W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 07:38 PM GMT

PDB ID : 1GLE
Title : CATION PROMOTED ASSOCIATION (CPA) OF A REGULATORY AND TARGET PROTEIN IS CONTROLLED BY PHOSPHORYLATION
Authors : Feese, M.D.; Meadow, N.D.; Roseman, S.; Pettigrew, D.W.; Remington, S.J.
Deposited on : 1994-03-07
Resolution : 2.94 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
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)	:	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 2.94 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	Percentile Ranks	Value
Clashscore		55
Ramachandran outliers		3.6%
Sidechain outliers		24.6%

Worse   *Better*

█ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
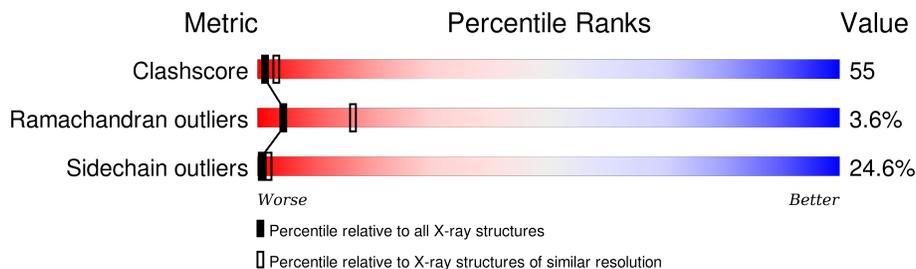
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2308 (2.98-2.90)
Ramachandran outliers	100387	2245 (2.98-2.90)
Sidechain outliers	100360	2247 (2.98-2.90)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	F	168	24% 48% 19% 5% ·
2	G	501	29% 43% 20% 5% ·

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
4	G3H	G	503	X	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4996 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 GLUCOSE-SPECIFIC PROTEIN IIIGlc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	161	Total	C	N	O	S	0	0	0
			1157	741	181	233	2			

- Molecule 2 is a protein called GLYCEROL KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	489	Total	C	N	O	S	0	0	0
			3752	2379	644	710	19			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		

- Molecule 4 is GLYCERALDEHYDE-3-PHOSPHATE (three-letter code: G3H) (formula: $C_3H_7O_6P$).
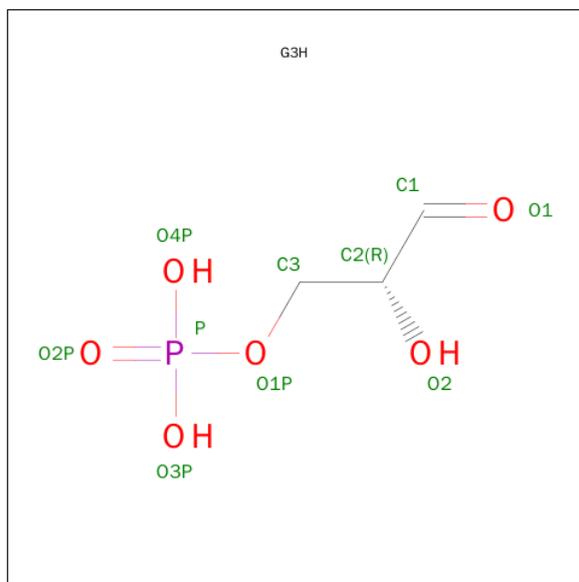
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	G	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
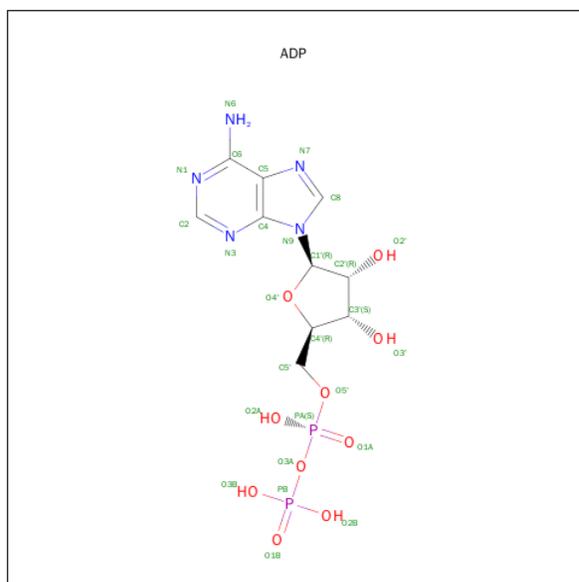
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	7	Total 7	O 7	0	0
6	G	41	Total 41	O 41	0	0

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.

