wwPDB X-ray Structure Validation Summary Report (i)

Jun 4, 2020 – 11:41 pm BST

PDB ID	:	1RUS
Title	:	CRYSTAL STRUCTURE OF THE BINARY COMPLEX OF RIBULOSE-1, 5-BISPHOSPHATE CARBOXYLASE AND ITS PRODUCT, 3-PHOSPHO-D-GLYCERATE
Authors	:	Lundqvist, T.; Schneider, G.
Deposited on	:	1991-10-10
Resolution	:	2.90 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 (i) symbol.

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

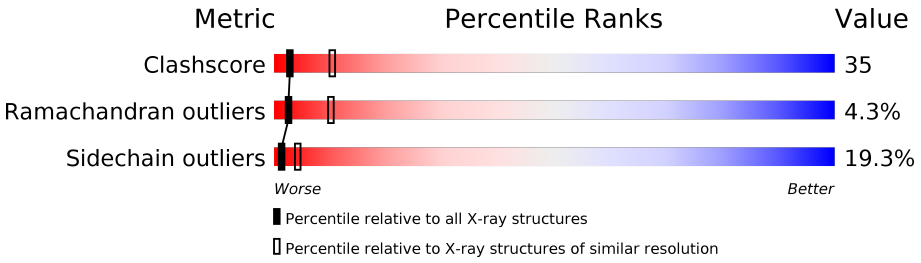
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.90 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	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	490	32% 33% 17% 7% 11%
1	B	490	33% 36% 17% • 11%

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
2	3PG	A	500	-	X	X	-
2	3PG	B	500	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6677 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.

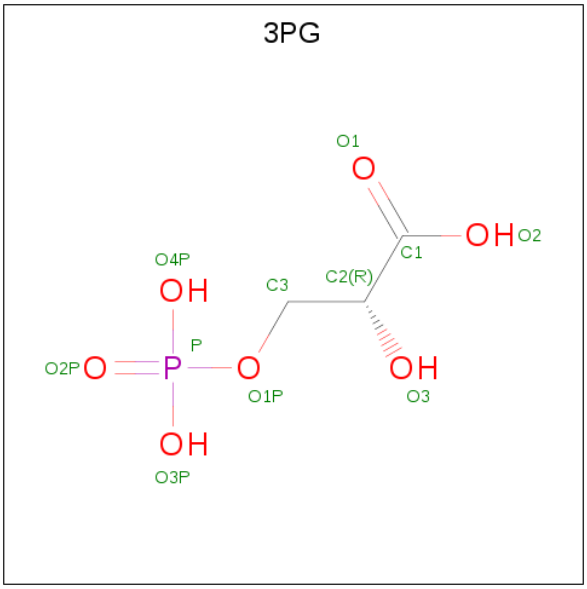
- Molecule 1 is a protein called RUBISCO (RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE(SLASH)OXYGENASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	7	0	0
			3337	2115	589	617	16			
1	B	435	Total	C	N	O	S	10	0	0
			3318	2105	584	613	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	ASP	HIS	CONFLICT	UNP P04718
B	91	ASP	HIS	CONFLICT	UNP P04718

- Molecule 2 is 3-PHOSPHOGLYCERIC ACID (three-letter code: 3PG) (formula: $C_3H_7O_7P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			11	3	7	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			11	3	7	1		

