



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 11:59 PM UTC

PDB ID : 7XGX / pdb_00007xgx
Title : Glucosyltransferase
Authors : Chen, T.T.; Ouyang, S.Y.
Deposited on : 2022-04-07
Resolution : 2.39 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

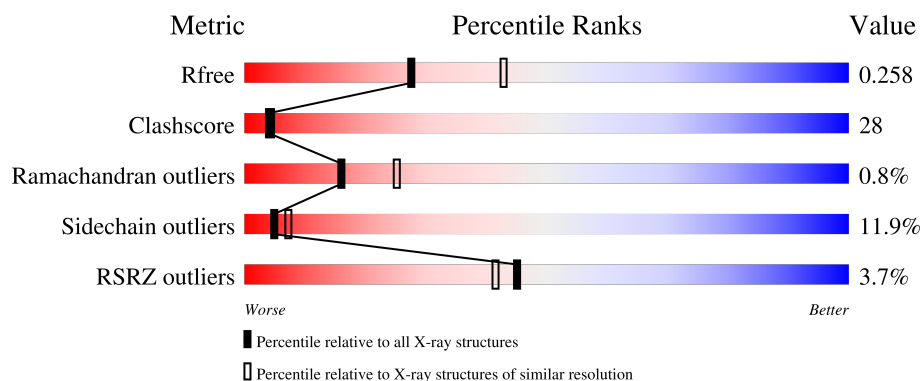
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	655	 4% 53% 31% 8% • 7%
1	B	655	 3% 48% 33% 8% • 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9711 atoms, of which 44 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 Lgt2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	607	Total	C	N	O	S	0	0	0
			4801	3040	828	907	26			
1	B	591	Total	C	N	O	S	0	0	0
			4674	2964	802	882	26			

There are 38 discrepancies between the modelled and reference sequences:

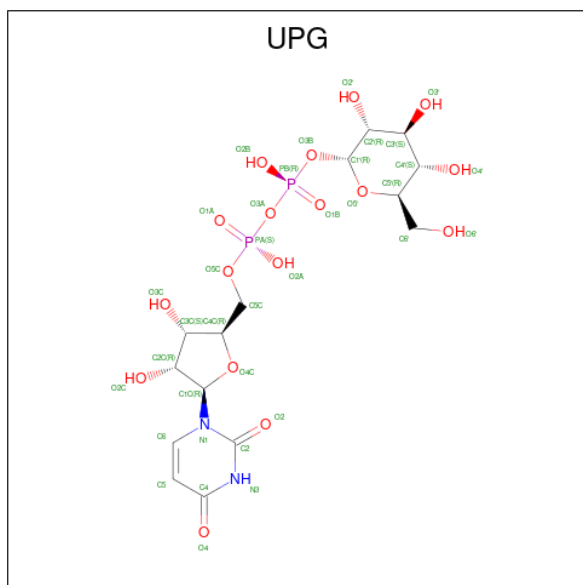
Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP A0A2S6F0H5
A	-17	GLY	-	expression tag	UNP A0A2S6F0H5
A	-16	SER	-	expression tag	UNP A0A2S6F0H5
A	-15	SER	-	expression tag	UNP A0A2S6F0H5
A	-14	HIS	-	expression tag	UNP A0A2S6F0H5
A	-13	HIS	-	expression tag	UNP A0A2S6F0H5
A	-12	HIS	-	expression tag	UNP A0A2S6F0H5
A	-11	HIS	-	expression tag	UNP A0A2S6F0H5
A	-10	HIS	-	expression tag	UNP A0A2S6F0H5
A	-9	HIS	-	expression tag	UNP A0A2S6F0H5
A	-8	SER	-	expression tag	UNP A0A2S6F0H5
A	-7	SER	-	expression tag	UNP A0A2S6F0H5
A	-6	GLY	-	expression tag	UNP A0A2S6F0H5
A	-5	LEU	-	expression tag	UNP A0A2S6F0H5
A	-4	VAL	-	expression tag	UNP A0A2S6F0H5
A	-3	PRO	-	expression tag	UNP A0A2S6F0H5
A	-2	ARG	-	expression tag	UNP A0A2S6F0H5
A	-1	GLY	-	expression tag	UNP A0A2S6F0H5
A	0	SER	-	expression tag	UNP A0A2S6F0H5
B	-18	MET	-	initiating methionine	UNP A0A2S6F0H5
B	-17	GLY	-	expression tag	UNP A0A2S6F0H5
B	-16	SER	-	expression tag	UNP A0A2S6F0H5
B	-15	SER	-	expression tag	UNP A0A2S6F0H5
B	-14	HIS	-	expression tag	UNP A0A2S6F0H5
B	-13	HIS	-	expression tag	UNP A0A2S6F0H5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP A0A2S6F0H5
B	-11	HIS	-	expression tag	UNP A0A2S6F0H5
B	-10	HIS	-	expression tag	UNP A0A2S6F0H5
B	-9	HIS	-	expression tag	UNP A0A2S6F0H5
B	-8	SER	-	expression tag	UNP A0A2S6F0H5
B	-7	SER	-	expression tag	UNP A0A2S6F0H5
B	-6	GLY	-	expression tag	UNP A0A2S6F0H5
B	-5	LEU	-	expression tag	UNP A0A2S6F0H5
B	-4	VAL	-	expression tag	UNP A0A2S6F0H5
B	-3	PRO	-	expression tag	UNP A0A2S6F0H5
B	-2	ARG	-	expression tag	UNP A0A2S6F0H5
B	-1	GLY	-	expression tag	UNP A0A2S6F0H5
B	0	SER	-	expression tag	UNP A0A2S6F0H5

