



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:59 PM UTC

PDB ID : 2ICY / pdb_00002icy
Title : Crystal Structure of a Putative UDP-glucose Pyrophosphorylase from Arabidopsis Thaliana with Bound UDP-glucose
Authors : McCoy, J.G.; Wesenberg, G.E.; Phillips Jr., G.N.; Bitto, E.; Bingman, C.A.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2006-09-13
Resolution : 1.64 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 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

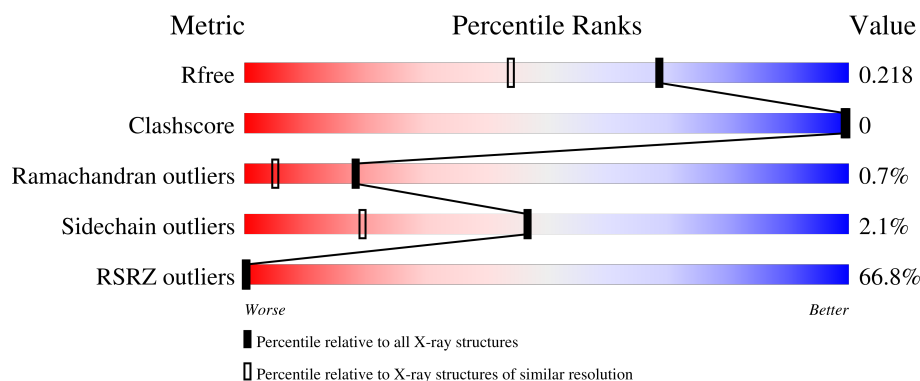
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	1-A	469	77% 94%
1	1-B	469	54% 95%
1	2-A	469	94%
1	2-B	469	96%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16171 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.

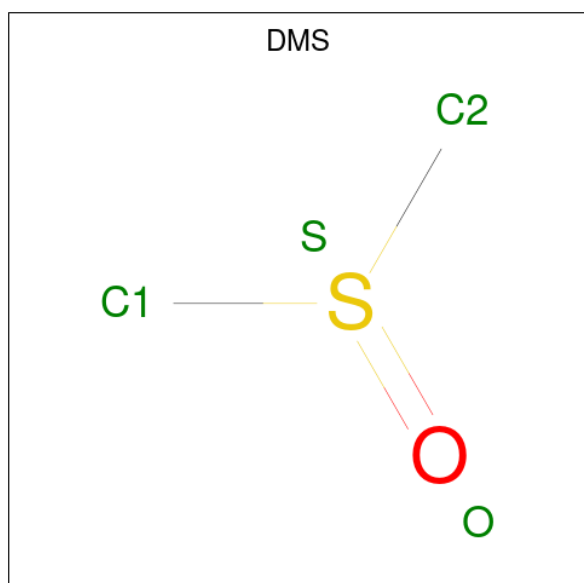
- Molecule 1 is a protein called Probable UTP-glucose-1-phosphate uridylyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	456	Total	C	N	O	S	0	0	0
			3550	2275	587	678	10			
1	2-A	459	Total	C	N	O	S	0	0	0
			3574	2289	593	682	10			
1	1-B	463	Total	C	N	O	S	0	0	0
			3602	2305	597	690	10			
1	2-B	463	Total	C	N	O	S	0	0	0
			3602	2305	597	690	10			

There are 2 discrepancies between the modelled and reference sequences:

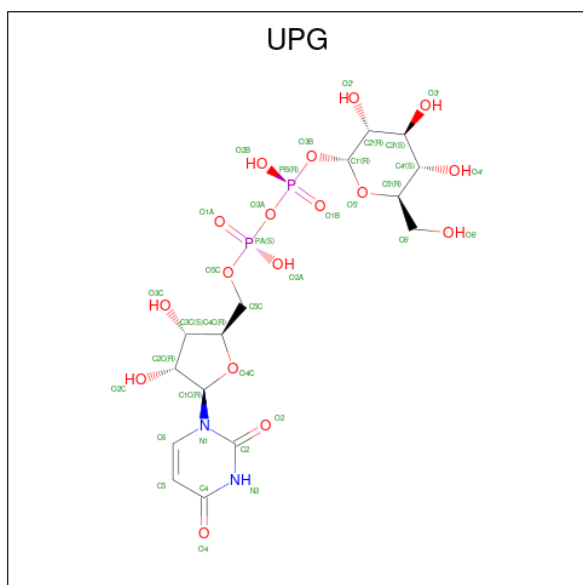
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	cloning artifact	UNP Q9M9P3
B	1	SER	-	cloning artifact	UNP Q9M9P3

- Molecule 2 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	1-A	1	Total	C	O	S	0	0
			4	2	1	1		
2	2-A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (CCD ID: UPG) (formula: $C_{15}H_{24}N_2O_{17}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	1-A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	2-A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	1-B	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

- Molecule 4

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1-A	356	Total	O	0	0
			356	356		
5	2-A	356	Total	O	0	0
			356	356		

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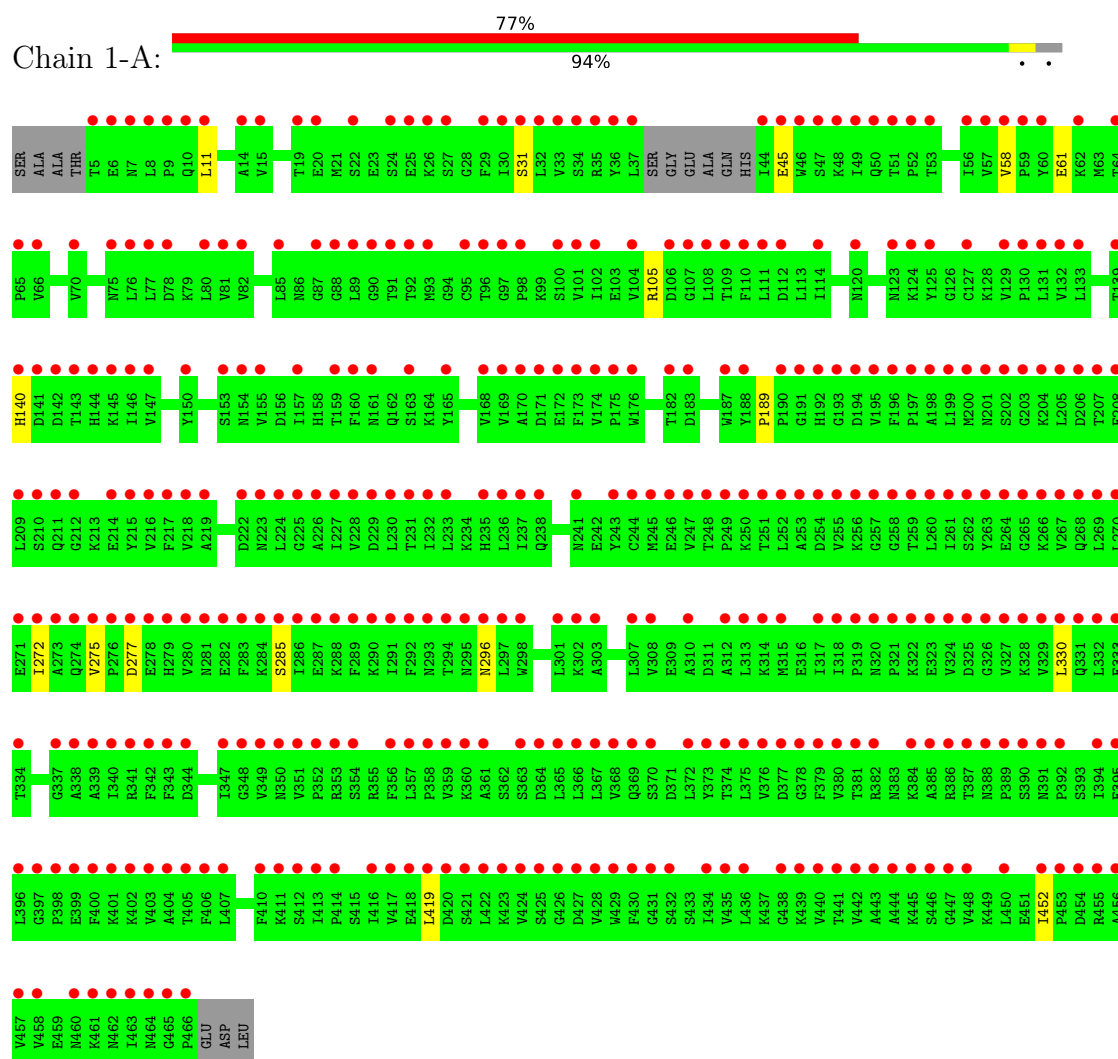
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1-B	492	Total 492	O 492	0	0
5	2-B	502	Total 502	O 502	0	0

