



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 06:19 PM GMT

PDB ID : 1L5R
Title : Human liver glycogen phosphorylase a complexed with riboflavin, N-Acetyl-beta-D-Glucopyranosylamine and CP-403,700
Authors : Ekstrom, J.L.; Pauly, T.A.; Carty, M.D.; Soeller, W.C.; Culp, J.; Danley, D.E.; Hoover, D.J.; Treadway, J.L.; Gibbs, E.M.; Fletterick, R.J.; Day, Y.S.N.; Myszka, D.G.; Rath, V.L.
Deposited on : 2002-03-07
Resolution : 2.10 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

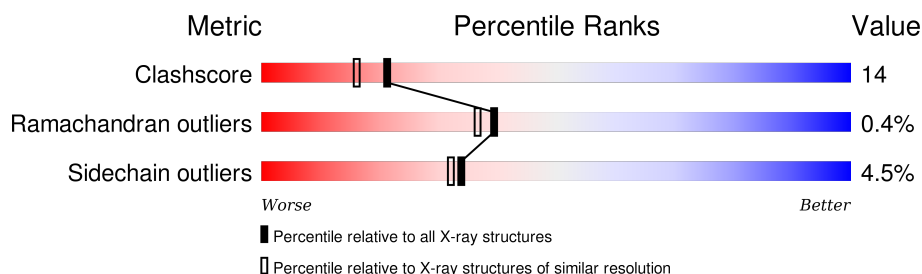
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	847	
1	B	847	

2 Entry composition [i](#)

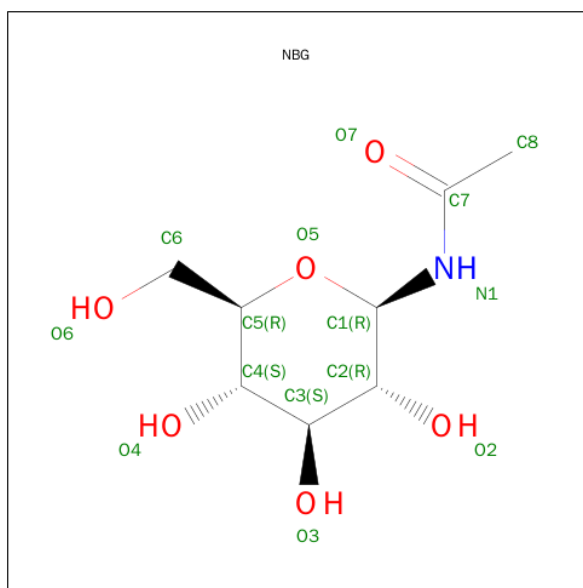
There are 7 unique types of molecules in this entry. The entry contains 13497 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 glycogen phosphorylase, liver form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	790	Total	C	N	O	S	0	0	0
			6417	4125	1089	1174	29			
1	B	791	Total	C	N	O	S	0	0	0
			6423	4128	1090	1176	29			

- Molecule 2 is SUGAR (1-N-ACETYL-BETA-D-GLUCOSAMINE) (three-letter code: NBG) (formula: $C_8H_{15}NO_6$).



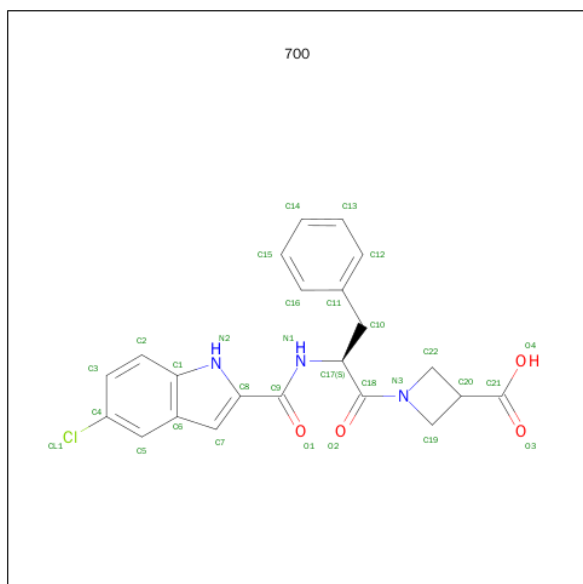
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



