



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 10:24 AM UTC

PDB ID : 1BWF / pdb_00001bwf
Title : ESCHERICHIA COLI GLYCEROL KINASE MUTANT WITH BOUND ATP
ANALOG SHOWING SUBSTANTIAL DOMAIN MOTION
Authors : Bystrom, C.E.; Pettigrew, D.W.; Branchaud, B.P.; Remington, S.J.
Deposited on : 1998-09-23
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

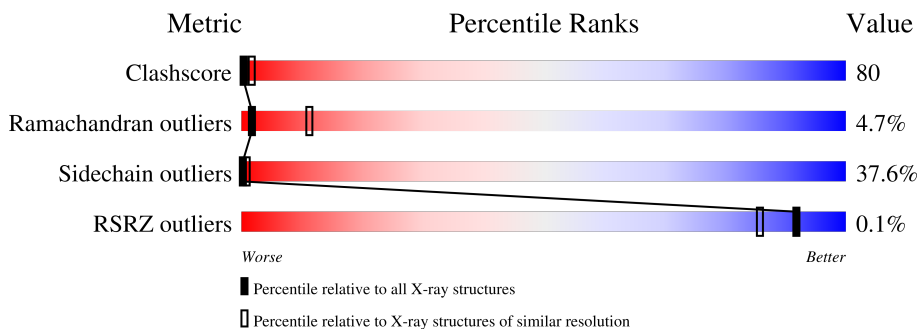
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	O	501	
1	Y	501	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7900 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 GLYCEROL KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Y	494	Total	C	N	O	S	0	0	0
			3910	2470	683	738	19			
1	O	494	Total	C	N	O	S	0	0	0
			3910	2470	683	738	19			

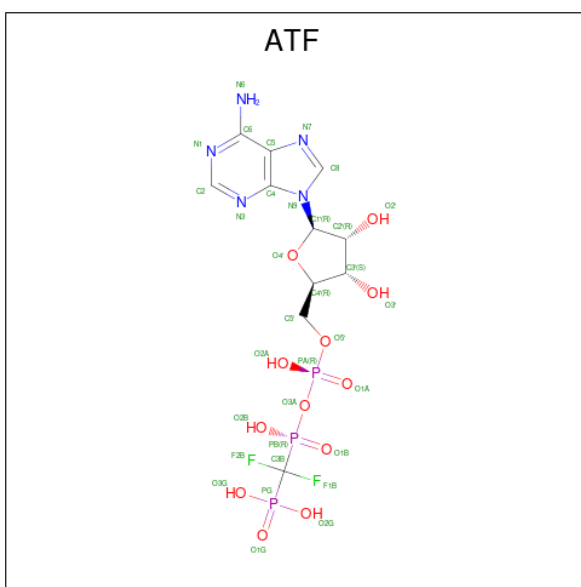
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	58	TRP	SER	engineered mutation	UNP P0A6F3
O	58	TRP	SER	engineered mutation	UNP P0A6F3

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

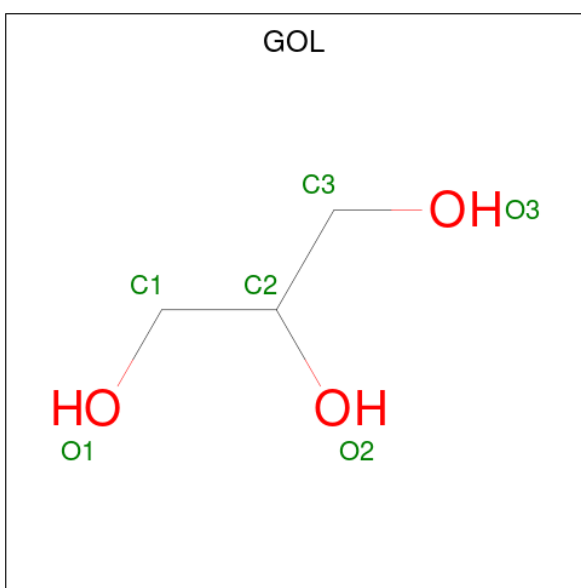
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	Y	1	Total	Mg	0	0
			1	1		
2	O	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHODIFLUOROMETHYLPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ATF) (formula: C₁₁H₁₆F₂N₅O₁₂P₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	Y	1	Total 33	C 11	F 2	N 5	O 12	P 3	0	0
3	O	1	Total 33	C 11	F 2	N 5	O 12	P 3	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).

