.49
1:B:133:ARG:O	1:B:134:ARG:HG3	2.13	0.49
1:B:139:SER:OG	1:B:336:HIS:HB2	2.13	0.49
1:A:182:TRP:O	1:A:186:VAL:HG22	2.13	0.49
1:A:449:ARG:HH11	1:A:449:ARG:HG2	1.78	0.49
1:A:262:GLN:O	1:A:266:ILE:HG12	2.13	0.48
1:B:112:ILE:CB	1:B:138:PHE:O	2.61	0.48
1:B:321:ARG:HB3	1:B:331:LYS:HE2	1.95	0.48
1:A:87:PRO:HD3	1:A:315:PRO:HG2	1.94	0.48
1:A:369:LYS:HG3	1:A:370:THR:N	2.28	0.48
1:B:149:ALA:HA	1:B:154:LYS:HE3	1.96	0.48
1:A:199:GLU:HB2	1:A:280:PHE:CE1	2.48	0.48
1:A:395:ASP:O	1:A:401:MSE:HE3	2.13	0.48
1:A:381:ARG:HG2	1:A:381:ARG:HH11	1.78	0.48
1:B:228:ASP:HB3	1:B:231:LYS:HE2	1.96	0.48
1:B:98:ILE:HG23	1:B:99:ASP:N	2.29	0.48
1:B:143:MSE:CE	1:B:146:VAL:HB	2.38	0.48
1:A:97:GLY:HA2	1:A:346:ALA:O	2.14	0.48
1:A:280:PHE:HA	1:A:283:ILE:HD13	1.95	0.48
1:A:95:ALA:HA	1:A:347:GLN:HE21	1.75	0.47
1:A:170:HIS:ND1	1:A:350:MSE:SE	2.97	0.47
1:A:384:ILE:O	1:A:388:ARG:HG2	2.14	0.47
1:B:388:ARG:HH21	1:B:426:LEU:HD11	1.79	0.47
1:A:119:ARG:HG2	1:A:147:LEU:HD13	1.95	0.47
1:A:318:ARG:HB3	4:A:1041:HOH:O	2.13	0.47
1:A:426:LEU:C	1:A:428:GLY:N	2.64	0.47
1:B:149:ALA:O	1:B:154:LYS:HB2	2.15	0.47
1:B:104:ILE:CG2	4:B:1080:HOH:O	2.57	0.47
1:A:138:PHE:H	1:A:138:PHE:HD2	1.61	0.47
1:A:196:THR:HB	1:A:199:GLU:HB3	1.96	0.47
1:A:314:ASP:N	1:A:315:PRO:CD	2.78	0.47
1:B:435:ILE:O	1:B:439:GLN:HG3	2.14	0.47
1:B:104:ILE:HG23	1:B:105:VAL:N	2.29	0.46
1:B:393:ASN:OD1	1:B:395:ASP:HB2	2.15	0.46
1:B:394:CYS:HB3	1:B:400:PHE:CD2	2.51	0.46
1:A:206:LEU:C	1:A:206:LEU:HD12	2.36	0.46
1:A:259:THR:OG1	1:A:262:GLN:HG3	2.15	0.46
1:B:184:GLN:HE22	1:B:227:PHE:HD1	1.64	0.46
1:A:169:MSE:HG3	1:A:361:LEU:HD22	1.97	0.46
1:B:100:TYR:CD1	1:B:103:LEU:HD12	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:ILE:O	1:B:287:PRO:HD3	2.15	0.46
1:A:418:LYS:HB2	1:A:418:LYS:HZ2	1.78	0.46
1:B:381:ARG:HG3	1:B:386:GLU:O	2.16	0.45
1:A:100:TYR:CZ	1:A:338:THR:HB	2.51	0.45
1:A:207:THR:H	1:A:210:GLN:NE2	2.15	0.45
1:B:104:ILE:HG23	1:B:105:VAL:HG13	1.99	0.45
1:B:311:ILE:HG23	1:B:312:ASP:N	2.31	0.45
1:B:300:ARG:HG2	1:B:300:ARG:NH1	2.27	0.45
1:A:206:LEU:HD11	1:A:211:ALA:HB2	1.99	0.45
1:A:201:TYR:HE1	3:A:601:GOL:HO2	1.62	0.45
1:A:259:THR:HA	1:B:274:CYS:HA	1.99	0.45
1:A:372:VAL:O	1:A:376:ALA:HB3	2.16	0.45
1:B:163:GLY:HA3	1:B:200:LYS:HE2	1.99	0.45
1:B:184:GLN:NE2	1:B:227:PHE:HD1	2.15	0.45
1:A:435:ILE:O	1:A:439:GLN:HG3	2.17	0.45
1:B:98:ILE:HG23	1:B:99:ASP:H	1.82	0.45
1:B:414:GLU:OE2	1:B:417:ARG:NH2	2.51	0.44
1:A:139:SER:HB3	1:A:336:HIS:HB2	1.99	0.44
1:A:216:VAL:O	1:A:219:ALA:HB3	2.18	0.44
1:A:100:TYR:O	1:A:101:ASP:CB	2.66	0.44
1:A:114:LYS:HE3	1:A:114:LYS:HA	2.00	0.44
