



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:11 PM GMT

PDB ID : 1EFK
Title : STRUCTURE OF HUMAN MALIC ENZYME IN COMPLEX WITH KE-
TOMALONATE
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

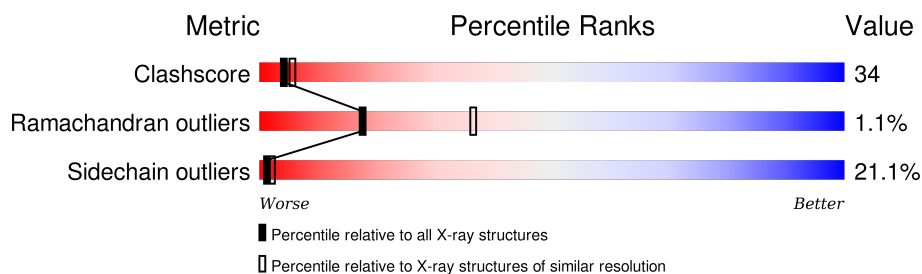
1 Overall quality at a glance

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 17931 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
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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
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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).

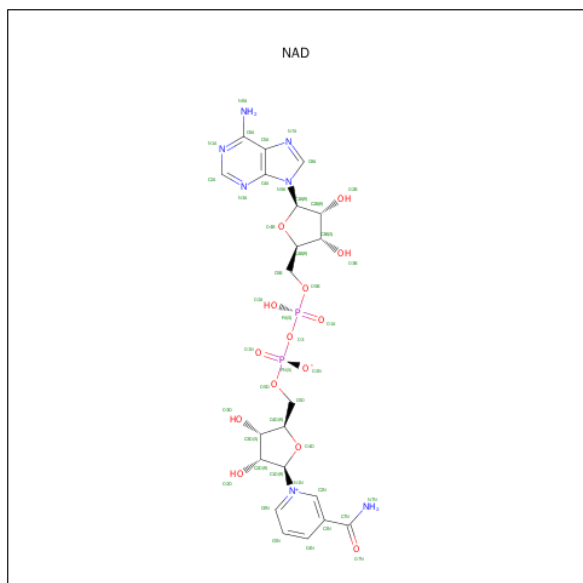
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0

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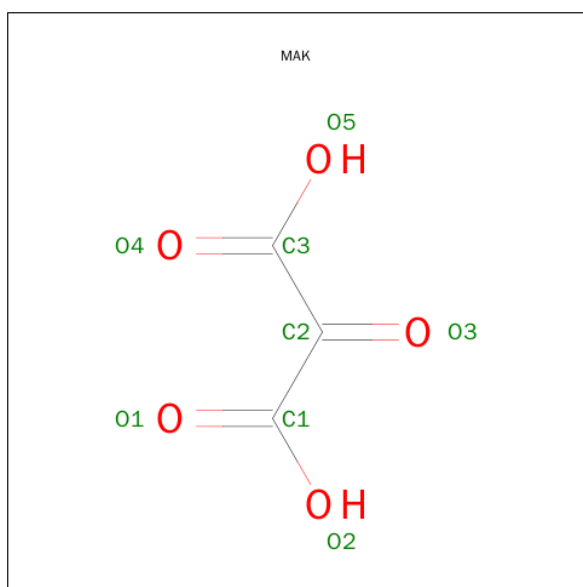
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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 ALPHA-KETOMALONIC ACID (three-letter code: MAK) (formula: $C_3H_2O_5$).



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.