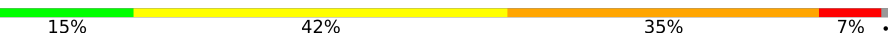


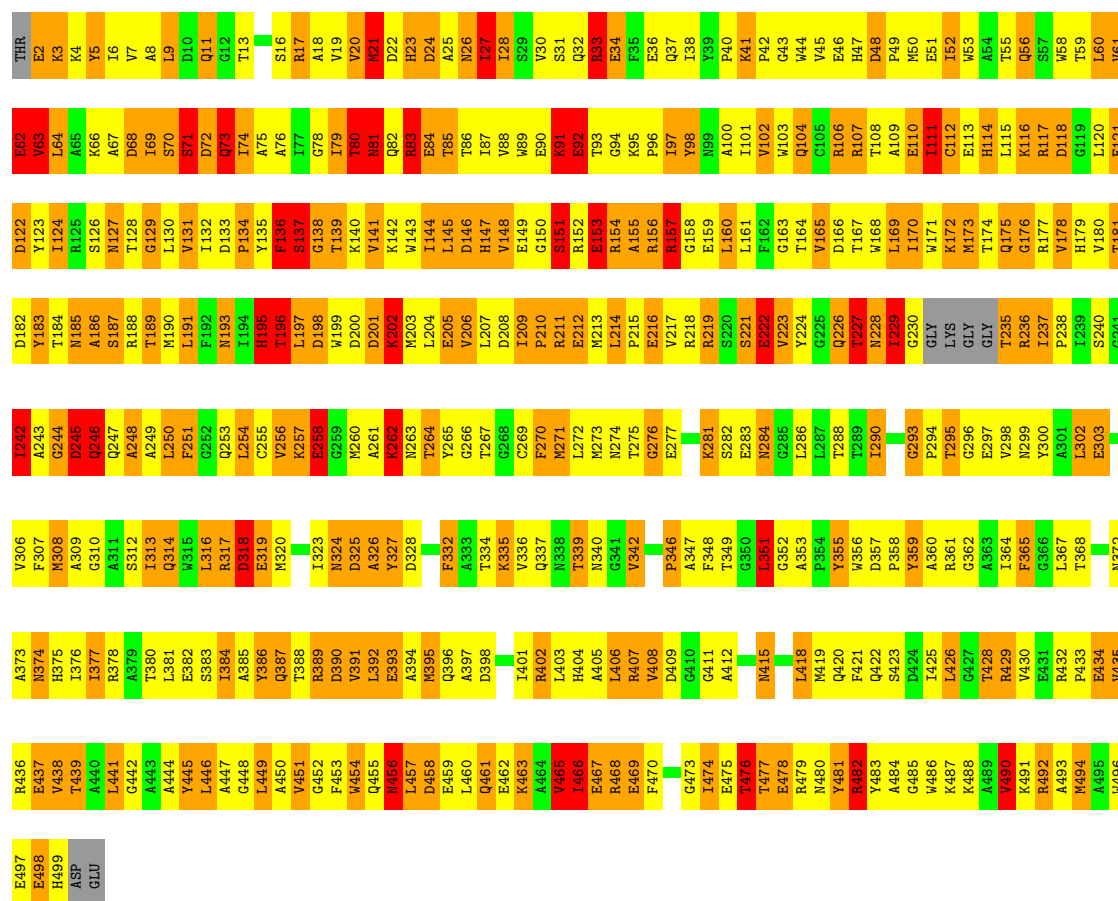
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Y	1	Total C O 6 3 3	0	0
4	O	1	Total C O 6 3 3	0	0

3 Residue-property plots

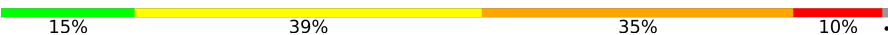
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Chain Y: 



• Molecule 1: GLYCEROL KINASE

Chain O: 



