wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 06:37 PM GMT

PDB ID	:	1BO5
Title	:	CRYSTAL STRUCTURE OF THE COMPLEX BETWEEN ESCHERICHIA COLI GLYCEROL KINASE AND THE ALLOSTERIC REGULATOR FRUCTOSE 1,6-BISPHOSPHATE.
Authors	:	Ormo, M.; Bystrom, C.E.; Remington, S.J.
Deposited on	:	1998-08-10
Resolution	:	3.20 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

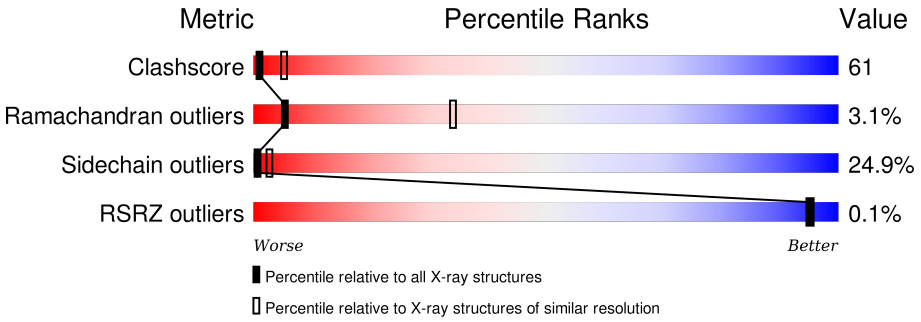
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 <=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	23% 50% 22%
1	Z	501	21% 52% 22%

2 Entry composition

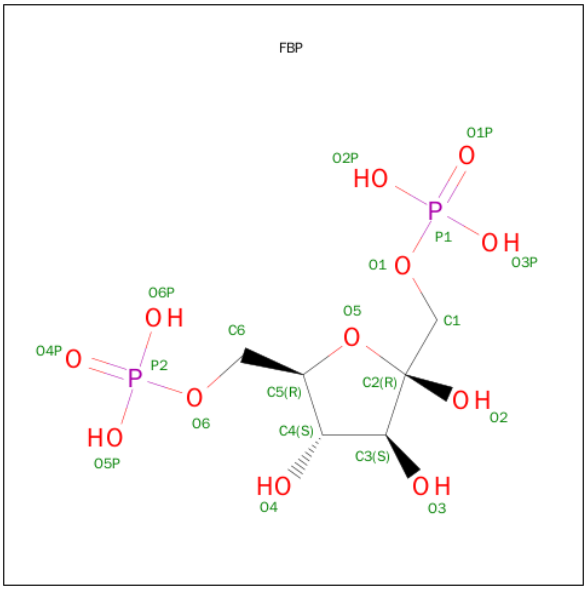
There are 3 unique types of molecules in this entry. The entry contains 7818 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (GLYCEROL KINASE).

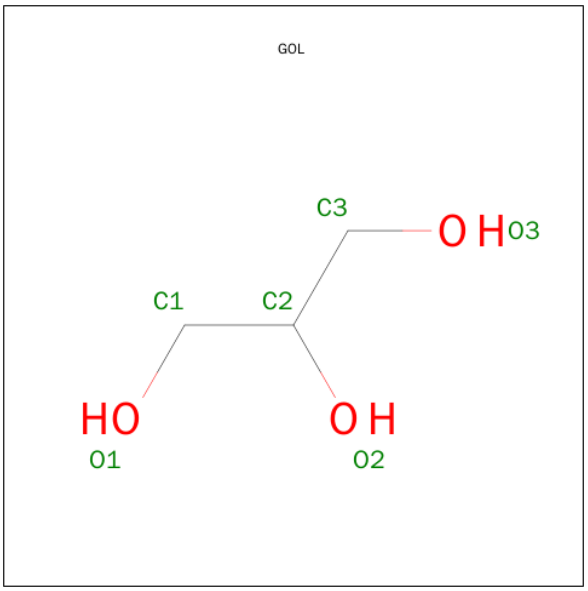
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	498	Total	C	N	O	S	0	0	0
			3878	2453	671	735	19			
1	Z	498	Total	C	N	O	S	0	0	0
			3888	2456	674	739	19			

- Molecule 2 is FRUCTOSE-1,6-DIPHOSPHATE (three-letter code: FBP) (formula: $C_6H_{14}O_{12}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	O	1	Total	C	O	P	0	1
			40	12	24	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



