



wwPDB X-ray Structure Validation Summary Report (i)

Feb 28, 2014 – 06:47 AM GMT

PDB ID : 2A7K
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 validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

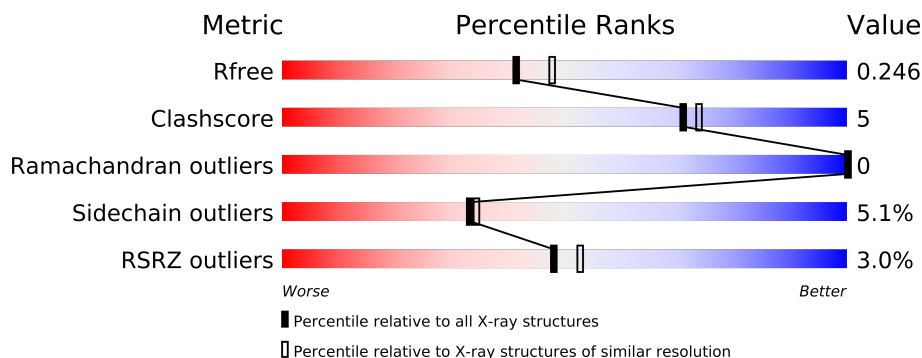
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1112 (2.26-2.22)
Clashscore	79885	1317 (2.26-2.22)
Ramachandran outliers	78287	1282 (2.26-2.22)
Sidechain outliers	78261	1282 (2.26-2.22)
RSRZ outliers	66119	1112 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	250	
1	B	250	
1	C	250	
1	D	250	
1	E	250	
1	F	250	
1	G	250	
1	H	250	
1	I	250	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16704 atoms, of which 0 are hydrogen and 0 are deuterium.

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

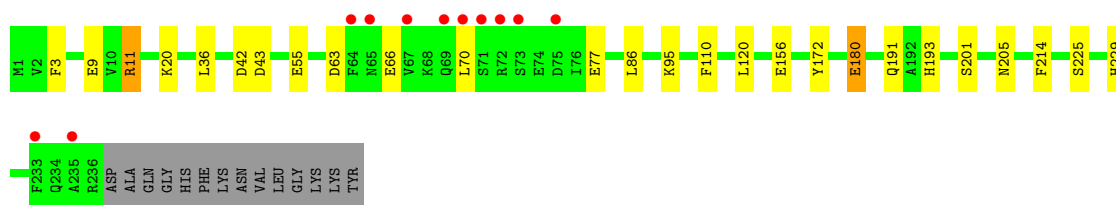
- Molecule 2 is water.

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

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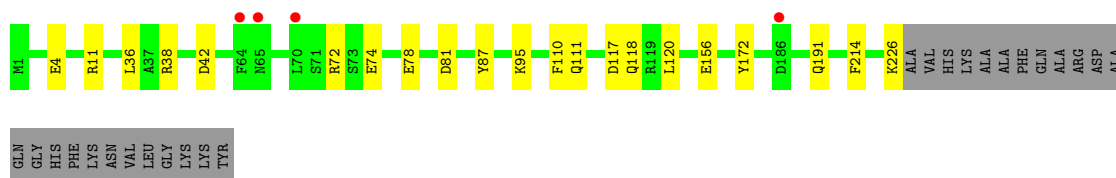
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	83	Total 83	O 83	0	0
2	G	77	Total 77	O 77	0	0
2	H	80	Total 80	O 80	0	0
2	I	89	Total 89	O 89	0	0



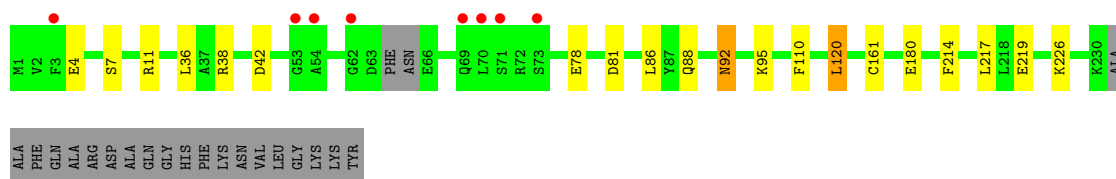
• Molecule 1: CarB

Chain F:



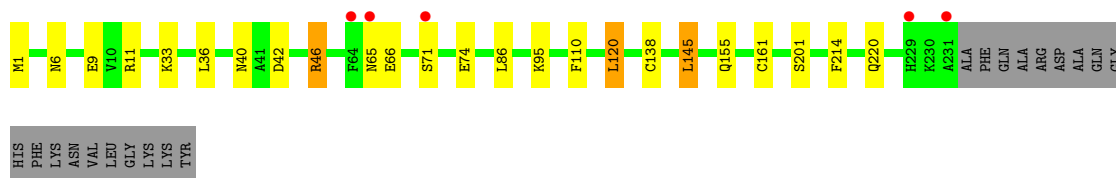
• Molecule 1: CarB

Chain G:



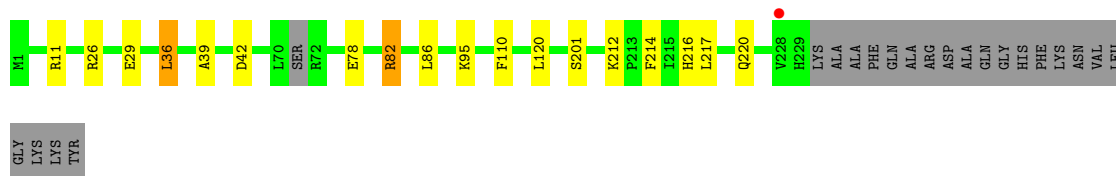
• Molecule 1: CarB

Chain H:



• Molecule 1: CarB

Chain I:



4 Data and refinement statistics

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)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.185 , 0.238 0.197 , 0.246	Depositor DCC
R_{free} test set	5084 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 38.1	EDS
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 100451 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16704	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage'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.

