



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5Z9A / pdb_00005z9a
Title : Crystal structure of chorismate synthase from *Pseudomonas aeruginosa*
Authors : Iqbal, N.; Chaudhary, A.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2018-02-02
Resolution : 2.79 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

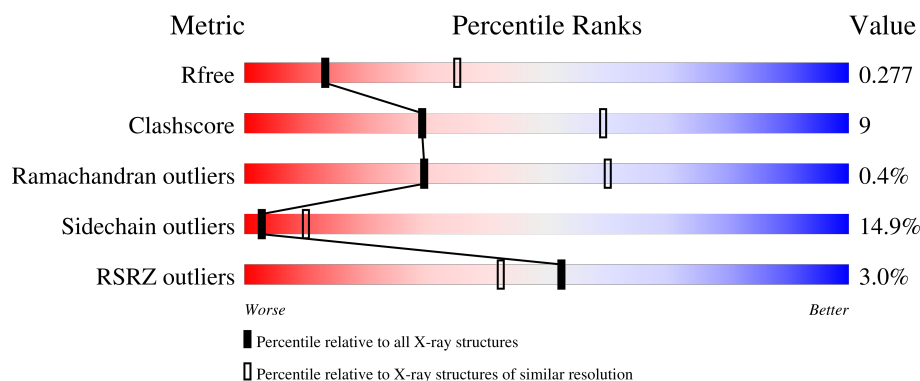
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	A	363	3% 48% 17% • • 32%
1	B	363	% 51% 14% • • 31%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3704 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 Chorismate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			1830	1153	321	348	8			
1	B	250	Total	C	N	O	S	0	0	0
			1854	1166	327	353	8			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total	O	0	0
			9	9		
2	B	11	Total	O	0	0
			11	11		

- Molecule 1: Chorismate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	76.53Å 76.53Å 389.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	66.28 – 2.79 66.28 – 2.79	Depositor EDS
% Data completeness (in resolution range)	96.4 (66.28-2.79) 96.4 (66.28-2.79)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.207 , 0.276 0.212 , 0.277	Depositor DCC
R_{free} test set	865 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	89.5	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 76.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3704	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.84% 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	A	1.15	8/1856 (0.4%)	1.24	14/2508 (0.6%)
1	B	1.22	8/1880 (0.4%)	1.33	21/2540 (0.8%)
All	All	1.18	16/3736 (0.4%)	1.28	35/5048 (0.7%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	77	THR	C-O	-8.81	1.14	1.23
1	A	28	ASP	C-O	-7.76	1.14	1.23
1	B	77	THR	C-O	-7.35	1.14	1.24
1	A	86	ARG	C-O	-6.70	1.15	1.24
1	A	347	ARG	N-CA	-6.58	1.38	1.46
1	B	28	ASP	C-O	-6.44	1.16	1.24
1	A	344	LEU	C-O	-6.43	1.16	1.24
1	A	46	ASP	C-O	-5.91	1.16	1.24
1	B	270	ASN	CG-ND2	-5.83	1.21	1.33
1	A	249	ALA	C-O	-5.76	1.16	1.23
1	A	343	LEU	C-O	-5.73	1.17	1.24
1	B	249	ALA	C-O	-5.71	1.16	1.24
1	B	83	LEU	C-O	5.45	1.30	1.24
1	B	345	ARG	C-O	-5.38	1.17	1.24
1	B	158	GLN	C-O	-5.32	1.17	1.23
1	B	252	ALA	CA-C	5.16	1.59	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	ILE	N-CA-C	-10.30	98.17	111.05
1	A	272	ALA	N-CA-C	-9.78	101.48	113.50
1	B	191	TYR	N-CA-C	-8.70	101.80	111.28
1	B	193	ASP	N-CA-C	-8.34	103.01	113.02
1	A	87	ASN	N-CA-C	7.95	122.41	112.24
1	A	86	ARG	N-CA-C	7.66	121.89	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	GLN	N-CA-C	-7.42	103.85	113.12
1	B	64	GLU	N-CA-C	7.13	119.13	111.36
1	B	251	ILE	N-CA-C	-7.02	103.68	110.42
1	A	28	ASP	O-C-N	-6.98	114.04	122.48
1	A	346	GLN	N-CA-C	6.89	118.87	111.36
1	A	164	ILE	CB-CA-C	-6.46	103.42	110.85
1	B	189	GLU	CA-C-N	6.39	130.03	120.31
1	B	189	GLU	C-N-CA	6.39	130.03	120.31
1	B	87	ASN	N-CA-C	6.32	120.21	111.55
1	B	8	LYS	CG-CD-CE	6.25	125.67	111.30
1	A	41	LEU	CD1-CG-CD2	-6.10	97.39	110.80
1	A	270	ASN	N-CA-C	5.97	118.85	108.76
1	B	189	GLU	N-CA-C	5.77	117.24	111.07
1	A	77	THR	O-C-N	-5.75	114.22	121.74
1	A	2	SER	N-CA-C	5.73	120.27	113.16
1	B	271	ASN	CA-C-N	5.41	131.87	121.54
1	B	271	ASN	C-N-CA	5.41	131.87	121.54
1	B	7	GLY	CA-C-O	-5.40	118.71	122.22
1	B	271	ASN	N-CA-C	-5.39	98.45	107.99
1	B	192	MET	N-CA-C	5.28	117.94	111.82
1	B	252	ALA	N-CA-C	5.27	122.03	110.80
1	A	347	ARG	N-CA-C	-5.17	105.64	111.28
1	A	77	THR	N-CA-C	-5.16	101.73	109.79
1	B	78	GLY	N-CA-C	-5.14	107.89	114.37
1	B	192	MET	CA-CB-CG	5.14	124.38	114.10
1	A	271	ASN	CB-CA-C	-5.12	103.19	111.28
1	B	28	ASP	O-C-N	-5.08	117.25	123.30
1	B	14	THR	CA-CB-CG2	5.08	119.13	110.50
1	B	41	LEU	CD1-CG-CD2	-5.07	99.64	110.80