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (CCD ID: UPG) (formula: $C_{15}H_{24}N_2O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).

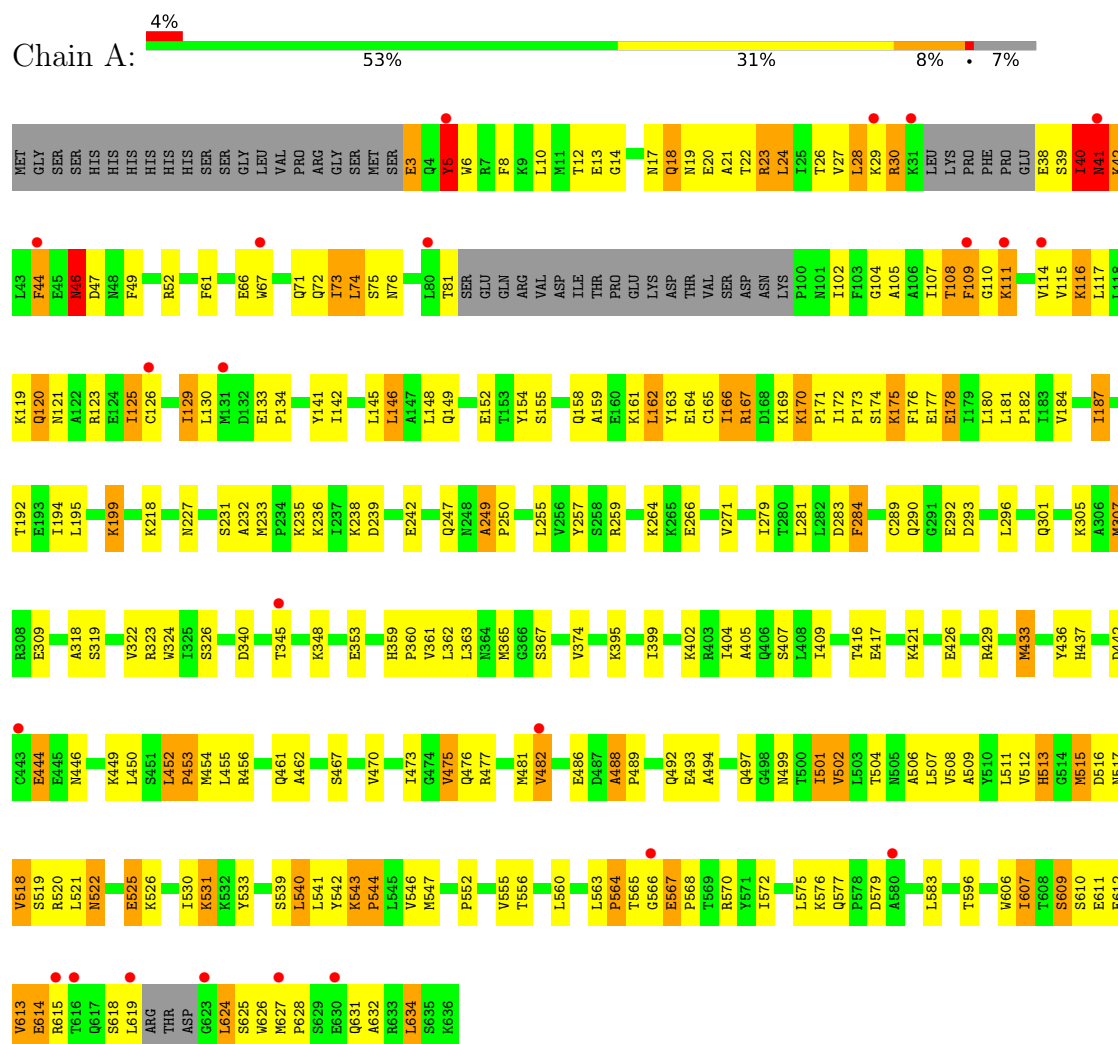


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	52	Total 52	O 52	0	0
3	B	68	Total 68	O 68	0	0

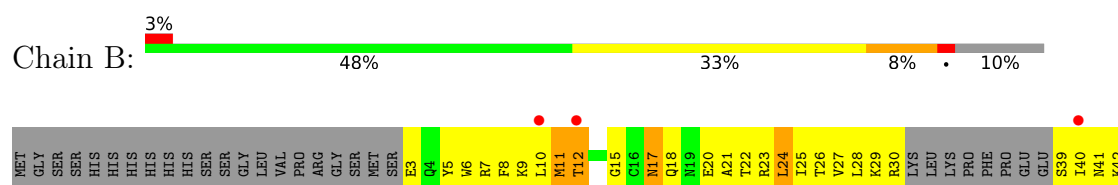
3 Residue-property plots [i](#)

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: Lgt2



• Molecule 1: Lgt2



N597	F598	T599	I603	P604	M605	M606	T607	T608	S609	S610	E611	E612	VAL	GLU	ARG	THR	GLN	SER	LEU	ARG	THR	ASP	GLY	L624	S625	W626	P628	S629	E630	GLN	ALA	ARG	LEU	SER	LYS																					
A506	L507	V508	Y509	L510	V511	V512	H513	M514	M515	D516	N517	V518	S519	R520	L521	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	O567	P568	T569	R570	K576	I582	L583	V592	K595	T596						
D285	E286	C289	D293	K307	N314	D320	W324	D340	N341	P342	K343	L344	T345	K348	K351	Y356	H359	P360	L363	K364	G365	G366	S367	A368	L369	V370	G373	V374	K378	E379	N380	N389	E493	A494	L495	Q496	Q497	G498	I501	V502	L503	T504	N505													
