



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 02:28 AM UTC

PDB ID : 1Q1L / pdb_00001q1l
Title : Crystal Structure of Chorismate Synthase
Authors : Viola, C.M.; Saridakis, V.; Christendat, D.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2003-07-21
Resolution : 2.05 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

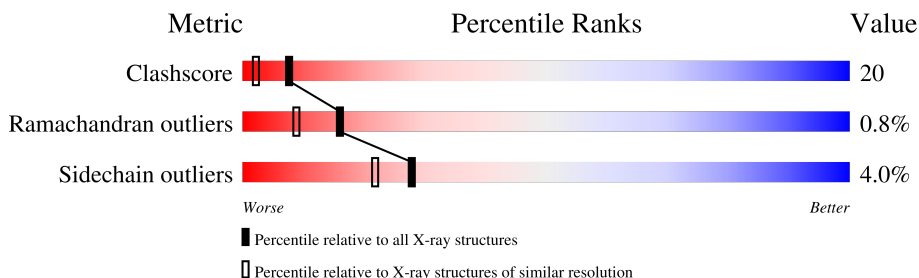
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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))
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	401	57% 24% • 16%
1	B	401	56% 25% • 16%
1	C	401	55% 26% • 17%
1	D	401	57% 24% • 17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11091 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	336	Total	C	N	O	S	Se	0	1	0
			2635	1674	465	489	1	6			
1	B	336	Total	C	N	O	S	Se	0	2	0
			2640	1675	465	493	1	6			
1	C	333	Total	C	N	O	S	Se	0	2	0
			2622	1662	462	491	1	6			
1	D	334	Total	C	N	O	S	Se	0	3	0
			2634	1670	465	492	1	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP O66493
A	-1	SER	-	expression tag	UNP O66493
A	0	HIS	-	expression tag	UNP O66493
A	1	MSE	MET	modified residue	UNP O66493
A	257	MSE	MET	modified residue	UNP O66493
A	258	MSE	MET	modified residue	UNP O66493
A	312	MSE	MET	modified residue	UNP O66493
A	320	MSE	MET	modified residue	UNP O66493
A	363	MSE	MET	modified residue	UNP O66493
A	381	MSE	MET	modified residue	UNP O66493
B	-2	GLY	-	expression tag	UNP O66493
B	-1	SER	-	expression tag	UNP O66493
B	0	HIS	-	expression tag	UNP O66493
B	1	MSE	MET	modified residue	UNP O66493
B	257	MSE	MET	modified residue	UNP O66493
B	258	MSE	MET	modified residue	UNP O66493
B	312	MSE	MET	modified residue	UNP O66493
B	320	MSE	MET	modified residue	UNP O66493
B	363	MSE	MET	modified residue	UNP O66493
B	381	MSE	MET	modified residue	UNP O66493
C	-2	GLY	-	expression tag	UNP O66493

