



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:12 PM GMT

PDB ID : 1EFL
Title : HUMAN MALIC ENZYME IN A QUATERNARY COMPLEX WITH NAD,
MG, AND TARTRONATE
Authors : Yang, Z.; Floyd, D.L.; Loeber, G.; Tong, L.
Deposited on : 2000-02-09
Resolution : 2.60 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

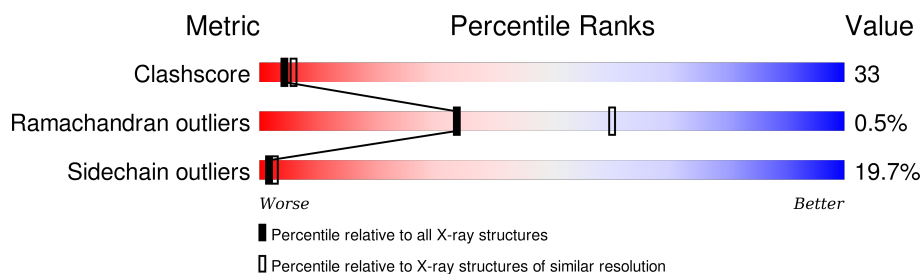
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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	584	
1	B	584	
1	C	584	
1	D	584	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17947 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 MALIC ENZYME.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			
1	B	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			
1	C	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			
1	D	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	38	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	47	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	75	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	86	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	108	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	177	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	219	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	239	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	325	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	327	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	343	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	407	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	539	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	29	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	38	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	47	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	75	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	86	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	108	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	177	MSE	MET	MODIFIED RESIDUE	UNP P23368

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Chain	Residue	Modelled	Actual	Comment	Reference
B	219	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	239	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	325	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	327	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	343	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	407	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	539	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	29	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	38	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	47	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	75	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	86	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	108	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	177	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	219	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	239	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	325	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	327	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	343	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	407	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	539	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	29	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	38	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	47	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	75	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	86	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	108	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	177	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	219	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	239	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	325	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	327	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	343	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	407	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	539	MSE	MET	MODIFIED RESIDUE	UNP P23368

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

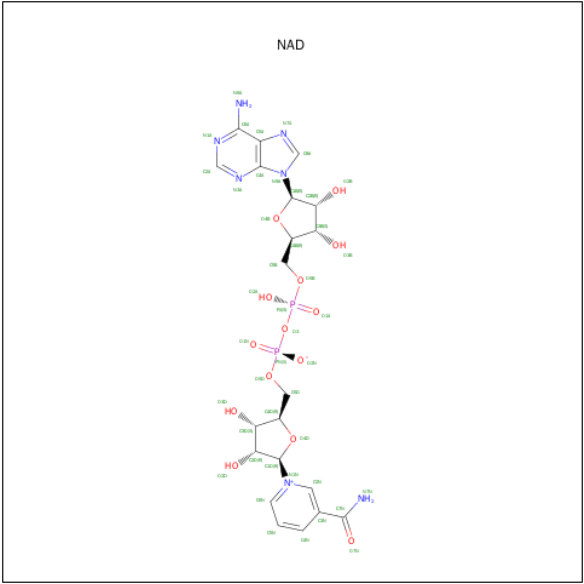
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0

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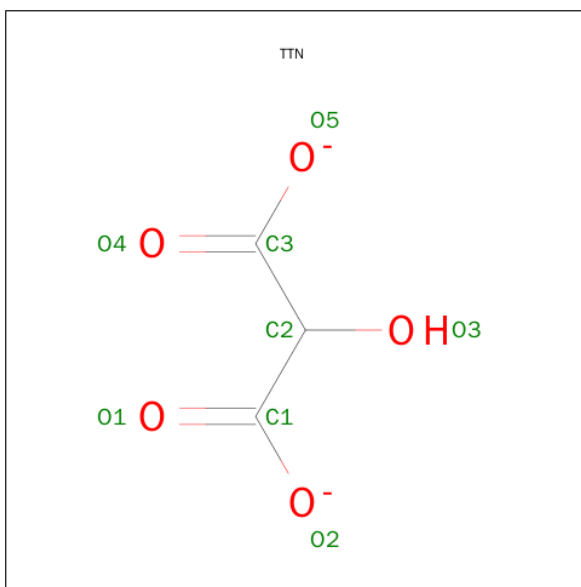
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	A	1	Total	C	N	O	P	9	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	9	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	9	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	9	0
			44	21	7	14	2		

