



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:32 AM UTC

PDB ID : 4M2B / pdb_00004m2b
Title : Crystal structure of L281D mutant of udp-glucose pyrophosphorylase from leishmania major in complex with udp-glc
Authors : Fuehring, J.; Routier, F.H.; Lamerz, A.-C.; Baruch, P.; Gerardy-Schahn, R.; Fedorov, R.
Deposited on : 2013-08-05
Resolution : 2.20 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

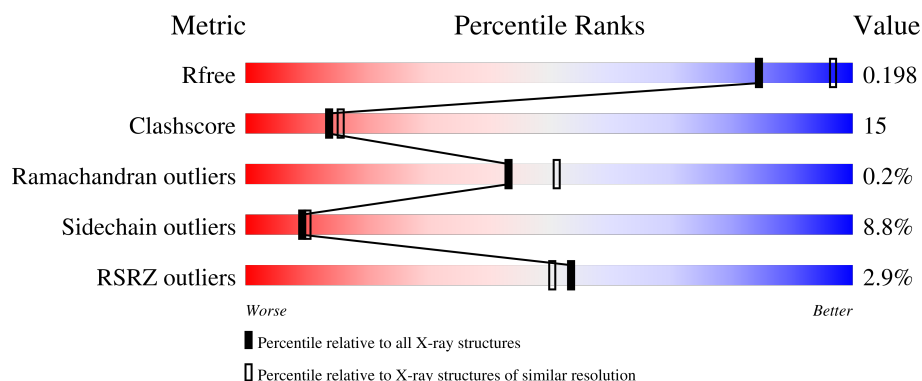
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	505	 3% 47% 37% 9% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4159 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.

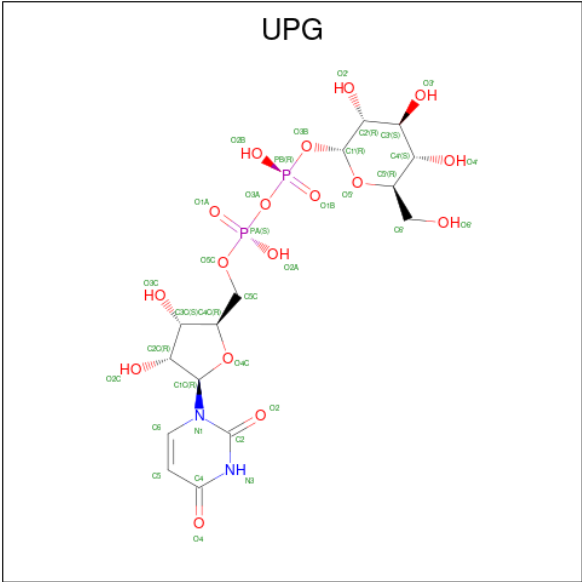
- Molecule 1 is a protein called UDP-glucose pyrophosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	0	0
			3730	2349	636	719	26			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	281	ASP	LEU	engineered mutation	UNP Q4QDU3
A	495	MET	-	expression tag	UNP Q4QDU3
A	496	ARG	-	expression tag	UNP Q4QDU3
A	497	PRO	-	expression tag	UNP Q4QDU3
A	498	LEU	-	expression tag	UNP Q4QDU3
A	499	GLU	-	expression tag	UNP Q4QDU3
A	500	HIS	-	expression tag	UNP Q4QDU3
A	501	HIS	-	expression tag	UNP Q4QDU3
A	502	HIS	-	expression tag	UNP Q4QDU3
A	503	HIS	-	expression tag	UNP Q4QDU3
A	504	HIS	-	expression tag	UNP Q4QDU3
A	505	HIS	-	expression tag	UNP Q4QDU3

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (CCD ID: UPG) (formula: C₁₅H₂₄N₂O₁₇P₂).