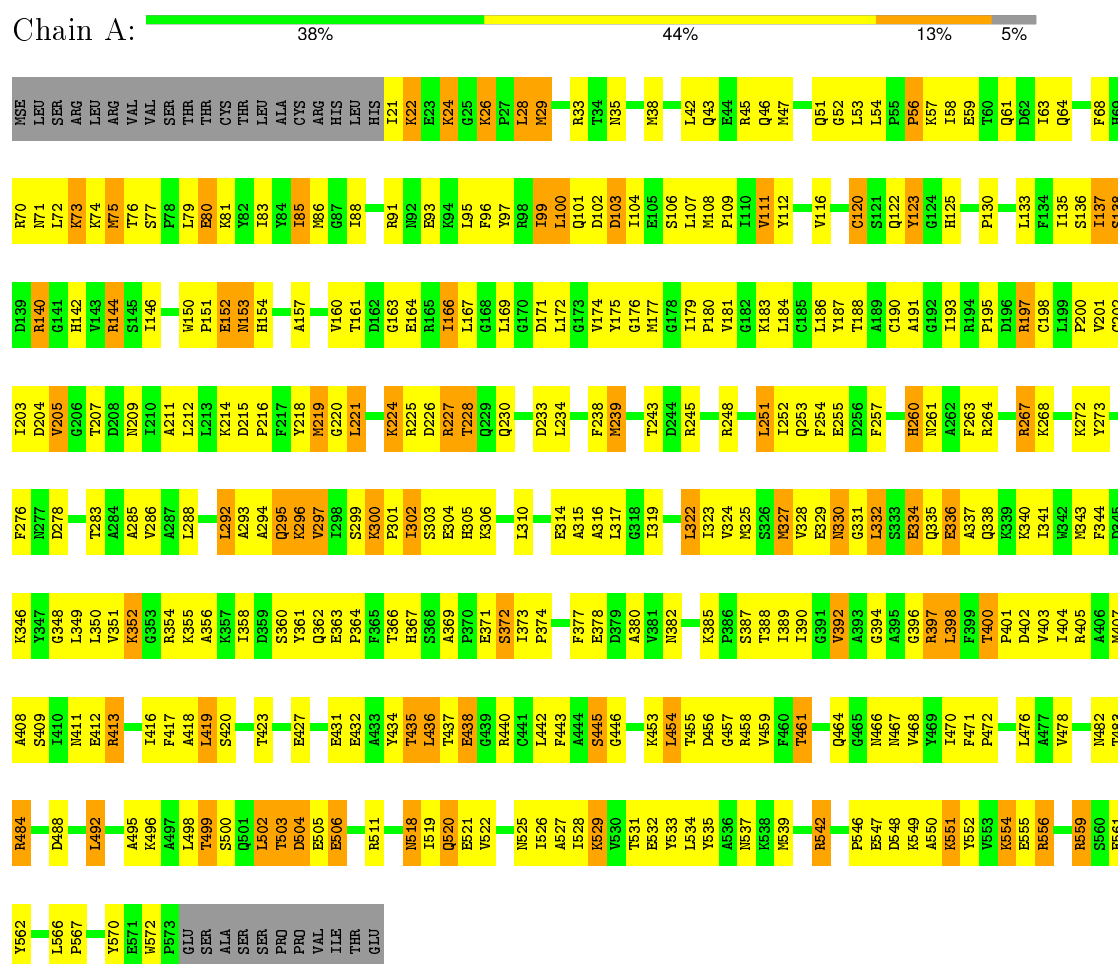
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	25	Total	O	0	0
			25	25		
5	B	18	Total	O	0	0
			18	18		
5	C	16	Total	O	0	0
			16	16		
5	D	16	Total	O	0	0
			16	16		

3 Residue-property plots

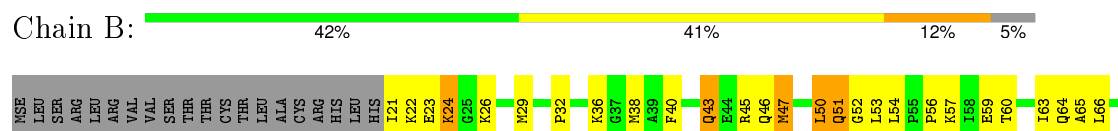
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