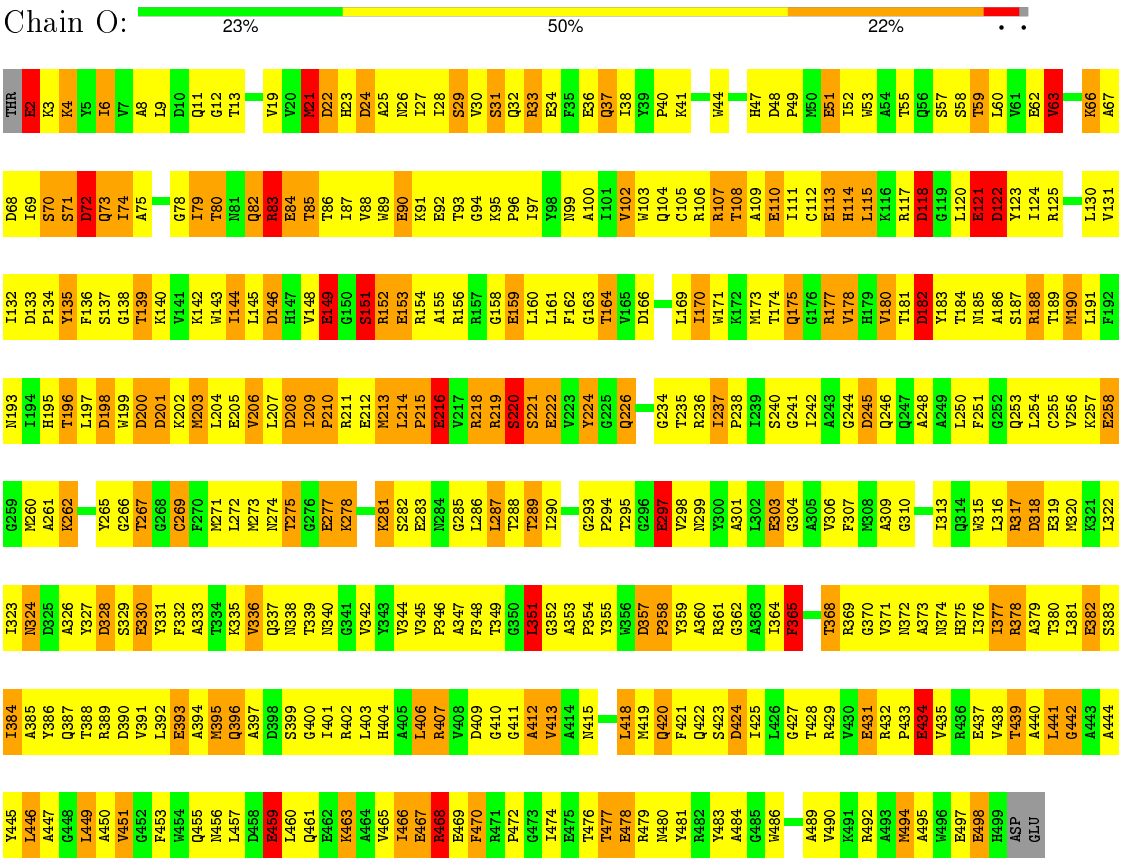
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	O	1	Total	C	O	0	0
			6	3	3		
3	Z	1	Total	C	O	0	0
			6	3	3		

3 Residue-property plots (i)

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.

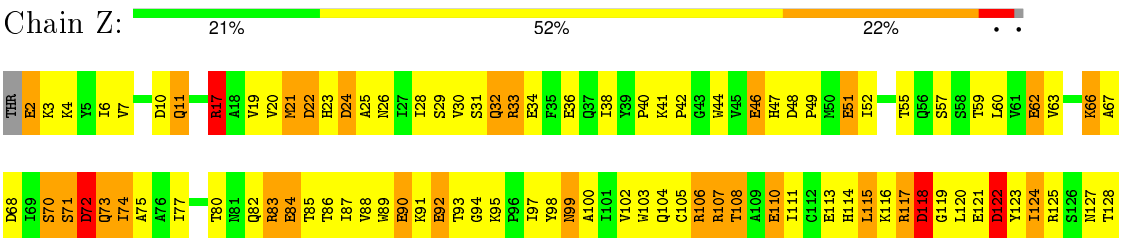
- Molecule 1: PROTEIN (GLYCEROL KINASE)

