



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:48 PM UTC

PDB ID : 5SUL / pdb_00005sul
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 ⓘ 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

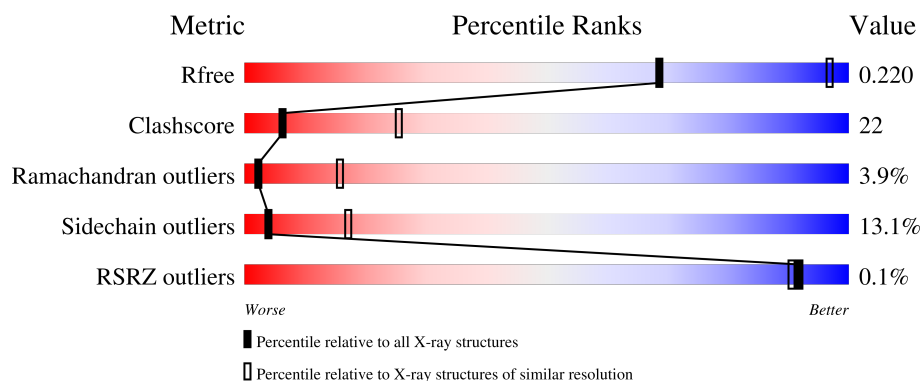
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	725	
1	B	725	

2 Entry composition

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:

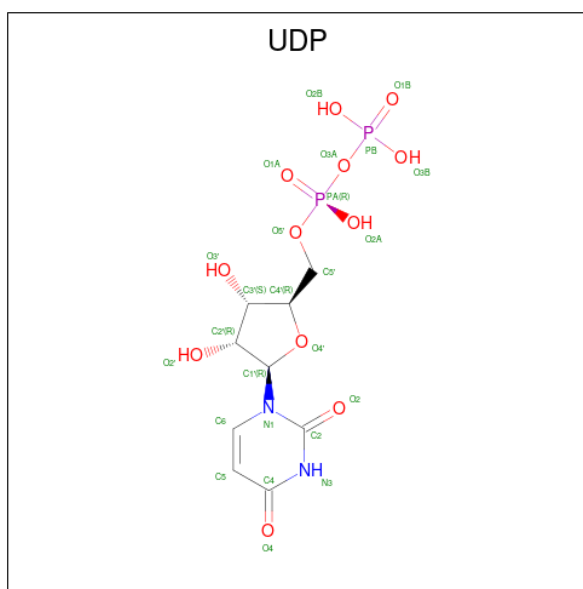
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P27472
A	-18	GLY	-	expression tag	UNP P27472
A	-17	SER	-	expression tag	UNP P27472
A	-16	SER	-	expression tag	UNP P27472
A	-15	HIS	-	expression tag	UNP P27472
A	-14	HIS	-	expression tag	UNP P27472
A	-13	HIS	-	expression 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

Continued on next page...

Continued from previous page...

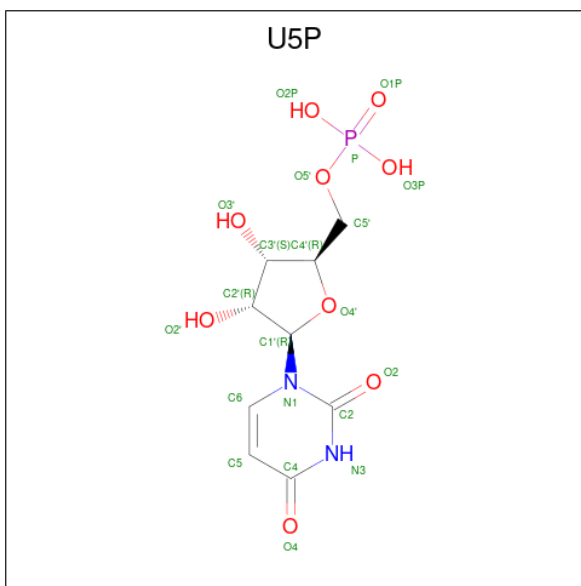
Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP P27472
B	-16	SER	-	expression tag	UNP P27472
B	-15	HIS	-	expression tag	UNP P27472
B	-14	HIS	-	expression tag	UNP P27472
B	-13	HIS	-	expression tag	UNP P27472
B	-12	HIS	-	expression tag	UNP P27472
B	-11	HIS	-	expression tag	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 (CCD ID: 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 (CCD ID: U5P) (formula: $C_9H_{13}N_2O_9P$).



