



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2025 – 01:04 PM EDT

PDB ID : 1GPA
Title : STRUCTURAL MECHANISM FOR GLYCOGEN PHOSPHORYLASE
CONTROL BY PHOSPHORYLATION AND AMP
Authors : Barford, D.; Hu, S.-H.; Johnson, L.N.
Deposited on : 1990-11-13
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

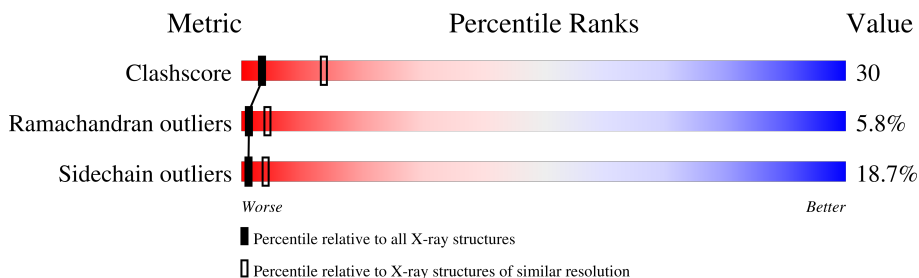
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (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 of 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	842	<div> <div>35%</div> <div>42%</div> <div>16%</div> <div>5%</div> <div>.</div> </div>
1	B	842	<div> <div>37%</div> <div>41%</div> <div>16%</div> <div>.</div> <div>.</div> </div>
1	C	842	<div> <div>35%</div> <div>40%</div> <div>18%</div> <div>6%</div> <div>.</div> </div>
1	D	842	<div> <div>31%</div> <div>42%</div> <div>20%</div> <div>6%</div> <div>.</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27029 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 A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	828	Total	C	N	O	P	S	44	0	0
			6732	4287	1190	1224	1	30			
1	B	827	Total	C	N	O	P	S	24	0	0
			6733	4286	1189	1227	1	30			
1	C	828	Total	C	N	O	P	S	0	0	0
			6732	4287	1190	1224	1	30			
1	D	828	Total	C	N	O	P	S	0	0	0
			6732	4287	1190	1224	1	30			

There are 4 discrepancies between the modelled and reference sequences:

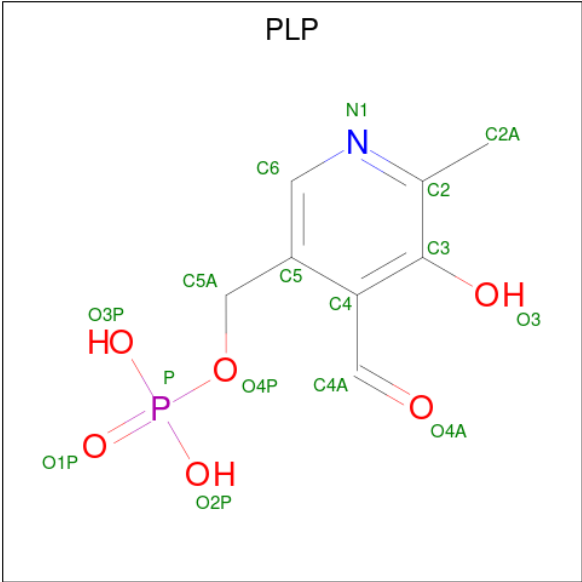
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	conflict	UNP P00489
B	380	ILE	LEU	conflict	UNP P00489
C	380	ILE	LEU	conflict	UNP P00489
D	380	ILE	LEU	conflict	UNP P00489