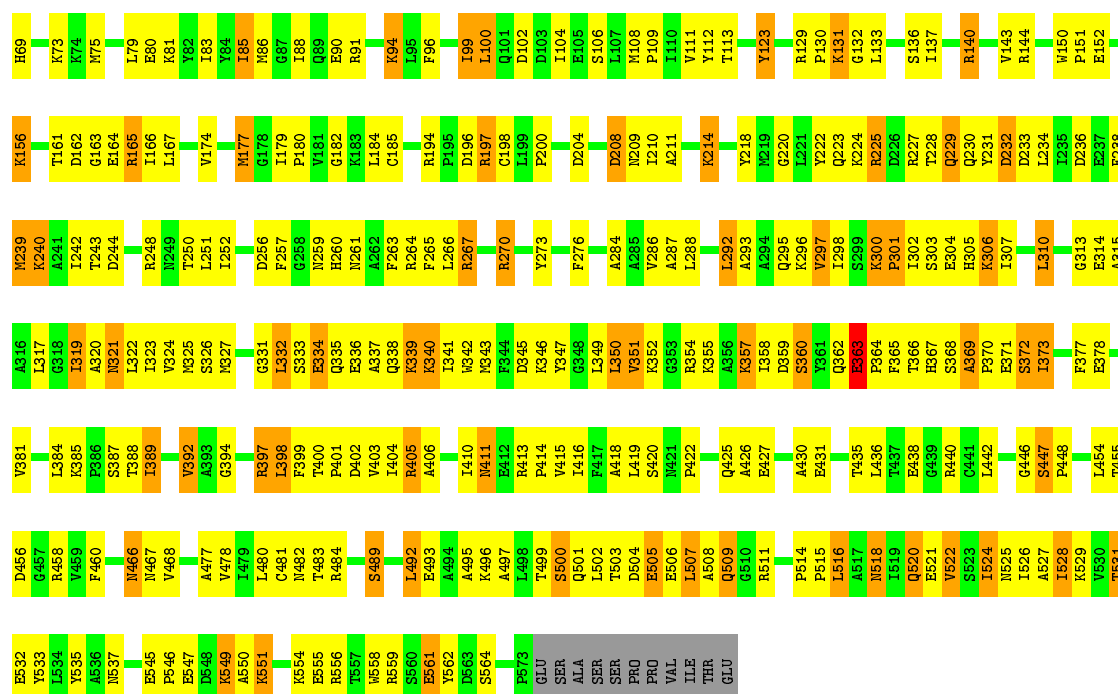
Note EDS was not executed.

