



wwPDB X-ray Structure Validation Summary Report

Mar 20, 2026 – 12:18 AM UTC

PDB ID : 2A7K / pdb_00002a7k
Title : carboxymethylproline synthase (CarB) from pectobacterium carotovora, apo enzyme
Authors : Sleeman, M.C.; Sorensen, J.L.; Batchelar, E.T.; McDonough, M.A.; Schofield, C.J.
Deposited on : 2005-07-05
Resolution : 2.24 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
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

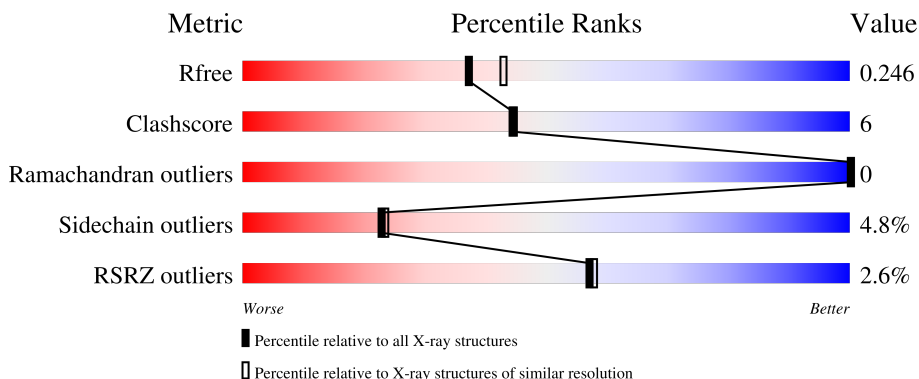
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	250	 3% 77% 15% 8%
1	B	250	 3% 78% 12% 8%
1	C	250	 0% 82% 13% 5%
1	D	250	 2% 74% 16% 9%
1	E	250	 2% 75% 18% 6%

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Mol	Chain	Length	Quality of chain
1	F	250	 76% 14% • 10%
1	G	250	 4% 77% 14% 9%
1	H	250	 3% 76% 15% • 8%
1	I	250	 3% 77% 13% • 9%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 16704 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 CarB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	229	Total 1756	C 1104	N 305	O 337	S 10	0	0	0
1	B	230	Total 1764	C 1108	N 310	O 336	S 10	0	0	0
1	C	238	Total 1833	C 1152	N 320	O 351	S 10	0	0	0
1	D	228	Total 1752	C 1102	N 305	O 335	S 10	0	0	0
1	E	236	Total 1798	C 1134	N 311	O 343	S 10	0	0	0
1	F	226	Total 1745	C 1097	N 303	O 335	S 10	0	0	0
1	G	228	Total 1726	C 1087	N 302	O 327	S 10	0	0	0
1	H	231	Total 1769	C 1114	N 305	O 340	S 10	0	0	0
1	I	228	Total 1755	C 1105	N 305	O 335	S 10	0	0	0

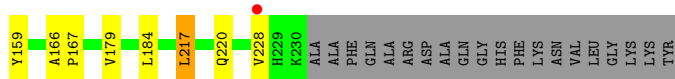
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	82	Total 82	O 82	0	0
2	B	102	Total 102	O 102	0	0
2	C	96	Total 96	O 96	0	0
2	D	117	Total 117	O 117	0	0
2	E	80	Total 80	O 80	0	0

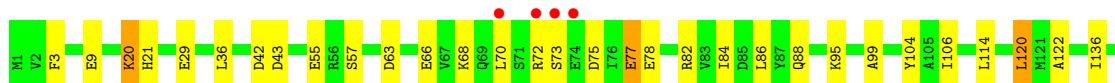
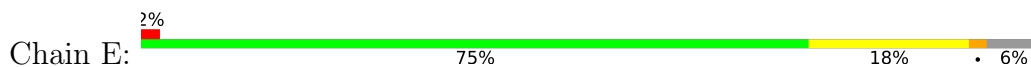
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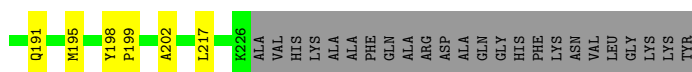
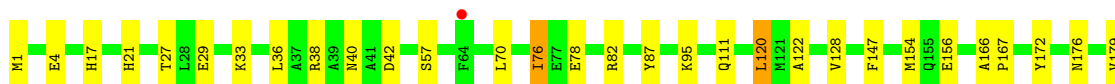
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	83	Total 83	O 83	0	0
2	G	77	Total 77	O 77	0	0
2	H	80	Total 80	O 80	0	0
2	I	89	Total 89	O 89	0	0



