wwPDB X-ray Structure Validation Summary Report (i)

Sep 23, 2023 – 02:05 PM EDT

PDB ID	:	5SUL
Title	:	Inhibited state structure of yGsy2p
Authors	:	Mahalingan, K.K.; Hurley, T.D.
Deposited on	:	2016-08-03
Resolution	:	3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

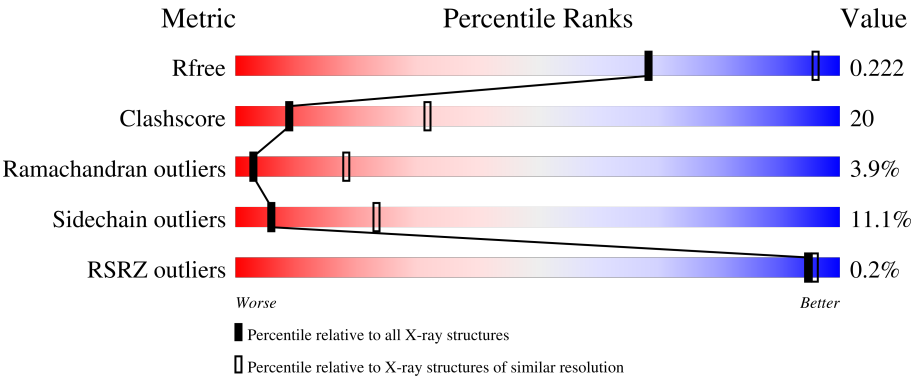
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	725	51% 30% 5% 15%
1	B	725	46% 32% 6% 16%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9615 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 Glycogen [starch] synthase isoform 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	619	Total	C	N	O	S	0	0	0
			4849	3087	838	905	19			
1	B	606	Total	C	N	O	S	0	0	0
			4720	3016	806	880	18			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P27472
A	-18	GLY	-	expression tag	UNP P27472
A	-17	SER	-	expression tag	UNP P27472
A	-16	SER	-	expression tag	UNP P27472
A	-15	HIS	-	expression tag	UNP P27472
A	-14	HIS	-	expression tag	UNP P27472
A	-13	HIS	-	expression tag	UNP P27472
A	-12	HIS	-	expression tag	UNP P27472
A	-11	HIS	-	expression tag	UNP P27472
A	-10	HIS	-	expression tag	UNP P27472
A	-9	SER	-	expression tag	UNP P27472
A	-8	SER	-	expression tag	UNP P27472
A	-7	GLY	-	expression tag	UNP P27472
A	-6	LEU	-	expression tag	UNP P27472
A	-5	VAL	-	expression tag	UNP P27472
A	-4	PRO	-	expression tag	UNP P27472
A	-3	ARG	-	expression tag	UNP P27472
A	-2	GLY	-	expression tag	UNP P27472
A	-1	SER	-	expression tag	UNP P27472
A	0	HIS	-	expression tag	UNP P27472
A	535	SER	ALA	conflict	UNP P27472
A	589	ALA	ARG	conflict	UNP P27472
A	592	ALA	ARG	conflict	UNP P27472
B	-19	MET	-	initiating methionine	UNP P27472
B	-18	GLY	-	expression tag	UNP P27472