• Molecule 1: MALIC ENZYME



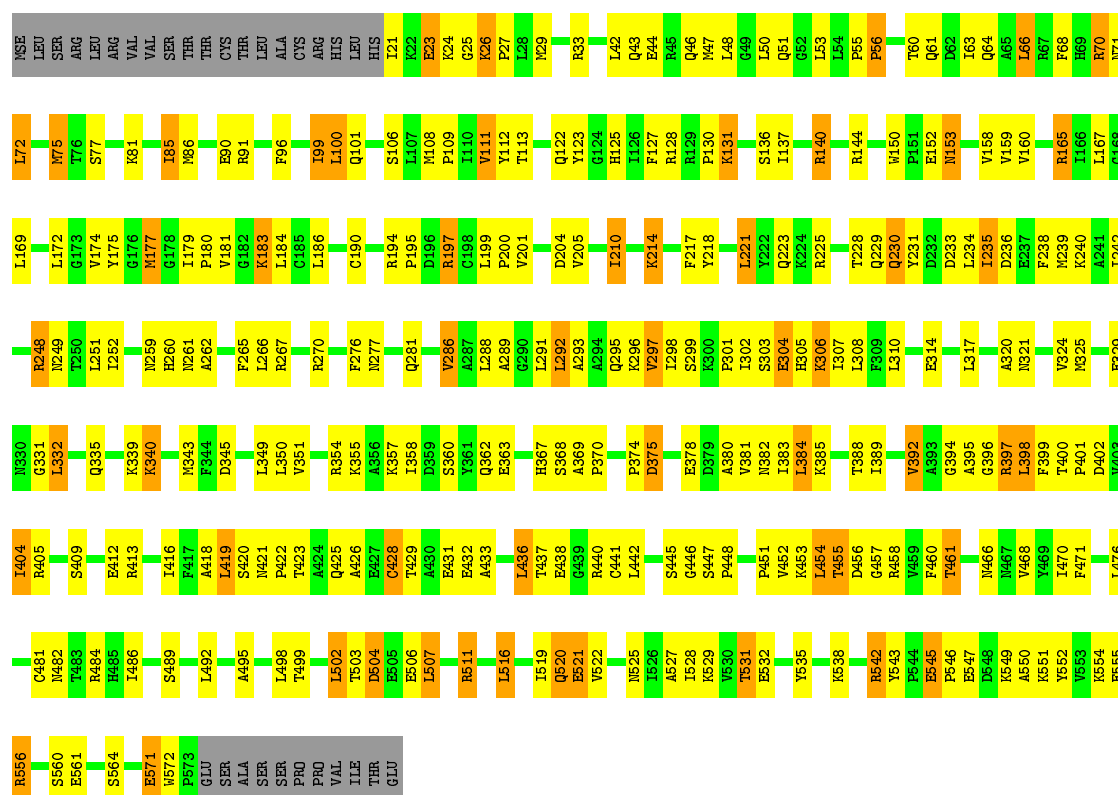
• Molecule 1: MALIC ENZYME





• Molecule 1: MALIC ENZYME

Chain C: 47% 38% 9% 5%



• Molecule 1: MALIC ENZYME

Chain D: 41% 39% 14% 5%

PRO	PRO	VAL	ILE	THR	GLU	Q510	R511	L512	L516	A517	R518	L519	Q520	E521	V522	N526	L526	A527	L528	R529	V530	T531	E532	L533	L534	Y535	A536	N537	K538	R542	Y543	P546	D547	K549	A550	K551	Y552	E553	K554	E555	R556	T557	R558	R559	S560	E561	Y562	L566	P567	D568	E571	R572	P573	GLU	SER	ALA	SER	SER																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
E431	E432	T435	L436	T437	E438	G439	R440	C441	L442	F443	A444	S445	G446	S447	P448	V4452	K4453	L4454	T4455	D4456	G4457	R4458	V4459	F4460	T4461	Q4464	G4465	N4466	N4467	V4468	F4471	P4472	G4473	V4474	A4475	L4476	A4477	V4478	I4479	S4489	L4492	E4493	S500	Q501	L502	T503	D504	E505	E506	L507	A508	Q509	E362	E363	P364	T366	E367	S368	A369	P370	E371	P374	D375	T376	F377	E378	D379	A380	V381	R382	L383	L384	S387	T388	I389	V392	A393	G394	R397	L398	F399	T400	P401	P402	V403	I404	R405	A406	M407	N408	S409	E412	R413	P414	V415	I416	S420	T423	A426	E427	C428	T429	A430	V297	L298	S299	K300	L301	I302	S303	E304	H305	K306	L307	L308	G313	E314	A315	A316	L319	A320	N321	L322	L323	D324	R245	R248	M249	L251	P254	L331	L332	S333	E334	Q335	E336	A337	Q338	K339	K340	L341	N342	N343	F344	D345	K346	Y347	G348	L349	L350	V351	G352	G353	K354	K355	I358	D359	S360	Y361	F217	Y218	M219	G220	L221	K224	R225	D226	R227	T228	Q229	Q230	D233	D236	E237	F238	M239	T243	D244	Y175	G176	M177	G178	I179	P180	V181	G182	K183	L184	C185	L186	G190	A191	G192	I193	R194	R197	G198	L199	P200	C202	L203	D204	V205	G206	T207	D208	N209	L210	A211	K214	K215	L216	F134	I135	S136	L137	R140	V143	R144	W150	L151	E152	N153	K156	A157	T161	D162	G163	E164	I166	L169	G170	D171	L172	G173	V174	Y175	G176	M177	G178	I179	P180	V181	G182	K183	L184	C185	L186	G190	A191	G192	I193	R194	R197	G198	L199	P200	C202	L203	D204	V205	G206	T207	D208	N209	