



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:56 PM GMT

PDB ID : 1HWY
Title : BOVINE GLUTAMATE DEHYDROGENASE COMPLEXED WITH NAD
AND 2-OXOGLUTARATE
Authors : Smith, T.J.; Peterson, P.E.; Schmidt, T.; Fang, J.; Stanley, C.A.
Deposited on : 2001-01-10
Resolution : 3.20 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

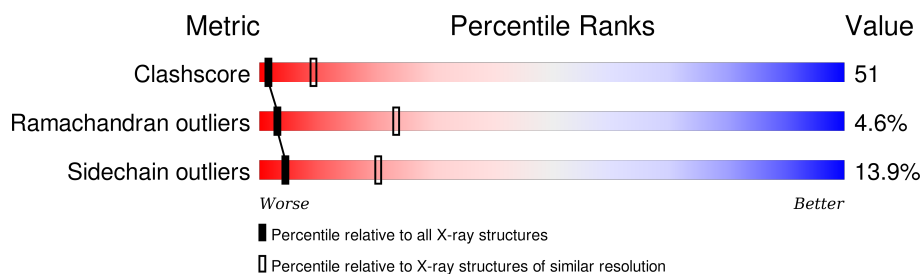
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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	501	<div> <div>34%</div> <div>52%</div> <div>12%</div> <div>.</div> </div>
1	B	501	<div> <div>32%</div> <div>54%</div> <div>12%</div> <div>.</div> </div>
1	C	501	<div> <div>32%</div> <div>55%</div> <div>12%</div> <div>.</div> </div>
1	D	501	<div> <div>33%</div> <div>53%</div> <div>12%</div> <div>.</div> </div>
1	E	501	<div> <div>32%</div> <div>54%</div> <div>13%</div> <div>.</div> </div>
1	F	501	<div> <div>32%</div> <div>54%</div> <div>12%</div> <div>.</div> </div>

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
2	PO4	A	502	-	-	X	-
2	PO4	A	504	-	-	X	-
2	PO4	B	503	-	-	X	-
2	PO4	B	505	-	-	X	-
2	PO4	C	503	-	-	X	-
2	PO4	C	505	-	-	X	-
2	PO4	D	503	-	-	X	-
2	PO4	D	504	-	-	X	-
2	PO4	E	503	-	-	X	-
2	PO4	E	504	-	-	X	-
2	PO4	F	502	-	-	X	-
2	PO4	F	504	-	-	X	-
3	AKG	A	506	-	-	X	-
3	AKG	B	506	-	-	X	-
3	AKG	C	506	-	-	X	-
3	AKG	D	506	-	-	X	-
3	AKG	E	506	-	-	X	-
3	AKG	F	506	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24468 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 GLUTAMATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			3910	2468	690	733	19			
1	B	501	Total	C	N	O	S	0	0	0
			3910	2468	690	733	19			
1	C	501	Total	C	N	O	S	0	0	0
			3910	2468	690	733	19			
1	D	501	Total	C	N	O	S	0	0	0
			3910	2468	690	733	19			
1	E	501	Total	C	N	O	S	0	0	0
			3910	2468	690	733	19			
1	F	501	Total	C	N	O	S	0	0	0
			3910	2468	690	733	19			

There are 30 discrepancies between the modelled and reference sequences:

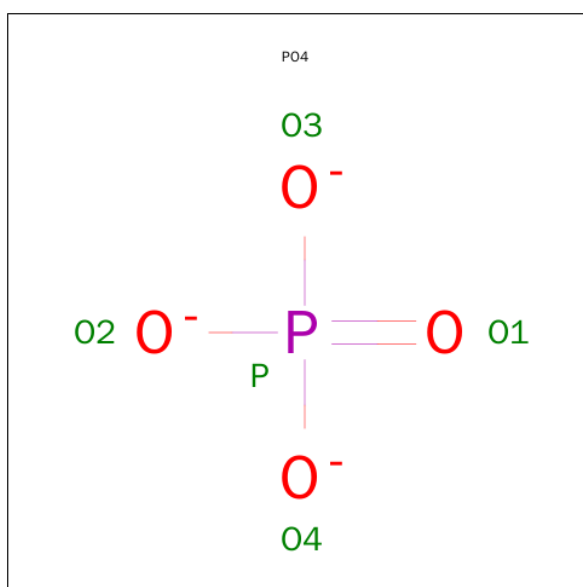
Chain	Residue	Modelled	Actual	Comment	Reference
A	200	GLY	LYS	SEE REMARK 999	UNP P00366
A	201	LYS	PRO	SEE REMARK 999	UNP P00366
A	202	PRO	GLY	SEE REMARK 999	UNP P00366
A	221	HIS	GLY	SEE REMARK 999	UNP P00366
A	222	GLY	HIS	SEE REMARK 999	UNP P00366
B	200	GLY	LYS	SEE REMARK 999	UNP P00366
B	201	LYS	PRO	SEE REMARK 999	UNP P00366
B	202	PRO	GLY	SEE REMARK 999	UNP P00366
B	221	HIS	GLY	SEE REMARK 999	UNP P00366
B	222	GLY	HIS	SEE REMARK 999	UNP P00366
C	200	GLY	LYS	SEE REMARK 999	UNP P00366
C	201	LYS	PRO	SEE REMARK 999	UNP P00366
C	202	PRO	GLY	SEE REMARK 999	UNP P00366
C	221	HIS	GLY	SEE REMARK 999	UNP P00366
C	222	GLY	HIS	SEE REMARK 999	UNP P00366
D	200	GLY	LYS	SEE REMARK 999	UNP P00366
D	201	LYS	PRO	SEE REMARK 999	UNP P00366