1:A:310:ALA:HB3	2:A:501:TYM:O2'	2.18	0.44
1:B:136:ILE:O	1:B:337:SER:HA	2.17	0.44
1:A:307:ILE:HD13	1:A:317:PHE:CE1	2.52	0.44
1:A:218:ASN:N	1:A:218:ASN:HD22	2.16	0.44
1:A:349:LYS:HB2	2:A:501:TYM:N6	2.32	0.44
1:A:274:CYS:HB2	1:B:255:GLN:O	2.18	0.43
1:B:104:ILE:CD1	1:B:139:SER:HB3	2.47	0.43
1:A:339:PHE:O	1:A:341:PRO:HD3	2.18	0.43
1:A:207:THR:OG1	1:A:210:GLN:HG3	2.19	0.43
1:A:397:ASP:OD1	1:A:399:SER:HB2	2.18	0.43
1:A:403:LEU:HD21	1:A:434:LEU:HA	2.00	0.43
1:A:130:HIS:CD2	1:A:130:HIS:H	2.37	0.43
1:B:260:PHE:CE2	1:B:264:LYS:HD2	2.54	0.43
1:A:228:ASP:OD1	1:A:231:LYS:HE3	2.19	0.43
1:B:142:ASP:OD1	1:B:321:ARG:NH2	2.52	0.43
1:B:314:ASP:N	1:B:315:PRO:CD	2.82	0.43
1:A:165:SER:CB	1:A:168:ALA:HB3	2.49	0.43
1:B:373:ASN:HD21	1:B:432:LYS:HE2	1.84	0.43
1:B:388:ARG:NH2	1:B:426:LEU:HD11	2.34	0.43
1:A:428:GLY:O	1:A:429:GLU:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LEU:CD2	1:A:311:ILE:HD13	2.49	0.43
1:A:165:SER:HB3	1:A:168:ALA:HB3	2.01	0.43
1:B:384:ILE:HG23	1:B:385:GLU:CD	2.38	0.43
1:B:412:LYS:O	1:B:416:ILE:HG13	2.18	0.43
1:A:191:LEU:HD23	1:A:232:THR:HG23	2.00	0.42
1:A:162:ARG:HG3	2:A:501:TYM:O1P	2.18	0.42
1:B:326:ARG:HG3	1:B:326:ARG:NH1	2.34	0.42
1:A:101:ASP:HA	1:A:104:ILE:HD12	2.01	0.42
1:A:167:GLU:O	1:A:168:ALA:O	2.37	0.42
1:B:104:ILE:CG2	1:B:105:VAL:N	2.82	0.42
1:B:160:THR:O	1:B:193:ILE:HA	2.19	0.42
1:A:160:THR:O	1:A:193:ILE:HA	2.19	0.42
1:B:216:VAL:O	1:B:219:ALA:HB3	2.19	0.42
1:B:250:ASN:ND2	1:B:291:ASN:ND2	2.55	0.42
1:B:98:ILE:O	1:B:99:ASP:HB3	2.20	0.42
1:A:162:ARG:HG3	1:A:162:ARG:NH1	2.35	0.42
1:A:92:THR:HG23	1:A:347:GLN:HA	2.02	0.42
1:B:300:ARG:NH2	1:B:302:ASP:OD2	2.53	0.41
1:A:138:PHE:CD2	1:A:138:PHE:N	2.86	0.41
1:B:391:GLY:HA3	1:B:421:THR:O	2.20	0.41
1:B:164:PRO:HG3	1:B:195:MSE:HE3	2.01	0.41
1:A:162:ARG:NE	1:A:218:ASN:OD1	2.45	0.41
1:A:414:GLU:OE2	1:A:417:ARG:NH1	2.52	0.41
1:A:218:ASN:O	1:A:222:ILE:HG12	2.21	0.41
1:B:399:SER:HA	1:B:434:LEU:HD22	2.03	0.41
1:B:170:HIS:HA	1:B:360:PHE:HA	2.02	0.41
1:B:344:GLN:HE21	1:B:344:GLN:HB2	1.67	0.41
1:A:426:LEU:O	1:A:427:THR:C	2.59	0.41
1:B:240:TYR:HA	1:B:243:MSE:HG2	2.03	0.41
1:A:313:GLN:O	1:A:317:PHE:CD2	2.74	0.41
1:B:368:ILE:HD13	1:B:442:ILE:HD12	2.02	0.41
1:A:290:SER:HB3	1:A:303:ILE:HB	2.02	0.40
1:A:125:GLY:O	1:A:126:GLN:HG2	2.21	0.40
1:B:367:GLN:O	1:B:371:LYS:HG2	2.21	0.40
1:B:115:GLU:OE1	1:B:115:GLU:O	2.39	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	386/437 (88%)	360 (93%)	20 (5%)	6 (2%)	9 4
1	B	358/437 (82%)	336 (94%)	18 (5%)	4 (1%)	14 8
All	All	744/874 (85%)	696 (94%)	38 (5%)	10 (1%)	12 6

