



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 20, 2025 – 06:04 pm GMT

PDB ID : 8RP7
Title : Glutaminase subunit of aminodeoxychorismate synthase from Escherichia coli
Authors : Sung, S.; Franziska, J.F.; Schlee, S.; Sterner, R.; Wilmanns, M.
Deposited on : 2024-01-12
Resolution : 2.82 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
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

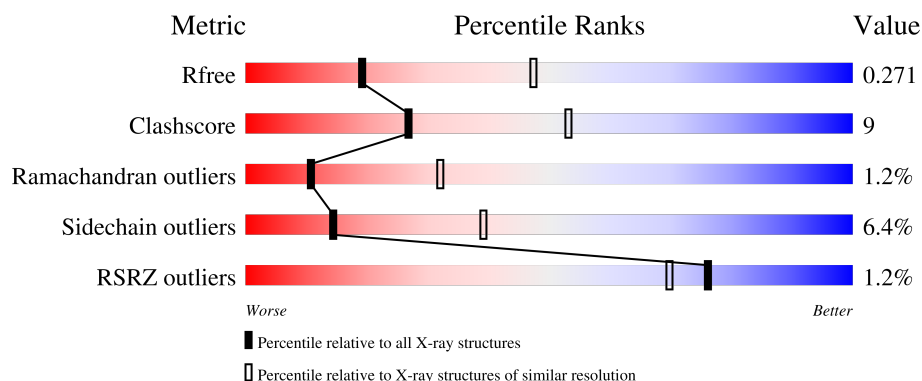
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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}	164625	4293 (2.84-2.80)
Clashscore	180529	4801 (2.84-2.80)
Ramachandran outliers	177936	4739 (2.84-2.80)
Sidechain outliers	177891	4741 (2.84-2.80)
RSRZ outliers	164620	4295 (2.84-2.80)

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	AAA	189	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>..</div> </div> </div>
1	BBB	189	<div> <div></div> <div> <div>72%</div> <div>25%</div> <div>..</div> </div> </div>
1	CCC	189	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>22%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8835 atoms, of which 4409 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 Aminodeoxychorismate synthase component 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	189	Total	C	H	N	O	S	73	0	0
			2938	936	1467	260	267	8			
1	BBB	189	Total	C	H	N	O	S	73	0	0
			2938	936	1467	260	267	8			
1	CCC	189	Total	C	H	N	O	S	75	1	0
			2956	942	1475	263	268	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-1	GLY	-	expression tag	UNP P00903
AAA	0	GLY	-	expression tag	UNP P00903
BBB	-1	GLY	-	expression tag	UNP P00903
BBB	0	GLY	-	expression tag	UNP P00903
CCC	-1	GLY	-	expression tag	UNP P00903
CCC	0	GLY	-	expression tag	UNP P00903

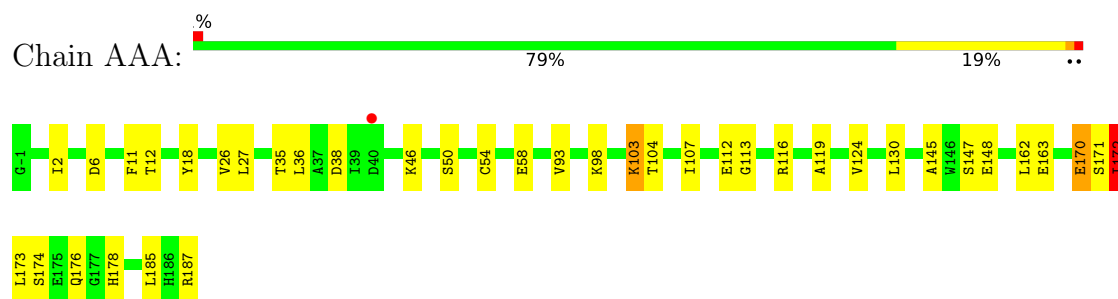
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	BBB	1	Total	O	0	0
			1	1		
2	CCC	2	Total	O	0	0
			2	2		

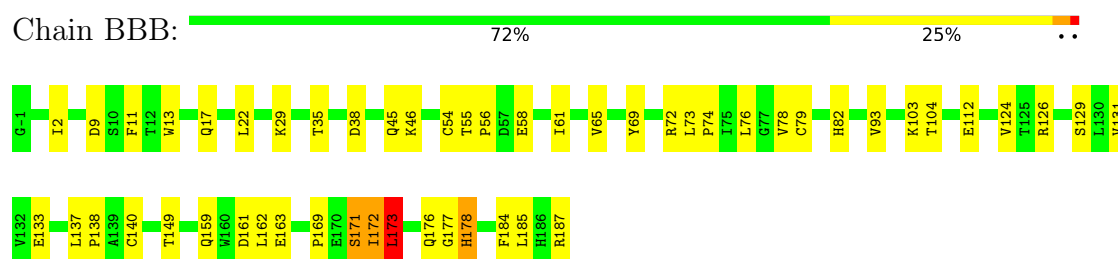
3 Residue-property plots [i](#)

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 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.

