



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 06:26 pm BST

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 ⓘ 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	:	2.11
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)	:	2.11

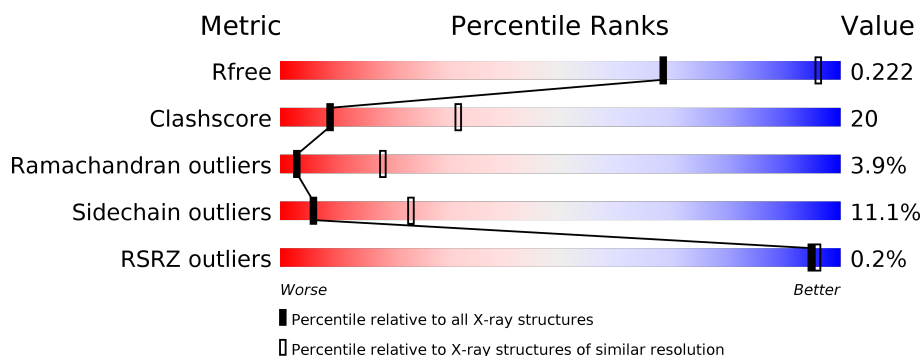
1 Overall quality at a glance ⓘ

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}	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 on 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:

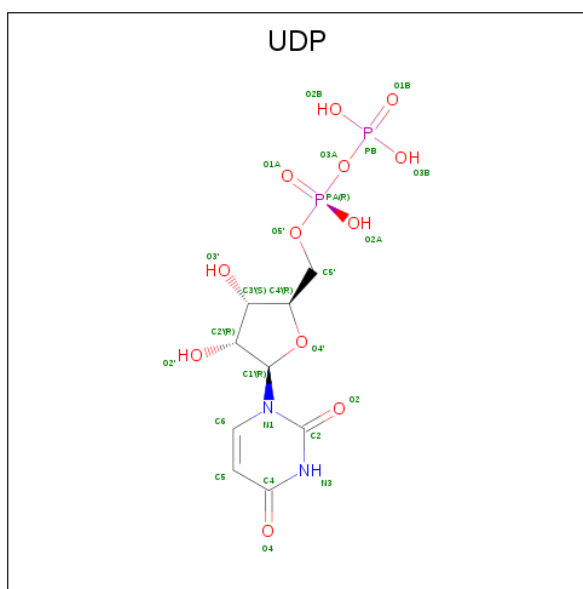
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P27472
A	-18	GLY	-	expression tag	UNP P27472
A	-17	SER	-	expression tag	UNP P27472
A	-16	SER	-	expression tag	UNP P27472
A	-15	HIS	-	expression tag	UNP P27472
A	-14	HIS	-	expression tag	UNP P27472
A	-13	HIS	-	expression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

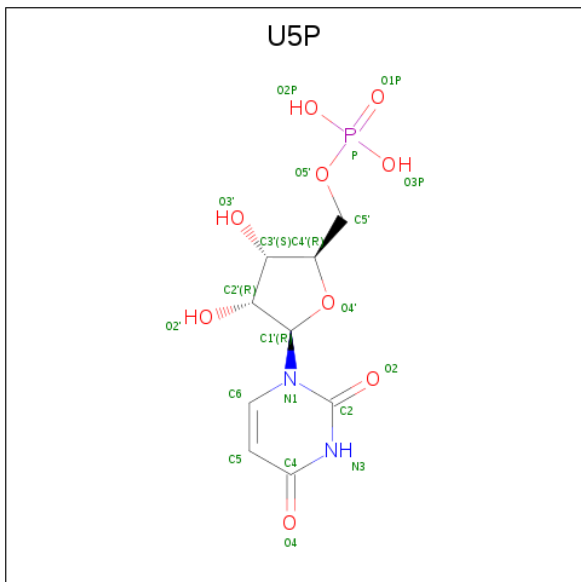
Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP P27472
B	-16	SER	-	expression tag	UNP P27472
B	-15	HIS	-	expression tag	UNP P27472
B	-14	HIS	-	expression tag	UNP P27472
B	-13	HIS	-	expression tag	UNP P27472
B	-12	HIS	-	expression tag	UNP P27472
B	-11	HIS	-	expression tag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

