



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:33 PM UTC

PDB ID : 1GLL / pdb_00001gll
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 : 1998-09-24
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

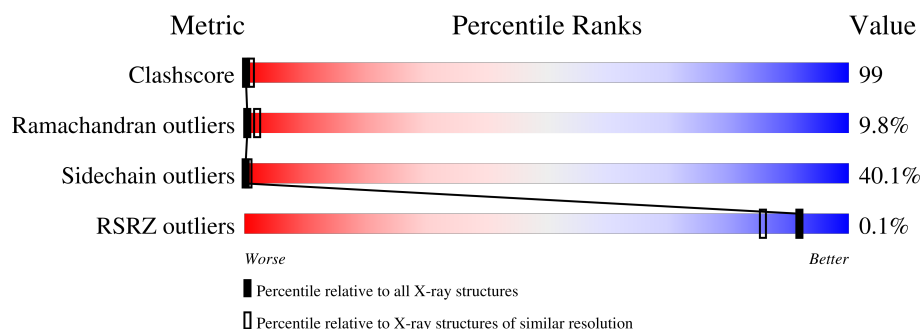
1 Overall quality at a glance

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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	O	600	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7896 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			

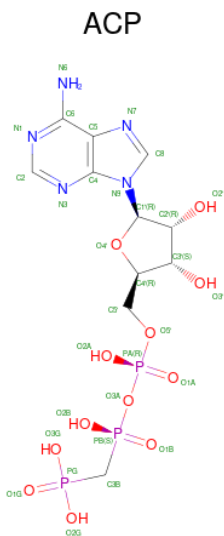
There are 2 discrepancies between the modelled and reference sequences:

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).

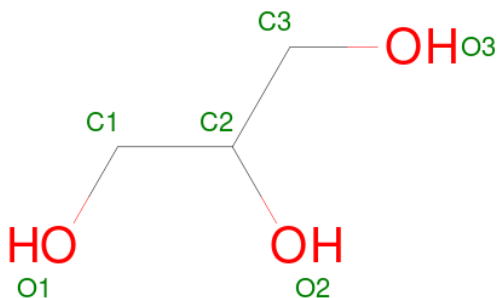
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	Y	1	Total	Mg	0	0
			1	1		
2	O	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	Y	1	Total 31	C 11	N 5	O 12	P 3	0	0
3	O	1	Total 31	C 11	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