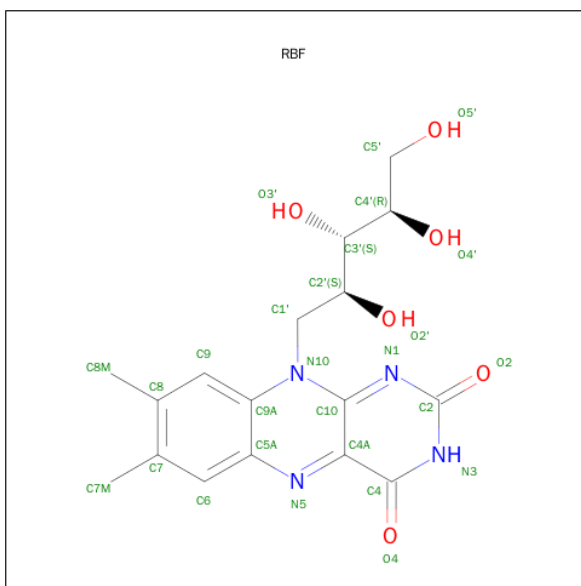
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is [5-CHLORO-1H-INDOL-2-CARBONYL-PHENYLALANINYL]-AZETIDINE-3-CARBOXYLIC ACID (three-letter code: 700) (formula: C₂₂H₂₀ClN₃O₄).



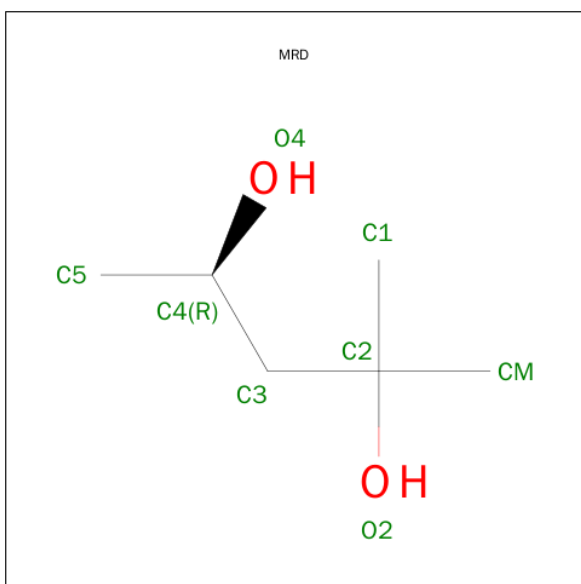
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			30	22	1	3	4		

- Molecule 5 is RIBOFLAVIN (three-letter code: RBF) (formula: $C_{17}H_{20}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			27	17	4	6		

- Molecule 6 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is water.

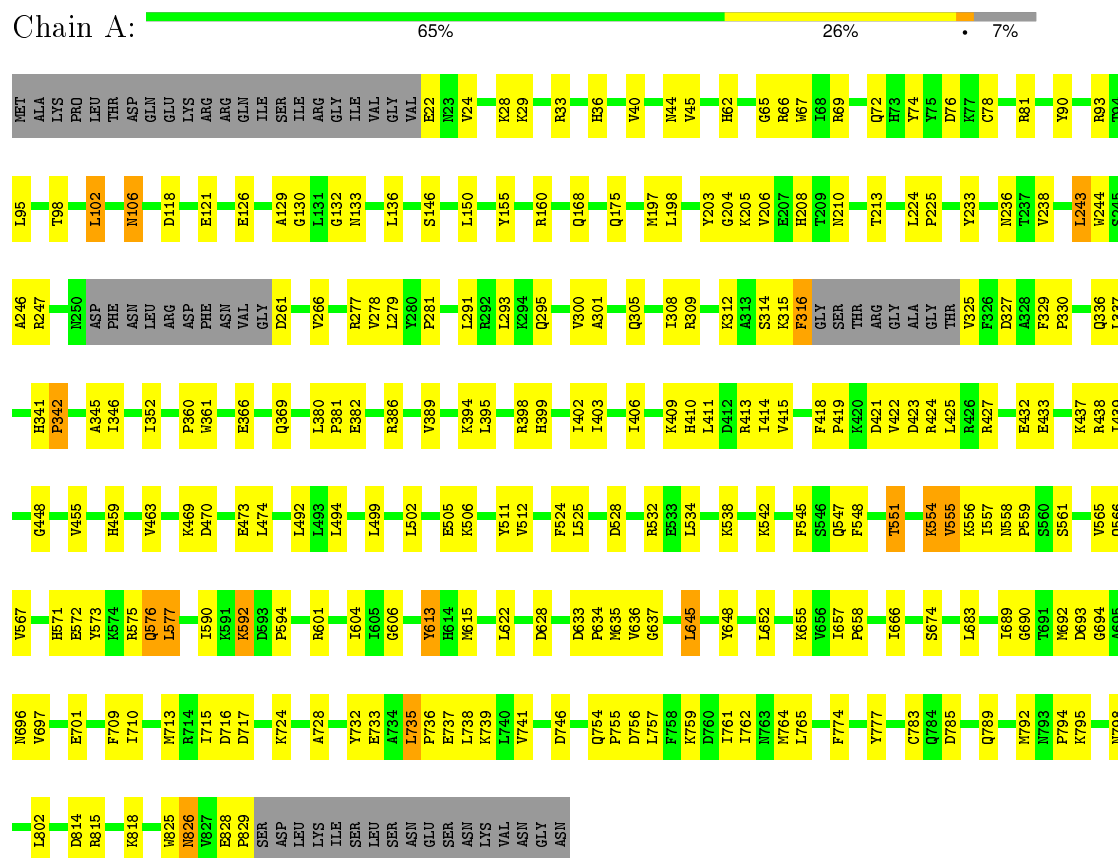
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	307	Total 307	O 307	0	0
7	B	240	Total 240	O 240	0	0