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Chain	Residue	Modelled	Actual	Comment	Reference
D	202	PRO	GLY	SEE REMARK 999	UNP P00366
D	221	HIS	GLY	SEE REMARK 999	UNP P00366
D	222	GLY	HIS	SEE REMARK 999	UNP P00366
E	200	GLY	LYS	SEE REMARK 999	UNP P00366
E	201	LYS	PRO	SEE REMARK 999	UNP P00366
E	202	PRO	GLY	SEE REMARK 999	UNP P00366
E	221	HIS	GLY	SEE REMARK 999	UNP P00366
E	222	GLY	HIS	SEE REMARK 999	UNP P00366
F	200	GLY	LYS	SEE REMARK 999	UNP P00366
F	201	LYS	PRO	SEE REMARK 999	UNP P00366
F	202	PRO	GLY	SEE REMARK 999	UNP P00366
F	221	HIS	GLY	SEE REMARK 999	UNP P00366
F	222	GLY	HIS	SEE REMARK 999	UNP P00366

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



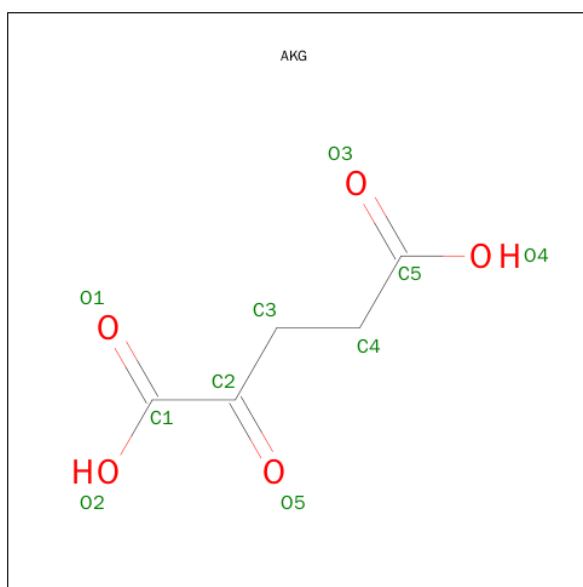
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		

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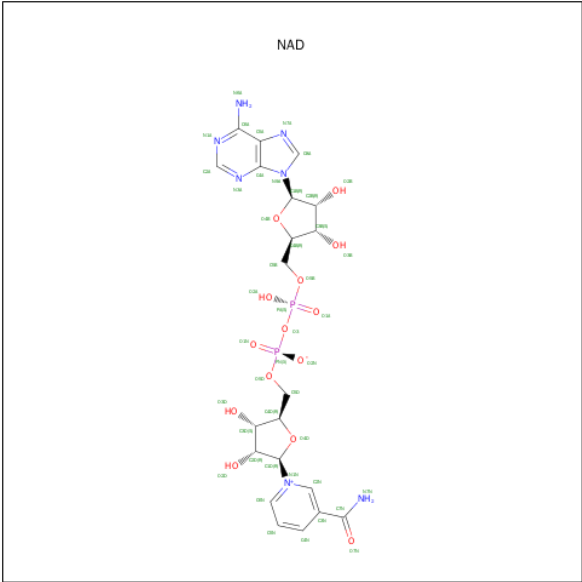
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: C₅H₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			10	5	5		
3	D	1	Total	C	O	0	0
			10	5	5		
3	C	1	Total	C	O	0	0
			10	5	5		
3	E	1	Total	C	O	0	0
			10	5	5		
3	B	1	Total	C	O	0	0
			10	5	5		
3	A	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
4	A	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
4	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	E	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
4	B	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
4	C	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
4	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	F	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is water.

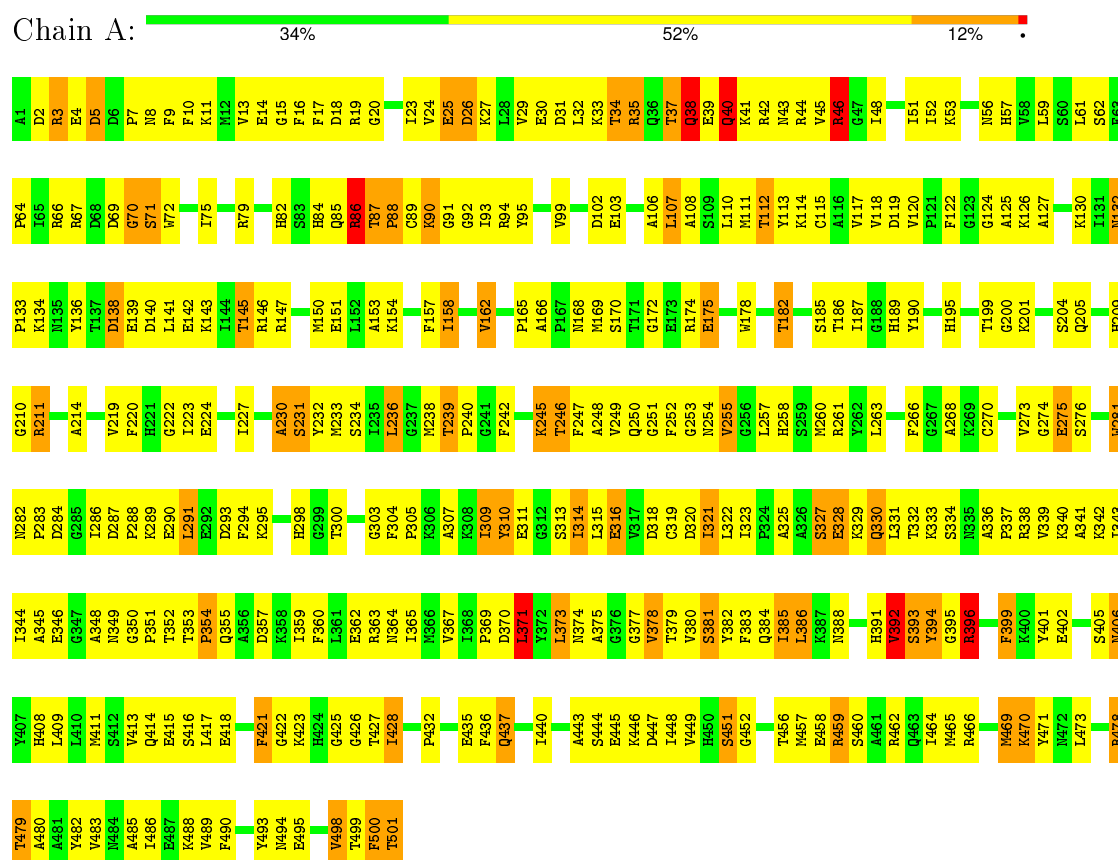
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total 6	O 6	0	0
5	B	6	Total 6	O 6	0	0
5	C	6	Total 6	O 6	0	0
5	D	6	Total 6	O 6	0	0
5	E	6	Total 6	O 6	0	0
5	F	6	Total 6	O 6	0	0