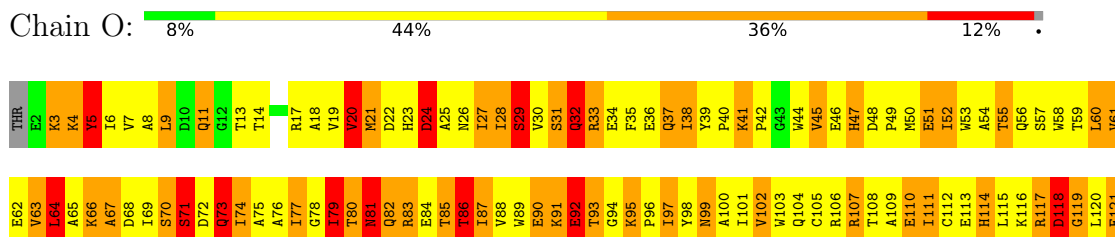
3 Residue-property plots

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



• Molecule 1: GLYCEROL KINASE



V490	K491	R492	A493	A494	A495	A496	E497	E498	H499	ASP	GLU
T428	R429	V430	E431	R432	P433	E434	V435	R436	E437	V438	T439
A440	L441	G442	A443	A444	V445	L446	A447	G448	L449	A450	V451
G452	F453	W454	Q455	N456	Y457	D458	E459	L460	Q461	E462	R463
A464	V465	L466	E467	R468	E469	F470	T474	E475	T476	T477	E478
R479	N480	Y481	R482	Y483	A484	C485	N486	K487	R488	A489	
F385	T386	R369	N372	A373	N374	H375	I376	I377	R378	A379	T380
L381	E382	S383	I384	A385	Y386	Q387	T388	R389	D390	Y391	L392
E393	A394	N395	Q396	D397	G398	G400	I401	R402	L403	H404	A405
L406	R407	V408	D409	G410	V413	A414	N415	N416	F417	L418	N419
Q420	F421	Q422	S423	D424	L425	L426	A427				
L302	E303	V306	F307	N308	A309	G310	A311	S312	I313	Q314	V315
L316	R317	D318	K321	L322	I323	N324	D325	A326	Y327	D328	S329
E330	Y331	F332	A333	T334	K335	V336	Q337	L401	R402	L403	H404
Y343	V344	V345	P346	A347	F348	T349	G350	L351	T288	G352	A353
P354	Y355	W356	D357	P358	Y359	A360	R361	G362	Y300	A363	I364
I242	A243	G244	N245	Q246	A248	A249	L250	F251	G252	D253	L254
C255	V256	E258	E259	H260	A261	K262	N263	T264	Y265	G266	T267
G268	C269	F270	M271	L272	M273	N274	T275	G276	E277	K278	A279
V280	K281	S282	E283	N284	C285	L286	L287	T288	T289	I290	A291
C292	G293	P294	T295	G296	E297	V298	N299	Y300	A301		
D182	Y183	T184	N185	A186	R187	T188	T189	M190	L191	F192	N193
D194	P195	F196	L197	D198	W199	D200	D201	K202	M203	L204	E205
V206	L207	D208	L209	P210	G211	R212	E213	L214	A215	E216	V217
R218	R219	S220	S221	E222	V223	Y224	G225	Q226	T227	N228	L229
I230	G231	L232	L233	Y234	L235	P236	P238	I239	G241		
Y123	I124	N125	A126	M127	T128	G129	L130	L131	I132	D133	P134
Y135	F136	S137	D138	K140	T139	D198	W199	D200	D201	K202	M203
W143	L204	E205	V206	L207	D208	L209	P210	G211	R212	E213	L214
A155	E156	R157	G158	E159	L160	L161	F162	G163	T164	W165	D166
T167	W168	L169	I170	W171	K172	M173	T174	Q175	R176	G177	V178
H179	V180	T181									

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 201.15Å 114.34Å 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) 82.3 (20.00-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	93.19 (at 2.97Å)	Xtriage
Refinement program	TNT 5F	Depositor
R, R_{free}	0.176 , (Not available) 0.166 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 205.0	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	7896	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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: ACP, GOL, MG

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	1.55	22/3991 (0.6%)	2.03	142/5412 (2.6%)
1	Y	1.71	49/3991 (1.2%)	2.15	153/5412 (2.8%)
All	All	1.63	71/7982 (0.9%)	2.09	295/10824 (2.7%)

The worst 5 of 71 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	300	TYR	CA-C	-7.75	1.43	1.52
1	Y	270	PHE	CA-C	-7.62	1.44	1.53
1	O	325	ASP	CA-C	-7.29	1.43	1.52
1	O	196	THR	CA-C	-6.66	1.44	1.52
1	O	331	TYR	C-O	6.61	1.31	1.24

The worst 5 of 295 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	83	ARG	CA-C-N	-17.81	94.28	122.24
1	Y	83	ARG	C-N-CA	-17.81	94.28	122.24
1	Y	390	ASP	CA-CB-CG	11.94	124.53	112.60
1	O	83	ARG	N-CA-C	10.84	126.84	113.50
1	Y	136	PHE	CA-CB-CG	-10.79	103.02	113.80

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	787	0
1	Y	3910	0	3841	771	0
2	O	1	0	0	0	0
2	Y	1	0	0	0	0
3	O	31	0	14	4	0
3	Y	31	0	14	5	0
4	O	6	0	8	7	0
4	Y	6	0	8	3	0
All	All	7896	0	7726	1550	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 99.

The worst 5 of 1550 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	1.25	1.13
1:O:48:ASP:HB3	1:O:51:GLU:HB3	1.16	1.13
1:O:415:ASN:ND2	1:O:418:LEU:H	1.48	1.11
1:Y:31:SER:HB2	1:Y:63:VAL:HG22	1.28	1.08
1:O:83:ARG:HB2	4:O:600:GOL:H12	1.11	1.08

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	O	490/501 (98%)	341 (70%)	102 (21%)	47 (10%)	0 2
1	Y	490/501 (98%)	354 (72%)	87 (18%)	49 (10%)	0 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	980/1002 (98%)	695 (71%)	189 (19%)	96 (10%)	0 2

5 of 96 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	58	TRP
1	Y	59	THR
1	Y	64	LEU
1	Y	151	SER
1	Y	165	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	O	408/412 (99%)	245 (60%)	163 (40%)	0 1
1	Y	408/412 (99%)	244 (60%)	164 (40%)	0 1
All	All	816/824 (99%)	489 (60%)	327 (40%)	0 1

5 of 327 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	173	MET
1	O	391	VAL
1	O	196	THR
1	O	256	VAL
1	O	434	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	37	GLN
1	O	179	HIS
1	O	73	GLN