3 Residue-property plots

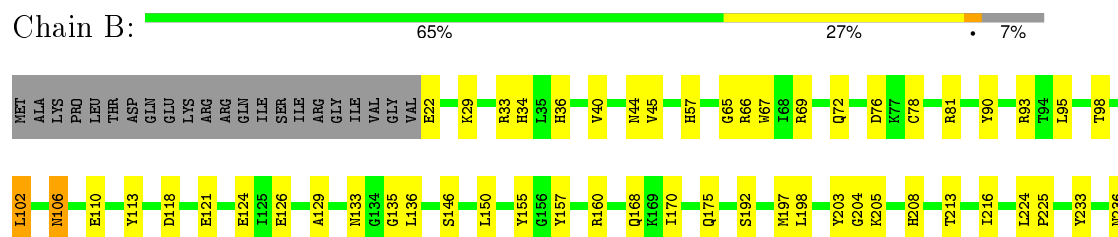
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

- Molecule 1: glycogen phosphorylase, liver form



- Molecule 1: glycogen phosphorylase, liver form



D785	K786	Q789	M792	N793	P794	L802	D814	R815	K818	W825	N826	N827	E828	P829	S830	ASP	LEU	LYS	ILE	SER	LEU	SER	SER	GLU	SER	ASN	LYS	VAL	ASN	GLY	D261	V266	E273	R277	V278	P281	N282	D283	N284	F285	V300	A301	A302	I303	L304	Q305	I308	R309	K310	F311	K312	D313	S314	K315	F316	GLY	SER	THR	ARG	GLY	ALA	GLY	THR	V325
T691	M692	D693	G694	A695	N696	V697	E701	L708	F709	I710	M713	R714	I715	D716	D717	K724	A728	V732	E733	A734	L735	P736	E737	L738	K739	L740	V741	D746	P752	K753	Q754	P755	D756	L757	N758	K759	D760	I761	I762	N763	N764	L765	D769	F774	Y777	C783	Q784																	
V565	Q566	V567	H571	E572	Y573	R574	R575	Q576	L577	K582	D593	P594	V599	P600	I604	I605	G606	Y613	H614	M615	M618	L622	D628	D633	P634	M635	V636	G637	L645	E646	N647	Y648	L652	F544	F545	K655	S656	Q546	F547	F548	T551	I554	V555	K556	I557	N558	S561																	
C445	G448	V455	H459	V463	K469	D470	E473	L474	T487	P488	R489	L492	L493	L494	L499	L502	E505	K506	V512	K513	F524	L525	D528	R532	K538	K542	L543	R544	F545	S546	Q547	F548	T551	I554	V555	K556	I557	N558	S561																									
F329	P330	L243	W244	S245	A246	R247	N250	ASP	PHE	ASN	LEU	ARG	ASP	PHE	ASN	VAL	GLY	D261	V266	E273	R277	V278	P281	N282	D283	N284	F285	K409	H410	L411	D412	R413	I414	V415	F418	P419	K420	D421	V422	D423	R424	L425	K426	R427	E432	E433	K437	R438	I439															