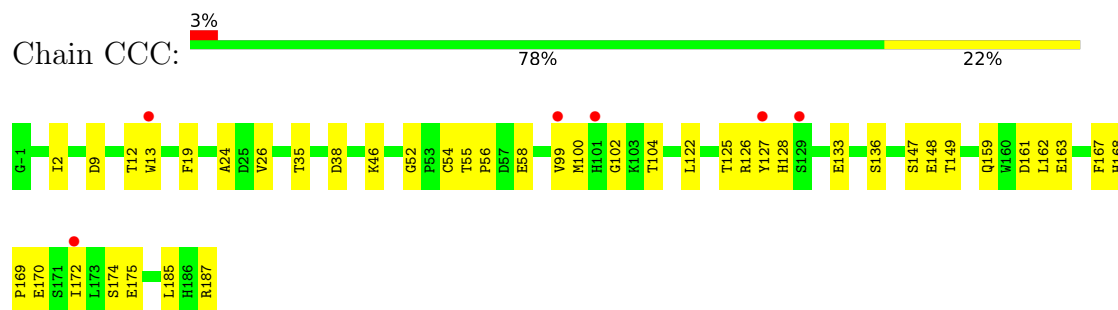
- Molecule 1: Aminodeoxychorismate synthase component 2



- Molecule 1: Aminodeoxychorismate synthase component 2



- Molecule 1: Aminodeoxychorismate synthase component 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	36.78Å 115.58Å 63.54Å 90.00° 101.06° 90.00°	Depositor
Resolution (Å)	42.42 – 2.82 42.42 – 2.82	Depositor EDS
% Data completeness (in resolution range)	98.7 (42.42-2.82) 98.7 (42.42-2.82)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.211 , 0.268 0.213 , 0.271	Depositor DCC
R_{free} test set	651 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 26.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8835	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

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	AAA	0.64	0/1507	0.80	1/2047 (0.0%)
1	BBB	0.63	0/1507	0.76	0/2047
1	CCC	0.64	0/1518	0.74	0/2063
All	All	0.63	0/4532	0.77	1/6157 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	148	GLU	CB-CA-C	5.69	121.78	110.40

There are no chirality outliers.

There are no planarity outliers.

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	AAA	1471	1467	1458	22	0
1	BBB	1471	1467	1458	32	0
1	CCC	1481	1475	1465	30	0
2	BBB	1	0	0	0	0
2	CCC	2	0	0	0	0
All	All	4426	4409	4381	80	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 9.

The worst 5 of 80 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:CCC:13:TRP:CD1	1:CCC:168[B]:HIS:NE2	2.00	1.28
1:CCC:13:TRP:HD1	1:CCC:168[B]:HIS:HE2	1.07	1.01
1:BBB:54:CYS:HB2	1:BBB:58:GLU:HG3	1.49	0.94
1:CCC:13:TRP:HD1	1:CCC:168[B]:HIS:NE2	1.52	0.93
1:AAA:103:LYS:HE3	1:AAA:104:THR:O	1.68	0.93

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	AAA	187/189 (99%)	173 (92%)	11 (6%)	3 (2%)	8	25
1	BBB	187/189 (99%)	176 (94%)	9 (5%)	2 (1%)	12	35
1	CCC	188/189 (100%)	172 (92%)	14 (7%)	2 (1%)	12	35
All	All	562/567 (99%)	521 (93%)	34 (6%)	7 (1%)	11	32

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	171	SER
1	AAA	170	GLU
1	AAA	172	ILE
1	BBB	172	ILE
1	BBB	173	LEU

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	AAA	157/157 (100%)	148 (94%)	9 (6%)	17	44
1	BBB	157/157 (100%)	145 (92%)	12 (8%)	11	31
1	CCC	158/157 (101%)	149 (94%)	9 (6%)	17	44
All	All	472/471 (100%)	442 (94%)	30 (6%)	14	39

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	149	THR
1	CCC	169	PRO
1	BBB	172	ILE
1	CCC	175	GLU
1	CCC	148	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

There are no ligands in this entry.

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	AAA	189/189 (100%)	-0.03	1 (0%) 87 83	28, 46, 82, 113	0
1	BBB	189/189 (100%)	0.03	0 100 100	31, 53, 89, 130	0
1	CCC	189/189 (100%)	0.06	6 (3%) 50 42	21, 53, 96, 153	1 (0%)
All	All	567/567 (100%)	0.02	7 (1%) 76 70	21, 49, 91, 153	1 (0%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	101	HIS	3.0
1	CCC	172	ILE	2.6
1	CCC	13	TRP	2.3
1	CCC	99	VAL	2.2
1	CCC	127	TYR	2.1

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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.