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

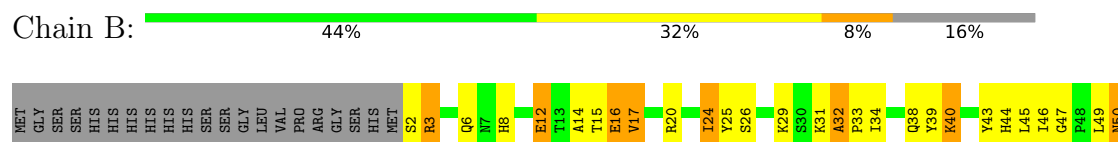
3 Residue-property plots

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



• Molecule 1: Glycogen [starch] synthase isoform 2



GLU	R615	G522	R447	E374	Y297	L213	L125	K51
VAL			V448	V375	R298		V126	A52
ASN	Y618	T528	D449	R376	G299	F225		Y54
ASN	F619	N529	D450	A377		G226	P129	
ALA	D620	V530	A451	L378	H302	I227	S130	I60
ASP	D621	S531	N452		F307	Y228	P131	L61
ASP	F622	G532	N453	T381	D308	H229	E132	D62
TYR	R623		L454	V382	L309	R230	N133	W63
PHE		R537				Y231	F135	K64
SER			K458	T386	T312	A237		K65
LEU		I541		T387	L313	A238	L142	P66
GLY		E542	V462	S388	Y314	H239	L143	E67
VAL		T543	O463	I389			G144	
ASN		N544	L464		I317	D242		S70
PRO			F465	R392		V243	V147	D71
ALA		Y549		D395	Y321	F244		R74
ASP		G550	S469		E322	T245	F150	P75
ALA		I551	D470	I398	Y323	T246		V76
ASP			R471	R399	K324		E153	Q77
ASP		V554	K473	Y400	N325	Q249	V154	H78
ASP		D555		P401	K326	I250	L157	A79
ASP		R556	F476	HIS	D328	F253	D158	L80
GLY		R557	H477	ASN	D329	E254		Q81
PRO		F558	P478	GLY	K330	A255	H161	T82
TYR		K559	E479	LEU		E256	A162	M83
ALA		A560	F480	THR	E333	H257	I163	
ASP			L481	THR	A334	L258		H88
ASP		E563		GLU	L335		H168	H89
SER		S564	V484	LEU	A336	R261		F90
		V565		PRO	R337	K262	V174	Y91
			L487	THR	L338		A175	Y92
ARG		L568	L488	ASP		G285	L176	G93
PRO		V569	G489	LEU	L342	I266	P177	W95
LEU			L490	GLY	K343	L267		I96
SER		M572			V344	P268	R180	I97
VAL			D491	E415	S345		K181	
PRO		R581	Y492	L416	G346	N272	K182	A100
GLY		Q582				V273	R183	P101
SER			R497	S419		I274	I184	K102
PRO		R587	G498	V423	K349	K275	D185	V103
ARG		N588	C499	M424	T350	F276	V186	I104
ASP		A589	H500	L425	V351		T188	L106
LEU		T590		K426	V352	ALA	F106	
ARG		E591	V503	R427		PHE	D107	
SER		A592	F504	R428	T355	HIS	L108	
ASN		L593	P505	I429	V356	GLU	D109	
SER		S594	S506	L430	N357	PHE	H193	V111
THR		D595	Y507		P358	GLN	A194	R112
VAL		L596			A359		G205	G113
TYR		L597	P510	R434		N284	Y114	S115
MET		D598		P435	N362	L285	G206	
THR		W599	Y513	E436	S363		F207	D208
PRO		K600	T514		F364	K289	F209	D121
GLY		R601	P515	P440		K290	Y210	L122
ASP		M602	A516	P441	L369	E291	N211	W123
LEU			E517	T442	K370		F209	S124
GLY		R610	C518	V443	G371	N294		
THR		Q611	T519	T444	Q372			
LEU			V520	H445				
GLN		L614	M521	N446	A373	F296	C212	