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	124.42Å 124.42Å 124.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	55.61 – 2.10	Depositor
% Data completeness (in resolution range)	95.5 (55.61-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13497	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

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: MRD, RBF, 700, NBG, PLP

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	0.44	0/6561	0.65	1/8873 (0.0%)
1	B	0.43	0/6567	0.65	1/8881 (0.0%)
All	All	0.43	0/13128	0.65	2/17754 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	ALA	N-CA-C	-5.82	95.29	111.00
1	A	129	ALA	N-CA-C	-5.38	96.47	111.00

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	A	6417	0	6412	191	0
1	B	6423	0	6417	183	0
2	A	15	0	15	0	0
3	A	15	0	7	0	0
3	B	15	0	7	0	0
4	A	30	0	18	0	0
5	A	27	0	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	8	0	14	0	0
7	A	307	0	0	28	0
7	B	240	0	0	18	0
All	All	13497	0	12910	368	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 14.

The worst 5 of 368 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:B:110:GLU:HA	7:B:2505:HOH:O	1.65	0.93
1:B:113:TYR:HB3	7:B:2505:HOH:O	1.69	0.93
1:A:213:THR:HB	7:A:2504:HOH:O	1.70	0.91
1:A:710:ILE:HD13	7:A:2205:HOH:O	1.72	0.89
1:A:798:ASN:HB3	7:A:2061:HOH:O	1.72	0.87

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	A	784/847 (93%)	742 (95%)	39 (5%)	3 (0%)	39	37
1	B	785/847 (93%)	742 (94%)	39 (5%)	4 (0%)	34	30
All	All	1569/1694 (93%)	1484 (95%)	78 (5%)	7 (0%)	39	37

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	555	VAL

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Mol	Chain	Res	Type
1	B	555	VAL
1	A	554	LYS
1	B	554	LYS
1	A	342	PRO

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	A	692/740 (94%)	662 (96%)	30 (4%)	35	34
1	B	693/740 (94%)	661 (95%)	32 (5%)	33	31
All	All	1385/1480 (94%)	1323 (96%)	62 (4%)	34	32

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	815	ARG
1	B	102	LEU
1	B	683	LEU
1	B	78	CYS
1	B	243	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	459	HIS
1	A	576	GLN
1	B	369	GLN
1	A	369	GLN
1	B	250	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 ⓘ

6 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	$\# Z > 2$
5	RBF	A	859	-	28,29,29	2.11	10 (35%)	30,43,43	3.18	9 (30%)
3	PLP	A	860	1	15,15,16	2.16	4 (26%)	21,22,23	1.44	4 (19%)
2	NBG	A	861	-	15,15,15	1.31	2 (13%)	21,21,21	1.19	2 (9%)
4	700	A	862	-	26,33,33	1.78	8 (30%)	33,47,47	1.51	6 (18%)
3	PLP	B	860	1	15,15,16	2.22	3 (20%)	21,22,23	1.02	1 (4%)
6	MRD	B	902	-	6,7,7	0.73	0	6,10,10	0.50	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
5	RBF	A	859	-	-	0/14/14/14	0/3/3/3
3	PLP	A	860	1	-	0/6/6/8	0/1/1/1
2	NBG	A	861	-	-	0/5/26/26	0/1/1/1
4	700	A	862	-	-	0/15/32/32	0/4/4/4
3	PLP	B	860	1	-	0/6/6/8	0/1/1/1
6	MRD	B	902	-	-	0/5/5/5	0/0/0/0

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	860	PLP	C4A-C4	-5.59	1.40	1.51
3	A	860	PLP	C4A-C4	-5.14	1.41	1.51
3	B	860	PLP	C3-C2	-4.97	1.37	1.40
3	A	860	PLP	P-O3P	-2.35	1.46	1.54
5	A	859	RBF	C4A-N5	-2.22	1.30	1.33

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	859	RBF	C4-C4A-C10	-7.02	115.45	119.94
5	A	859	RBF	N3-C2-N1	-6.70	116.41	127.69
5	A	859	RBF	C4A-C10-N10	-6.20	116.02	120.52
5	A	859	RBF	O5'-C5'-C4'	-5.66	98.52	111.07
4	A	862	700	C7-C6-C1	-4.40	102.44	106.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.