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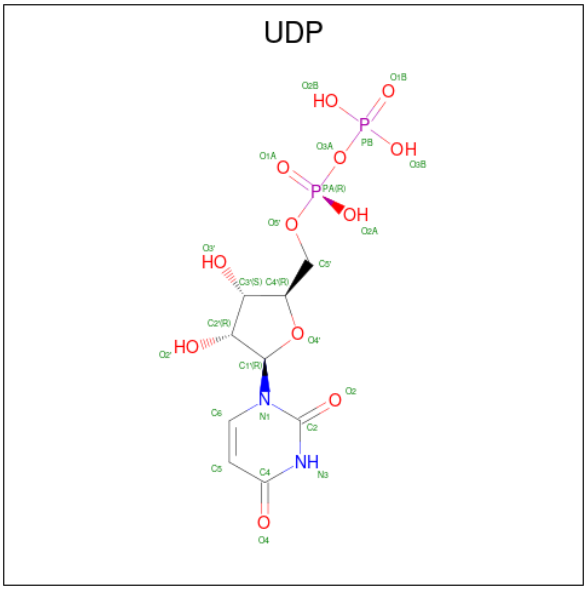
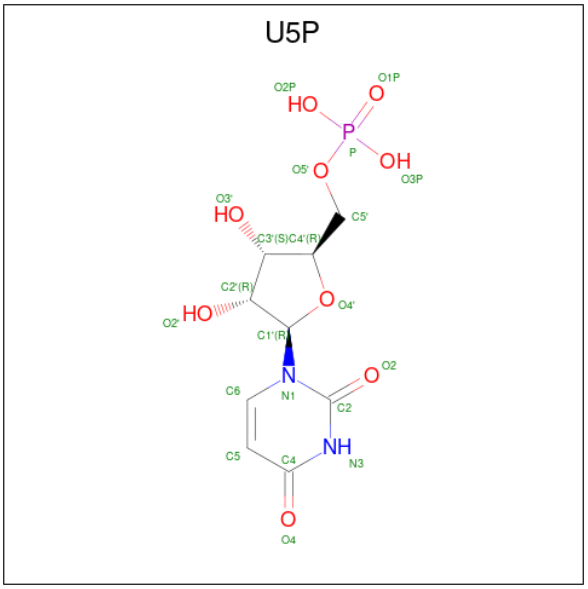
Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP P27472
B	-16	SER	-	expression tag	UNP P27472
B	-15	HIS	-	expression tag	UNP P27472
B	-14	HIS	-	expression tag	UNP P27472
B	-13	HIS	-	expression tag	UNP P27472
B	-12	HIS	-	expression tag	UNP P27472
B	-11	HIS	-	expression tag	UNP P27472
B	-10	HIS	-	expression tag	UNP P27472
B	-9	SER	-	expression tag	UNP P27472
B	-8	SER	-	expression tag	UNP P27472
B	-7	GLY	-	expression tag	UNP P27472
B	-6	LEU	-	expression tag	UNP P27472
B	-5	VAL	-	expression tag	UNP P27472
B	-4	PRO	-	expression tag	UNP P27472
B	-3	ARG	-	expression tag	UNP P27472
B	-2	GLY	-	expression tag	UNP P27472
B	-1	SER	-	expression tag	UNP P27472
B	0	HIS	-	expression tag	UNP P27472
B	535	SER	ALA	conflict	UNP P27472
B	589	ALA	ARG	conflict	UNP P27472
B	592	ALA	ARG	conflict	UNP P27472

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 3 is URIDINE-5'-MONOPHOSPHATE (three-letter code: U5P) (formula: $C_9H_{13}N_2O_9P$).