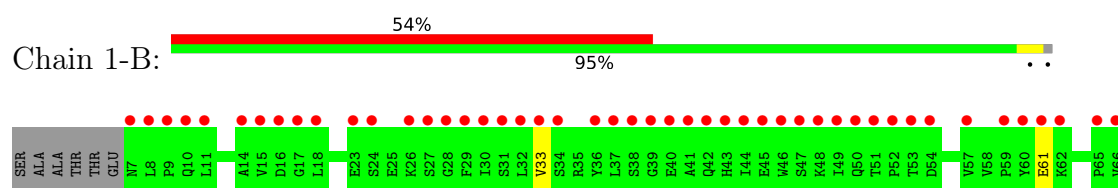
3 Residue-property plots

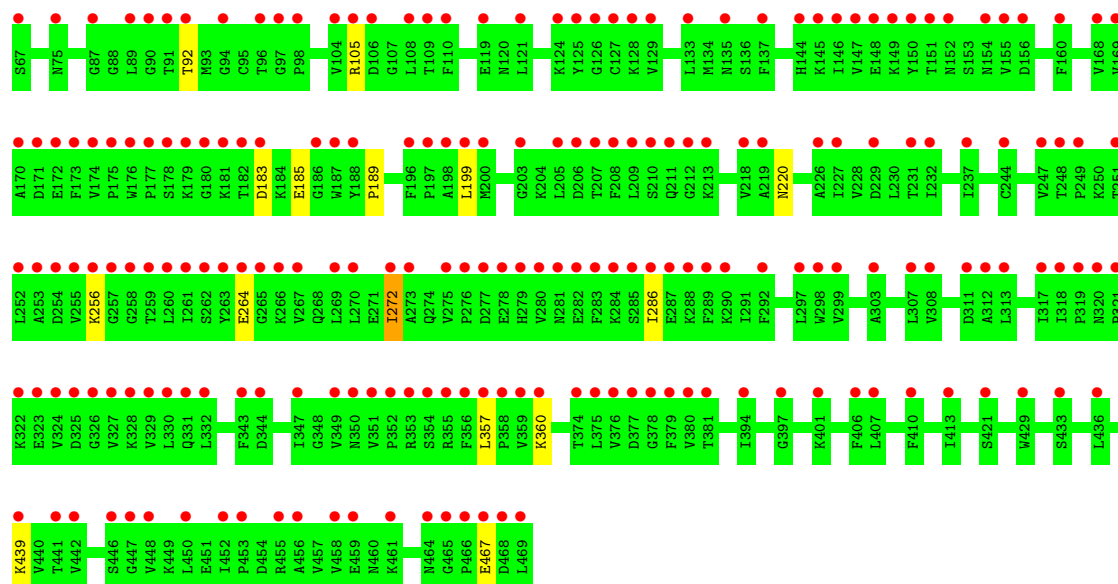
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Probable UTP-glucose-1-phosphate uridylyltransferase 2



- Molecule 1: Probable UTP-glucose-1-phosphate uridylyltransferase 2





- Molecule 1: Probable UTP-glucose-1-phosphate uridylyltransferase 2

Chain 2-A: 94%



- Molecule 1: Probable UTP-glucose-1-phosphate uridylyltransferase 2

Chain 2-B: 96%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	188.01Å 59.71Å 89.76Å 90.00° 100.32° 90.00°	Depositor
Resolution (Å)	38.25 – 1.64 38.25 – 1.64	Depositor EDS
% Data completeness (in resolution range)	99.4 (38.25-1.64) 99.4 (38.25-1.64)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 1.64Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.183 , 0.223 0.175 , 0.218	Depositor DCC
R_{free} test set	5964 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	16171	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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: U5P, DMS, 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	1-A	0.60	0/3617	0.79	5/4905 (0.1%)
1	1-B	0.67	0/3671	0.83	4/4979 (0.1%)
1	2-A	0.60	0/3642	0.80	5/4939 (0.1%)
1	2-B	0.67	0/3671	0.83	4/4979 (0.1%)
All	All	0.64	0/14601	0.81	18/19802 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-B	189	PRO	N-CA-C	-7.13	102.00	110.70
1	2-B	189	PRO	N-CA-C	-7.13	102.00	110.70
1	1-A	58	VAL	N-CA-C	6.29	114.03	108.63
1	2-A	58	VAL	N-CA-C	6.29	114.03	108.63
1	1-A	296	ASN	N-CA-C	-6.02	98.72	108.41
1	2-A	296	ASN	N-CA-C	-6.02	98.72	108.41
1	1-B	357	LEU	CA-C-N	-5.73	113.34	119.98
1	1-B	357	LEU	C-N-CA	-5.73	113.34	119.98
1	2-B	357	LEU	CA-C-N	-5.73	113.34	119.98
1	2-B	357	LEU	C-N-CA	-5.73	113.34	119.98
1	1-A	189	PRO	N-CA-C	-5.38	104.14	110.70
1	2-A	189	PRO	N-CA-C	-5.38	104.14	110.70
1	1-B	199	LEU	N-CA-C	-5.34	105.54	111.36
1	2-B	199	LEU	N-CA-C	-5.34	105.54	111.36
1	1-A	275	VAL	N-CA-C	5.33	113.14	107.76
1	2-A	275	VAL	N-CA-C	5.33	113.14	107.76
1	1-A	452	ILE	N-CA-C	-5.05	102.97	107.56
1	2-A	452	ILE	N-CA-C	-5.05	102.97	107.56

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	1-A	3550	0	3630	0	0
1	1-B	3602	0	3673	3	0
1	2-A	3574	0	3650	0	0
1	2-B	3602	0	3673	0	0
2	1-A	4	0	6	0	0
2	2-A	4	0	6	0	0
3	1-A	36	0	22	0	0
3	1-B	36	0	22	3	0
3	2-A	36	0	22	0	0
4	2-B	21	0	11	0	0
5	1-A	356	0	0	0	0
5	1-B	492	0	0	0	0
5	2-A	356	0	0	0	0
5	2-B	502	0	0	0	0
All	All	16171	0	14715	3	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 0.