L210	A211	K214	K215	L216	F134	I135	S136	L137	R140	V143	H69	R70	M71	L72	K73	E152	M75	T76	S77	K81	I83	Y84	I86	M86	Q89	R90	R91	N92	E93	K94	L95	G96	Y97	R98	I99	L100	D103	I104	E105	S106	G107	M108	P109	I110	V111	T115	G120	Y123	G124	H125	I126	K131	G132	L133	F134	I135	S136	L137	R140	V143	H69	R70	M71	L72	K73	E152	M75	T76	S77	K81	I83	Y84	I86	M86	Q89	R90	R91	N92	E93	K94	L95	G96	Y97	R98	I99	L100	D103	I104	E105	S106	G107	M108	P109	I110	V111	T115	G120	Y123	G124	H125	I126	K131	G132	L133	F134	I135	S136	L137	R140	V143	H69	R70	M71	L72	K73	E152	M75	T76	S77	K81	I83	Y84	I86	M86	Q89	R90	R91	N92	E93	K94	L95	G96	Y97	R98	I99	L100	D103	I104	E105	S106	G107	M108	P109	I110	V111	T115	G120	Y123	G124	H125	I126	K131	G132	L133	F134	I135	S136	L137	R140	V143	H69	R70	M71	L72	K73	E152	M75	T76	S77	K81	I83	Y84	I86	M86	Q89	R90	R91	N92	E93	K94	L95	G96	Y97	R98	I99	L100	D103	I104	E105	S106	G107	M108	P109	I110	V111	T115	G120	Y123	G124	H125	I126	K131	G132	L133	F134	I135	S136	L137	R140	V143	H69	R70	M71	L72	K73	E152	M75	T76	S77	K81	I83	Y84	I86	M86	Q89	R90	R91	N92	E93	K94	L95	G96	Y97	R98	I99	L100	D103	I104	E105	S106	G107	M108	P109	I110	V111	T115	G120	Y123	G124	H125	I126	K131	G132	L133	F134	I135	S136	L137	R140	V143	H69	R70	M71	L72	K73	E152	M75	T76	S77	K81	I83	Y84	I86	M86	Q89	R90	R91	N92	E93	K94	L95	G96	Y97	R98	I99	L100	D103	I104	E105	S106	G107	M108	P109	I110	V111	T115	G120	Y123	G124	H125	I126	K131	G132	L133	F134	I135	S136	L137	R140	V143	H69	R70	M71	L72	K73	E152	M75	T76	S77	K81	I83	Y84	I86	M86	Q89	R90	R91	N92	E93	K94	L95	G96	Y97	R98	I99	L100	D103	I104	E105	S106	G107	M108	P109	I110	V111	T115	G120	Y123	G124	H125	I126	K131	G132	L133	F134	I135	S136	L137	R140	V143	H69	R70	M71	L72	K73	E152	M75	T76	S77	K81	I83	Y84	I86	M86	Q89	R90	R91	N92	E93	K94	L95	G96	Y97	R98	I99	L100	D103	I104	E105	S106	G107	M108	P109	I110	V111	T115	G120	Y123	G124	H125	I126	K131	G132	L133	F134	I135	S136	L137	R140	V143	H69	R70	M71	L72	K73	E152	M75	T76	S77	K81	I83	Y84	I86	