E497	E498	E499	ASP	GLU	V435	A374	N374	F307	I242	A243	D182	D122	V63
					R436	R374	F307	I242	A243	D182	D122	V63	
					E437	H375			G244	T184	I124	L64	
					V438	I376	G310		D245	N185	R125	A65	
					T439	I377	A311		Q246	A186	S126	K66	
					A440	R378	S312		Q247	S187	N127	A67	
					L441				A248	R188	T128	D68	
					A444	L381	I313		A249	T189	G129	I69	
					V445	E382	Q314		L250	M190	L130	S70	
					L446	S383	L316		F251	L191	V131	S71	
					A447	Y386	R317		G252	F192	I132	D72	
					L448	Q387	D318		Q253	N193	D133	Q73	
					L449	T388	I322		L254	I194	P134	I74	
					A450	R389	I323		C255	H195	Y135	A75	
					V451	D390	I323		V256	T196	F136	A76	
					G452	V391	N324		K257	L197	S137	I77	
					F453	L392	D325		E258	D198	G138	G78	
					V454	E393	A326			W199	T139	I79	
					V455	A394	D328		K262	D200	K140	T80	
					Q455	R395	S329		T264	D201	V141	N81	
					V456	A397	E330		Y265	K202	K142	Q82	
					L457	D458	I331		G266	L204	W143	K83	
					E459	R398	F332		T267	L204	I144	E84	
					L460	S399	A333		G268	V206	L145	T85	
					Q461	G400	T334		C269	L207	D146	T86	
					E462	I401	K335		F270	L207	H147	I87	
					K463	R402			M271	D208	V148	W88	
					A464	L403	T339		L272	I209	E149	K89	
					V465	H404	N340		P210	G150	E90	E90	
					L466	A405	G341		R211	S151	R91	K91	
					E467	L406	V342		N274	E212	R152	E92	
					R468	R407			M213	E153	T93	K93	
					E469	V408			L214	R154	G94	G94	
					F470	G410			P215	A155	K95	K95	
					G473	E411			A279	R156	P96	P96	
					L474	A412			V280	V217	I97	I97	
					E475	V413			K281	E158	Y98	Y98	
					T476	L414			S282	R219	E159	N99	
					T477	N415			E283	S220	L160	A100	
					E478	A416			N284	S221	L161	T101	
					R479	F417			G285	E222	F162	V102	
					N480	L418			L286	V223	G163	W103	
					Y481	N419			T287	Y224	T164	Q104	
					R482	Q420			G225	G225	V165	C105	
					Y483	F421			T289	Q226	T167	R106	
					A484	Q422			I290	T227	T167	A107	
					G485	D423			N228	L169	T168	T108	
					Y486	D424			C291	L229	G168	A109	
					K487	I425			P294	L170	W170	E110	
					K488	L426			G296	K172	C112	C112	
					A489	G427			E297	GLY	H173	E113	
					V490	T428			T364	GLY	T174	R114	
					K491	R429			F365	T235	Q175	L115	
					R492	V430			G366	N299	G176	K116	
					L493	E431			L367	Y300	R177	R117	
					V494	R432			T368	A301	P178	D118	
					A495	P433			L302	T239	H179	G119	
					W496	E434			E303	S240	V180	L120	
									G304	G241	T181	E121	

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	99.77Å 200.29Å 114.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.0 (20.00-3.00) 94.4 (20.00-3.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	200.72 (at 2.92Å)	Xtriage
Refinement program	TNT 5F	Depositor
R, R_{free}	0.168 , (Not available) 0.160 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 171.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7900	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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: MG, GOL, ATF

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	O	1.50	18/3991 (0.5%)	2.12	166/5412 (3.1%)
1	Y	1.62	32/3991 (0.8%)	2.20	176/5412 (3.3%)
All	All	1.56	50/7982 (0.6%)	2.16	342/10824 (3.2%)

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	353	ALA	C-O	9.64	1.35	1.23
1	Y	353	ALA	CA-C	-8.35	1.43	1.53
1	Y	359	TYR	CA-C	-7.91	1.42	1.52
1	O	357	ASP	C-N	-7.18	1.26	1.34
1	Y	481	TYR	N-CA	-6.76	1.38	1.46