L439	L440	K441	E444	E445	N446	N447	L450	S451	L452	P453	M454	L455	R456	T460	Q461	S464	N465	L466	S467	S468	Y469	V470	R471	F472	I473	G474	V475	Q476	R477	G478	A479	E480	M481	V482	G483	A484	P485	E486	D487	A488	P489	E493	L494	Q496	Q497	G498	I501	V502	L503	T504	N505					
I187	K188	E189	N190	H191	T192	L195	N196	K199	R200	N201	C222	N227	N228	P229	A232	M233	P234	K235	K236	T237	K238	L241	E242	Q247	N248	K249	P250	E251	G251	V252	T253	K254	L255	V256	G257	V374	K378	E379	N380	N389	E493	L494	Q496	Q497	G498	I501	V502	L503	T504	N505						
K119	Q120	N121	A122	R123	E124	I125	C126	E127	S128	I129	L130	N131	D132	E133	P134	N135	L136	K137	Q138	I139	E140	Y141	I142	F143	K144	L145	L146	A147	L148	Y154	S155	G156	E157	Q158	A159	E160	K161	L162	Y163	E164	G165	I166	R167	D168	K169	K170	P171	S174	K175	F176	E177	E178	I179	V184	N185	R186
L73	L74	S75	N76	I77	Q78	P79	L80	SER	GLU	GLN	ARG	VAL	ASP	ILE	THR	PRO	THR	GLU	LYS	ASP	THR	VAL	SER	ASP	ASN	LYS	P100	N101	I102	F103	G104	I107	T108	F109	G110	K111	S112	P113	V114	V115	A116	L117	L118													