M86	Q89	R90	R91	N92	E93	K94	L95	G96	Y97	R98	I99	L100	D103	I104	E105	S106	G107	M108	P109	I110	V111	T115	G120	Y123	G124	H125	I126	K131	G132	L133	F134	I135	S136	L137	R140	V143	H69	R70	M71	L72	K73	E152	M75	T76	S77	K81	I83	Y84	I86	M86	Q89	R90	R91	N92	E93	K94	L95	G96	Y97	R98	I99	L100	D103	I104	E105	S106	G107	M108	P109	I110	V111	T115	G120	Y123	G124	H125	I126	K131	G132	L133	F134	I135	S136	L137	R140	V143	H69	R70	M71	L72	K73	E152	M75	T76	S77	K81	I83	Y84	I86	M86	Q89	R90	R91	N92	E93	K94	L95	G96	Y97	R98	I99	L100	D103	I104	E105	S106	G107	M108	P109	I110	V111	T115	G120	Y123	G124	H125	I126	K131	G132	L133	F134	I135	S136	L137	R140	V143	H69	R70	M71	L72	K73	E152	M75	T76	S77	K81	I83	Y84	I86	M86	Q89	R90	R91	N92	E93	K94	L95	G96	Y97	R98	I99	L100	D103	I104	E105	S106	G107	M108	P109	I110	V111	T115	G120	Y123	G124	H125	I126	K131	G132	L133	F134	I135	S136	L137	R140	V143	H69	R70	M71	L72	K73	E152	M75	T76	S77	K81	I83	Y84	I86	M86	Q89	R90	R91	N92	E93	K94	L95	G96	Y97	R98	I99	L100	D103	I104	E105	S106	G107	M108	P109	I110	V111	T115	G120	Y123	G124	H125	I126	K131	G132	L133	F134	I135	S136	L137	R140	V143	H69	R70	M71	L72	K73	E152	M75	T76	S77	K81	I83	Y84	I86	M86	Q89	R90	R91	N92	E93	K94	L95	G96	Y97	R98	I99	L100	D103	I104	E105	S106	G107	M108	P109	I110	V111	T115	G120	Y123	G124	H125	I126	K131	G132	L133	F134	I135	S136	L137	R140	V143	H69	R70	M71	L72	K73	E152	M75	T76	S77	K81	I83	Y84	I86	M86	Q89	R90	R91	N92	E93	K94	L95	G96	Y97	R98	I99	L100	D103	I104	E105	S106	G107	M108	P109	I110	V111	T115	G120	Y123	G124	H125	I126	K131	G132	L133	F134	I135	S136	L137	R140	V143	H69	R70	M71	L72	K73	E152	M75	T76	S77	K81	I83	Y84	I86	M86	Q89	R90	R91	N92	E93	K94	L95	G96	Y97	R98	I99	L100	D103	I104	E105	S106	G107	M108	P109	I110	V111	T115	G120	Y123	G124	H125	I126	K131	G132	L133	F134	I135	S136	L137	R140	V143	H69	R70	M71	L72	K73	E152	M75	T76	S77	K81	I83	Y84	I86	M86	Q89	R90	R91	N92	E93	K94	L95	G96	Y97	R98	I99	L100	D103	I104	E105	S106	G107	M108	P109	I110	V111	T115	G120	Y123	