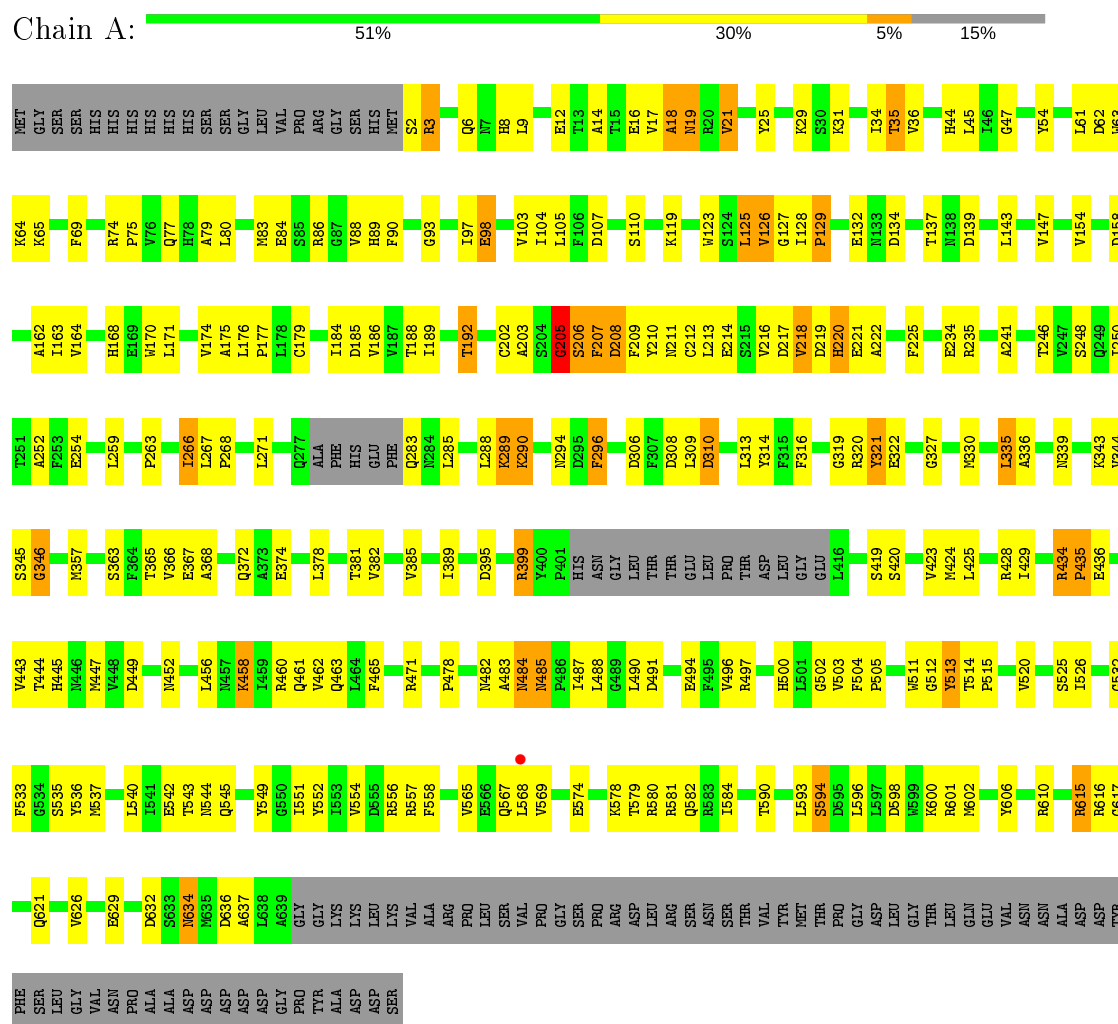


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	B	1	21	9	2	9	1	0	0

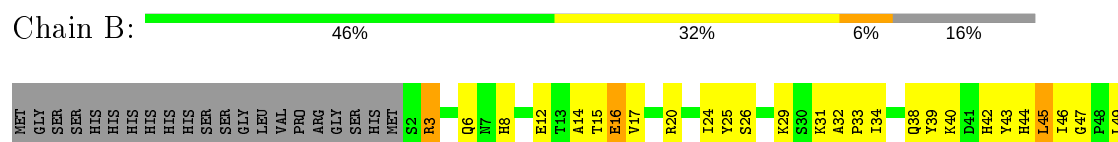
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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