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.06Å 75.86Å 126.64Å 90.00° 90.24° 90.00°	Depositor
Resolution (Å)	32.22 – 2.39 32.22 – 2.39	Depositor EDS
% Data completeness (in resolution range)	95.3 (32.22-2.39) 95.1 (32.22-2.39)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.215 , 0.265 0.227 , 0.258	Depositor DCC
R_{free} test set	1988 reflections (3.49%)	wwPDB-VP
Wilson B-factor (Å ²)	49.9	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.013 for -k,-h,-l 0.014 for k,h,-l 0.149 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9711	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UPG

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	1.12	34/4887 (0.7%)	0.91	26/6603 (0.4%)
1	B	1.04	32/4760 (0.7%)	0.96	30/6435 (0.5%)
All	All	1.08	66/9647 (0.7%)	0.94	56/13038 (0.4%)

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	543	LYS	C-O	-7.62	1.17	1.24
1	B	543	LYS	C-O	-7.46	1.17	1.24
1	A	544	PRO	C-O	-7.10	1.15	1.24
1	B	452	LEU	C-O	-6.87	1.18	1.24
1	A	14	GLY	C-O	-6.62	1.19	1.24

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	ASP	N-CA-C	19.88	153.15	110.80
1	A	29	LYS	CB-CA-C	-17.82	79.61	109.55
1	A	5	TYR	N-CA-C	14.91	130.57	112.38
1	B	47	ASP	CB-CA-C	-14.75	81.06	110.42
1	B	17	ASN	CB-CA-C	13.42	135.70	109.66

There are no chirality outliers.

There are no planarity outliers.

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	4801	0	4854	243	0
1	B	4674	0	4717	288	0
2	A	36	22	22	1	0
2	B	36	22	22	1	0
3	A	52	0	0	1	0
3	B	68	0	0	6	0
All	All	9667	44	9615	531	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 28.

The worst 5 of 531 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:129:ILE:CD1	1:A:192:THR:HG23	1.49	1.41
1:B:249:ALA:CB	1:B:250:PRO:CD	2.15	1.23
1:B:249:ALA:CB	1:B:250:PRO:HD2	1.71	1.21
1:B:249:ALA:HB1	1:B:250:PRO:CD	1.70	1.19
1:A:129:ILE:CD1	1:A:192:THR:CG2	2.20	1.19

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	599/655 (92%)	561 (94%)	33 (6%)	5 (1%)	16	25
1	B	583/655 (89%)	543 (93%)	35 (6%)	5 (1%)	14	22
All	All	1182/1310 (90%)	1104 (93%)	68 (6%)	10 (1%)	16	25

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	249	ALA
1	B	249	ALA
1	B	565	THR
1	B	519	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	533/578 (92%)	470 (88%)	63 (12%)	5	7
1	B	519/578 (90%)	457 (88%)	62 (12%)	5	7
All	All	1052/1156 (91%)	927 (88%)	125 (12%)	5	7

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	610	SER
1	B	518	VAL
1	B	46	ASN
1	B	516	ASP
1	B	567	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	461	GLN
1	B	513	HIS
1	A	517	ASN
1	A	537	GLN
1	B	121	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 oligosaccharides 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
2	UPG	B	701	-	37,38,38	1.10	2 (5%)	55,58,58	2.13	12 (21%)
2	UPG	A	701	-	37,38,38	1.19	6 (16%)	55,58,58	2.15	9 (16%)

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	UPG	B	701	-	-	2/23/59/59	0/3/3/3
2	UPG	A	701	-	-	3/23/59/59	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	UPG	C6-N1	-2.62	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	UPG	C6-N1	-2.42	1.32	1.38
2	A	701	UPG	C2-N1	2.41	1.42	1.38
2	B	701	UPG	PB-O2B	-2.37	1.44	1.55
2	A	701	UPG	PB-O2B	-2.34	1.44	1.55

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	UPG	O2-C2-N1	-7.76	112.70	122.80
2	A	701	UPG	O2-C2-N1	-7.25	113.36	122.80
2	A	701	UPG	C4-N3-C2	-6.83	118.14	126.61
2	B	701	UPG	C4-N3-C2	-6.48	118.57	126.61
2	B	701	UPG	N3-C2-N1	6.17	122.93	114.89

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	UPG	PB-O3A-PA-O1A
2	A	701	UPG	O5'-C1'-O3B-PB
2	B	701	UPG	C1'-O3B-PB-O1B
2	A	701	UPG	PB-O3A-PA-O2A
2	B	701	UPG	PB-O3A-PA-O2A