The worst 5 of 342 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	83	ARG	CA-C-N	-15.39	98.07	122.24
1	Y	83	ARG	C-N-CA	-15.39	98.07	122.24
1	Y	229	ILE	N-CA-C	-12.77	99.12	110.74
1	O	351	LEU	CA-C-N	-12.05	101.51	122.00
1	O	351	LEU	C-N-CA	-12.05	101.51	122.00

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	O	3910	0	3841	684	0
1	Y	3910	0	3841	575	1
2	O	1	0	0	0	0
2	Y	1	0	0	0	0
3	O	33	0	12	2	0
3	Y	33	0	12	3	0
4	O	6	0	8	2	0
4	Y	6	0	8	1	0
All	All	7900	0	7722	1254	1

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 80.

The worst 5 of 1254 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:Y:458:ASP:HA	1:Y:461:GLN:HG3	1.24	1.17
1:Y:74:ILE:HD11	1:Y:237:ILE:HG13	1.21	1.13
1:Y:229:ILE:HG21	1:Y:237:ILE:HG12	1.31	1.11
1:Y:124:ILE:HD13	1:Y:203:MET:HE1	1.26	1.09
1:Y:459:GLU:HB2	1:Y:460:LEU:HD12	1.32	1.07

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:58:TRP:CZ2	1:Y:58:TRP:CZ2[3_655]	2.10	0.10

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	O	490/501 (98%)	375 (76%)	87 (18%)	28 (6%)	1	8
1	Y	490/501 (98%)	404 (82%)	68 (14%)	18 (4%)	2	15
All	All	980/1002 (98%)	779 (80%)	155 (16%)	46 (5%)	2	11

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	71	SER
1	Y	151	SER
1	Y	153	GLU
1	Y	175	GLN
1	O	60	LEU

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	O	408/412 (99%)	251 (62%)	157 (38%)	0	1
1	Y	408/412 (99%)	258 (63%)	150 (37%)	0	1
All	All	816/824 (99%)	509 (62%)	307 (38%)	0	1

5 of 307 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	226	GLN
1	O	457	LEU
1	O	256	VAL
1	O	391	VAL
1	O	478	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	226	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	461	GLN
1	O	263	ASN
1	O	404	HIS
1	Y	246	GLN

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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
4	GOL	Y	600	-	5,5,5	0.65	0	5,5,5	0.95	0
3	ATF	O	601	2	31,35,35	2.04	7 (22%)	43,57,57	1.42	5 (11%)
3	ATF	Y	601	2	31,35,35	2.19	6 (19%)	43,57,57	1.80	7 (16%)
4	GOL	O	600	-	5,5,5	0.63	0	5,5,5	0.59	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
4	GOL	Y	600	-	-	2/4/4/4	-
3	ATF	O	601	2	-	5/19/50/50	0/3/3/3
3	ATF	Y	601	2	-	7/19/50/50	0/3/3/3
4	GOL	O	600	-	-	4/4/4/4	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	601	ATF	PB-O2B	6.64	1.69	1.56
3	O	601	ATF	PB-O2B	5.63	1.67	1.56
3	Y	601	ATF	PG-O3G	5.59	1.69	1.54
3	O	601	ATF	PG-O2G	5.32	1.68	1.54
3	Y	601	ATF	PG-O2G	5.05	1.68	1.54

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	601	ATF	PB-O3A-PA	-5.91	113.82	132.22
3	Y	601	ATF	O2'-C2'-C1'	-5.50	91.17	110.10
3	O	601	ATF	PB-O3A-PA	-3.77	120.49	132.22
3	O	601	ATF	O2'-C2'-C1'	-3.55	97.89	110.10
3	Y	601	ATF	O4'-C1'-N9	3.52	114.84	108.09