- Molecule 4 is TARTRONATE (three-letter code: TTN) (formula: C₃H₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	3	5		
4	B	1	Total	C	O	0	0
			8	3	5		
4	C	1	Total	C	O	0	0
			8	3	5		
4	D	1	Total	C	O	0	0
			8	3	5		

- Molecule 5 is water.

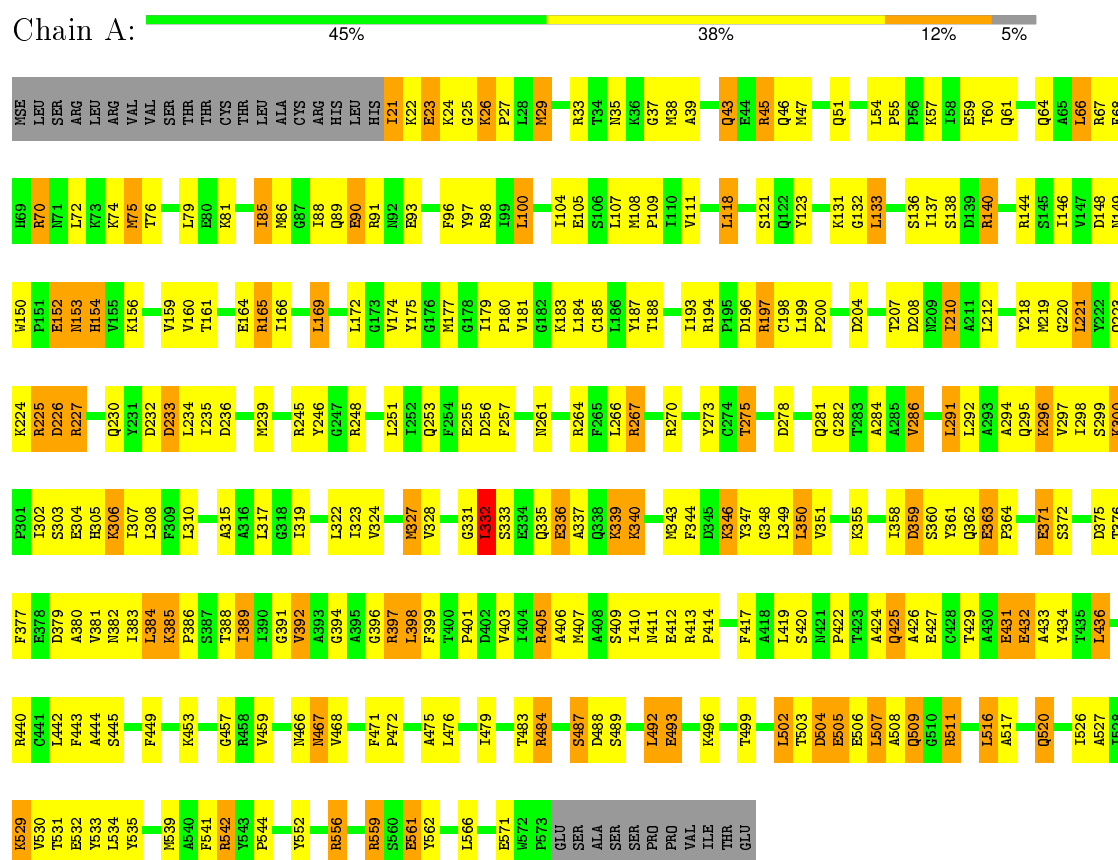
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	24	Total	O	0	0
			24	24		
5	B	17	Total	O	0	0
			17	17		
5	C	23	Total	O	0	0
			23	23		
5	D	27	Total	O	0	0
			27	27		

