



wwPDB X-ray Structure Validation Summary Report i

Feb 26, 2014 – 06:04 PM GMT

PDB ID : 2E37
Title : Structure of TT0471 protein from *Thermus thermophilus*
Authors : Lokanath, N.K.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2006-11-21
Resolution : 2.30 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

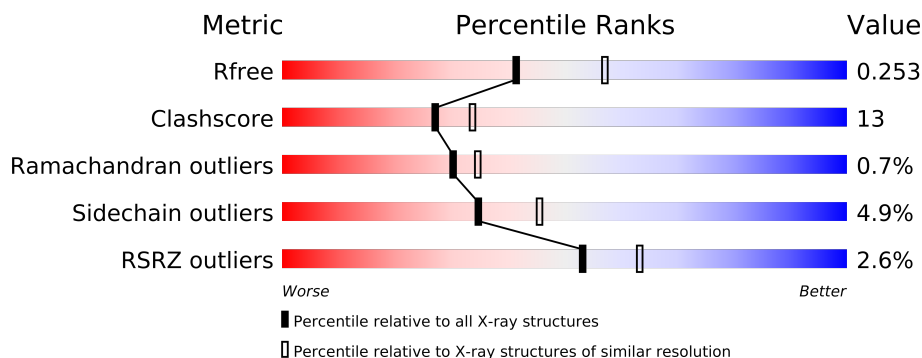
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	310	
1	B	310	
1	C	310	
1	D	310	
1	E	310	
1	F	310	
1	G	310	
1	H	310	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	B	1501	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19337 atoms, of which 0 are hydrogen and 0 are deuterium.

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 L-lactate dehydrogenase.

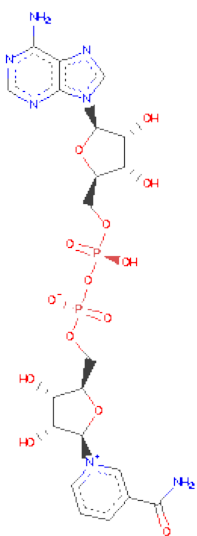
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	Se	0	0	0
			2300	1460	410	427	3			
1	B	304	Total	C	N	O	Se	0	0	0
			2268	1441	405	419	3			
1	C	310	Total	C	N	O	Se	0	0	0
			2315	1468	415	429	3			
1	D	302	Total	C	N	O	Se	0	0	0
			2253	1433	400	417	3			
1	E	304	Total	C	N	O	Se	0	0	0
			2271	1442	403	423	3			
1	F	308	Total	C	N	O	Se	0	0	0
			2300	1460	410	427	3			
1	G	310	Total	C	N	O	Se	0	0	0
			2315	1468	415	429	3			
1	H	308	Total	C	N	O	Se	0	0	0
			2300	1460	410	427	3			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	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		

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

- Molecule 4 is water.

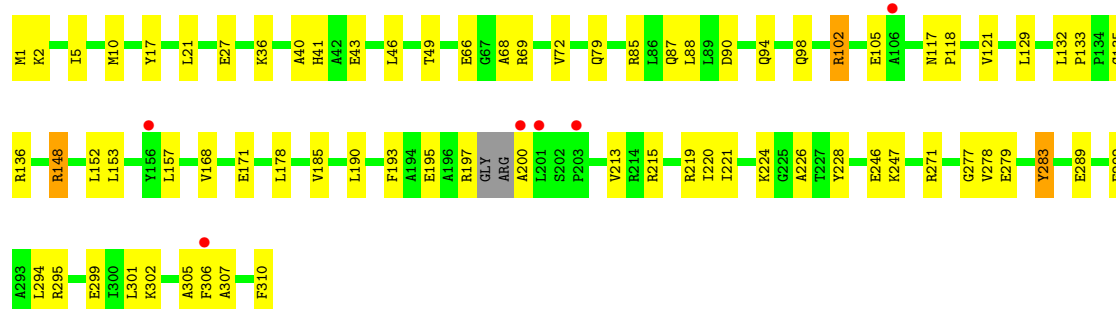
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	123	Total	O	0	0
			123	123		
4	B	76	Total	O	0	0
			76	76		
4	C	140	Total	O	0	0
			140	140		
4	D	60	Total	O	0	0
			60	60		
4	E	84	Total	O	0	0
			84	84		
4	F	100	Total	O	0	0
			100	100		
4	G	129	Total	O	0	0
			129	129		
4	H	117	Total	O	0	0
			117	117		

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.