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Mol	Chain	Res	Type
1	O	114	HIS
1	O	228	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 ⓘ

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	$\# Z > 2$
3	ACP	O	601	2	31,33,33	2.76	6 (19%)	47,52,52	2.25	5 (10%)
3	ACP	Y	601	2	31,33,33	2.76	5 (16%)	47,52,52	1.54	5 (10%)
4	GOL	O	600	-	5,5,5	0.64	0	5,5,5	0.38	0
4	GOL	Y	600	-	5,5,5	0.50	0	5,5,5	0.79	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	ACP	O	601	2	-	0/19/38/38	0/3/3/3
3	ACP	Y	601	2	-	4/19/38/38	0/3/3/3
4	GOL	O	600	-	-	2/4/4/4	-
4	GOL	Y	600	-	-	2/4/4/4	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	601	ACP	PG-O2G	9.66	1.76	1.55
3	Y	601	ACP	PA-O3A	9.25	1.69	1.59
3	O	601	ACP	PG-O3G	7.89	1.72	1.55
3	Y	601	ACP	PG-O3G	7.66	1.72	1.55
3	O	601	ACP	PG-O1G	6.50	1.63	1.50

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	601	ACP	C1'-N9-C8	-9.97	104.97	127.09
3	O	601	ACP	C4-N9-C1'	9.70	149.31	126.63
3	Y	601	ACP	C4-N9-C1'	5.44	139.36	126.63
3	Y	601	ACP	C1'-N9-C8	-4.40	117.32	127.09
3	Y	601	ACP	PB-O3A-PA	-3.43	121.17	132.37

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

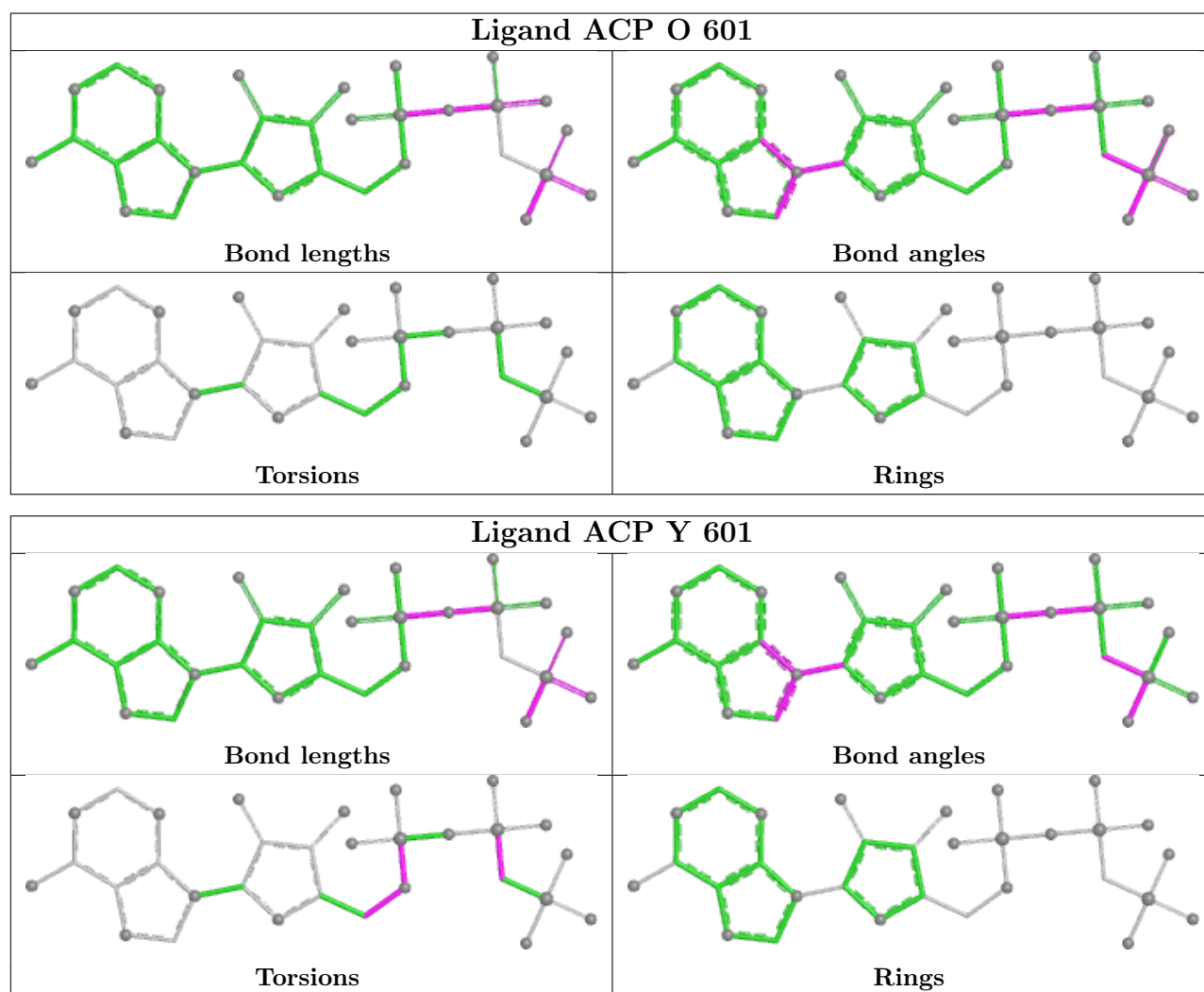
Mol	Chain	Res	Type	Atoms
3	Y	601	ACP	C5'-O5'-PA-O1A
3	Y	601	ACP	C5'-O5'-PA-O3A
4	Y	600	GOL	C1-C2-C3-O3
4	Y	600	GOL	O2-C2-C3-O3
4	O	600	GOL	C1-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	601	ACP	4	0
3	Y	601	ACP	5	0
4	O	600	GOL	7	0
4	Y	600	GOL	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.53	1 (0%) 91 83	13, 61, 94, 100	0
1	Y	494/501 (98%)	-0.76	0 100 100	7, 48, 81, 98	0
All	All	988/1002 (98%)	-0.65	1 (0%) 92 86	7, 54, 88, 100	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	160	LEU	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.