3 Residue-property plots

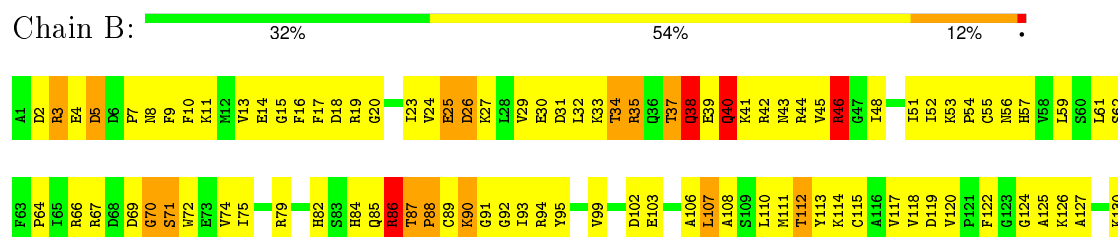
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

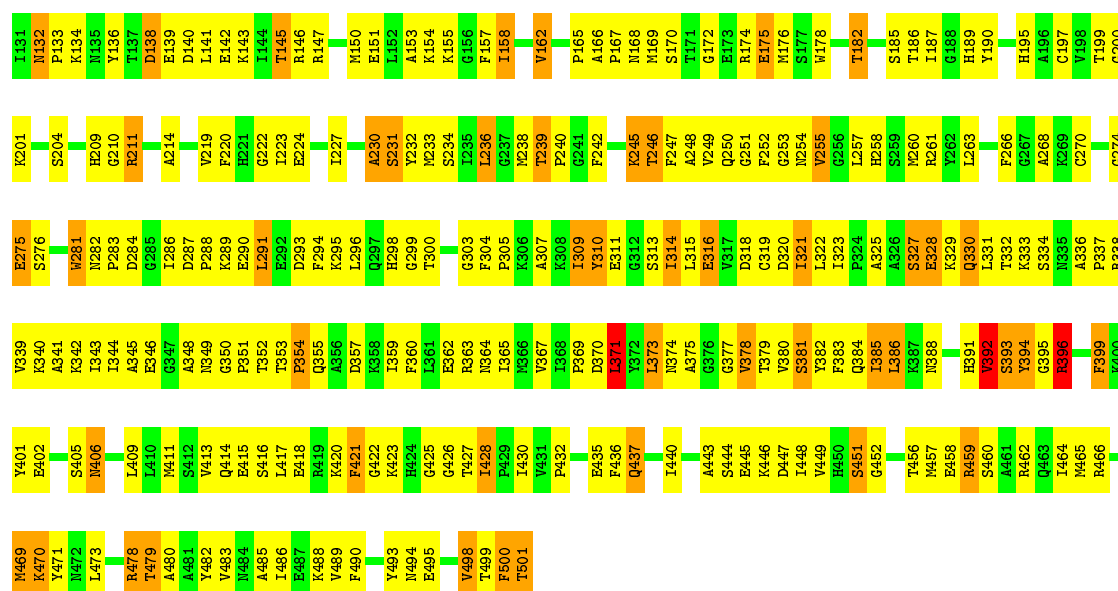
Note EDS was not executed.

