



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 17, 2018 – 10:04 pm GMT

PDB ID : 2CFC
Title : structural basis for stereo selectivity in the (R)- and (S)- hydroxypropylethane thiosulfonate dehydrogenases
Authors : Krishnakumar, A.M.; Nocek, B.P.; Clark, D.D.; Ensign, S.A.; Peters, J.W.
Deposited on : 2006-02-19
Resolution : 1.80 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

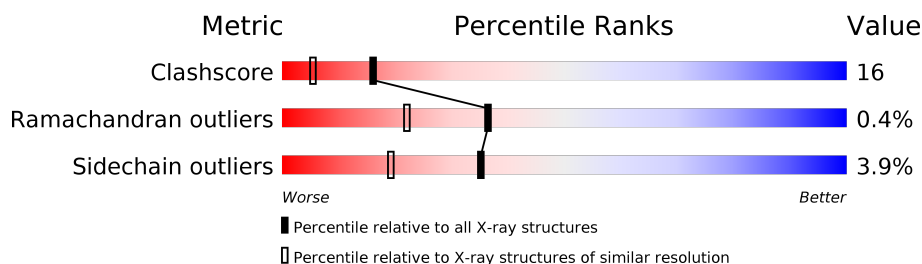
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	122078	6075 (1.80-1.80)
Ramachandran outliers	120005	6009 (1.80-1.80)
Sidechain outliers	119972	6008 (1.80-1.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	250	
1	B	250	
1	C	250	
1	D	250	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	KPC	A	1252	-	-	X	-

2 Entry composition ⓘ

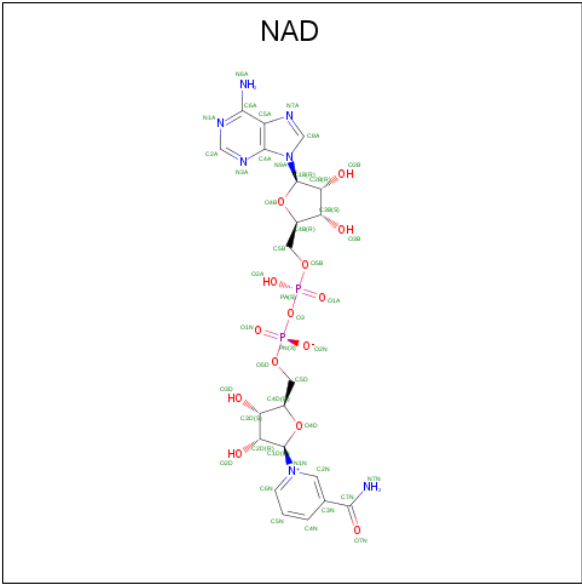
There are 4 unique types of molecules in this entry. The entry contains 8463 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2-(R)-HYDROXYPROPYL-COM DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1832	1144	325	352	11			
1	B	250	Total	C	N	O	S	0	0	0
			1832	1144	325	352	11			
1	C	250	Total	C	N	O	S	0	0	0
			1832	1144	325	352	11			
1	D	250	Total	C	N	O	S	0	0	0
			1832	1144	325	352	11			

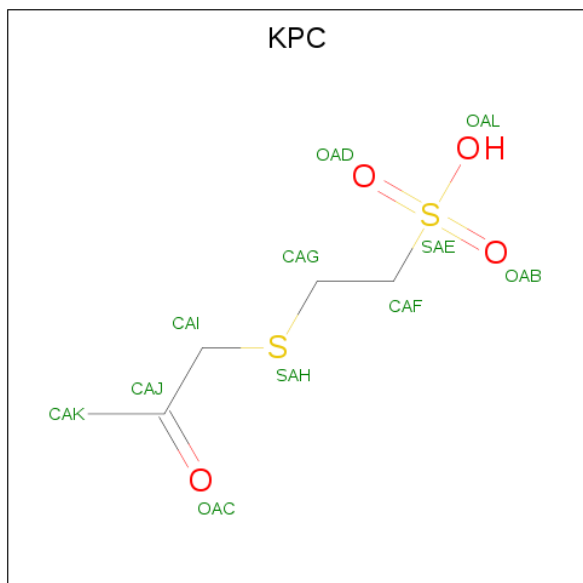
- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is (2-[2-KETOPROPYLTHIO]ETHANESULFONATE (three-letter code: KPC) (formula: C₅H₁₀O₄S₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			11	5	4	2		
3	B	1	Total	C	O	S	0	0
			11	5	4	2		
3	C	1	Total	C	O	S	0	0
			11	5	4	2		
3	D	1	Total	C	O	S	0	0
			11	5	4	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	246	Total	O	0	0
			246	246		
4	B	243	Total	O	0	0
			243	243		
4	C	201	Total	O	0	0
			201	201		