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

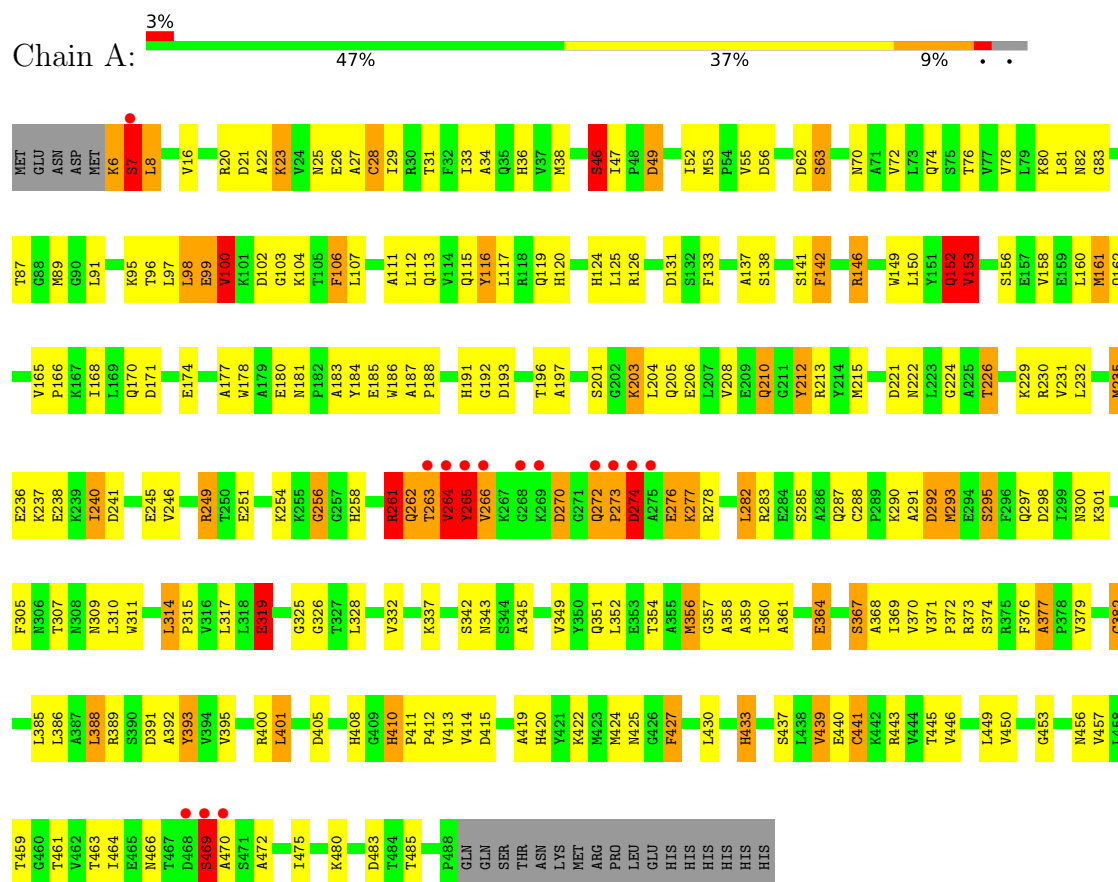
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	393	Total	O	0	0
			393	393		

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: UDP-glucose pyrophosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	78.79Å 86.90Å 138.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.40 – 2.20 23.40 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (23.40-2.20) 98.0 (23.40-2.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 2.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.175 , 0.242 (Not available) , 0.198	Depositor DCC
R_{free} test set	1204 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4159	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% 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: 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	2.14	161/3800 (4.2%)	1.33	25/5147 (0.5%)