All (3) 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:360:LYS:NZ	3:B:902:UPG:O1A	2.42	0.52
1:B:220:ASN:HD21	3:B:902:UPG:H5C1	1.85	0.42
1:B:220:ASN:OD1	3:B:902:UPG:H4C	2.20	0.42

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	1-A	452/469 (96%)	428 (95%)	22 (5%)	2 (0%)	30	14
1	1-B	461/469 (98%)	442 (96%)	14 (3%)	5 (1%)	11	1
1	2-A	455/469 (97%)	431 (95%)	23 (5%)	1 (0%)	43	27
1	2-B	461/469 (98%)	440 (95%)	17 (4%)	4 (1%)	14	2
All	All	1829/1876 (98%)	1741 (95%)	76 (4%)	12 (1%)	18	5

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2-B	40	GLU
1	2-B	181	LYS
1	1-A	45	GLU
1	1-B	264	GLU
1	2-B	70	VAL
1	1-B	272	ILE
1	1-A	285	SER
1	1-B	183	ASP
1	1-B	185	GLU
1	2-B	69	ASP
1	2-A	46	TRP
1	1-B	286	ILE

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	1-A	405/414 (98%)	396 (98%)	9 (2%)	45	18
1	1-B	410/414 (99%)	402 (98%)	8 (2%)	48	21
1	2-A	407/414 (98%)	397 (98%)	10 (2%)	42	14
1	2-B	410/414 (99%)	402 (98%)	8 (2%)	48	21
All	All	1632/1656 (99%)	1597 (98%)	35 (2%)	47	19

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	11	LEU
1	1-A	31	SER
1	1-A	61	GLU
1	1-A	105	ARG
1	1-A	140	HIS
1	1-A	272	ILE
1	1-A	277	ASP
1	1-A	330	LEU
1	1-A	419	LEU
1	1-B	33	VAL
1	1-B	61	GLU
1	1-B	92	THR
1	1-B	105	ARG
1	1-B	256	LYS
1	1-B	272	ILE
1	1-B	439	LYS
1	1-B	467	GLU
1	2-A	11	LEU
1	2-A	31	SER
1	2-A	42	GLN
1	2-A	61	GLU
1	2-A	105	ARG
1	2-A	140	HIS
1	2-A	272	ILE
1	2-A	277	ASP
1	2-A	330	LEU
1	2-A	419	LEU
1	2-B	33	VAL
1	2-B	61	GLU
1	2-B	92	THR
1	2-B	105	ARG
1	2-B	256	LYS
1	2-B	272	ILE

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Mol	Chain	Res	Type
1	2-B	439	LYS
1	2-B	467	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	140	HIS
1	1-A	238	GLN
1	1-B	274	GLN
1	1-B	350	ASN
1	2-A	42	GLN
1	2-A	43	HIS
1	2-A	86	ASN
1	2-A	135	ASN
1	2-A	320	ASN
1	2-B	86	ASN
1	2-B	135	ASN
1	2-B	279	HIS

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](#)

5 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	UPG	1-A	901	-	37,38,38	1.90	10 (27%)	55,58,58	1.28	7 (12%)
2	DMS	2-A	900	-	3,3,3	1.20	0	3,3,3	1.11	0
3	UPG	1-B	902	-	37,38,38	1.74	9 (24%)	55,58,58	1.40	8 (14%)
3	UPG	2-A	901	-	37,38,38	1.90	10 (27%)	55,58,58	1.28	7 (12%)
2	DMS	1-A	900	-	3,3,3	1.20	0	3,3,3	1.11	0

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	UPG	1-B	902	-	-	0/23/59/59	0/3/3/3
3	UPG	2-A	901	-	-	0/23/59/59	0/3/3/3
3	UPG	1-A	901	-	-	0/23/59/59	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-B	902	UPG	PA-O3A	4.50	1.64	1.59
3	1-A	901	UPG	PB-O3A	4.34	1.64	1.59
3	2-A	901	UPG	PB-O3A	4.34	1.64	1.59
3	1-A	901	UPG	PB-O3B	4.20	1.72	1.59
3	2-A	901	UPG	PB-O3B	4.20	1.72	1.59
3	1-A	901	UPG	PA-O3A	4.05	1.63	1.59
3	2-A	901	UPG	PA-O3A	4.05	1.63	1.59
3	1-B	902	UPG	PB-O3A	3.72	1.63	1.59
3	1-B	902	UPG	O5'-C5'	3.67	1.53	1.44
3	1-A	901	UPG	C6-N1	3.31	1.46	1.38
3	2-A	901	UPG	C6-N1	3.31	1.46	1.38
3	1-B	902	UPG	O3'-C3'	2.74	1.49	1.43
3	1-A	901	UPG	PA-O5C	-2.72	1.48	1.59
3	2-A	901	UPG	PA-O5C	-2.72	1.48	1.59
3	1-B	902	UPG	PB-O1B	-2.56	1.41	1.50
3	1-A	901	UPG	PB-O2B	-2.56	1.43	1.55
3	2-A	901	UPG	PB-O2B	-2.56	1.43	1.55
3	1-A	901	UPG	C2C-C1C	-2.38	1.46	1.53
3	2-A	901	UPG	C2C-C1C	-2.38	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-B	902	UPG	C2-N1	2.32	1.42	1.38
3	1-B	902	UPG	C5C-C4C	2.30	1.58	1.51
3	1-B	902	UPG	C4'-C5'	2.29	1.57	1.53
3	1-A	901	UPG	O3C-C3C	2.23	1.48	1.43
3	2-A	901	UPG	O3C-C3C	2.23	1.48	1.43
3	1-A	901	UPG	O4C-C4C	2.16	1.49	1.45
3	2-A	901	UPG	O4C-C4C	2.16	1.49	1.45
3	1-B	902	UPG	PA-O2A	-2.11	1.45	1.55
3	1-A	901	UPG	C4'-C5'	2.10	1.57	1.53
3	2-A	901	UPG	C4'-C5'	2.10	1.57	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-B	902	UPG	O5'-C1'-O3B	-3.51	106.78	111.36
3	1-B	902	UPG	C4'-C3'-C2'	-3.25	105.12	110.83
3	1-B	902	UPG	O3'-C3'-C2'	3.16	117.83	110.38
3	1-B	902	UPG	C2C-C3C-C4C	2.68	107.78	102.61
3	1-A	901	UPG	O3A-PA-O1A	-2.62	102.83	110.70
3	2-A	901	UPG	O3A-PA-O1A	-2.62	102.83	110.70
3	1-B	902	UPG	O4'-C4'-C3'	-2.58	104.29	110.38
3	1-A	901	UPG	C6'-C5'-C4'	-2.53	106.80	113.02
3	2-A	901	UPG	C6'-C5'-C4'	-2.53	106.80	113.02
3	1-A	901	UPG	O4'-C4'-C3'	-2.49	104.52	110.38
3	2-A	901	UPG	O4'-C4'-C3'	-2.49	104.52	110.38
3	1-B	902	UPG	C1'-C2'-C3'	2.48	115.23	110.01
3	1-B	902	UPG	PB-O3B-C1'	2.30	130.56	121.21
3	1-A	901	UPG	O3'-C3'-C2'	-2.27	105.04	110.38
3	2-A	901	UPG	O3'-C3'-C2'	-2.27	105.04	110.38
3	1-A	901	UPG	C4'-C3'-C2'	-2.25	106.88	110.83
3	2-A	901	UPG	C4'-C3'-C2'	-2.25	106.88	110.83
3	1-B	902	UPG	O6'-C6'-C5'	-2.12	104.13	111.33
3	1-A	901	UPG	C2C-C3C-C4C	2.09	106.64	102.61
3	2-A	901	UPG	C2C-C3C-C4C	2.09	106.64	102.61
3	1-A	901	UPG	O2B-PB-O1B	2.06	122.02	112.44
3	2-A	901	UPG	O2B-PB-O1B	2.06	122.02	112.44

There are no chirality outliers.

