



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:11 PM GMT

PDB ID : 1NVF
Title : Crystal structure of 3-dehydroquinase synthase (DHQS) in complex with ZN²⁺, ADP and carbaphosphonate
Authors : Nichols, C.E.; Ren, J.; Lamb, H.K.; Hawkins, A.R.; Stammers, D.K.
Deposited on : 2003-02-03
Resolution : 2.80 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

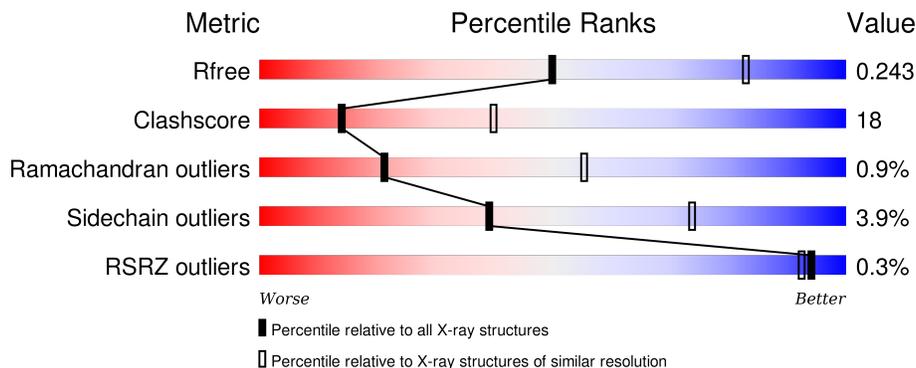
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	393	 61% 35% ..
1	B	393	 62% 34% ..
1	C	393	 67% 31% ..

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9500 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 3-DEHYDROQUINATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	388	2973	1887	516	558	12	0	0	0
1	B	388	2973	1887	516	558	12	0	0	0
1	C	388	2973	1887	516	558	12	0	0	0

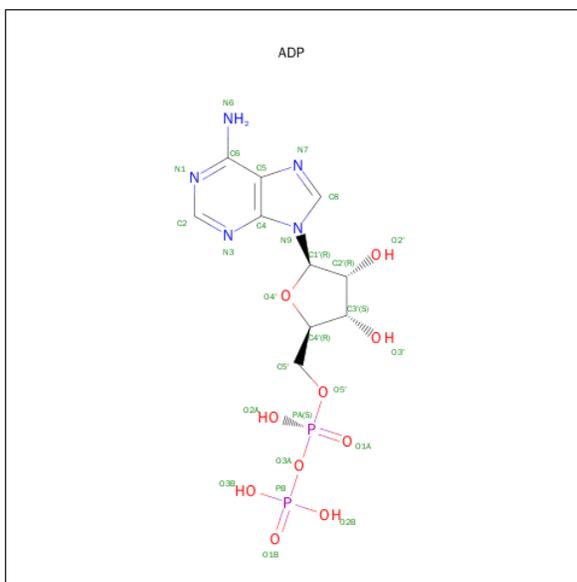
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

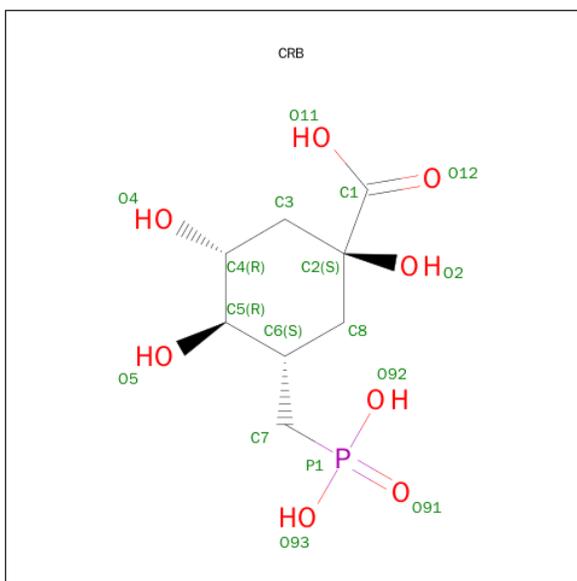
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	C	3	Total	Cl	0	0
			3	3		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is [1R-(1ALPHA,3BETA,4ALPHA,5BETA)]-5-(PHOSPHONOMETHYL)-1,3,4-TRIHYDROXYCYCLOHEXANE-1-CARBOXYLIC ACID (three-letter code: CRB) (formula: C₈H₁₅O₈P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			17	8	8	1		
5	B	1	Total	C	O	P	0	0
			17	8	8	1		
5	C	1	Total	C	O	P	0	0
			17	8	8	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	127	Total	O	0	0
			127	127		
6	B	116	Total	O	0	0
			116	116		
6	C	199	Total	O	0	0
			199	199		