G124	H125	I126	K131	G132	L133	F134	I135	S136	L137	R140	V143	H69	R70	M71	L72	K73	E152	M75	T76	S77	K81	I83	Y84	I86	M86	Q89	R90	R91	N92	E93	K94	L95	G96	Y97	R98	I99	L100	D103	I104	E105	S106	G107	M108	P109	I110	V111	T115	G120	Y123	G124	H125	I126	K131	G132	L133	F134	I135	S136	L137	R140	V143	H69	R70	M71	L72	K73	E152	M75	T76	S77	K81	I83	Y84	I86	M86	Q89	R90	R91	N92	E93	K94	L95	G96	Y97	R98	I99	L100	D103	I104	E105	S106	G107	M108	P109	I110	V111	T115	G120	Y123	G124	H125	I126	K131	G132	L133	F134	I135	S136	L137	R140	V143	H69	R70	M71	L72	K73	E152	M75	T76	S77	K81	I83	Y84	I86	M86	Q89	R90	R91	N92	E93	K94	L95	G96	Y97	R98	I99	L100	D103	I104	E105	S106	G107	M108	P109	I110	V111	T115	G120	Y123	G124	H125	I126	K131	G132	L133	F134	I135	S136	L137	R140	V143	H69	R70	M71	L72	K73	E152	M75	T76	S77	K81	I83	Y84	I86	M86	Q89	R90	R91	N92	E93	K94	L95	G96	Y97	R98	I99	L100	D103	I104	E105	S106	G107	M108	P109	I110	V111	T115	G120	Y123	G124	H125	I126	K131	G132	L133	F134	I135	S136	L137	R140	V143	H69	R70	M71	L72	K73	E152	M75	T76	S77	K81	I83	Y84	I86	M86	Q89	R90	R91	N92	E93	K94	L95	G96	Y97	R98	I99	L100	D103	I104	E105	S106	G107	M108	P109	I110	V111	T115	G120	Y123	G124	H125	I126	K131	G132	L133	F134	I135	S136	L137	R140	V143	H69	R70	M71	L72	K73	E152	M75	T76	S77	K81	I83	Y84	I86	M86	Q89	R90	R91	N92	E93	K94	L95	G96	Y97	R98	I99	L100	D103	I104	E105	S106	G107	M108	P109	I110	V111	T115	G120	Y123	G124	H125	I126	K131	G132	L133	F134	I135	S136	L137	R140	V143	H69	R70	M71	L72	K73	E152	M75	T76	S77	K81	I83	Y84	I86	M86	Q89	R90	R91	N92	E93	K94	L95	G96	Y97	R98	I99	L100	D103	I104	E105	S106	G107	M108	P109	I110	V111	T115	G120	Y123	G124	H125	I126	K131	G132	L133	F134	I135	S136	L137	R140	V143	H69	R70	M71	L72	K73	E152	M75	T76	S77	K81	I83	Y84	I86	M86	Q89	R90	R91	N92	E93	K94	L95	G96	Y97	R98	I99	L100	D103	I104	E105	S106	G107	M108	P109	I110	V111	T115	G120	Y123	G124	H125	I126	K131	G132	L133	F134	I135	S136	L137	R140	V143	H69	R70	M71	L72	K73	E152	M75	T76	S77	K81	I83	Y