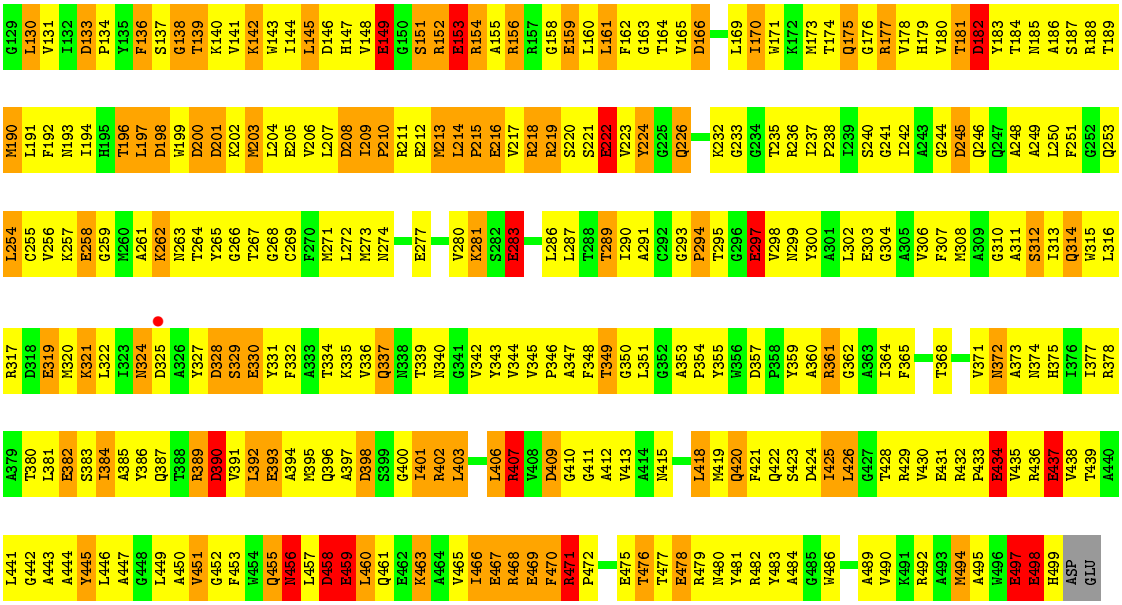
Chain O:



- Molecule 1: PROTEIN (GLYCEROL KINASE)

Chain Z:




G129 L130 V131 I132 D133 P134 Y135 F136 S137 G138 T139 K140 V141 K142 W143 I144 L145 D146 H147 V148 E149 G150 S151 R152 E153 R154 A155 R156 R157 G158 E159 L160 L161 F162 G163 T164 V165 D166 L169 I170 W171 K172 M173 T174 Q175 G176 R177 V178 H179 V180 T181 D182 Y183 T184 N185 A186 S187 R188 T189
M190 L191 F192 N193 I194 H195 T196 L197 D198 W199 D200 D201 K202 M203 L204 E205 V206 L207 D208 I209 P210 R211 E212 M213 L214 P215 E216 V217 R218 R219 S220 S221 E222 V223 Y224 G225 Q226 K232 G233 G234 T235 R236 I237 P238 I239 S240 G241 I242 A243 G244 D245 Q246 Q247 A248 A249 L250 F251 G252 Q253
L254 C255 V256 K257 E258 G259 M260 A261 K262 N263 T264 Y265 G266 T267 G268 C269 F270 M271 L272 M273 N274 E277 V280 K281 S282 E283 L286 L287 T288 T289 I290 A291 C292 G293 P294 T295 G296 E297 V298 N299 Y300 A301 L302 E303 G304 A305 V306 F307 M308 A309 G310 A311 S312 I313 Q314 W315 L316
R317 D318 E319 M320 K321 L322 I323 N324 D325 A326 Y327 D328 S329 E330 Y331 F332 A333 T334 K335 V336 Q337 N338 T339 N340 G341 V342 Y343 V344 V345 P346 A347 F348 T349 G350 L351 G352 A353 P354 Y355 W356 D357 P358 Y359 A360 R361 G362 A363 I364 F365 T368 V371 N372 A373 N374 H375 I376 I377 R378
A379 T380 L381 E382 S383 I384 A385 Y386 Q387 T388 R389 D390 V391 L392 E393 A394 M395 Q396 A397 D398 S399 G400 I401 R402 L403 L406 R407 V408 D409 G410 G411 A412 V413 A414 N415 L418 M419 Q420 F421 Q422 S423 D424 I425 L426 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 L460 Q461 E462 K463 A464 V465 I466 E467 R468 E469 F470 R471 P472 E475 T476 T477 E478 R479 N480 Y481 R482 Y483 A484 G485 W486 A489 V490 K491 R492 A493 M494 A495 W496 E497 E498 H499 ASP GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	169.41Å 169.41Å 204.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 19.97 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.0 (20.00-3.20) 90.3 (19.97-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 2.98Å)	Xtriage
Refinement program	TNT V. 5-F	Depositor
R, R_{free}	0.211 , (Not available) 0.190 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	44.4	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 94.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	1 of 54096 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7818	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, FBP

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	1.17	35/3958 (0.9%)	1.51	55/5373 (1.0%)
1	Z	1.18	32/3968 (0.8%)	1.53	55/5387 (1.0%)
All	All	1.18	67/7926 (0.8%)	1.52	110/10760 (1.0%)