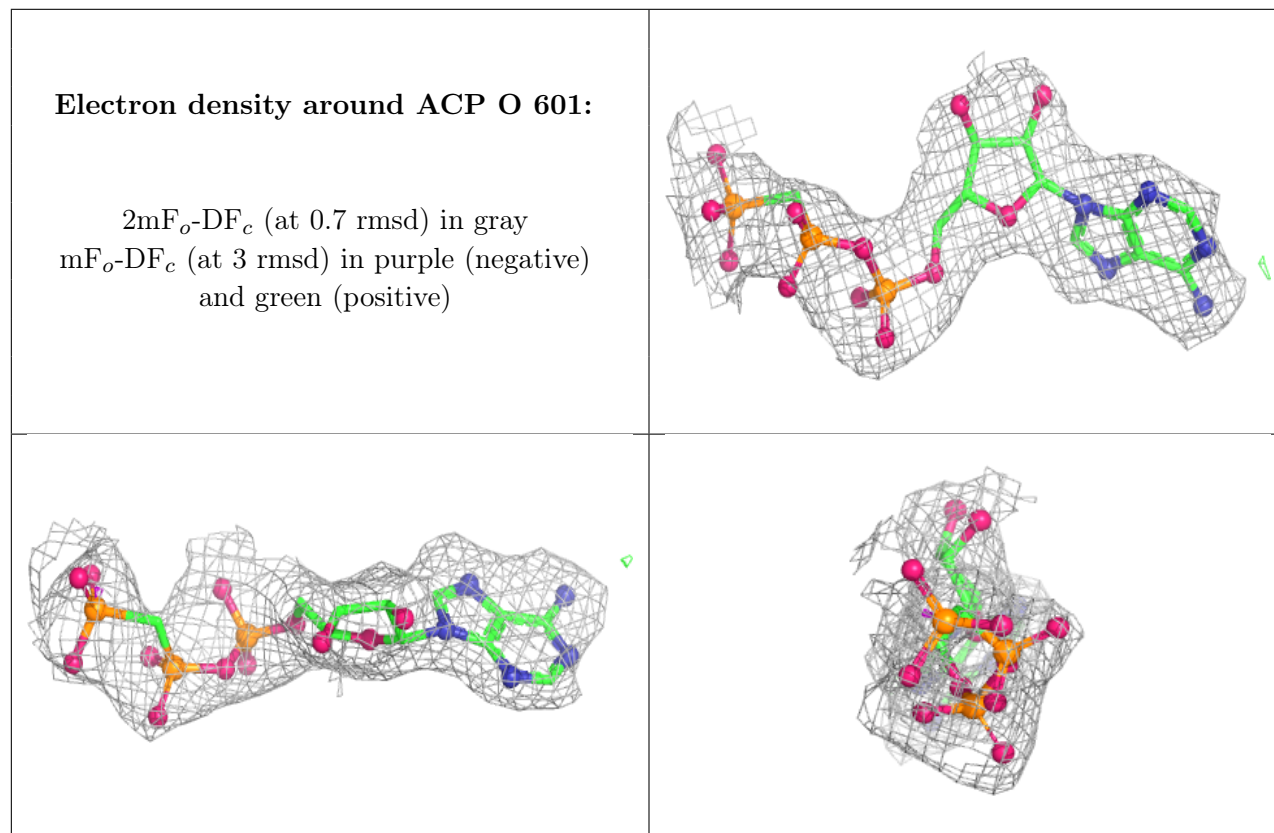
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ACP	O	601	31/31	0.94	0.09	60,60,60,60	0
3	ACP	Y	601	31/31	0.96	0.07	47,47,47,47	0
2	MG	O	602	1/1	0.96	0.12	65,65,65,65	0
4	GOL	Y	600	6/6	0.97	0.06	32,32,32,32	0