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	ALA
1	A	381	ARG
1	A	429	GLU
1	A	355	PRO
1	B	134	ARG
1	B	343	LEU
1	A	467	SER
1	B	303	ILE
1	B	372	VAL
1	A	87	PRO

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	343/369 (93%)	330 (96%)	13 (4%)	33 31
1	B	320/369 (87%)	313 (98%)	7 (2%)	52 55
All	All	663/738 (90%)	643 (97%)	20 (3%)	41 41

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ASP
1	A	114	LYS
1	A	159	TYR
1	A	195	MSE
1	A	204	LYS
1	A	229	ILE
1	A	236	SER
1	A	295	GLN
1	A	298	ARG
1	A	335	LEU
1	A	417	ARG
1	A	425	MSE
1	A	430	LEU
1	B	218	ASN
1	B	236	SER
1	B	239	ASP
1	B	291	ASN
1	B	344	GLN
1	B	432	LYS
1	B	455	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	130	HIS
1	A	152	ASN
1	A	210	GLN
1	A	255	GLN
1	A	373	ASN
1	A	389	GLN
1	A	415	GLN
1	A	446	GLN
1	B	118	ASN
1	B	126	GLN
1	B	184	GLN
1	B	257	HIS
1	B	261	ASN
1	B	291	ASN
1	B	344	GLN
1	B	356	ASN

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)

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	601	-	5,5,5	0.38	0	5,5,5	1.86	3 (60%)
3	GOL	A	602	-	5,5,5	0.32	0	5,5,5	1.84	3 (60%)
2	TYM	A	501	-	36,41,41	0.94	3 (8%)	39,61,61	0.82	1 (2%)

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	601	-	-	3/4/4/4	-
3	GOL	A	602	-	-	2/4/4/4	-
2	TYM	A	501	-	-	2/16/39/39	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	CZ3-CE3	2.39	1.42	1.36
2	A	501	TYM	C2-N3	2.28	1.35	1.32
2	A	501	TYM	CH2-CZ3	2.05	1.43	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	GOL	C3-C2-C1	2.65	121.99	111.70
3	A	602	GOL	C3-C2-C1	2.43	121.13	111.70
3	A	602	GOL	O2-C2-C1	2.38	119.61	109.12
3	A	601	GOL	O2-C2-C1	2.31	119.32	109.12
3	A	602	GOL	O2-C2-C3	2.30	119.26	109.12
3	A	601	GOL	O2-C2-C3	2.17	118.69	109.12
2	A	501	TYM	C5-C6-N6	2.02	123.42	120.35

There are no chirality outliers.