• Molecule 1: GLUTAMATE DEHYDROGENASE



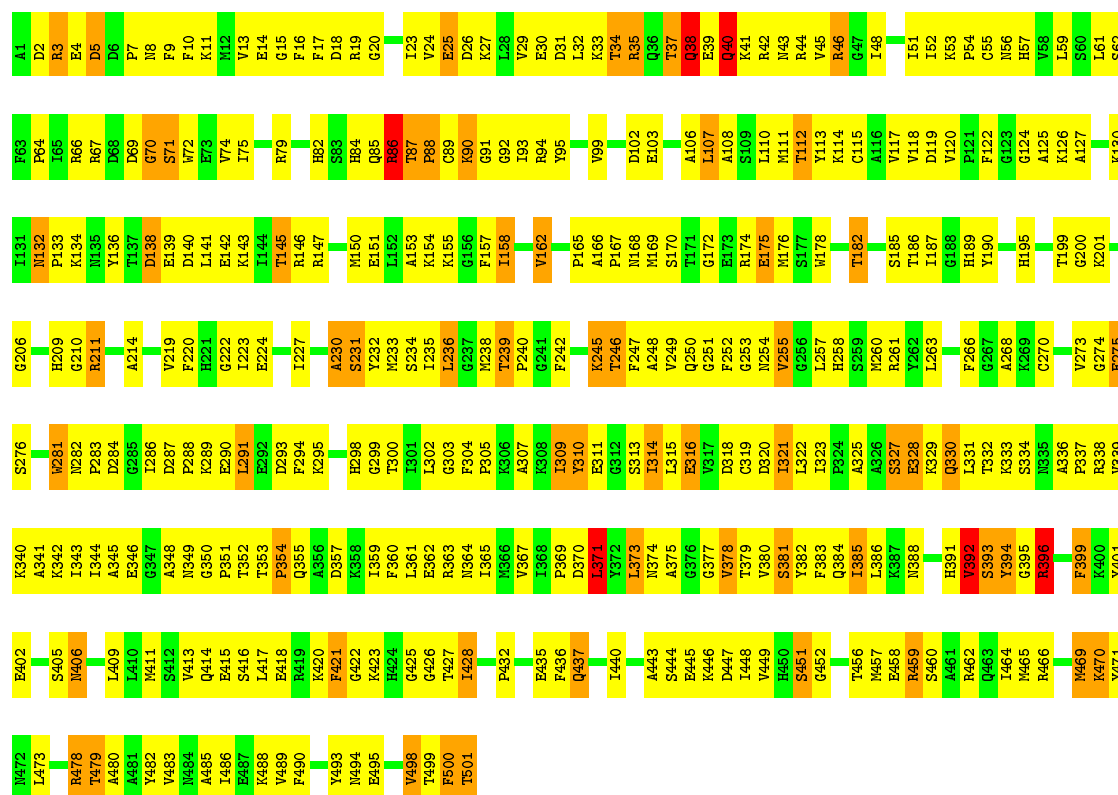
• Molecule 1: GLUTAMATE DEHYDROGENASE





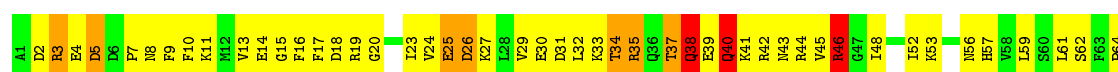
• Molecule 1: GLUTAMATE DEHYDROGENASE

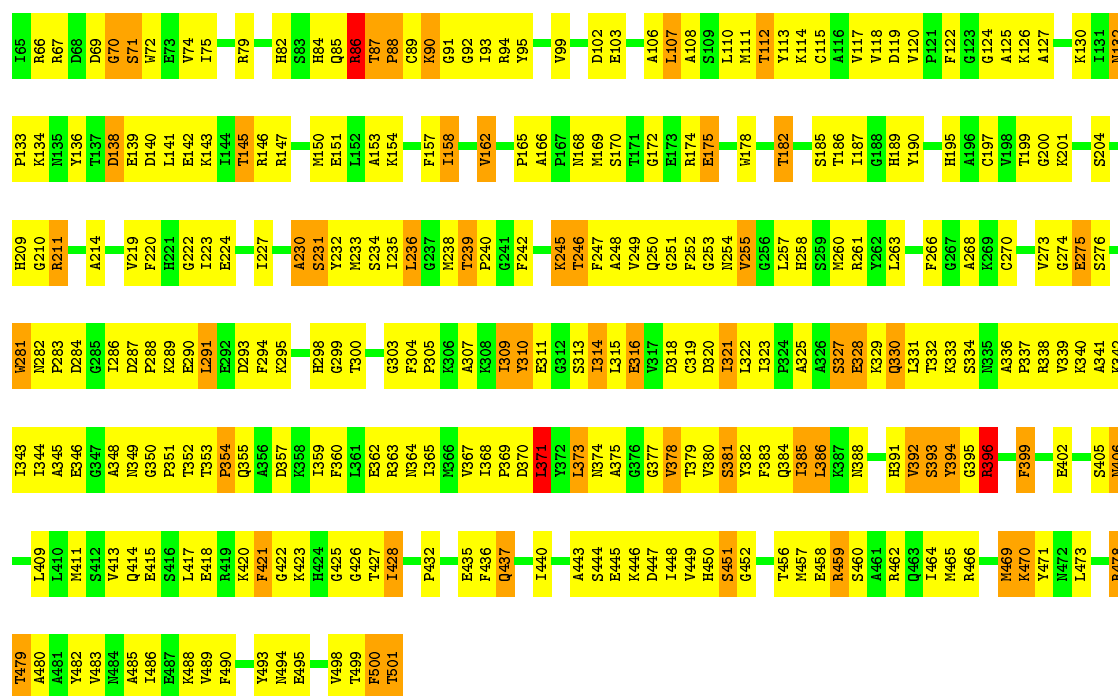
Chain C: 32% 55% 12%



• Molecule 1: GLUTAMATE DEHYDROGENASE

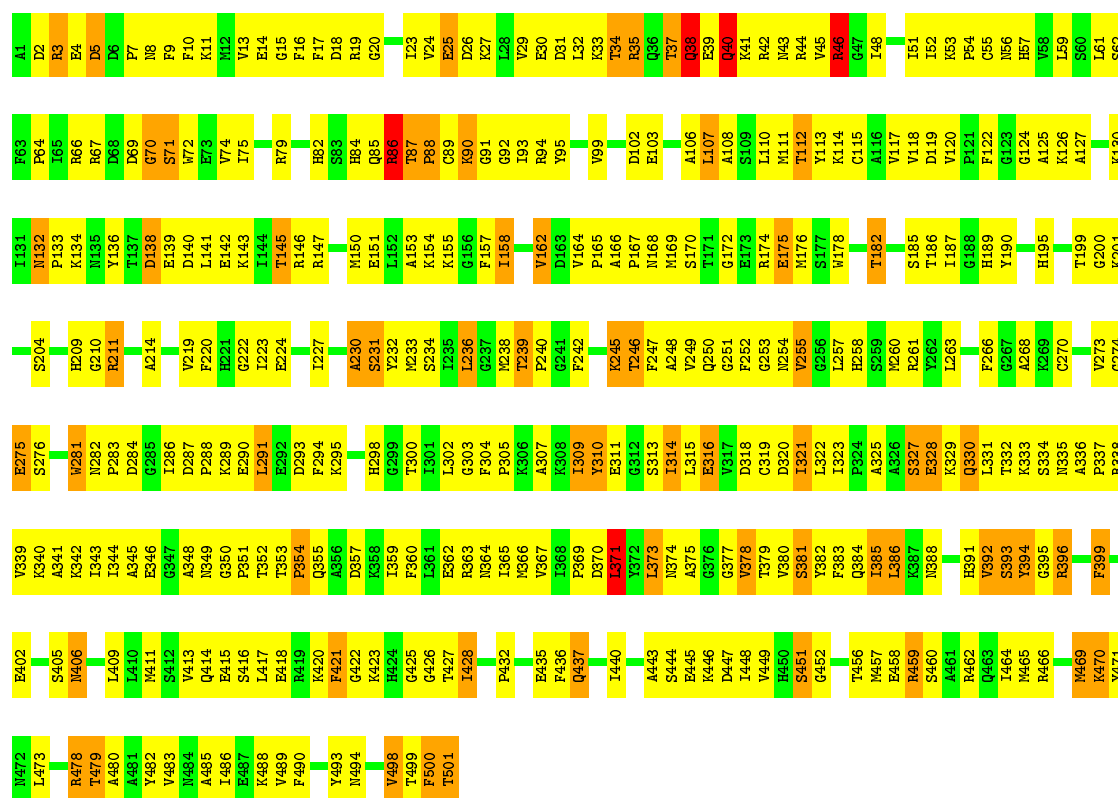
Chain D: 33% 53% 12%





• Molecule 1: GLUTAMATE DEHYDROGENASE

Chain E: 32% 54% 13%



• Molecule 1: GLUTAMATE DEHYDROGENASE

Chain F: 32% 54% 12%

V469	K470	Y471	M472	L473		R478	T479	A480	A481	Y482	Y483	M484	A485	I486	E487	K488	Y489	F490		Y493	M494	E495		Y498	T499	F500	T501																																	
V339	K340	A341	K342	I343	I344	A345	E346	G347	A348	N349	G350	P351	T352	T353	P354	Q355	A356	D357	K358	I359	F360	L361	E362	G363	N364	I365	M366	V367	P369	D370	L371	Y372	L373	N374	A375	G376	G377	V378	T379	V380	S381	Y382	F383	Q384	I385	L386	K387	N388		R391	V392	S393	Y394	G395	R396		F399	K400		
Y401	E402		S405	N406		L409	L410	M411	S412	Y413	Q414	E415	S416	L417	E418	R419	K420	F421	D422	K423	H424	G425	G426	T427	I428	P429	I430	V431	P432		E435	F436	Q437		I440		A443	S444	E445	K446	D447	I448	V449	H450	S451	G452		T456	M457	E458	R459	S460	A461	K462	Q463	I464	M465	R466		