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.158 , 0.223 0.155 , 0.220	Depositor DCC
R_{free} test set	1854 reflections (4.98%)	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 , 72.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	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.*

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: UDP, U5P

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	0.78	2/4964 (0.0%)	1.15	13/6752 (0.2%)
1	B	0.74	0/4836	1.16	12/6586 (0.2%)
All	All	0.76	2/9800 (0.0%)	1.15	25/13338 (0.2%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	GLY	C-O	7.04	1.33	1.23
1	A	129	PRO	N-CA	5.20	1.53	1.47

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	GLY	CA-C-N	-13.69	101.14	122.08
1	A	205	GLY	C-N-CA	-13.69	101.14	122.08
1	B	477	HIS	CA-C-N	8.30	130.21	119.84
1	B	477	HIS	C-N-CA	8.30	130.21	119.84
1	A	206	SER	O-C-N	7.43	129.97	122.10

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 [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	4849	0	4605	214	0
1	B	4720	0	4446	197	0
2	A	25	0	11	3	0
3	B	21	0	11	4	0
All	All	9615	0	9073	414	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 22.

The worst 5 of 414 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 [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	613/725 (85%)	512 (84%)	79 (13%)	22 (4%)	2	17
1	B	600/725 (83%)	502 (84%)	73 (12%)	25 (4%)	2	14
All	All	1213/1450 (84%)	1014 (84%)	152 (12%)	47 (4%)	2	16

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 ⓘ

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%)	449 (89%)	53 (11%)	6	24
1	B	484/623 (78%)	408 (84%)	76 (16%)	2	12
All	All	986/1246 (79%)	857 (87%)	129 (13%)	4	17

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	472	VAL
1	B	530	VAL
1	A	621	GLN
1	A	594	SER
1	B	554	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	302	HIS
1	B	611	GLN
1	B	325	ASN
1	B	482	ASN
1	A	485	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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$
2	UDP	A	801	-	25,26,26	1.05	1 (4%)	38,40,40	1.78	6 (15%)
3	U5P	B	801	-	22,22,22	2.55	5 (22%)	32,33,33	1.82	7 (21%)

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	UDP	A	801	-	-	2/16/32/32	0/2/2/2
3	U5P	B	801	-	-	9/10/26/26	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	8.70	1.38	1.23
3	B	801	U5P	O4-C4	5.93	1.36	1.24
3	B	801	U5P	C2-N1	3.50	1.43	1.38
3	B	801	U5P	C6-C5	2.56	1.41	1.35
2	A	801	UDP	C6-C5	2.31	1.40	1.35

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	UDP	C4-N3-C2	-5.58	119.68	126.61
3	B	801	U5P	C4-N3-C2	-4.68	120.81	126.61
2	A	801	UDP	N3-C2-N1	4.62	120.91	114.89
3	B	801	U5P	C5-C4-N3	4.43	121.00	114.80
2	A	801	UDP	C5-C4-N3	3.86	120.21	114.80

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'