3 Residue-property plots

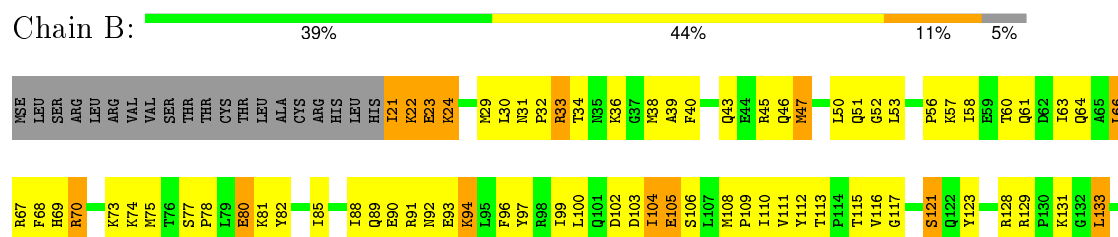
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

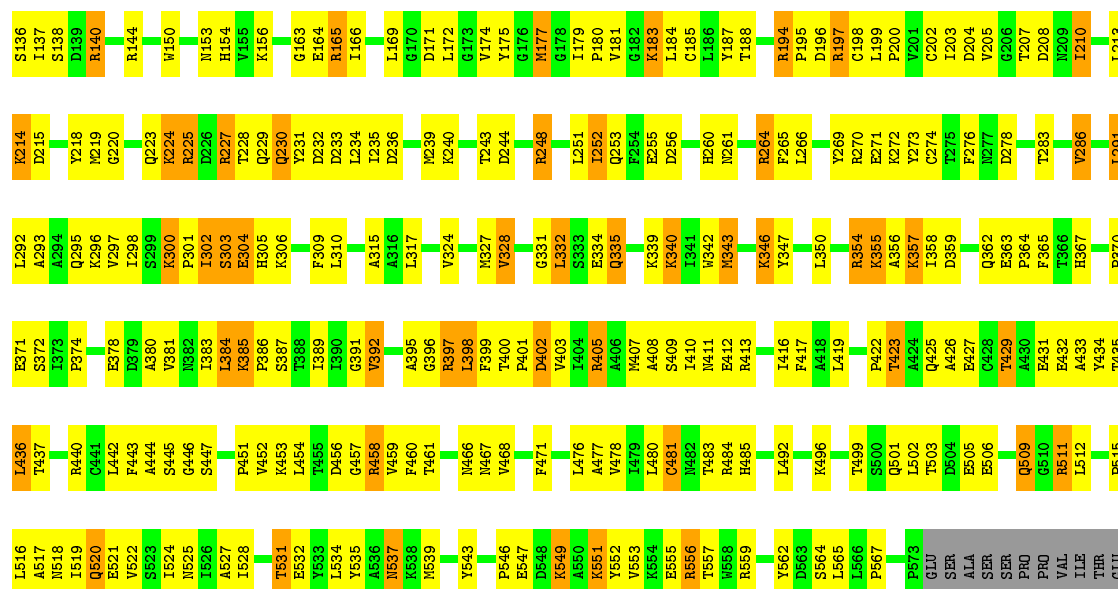
Note EDS was not executed.

