



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 08:04 AM EST

PDB ID : 1GLJ
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 : 1998-09-03
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030736

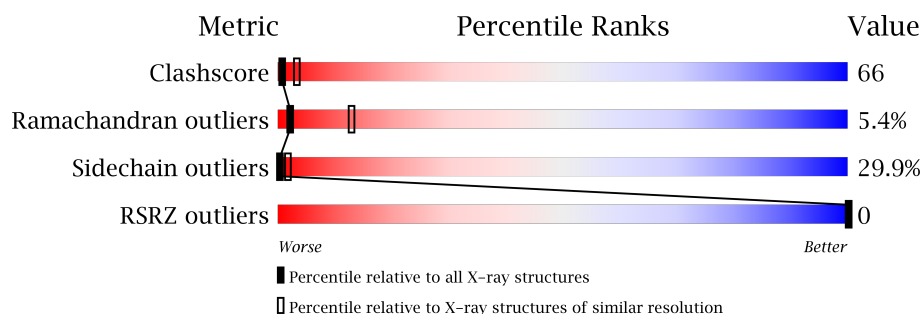
1 Overall quality at a glance

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	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (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 ≥ 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	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7895 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			

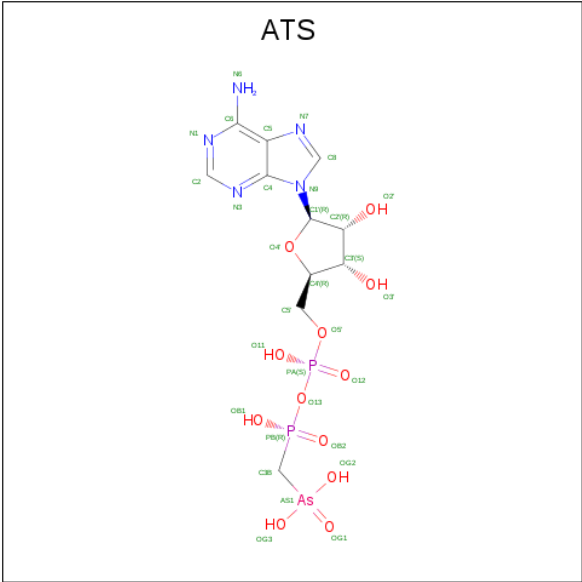
There are 2 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 3 is GAMMA-ARSONO-BETA, GAMMA-METHYLENEADENOSINE-5'-DIPHOSPHATE (three-letter code: ATS) (formula: C₁₁H₁₈AsN₅O₁₂P₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	Y	1	Total	As	C	N	O	P	0	0
			31	1	11	5	12	2		
3	O	1	Total	As	C	N	O	P	0	0
			31	1	11	5	12	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