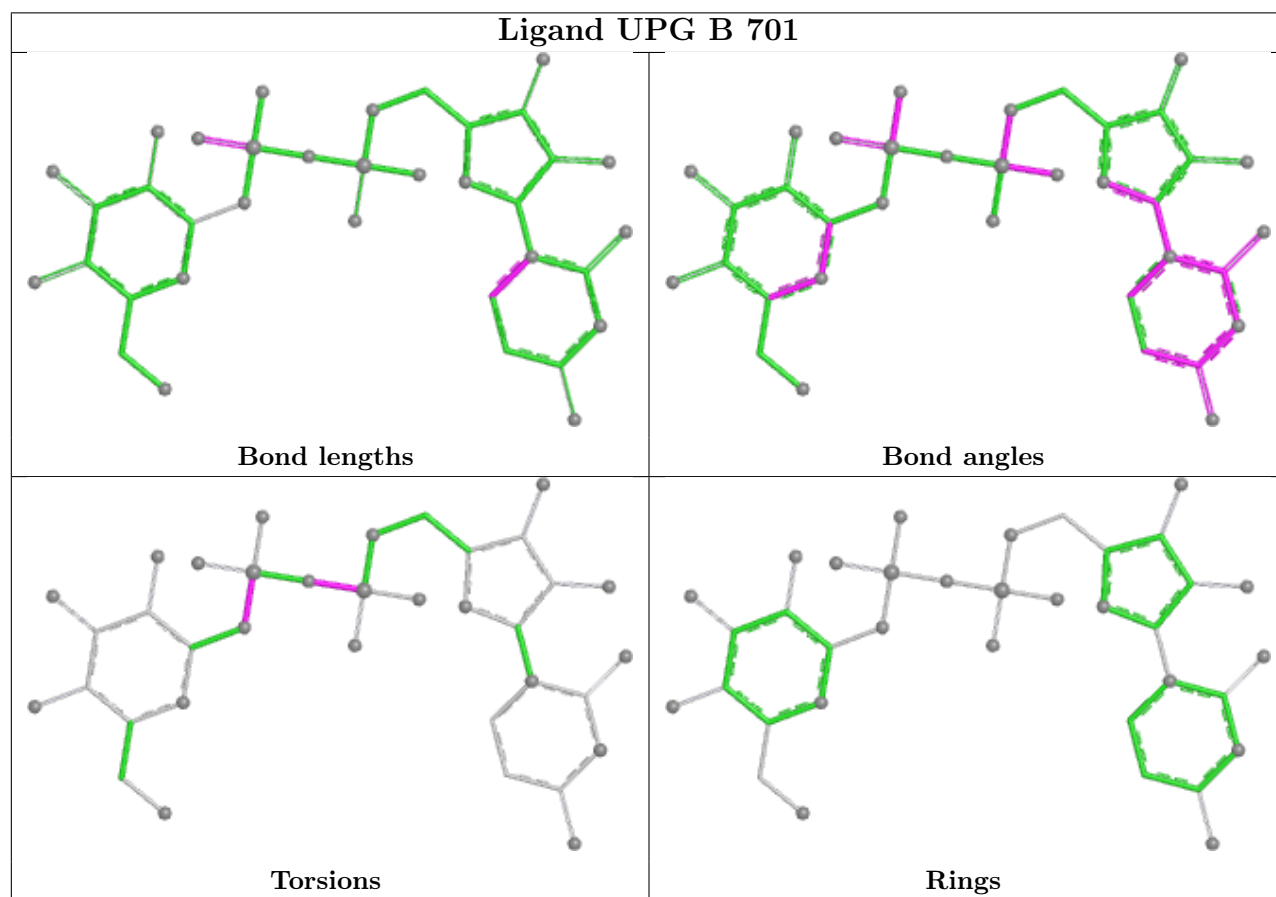
There are no ring outliers.