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

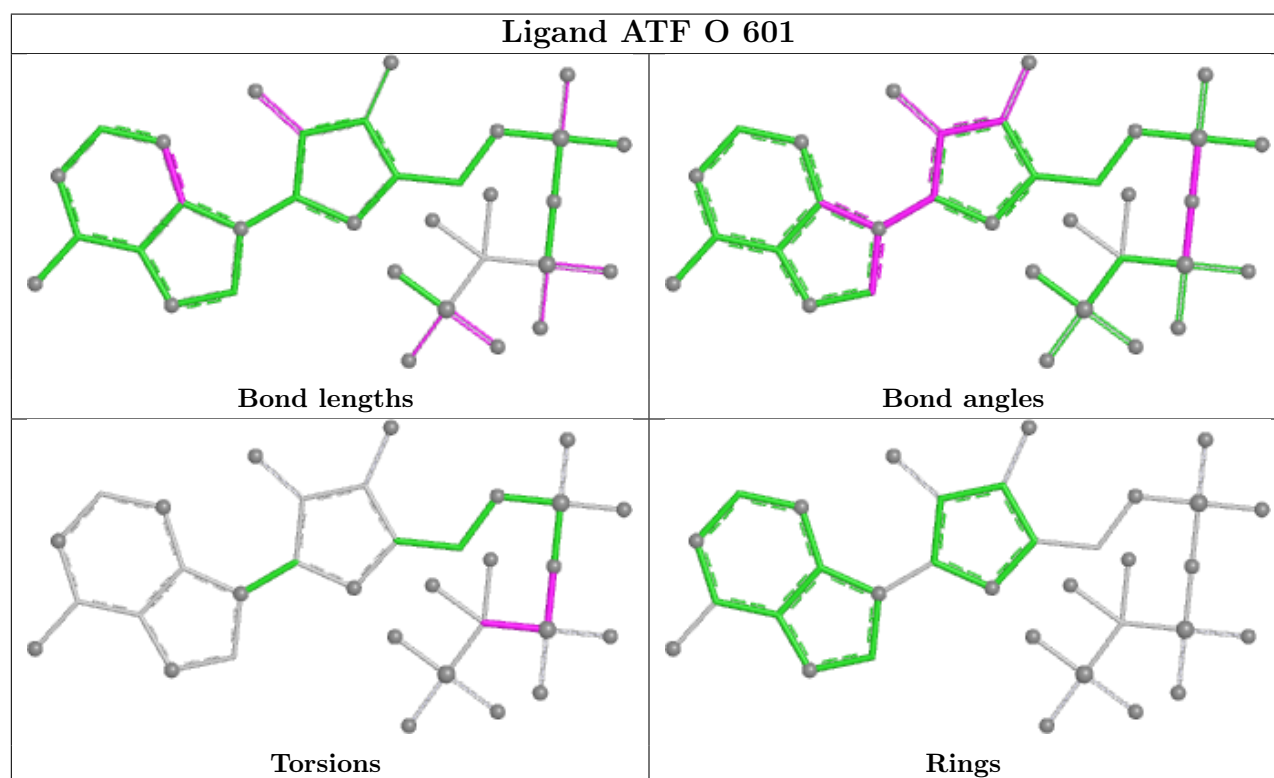
Mol	Chain	Res	Type	Atoms
3	Y	601	ATF	F1B-C3B-PB-O1B
3	Y	601	ATF	F2B-C3B-PB-O1B
3	Y	601	ATF	F1B-C3B-PB-O3A
3	Y	601	ATF	F2B-C3B-PB-O3A
3	Y	601	ATF	C5'-O5'-PA-O2A