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



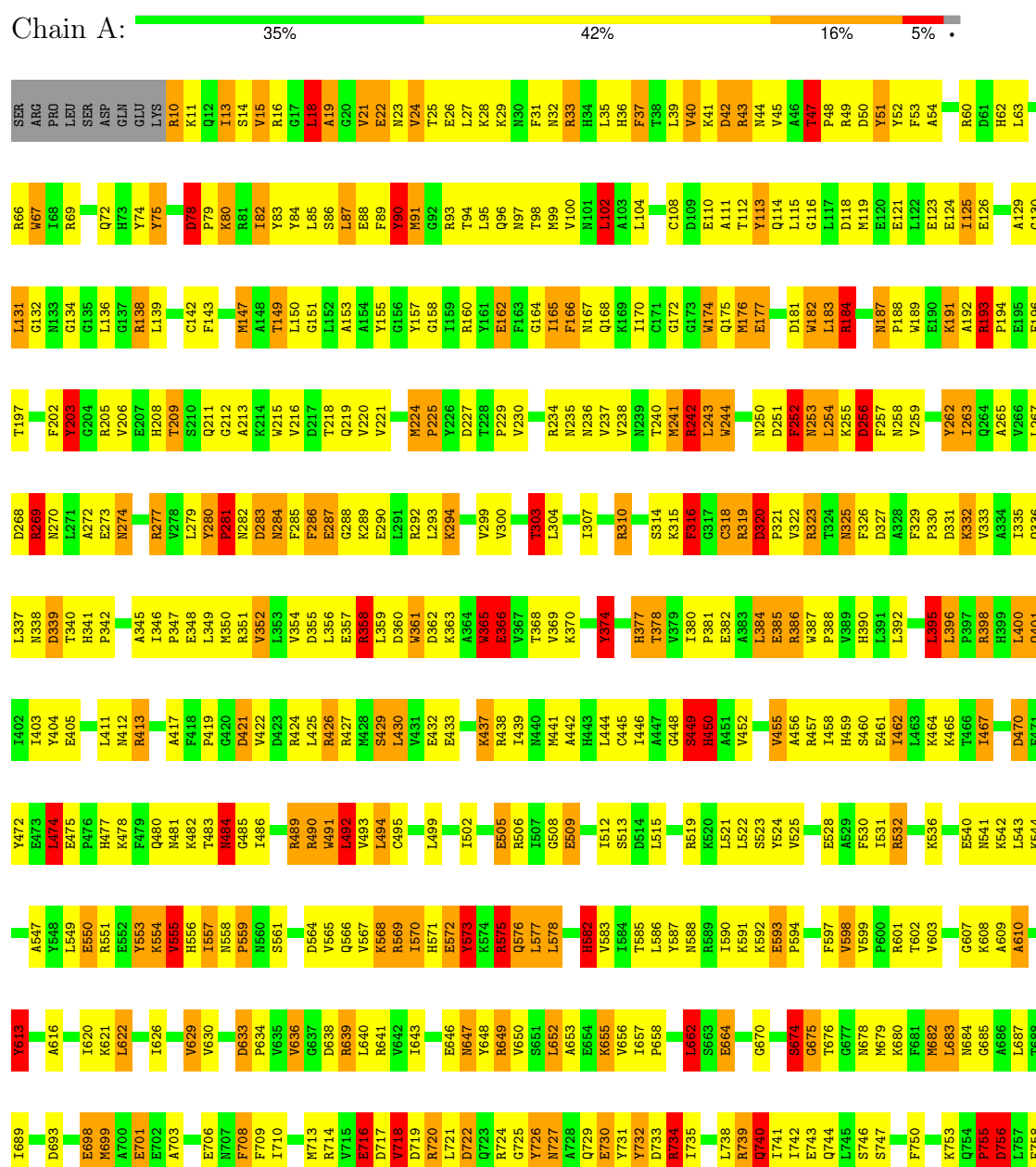
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

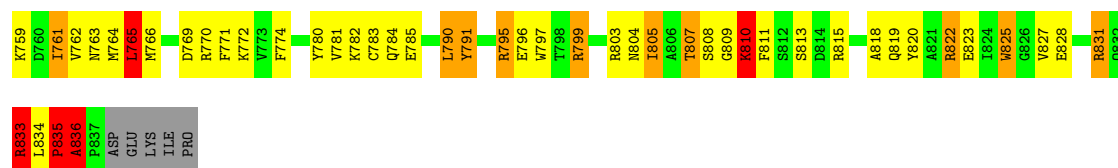
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