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	4

All (161) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	HIS	CG-ND1	-8.62	1.28	1.38
1	A	433	HIS	CG-ND1	-8.24	1.29	1.38
1	A	31	THR	C-O	-7.68	1.15	1.24
1	A	314	LEU	C-O	-7.55	1.17	1.24
1	A	391	ASP	C-O	-7.45	1.14	1.24
1	A	171	ASP	C-O	-7.38	1.15	1.24
1	A	72	VAL	C-O	-7.27	1.16	1.24
1	A	166	PRO	C-O	-7.23	1.15	1.23
1	A	433	HIS	CD2-NE2	-7.13	1.30	1.37
1	A	358	ALA	C-O	-7.11	1.15	1.24
1	A	29	ILE	C-O	-7.09	1.16	1.24
1	A	36	HIS	CD2-NE2	-7.04	1.30	1.37
1	A	97	LEU	C-O	-7.02	1.14	1.24
1	A	160	LEU	C-O	-7.00	1.15	1.24
1	A	411	PRO	C-O	-6.98	1.19	1.25
1	A	328	LEU	C-O	-6.93	1.18	1.25
1	A	420	HIS	CD2-NE2	-6.91	1.30	1.37
1	A	82	ASN	C-O	-6.88	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	HIS	CD2-NE2	-6.83	1.30	1.37
1	A	376	PHE	C-O	-6.79	1.16	1.23
1	A	120	HIS	CG-ND1	-6.77	1.30	1.38
1	A	450	VAL	C-O	-6.74	1.17	1.23
1	A	258	HIS	CG-ND1	-6.71	1.30	1.38
1	A	311	TRP	NE1-CE2	-6.65	1.30	1.37
1	A	408	HIS	CD2-NE2	-6.59	1.30	1.37
1	A	158	VAL	C-O	-6.59	1.17	1.24
1	A	36	HIS	CG-ND1	-6.58	1.31	1.38
1	A	231	VAL	C-O	-6.58	1.16	1.24
1	A	374	SER	C-O	-6.58	1.15	1.24
1	A	240	ILE	C-O	-6.56	1.16	1.24
1	A	8	LEU	C-O	-6.53	1.15	1.24
1	A	420	HIS	CG-ND1	-6.53	1.31	1.38
1	A	325	GLY	C-O	-6.46	1.17	1.24
1	A	356	MET	C-O	-6.44	1.16	1.24
1	A	168	ILE	C-O	-6.43	1.17	1.24
1	A	326	GLY	C-O	-6.37	1.17	1.24
1	A	236	GLU	C-O	-6.34	1.16	1.24
1	A	197	ALA	C-O	-6.34	1.16	1.24
1	A	28	CYS	C-O	-6.33	1.16	1.24
1	A	425	ASN	C-O	-6.31	1.16	1.24
1	A	370	VAL	C-O	-6.29	1.17	1.24
1	A	161	MET	C-O	-6.27	1.16	1.24
1	A	170	GLN	C-O	-6.27	1.16	1.24
1	A	352	LEU	C-O	-6.26	1.16	1.24
1	A	232	LEU	C-O	-6.21	1.16	1.24
1	A	288	CYS	C-O	-6.21	1.16	1.24
1	A	224	GLY	C-O	-6.19	1.16	1.23
1	A	208	VAL	C-O	-6.18	1.17	1.24
1	A	246	VAL	C-O	-6.14	1.17	1.24
1	A	319	GLU	C-O	-6.13	1.17	1.24
1	A	393	TYR	C-O	-6.13	1.16	1.24
1	A	360	ILE	C-O	-6.09	1.16	1.24
1	A	16	VAL	C-O	-6.08	1.17	1.24
1	A	184	TYR	C-O	-6.08	1.16	1.24
1	A	382	CYS	C-O	-6.04	1.16	1.24
1	A	368	ALA	C-O	-6.03	1.16	1.23
1	A	364	GLU	C-O	-6.02	1.17	1.24
1	A	63	SER	C-O	-5.99	1.16	1.24
1	A	180	GLU	C-O	-5.96	1.17	1.24
1	A	361	ALA	C-O	-5.95	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	ASP	C-O	-5.94	1.16	1.24
1	A	181	ASN	C-O	-5.94	1.18	1.24
1	A	81	LEU	C-O	-5.92	1.16	1.24
1	A	46	SER	C-O	-5.90	1.16	1.23
1	A	437	SER	C-O	-5.90	1.16	1.23
1	A	153	VAL	C-O	-5.87	1.17	1.24
1	A	112	LEU	C-O	-5.87	1.17	1.24
1	A	385	LEU	C-O	-5.84	1.17	1.24
1	A	191	HIS	CD2-NE2	-5.84	1.31	1.37
1	A	439	VAL	C-O	-5.84	1.17	1.24
1	A	238	GLU	C-O	-5.81	1.16	1.24
1	A	410	HIS	CG-ND1	-5.78	1.31	1.38
1	A	408	HIS	CG-ND1	-5.77	1.31	1.38
1	A	204	LEU	C-O	-5.77	1.17	1.24
1	A	413	VAL	C-O	-5.75	1.18	1.24
1	A	186	TRP	NE1-CE2	-5.75	1.31	1.37
1	A	317	LEU	C-O	-5.74	1.17	1.24
1	A	138	SER	C-O	-5.72	1.17	1.24
1	A	475	ILE	C-O	-5.72	1.17	1.24
1	A	47	ILE	C-O	-5.72	1.17	1.23
1	A	295	SER	C-O	-5.71	1.17	1.24
1	A	119	GLN	C-O	-5.70	1.17	1.24
1	A	183	ALA	C-O	-5.69	1.17	1.24
1	A	235	MET	C-O	-5.69	1.17	1.24
1	A	193	ASP	C-O	-5.68	1.16	1.24
1	A	292	ASP	C-O	-5.68	1.16	1.24
1	A	203	LYS	C-O	-5.67	1.17	1.24
1	A	185	GLU	C-O	-5.66	1.16	1.24
1	A	165	VAL	C-O	-5.64	1.17	1.24
1	A	196	THR	C-O	-5.64	1.17	1.24
1	A	405	ASP	C-O	-5.64	1.17	1.24
1	A	263	THR	CA-C	5.62	1.60	1.53
1	A	21	ASP	C-O	-5.61	1.17	1.24
1	A	427	PHE	C-O	-5.61	1.17	1.24
