



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:39 PM GMT

PDB ID : 1GLL  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

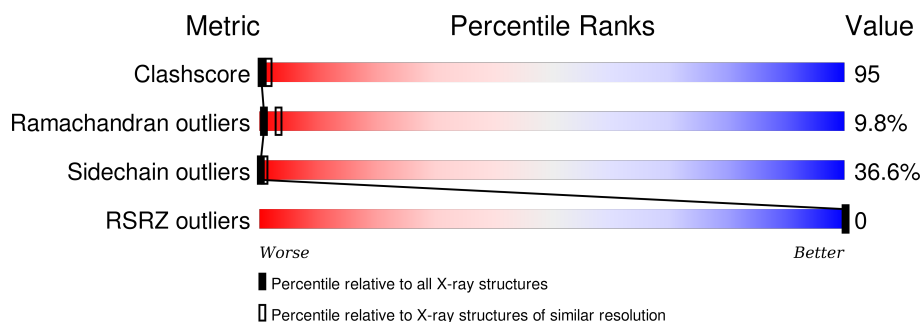
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


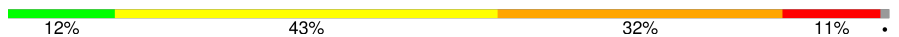
The reported resolution of this entry is 3.00 Å.

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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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			

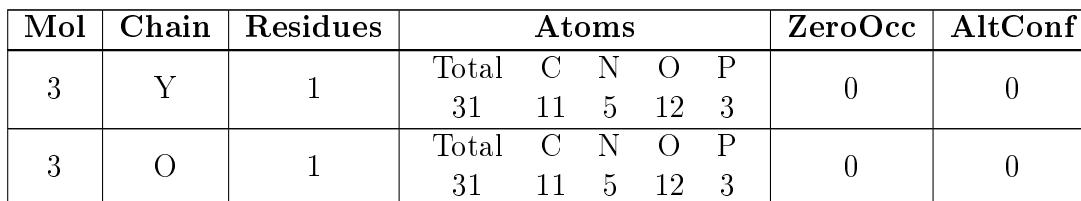
There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



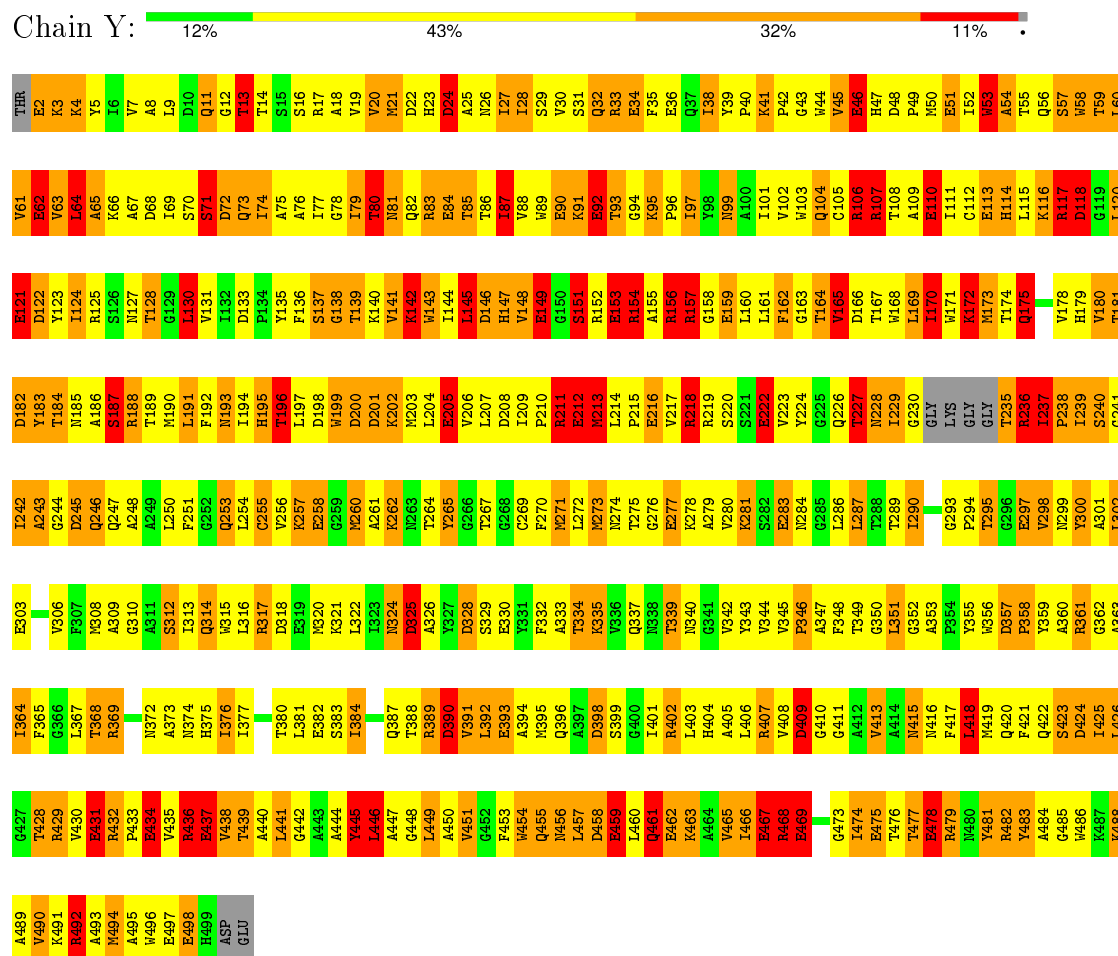
- GOL
- 
- The diagram shows a skeletal structure of 1,2,3-propanetriol (glycerol). The carbon atoms are labeled C1, C2, and C3 in green. The hydroxyl groups are shown as HO (red) and OH (red). The labels O1, O2, and O3 are in green below the respective oxygen atoms. The structure is drawn with black lines for the carbon backbone and red lines for the C-O and O-H bonds.