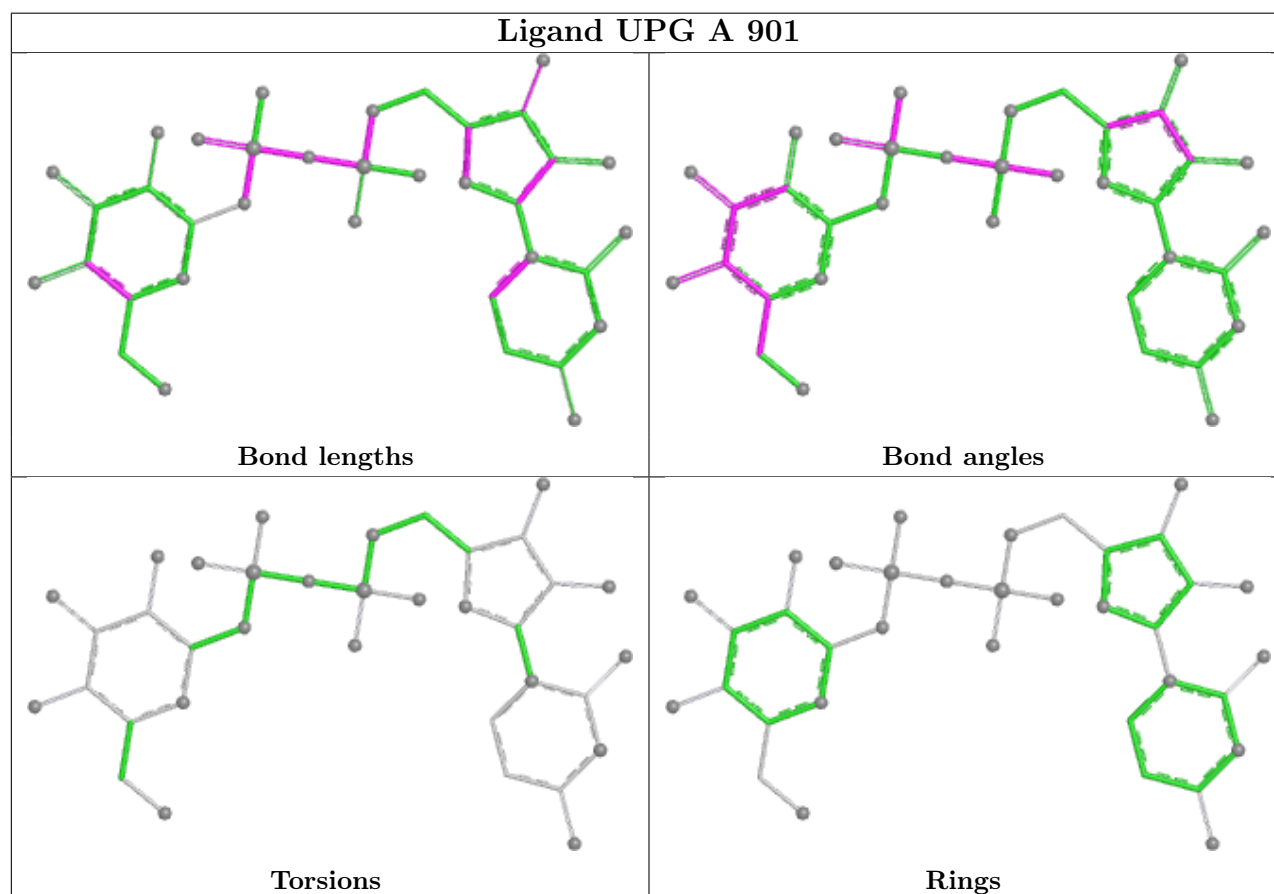
There are no torsion outliers.

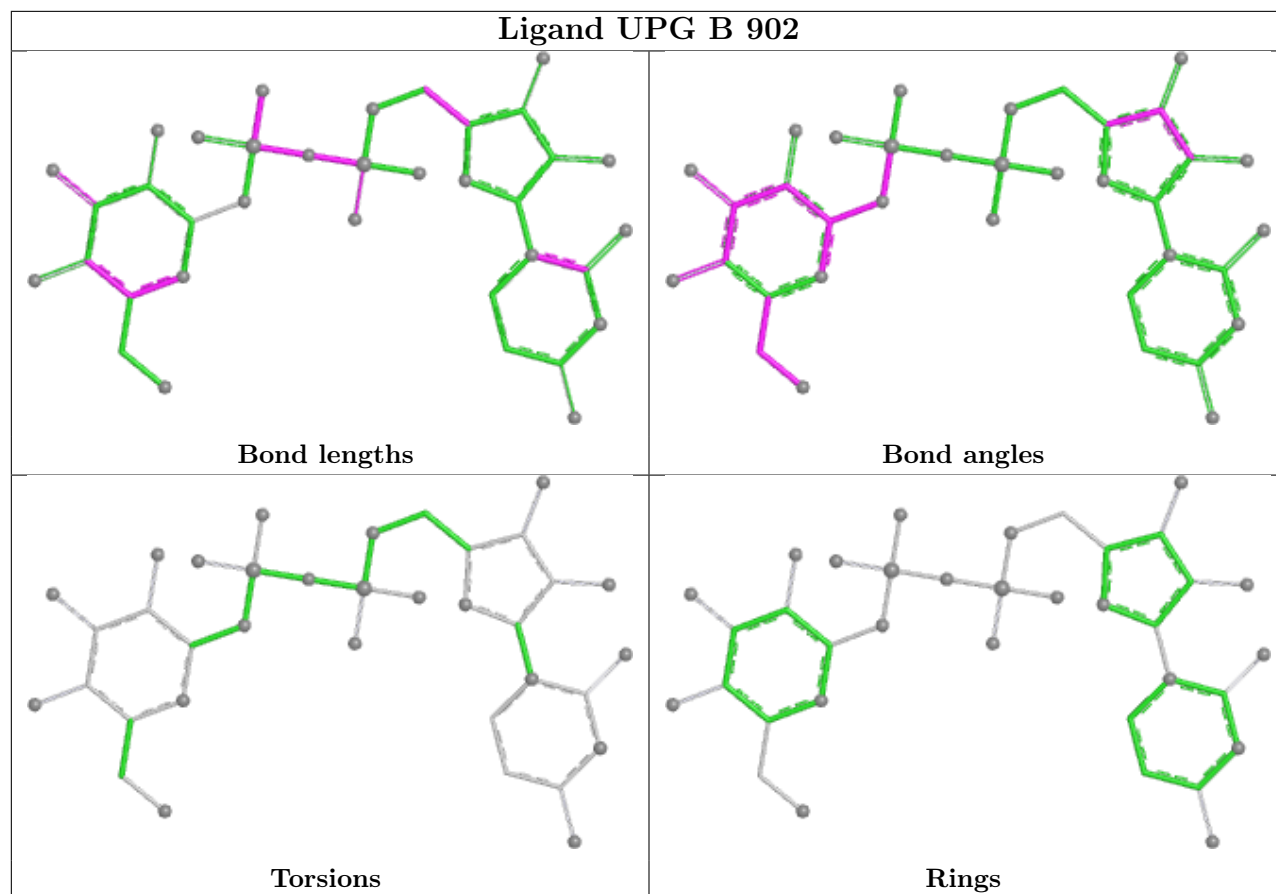
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	1-B	902	UPG	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