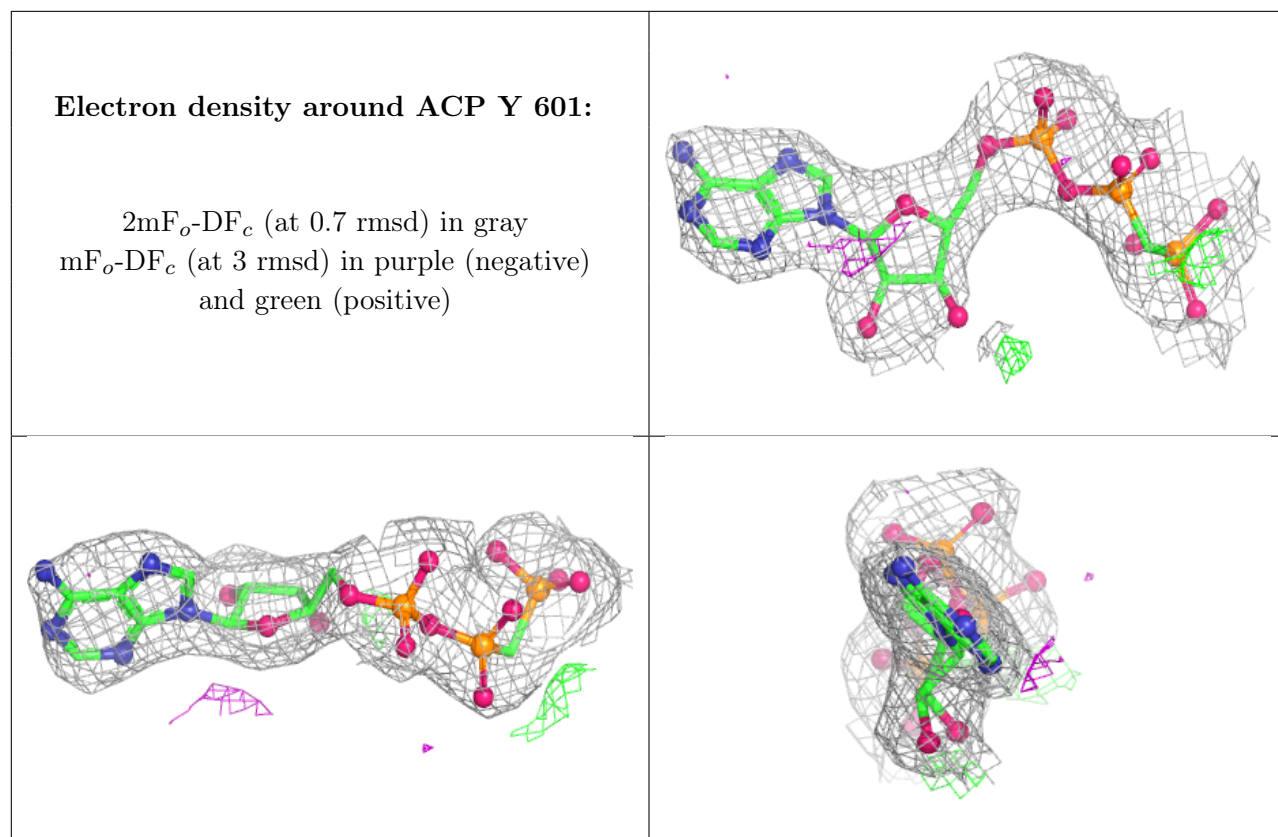
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	Y	602	1/1	0.98	0.03	40,40,40,40	0
4	GOL	O	600	6/6	0.98	0.04	29,29,29,29	0

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.