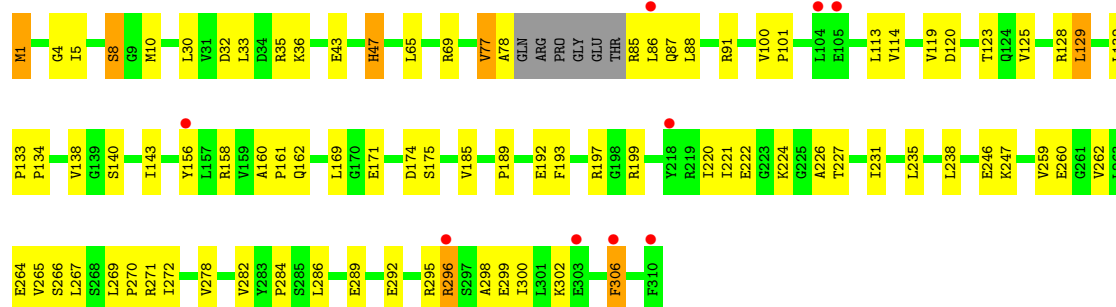
- Molecule 1: L-lactate dehydrogenase

Chain A: 



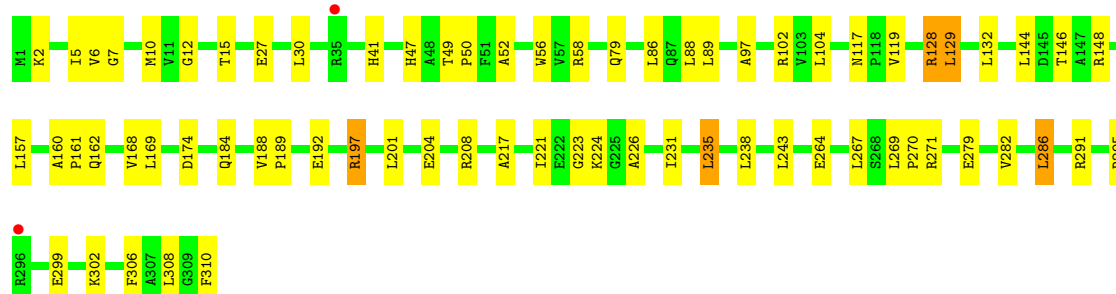
- Molecule 1: L-lactate dehydrogenase

Chain B: 

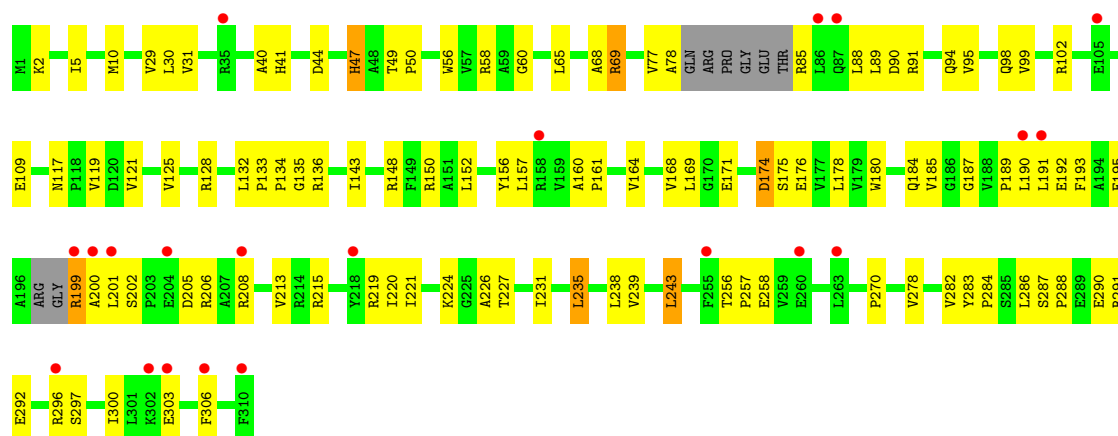


- Molecule 1: L-lactate dehydrogenase

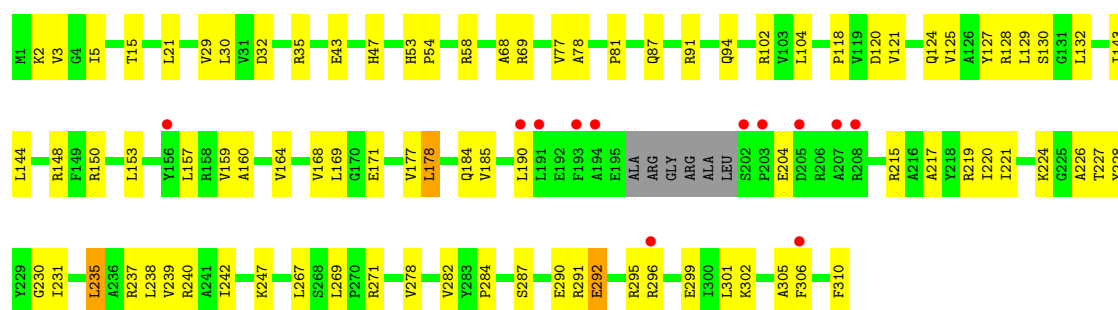
Chain C: 