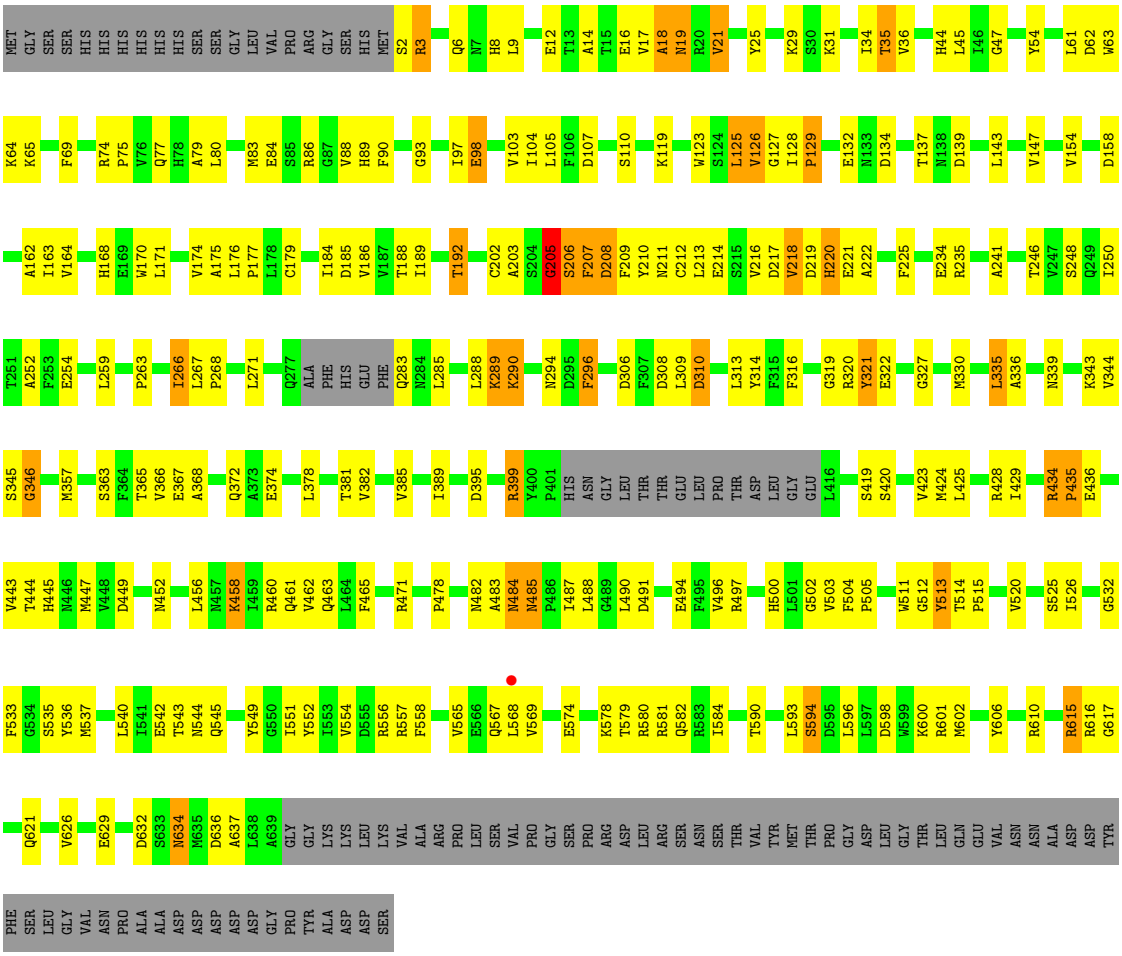
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			21	9	2	9	1		

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.

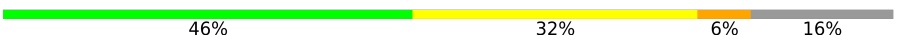
• Molecule 1: Glycogen [starch] synthase isoform 2

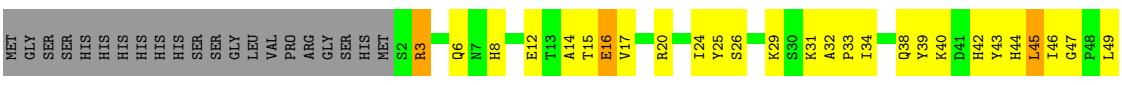
Chain A:

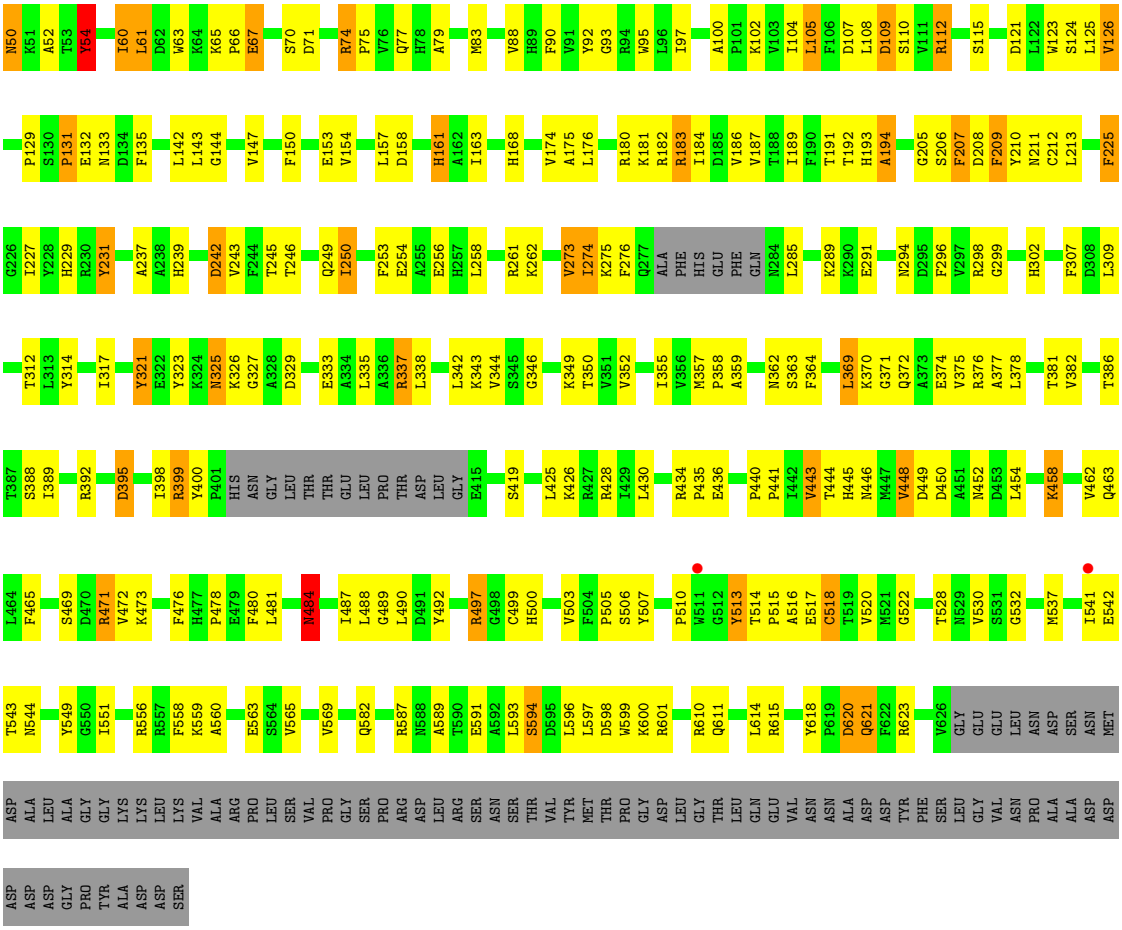


• Molecule 1: Glycogen [starch] synthase isoform 2

Chain B:






N50 K51 A52 T53 V54 I60 L61 D62 W63 K64 K65 P66 E67 S70 D71 R74 P75 V76 Q77 H78 A79 M83 V88 H89 F90 V91 Y92 G93 R94 W95 L96 I97 A100 P101 K102 V103 I104 L105 F106 D107 L108 D109 S110 V111 R112 S115 D121 L122 W123 S124 L125 V126
P129 S130 P131 E132 N133 D134 F135 L142 L143 G144 V147 F150 E153 V154 L157 D158 H161 A162 I163 H168 V174 A175 L176 R180 K181 R182 R183 I184 D185 V186 V187 T188 I189 F190 T191 T192 H193 A194 G205 S206 F207 D208 F209 Y210 N211 C212 L213 F225
G226 I227 Y228 H229 R230 Y231 A237 A238 H239 D242 V243 F244 T245 T246 Q249 I250 F253 E254 A255 E256 H257 L258 R261 K262 V273 I274 K275 F276 Q277 ALA PHE HIS GLU PHE GLN N284 L285 K289 K290 E291 N294 D296 F296 V297 R298 G299 H302 F307 D308 L309
T312 L313 Y314 I317 Y321 E322 Y323 K324 N326 K326 G327 A328 D329 E333 A334 L335 A336 R337 L338 L342 K343 V344 S345 G346 K349 T350 V351 V352 I355 V356 M357 P358 A359 N362 S363 F364 L369 K370 G371 Q372 A373 E374 V375 R376 A377 L378 T381 V382 T386
T387 S388 I389 R392 D396 I398 R399 Y400 P401 HIS ASN GLY LEU THR THR GLU LEU PRO THR ASP LEU GLY E415 S419 L425 K426 R427 R428 I429 L430 R434 P435 E436 P440 P441 I442 V443 T444 H445 N446 M447 V448 D449 D450 A451 N452 D453 L454 K458 V462 Q463
L464 F465 S469 D470 R471 V472 K473 F476 H477 P478 E479 F480 L481 N484 I487 L488 G489 L490 D491 Y492 R497 G498 C499 H500 V503 F504 P505 S506 Y507 P510 W511 G512 Y513 T514 P515 A516 E517 C518 T519 V520 M521 G522 T528 N529 V530 S531 G532 M537 I541 E542
T543 N544 Y549 G550 I551 R556 R557 F558 K559 A560 E563 S564 V565 V569 Q582 R587 N588 A589 T590 E591 A592 L593 S594 D595 L596 L597 D598 W599 K600 R601 R610 Q611 L614 R615 Y618 P619 D620 Q621 F622 R623 V626 GLY GLU GLU LEU ASN ASP SER ASN MET
ASP ALA LEU ALA GLY GLY LYS LYS LEU LYS VAL ALA ARG PRO LEU SER VAL PRO GLY SER PRO ARG ASP LEU ARG SER ASN SER THR VAL TYR MET THR PRO GLY ASP LEU GLY THR LEU GLN GLU VAL ASN ASN ALA ASP ASP TYR PHE SER LEU GLY VAL ASN PRO ALA ALA ASP ASP
ASP ASP ASP GLY PRO TYR ALA ASP ASP SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	122.45Å 122.45Å 279.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.04 – 3.30 46.04 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.04-3.30) 99.7 (46.04-3.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.158 , 0.223 0.158 , 0.222	Depositor DCC
R_{free} test set	1854 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	106.7	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 57.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.257 for -h,-k,l	Xtriage
Reported twinning fraction	0.681 for H, K, L 0.319 for -h,-k,l	Depositor
Outliers	0 of 37091 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9615	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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: U5P, UDP