1	A	111	ALA	C-O	-5.59	1.17	1.24
1	A	120	HIS	CD2-NE2	-5.59	1.31	1.37
1	A	261	ARG	C-O	-5.54	1.17	1.24
1	A	117	LEU	C-O	-5.50	1.17	1.24
1	A	332	VAL	C-O	-5.50	1.17	1.24
1	A	206	GLU	C-O	-5.49	1.17	1.24
1	A	113	GLN	C-O	-5.49	1.17	1.24
1	A	241	ASP	C-O	-5.49	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	GLN	C-O	-5.49	1.17	1.24
1	A	33	ILE	C-O	-5.48	1.17	1.24
1	A	20	ARG	C-O	-5.48	1.17	1.24
1	A	369	ILE	C-O	-5.47	1.18	1.24
1	A	106	PHE	C-O	-5.46	1.17	1.24
1	A	298	ASP	C-O	-5.43	1.17	1.24
1	A	124	HIS	CG-ND1	-5.42	1.32	1.38
1	A	230	ARG	C-O	-5.40	1.17	1.24
1	A	282	LEU	C-O	-5.40	1.17	1.24
1	A	290	LYS	C-O	-5.40	1.17	1.24
1	A	137	ALA	C-O	-5.38	1.18	1.24
1	A	464	ILE	C-O	-5.36	1.18	1.24
1	A	95	LYS	C-O	-5.35	1.17	1.24
1	A	237	LYS	C-O	-5.35	1.17	1.24
1	A	34	ALA	C-O	-5.34	1.17	1.24
1	A	52	ILE	C-O	-5.34	1.17	1.23
1	A	205	GLN	C-O	-5.33	1.17	1.24
1	A	307	THR	C-O	-5.30	1.17	1.24
1	A	441	CYS	C-O	-5.30	1.17	1.24
1	A	430	LEU	C-O	-5.30	1.17	1.24
1	A	177	ALA	C-O	-5.30	1.17	1.24
1	A	215	MET	C-O	-5.29	1.18	1.24
1	A	221	ASP	C-O	-5.29	1.17	1.24
1	A	78	VAL	C-O	-5.28	1.18	1.24
1	A	392	ALA	C-O	-5.28	1.17	1.24
1	A	359	ALA	C-O	-5.28	1.17	1.24
1	A	178	TRP	NE1-CE2	-5.26	1.31	1.37
1	A	388	LEU	C-O	-5.24	1.18	1.24
1	A	349	VAL	C-O	-5.24	1.18	1.23
1	A	249	ARG	C-O	-5.24	1.17	1.24
1	A	285	SER	C-O	-5.23	1.18	1.24
1	A	100	VAL	C-O	-5.23	1.18	1.23
1	A	445	THR	C-O	-5.22	1.18	1.24
1	A	410	HIS	CD2-NE2	-5.21	1.32	1.37
1	A	283	ARG	C-O	-5.19	1.18	1.24
1	A	142	PHE	C-O	-5.18	1.18	1.24
1	A	419	ALA	C-O	-5.17	1.18	1.24
1	A	377	ALA	C-O	-5.17	1.18	1.24
1	A	188	PRO	C-O	-5.16	1.18	1.24
1	A	415	ASP	C-O	-5.16	1.18	1.24
1	A	83	GLY	C-O	-5.16	1.17	1.23
1	A	26	GLU	C-O	-5.14	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	446	VAL	C-O	-5.12	1.18	1.24
1	A	201	SER	C-O	-5.11	1.17	1.24
1	A	373	ARG	C-O	-5.11	1.17	1.24
1	A	98	LEU	C-O	-5.11	1.17	1.23
1	A	287	GLN	C-O	-5.11	1.17	1.24
1	A	457	VAL	C-O	-5.11	1.18	1.24
1	A	76	THR	C-O	-5.10	1.17	1.24
1	A	345	ALA	C-O	-5.08	1.17	1.24
1	A	116	TYR	C-O	-5.07	1.18	1.24
1	A	70	ASN	C-O	-5.07	1.17	1.24
1	A	449	LEU	C-O	-5.07	1.17	1.24
1	A	174	GLU	C-O	-5.04	1.17	1.23
1	A	131	ASP	C-O	-5.04	1.17	1.23
1	A	27	ALA	C-O	-5.03	1.18	1.24
1	A	212	TYR	C-O	-5.02	1.17	1.23
1	A	422	LYS	C-O	-5.02	1.18	1.24
1	A	264	VAL	CA-C	5.01	1.58	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	THR	N-CA-C	17.08	134.81	111.24
1	A	270	ASP	N-CA-C	-12.83	89.01	108.52
1	A	264	VAL	N-CA-C	10.56	124.20	108.46
1	A	270	ASP	CB-CA-C	10.54	126.97	109.99
1	A	158	VAL	N-CA-C	8.70	118.60	110.42
1	A	156	SER	N-CA-C	8.52	120.64	111.36
1	A	469	SER	CB-CA-C	-8.19	94.12	110.42
1	A	152	GLN	N-CA-C	-7.12	99.90	110.23
1	A	265	TYR	CA-C-N	7.12	133.36	122.68
1	A	265	TYR	C-N-CA	7.12	133.36	122.68
1	A	470	ALA	N-CA-C	-6.95	104.79	113.55
1	A	7	SER	N-CA-C	6.67	119.56	110.55
1	A	367	SER	N-CA-C	6.43	117.05	108.38
1	A	319	GLU	N-CA-C	6.30	118.14	111.28
1	A	146	ARG	N-CA-C	6.19	120.96	113.41
1	A	469	SER	N-CA-C	6.02	123.62	110.80
1	A	141	SER	N-CA-C	5.94	117.75	111.28
1	A	263	THR	CB-CA-C	-5.78	103.19	112.09
1	A	256	GLY	N-CA-C	5.73	117.90	110.45
1	A	150	LEU	N-CA-C	5.47	117.32	111.36
1	A	87	THR	N-CA-C	5.33	118.00	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	GLN	N-CA-C	5.26	119.91	111.81
1	A	187	ALA	N-CA-C	5.25	116.74	108.23
1	A	293	MET	N-CA-C	5.19	117.67	111.71
1	A	63	SER	N-CA-C	5.13	117.78	111.82