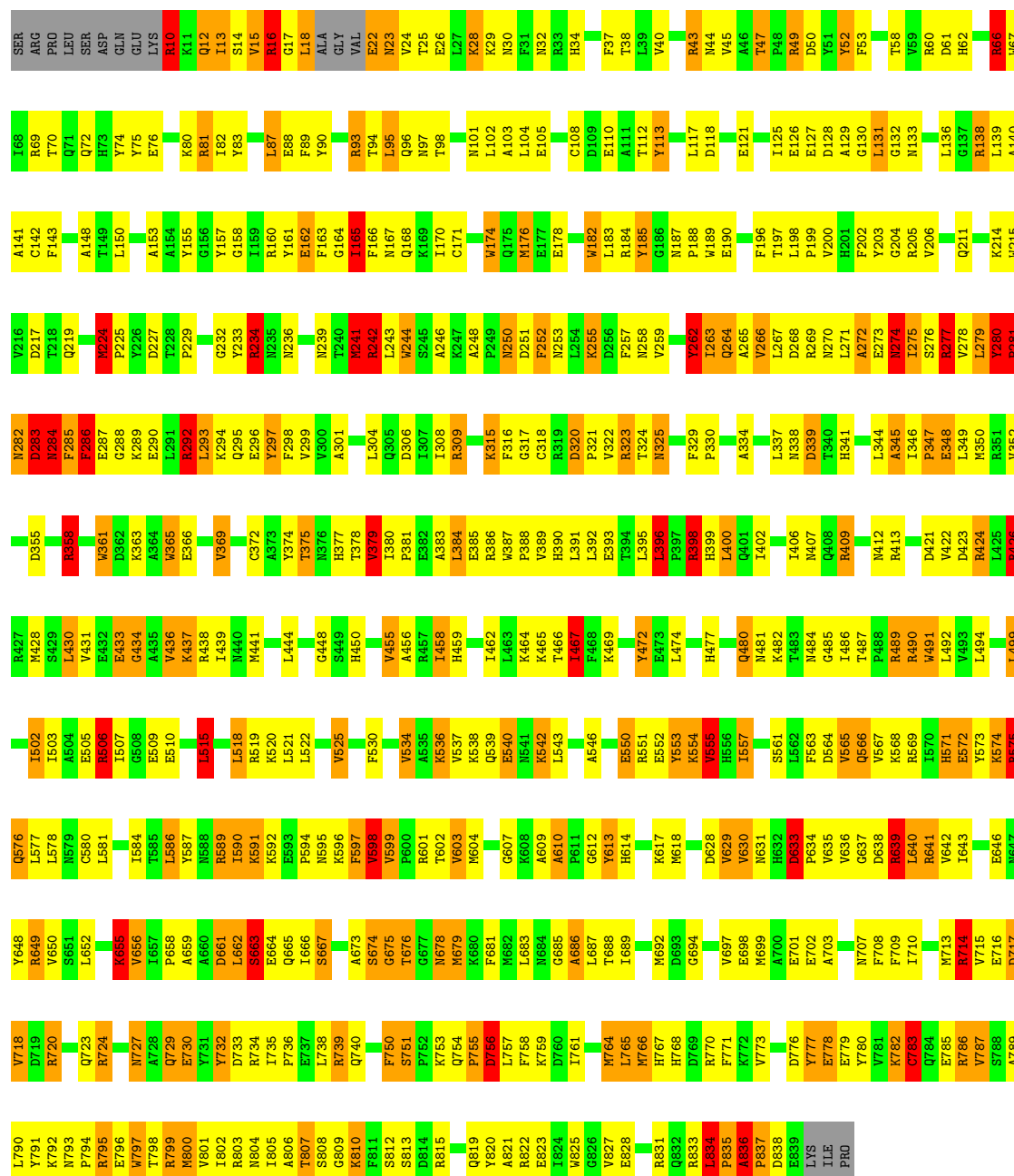
• Molecule 1: GLYCOGEN PHOSPHORYLASE A





• Molecule 1: GLYCOGEN PHOSPHORYLASE A

Chain B: 37% 41% 16%



• Molecule 1: GLYCOGEN PHOSPHORYLASE A

Chain C: 35% 40% 18% 6%



4 Data and refinement statistics

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	119.00Å 190.00Å 88.20Å 90.00° 109.35° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	27029	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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: SEP, SO4, 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	1.12	5/6873 (0.1%)	2.11	267/9300 (2.9%)
1	B	1.07	5/6873 (0.1%)	2.08	259/9298 (2.8%)
1	C	1.11	5/6873 (0.1%)	2.10	264/9300 (2.8%)
1	D	1.09	7/6873 (0.1%)	2.19	266/9300 (2.9%)
All	All	1.10	22/27492 (0.1%)	2.12	1056/37198 (2.8%)

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	A	0	11
1	B	0	11
1	C	0	9
1	D	0	15
All	All	0	46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	24	VAL	C-N	26.58	1.95	1.34
1	A	756	ASP	N-CA	15.44	1.77	1.46
1	A	47	THR	N-CA	-11.92	1.22	1.46
1	D	22	GLU	CD-OE2	6.78	1.33	1.25
1	A	543	LEU	N-CA	6.35	1.59	1.46

The worst 5 of 1056 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	24	VAL	O-C-N	26.50	165.09	122.70
1	D	251	ASP	CA-CB-CG	25.67	169.87	113.40
1	D	24	VAL	CA-C-N	-20.73	71.59	117.20
1	D	575	ARG	NE-CZ-NH1	18.09	129.35	120.30
1	D	281	PRO	O-C-N	17.08	150.02	122.70

There are no chirality outliers.

5 of 46 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	TYR	Sidechain
1	A	203	TYR	Sidechain
1	A	320	ASP	Peptide
1	A	380	ILE	Peptide
1	A	51	TYR	Sidechain

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	A	6732	0	6675	411	1