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	0.59	3/4964 (0.1%)	0.81	1/6752 (0.0%)
1	B	0.57	0/4836	0.79	1/6586 (0.0%)
All	All	0.58	3/9800 (0.0%)	0.80	2/13338 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	GLY	C-O	6.11	1.33	1.23
1	A	206	SER	CB-OG	5.92	1.50	1.42
1	A	206	SER	CA-CB	5.30	1.60	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	205	GLY	C-N-CA	-8.22	101.14	121.70
1	B	597	LEU	CA-CB-CG	5.44	127.81	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	GLY	Peptide
1	B	484	ASN	Peptide

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	4849	0	4605	190	0
1	B	4720	0	4446	186	0
2	A	25	0	11	3	0
3	B	21	0	11	4	0
All	All	9615	0	9073	379	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 20.

The worst 5 of 379 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:B:213:LEU:HD23	1:B:253:PHE:CE2	1.76	1.21
1:B:314:TYR:H	1:B:500:HIS:CD2	1.74	1.04
1:B:74:ARG:HE	1:B:77:GLN:NE2	1.56	1.04
1:B:213:LEU:HD23	1:B:253:PHE:HE2	0.87	0.99
1:B:213:LEU:CD2	1:B:253:PHE:HE2	1.77	0.97

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	613/725 (85%)	512 (84%)	79 (13%)	22 (4%)	3 20
1	B	600/725 (83%)	502 (84%)	73 (12%)	25 (4%)	3 17
All	All	1213/1450 (84%)	1014 (84%)	152 (12%)	47 (4%)	3 18

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	18	ALA
1	A	126	VAL
1	A	208	ASP
1	A	218	VAL

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	502/623 (81%)	457 (91%)	45 (9%)	9 32
1	B	484/623 (78%)	420 (87%)	64 (13%)	4 17
All	All	986/1246 (79%)	877 (89%)	109 (11%)	6 23

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	60	ILE
1	B	250	ILE
1	B	497	ARG
1	B	67	GLU
1	B	161	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	582	GLN

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Mol	Chain	Res	Type
1	B	484	ASN
1	B	7	ASN
1	B	611	GLN
1	B	325	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

2 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	U5P	B	801	-	22,22,22	2.50	5 (22%)	33,33,33	1.75	7 (21%)
2	UDP	A	801	-	24,26,26	0.99	1 (4%)	37,40,40	1.81	7 (18%)

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	U5P	B	801	-	-	9/10/26/26	0/2/2/2
2	UDP	A	801	-	-	2/16/32/32	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	U5P	O2-C2	8.44	1.38	1.23
3	B	801	U5P	O4-C4	5.95	1.36	1.24
3	B	801	U5P	C2-N1	3.43	1.43	1.38
3	B	801	U5P	C6-C5	2.58	1.41	1.35
2	A	801	UDP	C6-C5	2.33	1.40	1.35