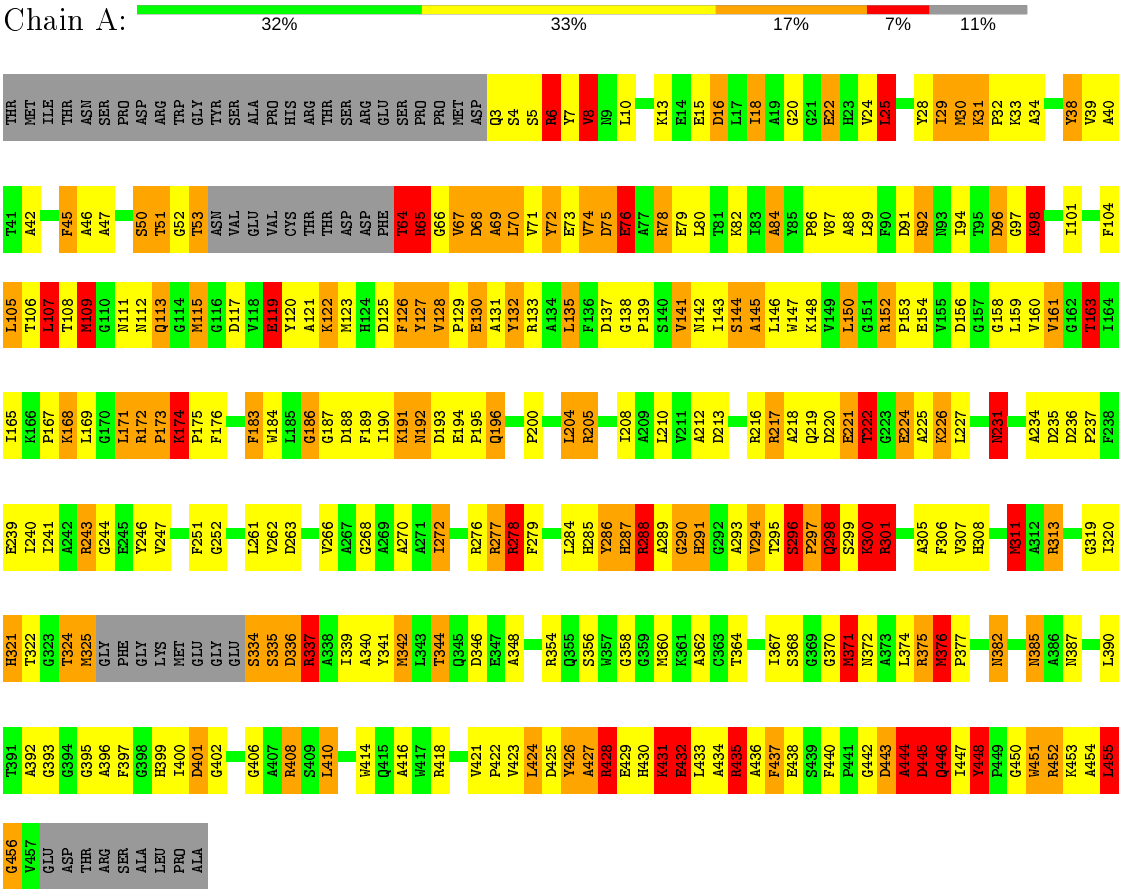
3 Residue-property plots (i)

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

Note EDS was not executed.

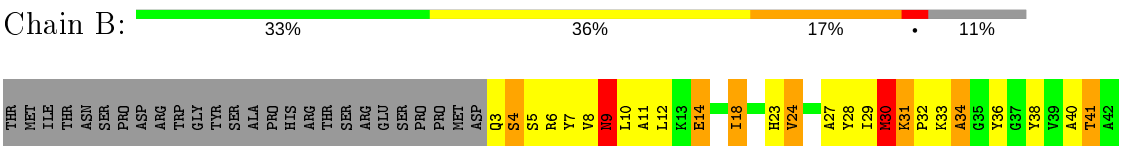
• Molecule 1: RUBISCO (RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE(SLASH)OXYGENASE)