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	272	GLN	Peptide
1	A	273	PRO	Peptide
1	A	274	ASP	Peptide
1	A	7	SER	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	3730	0	3713	109	0
2	A	36	0	22	2	0
3	A	393	0	0	19	0
All	All	4159	0	3735	109	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 15.

All (109) 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:265:TYR:CA	1:A:276:GLU:HB3	1.72	1.18
1:A:265:TYR:HA	1:A:276:GLU:HB3	1.22	1.15
1:A:126:ARG:HD2	3:A:2259:HOH:O	1.48	1.14
1:A:469:SER:HA	3:A:2129:HOH:O	1.51	1.06
1:A:273:PRO:HA	1:A:274:ASP:HB2	1.40	1.01
1:A:272:GLN:HE21	1:A:273:PRO:HD3	1.24	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:GLN:HE22	2:A:1001:UPG:HN3	1.05	0.99
1:A:115:GLN:HG3	1:A:149:TRP:CZ2	1.98	0.97
1:A:265:TYR:HA	1:A:276:GLU:CB	1.96	0.95
1:A:152:GLN:O	1:A:153:VAL:HG22	1.72	0.90
1:A:273:PRO:CA	1:A:274:ASP:HB2	2.02	0.88
1:A:265:TYR:CB	1:A:276:GLU:HB3	2.02	0.88
1:A:126:ARG:HH21	1:A:210:GLN:HE22	1.23	0.86
1:A:265:TYR:HB3	1:A:276:GLU:HB3	1.63	0.80
1:A:126:ARG:HH21	1:A:210:GLN:NE2	1.82	0.77
1:A:262:GLN:CG	1:A:262:GLN:O	2.36	0.74
1:A:229:LYS:NZ	3:A:2205:HOH:O	2.20	0.74
1:A:472:ALA:HB3	3:A:2362:HOH:O	1.87	0.73
1:A:272:GLN:NE2	1:A:273:PRO:HD3	2.02	0.73
1:A:115:GLN:HG3	1:A:149:TRP:HZ2	1.52	0.73
1:A:46:SER:HB3	3:A:2195:HOH:O	1.91	0.69
1:A:91:LEU:HD22	3:A:2134:HOH:O	1.93	0.69
1:A:266:VAL:HG23	1:A:277:LYS:H	1.62	0.65
1:A:301:LYS:NZ	3:A:2107:HOH:O	2.30	0.64
1:A:162:GLN:NE2	2:A:1001:UPG:HN3	1.87	0.62
1:A:410:HIS:HE1	3:A:2064:HOH:O	1.81	0.62
1:A:453:GLY:H	1:A:456:ASN:HD21	1.47	0.62
1:A:266:VAL:HG21	1:A:277:LYS:HB2	1.80	0.62
1:A:265:TYR:HA	1:A:276:GLU:CA	2.30	0.61
1:A:265:TYR:HB3	1:A:276:GLU:CB	2.31	0.61
1:A:152:GLN:O	1:A:153:VAL:CG2	2.48	0.60
1:A:22:ALA:C	1:A:23:LYS:HG2	2.26	0.60
1:A:261:ARG:HG3	1:A:278:ARG:HG3	1.83	0.59
1:A:265:TYR:HA	1:A:276:GLU:HA	1.85	0.58
1:A:262:GLN:O	1:A:262:GLN:HG3	2.05	0.56
1:A:89:MET:HE2	1:A:424:MET:CE	2.36	0.56
1:A:7:SER:OG	1:A:8:LEU:N	2.39	0.55
1:A:213:ARG:HD2	1:A:315:PRO:HG3	1.87	0.55
1:A:265:TYR:HB3	1:A:276:GLU:CG	2.37	0.55
1:A:96:THR:HA	1:A:106:PHE:HB2	1.89	0.54
1:A:100:VAL:O	1:A:389:ARG:HG2	2.07	0.54
1:A:133:PHE:HE2	3:A:2351:HOH:O	1.90	0.53
1:A:371:VAL:HB	1:A:372:PRO:HD2	1.90	0.53
1:A:293:MET:O	1:A:297:GLN:HG3	2.07	0.53
1:A:319:GLU:HG3	3:A:2257:HOH:O	2.09	0.53
1:A:89:MET:HE2	1:A:424:MET:HE1	1.91	0.53
1:A:104:LYS:HE2	3:A:2184:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ARG:NH2	3:A:2208:HOH:O	2.41	0.52
1:A:46:SER:CB	3:A:2195:HOH:O	2.52	0.52
1:A:222:ASN:ND2	1:A:377:ALA:H	2.07	0.52