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	UDP	C4-N3-C2	-5.23	119.68	126.58
2	A	801	UDP	N3-C2-N1	4.53	120.91	114.89
3	B	801	U5P	C4-N3-C2	-4.38	120.81	126.58
3	B	801	U5P	C5-C4-N3	4.12	121.00	114.84
2	A	801	UDP	C5-C4-N3	3.59	120.21	114.84

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	801	U5P	C5'-O5'-P-O1P
3	B	801	U5P	C5'-O5'-P-O2P
3	B	801	U5P	C5'-O5'-P-O3P
2	A	801	UDP	C3'-C4'-C5'-O5'
2	A	801	UDP	O4'-C4'-C5'-O5'

There are no ring outliers.

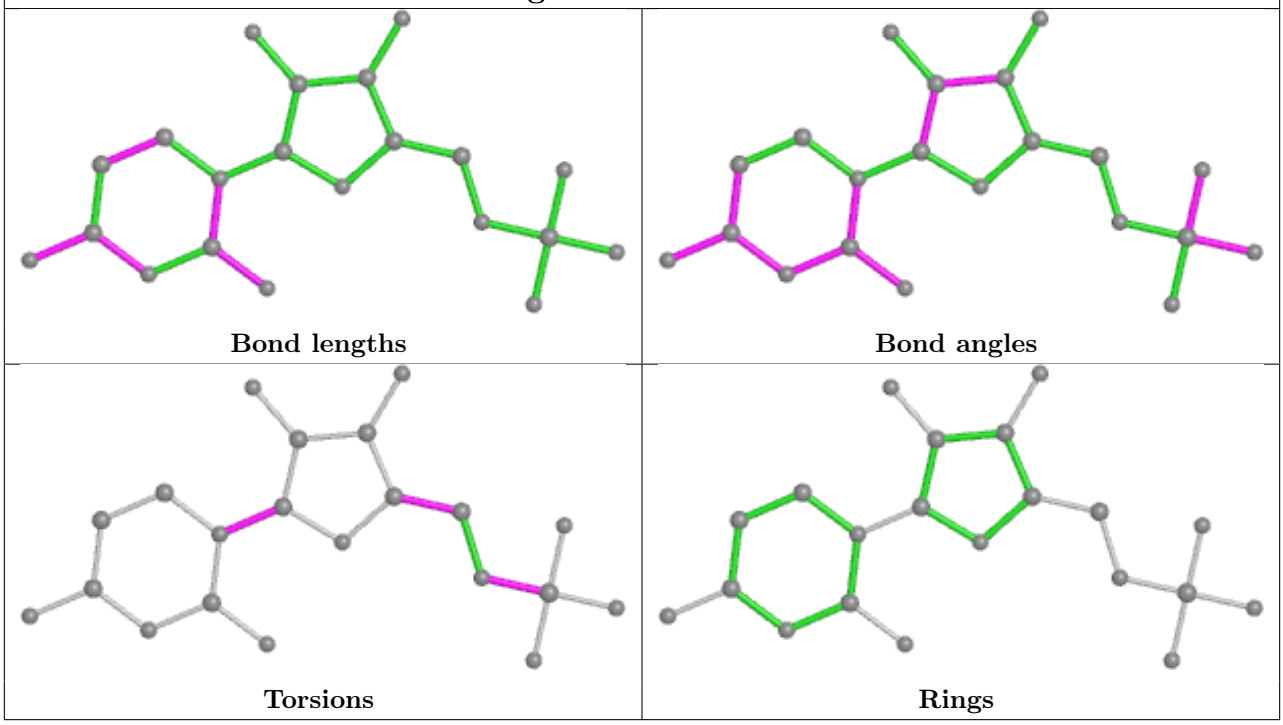
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	801	U5P	4	0
2	A	801	UDP	3	0