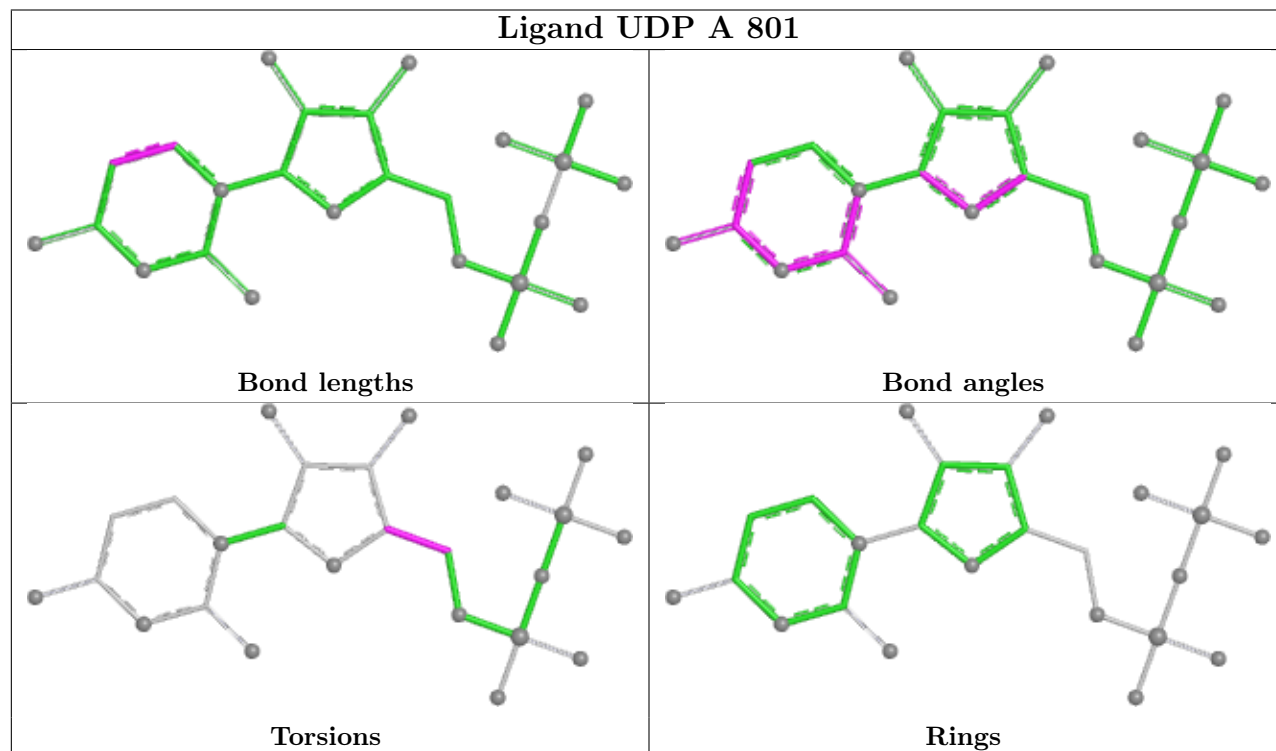
There are no ring outliers.