E275	S276		N281	P283	D284	G285	I286	D287	P288	K289	E290	L291	E292	F293	F294	K295		H298	G299	T300	I301	L302	G303	F304	K305	K306	A307	K308	I309	Y310	E311	G312	S313	I314	L315	E316	V317	D318	C319	D320	I321	L322	I323	P324	A325	A326	S327	E328	K329	Q330	L331	T332	K333	S334	H335	A336	P337	R338		
S204	Q205		R209	G210	R211		A214		V219	F220	H221	G222	I223	E224		I227		A230	S231	Y232	M233	S234	I235	L236	G237	M238	T239	P240	G241	F242		K245	T246	F247	A248	V249	Q250	G251	F252	G253	N254	V255	G256	L257	H258	S259	R260	R261	Y262	L263		F266	G267	A268	K269	G270		V273	G274	
L131	M132	P133	K134	N135	Y136	T137	D138	E139	L140	L141	E142	K143	L144	T145	R146	R147		M150	E151	L152	A153	K154	K155	G156	F157	T158		V162		P165	A166	P167	M168	M169	S170	T171	G172	E173	R174	E175	M176	S177	H178		T182		S185	T186	I187	G188	H189		F266	G267	A268	K269	G270		V273	G274
A1	D2	R3	E4	D5	D6	P7	M8	F9	F10	K11	M12	V13	E14	G15	F16	F17	D18	R19	G20		L23	V24	E25	D26	K27	L28	V29	E30	D31	L32	K33	T34	R35	Q36	T37	Q38	E39	Q40	K41	R42	N43	R44	V45	R46	G47	L48		I51	I52	K53	C55	F122	G123	H57	A125	V58	L59	S60	S62	
F63	P64	I65	R66	R67	D68	D69	G70	S71	W72	E73	W74	I75		R79		H82	S83	H84	Q85	R86	T87	P88	C89	K90	G91	G92	I93	R94	Y95		V99		D102	M103		A106	L107	A108	S109	L110	M111	T112	Y113	K114	C115	A116	V117	V118	D119	V120	P121	G123	G124	A125	K126	A127		K130		

