W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 26, 2014 – 03:47 PM GMT

PDB ID : 1R52
Title : Crystal structure of the bifunctional chorismate synthase from Saccharomyces cerevisiae
Authors : Quevillon-Cheruel, S.; Leulliot, N.; Meyer, P.; Graille, M.; Bremang, M.; Blondeau, K.; Sorel, I.; Poupon, A.; Janin, J.; van Tilbeurgh, H.
Deposited on : 2003-10-09
Resolution : 2.89 Å(reported)

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 2.89 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	Percentile Ranks	Value
Rfree		0.166
Clashscore		15
Ramachandran outliers		2.9%
Sidechain outliers		5.8%
RSRZ outliers		0.4%

Worse   Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
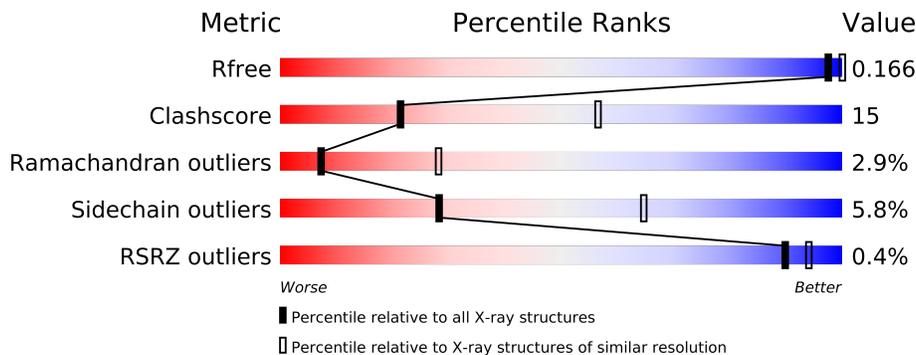
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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	382	
1	B	382	
1	C	382	
1	D	382	

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 8636 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 Chorismate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	45	0	0
			2138	1347	371	405	15			
1	B	282	Total	C	N	O	S	44	0	0
			2130	1340	373	402	15			
1	C	283	Total	C	N	O	S	46	0	0
			2139	1345	374	405	15			
1	D	282	Total	C	N	O	S	41	0	0
			2131	1341	373	402	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	377	HIS	-	EXPRESSION TAG	UNP P28777
A	378	HIS	-	EXPRESSION TAG	UNP P28777
A	379	HIS	-	EXPRESSION TAG	UNP P28777
A	380	HIS	-	EXPRESSION TAG	UNP P28777
A	381	HIS	-	EXPRESSION TAG	UNP P28777
A	382	HIS	-	EXPRESSION TAG	UNP P28777
B	377	HIS	-	EXPRESSION TAG	UNP P28777
B	378	HIS	-	EXPRESSION TAG	UNP P28777
B	379	HIS	-	EXPRESSION TAG	UNP P28777
B	380	HIS	-	EXPRESSION TAG	UNP P28777
B	381	HIS	-	EXPRESSION TAG	UNP P28777
B	382	HIS	-	EXPRESSION TAG	UNP P28777
C	377	HIS	-	EXPRESSION TAG	UNP P28777
C	378	HIS	-	EXPRESSION TAG	UNP P28777
C	379	HIS	-	EXPRESSION TAG	UNP P28777
C	380	HIS	-	EXPRESSION TAG	UNP P28777
C	381	HIS	-	EXPRESSION TAG	UNP P28777
C	382	HIS	-	EXPRESSION TAG	UNP P28777
D	377	HIS	-	EXPRESSION TAG	UNP P28777
D	378	HIS	-	EXPRESSION TAG	UNP P28777
D	379	HIS	-	EXPRESSION TAG	UNP P28777

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Chain	Residue	Modelled	Actual	Comment	Reference
D	380	HIS	-	EXPRESSION TAG	UNP P28777
D	381	HIS	-	EXPRESSION TAG	UNP P28777
D	382	HIS	-	EXPRESSION TAG	UNP P28777

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	25	Total 25	O 25	0	0
2	B	26	Total 26	O 26	0	0
2	C	27	Total 27	O 27	0	0
2	D	20	Total 20	O 20	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Chorismate synthase

Chain A:

• Molecule 1: Chorismate synthase

Chain B:

• Molecule 1: Chorismate synthase

Chain C:

• Molecule 1: Chorismate synthase

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	57.82Å 75.60Å 91.33Å 114.44° 108.43° 89.98°	Depositor
Resolution (Å)	29.75 – 2.89 29.73 – 2.89	Depositor EDS
% Data completeness (in resolution range)	89.6 (29.75-2.89) 89.6 (29.73-2.89)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.52 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.188 , 0.224 0.174 , 0.166	Depositor DCC
R_{free} test set	1344 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	47.8	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 20.9	EDS
Estimated twinning fraction	0.467 for h,-k,-h-l 0.467 for -h,k,-k-l 0.467 for -h,-k,h+k+l	Xtriage
L-test for twinning	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Outliers	0 of 26514 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8636	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities 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	1.15	10/2172 (0.5%)	1.12	16/2927 (0.5%)
1	B	1.13	7/2163 (0.3%)	1.14	14/2914 (0.5%)
1	C	1.18	6/2173 (0.3%)	1.41	20/2928 (0.7%)
1	D	1.12	7/2165 (0.3%)	1.15	17/2917 (0.6%)
All	All	1.15	30/8673 (0.3%)	1.21	67/11686 (0.6%)

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	313	VAL	CB-CG1	14.57	1.83	1.52
1	C	61	ASP	CB-CG	-12.56	1.25	1.51
1	C	286	THR	CB-OG1	11.37	1.66	1.43
1	A	276	TYR	CB-CG	-8.92	1.38	1.51
1	A	61	ASP	CB-CG	-8.44	1.34	1.51

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	276	TYR	CB-CG-CD1	-27.23	104.66	121.00
1	C	276	TYR	CB-CG-CD2	23.81	135.28	121.00
1	C	313	VAL	CA-CB-CG2	-18.45	83.22	110.90
1	C	313	VAL	CA-CB-CG1	-18.19	83.62	110.90
1	C	313	VAL	CG1-CB-CG2	-12.15	91.47	110.90

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	2138	0	2151	80	0
1	B	2130	0	2151	75	0
1	C	2139	0	2161	76	0
1	D	2131	0	2157	81	0
2	A	25	0	0	2	0
2	B	26	0	0	0	0
2	C	27	0	0	0	0
2	D	20	0	0	2	0
All	All	8636	0	8620	256	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 15.

The worst 5 of 256 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:187:MET:CE	1:C:187:MET:SD	2.05	1.44
1:A:187:MET:SD	1:A:187:MET:CE	2.08	1.41
1:D:187:MET:CE	1:D:187:MET:SD	2.08	1.40
1:B:368:ARG:HD3	2:D:385:HOH:O	1.68	0.92
1:A:367:ALA:HB2	1:C:367:ALA:HB2	1.61	0.81

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	273/382 (72%)	249 (91%)	16 (6%)	8 (3%)	7	28
1	B	272/382 (71%)	250 (92%)	14 (5%)	8 (3%)	7	28
1	C	273/382 (72%)	247 (90%)	18 (7%)	8 (3%)	7	28
1	D	272/382 (71%)	248 (91%)	16 (6%)	8 (3%)	7	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1090/1528 (71%)	994 (91%)	64 (6%)	32 (3%)	7 28

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	147	SER
1	A	234	CYS
1	A	339	ASP
1	B	16	SER

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	234/318 (74%)	220 (94%)	14 (6%)	27	63
1	B	233/318 (73%)	219 (94%)	14 (6%)	27	63
1	C	235/318 (74%)	223 (95%)	12 (5%)	33	72
1	D	234/318 (74%)	220 (94%)	14 (6%)	27	63
All	All	936/1272 (74%)	882 (94%)	54 (6%)	28	65

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	313	VAL
1	C	130	ILE
1	D	312	SER
1	B	339	ASP
1	B	369	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	148	ASN
1	B	365	GLN

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Mol	Chain	Res	Type
1	D	262	GLN
1	B	262	GLN
1	B	272	ASN

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(Å²)	Q<0.9
1	A	283/382 (74%)	-0.38	1 (0%)	90 94	10, 32, 57, 67	9 (3%)
1	B	282/382 (73%)	-0.37	0	100 100	9, 32, 57, 67	9 (3%)
1	C	283/382 (74%)	-0.38	1 (0%)	90 94	9, 32, 56, 67	10 (3%)
1	D	282/382 (73%)	-0.35	2 (0%)	84 90	10, 32, 57, 67	8 (2%)
All	All	1130/1528 (73%)	-0.37	4 (0%)	90 94	9, 32, 57, 67	36 (3%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	17	HIS	3.2
1	D	17	HIS	3.1
1	D	19	LYS	2.7
1	C	17	HIS	2.1

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 (i)

There are no such residues in this entry.