1:A:461:THR:O	1:A:483:ASP:HA	2.09	0.52
1:A:126:ARG:NH2	1:A:210:GLN:NE2	2.55	0.51
1:A:264:VAL:O	1:A:276:GLU:HB2	2.10	0.51
1:A:395:VAL:HG22	1:A:401:LEU:HD22	1.91	0.51
1:A:152:GLN:HG2	1:A:153:VAL:HG13	1.92	0.51
1:A:265:TYR:HB3	1:A:276:GLU:HG2	1.91	0.51
1:A:261:ARG:CG	1:A:278:ARG:HG3	2.39	0.51
1:A:251:GLU:OE1	1:A:443:ARG:NH2	2.38	0.50
1:A:273:PRO:CB	1:A:274:ASP:HB2	2.42	0.49
1:A:91:LEU:CD2	1:A:98:LEU:HD11	2.42	0.49
1:A:300:ASN:ND2	3:A:2326:HOH:O	2.44	0.49
1:A:210:GLN:HE21	1:A:212:TYR:HE1	1.61	0.49
1:A:273:PRO:HA	1:A:274:ASP:CB	2.27	0.49
1:A:266:VAL:CG2	1:A:277:LYS:H	2.25	0.49
1:A:262:GLN:O	1:A:262:GLN:HG2	2.12	0.48
1:A:343:ASN:C	1:A:343:ASN:HD22	2.20	0.48
1:A:386:LEU:HB2	1:A:427:PHE:HE1	1.78	0.48
1:A:125:LEU:HD12	3:A:2244:HOH:O	2.13	0.48
1:A:7:SER:HA	1:A:8:LEU:HG	1.95	0.47
1:A:386:LEU:HB2	1:A:427:PHE:CE1	2.48	0.47
1:A:466:ASN:C	1:A:466:ASN:OD1	2.56	0.47
1:A:99:GLU:OE1	1:A:103:GLY:HA2	2.14	0.46
1:A:249:ARG:NE	3:A:2115:HOH:O	2.47	0.46
1:A:439:VAL:HG13	1:A:440:GLU:HG3	1.96	0.46
1:A:379:VAL:CG2	1:A:388:LEU:HD22	2.46	0.46
1:A:264:VAL:O	1:A:276:GLU:CB	2.64	0.46
1:A:226:THR:HB	1:A:400:ARG:HD3	1.97	0.46
1:A:245:GLU:HB2	1:A:309:ASN:HB2	1.97	0.46
1:A:161:MET:HB2	1:A:161:MET:HE2	1.62	0.45
1:A:412:PRO:HB3	1:A:441:CYS:O	2.16	0.45
1:A:386:LEU:HD23	1:A:414:VAL:HG11	1.98	0.45
1:A:291:ALA:HB3	3:A:2308:HOH:O	2.16	0.45
1:A:256:GLY:HA3	1:A:305:PHE:CZ	2.51	0.45
1:A:49:ASP:OD2	1:A:292:ASP:HB3	2.16	0.45
1:A:6:LYS:HB3	1:A:7:SER:H	1.37	0.45
1:A:265:TYR:HD1	1:A:265:TYR:O	2.00	0.45
1:A:115:GLN:CG	1:A:149:TRP:CZ2	2.86	0.44
1:A:314:LEU:N	1:A:315:PRO:HD2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:TYR:N	1:A:276:GLU:HB3	2.27	0.44
1:A:146:ARG:HG2	3:A:2200:HOH:O	2.18	0.43
1:A:310:LEU:HD12	1:A:356:MET:HE3	2.00	0.43
1:A:7:SER:HA	1:A:8:LEU:CG	2.48	0.43
1:A:142:PHE:C	1:A:142:PHE:CD2	2.97	0.43
1:A:91:LEU:CD1	1:A:98:LEU:HD11	2.49	0.43
1:A:382:CYS:SG	1:A:424:MET:HE2	2.59	0.42
1:A:261:ARG:NH1	1:A:278:ARG:HA	2.34	0.42
1:A:337:LYS:HG3	1:A:351:GLN:NE2	2.34	0.42
1:A:282:LEU:HD22	1:A:357:GLY:HA3	2.02	0.42
1:A:388:LEU:HA	1:A:393:TYR:CD1	2.56	0.41
1:A:38:MET:HA	1:A:38:MET:HE2	2.01	0.41
1:A:266:VAL:HG11	1:A:277:LYS:HZ1	1.85	0.41
1:A:116:TYR:CD2	1:A:116:TYR:C	2.98	0.41
1:A:433:HIS:HE1	3:A:2171:HOH:O	2.04	0.41
1:A:107:LEU:HD23	1:A:142:PHE:CD2	2.55	0.41
1:A:192:GLY:HA3	1:A:354:THR:OG1	2.21	0.41
1:A:463:THR:O	1:A:485:THR:HA	2.21	0.40
1:A:7:SER:HA	1:A:8:LEU:HA	1.89	0.40
1:A:25:ASN:ND2	1:A:28:CYS:H	2.20	0.40
1:A:235:MET:HG2	1:A:240:ILE:HB	2.04	0.40