• Molecule 1: MALIC ENZYME

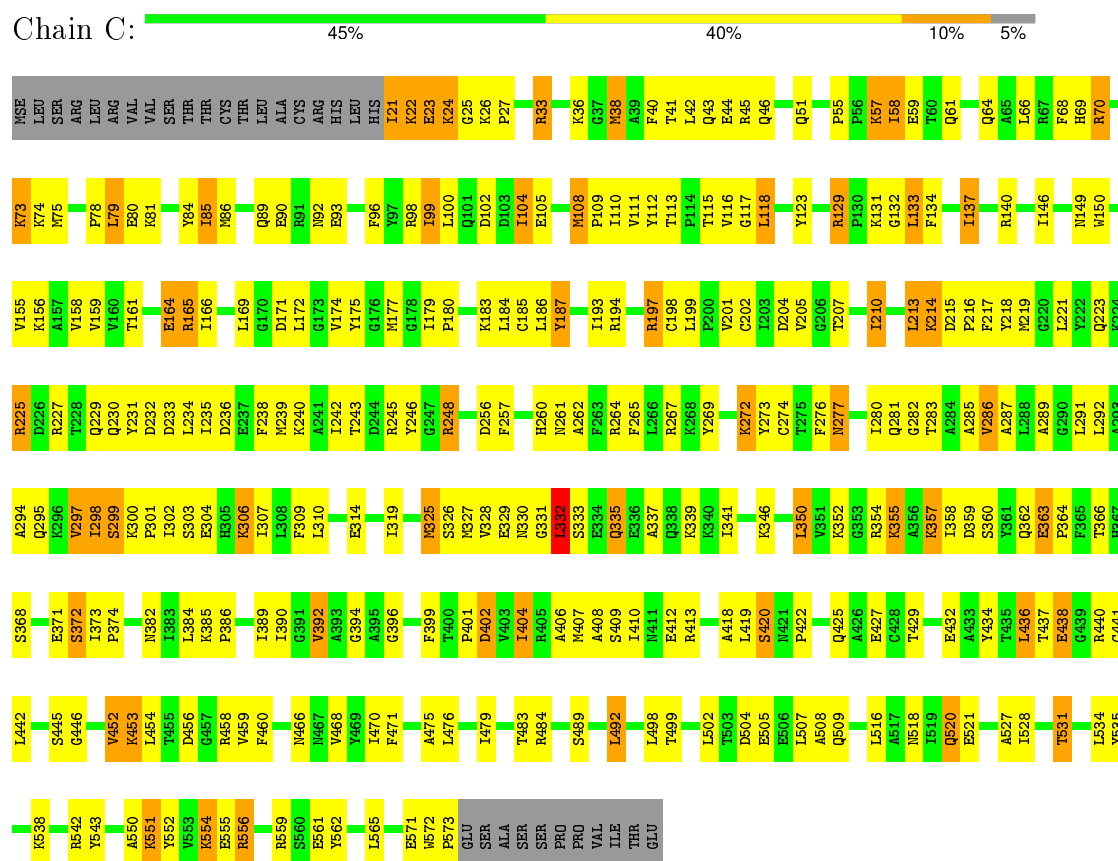


• Molecule 1: MALIC ENZYME

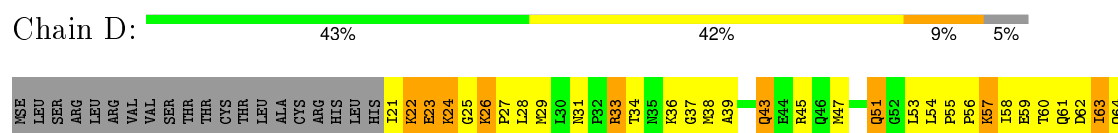




• Molecule 1: MALIC ENZYME



• Molecule 1: MALIC ENZYME



T531	E532	L533	L534	L535	A536	N537	A540	F541	B542	L543	P544	E545	D548	K549	A550	K551	K554	E555	B556	B559	S560	E561	L562	D563	S564	L565	L566	P572	P573	GLU	SER	ALA	SER	SER	PRO	PRO	VAL	ILE	THR	GLU														
Q457	R458	V459	F460	N466	N467	V468	V469	I470	F471	P472	A475	L476	A477	V478	I479	L480	C481	N482	T483	R484	H485	I486	S489	L492	K496	L497	L498	T499	S500	Q501	L502	T503	D504	E505	E506	L507	A508	Q509	G510	R511	P515	L516	A517	N518	I519	Q520	E521	I526	A527	K529	V530			
F377	E378	D379	A380	N381	N382	T383	L384	P385	P386	S387	T388	L389	G391	A392	G393	G394	R397	L398	F399	T400	P401	D402	V403	L404	R405	A406	N407	A408	S409	I410	L411	R412	R413	P414	V415	L416	F417	S420	T423	E427	E432	L436	T437	R440	C441	L442	F443	S447	D456					
A294	Q295	R296	V297	I298	S299	K300	F301	L302	S303	E304	H305	K306	I307	F309	L310	E314	A315	A316	T319	V324	M327	V328	L351	G331	T352	Q353	S333	E334	Q335	E336	A337	M342	M343	K346	Y347	L350	K355	A356	K357	L358	D359	S360	Y361	Q362	T366	E371	S372	I373						
L221	T222	Q223	K224	R225	D226	R227	T228	Q229	Q230	D233	L234	T235	D236	E237	F238	N239	K240	L241	T242	D244	R245	Y246	N249	T250	L251	T252	Q253	D256	N261	A262	F263	R264	F265	L266	R267	K268	Y269	R270	E271	K272	Y273	C274	T275	F276	A285	V286	L288	A289	G290	L291	L292	A293		
R144	S145	I146	V147	D148	N149	M150	F151	E152	N153	K156	R165	I166	L169	V174	Y175	G176	M177	G178	I179	P180	K183	L184	F185	A189	T197	C190	A191	G192	I193	R194	P195	D196	R197	C198	P199	P200	V201	C202	I203	D204	T207	D208	N209	I210	A211	L212	L213	K214	D215	P216	F217	Y218	M219	G220