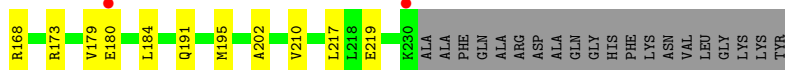
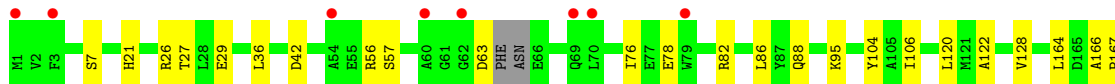
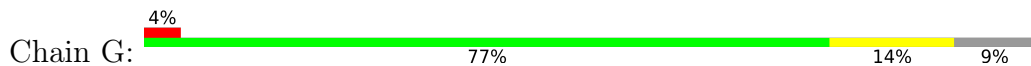
- Molecule 1: CarB



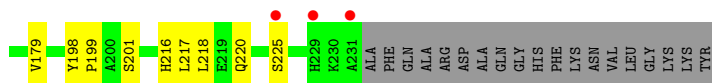
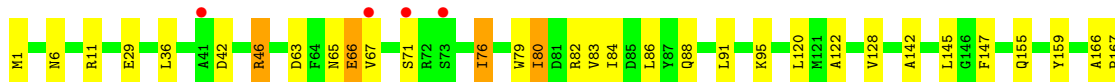
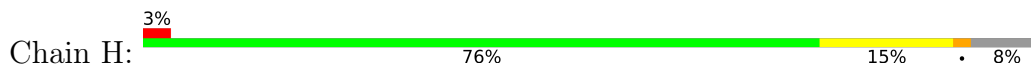
- Molecule 1: CarB



- Molecule 1: CarB



- Molecule 1: CarB



- Molecule 1: CarB



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.21Å 89.86Å 264.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.60 – 2.24 45.60 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.60-2.24) 99.7 (45.60-2.24)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.08 (at 2.24Å)	Xtrriage
Refinement program	REFMAC refmac_5.2.0005	Depositor
R, R_{free}	0.185 , 0.238 0.195 , 0.246	Depositor DCC
R_{free} test set	5084 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtrriage
Anisotropy	0.254	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.019 for k,h,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16704	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.22% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.96	1/1787 (0.1%)	0.96	0/2421
1	B	1.04	3/1796 (0.2%)	1.01	2/2434 (0.1%)
1	C	0.97	1/1867 (0.1%)	0.97	0/2530
1	D	1.03	0/1784	0.99	0/2418
1	E	0.94	1/1832 (0.1%)	0.96	0/2486
1	F	0.91	0/1777	0.94	1/2408 (0.0%)
1	G	0.90	0/1757	0.95	0/2384
1	H	0.93	0/1802	0.98	1/2444 (0.0%)
1	I	0.95	0/1787	1.00	2/2422 (0.1%)
All	All	0.96	6/16189 (0.0%)	0.97	6/21947 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	140	VAL	CA-CB	6.40	1.62	1.54
1	E	99	ALA	CA-CB	-6.14	1.45	1.53
1	A	210	VAL	CA-CB	5.84	1.61	1.54
1	B	94	ASN	CB-CG	5.53	1.65	1.52
1	B	210	VAL	CA-CB	5.46	1.60	1.54

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	228	VAL	N-CA-C	-11.31	99.30	110.72
1	I	76	ILE	CB-CA-C	-6.78	102.99	112.14
1	B	205	ASN	CB-CA-C	-5.66	101.39	110.79
1	B	186	ASP	N-CA-CB	-5.36	102.25	110.12
1	H	80	ILE	CB-CA-C	-5.26	105.23	111.97