All (7) torsion outliers are listed below:

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

There are no ring outliers.

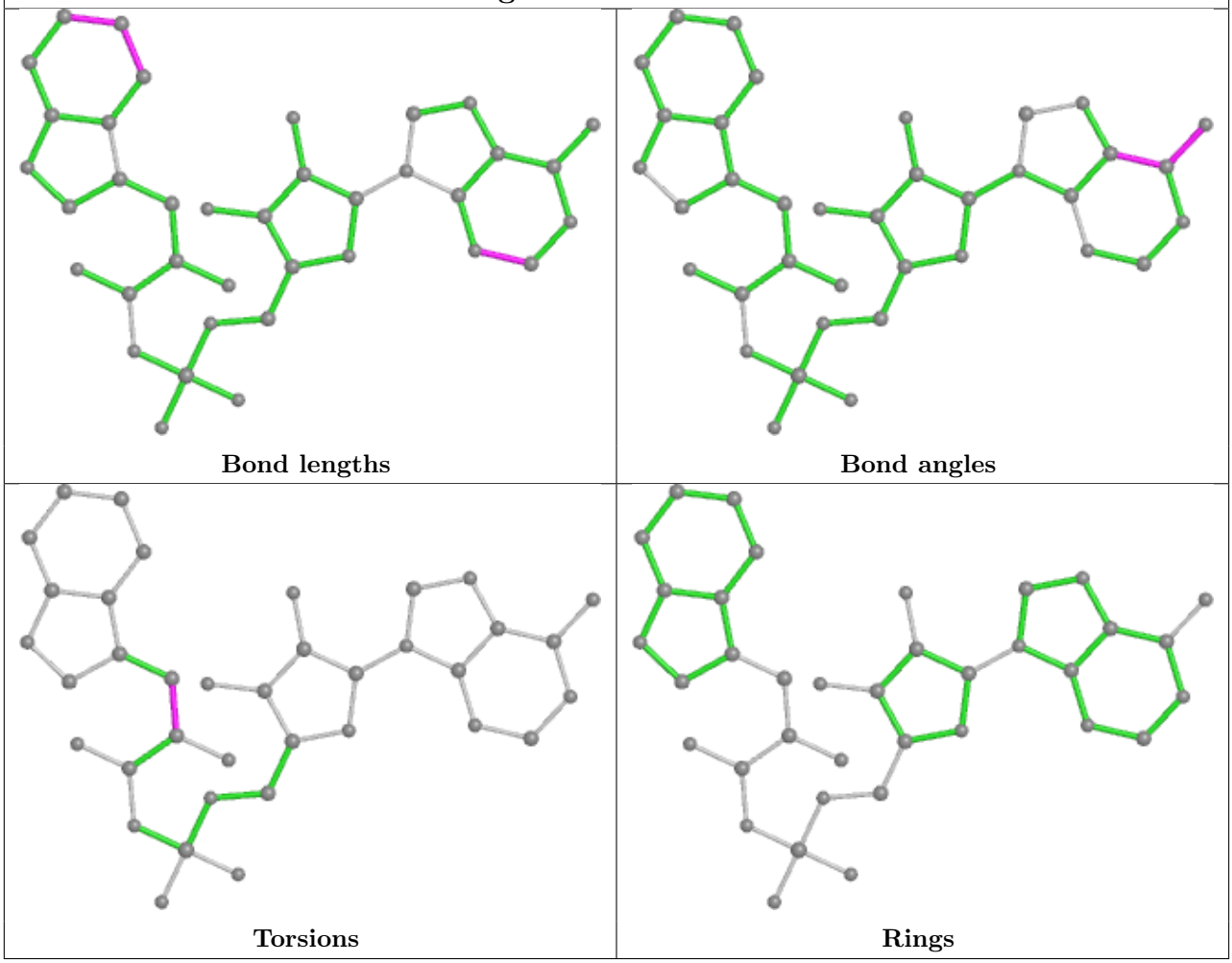
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	GOL	1	0
3	A	602	GOL	1	0
2	A	501	TYM	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 TYM A 501