ASP	T543	L464	T387	G226	T312	G226	P129	N50
ASP	N544	F465	S388	I227	L313	I227	S130	A51
ASP	Y549	S469	I389	I228	Y314	I228	P131	A52
GLY	G550	G550	R392	R230	D470	R230	E132	T53
GLY	I551	R471	R392	R230	D470	R230	E132	T53
LYS	R556	K472	D395	I231	Y321	A237	D134	T60
LYS	R557	K473	I398	E322	R399	A238	F135	L61
LYS	F558	F476	R399	E322	R399	A238	L142	N63
VAL	K559	H477	Y400	K324	Y323	E239	L143	D62
ALA	A560	P478	F401	N325	K326	D242	G144	K65
ARG	E563	E479	H15	K326	G327	V243	V147	P66
PRO	S564	F480	ASN	F244	G327	T245	F150	E67
LEU	S564	L481	GLY	A328	L338	T245	F150	S70
SER	V565	R384	LEU	D329	L342	T246	E153	D71
VAL	V569	I487	THR	E333	K343	Q249	E153	R74
PRO	Q582	G488	GLU	A334	L335	I250	V154	P75
SER	R587	G489	LEU	L488	PRQ	F253	L157	V76
ARG	N588	R490	THR	R490	R337	E254	D158	Q77
ASP	A589	D491	ASP	L338	ASP	E255	H161	H78
LEU	T590	Y492	LEU	E256	LEU	E256	A162	A79
ARG	S591	R497	GLY	E257	L342	E257	A162	M63
SER	A592	G498	E415	L258	K343	L258	I163	M63
ASN	C499	G499	S419	K261	S345	K261	H168	V68
SER	S594	H500	G346	R262	G346	R262	H168	H89
VAL	D595	V503	L425	V273	K349	V273	V174	F90
TYR	L596	F504	R426	I274	T350	I274	A175	V91
MET	L597	R427	F504	K275	V351	K275	L176	Y92
THR	D598	P505	R428	K276	V351	K276	G93	G93
PRO	N599	S506	I429	F276	V352	F276	R180	R94
GLY	K600	Y507	L430	Q277	V352	Q277	K181	R95
ASP	R601	P510	R434	ALA	T355	ALA	R182	L96
LEU	R610	M511	P435	PHE	V356	PHE	R183	I97
GLY	Q611	G512	E436	H15	M357	H15	I184	A100
LEU	L614	Y513	T514	PHE	G512	GLU	D185	P101
GLN	R615	P515	P440	GLN	A359	PHE	V186	K102
GLU	Y618	A516	P441	N362	N362	T284	V187	V103
VAL	P619	E517	I442	S363	S363	L285	T189	I104
ASN	D620	C618	V443	F364	F364	L285	F190	L105
ALA	Q621	T519	R445	L369	L369	K289	T191	F106
ASP	F622	V520	N446	K370	K370	K290	T192	D107
ASP	R623	M521	N447	G371	G371	E291	H193	L108
TYR	V626	G522	V448	Q372	Q372	N294	A194	D109
PHE	GLY	T528	D449	A373	A373	I295	G205	S110
SER	GLY	N529	D450	E374	E374	D295	S206	R112
LEU	GLU	V530	N451	V375	V375	V297	F207	G115
GLY	VAL	S531	N452	R376	R376	R298	D208	S115
VAL	ASN	G532	D453	A377	A377	G299	F209	D121
ASN	PRO	M537	L454	L378	L378	H502	N211	L122
ASP	ALA	R458	T381	V382	V382	F307	G212	M123
ALA	SER	I541	V462	T381	T381	G212	L213	S124
ASP	ASN	E542	D462	T386	T386	D308	C125	L125
ASP	MET						F205	R126

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 0.158 , 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	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	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.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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	0.59	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(°)	Ideal(°)
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 ⓘ

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	20	ARG
1	B	105	LEU
1	B	513	TYR
1	B	26	SER
1	B	50	ASN

Some 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	567	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	6	GLN
1	B	484	ASN
1	A	634	ASN
1	B	7	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 carbohydrates 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$
3	U5P	B	801	-	18,22,22	1.36	1 (5%)	21,33,33	1.40	2 (9%)
2	UDP	A	801	-	20,26,26	0.83	0	25,40,40	1.17	2 (8%)

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	-	-	6/8/26/26	0/2/2/2
2	UDP	A	801	-	-	2/14/32/32	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	U5P	O4-C4	4.58	1.36	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	UDP	PA-O3A-PB	-3.44	121.03	132.83
3	B	801	U5P	C3'-C2'-C1'	3.27	105.90	100.98
3	B	801	U5P	O3P-P-O2P	2.23	116.18	107.64
2	A	801	UDP	O4'-C1'-C2'	-2.05	103.94	106.93

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	801	U5P	C2'-C1'-N1-C6
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'