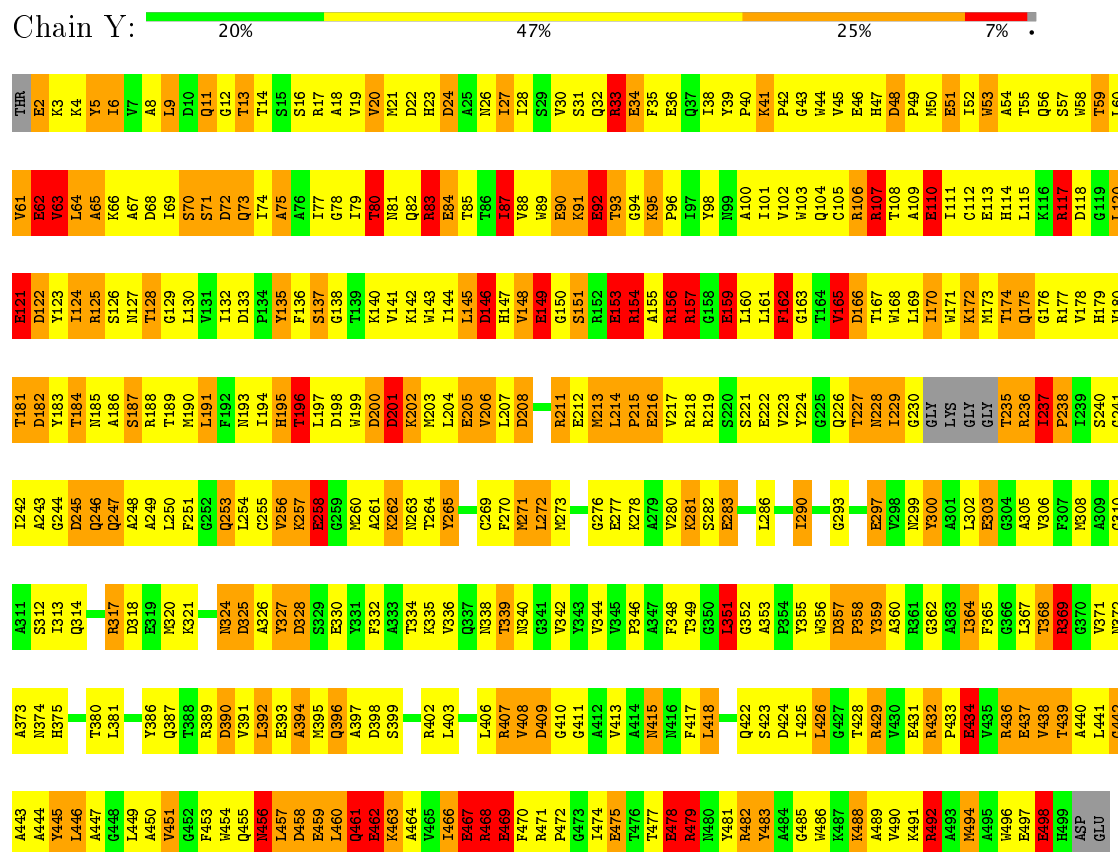


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	Y	1	Total	C	O	0	0
			6	3	3		
4	O	1	Total	C	O	0	0
			6	3	3		

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 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



L444	L381	L316	Q246	T184
Y445	E382	R317	Q247	N185
L446	S383	D318	A248	A186
A447		E319	A249	S187
G448	Y386	N320	L250	R188
L449	Q387	K321	P251	T189
A450	T388	L322	G352	N190
V451	R389	L323	Q253	L191
F453	D390	N324	L254	F192
N454	V391	D325	C255	N193
	L392	A326	V256	I194
Q455	E393	Y327	K257	H195
N456	A394	D328	E358	T196
L457	N395	S329		L197
D458	Q396	E330	K262	D198
E459	A397	Y331	N263	W199
L460	D398	F332	T264	D200
Q461	S399	A333	Y265	D201
E462	G400	T334		K202
K463	I401	K335	C269	N203
A464	R402		F270	L204
L466	L403		E271	E205
E467			L272	V206
B468	L406		N273	L207
E469	R407	N340	N274	D208
F470	V408	G343	T275	L209
P471	D409	Y343	G276	P210
P472	G410	V344	E277	R211
G473		V345	K278	E212
L474	V413	P346	A279	N213
E475	A414	A347	V280	L214
T476	N415	F348	K281	P215
T477	N416		S282	E216
E478	F417	L351	E283	V217
R479	L418	G352		R218
N480	N419	A353	L286	R219
Y481	Q420	P354	L287	S220
R482	P421	Y355	T288	S221
A484	Q422	N356	T289	E222
Q485	S423	D357	L290	
N486	D424	P358	A291	Q226
K487	I425	Y359	C292	T227
K488	L426	A360	G293	N228
A489	Q427	R361	P294	T229
K491	T428	G362	T295	G230
R492	R429	A363	G296	GLY
A493	V430	I364	E297	LYS
N494	E431		V298	GLY
A495	R432	L367	N299	T235
N496	P433	T368	X300	T236
E497	E434	R369	A301	K236
H498	V435		L302	T237
E499	R436	A373	E303	P238
H499	V438	N374		L239
	E497	H375	G310	S240
	E498	I376	A311	G241
	H499	I377	S312	T242
ASP	A440	R378	I313	A243
GLU	L441	A379	Q314	G244
	G442	T380	W315	D245

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	99.67Å 200.70Å 114.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 18.49 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.0 (20.00-3.00) 90.6 (18.49-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	246.72 (at 2.98Å)	Xtriage
Refinement program	TNT 5F, X-PLOR	Depositor
R, R_{free}	0.166 , (Not available) 0.159 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 130.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7895	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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: GOL, MG, ATS

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	1.29	39/3991 (1.0%)	1.72	80/5412 (1.5%)
1	Y	1.38	36/3991 (0.9%)	1.86	104/5412 (1.9%)
All	All	1.33	75/7982 (0.9%)	1.79	184/10824 (1.7%)