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	1830	0	1863	34	0
1	B	1854	0	1882	35	0
2	A	9	0	0	0	0
2	B	11	0	0	1	0
All	All	3704	0	3745	64	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.

All (64) 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:B:233:LEU:HD13	1:B:289:LEU:HD21	1.39	1.03
1:B:273:GLY:O	1:B:285:ILE:HA	1.70	0.91
1:A:253:GLN:H	1:B:202:VAL:HG23	1.39	0.88
1:B:45:LEU:O	1:B:48:ARG:HB2	1.81	0.80
1:A:253:GLN:N	1:B:202:VAL:HG23	1.99	0.76
1:A:253:GLN:H	1:B:202:VAL:CG2	2.03	0.71
1:A:328:THR:OG1	1:A:329:PRO:HD3	1.90	0.71
1:A:169:TRP:O	1:A:172:VAL:HG23	1.90	0.70
1:B:49:LYS:O	1:B:49:LYS:HD2	1.91	0.70
1:A:253:GLN:HG3	1:A:253:GLN:O	1.93	0.68
1:A:348:GLY:O	1:A:349:GLN:HB2	1.93	0.68
1:B:271:ASN:ND2	1:B:271:ASN:H	1.92	0.66
1:B:346:GLN:HA	1:B:346:GLN:OE1	1.96	0.66
1:B:348:GLY:O	1:B:349:GLN:HB3	1.95	0.66
1:B:233:LEU:HB3	1:B:289:LEU:CD2	2.29	0.62
1:B:202:VAL:HG22	1:B:203:GLY:N	2.17	0.58
1:B:233:LEU:HD13	1:B:289:LEU:CD2	2.24	0.57
1:B:233:LEU:CD1	1:B:289:LEU:HD21	2.25	0.56
1:A:240:LYS:HG3	1:A:292:LYS:HB3	1.86	0.56
1:A:224:ARG:HD3	1:A:278:GLY:HA3	1.89	0.55
1:B:194:GLN:HA	1:B:194:GLN:OE1	2.07	0.55
1:A:84:LEU:HD22	1:A:85:ILE:N	2.23	0.53
1:B:233:LEU:HB3	1:B:289:LEU:HD22	1.90	0.53
1:A:134:ARG:HB3	1:A:334:MET:HE3	1.90	0.53
1:A:11:THR:OG1	1:A:28:ASP:HB3	2.08	0.53
1:A:206:ILE:HG12	1:A:291:LEU:CD2	2.38	0.53
1:B:34:LEU:HD11	1:B:143:LYS:HG3	1.92	0.52
1:A:7:GLY:C	1:A:11:THR:HG22	2.36	0.51
1:B:224:ARG:HB2	2:B:403:HOH:O	2.09	0.51
1:B:155:TYR:HB2	1:B:180:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:GLN:C	1:B:348:GLY:N	2.70	0.50
1:A:334:MET:HE2	1:A:337:ILE:HD12	1.93	0.50
1:A:197:ARG:HG2	1:A:198:ASP:OD1	2.11	0.50
1:B:202:VAL:CG2	1:B:203:GLY:N	2.74	0.50
1:B:174:GLN:HE21	1:B:174:GLN:HA	1.77	0.49
1:B:346:GLN:C	1:B:348:GLY:H	2.20	0.49
1:A:155:TYR:HB2	1:A:180:PRO:HD3	1.95	0.49
1:A:158:GLN:NE2	1:B:251:ILE:HG13	2.28	0.48
1:B:49:LYS:HD2	1:B:49:LYS:C	2.39	0.47
1:B:346:GLN:O	1:B:348:GLY:N	2.48	0.47
1:A:246:ALA:HB2	1:A:271:ASN:HB3	1.97	0.47
1:A:346:GLN:NE2	1:A:346:GLN:HA	2.29	0.46
1:B:189:GLU:O	1:B:192:MET:HB2	2.15	0.46
1:A:84:LEU:HD22	1:A:85:ILE:H	1.81	0.46
1:B:23:LEU:HD11	1:B:129:ARG:HD2	1.98	0.45
1:A:206:ILE:HG12	1:A:291:LEU:HD21	1.99	0.45
1:A:247:GLY:O	1:A:249:ALA:O	2.35	0.45
1:A:15:ALA:HB3	1:A:24:VAL:HG12	1.99	0.44
1:B:349:GLN:HE21	1:B:349:GLN:HB2	1.69	0.44
1:A:48:ARG:O	1:A:49:LYS:C	2.60	0.44
1:A:348:GLY:O	1:A:349:GLN:CB	2.64	0.44
1:B:164:ILE:CD1	1:B:180:PRO:HD2	2.48	0.44
1:A:236:ILE:HG12	1:A:330:ILE:CD1	2.49	0.43
1:A:250:SER:C	1:A:252:ALA:N	2.74	0.43
1:A:239:VAL:HG22	1:A:291:LEU:HD11	2.01	0.43
1:A:292:LYS:HD2	1:A:293:PRO:O	2.19	0.42
1:B:251:ILE:H	1:B:251:ILE:HG12	1.47	0.42
1:A:34:LEU:HD11	1:A:143:LYS:HG3	2.00	0.42
1:B:330:ILE:O	1:B:334:MET:HG2	2.19	0.42
1:A:253:GLN:HG2	1:B:293:PRO:CG	2.50	0.42
1:A:236:ILE:HG12	1:A:330:ILE:HD12	2.02	0.41
1:B:174:GLN:HE21	1:B:174:GLN:CA	2.33	0.41
1:B:236:ILE:HG12	1:B:330:ILE:CD1	2.51	0.41
1:A:206:ILE:HG12	1:A:291:LEU:HD23	2.02	0.41