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	O	1	1

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Z	51	GLU	CD-OE1	8.97	1.35	1.25
1	Z	92	GLU	CD-OE1	8.22	1.34	1.25
1	Z	382	GLU	CD-OE2	8.19	1.34	1.25
1	O	51	GLU	CD-OE1	8.05	1.34	1.25
1	Z	212	GLU	CD-OE2	7.96	1.34	1.25

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Z	22	ASP	CB-CG-OD1	8.79	126.21	118.30
1	O	201	ASP	CB-CG-OD1	-8.59	110.57	118.30
1	Z	10	ASP	CB-CG-OD1	-8.38	110.76	118.30
1	Z	409	ASP	CB-CG-OD2	-8.35	110.79	118.30
1	O	24	ASP	CB-CG-OD1	-7.97	111.12	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	O	21	MET	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	O	351	LEU	Mainchain

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	3878	0	3774	472	0
1	Z	3888	0	3778	463	0
2	O	40	0	20	3	0
3	O	6	0	8	2	0
3	Z	6	0	8	0	0
All	All	7818	0	7588	935	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 61.

The worst 5 of 935 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:83:ARG:HH11	1:O:83:ARG:HG3	1.04	1.11
1:O:145:LEU:HD11	1:O:213:MET:HE1	1.30	1.11
1:Z:438:VAL:HA	1:Z:441:LEU:HD12	1.30	1.06
1:Z:71:SER:HB2	1:Z:235:THR:HG21	1.32	1.05
1:O:255:CYS:HB3	1:O:260:MET:HB3	1.39	1.03

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	496/501 (99%)	406 (82%)	74 (15%)	16 (3%)	5 33
1	Z	496/501 (99%)	414 (84%)	67 (14%)	15 (3%)	5 35
All	All	992/1002 (99%)	820 (83%)	141 (14%)	31 (3%)	5 34

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	99	ASN
1	O	121	GLU
1	O	151	SER
1	Z	149	GLU
1	O	72	ASP

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	396/412 (96%)	301 (76%)	95 (24%)	1 3
1	Z	398/412 (97%)	295 (74%)	103 (26%)	0 2
All	All	794/824 (96%)	596 (75%)	198 (25%)	1 3

5 of 198 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	466	ILE

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Mol	Chain	Res	Type
1	Z	74	ILE
1	Z	455	GLN
1	O	477	THR
1	Z	29	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	Z	11	GLN
1	Z	179	HIS
1	Z	461	GLN
1	Z	147	HIS
1	Z	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 carbohydrates in this entry.

5.6 Ligand geometry

4 ligands are 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	FBP	O	502[A]	-	18,20,20	1.07	0	21,32,32	1.51	2 (9%)
2	FBP	O	502[B]	-	18,20,20	1.00	0	21,32,32	1.18	2 (9%)
3	GOL	O	601	-	5,5,5	0.37	0	5,5,5	0.49	0
3	GOL	Z	601	-	5,5,5	0.30	0	5,5,5	0.36	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
2	FBP	O	502[A]	-	-	0/13/32/32	0/1/1/1
2	FBP	O	502[B]	-	-	0/13/32/32	0/1/1/1
3	GOL	O	601	-	-	0/4/4/4	0/0/0/0
3	GOL	Z	601	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	502[B]	FBP	O3P-P1-O2P	3.04	118.94	107.38
2	O	502[B]	FBP	O6P-P2-O5P	3.14	119.34	107.38
2	O	502[A]	FBP	O6P-P2-O5P	3.19	119.54	107.38
2	O	502[A]	FBP	O3P-P1-O2P	4.95	126.22	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	502[A]	FBP	2	0
2	O	502[B]	FBP	1	0
3	O	601	GOL	2	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

6.1 Protein, DNA and RNA chains

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^{th} 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	498/501 (99%)	-0.88	0 100 100	12, 28, 62, 90	0
1	Z	498/501 (99%)	-0.92	1 (0%) 95 94	10, 26, 60, 89	0
All	All	996/1002 (99%)	-0.90	1 (0%) 95 95	10, 27, 61, 90	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Z	325	ASP	2.3

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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^{th} 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
2	FBP	O	502[B]	20/20	0.88	0.26	1.93	49,49,49,49	20
2	FBP	O	502[A]	20/20	0.88	0.26	1.81	49,49,49,49	20

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	Z	601	6/6	0.98	0.13	0.87	10,11,15,34	0
3	GOL	O	601	6/6	0.97	0.14	0.86	10,18,32,41	0

6.5 Other polymers (i)

There are no such residues in this entry.