MET	Q99	R222	R335
SER	M100	R223	R336
ASN	V109	E224	L337
P4	I117	V225	T338
I9	L120	E229	A339
L10	T121	R230	N358
G11	F122	R231	K362
R12	G123	E232	K363
I15	F124	G233	K364
I16	V124	T234	S369
M22	Y134	E235	A370
Y25	V135	E237	I371
K28	P138	L238	E376
D29	T139	L239	T377
L30	T140	K240	R378
I31	L141	L244	A379
C34	L142	D257	V381
T43	A143	E258	S380
D44	M144	R259	V381
T45	M145	E260	D386
M46	V146	G261	I387
I47	S147	G262	R388
G48	S148	M268	V389
T52	I149	I273	V390
P63	T153	A291	L391
S54	A154	A292	ALA
F55	I155	V291	PRD
R60	D156	A292	
R61	K161	M295	
R62	I164	V296	
S69	K172	R297	
L73	I173	E298	
M76	Y174	A299	
R77	L180	E300	
P78	M192	I307	
P79	I196	L308	
G80	I196	K309	
E81	E205	G310	
V82	E205	V311	
S83	T208	A312	
K84	E212	R315	
T88	M213	I316	
K89	A214	P326	
I92	L218	D331	
E93	K219	I334	
	A220		
	V221		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	206.50 Å 136.40 Å 40.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.07 – 2.80 39.65 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.7 (26.07-2.80) 94.7 (39.65-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.94 (at 2.81 Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.184 , 0.242 0.185 , 0.243	Depositor DCC
R_{free} test set	1347 reflections (4.89%)	DCC
Wilson B-factor (Å ²)	39.3	Xtrriage
Anisotropy	0.727	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.0	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Outliers	1 of 27531 reflections (0.004%)	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9500	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CRB, ZN, ADP, CL

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	0.40	0/3023	0.63	0/4097
1	B	0.39	0/3023	0.63	0/4097
1	C	0.40	0/3023	0.64	0/4097
All	All	0.40	0/9069	0.63	0/12291

There are no bond length outliers.

There are no bond angle outliers.

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	2973	0	3061	118	0
1	B	2973	0	3061	120	0
1	C	2973	0	3061	100	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	1	0	0	0	0
3	C	3	0	0	0	0
4	A	27	0	12	1	0
4	B	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	27	0	12	0	0
5	A	17	0	11	1	0
5	B	17	0	10	1	0
5	C	17	0	11	0	0
6	A	127	0	0	9	0
6	B	116	0	0	5	0
6	C	199	0	0	16	0
All	All	9500	0	9251	335	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 18.

The worst 5 of 335 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:A:280:ILE:HD11	1:A:351:ASN:HD21	1.41	0.86
1:B:296:VAL:O	1:B:300:GLU:HG3	1.76	0.85
1:C:31:ILE:HD12	1:C:62:ARG:HB3	1.60	0.84
1:C:45:THR:HB	1:C:79:PRO:HD3	1.57	0.84
1:A:334:ILE:O	1:A:338:THR:HG22	1.77	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	386/393 (98%)	358 (93%)	23 (6%)	5 (1%)	15 44
1	B	386/393 (98%)	355 (92%)	26 (7%)	5 (1%)	15 44
1	C	386/393 (98%)	364 (94%)	21 (5%)	1 (0%)	46 79
All	All	1158/1179 (98%)	1077 (93%)	70 (6%)	11 (1%)	21 55

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	TYR
1	B	25	TYR
1	B	214	ALA
1	B	227	PRO
1	A	260	GLU