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.50Å 101.00Å 164.60Å 90.00° 102.20° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.230 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24468	wwPDB-VP
Average B, all atoms (Å ²)	10.0	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: PO4, AKG, 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	0.62	0/3991	0.84	10/5384 (0.2%)
1	B	0.62	0/3991	0.84	10/5384 (0.2%)
1	C	0.62	0/3991	0.84	9/5384 (0.2%)
1	D	0.62	0/3991	0.84	10/5384 (0.2%)
1	E	0.62	0/3991	0.84	10/5384 (0.2%)
1	F	0.62	0/3991	0.84	10/5384 (0.2%)
All	All	0.62	0/23946	0.84	59/32304 (0.2%)

There are no bond length outliers.

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	478	ARG	NE-CZ-NH1	-6.37	117.11	120.30
1	B	478	ARG	NE-CZ-NH1	-6.35	117.12	120.30
1	A	478	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	E	478	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	C	478	ARG	NE-CZ-NH1	-6.28	117.16	120.30

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	3910	0	3888	431	1
1	B	3910	0	3888	453	2
1	C	3910	0	3888	431	2
1	D	3910	0	3888	419	0
1	E	3910	0	3888	437	1
1	F	3910	0	3888	444	0
2	A	20	0	0	6	0
2	B	20	0	0	6	0
2	C	20	0	0	6	0
2	D	20	0	0	6	0
2	E	20	0	0	6	0
2	F	20	0	0	6	0
3	A	10	0	4	6	0
3	B	10	0	4	7	0
3	C	10	0	4	7	0
3	D	10	0	4	7	0
3	E	10	0	4	7	0
3	F	10	0	4	7	0
4	A	132	0	78	32	0
4	B	132	0	78	35	0
4	C	132	0	78	38	0
4	D	132	0	77	34	0
4	E	132	0	77	30	0
4	F	132	0	77	33	0
5	A	6	0	0	4	0
5	B	6	0	0	4	0
5	C	6	0	0	4	0
5	D	6	0	0	5	0
5	E	6	0	0	4	0
5	F	6	0	0	4	0
All	All	24468	0	23817	2472	3

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 51.

The worst 5 of 2472 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:D:391:HIS:CA	4:D:507[A]:NAD:O3D	1.66	1.41
1:F:391:HIS:CA	4:F:508[A]:NAD:O3D	1.66	1.41
1:B:391:HIS:CA	4:B:507[A]:NAD:O3D	1.69	1.40
1:C:391:HIS:CA	4:C:507[A]:NAD:O3D	1.70	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:HIS:CA	4:A:507[A]:NAD:O3D	1.69	1.38

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ILE:CG1	1:C:284:ASP:OD1[2_545]	2.14	0.06
1:A:3:ARG:CZ	1:E:298:HIS:NE2[2_556]	2.14	0.06
1:B:69:ASP:O	1:C:3:ARG:NH2[2_545]	2.19	0.01

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	499/501 (100%)	417 (84%)	59 (12%)	23 (5%)	3	23
1	B	499/501 (100%)	417 (84%)	59 (12%)	23 (5%)	3	23
1	C	499/501 (100%)	417 (84%)	59 (12%)	23 (5%)	3	23
1	D	499/501 (100%)	417 (84%)	59 (12%)	23 (5%)	3	23
1	E	499/501 (100%)	417 (84%)	59 (12%)	23 (5%)	3	23
1	F	499/501 (100%)	417 (84%)	59 (12%)	23 (5%)	3	23
All	All	2994/3006 (100%)	2502 (84%)	354 (12%)	138 (5%)	3	23

5 of 138 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	35	ARG
1	A	70	GLY
1	B	5	ASP
1	B	35	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	417/417 (100%)	359 (86%)	58 (14%)	4	20
1	B	417/417 (100%)	359 (86%)	58 (14%)	4	20
1	C	417/417 (100%)	359 (86%)	58 (14%)	4	20
1	D	417/417 (100%)	359 (86%)	58 (14%)	4	20
1	E	417/417 (100%)	359 (86%)	58 (14%)	4	20
1	F	417/417 (100%)	359 (86%)	58 (14%)	4	20
All	All	2502/2502 (100%)	2154 (86%)	348 (14%)	4	20

5 of 348 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	392	VAL
1	D	236	LEU
1	F	321	ILE
1	C	405	SER
1	D	38	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 103 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	282	ASN
1	D	168	ASN
1	F	254	ASN
1	C	388	ASN
1	D	43	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