1	B	6733	0	6667	363	0
1	C	6732	0	6674	391	0
1	D	6732	0	6674	454	1
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	1	0
2	D	10	0	0	0	0
3	A	15	0	7	1	0
3	B	15	0	7	1	0
3	C	15	0	7	1	0
3	D	15	0	6	1	0
All	All	27029	0	26717	1582	1

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 30.

The worst 5 of 1582 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:756:ASP:N	1:A:756:ASP:CA	1.77	1.46
1:C:279:LEU:HD22	1:C:281:PRO:CD	1.62	1.28
1:C:279:LEU:HD22	1:C:281:PRO:CG	1.70	1.22
1:B:283:ASP:OD2	1:B:383:ALA:HB1	1.39	1.21
1:C:283:ASP:OD2	1:C:383:ALA:HB1	1.37	1.19

All (1) 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:21:VAL:O	1:D:370:LYS:NZ[2_646]	1.97	0.23

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	825/842 (98%)	656 (80%)	130 (16%)	39 (5%)	2	7
1	B	822/842 (98%)	674 (82%)	105 (13%)	43 (5%)	1	5
1	C	825/842 (98%)	673 (82%)	100 (12%)	52 (6%)	1	3
1	D	825/842 (98%)	635 (77%)	133 (16%)	57 (7%)	1	2
All	All	3297/3368 (98%)	2638 (80%)	468 (14%)	191 (6%)	1	4

5 of 191 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ALA
1	A	166	PHE
1	A	252	PHE
1	A	256	ASP
1	A	265	ALA

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	714/730 (98%)	585 (82%)	129 (18%)	1	4
1	B	715/730 (98%)	600 (84%)	115 (16%)	2	6
1	C	714/730 (98%)	574 (80%)	140 (20%)	1	3
1	D	714/730 (98%)	563 (79%)	151 (21%)	1	2
All	All	2857/2920 (98%)	2322 (81%)	535 (19%)	1	4

5 of 535 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	400	LEU
1	D	490	ARG
1	D	398	ARG
1	D	727	ASN
1	B	555	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	481	ASN
1	D	377	HIS
1	C	576	GLN
1	D	23	ASN
1	D	450	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](#)