Note EDS was not executed.

• Molecule 1: GLUCOSE-SPECIFIC PROTEIN IIIGlc
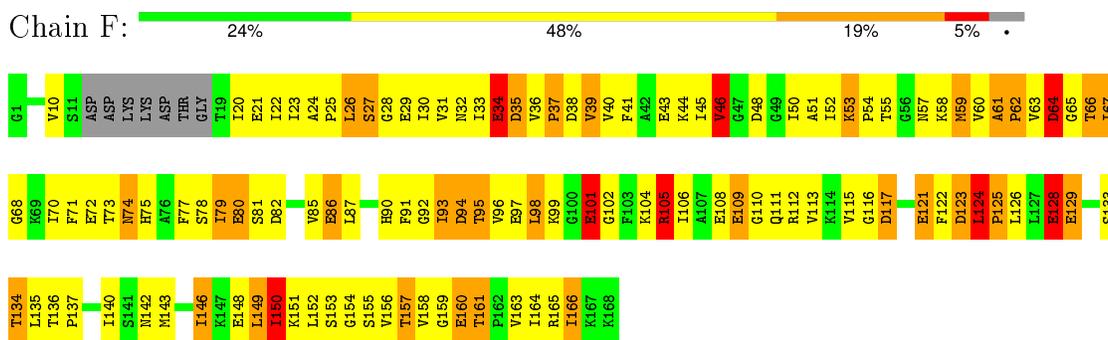
• Molecule 2: GLYCEROL KINASE
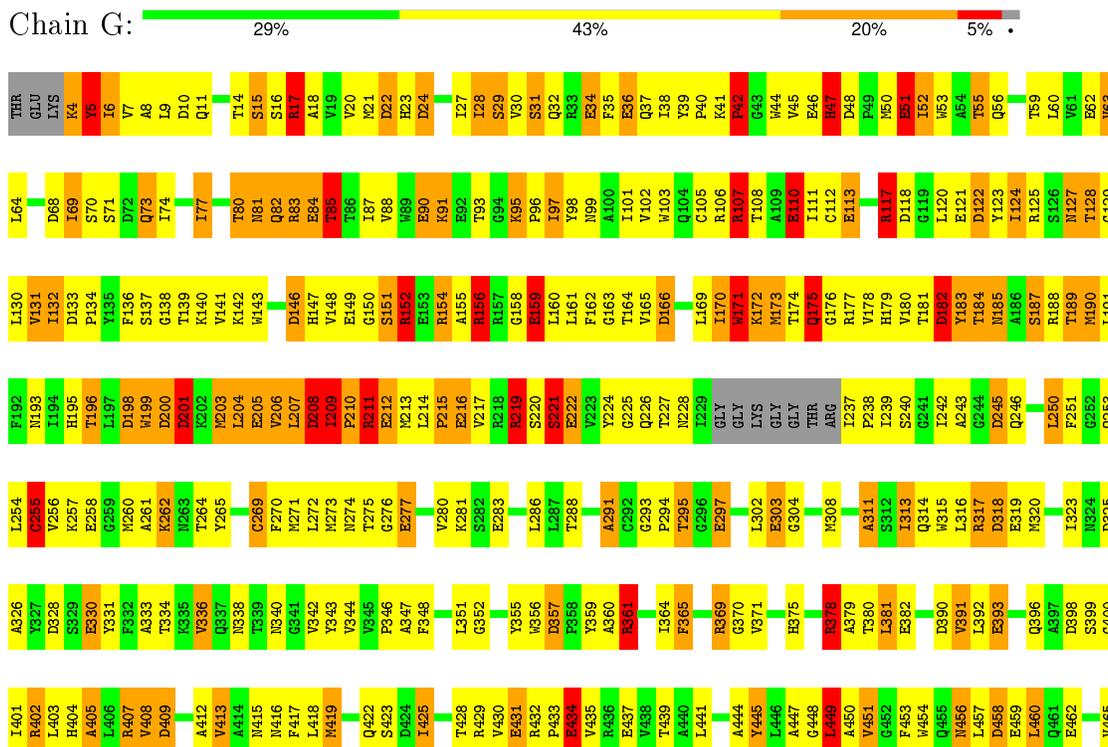
I466 E467 R468 E469 F470 R471 P472 G473 I474 E475 T476 T477 E478 R479 N480 Y481 R482 G485 K488 A489 V490 K491 M494 A495 W496 E497 E498 H499 ASP GLU