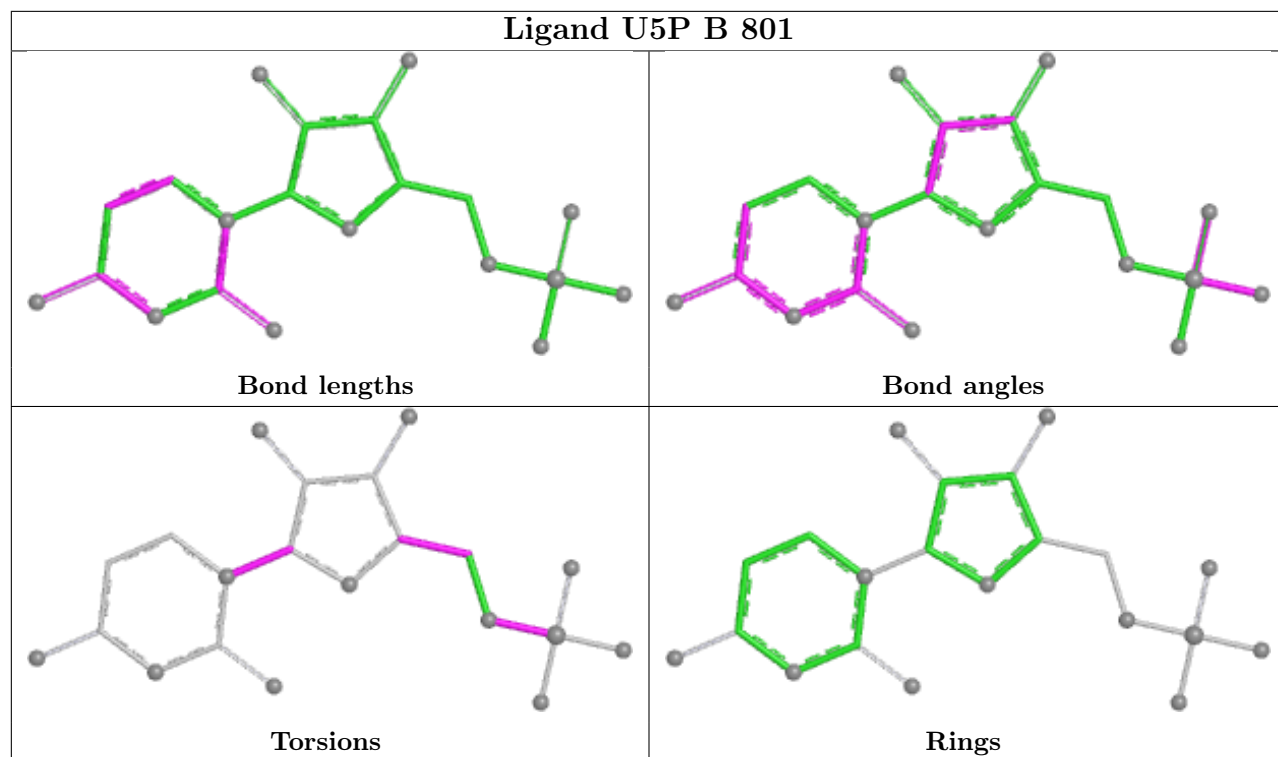
2 monomers are involved in 7 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	619/725 (85%)	-1.36	0	100 100	71, 106, 145, 176	0
1	B	606/725 (83%)	-1.30	1 (0%)	91 86	73, 110, 154, 204	0
All	All	1225/1450 (84%)	-1.33	1 (0%)	92 90	71, 108, 150, 204	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	277	GLN	2.5

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.

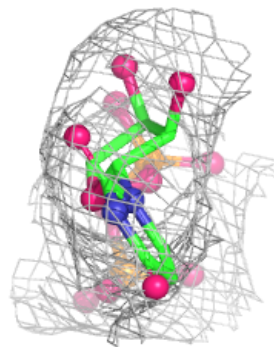
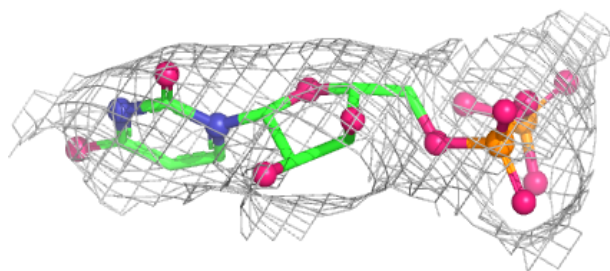
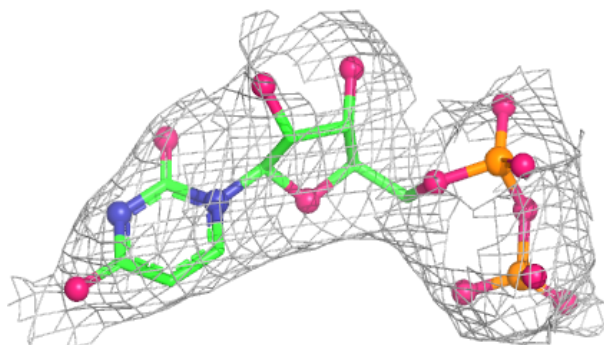
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	UDP	A	801	25/25	0.99	0.03	92,121,165,169	0
3	U5P	B	801	21/21	0.99	0.04	88,108,120,130	0