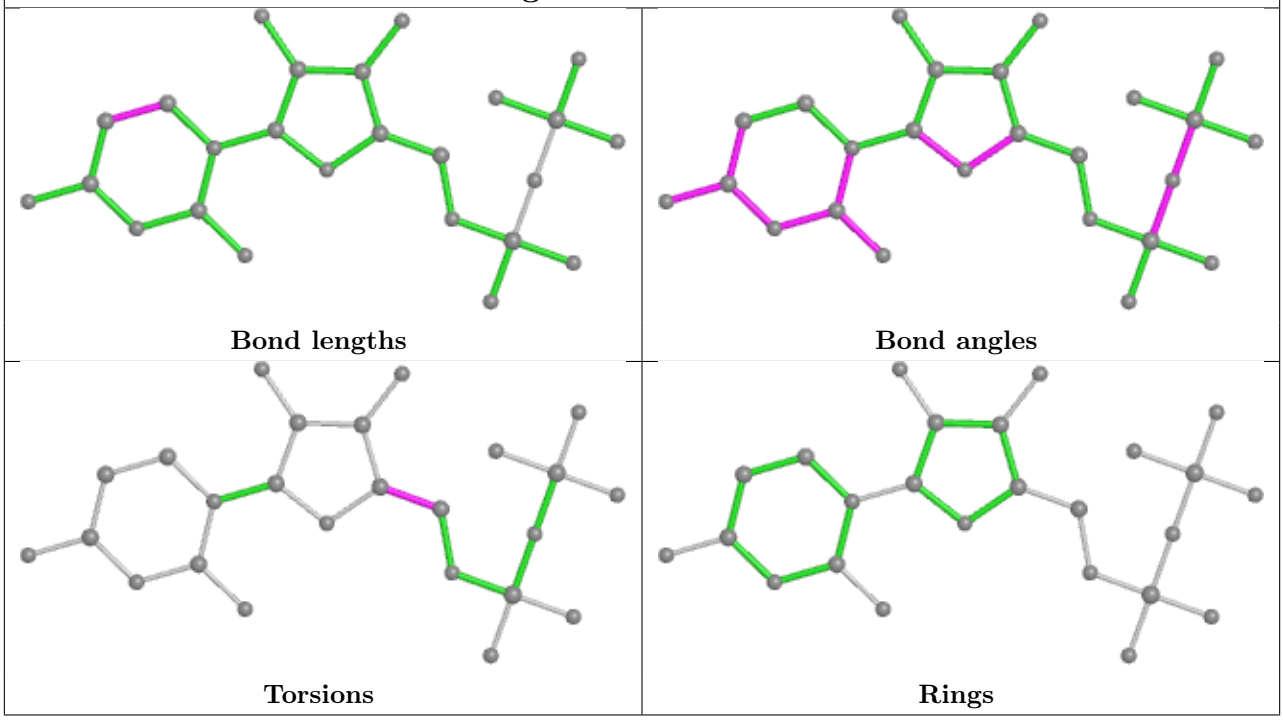
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 U5P B 801



Ligand UDP A 801



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	619/725 (85%)	-0.07	1 (0%)	95	96	71, 106, 145, 176	0
1	B	606/725 (83%)	-0.09	2 (0%)	94	94	73, 110, 154, 204	0
All	All	1225/1450 (84%)	-0.08	3 (0%)	95	96	71, 108, 150, 204	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	541	ILE	2.3
1	A	568	LEU	2.0
1	B	511	TRP	2.0

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

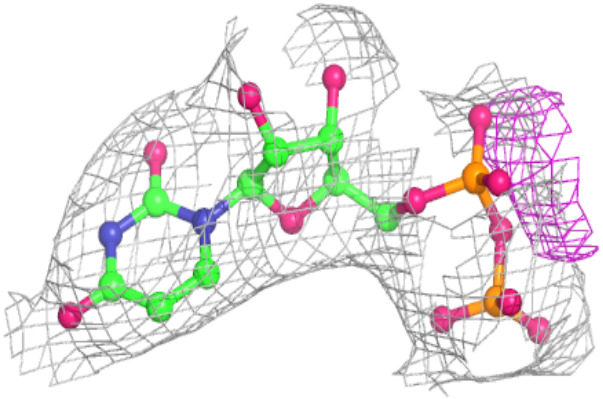
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

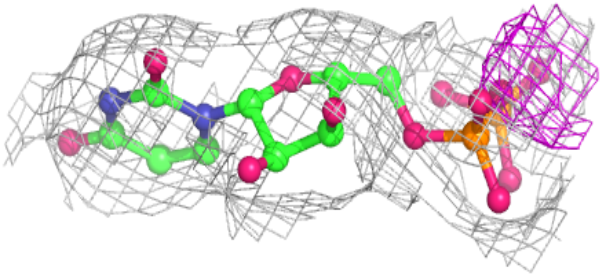
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	UDP	A	801	25/25	0.94	0.18	92,121,165,169	0
3	U5P	B	801	21/21	0.96	0.16	88,108,120,130	0