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	124.03Å 125.11Å 133.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.80 – 2.94	Depositor
% Data completeness (in resolution range)	(Not available) (21.80-2.94)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.149 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4996	wwPDB-VP
Average B, all atoms (Å^2)	39.0	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: G3H, ZN, ADP

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	F	1.45	15/1172 (1.3%)	1.81	24/1592 (1.5%)
2	G	1.31	31/3831 (0.8%)	1.77	93/5211 (1.8%)
All	All	1.34	46/5003 (0.9%)	1.78	117/6803 (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
2	G	2	0

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	110	GLU	CD-OE2	11.00	1.37	1.25
2	G	393	GLU	CD-OE1	9.82	1.36	1.25
2	G	62	GLU	CD-OE2	9.63	1.36	1.25
1	F	101	GLU	CD-OE2	9.56	1.36	1.25
2	G	216	GLU	CD-OE2	9.46	1.36	1.25

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	209	ILE	C-N-CD	-12.36	93.41	120.60
2	G	369	ARG	NE-CZ-NH1	11.41	126.00	120.30
1	F	124	LEU	C-N-CD	-10.71	97.05	120.60
2	G	361	ARG	NE-CZ-NH1	10.68	125.64	120.30
1	F	94	ASP	CB-CG-OD2	-10.02	109.29	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	255	CYS	CA
2	G	480	ASN	CA

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	F	1157	0	1133	138	0
2	G	3752	0	3605	392	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	G	10	0	5	5	0
5	G	27	0	12	0	0
6	F	7	0	0	1	0
6	G	41	0	0	5	0
All	All	4996	0	4755	530	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 55.

The worst 5 of 530 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:F:40:VAL:HA	1:F:45:ILE:HD12	1.18	1.10
2:G:7:VAL:HG22	2:G:20:VAL:HG22	1.32	1.09
1:F:30:ILE:HD11	1:F:163:VAL:HG12	1.38	1.03
2:G:152:ARG:HH21	2:G:208:ASP:HB3	1.32	0.95
1:F:140:ILE:HD13	1:F:149:LEU:HD12	1.46	0.94

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	F	157/168 (94%)	133 (85%)	18 (12%)	6 (4%)	4	15
2	G	485/501 (97%)	410 (84%)	58 (12%)	17 (4%)	4	17
All	All	642/669 (96%)	543 (85%)	76 (12%)	23 (4%)	4	16

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	109	GLU
1	F	124	LEU
2	G	42	PRO
2	G	175	GLN
2	G	255	CYS

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	F	123/145 (85%)	88 (72%)	35 (28%)	0	1
2	G	378/412 (92%)	290 (77%)	88 (23%)	1	2
All	All	501/557 (90%)	378 (75%)	123 (25%)	1	2

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	73	GLN

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Mol	Chain	Res	Type
2	G	122	ASP
2	G	434	GLU
2	G	80	THR
2	G	91	LYS

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

Mol	Chain	Res	Type
2	G	81	ASN
2	G	185	ASN
2	G	404	HIS
2	G	56	GLN
2	G	396	GLN

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	G3H	G	503	-	9,9,9	2.07	2 (22%)	10,12,12	2.08	1 (10%)
5	ADP	G	504	-	22,29,29	0.79	0	27,45,45	2.82	6 (22%)

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	G3H	G	503	-	1/1/2/3	0/6/8/8	0/0/0/0
5	ADP	G	504	-	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	503	G3H	C2-C1	2.69	1.55	1.50
4	G	503	G3H	O1-C1	5.23	1.44	1.19

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	504	ADP	C1'-N9-C4	-9.80	112.16	126.94
4	G	503	G3H	O1-C1-C2	-5.73	110.85	125.35
5	G	504	ADP	O3A-PA-O5'	-4.16	91.90	102.94
5	G	504	ADP	PA-O3A-PB	-3.93	119.48	132.67
5	G	504	ADP	O2'-C2'-C3'	-3.15	101.59	111.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	G	503	G3H	C2

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	503	G3H	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 (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.