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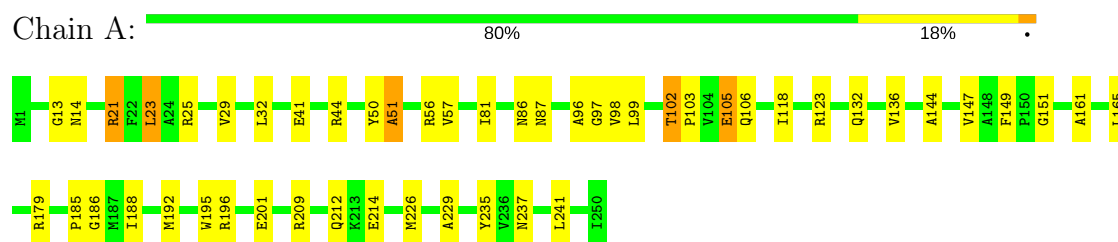
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	225	Total 225	O 225	0	0

3 Residue-property plots

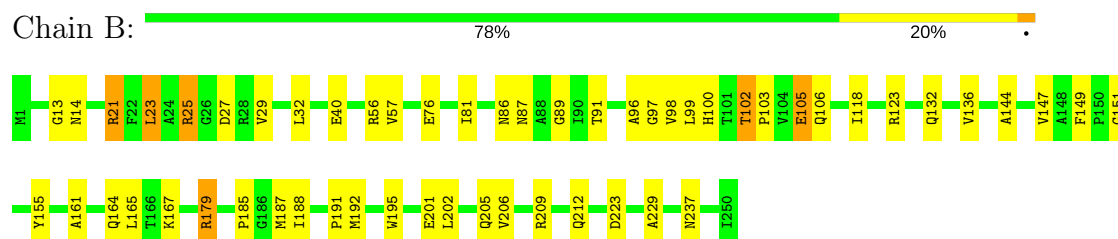
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

• Molecule 1: 2-(R)-HYDROXYPROPYL-COM DEHYDROGENASE



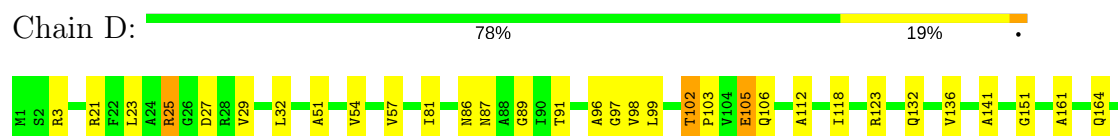
• Molecule 1: 2-(R)-HYDROXYPROPYL-COM DEHYDROGENASE



• Molecule 1: 2-(R)-HYDROXYPROPYL-COM DEHYDROGENASE



• Molecule 1: 2-(R)-HYDROXYPROPYL-COM DEHYDROGENASE





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.44Å 110.28Å 68.98Å 90.00° 93.88° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80	Depositor
% Data completeness (in resolution range)	76.1 (50.00-1.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.197 , 0.227	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8463	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

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: KPC, NAD

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	0.57	0/1857	0.72	0/2526
1	B	0.57	0/1857	0.74	0/2526
1	C	0.51	0/1857	0.71	0/2526
1	D	0.51	0/1857	0.72	0/2526
All	All	0.54	0/7428	0.72	0/10104

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	1832	0	1845	59	0
1	B	1832	0	1845	51	0
1	C	1832	0	1845	60	0
1	D	1832	0	1845	55	0
2	A	44	0	26	11	0
2	B	44	0	26	17	0
2	C	44	0	26	11	0
2	D	44	0	26	17	0
3	A	11	0	10	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	11	0	10	5	0
3	C	11	0	10	4	0
3	D	11	0	10	5	0
4	A	246	0	0	4	0
4	B	243	0	0	4	0
4	C	201	0	0	4	0
4	D	225	0	0	6	0
All	All	8463	0	7524	234	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 16.