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, 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	1-A	456/469 (97%)	3.21	363 (79%)  	5, 12, 25, 36	456 (100%)
1	1-B	463/469 (98%)	2.55	251 (54%)  	4, 10, 23, 35	463 (100%)
1	2-A	0/469	-	-	-	-
1	2-B	0/469	-	-	-	-
All	All	919/1876 (48%)	2.88	614 (66%)  	4, 11, 24, 36	919 (100%)

All (614) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	366	LEU	10.8
1	1-A	44	ILE	9.4
1	1-B	376	VAL	8.6
1	1-B	378	GLY	8.5
1	1-B	176	TRP	8.3
1	1-B	324	VAL	8.3
1	1-B	379	PHE	8.2
1	1-A	89	LEU	8.0
1	1-B	41	ALA	7.7
1	1-A	283	PHE	7.5
1	1-B	283	PHE	7.4
1	1-B	380	VAL	7.4
1	1-A	276	PRO	7.3
1	1-A	324	VAL	7.3
1	1-A	46	TRP	7.1
1	1-A	392	PRO	7.0
1	1-A	441	THR	7.0
1	1-A	273	ALA	6.9
1	1-A	272	ILE	6.9
1	1-A	458	VAL	6.9
1	1-B	327	VAL	6.9
1	1-A	434	ILE	6.9

