



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:36 PM UTC

PDB ID : 3SS4 / pdb_00003ss4
Title : Crystal structure of mouse Glutaminase C, phosphate-bound form
Authors : Ambrosio, A.L.B.; Dias, S.M.G.; Cerione, R.A.
Deposited on : 2011-07-07
Resolution : 2.85 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

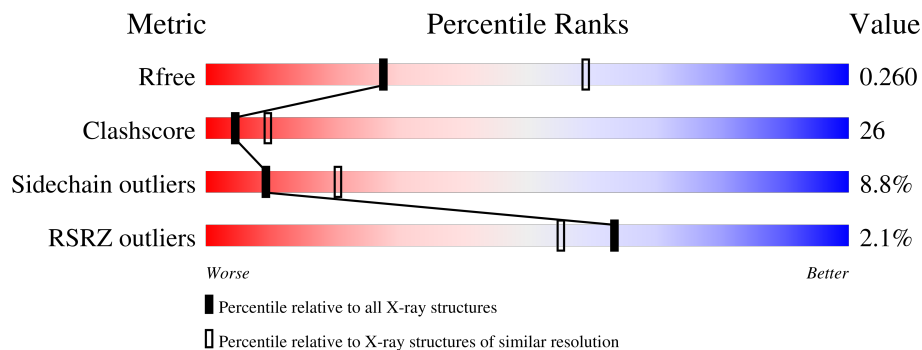
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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))
R_{free}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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 $\leq 5\%$. 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	A	479	 2% 49% 28% • 19%
1	B	479	 2% 49% 29% • 19%
1	C	479	 2% 43% 34% 5% 18%
1	D	479	 2% 43% 34% • 19%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12470 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 Glutaminase C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	390	3051	1952	513	558	28	4	0	0
1	B	388	3036	1941	511	556	28	4	0	0
1	C	394	3083	1970	519	566	28	5	0	0
1	D	387	3025	1930	510	557	28	4	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	125	GLY	-	expression tag	UNP Q69ZX9
A	126	SER	-	expression tag	UNP Q69ZX9
A	127	HIS	-	expression tag	UNP Q69ZX9
B	125	GLY	-	expression tag	UNP Q69ZX9
B	126	SER	-	expression tag	UNP Q69ZX9
B	127	HIS	-	expression tag	UNP Q69ZX9
C	125	GLY	-	expression tag	UNP Q69ZX9
C	126	SER	-	expression tag	UNP Q69ZX9
C	127	HIS	-	expression tag	UNP Q69ZX9
D	125	GLY	-	expression tag	UNP Q69ZX9
D	126	SER	-	expression tag	UNP Q69ZX9
D	127	HIS	-	expression tag	UNP Q69ZX9

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



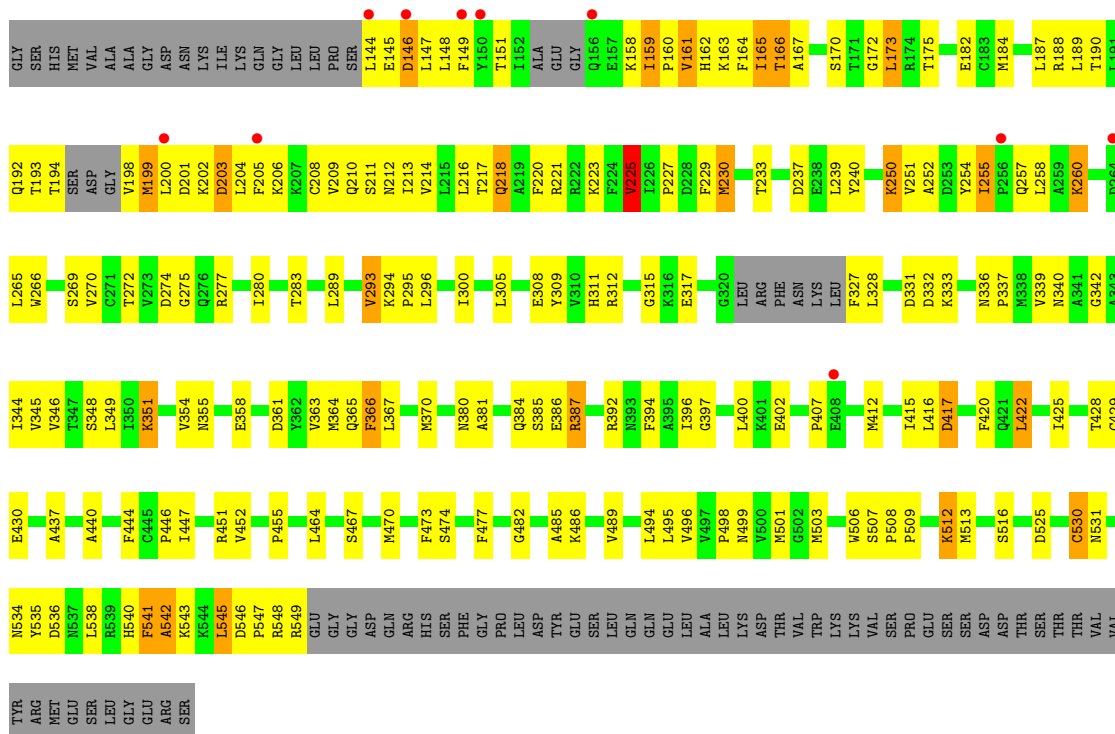
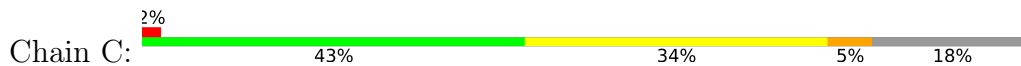
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0