The worst 5 of 234 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)
3:D:1252:KPC:HAG1	3:D:1252:KPC:HAK1	1.49	0.92
1:B:21:ARG:NH2	1:B:223:ASP:OD1	2.04	0.91
1:D:87:ASN:O	2:D:1251:NAD:H4D	1.73	0.89
3:C:1252:KPC:HAG1	3:C:1252:KPC:HAK1	1.54	0.88
1:A:179:ARG:HG3	1:A:179:ARG:HH11	1.43	0.83

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	248/250 (99%)	240 (97%)	7 (3%)	1 (0%)	36 22
1	B	248/250 (99%)	242 (98%)	6 (2%)	0	100 100
1	C	248/250 (99%)	239 (96%)	7 (3%)	2 (1%)	21 8
1	D	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	36 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	992/1000 (99%)	960 (97%)	28 (3%)	4 (0%)	36	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	ALA
1	C	51	ALA
1	C	2	SER
1	D	51	ALA

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	186/186 (100%)	180 (97%)	6 (3%)	42	27
1	B	186/186 (100%)	177 (95%)	9 (5%)	28	13
1	C	186/186 (100%)	180 (97%)	6 (3%)	42	27
1	D	186/186 (100%)	178 (96%)	8 (4%)	32	16
All	All	744/744 (100%)	715 (96%)	29 (4%)	35	19

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	179	ARG
1	C	25	ARG
1	D	179	ARG
1	B	195	TRP
1	C	56	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	164	GLN

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Mol	Chain	Res	Type
1	C	14	ASN
1	D	199	GLN
1	B	205	GLN
1	B	212	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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	$\# Z > 2$
2	NAD	A	1251	-	40,48,48	1.34	4 (10%)	44,73,73	2.03	5 (11%)
3	KPC	A	1252	-	10,10,10	1.72	1 (10%)	9,13,13	1.39	2 (22%)
2	NAD	B	1251	-	40,48,48	1.35	5 (12%)	44,73,73	1.93	5 (11%)
3	KPC	B	1252	-	10,10,10	1.71	1 (10%)	9,13,13	1.32	2 (22%)
2	NAD	C	1251	-	40,48,48	1.36	4 (10%)	44,73,73	1.88	4 (9%)
3	KPC	C	1252	-	10,10,10	1.72	1 (10%)	9,13,13	1.32	2 (22%)
2	NAD	D	1251	-	40,48,48	1.36	4 (10%)	44,73,73	1.86	4 (9%)
3	KPC	D	1252	-	10,10,10	1.72	1 (10%)	9,13,13	1.34	2 (22%)

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
2	NAD	A	1251	-	-	0/22/62/62	0/5/5/5
3	KPC	A	1252	-	-	0/8/8/8	0/0/0/0
2	NAD	B	1251	-	-	0/22/62/62	0/5/5/5
3	KPC	B	1252	-	-	0/8/8/8	0/0/0/0
2	NAD	C	1251	-	-	0/22/62/62	0/5/5/5
3	KPC	C	1252	-	-	0/8/8/8	0/0/0/0
2	NAD	D	1251	-	-	0/22/62/62	0/5/5/5
3	KPC	D	1252	-	-	0/8/8/8	0/0/0/0

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1251	NAD	C8A-N9A	-2.84	1.33	1.36
2	D	1251	NAD	C8A-N9A	-2.79	1.33	1.36
2	B	1251	NAD	C8A-N9A	-2.78	1.33	1.36
2	A	1251	NAD	C8A-N9A	-2.67	1.33	1.36
2	C	1251	NAD	C6N-N1N	2.00	1.40	1.35

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1251	NAD	N3A-C2A-N1A	-9.13	121.05	128.86
2	A	1251	NAD	N3A-C2A-N1A	-9.02	121.14	128.86
2	D	1251	NAD	N3A-C2A-N1A	-9.00	121.16	128.86
2	C	1251	NAD	N3A-C2A-N1A	-8.76	121.37	128.86
2	A	1251	NAD	C4D-O4D-C1D	-6.41	103.15	109.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 77 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1251	NAD	11	0
3	A	1252	KPC	7	0
2	B	1251	NAD	17	0
3	B	1252	KPC	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1251	NAD	11	0
3	C	1252	KPC	4	0
2	D	1251	NAD	17	0
3	D	1252	KPC	5	0

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.