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Mol	Chain	Res	Type	RSRZ
1	1-A	255	VAL	6.8
1	1-A	280	VAL	6.7
1	1-A	327	VAL	6.7
1	1-A	444	ALA	6.6
1	1-A	37	LEU	6.6
1	1-B	286	ILE	6.6
1	1-A	253	ALA	6.6
1	1-A	286	ILE	6.5
1	1-A	436	LEU	6.5
1	1-A	443	ALA	6.4
1	1-B	252	LEU	6.3
1	1-A	252	LEU	6.2
1	1-B	375	LEU	6.2
1	1-A	251	THR	6.1
1	1-B	280	VAL	6.0
1	1-A	406	PHE	6.0
1	1-B	275	VAL	6.0
1	1-A	365	LEU	5.9
1	1-A	394	ILE	5.8
1	1-B	255	VAL	5.8
1	1-A	356	PHE	5.8
1	1-A	379	PHE	5.8
1	1-B	285	SER	5.8
1	1-A	275	VAL	5.7
1	1-B	272	ILE	5.7
1	1-A	258	GLY	5.7
1	1-A	361	ALA	5.7
1	1-A	417	VAL	5.6
1	1-A	225	GLY	5.5
1	1-A	47	SER	5.5
1	1-B	182	THR	5.5
1	1-A	368	VAL	5.4
1	1-A	422	LEU	5.4
1	1-A	430	PHE	5.4
1	1-B	357	LEU	5.4
1	1-A	291	ILE	5.3
1	1-A	452	ILE	5.3
1	1-B	33	VAL	5.3
1	1-B	92	THR	5.3
1	1-B	326	GLY	5.3
1	1-B	50	GLN	5.3
1	1-A	226	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
1	1-B	377	ASP	5.3
1	1-A	453	PRO	5.2
1	1-A	372	LEU	5.2
1	1-B	205	LEU	5.2
1	1-B	171	ASP	5.2
1	1-A	88	GLY	5.2
1	1-B	44	ILE	5.2
1	1-B	174	VAL	5.2
1	1-B	34	SER	5.2
1	1-B	151	THR	5.2
1	1-A	376	VAL	5.1
1	1-B	356	PHE	5.1
1	1-A	171	ASP	5.1
1	1-B	49	ILE	5.1
1	1-A	33	VAL	5.1
1	1-A	351	VAL	5.1
1	1-A	440	VAL	5.1
1	1-A	442	VAL	5.1
1	1-B	173	PHE	5.1
1	1-A	420	ASP	5.1
1	1-B	281	ASN	5.0
1	1-B	46	TRP	5.0
1	1-A	90	GLY	5.0
1	1-B	279	HIS	5.0
1	1-A	462	ASN	5.0
1	1-A	254	ASP	5.0
1	1-A	374	THR	5.0
1	1-A	389	PRO	5.0
1	1-A	410	PHE	5.0
1	1-A	435	VAL	5.0
1	1-A	419	LEU	5.0
1	1-A	289	PHE	5.0
1	1-B	289	PHE	4.9
1	1-A	326	GLY	4.9
1	1-B	320	ASN	4.9
1	1-B	253	ALA	4.9
1	1-A	438	GLY	4.9
1	1-A	32	LEU	4.9
1	1-B	32	LEU	4.9
1	1-A	5	THR	4.8
1	1-B	276	PRO	4.8
1	1-B	209	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	1-A	203	GLY	4.8
1	1-B	177	PRO	4.8
1	1-B	284	LYS	4.8
1	1-A	385	ALA	4.8
1	1-B	179	LYS	4.8
1	1-A	400	PHE	4.8
1	1-A	421	SER	4.7
1	1-B	30	ILE	4.7
1	1-A	8	LEU	4.7
1	1-B	256	LYS	4.7
1	1-A	257	GLY	4.7
1	1-A	210	SER	4.7
1	1-B	208	PHE	4.6
1	1-A	450	LEU	4.6
1	1-A	431	GLY	4.6
1	1-B	277	ASP	4.6
1	1-A	279	HIS	4.6
1	1-B	212	GLY	4.6
1	1-B	325	ASP	4.6
1	1-A	330	LEU	4.5
1	1-B	149	LYS	4.5
1	1-A	96	THR	4.5
1	1-A	259	THR	4.5
1	1-B	207	THR	4.5
1	1-B	381	THR	4.5
1	1-B	43	HIS	4.5
1	1-B	354	SER	4.5
1	1-A	357	LEU	4.5
1	1-A	227	ILE	4.5
1	1-A	413	ILE	4.5
1	1-A	352	PRO	4.4
1	1-A	11	LEU	4.4
1	1-B	328	LYS	4.4
1	1-B	128	LYS	4.4
1	1-A	391	ASN	4.4
1	1-A	329	VAL	4.4
1	1-A	349	VAL	4.4
1	1-A	202	SER	4.4
1	1-A	390	SER	4.4
1	1-A	463	ILE	4.4
1	1-B	152	ASN	4.3
1	1-B	358	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	1-B	273	ALA	4.3
1	1-B	292	PHE	4.3
1	1-B	183	ASP	4.3
1	1-A	456	ALA	4.3
1	1-B	330	LEU	4.3
1	1-B	351	VAL	4.3
1	1-A	284	LYS	4.3
1	1-A	375	LEU	4.2
1	1-B	89	LEU	4.2
1	1-B	48	LYS	4.2
1	1-B	169	VAL	4.2
1	1-A	350	ASN	4.2
1	1-B	261	ILE	4.2
1	1-A	48	LYS	4.2
1	1-A	36	TYR	4.2
1	1-A	377	ASP	4.2
1	1-A	454	ASP	4.2
1	1-B	175	PRO	4.2
1	1-A	228	VAL	4.2
1	1-A	397	GLY	4.2
1	1-A	285	SER	4.1
1	1-B	282	GLU	4.1
1	1-A	321	PRO	4.1
1	1-A	292	PHE	4.1
1	1-B	8	LEU	4.1
1	1-A	93	MET	4.1
1	1-B	91	THR	4.1
1	1-B	181	LYS	4.1
1	1-A	418	GLU	4.1
1	1-A	64	THR	4.1
1	1-B	104	VAL	4.1
1	1-B	170	ALA	4.0
1	1-B	329	VAL	4.0
1	1-A	358	PRO	4.0
1	1-B	319	PRO	4.0
1	1-A	34	SER	4.0
1	1-A	237	ILE	4.0
1	1-A	298	TRP	4.0
1	1-B	198	ALA	4.0
1	1-B	322	LYS	4.0
1	1-A	49	ILE	3.9
1	1-A	98	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	1-A	464	ASN	3.9
1	1-A	209	LEU	3.9
1	1-A	263	TYR	3.9
1	1-B	150	TYR	3.9
1	1-B	146	ILE	3.9
1	1-B	37	LEU	3.9
1	1-A	278	GLU	3.9
1	1-B	203	GLY	3.9
1	1-A	398	PRO	3.9
1	1-A	30	ILE	3.9
1	1-A	57	VAL	3.9
1	1-A	387	THR	3.9
1	1-B	210	SER	3.9
1	1-A	447	GLY	3.9
1	1-B	465	GLY	3.9
1	1-B	469	LEU	3.8
1	1-A	266	LYS	3.8
1	1-A	414	PRO	3.8
1	1-A	405	THR	3.8
1	1-B	178	SER	3.8
1	1-A	388	ASN	3.8
1	1-A	360	LYS	3.8
1	1-A	439	LYS	3.8
1	1-B	288	LYS	3.8
1	1-B	10	GLN	3.8
1	1-B	31	SER	3.8
1	1-A	45	GLU	3.8
1	1-B	172	GLU	3.8
1	1-A	322	LYS	3.7
1	1-A	87	GLY	3.7
1	1-A	174	VAL	3.7
1	1-A	141	ASP	3.7
1	1-A	455	ARG	3.7
1	1-A	342	PHE	3.7
1	1-B	249	PRO	3.7
1	1-B	260	LEU	3.7
1	1-A	426	GLY	3.7
1	1-A	317	ILE	3.7
1	1-A	457	VAL	3.7
1	1-A	143	THR	3.7
1	1-A	231	THR	3.7
1	1-A	248	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	1-A	142	ASP	3.7
1	1-B	36	TYR	3.7
1	1-A	359	VAL	3.6
1	1-B	247	VAL	3.6
1	1-A	233	LEU	3.6
1	1-A	277	ASP	3.6
1	1-A	127	CYS	3.6
1	1-A	288	LYS	3.6
1	1-A	173	PHE	3.6
1	1-A	287	GLU	3.6
1	1-B	53	THR	3.6
1	1-A	15	VAL	3.6
1	1-A	111	LEU	3.6
1	1-A	269	LEU	3.6
1	1-A	396	LEU	3.6
1	1-B	39	GLY	3.6
1	1-B	121	LEU	3.6
1	1-A	339	ALA	3.6
1	1-A	274	GLN	3.6
1	1-A	320	ASN	3.5
1	1-A	446	SER	3.5
1	1-A	337	GLY	3.5
1	1-A	217	PHE	3.5
1	1-B	29	PHE	3.5
1	1-B	450	LEU	3.5
1	1-A	423	LYS	3.5
1	1-A	161	ASN	3.5
1	1-B	90	GLY	3.5
1	1-A	429	TRP	3.5
1	1-A	247	VAL	3.5
1	1-A	144	HIS	3.5
1	1-A	416	ILE	3.5
1	1-A	29	PHE	3.5
1	1-B	18	LEU	3.5
1	1-A	448	VAL	3.5
1	1-A	92	THR	3.5
1	1-A	35	ARG	3.5
1	1-A	325	ASP	3.4
1	1-A	6	GLU	3.4
1	1-A	66	VAL	3.4
1	1-A	70	VAL	3.4
1	1-A	424	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	1-B	155	VAL	3.4
1	1-A	19	THR	3.4
1	1-A	465	GLY	3.4
1	1-B	97	GLY	3.4
1	1-B	180	GLY	3.4
1	1-A	59	PRO	3.4
1	1-B	106	ASP	3.4
1	1-A	50	GLN	3.4
1	1-A	170	ALA	3.4
1	1-A	363	SER	3.4
1	1-B	47	SER	3.4
1	1-A	31	SER	3.4
1	1-B	360	LYS	3.4
1	1-A	282	GLU	3.4
1	1-A	428	VAL	3.4
1	1-B	267	VAL	3.4
1	1-A	56	ILE	3.3
1	1-A	230	LEU	3.3
1	1-B	51	THR	3.3
1	1-B	248	THR	3.3
1	1-B	321	PRO	3.3
1	1-A	267	VAL	3.3
1	1-A	14	ALA	3.3
1	1-B	94	GLY	3.3
1	1-A	460	ASN	3.3
1	1-B	96	THR	3.3
1	1-A	297	LEU	3.3
1	1-A	301	LEU	3.3
1	1-A	256	LYS	3.3
1	1-B	211	GLN	3.3
1	1-B	452	ILE	3.3
1	1-B	352	PRO	3.3
1	1-A	140	HIS	3.3
1	1-A	132	VAL	3.3
1	1-B	15	VAL	3.3
1	1-A	261	ILE	3.2
1	1-A	340	ILE	3.2
1	1-A	9	PRO	3.2
1	1-B	54	ASP	3.2
1	1-A	341	ARG	3.2
1	1-A	7	ASN	3.2
1	1-B	168	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	1-B	200	MET	3.2
1	1-B	186	GLY	3.2
1	1-A	262	SER	3.2
1	1-A	370	SER	3.2
1	1-B	38	SER	3.2
1	1-A	76	LEU	3.2
1	1-A	238	GLN	3.2
1	1-B	257	GLY	3.2
1	1-A	60	TYR	3.2
1	1-B	264	GLU	3.2
1	1-B	466	PRO	3.2
1	1-A	281	ASN	3.2
1	1-A	205	LEU	3.2
1	1-B	42	GLN	3.2
1	1-B	269	LEU	3.2
1	1-A	386	ARG	3.2
1	1-A	199	LEU	3.1
1	1-A	395	GLU	3.1
1	1-A	101	VAL	3.1
1	1-A	104	VAL	3.1
1	1-A	466	PRO	3.1
1	1-A	243	TYR	3.1
1	1-A	373	TYR	3.1
1	1-B	413	ILE	3.1
1	1-A	77	LEU	3.1
1	1-A	407	LEU	3.1
1	1-B	374	THR	3.1
1	1-B	9	PRO	3.1
1	1-B	98	PRO	3.1
1	1-A	24	SER	3.1
1	1-A	125	TYR	3.1
1	1-A	97	GLY	3.1
1	1-B	258	GLY	3.1
1	1-A	332	LEU	3.1
1	1-B	105	ARG	3.1
1	1-A	51	THR	3.1
1	1-B	433	SER	3.1
1	1-B	206	ASP	3.1
1	1-A	58	VAL	3.0
1	1-A	380	VAL	3.0
1	1-B	439	LYS	3.0
1	1-A	80	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	1-A	224	LEU	3.0
1	1-A	270	LEU	3.0
1	1-A	354	SER	3.0
1	1-A	245	MET	3.0
1	1-A	461	LYS	3.0
1	1-A	308	VAL	3.0
1	1-B	265	GLY	3.0
1	1-B	353	ARG	3.0
1	1-A	236	LEU	3.0
1	1-A	312	ALA	3.0
1	1-B	127	CYS	3.0
1	1-A	271	GLU	3.0
1	1-B	7	ASN	3.0
1	1-A	307	LEU	3.0
1	1-B	11	LEU	3.0
1	1-B	287	GLU	3.0
1	1-A	197	PRO	3.0
1	1-B	27	SER	2.9
1	1-B	278	GLU	2.9
1	1-A	157	ILE	2.9
1	1-A	232	ILE	2.9
1	1-A	319	PRO	2.9
1	1-A	110	PHE	2.9
1	1-B	229	ASP	2.9
1	1-B	332	LEU	2.9
1	1-A	212	GLY	2.9
1	1-A	249	PRO	2.9
1	1-A	369	GLN	2.9
1	1-A	427	ASP	2.9
1	1-A	302	LYS	2.9
1	1-A	207	THR	2.9
1	1-B	259	THR	2.9
1	1-A	195	VAL	2.9
1	1-B	14	ALA	2.9
1	1-A	318	ILE	2.9
1	1-B	317	ILE	2.9
1	1-B	231	THR	2.8
1	1-A	250	LYS	2.8
1	1-A	52	PRO	2.8
1	1-A	131	LEU	2.8
1	1-A	260	LEU	2.8
1	1-B	24	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	1-B	262	SER	2.8
1	1-A	201	ASN	2.8
1	1-A	208	PHE	2.8
1	1-B	87	GLY	2.8
1	1-B	303	ALA	2.8
1	1-A	403	VAL	2.8
1	1-B	147	VAL	2.8
1	1-A	445	LYS	2.8
1	1-B	145	LYS	2.8
1	1-B	156	ASP	2.8
1	1-A	265	GLY	2.8
1	1-A	310	ALA	2.8
1	1-A	338	ALA	2.8
1	1-A	244	CYS	2.8
1	1-B	199	LEU	2.8
1	1-A	411	LYS	2.8
1	1-B	318	ILE	2.8
1	1-A	91	THR	2.8
1	1-B	109	THR	2.8
1	1-B	126	GLY	2.8
1	1-A	404	ALA	2.7
1	1-B	467	GLU	2.7
1	1-B	442	VAL	2.7
1	1-A	367	LEU	2.7
1	1-B	125	TYR	2.7
1	1-B	188	TYR	2.7
1	1-A	192	HIS	2.7
1	1-A	107	GLY	2.7
1	1-A	78	ASP	2.7
1	1-A	108	LEU	2.7
1	1-A	53	THR	2.7
1	1-B	397	GLY	2.7
1	1-A	75	ASN	2.7
1	1-A	303	ALA	2.7
1	1-A	344	ASP	2.7
1	1-B	52	PRO	2.7
1	1-B	61	GLU	2.7
1	1-A	95	CYS	2.7
1	1-B	407	LEU	2.7
1	1-B	263	TYR	2.7
1	1-A	204	LYS	2.7
1	1-A	328	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	1-A	229	ASP	2.7
1	1-B	455	ARG	2.6
1	1-B	197	PRO	2.6
1	1-A	153	SER	2.6
1	1-B	251	THR	2.6
1	1-A	85	LEU	2.6
1	1-B	108	LEU	2.6
1	1-A	147	VAL	2.6
1	1-B	359	VAL	2.6
1	1-A	347	ILE	2.6
1	1-B	344	ASP	2.6
1	1-A	402	LYS	2.6
1	1-B	464	ASN	2.6
1	1-A	378	GLY	2.6
1	1-A	172	GLU	2.6
1	1-B	133	LEU	2.6
1	1-B	254	ASP	2.6
1	1-A	155	VAL	2.6
1	1-A	102	ILE	2.6
1	1-B	394	ILE	2.6
1	1-A	223	ASN	2.6
1	1-B	468	ASP	2.6
1	1-A	196	PHE	2.6
1	1-A	235	HIS	2.6
1	1-B	270	LEU	2.6
1	1-A	150	TYR	2.6
1	1-B	57	VAL	2.6
1	1-A	432	SER	2.6
1	1-A	123	ASN	2.6
1	1-A	130	PRO	2.6
1	1-A	20	GLU	2.6
1	1-A	264	GLU	2.6
1	1-B	311	ASP	2.5
1	1-B	160	PHE	2.5
1	1-A	145	LYS	2.5
1	1-A	216	VAL	2.5
1	1-A	218	VAL	2.5
1	1-A	246	GLU	2.5
1	1-A	333	GLU	2.5
1	1-B	66	VAL	2.5
1	1-B	119	GLU	2.5
1	1-B	59	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	1-A	10	GLN	2.5
1	1-B	331	GLN	2.5
1	1-B	447	GLY	2.5
1	1-B	45	GLU	2.5
1	1-A	364	ASP	2.5
1	1-B	347	ILE	2.5
1	1-A	323	GLU	2.5
1	1-A	313	LEU	2.5
1	1-A	343	PHE	2.5
1	1-B	110	PHE	2.5
1	1-B	456	ALA	2.5
1	1-A	146	ILE	2.5
1	1-B	129	VAL	2.5
1	1-B	266	LYS	2.5
1	1-A	425	SER	2.5
1	1-B	154	ASN	2.4
1	1-A	183	ASP	2.4
1	1-A	191	GLY	2.4
1	1-A	382	ARG	2.4
1	1-A	198	ALA	2.4
1	1-B	227	ILE	2.4
1	1-A	296	ASN	2.4
1	1-B	350	ASN	2.4
1	1-B	124	LYS	2.4
1	1-B	148	GLU	2.4
1	1-B	144	HIS	2.4
1	1-B	429	TRP	2.4
1	1-B	137	PHE	2.4
1	1-A	219	ALA	2.4
1	1-A	159	THR	2.4
1	1-A	211	GLN	2.4
1	1-A	215	TYR	2.4
1	1-B	23	GLU	2.4
1	1-B	65	PRO	2.4
1	1-B	453	PRO	2.4
1	1-A	381	THR	2.4
1	1-B	441	THR	2.4
1	1-B	232	ILE	2.4
1	1-B	237	ILE	2.4
1	1-A	169	VAL	2.4
1	1-A	193	GLY	2.3
1	1-A	133	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	1-A	194	ASP	2.3
1	1-A	294	THR	2.3
1	1-B	213	LYS	2.3
1	1-B	343	PHE	2.3
1	1-A	315	MET	2.3
1	1-B	187	TRP	2.3
1	1-B	299	VAL	2.3
1	1-B	308	VAL	2.3
1	1-A	399	GLU	2.3
1	1-B	459	GLU	2.3
1	1-A	26	LYS	2.3
1	1-A	124	LYS	2.3
1	1-A	384	LYS	2.3
1	1-B	410	PHE	2.3
1	1-A	176	TRP	2.3
1	1-A	412	SER	2.3
1	1-B	355	ARG	2.3
1	1-B	448	VAL	2.3
1	1-B	458	VAL	2.3
1	1-A	112	ASP	2.3
1	1-A	139	THR	2.3
1	1-B	307	LEU	2.3
1	1-B	313	LEU	2.3
1	1-A	120	ASN	2.3
1	1-B	446	SER	2.3
1	1-B	26	LYS	2.3
1	1-B	60	TYR	2.3
1	1-A	82	VAL	2.3
1	1-A	25	GLU	2.2
1	1-A	214	GLU	2.2
1	1-B	244	CYS	2.2
1	1-A	295	ASN	2.2
1	1-B	75	ASN	2.2
1	1-B	436	LEU	2.2
1	1-A	314	LYS	2.2
1	1-A	160	PHE	2.2
1	1-A	165	TYR	2.2
1	1-B	349	VAL	2.2
1	1-A	182	THR	2.2
1	1-A	334	THR	2.2
1	1-B	298	TRP	2.2
1	1-B	226	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	1-B	461	LYS	2.2
1	1-B	17	GLY	2.2
1	1-B	28	GLY	2.2
1	1-A	188	TYR	2.2
1	1-A	65	PRO	2.2
1	1-B	67	SER	2.2
1	1-A	353	ARG	2.2
1	1-A	241	ASN	2.2
1	1-A	293	ASN	2.2
1	1-B	290	LYS	2.2
1	1-A	114	ILE	2.2
1	1-A	109	THR	2.2
1	1-A	190	PRO	2.2
1	1-A	163	SER	2.2
1	1-B	218	VAL	2.1
1	1-A	331	GLN	2.1
1	1-B	297	LEU	2.1
1	1-B	62	LYS	2.1
1	1-A	206	ASP	2.1
1	1-B	196	PHE	2.1
1	1-A	81	VAL	2.1
1	1-B	312	ALA	2.1
1	1-A	22	SER	2.1
1	1-A	187	TRP	2.1
1	1-B	40	GLU	2.1
1	1-B	323	GLU	2.1
1	1-B	421	SER	2.1
1	1-A	62	LYS	2.1
1	1-B	401	LYS	2.1
1	1-A	154	ASN	2.1
1	1-A	100	SER	2.1
1	1-A	222	ASP	2.1
1	1-B	16	ASP	2.1
1	1-A	290	LYS	2.1
1	1-A	401	LYS	2.1
1	1-A	348	GLY	2.0
1	1-A	200	MET	2.0
1	1-A	268	GLN	2.0
1	1-A	106	ASP	2.0
1	1-A	27	SER	2.0
1	1-A	129	VAL	2.0
1	1-A	168	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	1-A	175	PRO	2.0
1	1-B	135	ASN	2.0
1	1-B	406	PHE	2.0
1	1-B	219	ALA	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