- Molecule 3 is water.

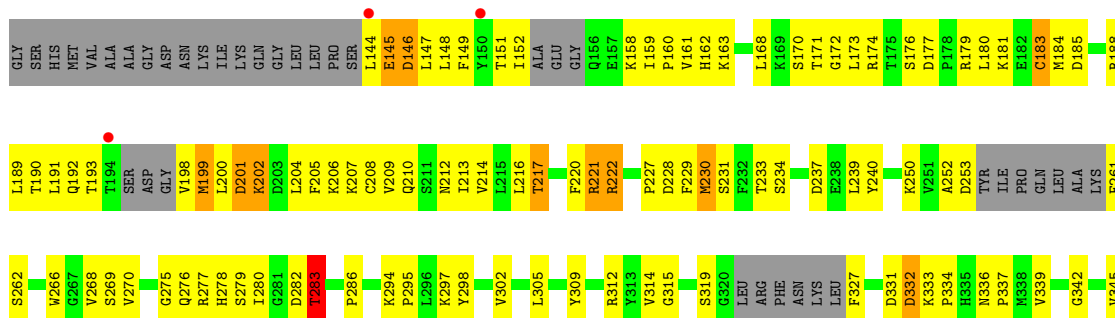
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	63	Total O 63 63	0	0
3	B	71	Total O 71 71	0	0
3	C	53	Total O 53 53	0	0
3	D	68	Total O 68 68	0	0

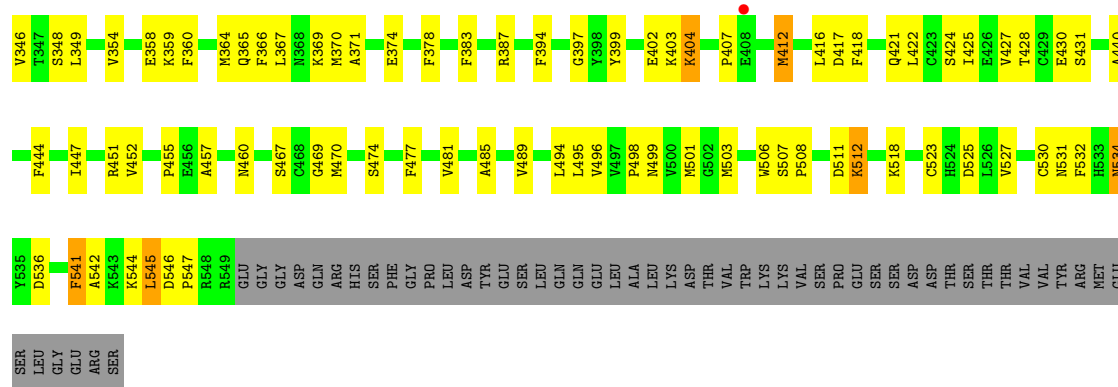


● Molecule 1: Glutaminase C



● Molecule 1: Glutaminase C





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.72Å 136.28Å 176.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 2.85 19.91 – 2.85	Depositor EDS
% Data completeness (in resolution range)	93.3 (19.91-2.85) 92.8 (19.91-2.85)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.85Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.227 , 0.270 (Not available) , 0.260	Depositor DCC
R_{free} test set	2640 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtrriage
Anisotropy	0.321	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12470	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.35 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.9224e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: PO4