L65	L66	R67	F68	B69	H70	N71	L72	K73	K74	T75	T76	S77	F78	L79	E80	K81	Y82	I83	T84	L85	H86	R91	N92	E93	R94	F96	Y97	R98	I99	L100	Q101	I104	L107	M108	P109	I110	V111	Y112	T115	H125	R128	K131	G132	L133	S136	I137	S138	D139	R140					

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	228.80 Å 117.00 Å 114.30 Å 90.00° 109.20° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.60)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.206 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17947	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: MG, TTN, 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	0.46	0/4447	0.65	0/5998
1	B	0.46	0/4447	0.66	0/5998
1	C	0.45	0/4447	0.65	1/5998 (0.0%)
1	D	0.46	0/4447	0.65	0/5998
All	All	0.46	0/17788	0.65	1/23992 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	310	LEU	N-CA-C	-5.09	97.27	111.00

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	4367	0	4407	333	0
1	B	4367	0	4407	331	0
1	C	4367	0	4407	252	0
1	D	4367	0	4407	314	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	88	0	52	6	0
3	B	88	0	52	2	0
3	C	88	0	52	5	0
3	D	88	0	52	4	0
4	A	8	0	1	0	0
4	B	8	0	1	1	0
4	C	8	0	1	2	0
4	D	8	0	2	1	0
5	A	24	0	0	5	0
5	B	17	0	0	9	0
5	C	23	0	0	5	0
5	D	27	0	0	3	0
All	All	17947	0	17841	1185	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 33.

The worst 5 of 1185 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:227:ARG:HH11	1:A:227:ARG:HG2	1.03	1.11
1:D:520:GLN:HE22	1:D:521:GLU:HG2	1.13	1.07
1:A:511:ARG:HB3	1:A:511:ARG:HH11	1.20	1.02
1:C:355:LYS:HA	1:C:355:LYS:HE2	1.42	1.01
1:B:227:ARG:HH11	1:B:227:ARG:HG2	1.24	1.00

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	551/584 (94%)	516 (94%)	33 (6%)	2 (0%)	39	65
1	B	551/584 (94%)	513 (93%)	35 (6%)	3 (0%)	34	60
1	C	551/584 (94%)	525 (95%)	23 (4%)	3 (0%)	34	60
1	D	551/584 (94%)	515 (94%)	32 (6%)	4 (1%)	26	51
All	All	2204/2336 (94%)	2069 (94%)	123 (6%)	12 (0%)	34	60