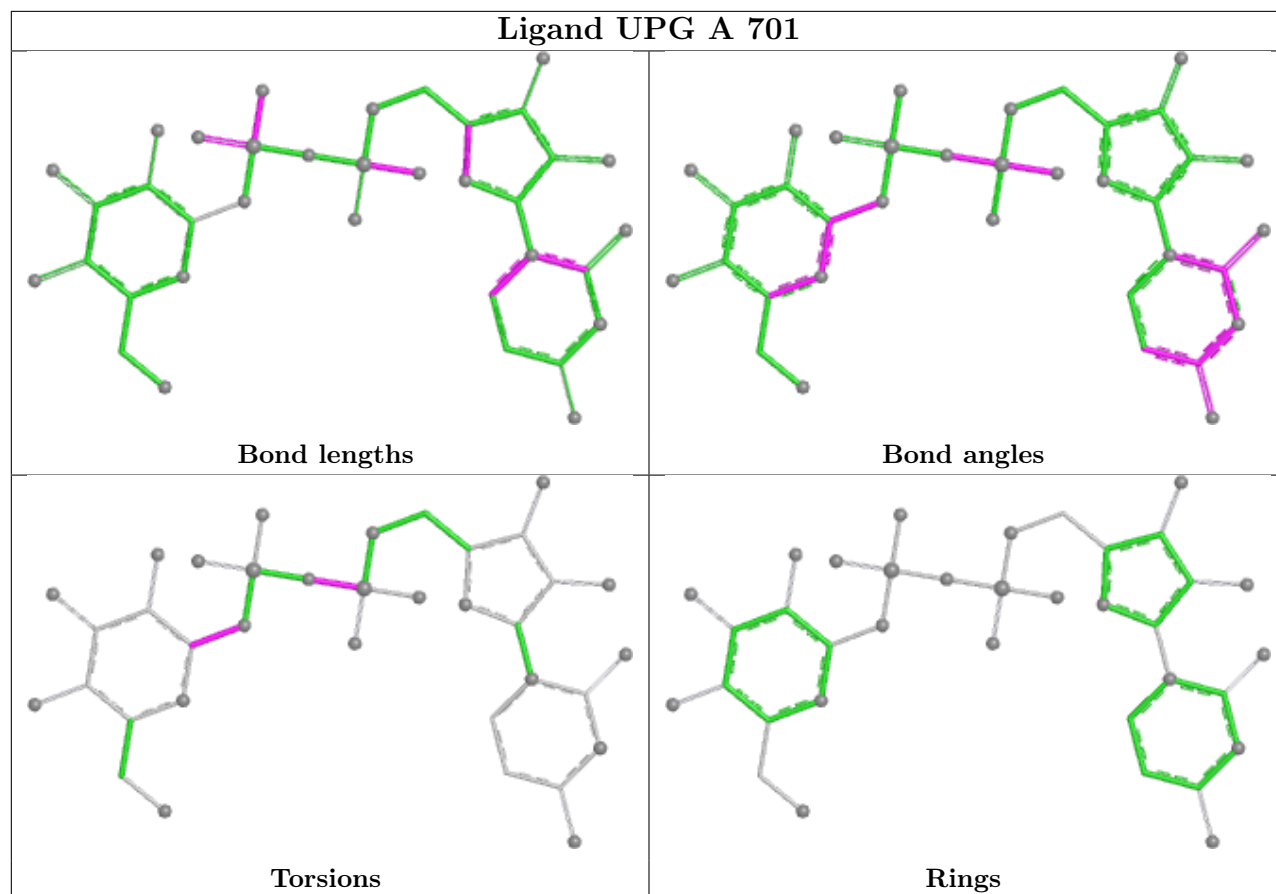
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	UPG	1	0
2	A	701	UPG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [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	607/655 (92%)	0.45	23 (3%) 44 40	38, 63, 96, 120	0
1	B	591/655 (90%)	0.46	21 (3%) 46 42	37, 60, 97, 109	0
All	All	1198/1310 (91%)	0.45	44 (3%) 45 41	37, 62, 97, 120	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	521	LEU	4.6
1	A	109	PHE	4.0
1	B	44	PHE	3.9
1	B	47	ASP	3.5
1	A	5	TYR	3.3

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](#)