4 non-standard protein/DNA/RNA residues 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
1	SEP	A	14	1	8,9,10	1.20	0	7,12,14	3.04	2 (28%)
1	SEP	C	14	1	8,9,10	1.35	1 (12%)	7,12,14	4.36	2 (28%)
1	SEP	B	14	1	8,9,10	1.12	0	7,12,14	2.68	2 (28%)
1	SEP	D	14	1	8,9,10	1.26	0	7,12,14	14.68	1 (14%)

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
1	SEP	A	14	1	-	5/6/8/10	-
1	SEP	C	14	1	-	3/6/8/10	-
1	SEP	B	14	1	-	6/6/8/10	-
1	SEP	D	14	1	-	5/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	14	SEP	CA-N	-2.24	1.41	1.48

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	14	SEP	OG-CB-CA	-38.78	70.41	108.14
1	C	14	SEP	OG-CB-CA	11.01	118.86	108.14
1	A	14	SEP	OG-CB-CA	7.29	115.24	108.14
1	B	14	SEP	OG-CB-CA	6.21	114.19	108.14
1	A	14	SEP	O2P-P-OG	2.96	114.38	106.67

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	14	SEP	N-CA-CB-OG
1	A	14	SEP	CA-CB-OG-P
1	A	14	SEP	CB-OG-P-O2P
1	A	14	SEP	CB-OG-P-O3P
1	B	14	SEP	C-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	14	SEP	1	0
1	D	14	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	SO4	B	901	-	4,4,4	0.40	0	6,6,6	0.41	0
2	SO4	D	901	-	4,4,4	0.36	0	6,6,6	0.70	0
3	PLP	A	999	1	15,15,16	2.23	4 (26%)	21,22,23	1.54	5 (23%)
3	PLP	D	999	1	15,15,16	1.49	3 (20%)	21,22,23	1.21	2 (9%)
2	SO4	D	902	-	4,4,4	0.61	0	6,6,6	0.31	0
2	SO4	B	902	-	4,4,4	0.54	0	6,6,6	0.36	0
2	SO4	C	902	-	4,4,4	0.50	0	6,6,6	0.43	0
3	PLP	B	999	1	15,15,16	1.33	2 (13%)	21,22,23	1.73	2 (9%)
2	SO4	C	901	-	4,4,4	0.35	0	6,6,6	0.44	0
3	PLP	C	999	1	15,15,16	1.37	1 (6%)	21,22,23	1.22	2 (9%)
2	SO4	A	901	-	4,4,4	0.46	0	6,6,6	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	902	-	4,4,4	0.47	0	6,6,6	0.32	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
3	PLP	C	999	1	-	1/6/6/8	0/1/1/1
3	PLP	B	999	1	-	2/6/6/8	0/1/1/1
3	PLP	A	999	1	-	3/6/6/8	0/1/1/1
3	PLP	D	999	1	-	2/6/6/8	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	PLP	C5-C4	-5.43	1.34	1.40
3	C	999	PLP	C3-C2	-3.85	1.37	1.41
3	A	999	PLP	C3-C2	-3.52	1.37	1.41
3	D	999	PLP	C3-C2	-3.39	1.37	1.41
3	A	999	PLP	C2A-C2	-3.34	1.45	1.50

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	999	PLP	O4P-C5A-C5	5.48	119.62	109.36
3	A	999	PLP	C4A-C4-C5	-4.17	116.64	120.94
3	C	999	PLP	O4P-C5A-C5	3.58	116.08	109.36
3	D	999	PLP	O4P-C5A-C5	2.73	114.47	109.36
3	C	999	PLP	O3P-P-O4P	2.71	113.75	106.67

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	PLP	C5A-O4P-P-O2P
3	A	999	PLP	C5A-O4P-P-O3P
3	B	999	PLP	C5A-O4P-P-O2P
3	B	999	PLP	C5A-O4P-P-O3P
3	D	999	PLP	C5A-O4P-P-O2P

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	PLP	1	0
3	D	999	PLP	1	0
2	C	902	SO4	1	0
3	B	999	PLP	1	0
3	C	999	PLP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	24:VAL	C	25:THR	N	1.95

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.