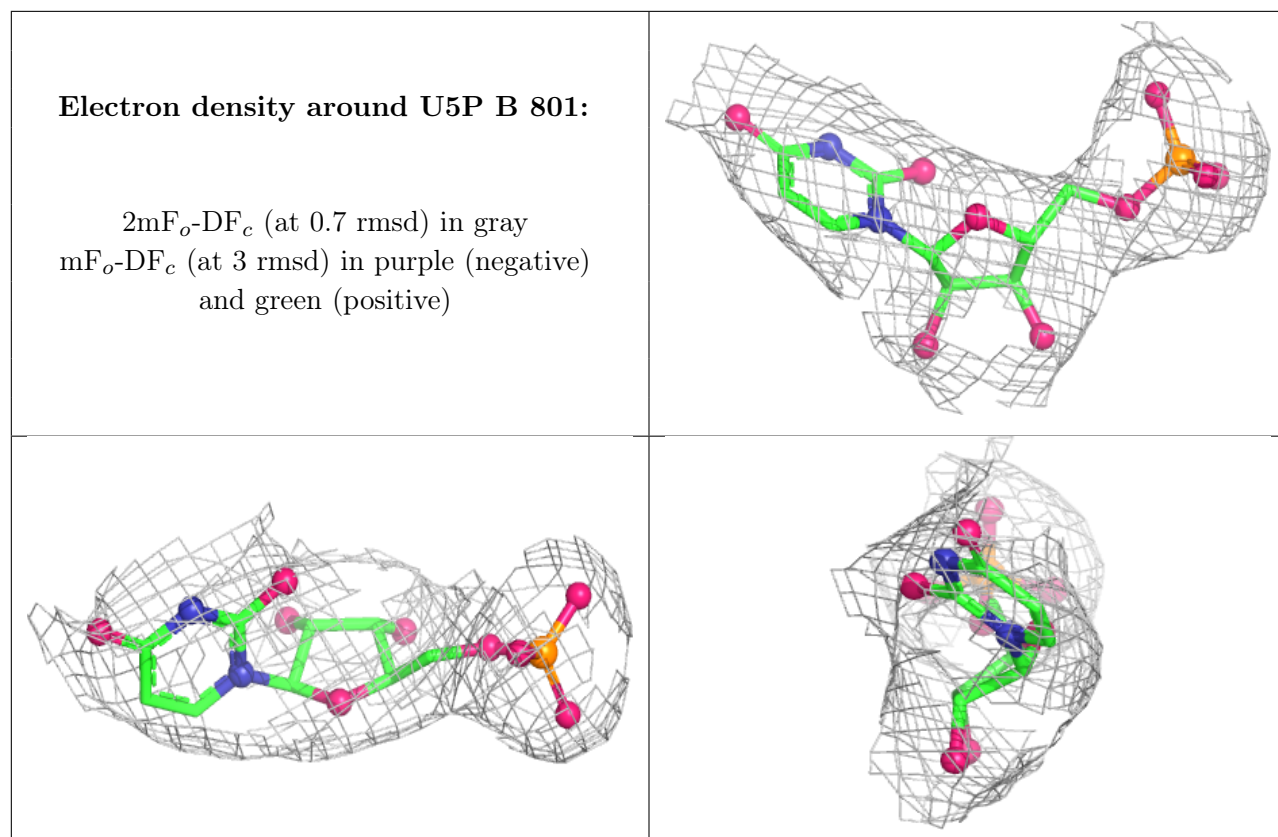
The following is a graphical depiction of the model fit to experimental electron density of all

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)





6.5 Other polymers [i](#)

There are no such residues in this entry.