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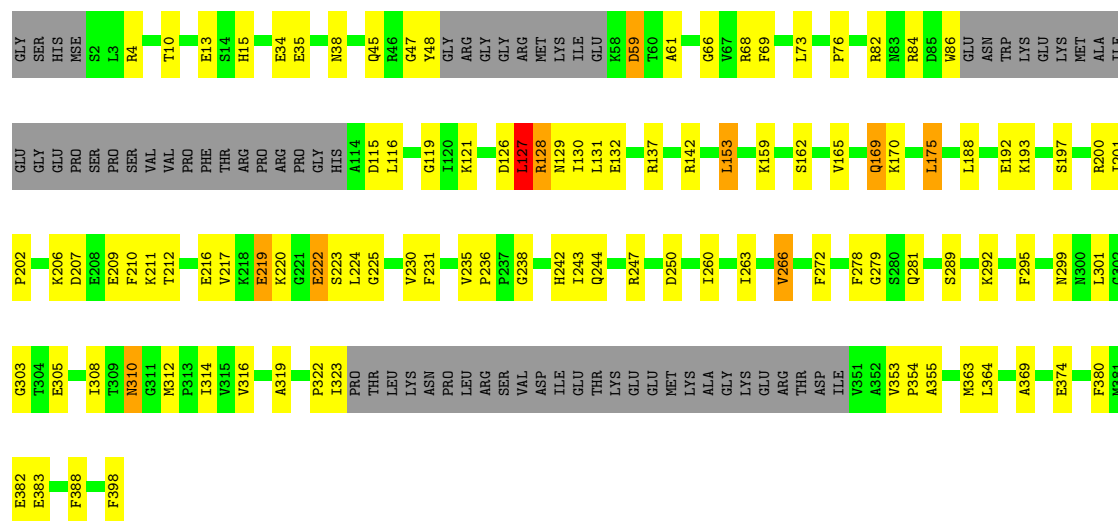
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP O66493
C	0	HIS	-	expression tag	UNP O66493
C	1	MSE	MET	modified residue	UNP O66493
C	257	MSE	MET	modified residue	UNP O66493
C	258	MSE	MET	modified residue	UNP O66493
C	312	MSE	MET	modified residue	UNP O66493
C	320	MSE	MET	modified residue	UNP O66493
C	363	MSE	MET	modified residue	UNP O66493
C	381	MSE	MET	modified residue	UNP O66493
D	-2	GLY	-	expression tag	UNP O66493
D	-1	SER	-	expression tag	UNP O66493
D	0	HIS	-	expression tag	UNP O66493
D	1	MSE	MET	modified residue	UNP O66493
D	257	MSE	MET	modified residue	UNP O66493
D	258	MSE	MET	modified residue	UNP O66493
D	312	MSE	MET	modified residue	UNP O66493
D	320	MSE	MET	modified residue	UNP O66493
D	363	MSE	MET	modified residue	UNP O66493
D	381	MSE	MET	modified residue	UNP O66493

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	157	Total O 157 157	0	0
2	B	137	Total O 137 137	0	0
2	C	127	Total O 127 127	0	0
2	D	139	Total O 139 139	0	0

M363	Q281	P202	LVS	GLY
L372	S289	F203	GLU	SER
D379	K282	E209	LYS	NSE
F380	F295	F210	ALA	S2
E382	N299	K211	ILE	L3
E383	G303	T212	GLY	R4
V392	T304	G211	GLU	Y5
K396	G306	Y213	PRO	L6
S397	K308	I214	SER	R7
F398	T309	V217	PRO	F8
	N310	K220	VAL	L9
	G311	E222	VAL	T10
	M312	S223	PHE	G18
	P313	L224	THR	L22
	I314	G225	ARG	L23
	R317	F231	PRO	E24
	V318	V235	ARG	L30
	A319	P236	PRO	P31
	P322	S241	GLY	E34
	I323	H242	ALA	L41
	PRO	I243	LYS	R44
THR	LYS	Q244	GLU	Q45
LEU	ASN	E245	LYS	Y48
LEU	PRO	D246	LYS	GLY
LEU	ASN	R247	ARG	GLY
ASN	PRO	R248	MET	GLY
PRO	LEU	I249	LYS	ARG
LEU	ARG	D250	LYS	MET
ARG	SER	Q255	ILE	LYS
SER	VAL	A256	ILE	ILE
ASP	ASP	M257	GLU	GLU
ILE	ILE	M258	GLU	GLU
GLU	GLU	S259	GLU	V58
THR	THR	I260	GLU	D59
LYS	GLU	Q261	GLU	T60
GLU	GLU	A262	GLU	I63
GLU	GLU	I263	GLU	L64
MET	LYS	V266	GLU	S65
LYS	ALA	E267	GLY	R68
ALA	GLY	L270	GLY	F69
GLY	GLY	G271	GLY	L73
GLU	GLU	F272	ARG	R82
ARG	THR	E273	THR	N83
THR	ASP	A274	ILE	R84
ASP	ILE	R275	VAL	E87
ILE	VAL	R276	ALA	ASN
VAL	ALA	R277	ALA	THR
ALA	P353	F278	P354	THR
P354	P354	G279	P354	THR
		S280		