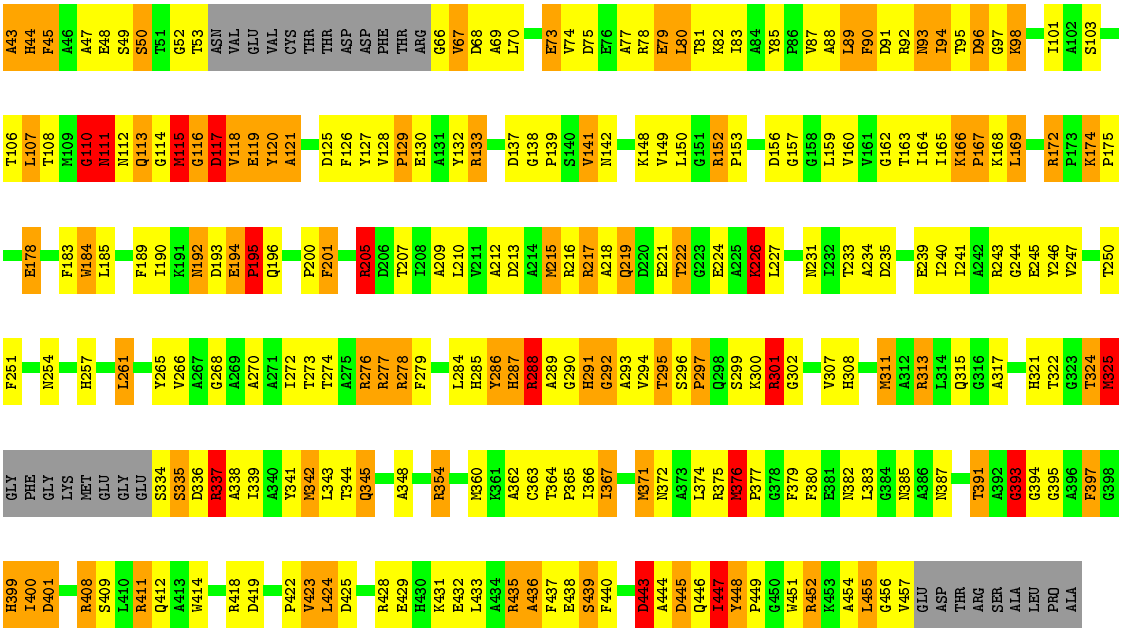
Chain A:



• Molecule 1: RUBISCO (RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE(SLASH)OXYGENASE)

Chain B:




A43 H44 F45 A46 A47 E48 S49 S50 T51 G52 T53 ASN VAL GLU VAL CYS THR THR ASP ASP PHE THR ARG G66 V67 D68 A69 L70 E73 V74 D75 E76 A77 R78 E79 L80 T81 K82 I83 A84 Y85 P86 V87 A88 L89 F90 D91 R92 N93 I94 T95 D96 G97 K98 I101 A102 S103
T106 L107 T108 M109 G110 N111 N112 Q113 G114 M115 G116 D117 V118 E119 Y120 A121 D125 F126 Y127 V128 P129 E130 A131 Y132 R133 D137 G138 P139 S140 V141 N142 K148 V149 L150 G151 R152 P153 D156 G157 G158 L159 V160 V161 G162 T163 I164 I165 K166 P167 K168 L169 R172 P173 K174 P175
E178 F183 W184 L185 F189 I190 K191 N192 D193 E194 P195 Q196 P200 F201 R205 D206 T207 I208 A209 L210 V211 A212 D213 A214 M215 R216 R217 A218 Q219 D220 E221 T222 G223 E224 A225 K226 L227 N231 I232 T233 A234 D235 E239 I240 I241 A242 R243 G244 E245 Y246 V247 T250
F251 N254 H257 L261 Y265 V266 A267 G268 A269 A270 A271 I272 T273 T274 A275 R276 R277 R278 F279 L284 H285 Y286 H287 R288 A289 G290 H291 G292 A293 V294 T295 S296 P297 Q298 S299 K300 R301 G302 V307 H308 M311 A312 R313 L314 Q315 G316 A317 H321 T322 G323 T324 M325
GLY PHE GLY LYS MET GLU GLY GLU S334 S335 D336 R337 A338 I339 A340 Y341 M342 L343 T344 Q345 A348 R354 M360 K361 A362 C363 T364 P365 I366 I367 M371 N372 A373 L374 R375 N376 P377 G378 F379 F380 E381 N382 L383 G384 N385 A386 N387 T391 A392 G393 G394 G395 A396 F397 G398
H399 I400 D401 R408 S409 L410 R411 Q412 A413 W414 R418 D419 P422 V423 L424 D425 R428 E429 H430 K431 E432 L433 A434 R435 A436 F437 E438 S439 F440 D443 A444 D445 Q446 T447 Y448 P449 G450 W451 R452 K453 A454 L455 G456 V457 GLU ASP THR ARG SER ALA LEU PRO ALA

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.50Å 70.60Å 104.10Å 90.00° 92.10° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.203 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6677	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PG