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	A	0.74	1/1787 (0.1%)	0.83	7/2421 (0.3%)
1	B	0.78	1/1796 (0.1%)	0.83	5/2434 (0.2%)
1	C	0.76	0/1867	0.83	3/2530 (0.1%)
1	D	0.83	0/1784	0.87	6/2418 (0.2%)
1	E	0.72	0/1832	0.78	2/2486 (0.1%)
1	F	0.73	1/1777 (0.1%)	0.76	0/2408
1	G	0.72	2/1757 (0.1%)	0.80	1/2384 (0.0%)
1	H	0.75	2/1802 (0.1%)	0.80	2/2444 (0.1%)
1	I	0.74	0/1787	0.78	2/2422 (0.1%)
All	All	0.75	7/16189 (0.0%)	0.81	28/21947 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	94	ASN	CB-CG	6.45	1.65	1.51
1	G	161	CYS	CB-SG	-6.35	1.71	1.82
1	F	74	GLU	CD-OE2	5.97	1.32	1.25
1	G	92	ASN	CB-CG	5.23	1.63	1.51
1	H	161	CYS	CB-SG	-5.21	1.73	1.81

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	11	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	A	42	ASP	CB-CG-OD1	6.68	124.31	118.30
1	E	11	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	H	120	LEU	CA-CB-CG	6.34	129.87	115.30
1	A	82	ARG	NE-CZ-NH1	6.29	123.45	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1756	0	0	11	0
1	B	1764	0	0	8	0
1	C	1833	0	0	9	0
1	D	1752	0	1	10	0
1	E	1798	0	0	8	0
1	F	1745	0	0	8	0
1	G	1726	0	0	5	0
1	H	1769	0	0	10	0
1	I	1755	0	0	5	0
2	A	82	0	0	3	0
2	B	102	0	0	1	0
2	C	96	0	0	5	0
2	D	117	0	0	3	0
2	E	80	0	0	1	0
2	F	83	0	0	1	0
2	G	77	0	0	1	0
2	H	80	0	0	5	0
2	I	89	0	0	1	0
All	All	16704	0	1	72	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

The worst 5 of 72 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:4:GLU:OE2	1:F:38:ARG:NH2	2.11	0.84
1:A:42:ASP:O	1:A:95:LYS:NZ	2.19	0.75
1:D:68:LYS:NZ	2:D:367:HOH:O	2.23	0.71
1:I:29:GLU:OE2	1:I:82:ARG:NH1	2.27	0.67
1:E:225:SER:O	1:E:229:HIS:CD2	2.49	0.66

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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 ⓘ

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%)	177 (96%)	8 (4%)	40	45
1	B	186/205 (91%)	177 (95%)	9 (5%)	35	38
1	C	194/205 (95%)	186 (96%)	8 (4%)	41	48
1	D	186/205 (91%)	177 (95%)	9 (5%)	35	38
1	E	188/205 (92%)	175 (93%)	13 (7%)	22	19
1	F	187/205 (91%)	181 (97%)	6 (3%)	51	61
1	G	180/205 (88%)	170 (94%)	10 (6%)	30	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	188/205 (92%)	176 (94%)	12 (6%)	25	23
1	I	187/205 (91%)	176 (94%)	11 (6%)	28	27
All	All	1681/1845 (91%)	1595 (95%)	86 (5%)	33	34

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	43	ASP
1	F	78	GLU
1	I	86	LEU
1	E	70	LEU
1	E	110	PHE

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

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.06	11 (4%)	29 31	21, 34, 63, 84	0
1	B	230/250 (92%)	-0.01	13 (5%)	23 26	19, 31, 68, 92	0
1	C	238/250 (95%)	-0.09	1 (0%)	90 93	20, 34, 52, 69	1 (0%)
1	D	228/250 (91%)	-0.13	8 (3%)	42 46	19, 30, 58, 78	0
1	E	236/250 (94%)	-0.04	11 (4%)	30 32	21, 36, 66, 82	0
1	F	226/250 (90%)	-0.16	4 (1%)	65 69	23, 38, 55, 72	0
1	G	228/250 (91%)	0.00	8 (3%)	42 46	21, 39, 65, 96	1 (0%)
1	H	231/250 (92%)	0.06	5 (2%)	59 63	21, 39, 76, 99	0
1	I	228/250 (91%)	-0.19	1 (0%)	90 93	19, 34, 56, 68	0
All	All	2074/2250 (92%)	-0.07	62 (2%)	48 53	19, 35, 63, 99	2 (0%)

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	71	SER	5.8
1	G	70	LEU	5.6
1	A	64	PHE	5.1
1	B	67	VAL	5.1
1	E	70	LEU	5.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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.