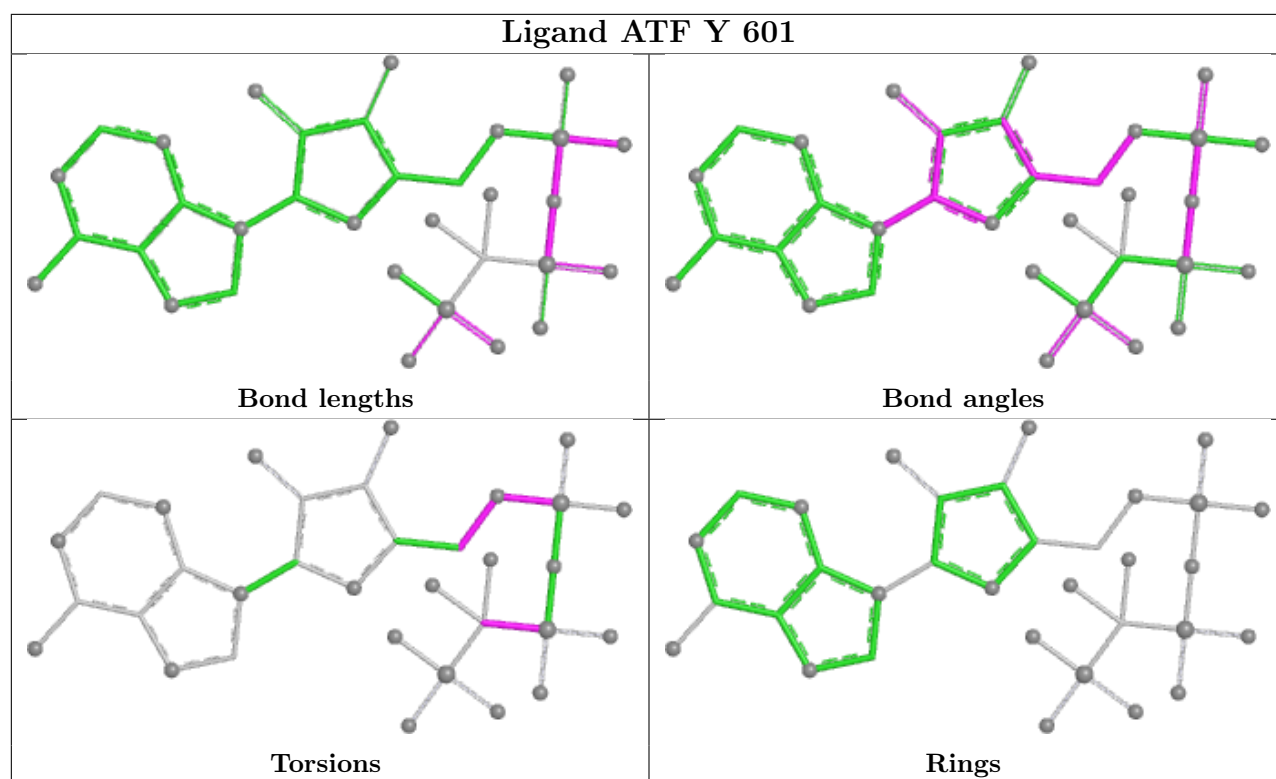
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Y	600	GOL	1	0
3	O	601	ATF	2	0
3	Y	601	ATF	3	0
4	O	600	GOL	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	O	494/501 (98%)	-0.58	1 (0%) 91 83	9, 52, 92, 100	0
1	Y	494/501 (98%)	-0.79	0 100 100	7, 41, 80, 100	0
All	All	988/1002 (98%)	-0.69	1 (0%) 92 86	7, 47, 88, 100	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	296	GLY	2.6

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	Y	602	1/1	0.80	0.16	43,43,43,43	0
2	MG	O	602	1/1	0.87	0.18	56,56,56,56	0
3	ATF	Y	601	33/33	0.92	0.10	42,42,42,42	0
3	ATF	O	601	33/33	0.95	0.08	56,56,56,56	0