48 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	PO4	A	502	-	4,4,4	1.13	1 (25%)	6,6,6	0.29	0
2	PO4	A	503	-	4,4,4	1.13	1 (25%)	6,6,6	0.29	0
2	PO4	A	504	-	4,4,4	1.13	1 (25%)	6,6,6	0.29	0
2	PO4	A	505	-	4,4,4	1.67	1 (25%)	6,6,6	0.29	0
3	AKG	A	506	-	3,9,9	1.06	0	4,11,11	3.18	3 (75%)
4	NAD	A	507[A]	-	38,48,48	2.28	11 (28%)	47,73,73	2.77	16 (34%)
4	NAD	A	507[B]	-	38,48,48	2.47	11 (28%)	47,73,73	2.35	16 (34%)
4	NAD	A	508	-	38,48,48	2.23	12 (31%)	47,73,73	2.78	16 (34%)
2	PO4	B	502	-	4,4,4	1.13	1 (25%)	6,6,6	0.29	0
2	PO4	B	503	-	4,4,4	1.13	1 (25%)	6,6,6	0.29	0
2	PO4	B	504	-	4,4,4	1.67	1 (25%)	6,6,6	0.29	0
2	PO4	B	505	-	4,4,4	1.12	1 (25%)	6,6,6	0.29	0
3	AKG	B	506	-	3,9,9	1.05	0	4,11,11	3.17	3 (75%)
4	NAD	B	507[A]	-	38,48,48	2.27	11 (28%)	47,73,73	2.77	16 (34%)
4	NAD	B	507[B]	-	38,48,48	2.47	11 (28%)	47,73,73	2.35	16 (34%)
4	NAD	B	508	-	38,48,48	2.22	12 (31%)	47,73,73	2.78	15 (31%)
2	PO4	C	502	-	4,4,4	1.13	1 (25%)	6,6,6	0.29	0
2	PO4	C	503	-	4,4,4	1.13	1 (25%)	6,6,6	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	C	504	-	4,4,4	1.68	1 (25%)	6,6,6	0.29	0
2	PO4	C	505	-	4,4,4	1.13	1 (25%)	6,6,6	0.29	0
3	AKG	C	506	-	3,9,9	1.07	0	4,11,11	3.18	3 (75%)
4	NAD	C	507[A]	-	38,48,48	2.27	11 (28%)	47,73,73	2.77	16 (34%)
4	NAD	C	507[B]	-	38,48,48	2.47	11 (28%)	47,73,73	2.35	16 (34%)
4	NAD	C	508	-	38,48,48	2.23	12 (31%)	47,73,73	2.78	16 (34%)
2	PO4	D	502	-	4,4,4	1.13	1 (25%)	6,6,6	0.29	0
2	PO4	D	503	-	4,4,4	1.12	1 (25%)	6,6,6	0.29	0
2	PO4	D	504	-	4,4,4	1.13	1 (25%)	6,6,6	0.29	0
2	PO4	D	505	-	4,4,4	1.67	1 (25%)	6,6,6	0.29	0
3	AKG	D	506	-	3,9,9	1.04	0	4,11,11	3.18	3 (75%)
4	NAD	D	507[A]	-	38,48,48	2.27	11 (28%)	47,73,73	2.77	16 (34%)
4	NAD	D	507[B]	-	38,48,48	2.47	11 (28%)	47,73,73	2.35	16 (34%)
4	NAD	D	508	-	38,48,48	2.24	12 (31%)	47,73,73	2.79	16 (34%)
2	PO4	E	502	-	4,4,4	1.12	1 (25%)	6,6,6	0.29	0
2	PO4	E	503	-	4,4,4	1.14	1 (25%)	6,6,6	0.29	0
2	PO4	E	504	-	4,4,4	1.13	1 (25%)	6,6,6	0.29	0
2	PO4	E	505	-	4,4,4	1.67	1 (25%)	6,6,6	0.29	0
3	AKG	E	506	-	3,9,9	1.08	0	4,11,11	3.18	3 (75%)
4	NAD	E	507[A]	-	38,48,48	2.27	11 (28%)	47,73,73	2.76	16 (34%)
4	NAD	E	507[B]	-	38,48,48	2.47	11 (28%)	47,73,73	2.35	16 (34%)
4	NAD	E	508	-	38,48,48	2.24	12 (31%)	47,73,73	2.79	15 (31%)
2	PO4	F	502	-	4,4,4	1.13	1 (25%)	6,6,6	0.29	0
2	PO4	F	503	-	4,4,4	1.13	1 (25%)	6,6,6	0.29	0
2	PO4	F	504	-	4,4,4	1.13	1 (25%)	6,6,6	0.29	0
2	PO4	F	505	-	4,4,4	1.67	1 (25%)	6,6,6	0.29	0
3	AKG	F	506	-	3,9,9	1.08	0	4,11,11	3.19	3 (75%)
4	NAD	F	507	-	38,48,48	2.23	12 (31%)	47,73,73	2.78	16 (34%)
4	NAD	F	508[A]	-	38,48,48	2.27	11 (28%)	47,73,73	2.77	16 (34%)
4	NAD	F	508[B]	-	38,48,48	2.47	11 (28%)	47,73,73	2.35	16 (34%)