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

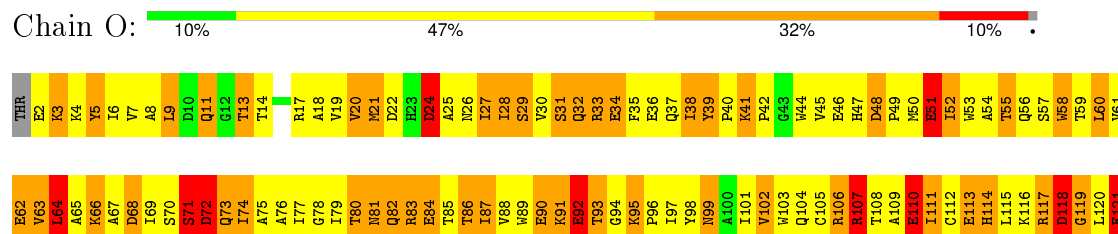
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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



A489	A490	A491	A492	A493	A494	A495	A496	A497	A498	A499	ASP	GLU																																																		
G427	T428	R429	V430	E431	R432	P433	E434	V435	R436	E437	V438	T439	A440	L441	G442	A443	A444	Y445	L446	A447	G448	L449	A450	V451	G452	F453	W454	Q455	N456	L457	D458	E459	Q460	E461	E462	K463	A464	V465	I466	E467	R468	E469	F470	I471	E472	T473	E474	R475	N476	Y477	Q478	A479	N480	Y481	R482	Y483	A484	G485	W486	K487	K488	
A363	I364	F365		T366	R369		N372	A373	N374	H375	I376	I377	R378	A379	T380	L381	E382	S383	I384	A385	G386	Q387	T388	R389	D390	V391	L392	E393	Q394	N395	Q396	A397	D398		I401	R402	L403	H404	L405	E406	R407	V408	D409	G410		V413	A414	N415	W416	F417	N418	Y419	Q420	Y421	Q422	S423	D424	I425	L426			
L302	E303		V306	F307	N308	A309	G310	A311	S312	I313	Q314	R315	L316	R317	D318	E319	R320	G321	K322	L323	N324	D325	A326	Y327	D328	S329	E330	F331	F332	F333	A334	T334	K335	V336	Q337	N338	T339	N340	G341	V342	Y343	S344	V345	P346	A347	F348	T349	G350	T351	L352	G353	A354	P355	Y356	W357	D358	P359	Y360	R361	G362		
T242	A243	G244	D245	Q246	Q247	A248	A249	L250	F251	G252	Q253	L254	C255	V256	K257	E258	G259	N260	A261	K262	N263	T264	Y265	G266	T267	G268	C269	F270	N271	L272	N273	N274	T275	G276	E277	K278	A279	V280	K281	S282	E283	N284	C285	L286	L287	T288	T289	T290	A291	C292	G293	T294	T295	G296	E297	V298	N299	Y300	A301			
D182	Y183	T184	N185	R125	S126	N127	R188	T189	M190	L191	F192	N193	L194	H195	T196	L197	D198	W199	D200	E201	K202	M203	L204	E205	V206	L207	D208	I209	P210	G150	R211	E212	N213	L214	P215	E216	V217	R218	R219	S220	S221	F162	G163	Y224	G225	Q226	T227	N228	I229	G230	GLY	LYS	GLY	GLY	T235	Q175	R236	I237	P238	I239	S240	G241
D122	Y123	I124	R125	S126	N127	T128	L129	L130	V131	I132	D133	P134	Y135	F136	S137	G138	T139	D200	K140	V141	K142	W143	I144	E145	D146	H147	V148	E149	P210	G150	R211	E212	N213	L214	P215	E216	V217	R218	R219	S220	S221	F162	G163	Y224	G225	Q226	T227	N228	I229	G230	GLY	LYS	GLY	GLY	T235	Q175	R236	I237	P238	I239	S240	G241