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	229.60 Å 118.60 Å 113.10 Å 90.00° 109.60° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	94.0 (20.00-2.60)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.218 , 0.301	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17931	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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, MAK, 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	0.44	0/4447	0.64	0/5998
1	B	0.45	0/4447	0.64	0/5998
1	C	0.46	0/4447	0.65	0/5998
1	D	0.45	1/4447 (0.0%)	0.64	0/5998
All	All	0.45	1/17788 (0.0%)	0.64	0/23992

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	185	CYS	CB-SG	-5.57	1.72	1.81

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	4367	0	4407	359	0
1	B	4367	0	4407	313	0
1	C	4367	0	4407	217	0
1	D	4367	0	4407	334	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	4	0
3	B	88	0	52	5	0
3	C	88	0	52	3	0
3	D	88	0	52	3	0
4	A	8	0	0	1	0
4	B	8	0	0	1	0
4	C	8	0	0	1	0
4	D	8	0	0	2	0
5	A	25	0	0	4	0
5	B	18	0	0	4	0
5	C	16	0	0	3	0
5	D	16	0	0	1	0
All	All	17931	0	17836	1198	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 34.

The worst 5 of 1198 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:C:210:ILE:H	1:C:210:ILE:HD13	1.00	1.10
1:D:140:ARG:HH22	1:D:233:ASP:HB3	1.15	1.09
1:D:177:MSE:HE1	1:D:181:VAL:HG23	1.34	1.06
1:A:327:MSE:HE3	1:A:337:ALA:HB1	1.38	1.06
1:B:354:ARG:HE	1:B:358:ILE:HD11	1.21	1.06

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%)	512 (93%)	34 (6%)	5 (1%)	21	42
1	B	551/584 (94%)	512 (93%)	32 (6%)	7 (1%)	15	30
1	C	551/584 (94%)	513 (93%)	34 (6%)	4 (1%)	26	51
1	D	551/584 (94%)	499 (91%)	43 (8%)	9 (2%)	12	24
All	All	2204/2336 (94%)	2036 (92%)	143 (6%)	25 (1%)	17	36

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	332	LEU
1	B	332	LEU
1	C	332	LEU
1	D	270	ARG
1	D	332	LEU

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%)	374 (80%)	95 (20%)	1	2
1	C	469/483 (97%)	380 (81%)	89 (19%)	2	3
1	D	469/483 (97%)	356 (76%)	113 (24%)	1	1
All	All	1876/1932 (97%)	1481 (79%)	395 (21%)	1	2

5 of 395 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	511	ARG
1	C	223	GLN
1	D	445	SER
1	B	522	VAL
1	C	75	MSE

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	518	ASN
1	C	229	GLN
1	D	425	GLN
1	B	520	GLN
1	C	69	HIS

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	1.80	9 (23%)	47,73,73	1.90	4 (8%)
3	NAD	A	602	-	38,48,48	1.85	9 (23%)	47,73,73	1.92	5 (10%)
4	MAK	A	603	2	1,7,7	3.34	1 (100%)	0,9,9	0.00	-
3	NAD	B	1601	-	38,48,48	1.68	7 (18%)	47,73,73	2.06	6 (12%)
3	NAD	B	1602	-	38,48,48	1.92	10 (26%)	47,73,73	1.89	5 (10%)
4	MAK	B	1603	2	1,7,7	3.20	1 (100%)	0,9,9	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	C	2601	-	38,48,48	1.68	8 (21%)	47,73,73	1.96	8 (17%)
3	NAD	C	2602	-	38,48,48	2.01	9 (23%)	47,73,73	1.90	5 (10%)
4	MAK	C	2603	2	1,7,7	3.22	1 (100%)	0,9,9	0.00	-
3	NAD	D	3601	-	38,48,48	1.95	8 (21%)	47,73,73	1.98	4 (8%)
3	NAD	D	3602	-	38,48,48	1.80	9 (23%)	47,73,73	1.96	4 (8%)
4	MAK	D	3603	2	1,7,7	3.16	1 (100%)	0,9,9	0.00	-

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	MAK	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	MAK	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	MAK	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	MAK	D	3603	2	-	0/0/8/8	0/0/0/0

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3601	NAD	C5A-C4A	-3.33	1.33	1.40
3	B	1601	NAD	C5A-C4A	-3.18	1.33	1.40
3	C	2601	NAD	C5A-C4A	-3.18	1.33	1.40
3	A	601	NAD	C5A-C4A	-2.98	1.33	1.40
3	D	3602	NAD	C5A-C4A	-2.88	1.34	1.40

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1601	NAD	N3A-C2A-N1A	-11.17	120.34	128.89
3	D	3602	NAD	N3A-C2A-N1A	-10.69	120.71	128.89
3	D	3601	NAD	N3A-C2A-N1A	-10.63	120.76	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2601	NAD	N3A-C2A-N1A	-10.40	120.94	128.89
3	A	602	NAD	N3A-C2A-N1A	-10.36	120.96	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	NAD	3	0
3	A	602	NAD	1	0
4	A	603	MAK	1	0
3	B	1601	NAD	4	0
3	B	1602	NAD	1	0
4	B	1603	MAK	1	0
3	C	2601	NAD	3	0
4	C	2603	MAK	1	0
3	D	3601	NAD	3	0
4	D	3603	MAK	2	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.