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	321/326 (98%)	311 (97%)	10 (3%)	47 81
1	B	321/326 (98%)	304 (95%)	17 (5%)	28 61
1	C	321/326 (98%)	310 (97%)	11 (3%)	44 78
All	All	963/978 (98%)	925 (96%)	38 (4%)	39 74

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	100	ASN
1	B	244	LEU
1	C	268	ASN
1	B	205	GLU
1	B	268	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	351	ASN
1	B	24	ASN
1	B	351	ASN
1	A	275	HIS
1	B	100	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ADP	A	400	-	22,29,29	1.87	5 (22%)	27,45,45	1.45	5 (18%)
5	CRB	A	500	2	13,17,17	2.18	3 (23%)	17,27,27	0.66	0
4	ADP	B	401	-	22,29,29	1.94	5 (22%)	27,45,45	1.41	5 (18%)
5	CRB	B	501	2	13,17,17	1.54	3 (23%)	17,27,27	0.98	0
4	ADP	C	402	-	22,29,29	2.01	5 (22%)	27,45,45	1.53	5 (18%)
5	CRB	C	502	2	13,17,17	1.68	4 (30%)	17,27,27	1.00	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	A	400	-	-	0/12/32/32	0/3/3/3
5	CRB	A	500	2	-	0/5/29/29	0/1/1/1
4	ADP	B	401	-	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CRB	B	501	2	-	0/5/29/29	0/1/1/1
4	ADP	C	402	-	-	0/12/32/32	0/3/3/3
5	CRB	C	502	2	-	0/5/29/29	0/1/1/1

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	502	CRB	C6-C5	2.15	1.55	1.53
5	A	500	CRB	C8-C2	2.16	1.55	1.53
5	B	501	CRB	C8-C6	2.19	1.57	1.53
5	C	502	CRB	C8-C6	2.26	1.58	1.53
5	B	501	CRB	C4-C5	2.28	1.55	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	400	ADP	O4'-C1'-N9	-3.17	101.45	108.10
4	B	401	ADP	O4'-C1'-N9	-2.90	102.04	108.10
4	C	402	ADP	O4'-C1'-N9	-2.50	102.86	108.10
4	B	401	ADP	C2'-C3'-C4'	2.00	106.73	102.61
5	C	502	CRB	O5-C5-C6	2.20	113.73	110.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	400	ADP	1	0
5	A	500	CRB	1	0
4	B	401	ADP	1	0
5	B	501	CRB	1	0

5.7 Other polymers [i](#)

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 [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	388/393 (98%)	-0.51	4 (1%) 84 77	18, 37, 72, 106	0
1	B	388/393 (98%)	-0.54	0 100 100	13, 37, 75, 107	0
1	C	388/393 (98%)	-0.72	0 100 100	10, 27, 55, 91	0
All	All	1164/1179 (98%)	-0.59	4 (0%) 94 92	10, 33, 70, 107	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	339	ALA	3.5
1	A	342	HIS	3.0
1	A	234	GLY	2.6
1	A	340	GLY	2.2

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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	C	602	1/1	0.98	0.13	1.01	33,33,33,33	0
5	CRB	A	500	17/17	0.97	0.15	0.49	24,32,49,55	0
5	CRB	C	502	17/17	0.98	0.12	-0.07	5,18,27,32	0
4	ADP	B	401	27/27	0.97	0.14	-0.10	27,40,51,56	0
4	ADP	C	402	27/27	0.97	0.12	-0.34	15,28,39,41	0
5	CRB	B	501	17/17	0.98	0.12	-0.37	5,16,29,30	0
4	ADP	A	400	27/27	0.97	0.13	-0.39	8,27,36,45	0
3	CL	A	604	1/1	0.97	0.12	-1.44	42,42,42,42	0
2	ZN	B	601	1/1	0.99	0.10	-2.11	29,29,29,29	0
2	ZN	A	600	1/1	0.99	0.08	-6.81	32,32,32,32	0
3	CL	C	603	1/1	0.93	0.14	-	36,36,36,36	1
3	CL	C	2605	1/1	0.81	0.21	-	63,63,63,63	0
3	CL	C	2606	1/1	0.88	0.16	-	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.