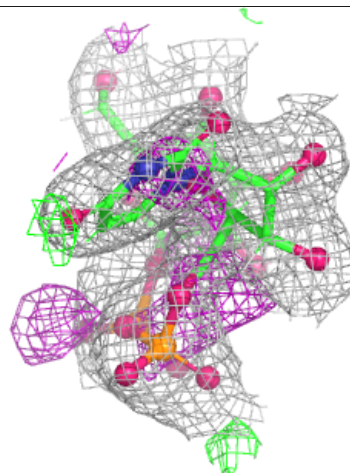
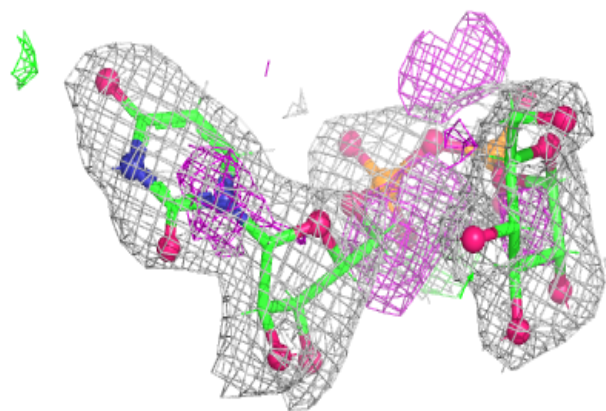
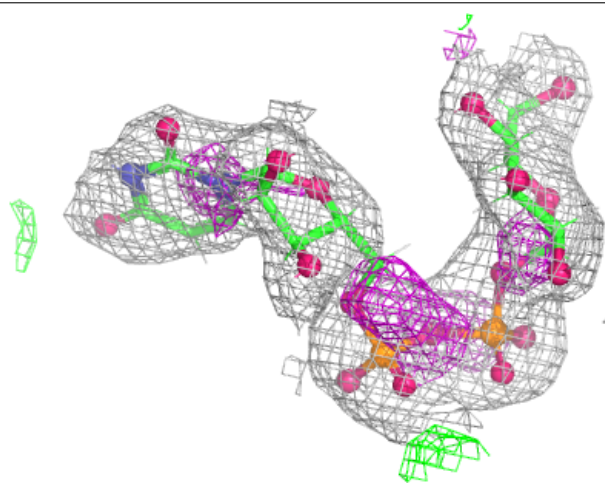
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	UPG	A	701	36/36	0.90	0.08	41,62,76,79	0
2	UPG	B	701	36/36	0.91	0.09	44,61,73,77	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.

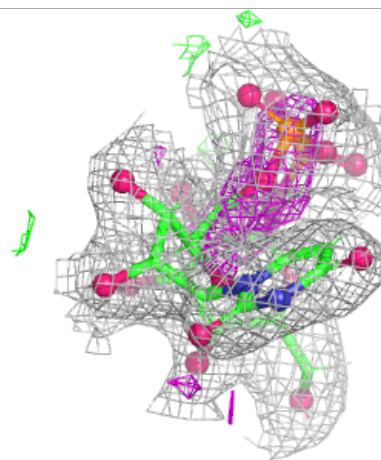
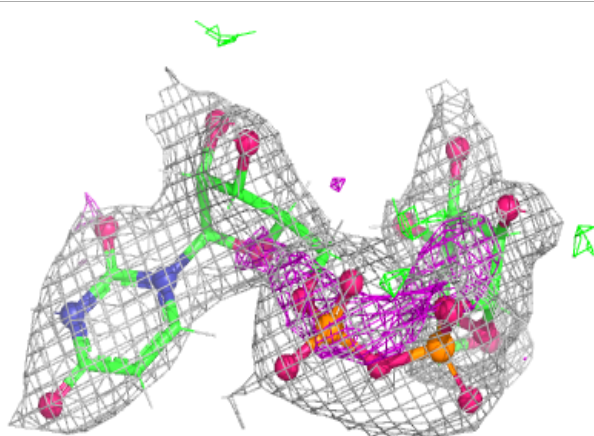
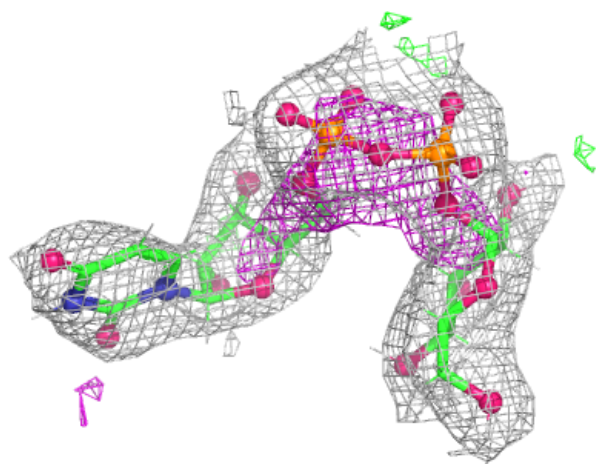
Electron density around UPG A 701:

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 UPG B 701:

$2mF_o-DF_c$ (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.