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	A	1756	0	1710	22	0
1	B	1764	0	1724	25	0
1	C	1833	0	1793	16	0
1	D	1752	0	1707	29	0
1	E	1798	0	1747	28	0
1	F	1745	0	1710	22	0
1	G	1726	0	1677	15	0
1	H	1769	0	1727	24	0
1	I	1755	0	1716	18	0
2	A	82	0	0	2	0
2	B	102	0	0	3	0
2	C	96	0	0	1	0
2	D	117	0	0	4	0
2	E	80	0	0	0	0
2	F	83	0	0	0	0
2	G	77	0	0	2	0
2	H	80	0	0	4	0
2	I	89	0	0	2	0
All	All	16704	0	15511	187	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 6.

The worst 5 of 187 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:H:46:ARG:HH11	1:H:46:ARG:HG2	1.32	0.94
1:D:17:HIS:HD2	1:D:19:ASN:H	1.14	0.93
1:A:6:ASN:HD21	1:A:11:ARG:HH11	1.17	0.92
1:B:6:ASN:HD21	1:B:11:ARG:HE	1.25	0.84
1:F:4:GLU:OE2	1:F:38:ARG:NH2	2.11	0.84

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	225/250 (90%)	220 (98%)	5 (2%)	0	100	100
1	B	228/250 (91%)	221 (97%)	7 (3%)	0	100	100
1	C	236/250 (94%)	232 (98%)	4 (2%)	0	100	100
1	D	224/250 (90%)	219 (98%)	5 (2%)	0	100	100
1	E	234/250 (94%)	230 (98%)	4 (2%)	0	100	100
1	F	224/250 (90%)	221 (99%)	3 (1%)	0	100	100
1	G	224/250 (90%)	219 (98%)	5 (2%)	0	100	100
1	H	229/250 (92%)	223 (97%)	6 (3%)	0	100	100
1	I	224/250 (90%)	221 (99%)	3 (1%)	0	100	100
All	All	2048/2250 (91%)	2006 (98%)	42 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	185/205 (90%)	179 (97%)	6 (3%)	34	40
1	B	186/205 (91%)	179 (96%)	7 (4%)	29	34
1	C	194/205 (95%)	187 (96%)	7 (4%)	31	36
1	D	186/205 (91%)	175 (94%)	11 (6%)	18	16
1	E	188/205 (92%)	178 (95%)	10 (5%)	20	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	187/205 (91%)	182 (97%)	5 (3%)	39	47
1	G	180/205 (88%)	167 (93%)	13 (7%)	13	10
1	H	188/205 (92%)	176 (94%)	12 (6%)	16	14
1	I	187/205 (91%)	177 (95%)	10 (5%)	20	20
All	All	1681/1845 (91%)	1600 (95%)	81 (5%)	23	23

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	191	GLN
1	I	26	ARG
1	H	1	MET
1	H	76	ILE
1	I	86	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	94	ASN
1	I	191	GLN
1	F	111	GLN
1	I	220	GLN
1	I	118	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 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	A	229/250 (91%)	-0.04	8 (3%) 47 46	21, 34, 63, 84	0
1	B	230/250 (92%)	-0.04	8 (3%) 47 46	19, 31, 68, 92	0
1	C	238/250 (95%)	-0.13	2 (0%) 82 84	16, 34, 52, 69	1 (0%)
1	D	228/250 (91%)	-0.12	5 (2%) 62 64	19, 30, 58, 78	0
1	E	236/250 (94%)	0.01	6 (2%) 58 59	21, 36, 66, 82	0
1	F	226/250 (90%)	-0.04	1 (0%) 88 90	23, 38, 55, 72	0
1	G	228/250 (91%)	0.16	10 (4%) 39 37	21, 39, 65, 96	1 (0%)
1	H	231/250 (92%)	0.17	7 (3%) 52 52	21, 39, 76, 99	0
1	I	228/250 (91%)	-0.05	7 (3%) 51 51	19, 34, 56, 68	0
All	All	2074/2250 (92%)	-0.01	54 (2%) 57 58	16, 35, 63, 99	2 (0%)

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	228	VAL	4.2
1	A	72	ARG	4.2
1	H	231	ALA	3.9
1	G	69	GLN	3.8
1	G	230	LYS	3.8

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.