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	481/505 (95%)	472 (98%)	8 (2%)	1 (0%)	43 51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	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	410/432 (95%)	374 (91%)	36 (9%)	9 10

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	7	SER
1	A	23	LYS
1	A	46	SER
1	A	49	ASP
1	A	53	MET
1	A	55	VAL
1	A	56	ASP
1	A	63	SER
1	A	74	GLN
1	A	80	LYS
1	A	99	GLU
1	A	100	VAL
1	A	102	ASP
1	A	152	GLN
1	A	203	LYS
1	A	226	THR
1	A	254	LYS
1	A	261	ARG
1	A	263	THR
1	A	264	VAL
1	A	265	TYR
1	A	266	VAL
1	A	270	ASP
1	A	274	ASP
1	A	276	GLU

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Mol	Chain	Res	Type
1	A	277	LYS
1	A	295	SER
1	A	319	GLU
1	A	342	SER
1	A	364	GLU
1	A	367	SER
1	A	401	LEU
1	A	459	THR
1	A	469	SER
1	A	480	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	25	ASN
1	A	35	GLN
1	A	82	ASN
1	A	119	GLN
1	A	152	GLN
1	A	162	GLN
1	A	163	ASN
1	A	164	GLN
1	A	205	GLN
1	A	210	GLN
1	A	222	ASN
1	A	262	GLN
1	A	272	GLN
1	A	300	ASN
1	A	322	GLN
1	A	343	ASN
1	A	351	GLN
1	A	410	HIS
1	A	456	ASN

5.3.3 RNA ⓘ

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](#)

1 ligand is 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	A	1001	-	37,38,38	1.11	4 (10%)	55,58,58	1.50	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	A	1001	-	-	1/23/59/59	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	UPG	O5'-C1'	2.51	1.48	1.41
2	A	1001	UPG	O2-C2	2.44	1.27	1.23
2	A	1001	UPG	C2-N1	2.44	1.42	1.38
2	A	1001	UPG	C2-N3	-2.33	1.33	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	UPG	C4-N3-C2	-4.56	120.96	126.61
2	A	1001	UPG	C5-C4-N3	4.26	120.77	114.80
2	A	1001	UPG	N3-C2-N1	3.84	119.90	114.89
2	A	1001	UPG	O5'-C1'-O3B	-2.67	107.87	111.36
2	A	1001	UPG	O4-C4-C5	-2.49	120.87	125.16
2	A	1001	UPG	O3A-PA-O1A	-2.44	103.37	110.70
2	A	1001	UPG	O3C-C3C-C4C	-2.36	104.29	111.08
2	A	1001	UPG	O2B-PB-O3B	-2.28	97.41	106.70
2	A	1001	UPG	O2B-PB-O3A	2.05	112.83	107.27

There are no chirality outliers.

All (1) torsion outliers are listed below:

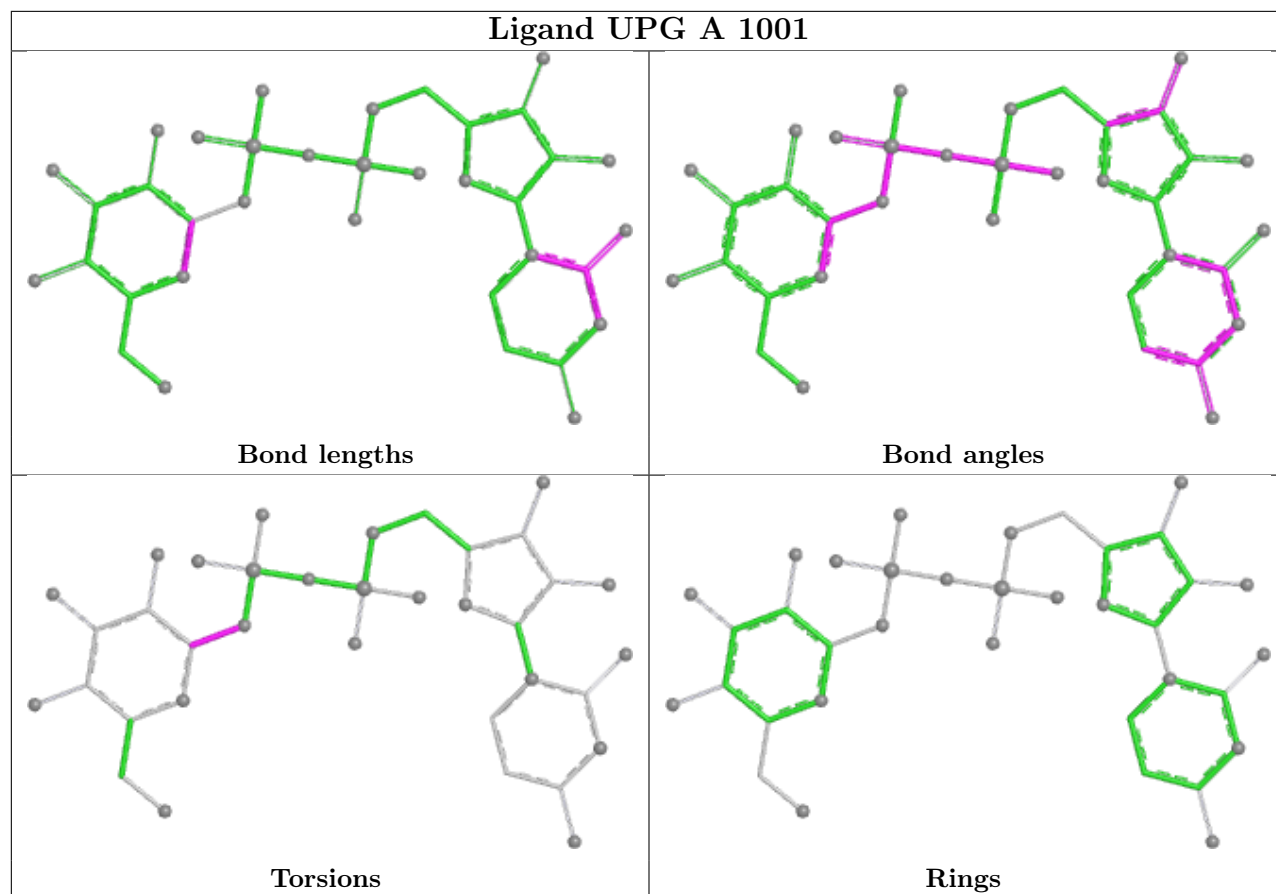
Mol	Chain	Res	Type	Atoms
2	A	1001	UPG	O5'-C1'-O3B-PB