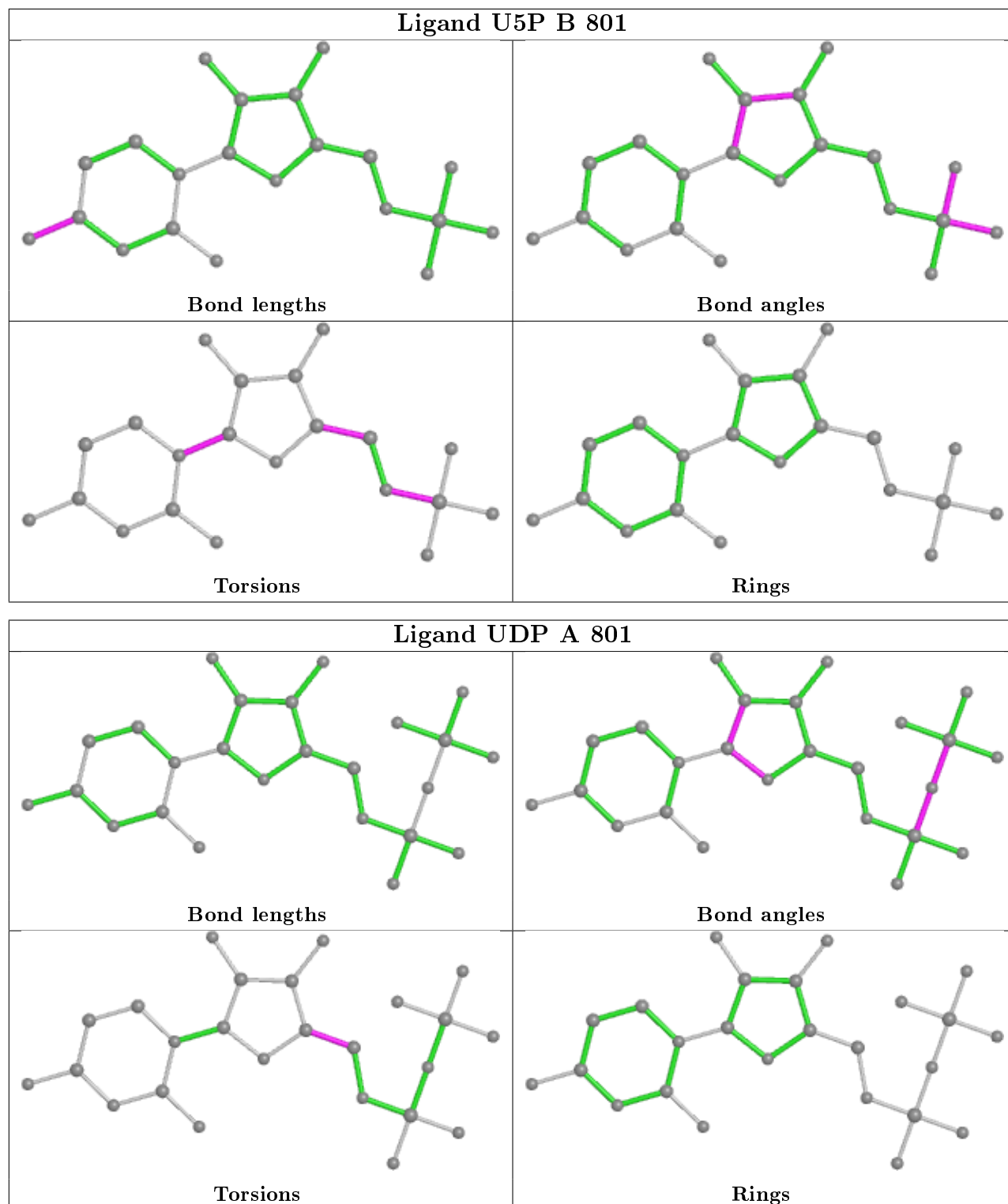
There are no ring outliers.

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 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%)	-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 [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

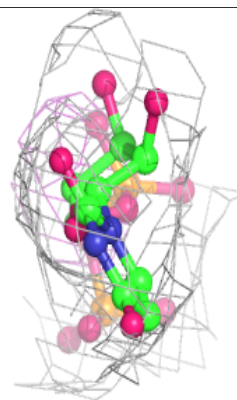
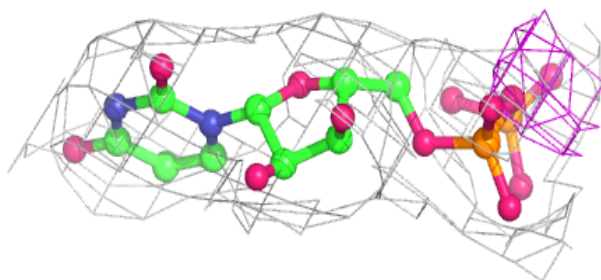
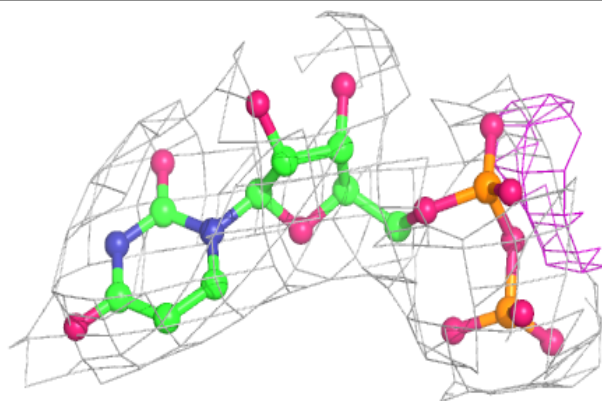
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