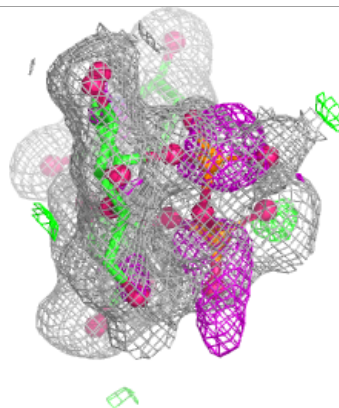
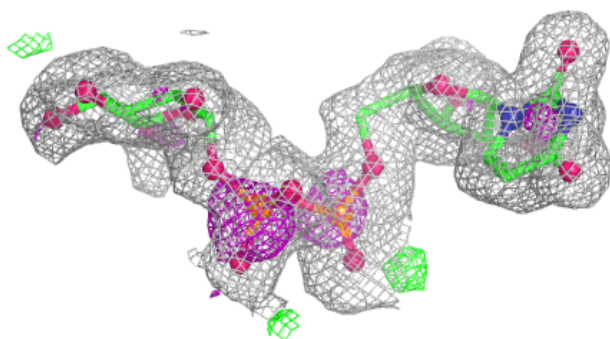
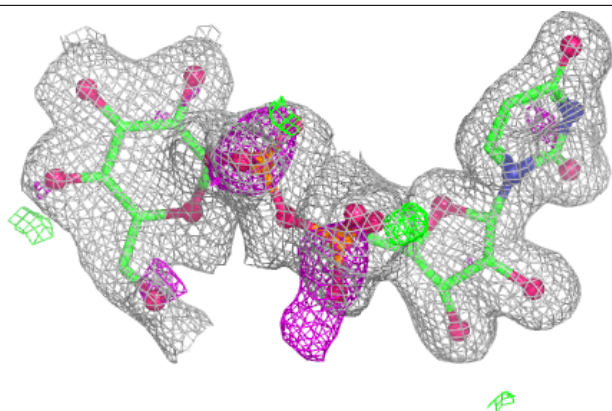
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	DMS	1-A	900	4/4	0.88	0.15	28,36,37,39	4
2	DMS	2-A	900	4/4	-	-	28,36,37,39	4
3	UPG	1-B	902	36/36	0.88	0.09	13,22,29,31	36
3	UPG	2-A	901	36/36	-	-	19,22,27,28	36
3	UPG	1-A	901	36/36	0.91	0.12	19,22,27,28	36