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	237/363 (65%)	230 (97%)	7 (3%)	0	100	100
1	B	240/363 (66%)	232 (97%)	6 (2%)	2 (1%)	16	44
All	All	477/726 (66%)	462 (97%)	13 (3%)	2 (0%)	30	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	272	ALA
1	B	347	ARG

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	190/289 (66%)	160 (84%)	30 (16%)	2	9
1	B	192/289 (66%)	165 (86%)	27 (14%)	3	12
All	All	382/578 (66%)	325 (85%)	57 (15%)	3	10

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	8	LYS
1	A	9	LEU
1	A	14	THR

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Mol	Chain	Res	Type
1	A	24	VAL
1	A	35	GLU
1	A	42	GLN
1	A	47	ARG
1	A	49	LYS
1	A	64	GLU
1	A	73	GLU
1	A	79	THR
1	A	84	LEU
1	A	86	ARG
1	A	148	LEU
1	A	192	MET
1	A	195	LEU
1	A	202	VAL
1	A	208	VAL
1	A	213	VAL
1	A	251	ILE
1	A	253	GLN
1	A	271	ASN
1	A	276	LEU
1	A	291	LEU
1	A	292	LYS
1	A	294	THR
1	A	330	ILE
1	A	346	GLN
1	A	347	ARG
1	B	1	MET
1	B	8	LYS
1	B	9	LEU
1	B	24	VAL
1	B	42	GLN
1	B	49	LYS
1	B	73	GLU
1	B	86	ARG
1	B	88	THR
1	B	148	LEU
1	B	164	ILE
1	B	174	GLN
1	B	194	GLN
1	B	200	ASP
1	B	208	VAL
1	B	213	VAL

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Mol	Chain	Res	Type
1	B	251	ILE
1	B	253	GLN
1	B	270	ASN
1	B	271	ASN
1	B	276	LEU
1	B	289	LEU
1	B	291	LEU
1	B	326	ARG
1	B	330	ILE
1	B	346	GLN
1	B	349	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	346	GLN
1	A	349	GLN
1	B	42	GLN
1	B	174	GLN
1	B	271	ASN
1	B	288	HIS
1	B	349	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	247/363 (68%)	0.24	10 (4%) 42 33	70, 97, 146, 175	0
1	B	250/363 (68%)	0.09	5 (2%) 65 56	62, 82, 136, 160	0
All	All	497/726 (68%)	0.17	15 (3%) 52 42	62, 89, 142, 175	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	4.9
1	A	1	MET	4.5
1	A	270	ASN	4.4
1	B	192	MET	3.7
1	B	251	ILE	3.1
1	B	88	THR	3.1
1	A	46	ASP	3.0
1	A	172	VAL	2.7
1	A	252	ALA	2.7
1	A	253	GLN	2.6
1	A	328	THR	2.5
1	B	49	LYS	2.2
1	A	251	ILE	2.2
1	A	49	LYS	2.1
1	A	131	THR	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 oligosaccharides 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.