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	UPG	2	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	483/505 (95%)	-0.41	14 (2%) 53 50	12, 24, 52, 133	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	273	PRO	4.3
1	A	469	SER	3.9
1	A	7	SER	3.9
1	A	275	ALA	3.6
1	A	266	VAL	3.4
1	A	268	GLY	3.2
1	A	263	THR	2.9
1	A	272	GLN	2.9
1	A	265	TYR	2.8
1	A	264	VAL	2.7
1	A	468	ASP	2.6
1	A	269	LYS	2.5
1	A	470	ALA	2.4
1	A	274	ASP	2.3

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](#)

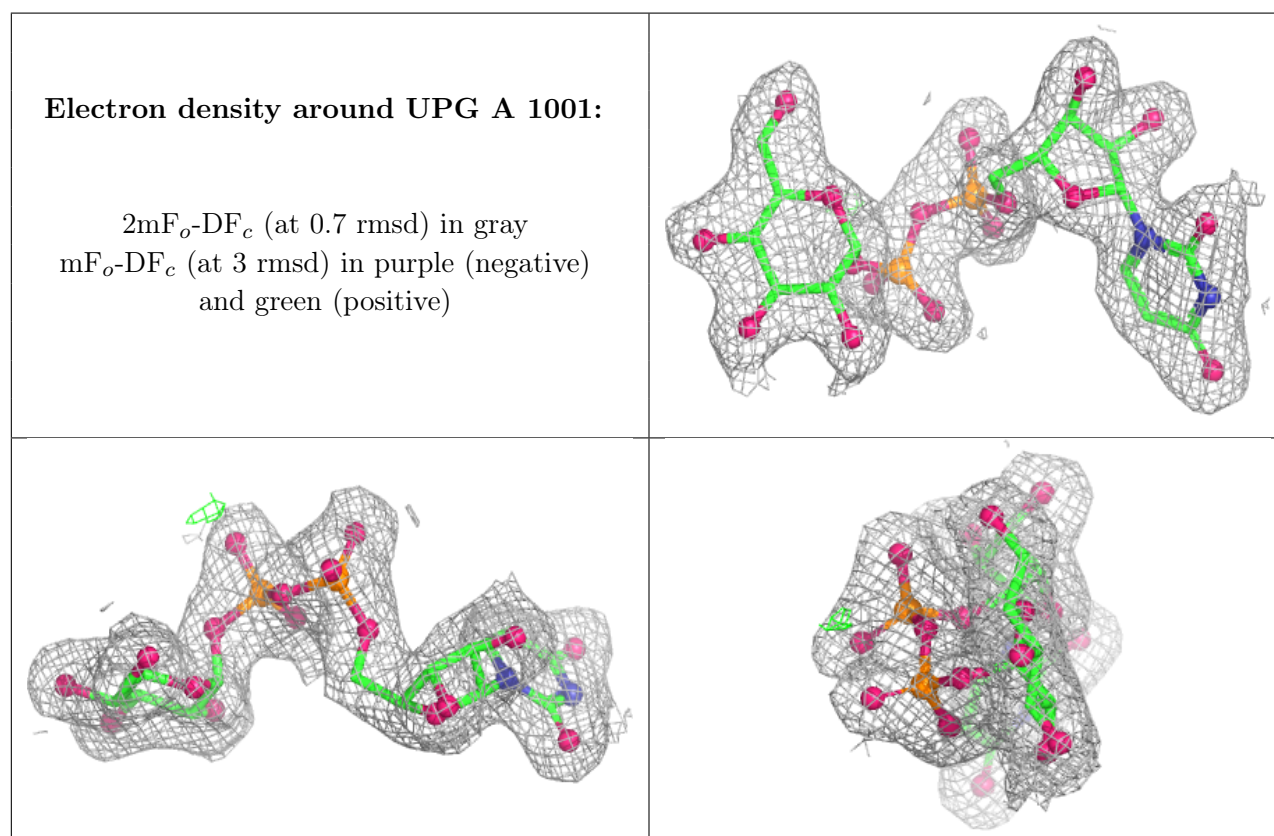
There are no oligosaccharides in this entry.

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	1001	36/36	0.99	0.04	14,15,18,19	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.