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	332	LEU
1	C	332	LEU
1	C	392	VAL
1	A	332	LEU
1	D	270	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	469/483 (97%)	371 (79%)	98 (21%)	1	2
1	B	469/483 (97%)	373 (80%)	96 (20%)	1	2
1	C	469/483 (97%)	379 (81%)	90 (19%)	2	3
1	D	469/483 (97%)	384 (82%)	85 (18%)	2	3
All	All	1876/1932 (97%)	1507 (80%)	369 (20%)	1	2

5 of 369 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	385	LYS
1	C	74	LYS
1	D	358	ILE
1	B	409	SER
1	B	547	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	525	ASN
1	C	230	GLN
1	D	482	ASN
1	B	537	ASN
1	C	64	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](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\# Z > 2$
3	NAD	A	601	-	38,48,48	1.69	8 (21%)	47,73,73	2.07	7 (14%)
3	NAD	A	602	-	38,48,48	1.96	9 (23%)	47,73,73	1.98	5 (10%)
4	TTN	A	603	2	1,7,7	0.34	0	2,9,9	0.36	0
3	NAD	B	1601	-	38,48,48	1.75	9 (23%)	47,73,73	2.07	8 (17%)
3	NAD	B	1602	-	38,48,48	1.90	10 (26%)	47,73,73	1.88	5 (10%)
4	TTN	B	1603	2	1,7,7	0.37	0	2,9,9	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	C	2601	-	38,48,48	1.75	9 (23%)	47,73,73	2.10	6 (12%)
3	NAD	C	2602	-	38,48,48	2.09	11 (28%)	47,73,73	1.86	5 (10%)
4	TTN	C	2603	2	1,7,7	0.13	0	2,9,9	0.95	0
3	NAD	D	3601	-	38,48,48	1.84	9 (23%)	47,73,73	2.02	7 (14%)
3	NAD	D	3602	-	38,48,48	2.01	11 (28%)	47,73,73	1.94	4 (8%)
4	TTN	D	3603	2	1,7,7	0.40	0	2,9,9	0.58	0

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
3	NAD	A	601	-	-	0/22/62/62	0/5/5/5
3	NAD	A	602	-	-	0/22/62/62	0/5/5/5
4	TTN	A	603	2	-	0/0/8/8	0/0/0/0
3	NAD	B	1601	-	-	0/22/62/62	0/5/5/5
3	NAD	B	1602	-	-	0/22/62/62	0/5/5/5
4	TTN	B	1603	2	-	0/0/8/8	0/0/0/0
3	NAD	C	2601	-	-	0/22/62/62	0/5/5/5
3	NAD	C	2602	-	-	0/22/62/62	0/5/5/5
4	TTN	C	2603	2	-	0/0/8/8	0/0/0/0
3	NAD	D	3601	-	-	0/22/62/62	0/5/5/5
3	NAD	D	3602	-	-	0/22/62/62	0/5/5/5
4	TTN	D	3603	2	-	0/0/8/8	0/0/0/0

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2601	NAD	C5A-C4A	-3.50	1.32	1.40
3	A	601	NAD	C5A-C4A	-3.29	1.33	1.40
3	A	602	NAD	C5A-C4A	-3.10	1.33	1.40
3	B	1602	NAD	C5A-C4A	-3.03	1.33	1.40
3	B	1601	NAD	C5A-C4A	-2.91	1.33	1.40

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2601	NAD	N3A-C2A-N1A	-11.20	120.32	128.89
3	A	602	NAD	N3A-C2A-N1A	-10.87	120.57	128.89
3	A	601	NAD	N3A-C2A-N1A	-10.79	120.64	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1601	NAD	N3A-C2A-N1A	-10.64	120.75	128.89
3	D	3601	NAD	N3A-C2A-N1A	-10.60	120.78	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	NAD	4	0
3	A	602	NAD	2	0
3	B	1601	NAD	1	0
3	B	1602	NAD	1	0
4	B	1603	TTN	1	0
3	C	2601	NAD	4	0
3	C	2602	NAD	1	0
4	C	2603	TTN	2	0
3	D	3601	NAD	1	0
3	D	3602	NAD	3	0
4	D	3603	TTN	1	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 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.