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.77Å 201.15Å 114.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 18.03 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.0 (20.00-3.00) 82.7 (18.03-3.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	93.19 (at 2.97Å)	Xtriage
Refinement program	TNT V. 5-F	Depositor
R, $R_{free}$	0.176 , (Not available) 0.166 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	53.7	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.21 , 157.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 19426 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7896	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, MG, ACP

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	1.27	37/3991 (0.9%)	1.68	72/5412 (1.3%)
1	Y	1.38	35/3991 (0.9%)	1.76	90/5412 (1.7%)
All	All	1.33	72/7982 (0.9%)	1.72	162/10824 (1.5%)

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	478	GLU	CD-OE2	9.70	1.36	1.25
1	Y	153	GLU	CD-OE1	9.27	1.35	1.25
1	O	258	GLU	CD-OE2	9.23	1.35	1.25
1	Y	34	GLU	CD-OE1	9.09	1.35	1.25
1	Y	478	GLU	CD-OE2	9.08	1.35	1.25

The worst 5 of 162 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	237	ILE	C-N-CD	-15.74	85.98	120.60
1	Y	83	ARG	C-N-CA	-10.97	94.28	121.70
1	Y	200	ASP	CB-CG-OD2	-10.81	108.57	118.30
1	Y	492	ARG	NE-CZ-NH1	10.66	125.63	120.30
1	O	468	ARG	NE-CZ-NH1	9.89	125.25	120.30

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	O	3910	0	3841	747	0
1	Y	3910	0	3841	743	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	2	0
All	All	7896	0	7726	1482	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 95.

The worst 5 of 1482 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%)	<b>1</b> <b>3</b>
1	Y	490/501 (98%)	354 (72%)	87 (18%)	49 (10%)	<b>1</b> <b>3</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	980/1002 (98%)	695 (71%)	189 (19%)	96 (10%)	<b>1</b> <b>3</b>

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%)	258 (63%)	150 (37%)	<b>0</b> <b>1</b>
1	Y	408/412 (99%)	259 (64%)	149 (36%)	<b>0</b> <b>1</b>
All	All	816/824 (99%)	517 (63%)	299 (37%)	<b>0</b> <b>1</b>

5 of 299 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	461	GLN
1	O	60	LEU
1	O	435	VAL
1	Y	467	GLU
1	O	5	TYR

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

Mol	Chain	Res	Type
1	Y	420	GLN
1	O	23	HIS
1	O	387	GLN

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Mol	Chain	Res	Type
1	Y	422	GLN
1	Y	461	GLN

### 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 carbohydrates 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	$\# Z  > 2$
4	GOL	O	600	-	5,5,5	0.58	0	5,5,5	0.28	0
3	ACP	O	601	2	25,33,33	2.81	6 (24%)	31,52,52	2.92	4 (12%)
4	GOL	Y	600	-	5,5,5	0.42	0	5,5,5	0.70	0
3	ACP	Y	601	2	25,33,33	2.32	4 (16%)	31,52,52	2.03	4 (12%)

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	O	600	-	-	0/4/4/4	0/0/0/0
3	ACP	O	601	2	-	0/15/38/38	0/3/3/3
4	GOL	Y	600	-	-	0/4/4/4	0/0/0/0
3	ACP	Y	601	2	-	0/15/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	601	ACP	C4-N3	-2.02	1.32	1.35
3	O	601	ACP	PB-O1B	2.18	1.57	1.51
3	O	601	ACP	PB-O3A	3.88	1.62	1.58
3	Y	601	ACP	PG-O1G	4.13	1.59	1.50
3	Y	601	ACP	PB-O3A	5.07	1.64	1.58

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	601	ACP	PA-O3A-PB	-4.11	121.17	132.73
3	O	601	ACP	PA-O3A-PB	-3.73	122.25	132.73
3	Y	601	ACP	O1G-PG-C3B	-3.13	104.00	111.13
3	O	601	ACP	O1G-PG-C3B	-2.34	105.80	111.13
3	O	601	ACP	C2'-C1'-N9	2.60	118.27	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	O	600	GOL	7	0
3	O	601	ACP	4	0
4	Y	600	GOL	2	0
3	Y	601	ACP	5	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	O	494/501 (98%)	-0.78	0 100 100	13, 61, 94, 100	0
1	Y	494/501 (98%)	-0.98	0 100 100	7, 48, 81, 98	0
All	All	988/1002 (98%)	-0.88	0 100 100	7, 54, 88, 100	0

There are no RSRZ outliers to report.

### 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	Y	600	6/6	0.96	0.13	1.01	32,32,32,32	0
3	ACP	O	601	31/31	0.96	0.13	0.58	60,60,60,60	0
3	ACP	Y	601	31/31	0.97	0.11	0.17	47,47,47,47	0
4	GOL	O	600	6/6	0.98	0.09	-1.83	29,29,29,29	0
2	MG	O	602	1/1	0.90	0.56	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	Y	602	1/1	0.99	0.20	-	40,40,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.