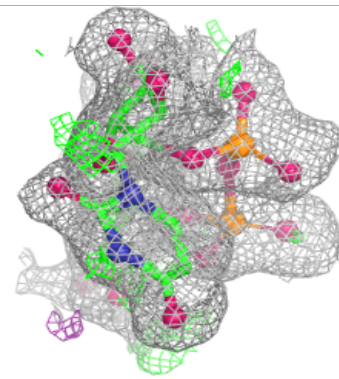
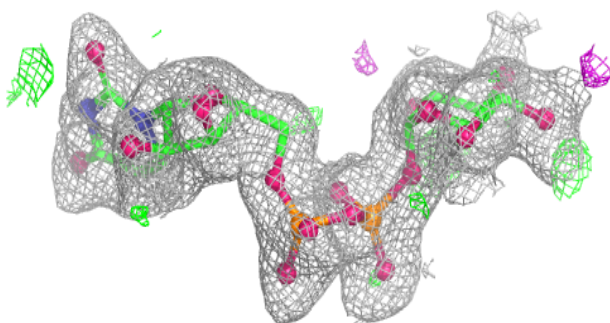
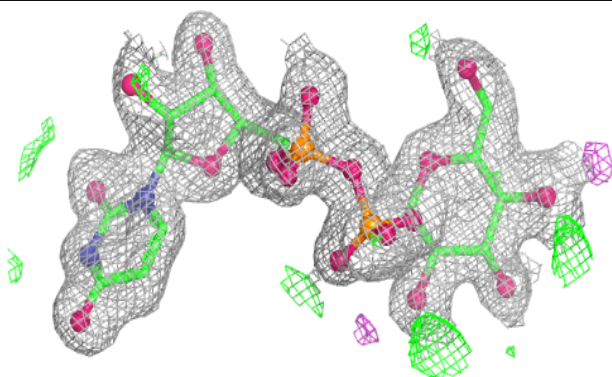
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UPG B 902:

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

**Electron density around UPG A 901:**

$2mF_o-DF_c$ (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.