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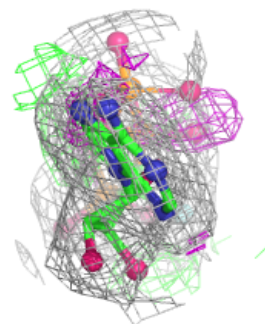
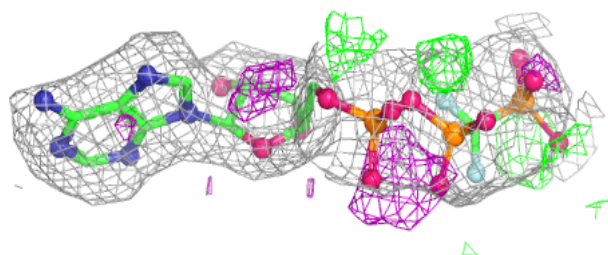
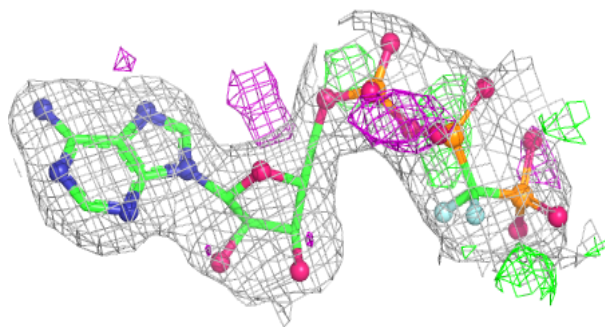
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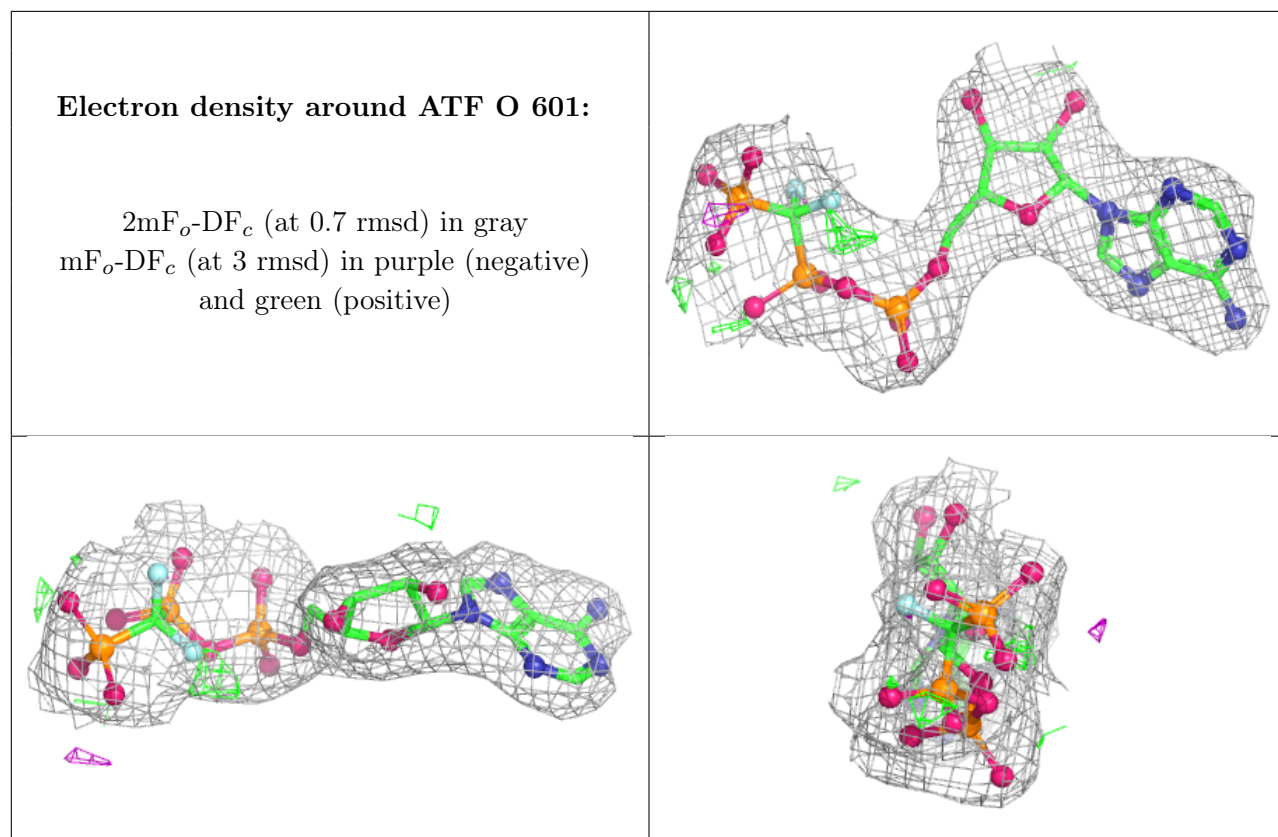
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	O	600	6/6	0.96	0.07	31,31,31,31	0
4	GOL	Y	600	6/6	0.98	0.05	14,14,14,14	0

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 ATF Y 601:

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.