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	0.76	3/3118 (0.1%)	0.83	8/4205 (0.2%)
1	B	0.74	2/3101 (0.1%)	0.82	0/4179
1	C	0.78	1/3150 (0.0%)	0.87	7/4249 (0.2%)
1	D	0.75	1/3089 (0.0%)	0.82	1/4164 (0.0%)
All	All	0.76	7/12458 (0.1%)	0.84	16/16797 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	225	VAL	CA-CB	-6.38	1.47	1.54
1	A	199	MET	C-N	-6.37	1.24	1.33
1	B	159	ILE	CA-CB	-5.74	1.46	1.54
1	C	175	THR	CA-CB	-5.50	1.43	1.53
1	A	366	PHE	C-O	-5.33	1.17	1.24

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	159	ILE	N-CA-C	11.84	120.27	107.60
1	C	331	ASP	N-CA-C	-6.55	104.86	112.92
1	A	200	LEU	O-C-N	-6.16	115.19	123.19
1	D	469	GLY	N-CA-C	5.67	120.97	113.37
1	A	469	GLY	N-CA-C	5.47	119.78	112.77

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	3051	0	3036	159	0
1	B	3036	0	3017	136	0
1	C	3083	0	3066	181	0
1	D	3025	0	3001	168	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	63	0	0	0	0
3	B	71	0	0	0	0
3	C	53	0	0	2	0
3	D	68	0	0	0	0
All	All	12470	0	12120	634	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 26.

The worst 5 of 634 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:200:LEU:HD12	1:A:204:LEU:CD2	1.62	1.28
1:C:148:LEU:HD13	1:C:148:LEU:O	1.41	1.18
1:C:387:ARG:HG2	1:C:387:ARG:HH11	1.01	1.15
1:A:200:LEU:HD12	1:A:204:LEU:HD21	1.19	1.14
1:A:548:ARG:HG3	1:A:548:ARG:HH11	1.08	1.13

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	339/415 (82%)	312 (92%)	27 (8%)	11	24
1	B	337/415 (81%)	305 (90%)	32 (10%)	8	17
1	C	343/415 (83%)	312 (91%)	31 (9%)	9	19
1	D	337/415 (81%)	307 (91%)	30 (9%)	9	20
All	All	1356/1660 (82%)	1236 (91%)	120 (9%)	9	20

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	541	PHE
1	D	327	PHE
1	C	225	VAL
1	D	319	SER
1	D	541	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	373	ASN
1	C	421	GLN
1	D	373	ASN
1	C	540	HIS
1	A	521	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	PO4	A	1	-	4,4,4	0.91	0	6,6,6	0.51	0
2	PO4	D	4	-	4,4,4	0.90	0	6,6,6	0.50	0
2	PO4	C	3	-	4,4,4	0.91	0	6,6,6	0.41	0
2	PO4	B	2	-	4,4,4	0.93	0	6,6,6	0.43	0

There are no bond length outliers.

There are no bond angle outliers.

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](#)

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, 95th 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	A	390/479 (81%)	-0.11	8 (2%) 63 55	26, 40, 75, 88	4 (1%)
1	B	388/479 (81%)	-0.02	10 (2%) 57 48	26, 40, 78, 94	4 (1%)
1	C	394/479 (82%)	-0.01	10 (2%) 58 49	24, 43, 82, 105	4 (1%)
1	D	387/479 (80%)	-0.03	4 (1%) 79 74	24, 41, 77, 95	4 (1%)
All	All	1559/1916 (81%)	-0.04	32 (2%) 63 55	24, 41, 78, 105	16 (1%)

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	257	GLN	4.5
1	C	149	PHE	4.0
1	A	200	LEU	4.0
1	A	144	LEU	3.3
1	C	200	LEU	3.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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. The B-factors column lists the minimum, median, 95th 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	B-factors(\AA^2)	Q<0.9
2	PO4	D	4	5/5	0.90	0.09	43,52,68,84	0
2	PO4	C	3	5/5	0.93	0.07	45,49,58,74	0
2	PO4	B	2	5/5	0.93	0.08	49,50,67,69	0
2	PO4	A	1	5/5	0.94	0.06	40,49,56,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.