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	Y	0	1

The worst 5 of 75 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	258	GLU	CD-OE2	8.77	1.35	1.25
1	Y	283	GLU	CD-OE1	8.74	1.35	1.25
1	Y	462	GLU	CD-OE2	8.57	1.35	1.25
1	O	153	GLU	CD-OE1	8.19	1.34	1.25
1	Y	498	GLU	CD-OE2	8.11	1.34	1.25

The worst 5 of 184 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	106	ARG	NE-CZ-NH2	-14.77	112.92	120.30
1	Y	117	ARG	NE-CZ-NH1	13.46	127.03	120.30
1	O	471	ARG	NE-CZ-NH1	13.00	126.80	120.30
1	Y	245	ASP	CB-CG-OD2	-11.70	107.77	118.30
1	Y	196	THR	N-CA-CB	-11.20	89.02	110.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Y	196	THR	Mainchain

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	558	0
1	Y	3910	0	3841	486	0
2	Y	1	0	0	0	0
3	O	31	0	12	2	0
3	Y	31	0	12	2	0
4	O	6	0	8	2	0
4	Y	6	0	8	3	0
All	All	7895	0	7722	1036	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 66.

The worst 5 of 1036 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:O:22:ASP:HB3	1:O:28:ILE:HD11	1.30	1.13
1:O:47:HIS:HB3	1:O:52:ILE:HD11	1.32	1.09
1:O:5:TYR:HB2	1:O:74:ILE:HG22	1.37	1.07
1:Y:193:ASN:HB3	1:Y:196:THR:HG21	1.37	1.06
1:Y:458:ASP:HA	1:Y:461:GLN:HG3	1.34	1.06

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%)	375 (76%)	85 (17%)	30 (6%)	2	10
1	Y	490/501 (98%)	391 (80%)	76 (16%)	23 (5%)	3	16
All	All	980/1002 (98%)	766 (78%)	161 (16%)	53 (5%)	2	13

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	61	VAL
1	Y	64	LEU
1	Y	65	ALA
1	Y	75	ALA
1	Y	151	SER

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	O	408/412 (99%)	283 (69%)	125 (31%)	0	2
1	Y	408/412 (99%)	289 (71%)	119 (29%)	0	2
All	All	816/824 (99%)	572 (70%)	244 (30%)	0	2

5 of 244 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	469	GLU

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Mol	Chain	Res	Type
1	O	82	GLN
1	O	454	TRP
1	Y	479	ARG
1	O	20	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	Y	456	ASN
1	O	37	GLN
1	O	396	GLN
1	O	11	GLN
1	O	47	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is 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	0.46	0	5,5,5	0.26	0
3	ATS	O	601	-	25,33,33	1.35	4 (16%)	27,52,52	1.16	2 (7%)
4	GOL	Y	600	-	5,5,5	0.58	0	5,5,5	0.80	0
3	ATS	Y	601	2	25,33,33	1.08	2 (8%)	27,52,52	1.34	3 (11%)

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	ATS	O	601	-	-	0/9/38/38	0/3/3/3
4	GOL	Y	600	-	-	0/4/4/4	0/0/0/0
3	ATS	Y	601	2	-	0/9/38/38	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	601	ATS	C4-N3	-3.08	1.31	1.35
3	O	601	ATS	C8-N7	-2.56	1.29	1.34
3	Y	601	ATS	O2'-C2'	-2.31	1.37	1.43
3	Y	601	ATS	O3'-C3'	-2.22	1.37	1.43
3	O	601	ATS	C5-C4	-2.14	1.35	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	601	ATS	PA-O13-PB	-3.34	121.61	132.39
3	O	601	ATS	PA-O13-PB	-2.28	125.03	132.39
3	Y	601	ATS	N6-C6-N1	-2.10	114.59	118.77
3	O	601	ATS	C1'-N9-C4	3.55	132.77	126.64
3	Y	601	ATS	C5-C6-N6	3.78	128.17	120.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

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

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%)	-0.73	0 100 100	7, 52, 91, 100	0
1	Y	494/501 (98%)	-0.94	0 100 100	5, 38, 78, 100	0
All	All	988/1002 (98%)	-0.83	0 100 100	5, 45, 86, 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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	ATS	Y	601	31/31	0.97	0.12	0.72	50,50,50,50	0
3	ATS	O	601	31/31	0.95	0.14	0.61	64,64,64,64	0
4	GOL	Y	600	6/6	0.98	0.11	-0.48	17,17,17,17	0
4	GOL	O	600	6/6	0.98	0.12	-0.49	45,45,45,45	0
2	MG	Y	602	1/1	0.95	0.16	-	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.