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	153.43Å 95.96Å 113.46Å 90.00° 93.04° 90.00°	Depositor
Resolution (Å)	24.63 – 2.05	Depositor
% Data completeness (in resolution range)	81.2 (24.63-2.05)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.209 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11091	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

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	0.80	16/2675 (0.6%)	0.85	3/3579 (0.1%)
1	B	1.06	28/2680 (1.0%)	0.81	1/3588 (0.0%)
1	C	1.02	24/2661 (0.9%)	0.82	1/3560 (0.0%)
1	D	1.20	42/2673 (1.6%)	0.81	6/3577 (0.2%)
All	All	1.03	110/10689 (1.0%)	0.83	11/14304 (0.1%)

The worst 5 of 110 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	266[A]	VAL	CA-CB	20.41	1.83	1.54
1	D	266[B]	VAL	CA-CB	20.41	1.83	1.54
1	B	266[A]	VAL	CA-CB	20.24	1.82	1.54
1	B	266[B]	VAL	CA-CB	20.24	1.82	1.54
1	C	266[A]	VAL	CA-CB	20.10	1.82	1.54

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	GLY	N-CA-C	-10.55	102.13	114.69
1	C	225	GLY	N-CA-C	-5.91	104.66	112.81
1	B	243	ILE	N-CA-C	5.84	118.39	111.09
1	D	225	GLY	N-CA-C	-5.68	104.79	112.57
1	A	243	ILE	N-CA-C	5.64	118.10	111.05

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2635	0	2653	108	0
1	B	2640	0	2648	120	0
1	C	2622	0	2624	117	0
1	D	2634	0	2639	130	0
2	A	157	0	0	1	0
2	B	137	0	0	4	0
2	C	127	0	0	6	0
2	D	139	0	0	5	0
All	All	11091	0	10564	425	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 20.

The worst 5 of 425 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:266[A]:VAL:CA	1:B:266[A]:VAL:CB	1.82	1.56
1:B:266[B]:VAL:CB	1:B:266[B]:VAL:CA	1.82	1.56
1:C:266[A]:VAL:CB	1:C:266[A]:VAL:CA	1.82	1.55
1:C:266[B]:VAL:CB	1:C:266[B]:VAL:CA	1.82	1.55
1:A:159[A]:LYS:CG	1:A:159[A]:LYS:CB	1.84	1.54

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	329/401 (82%)	313 (95%)	12 (4%)	4 (1%)	10 4
1	B	330/401 (82%)	312 (94%)	13 (4%)	5 (2%)	8 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	327/401 (82%)	316 (97%)	10 (3%)	1 (0%)	36	30
1	D	329/401 (82%)	320 (97%)	8 (2%)	1 (0%)	36	30
All	All	1315/1604 (82%)	1261 (96%)	43 (3%)	11 (1%)	16	9

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	PRO
1	B	84	ARG
1	B	324	PRO
1	A	292	LYS
1	B	135	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	274/322 (85%)	261 (95%)	13 (5%)	23	17
1	B	275/322 (85%)	265 (96%)	10 (4%)	31	26
1	C	273/322 (85%)	259 (95%)	14 (5%)	21	14
1	D	274/322 (85%)	266 (97%)	8 (3%)	37	33
All	All	1096/1288 (85%)	1051 (96%)	45 (4%)	28	21

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	165	VAL
1	C	310	ASN
1	C	170	LYS
1	C	250[A]	ASP
1	D	35	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	299	ASN
1	D	299	ASN
1	C	310	ASN
1	D	124	GLN
1	D	310	ASN

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](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.