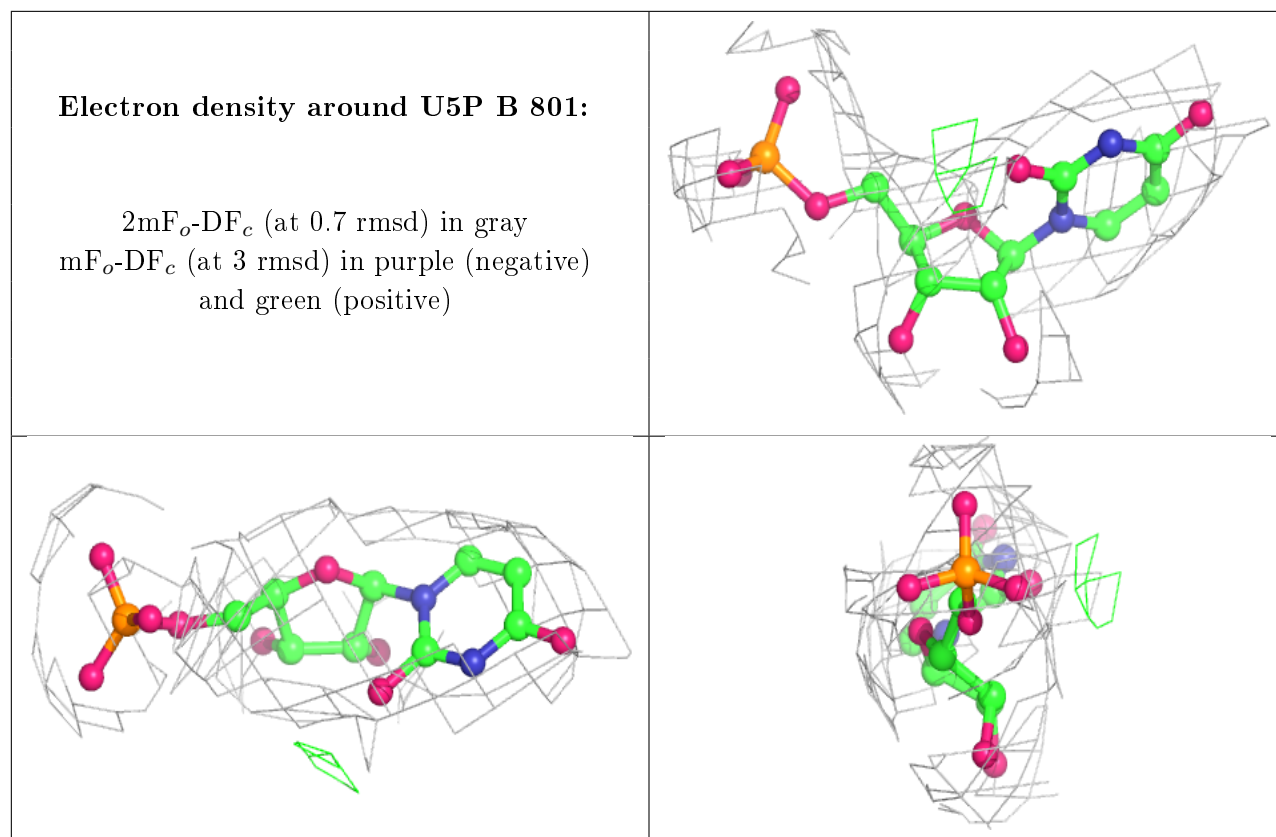
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	UDP	A	801	25/25	0.94	0.18	92,121,165,169	0
3	U5P	B	801	21/21	0.96	0.16	88,108,120,130	0

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)





6.5 Other polymers [i](#)

There are no such residues in this entry.