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	378/437 (86%)	0.82	59 (15%)	2	1	22, 49, 76, 84	11 (2%)
1	B	353/437 (80%)	0.55	37 (10%)	6	5	20, 51, 77, 88	6 (1%)
All	All	731/874 (83%)	0.69	96 (13%)	3	3	20, 50, 76, 88	17 (2%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	353	SER	5.4
1	A	167	GLU	5.3
1	A	390	PHE	5.2
1	B	390	PHE	5.2
1	B	384	ILE	5.0
1	A	355	PRO	5.0
1	B	98	ILE	4.7
1	A	352	ALA	4.6
1	B	100	TYR	4.4
1	A	90	VAL	4.3
1	A	168	ALA	4.2
1	A	85	VAL	4.2
1	B	166	SER	4.1
1	B	389	GLN	4.1
1	B	102	LYS	4.0
1	A	98	ILE	3.8
1	A	160	THR	3.8
1	A	161	GLY	3.7
1	B	97	GLY	3.7
1	A	283	ILE	3.7
1	B	103	LEU	3.7
1	A	469	ASP	3.6
1	A	391	GLY	3.5
1	A	374	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	385	GLU	3.4
1	A	159	TYR	3.3
1	A	166	SER	3.3
1	B	167	GLU	3.3
1	B	104	ILE	3.3
1	B	168	ALA	3.3
1	A	93	SER	3.2
1	A	360	PHE	3.2
1	B	426	LEU	3.2
1	B	311	ILE	3.2
1	A	172	GLY	3.2
1	A	175	ILE	3.1
1	A	94	SER	3.1
1	A	282	ALA	3.0
1	A	176	PRO	3.0
1	B	344	GLN	3.0
1	A	177	PHE	3.0
1	B	383	THR	3.0
1	A	107	PHE	3.0
1	A	192	VAL	2.9
1	A	84	PHE	2.9
1	A	308	PRO	2.8
1	A	354	ASP	2.8
1	A	351	SER	2.8
1	A	392	GLY	2.8
1	A	251	VAL	2.8
1	A	307	ILE	2.8
1	A	298	ARG	2.7
1	B	382	ASP	2.7
1	A	382	ASP	2.7
1	A	82	GLU	2.7
1	A	92	THR	2.6
1	A	103	LEU	2.6
1	A	384	ILE	2.6
1	A	97	GLY	2.6
1	B	366	LYS	2.6
1	A	383	THR	2.5
1	B	283	ILE	2.5
1	B	393	ASN	2.5
1	B	343	LEU	2.5
1	B	396	VAL	2.5
1	B	339	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	251	VAL	2.5
1	B	356	ASN	2.4
1	A	89	THR	2.4
1	A	309	CYS	2.4
1	B	409	ASP	2.4
1	B	388	ARG	2.4
1	B	114	LYS	2.4
1	B	99	ASP	2.4
1	B	377	PHE	2.3
1	A	285	ALA	2.3
1	A	430	LEU	2.3
1	A	287	PRO	2.3
1	A	422	SER	2.3
1	A	348	THR	2.3
1	B	387	HIS	2.3
1	A	171	VAL	2.3
1	B	316	TYR	2.2
1	A	418	LYS	2.2
1	B	265	GLY	2.2
1	A	193	ILE	2.2
1	A	180	THR	2.2
1	A	153	LYS	2.2
1	A	356	ASN	2.2
1	A	102	LYS	2.1
1	A	358	SER	2.1
1	B	308	PRO	2.1
1	A	206	LEU	2.1
1	B	424	ALA	2.1
1	A	405	PHE	2.0
1	B	105	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 monosaccharides in this entry.