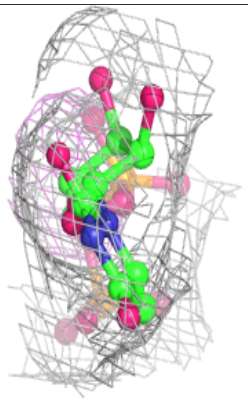
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UDP A 801:

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

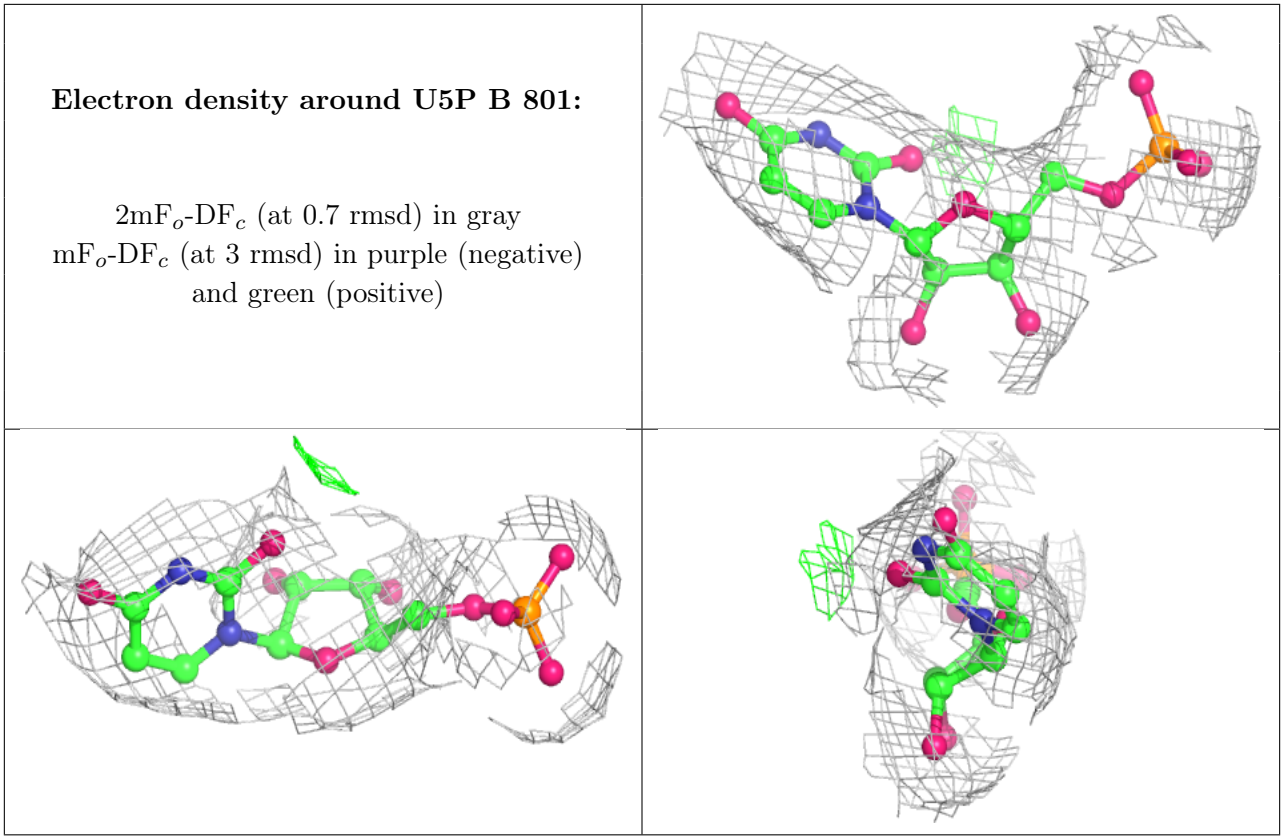






Electron density around U5P B 801:

$2mF_o$-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.