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	A	1.04	2/3417 (0.1%)	2.34	189/4629 (4.1%)
1	B	1.13	6/3398 (0.2%)	2.37	182/4604 (4.0%)
All	All	1.08	8/6815 (0.1%)	2.35	371/9233 (4.0%)

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	B	0	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	14	GLU	CD-OE1	-6.38	1.18	1.25
1	B	195	PRO	N-CD	-5.90	1.39	1.47
1	B	194	GLU	CG-CD	5.88	1.60	1.51
1	B	288	ARG	CD-NE	5.87	1.56	1.46
1	B	288	ARG	NE-CZ	5.71	1.40	1.33

The worst 5 of 371 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	216	ARG	NE-CZ-NH1	31.64	136.12	120.30
1	B	418	ARG	NE-CZ-NH1	29.99	135.30	120.30
1	B	418	ARG	CD-NE-CZ	23.09	155.92	123.60
1	B	429	GLU	CA-CB-CG	22.29	162.44	113.40
1	A	428	ARG	NE-CZ-NH1	21.75	131.17	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	111	ASN	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	A	3337	0	3242	258	2
1	B	3318	0	3220	237	0
2	A	11	0	4	7	0
2	B	11	0	4	5	0
All	All	6677	0	6470	464	2

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 35.

The worst 5 of 464 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:A:196:GLN:O	1:A:231:ASN:ND2	1.67	1.28
1:A:288:ARG:HD3	1:A:291:HIS:NE2	1.52	1.23
1:B:3:GLN:NE2	1:B:44:HIS:HA	1.50	1.22
1:B:321:HIS:HB3	2:B:500:3PG:O4P	1.41	1.17
1:B:335:SER:O	1:B:339:ILE:CG1	1.93	1.14

All (2) 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:A:346:ASP:OD2	1:A:408:ARG:NH2[2_646]	1.89	0.31
1:A:358:GLY:O	1:A:431:LYS:CD[2_646]	2.07	0.13

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	A	431/490 (88%)	374 (87%)	38 (9%)	19 (4%)	2 10
1	B	429/490 (88%)	365 (85%)	46 (11%)	18 (4%)	3 10
All	All	860/980 (88%)	739 (86%)	84 (10%)	37 (4%)	2 10

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	298	GLN
1	A	372	ASN
1	B	4	SER
1	B	5	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	A	330/376 (88%)	254 (77%)	76 (23%)	1 2
1	B	327/376 (87%)	276 (84%)	51 (16%)	2 8
All	All	657/752 (87%)	530 (81%)	127 (19%)	1 4

5 of 127 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	334	SER

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Mol	Chain	Res	Type
1	A	435	ARG
1	B	400	ILE
1	A	337	ARG
1	A	376	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	415	GLN
1	B	9	ASN
1	B	315	GLN
1	A	385	ASN
1	B	231	ASN

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)

2 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	3PG	A	500	-	7,10,10	4.60	6 (85%)	10,14,14	3.58	8 (80%)
2	3PG	B	500	-	7,10,10	1.91	2 (28%)	10,14,14	2.07	1 (10%)

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	3PG	A	500	-	-	3/6/10/10	-
2	3PG	B	500	-	-	4/6/10/10	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	3PG	P-O1P	8.17	1.86	1.60
2	A	500	3PG	C3-C2	6.31	1.72	1.50
2	A	500	3PG	O1P-C3	3.78	1.59	1.44
2	A	500	3PG	P-O2P	3.72	1.62	1.50
2	B	500	3PG	P-O2P	3.32	1.61	1.50

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	3PG	P-O1P-C3	5.82	134.32	118.30
2	B	500	3PG	O1P-C3-C2	5.15	122.81	107.94
2	A	500	3PG	O1P-C3-C2	4.65	121.36	107.94
2	A	500	3PG	O3-C2-C1	-3.91	99.88	111.66
2	A	500	3PG	O1P-P-O2P	3.91	117.44	106.47

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	3PG	C1-C2-C3-O1P
2	A	500	3PG	O3-C2-C3-O1P
2	B	500	3PG	C2-C3-O1P-P
2	B	500	3PG	C3-O1P-P-O2P
2	B	500	3PG	C3-O1P-P-O3P

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	3PG	7	0
2	B	500	3PG	5	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.