6.4 Ligands

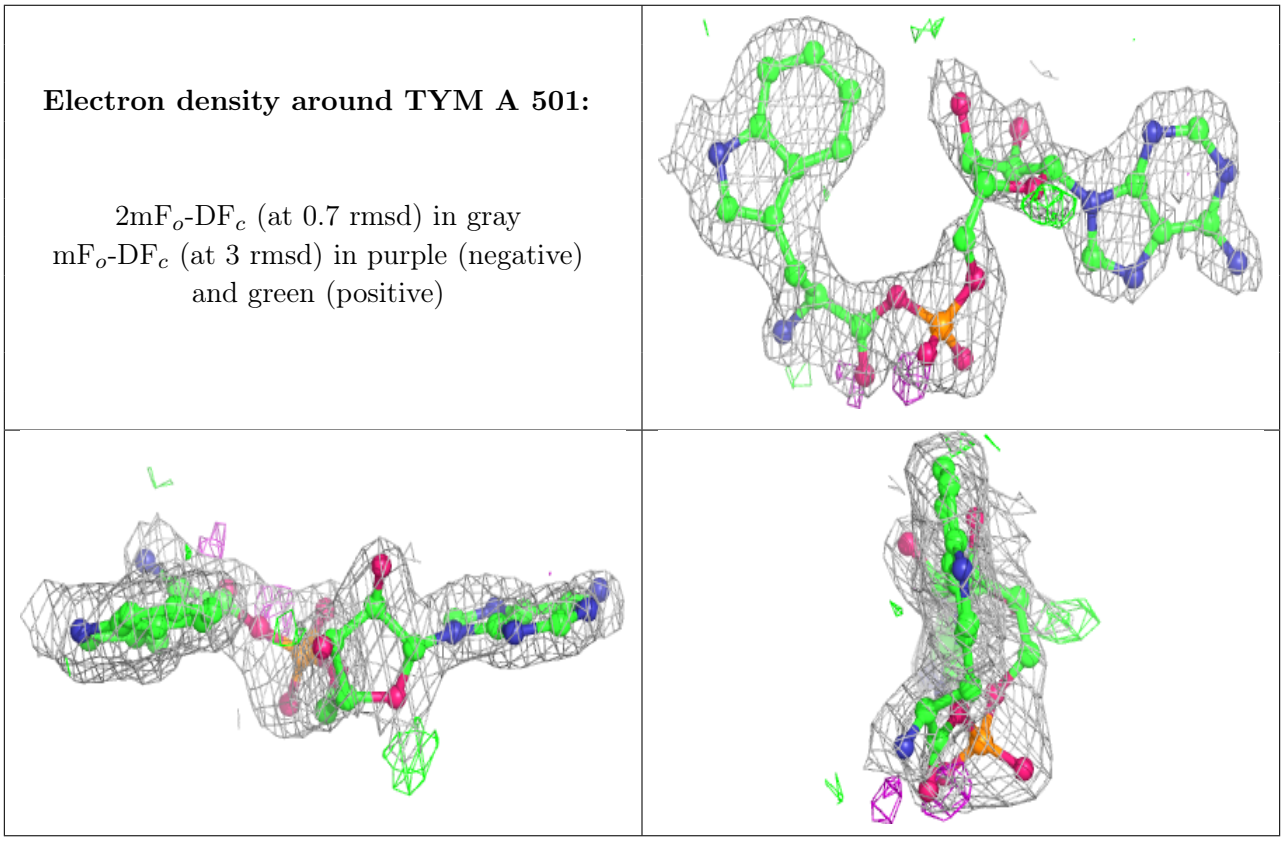
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	GOL	A	602	6/6	0.62	0.33	55,57,57,57	0
3	GOL	A	601	6/6	0.80	0.29	52,54,54,55	0
2	TYM	A	501	37/37	0.87	0.24	45,53,60,60	8

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 TYM 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

There are no such residues in this entry.