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	PO4	A	502	-	-	0/0/0/0	0/0/0/0
2	PO4	A	503	-	-	0/0/0/0	0/0/0/0
2	PO4	A	504	-	-	0/0/0/0	0/0/0/0
2	PO4	A	505	-	-	0/0/0/0	0/0/0/0
3	AKG	A	506	-	-	0/3/9/9	0/0/0/0
4	NAD	A	507[A]	-	-	0/22/62/62	0/5/5/5
4	NAD	A	507[B]	-	-	0/22/62/62	0/5/5/5
4	NAD	A	508	-	-	0/22/62/62	0/5/5/5
2	PO4	B	502	-	-	0/0/0/0	0/0/0/0
2	PO4	B	503	-	-	0/0/0/0	0/0/0/0
2	PO4	B	504	-	-	0/0/0/0	0/0/0/0
2	PO4	B	505	-	-	0/0/0/0	0/0/0/0
3	AKG	B	506	-	-	0/3/9/9	0/0/0/0
4	NAD	B	507[A]	-	-	0/22/62/62	0/5/5/5
4	NAD	B	507[B]	-	-	0/22/62/62	0/5/5/5
4	NAD	B	508	-	-	0/22/62/62	0/5/5/5
2	PO4	C	502	-	-	0/0/0/0	0/0/0/0
2	PO4	C	503	-	-	0/0/0/0	0/0/0/0
2	PO4	C	504	-	-	0/0/0/0	0/0/0/0
2	PO4	C	505	-	-	0/0/0/0	0/0/0/0
3	AKG	C	506	-	-	0/3/9/9	0/0/0/0
4	NAD	C	507[A]	-	-	0/22/62/62	0/5/5/5
4	NAD	C	507[B]	-	-	0/22/62/62	0/5/5/5
4	NAD	C	508	-	-	0/22/62/62	0/5/5/5
2	PO4	D	502	-	-	0/0/0/0	0/0/0/0
2	PO4	D	503	-	-	0/0/0/0	0/0/0/0
2	PO4	D	504	-	-	0/0/0/0	0/0/0/0
2	PO4	D	505	-	-	0/0/0/0	0/0/0/0
3	AKG	D	506	-	-	0/3/9/9	0/0/0/0
4	NAD	D	507[A]	-	-	0/22/62/62	0/5/5/5
4	NAD	D	507[B]	-	-	0/22/62/62	0/5/5/5
4	NAD	D	508	-	-	0/22/62/62	0/5/5/5
2	PO4	E	502	-	-	0/0/0/0	0/0/0/0
2	PO4	E	503	-	-	0/0/0/0	0/0/0/0
2	PO4	E	504	-	-	0/0/0/0	0/0/0/0
2	PO4	E	505	-	-	0/0/0/0	0/0/0/0
3	AKG	E	506	-	-	0/3/9/9	0/0/0/0
4	NAD	E	507[A]	-	-	0/22/62/62	0/5/5/5
4	NAD	E	507[B]	-	-	0/22/62/62	0/5/5/5
4	NAD	E	508	-	-	0/22/62/62	0/5/5/5
2	PO4	F	502	-	-	0/0/0/0	0/0/0/0
2	PO4	F	503	-	-	0/0/0/0	0/0/0/0
2	PO4	F	504	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	F	505	-	-	0/0/0/0	0/0/0/0
3	AKG	F	506	-	-	0/3/9/9	0/0/0/0
4	NAD	F	507	-	-	0/22/62/62	0/5/5/5
4	NAD	F	508[A]	-	-	0/22/62/62	0/5/5/5
4	NAD	F	508[B]	-	-	0/22/62/62	0/5/5/5

The worst 5 of 228 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	507[B]	NAD	C2N-C3N	-4.30	1.32	1.39
4	B	507[B]	NAD	C2N-C3N	-4.29	1.32	1.39
4	E	507[B]	NAD	C2N-C3N	-4.27	1.32	1.39
4	F	508[B]	NAD	C2N-C3N	-4.27	1.32	1.39
4	C	507[B]	NAD	C2N-C3N	-4.25	1.32	1.39

The worst 5 of 304 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	507	NAD	N3A-C2A-N1A	-11.36	120.20	128.89
4	D	508	NAD	N3A-C2A-N1A	-11.35	120.20	128.89
4	C	508	NAD	N3A-C2A-N1A	-11.35	120.21	128.89
4	A	508	NAD	N3A-C2A-N1A	-11.34	120.21	128.89
4	B	508	NAD	N3A-C2A-N1A	-11.34	120.22	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

48 monomers are involved in 257 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	PO4	2	0
2	A	503	PO4	1	0
2	A	504	PO4	2	0
2	A	505	PO4	1	0
3	A	506	AKG	6	0
4	A	507[A]	NAD	16	0
4	A	507[B]	NAD	6	0
4	A	508	NAD	10	0
2	B	502	PO4	1	0
2	B	503	PO4	2	0
2	B	504	PO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	505	PO4	2	0
3	B	506	AKG	7	0
4	B	507[A]	NAD	17	0
4	B	507[B]	NAD	7	0
4	B	508	NAD	11	0
2	C	502	PO4	1	0
2	C	503	PO4	2	0
2	C	504	PO4	1	0
2	C	505	PO4	2	0
3	C	506	AKG	7	0
4	C	507[A]	NAD	19	0
4	C	507[B]	NAD	7	0
4	C	508	NAD	12	0
2	D	502	PO4	1	0
2	D	503	PO4	2	0
2	D	504	PO4	2	0
2	D	505	PO4	1	0
3	D	506	AKG	7	0
4	D	507[A]	NAD	16	0
4	D	507[B]	NAD	7	0
4	D	508	NAD	11	0
2	E	502	PO4	1	0
2	E	503	PO4	2	0
2	E	504	PO4	2	0
2	E	505	PO4	1	0
3	E	506	AKG	7	0
4	E	507[A]	NAD	12	0
4	E	507[B]	NAD	7	0
4	E	508	NAD	11	0
2	F	502	PO4	2	0
2	F	503	PO4	1	0
2	F	504	PO4	2	0
2	F	505	PO4	1	0
3	F	506	AKG	7	0
4	F	507	NAD	12	0
4	F	508[A]	NAD	14	0
4	F	508[B]	NAD	7	0

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.