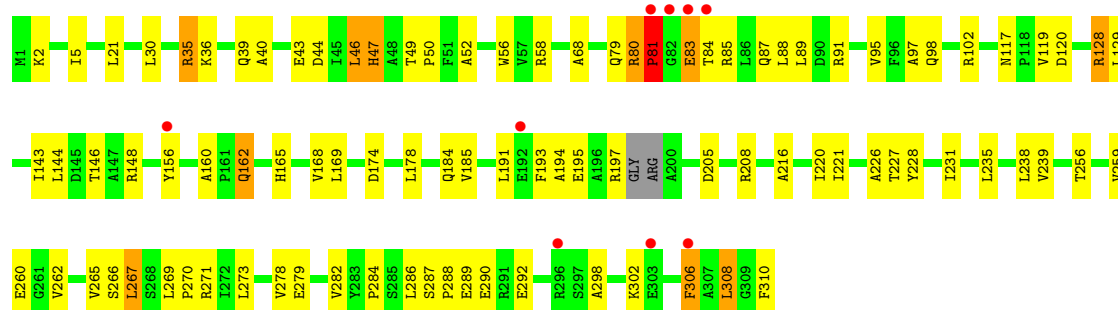
- Molecule 1: L-lactate dehydrogenase

Chain D: 

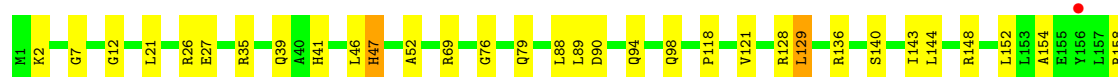
- Molecule 1: L-lactate dehydrogenase

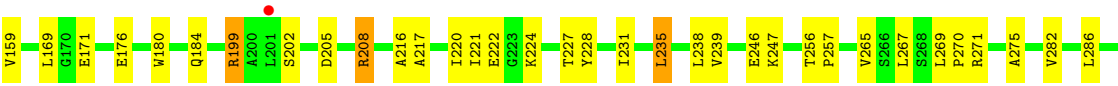
Chain E: 

- Molecule 1: L-lactate dehydrogenase

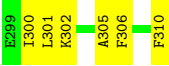
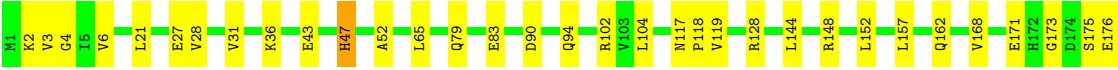
Chain F: 

- Molecule 1: L-lactate dehydrogenase

Chain G: 



● Molecule 1: L-lactate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.74Å 135.64Å 162.06Å 90.00° 113.79° 90.00°	Depositor
Resolution (Å)	44.01 – 2.30 44.01 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.1 (44.01-2.30) 95.2 (44.01-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.255 0.214 , 0.253	Depositor DCC
R_{free} test set	6900 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.609	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 135809 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19337	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	0.39	0/2337	0.65	0/3175
1	B	0.41	0/2304	0.69	0/3129
1	C	0.40	0/2353	0.67	0/3197
1	D	0.39	0/2288	0.66	0/3107
1	E	0.39	0/2308	0.66	0/3136
1	F	0.43	0/2337	0.71	0/3175
1	G	0.47	1/2353 (0.0%)	0.71	0/3197
1	H	0.44	0/2337	0.70	0/3175
All	All	0.42	1/18617 (0.0%)	0.68	0/25291

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	180	TRP	NE1-CE2	8.71	1.48	1.37

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2300	0	2350	61	0
1	B	2268	0	2322	71	0
1	C	2315	0	2367	47	0
1	D	2253	0	2305	89	0
1	E	2271	0	2316	71	0
1	F	2300	0	2350	84	0
1	G	2315	0	2367	50	0
1	H	2300	0	2350	49	0
2	B	5	0	0	1	0
2	H	5	0	0	0	0
3	A	44	0	26	0	0
3	C	44	0	26	0	0
3	E	44	0	26	0	0
3	G	44	0	26	1	0
4	A	123	0	0	4	0
4	B	76	0	0	2	0
4	C	140	0	0	4	0
4	D	60	0	0	0	0
4	E	84	0	0	3	0
4	F	100	0	0	5	0
4	G	129	0	0	2	0
4	H	117	0	0	2	0
All	All	19337	0	18831	484	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

The worst 5 of 484 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:79:GLN:HE22	1:F:84:THR:HA	1.14	1.09
1:D:156:TYR:CE2	1:D:201:LEU:HD23	1.96	1.01
1:D:69:ARG:HH11	1:D:69:ARG:HB3	1.24	0.99
1:D:192:GLU:HG3	1:D:193:PHE:H	1.32	0.93
1:D:192:GLU:HG3	1:D:193:PHE:N	1.85	0.92

There are no symmetry-related clashes.

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	304/310 (98%)	290 (95%)	14 (5%)	0	100	100
1	B	300/310 (97%)	279 (93%)	19 (6%)	2 (1%)	30	34
1	C	308/310 (99%)	295 (96%)	10 (3%)	3 (1%)	22	23
1	D	296/310 (96%)	282 (95%)	13 (4%)	1 (0%)	50	60
1	E	300/310 (97%)	282 (94%)	16 (5%)	2 (1%)	30	34
1	F	304/310 (98%)	288 (95%)	12 (4%)	4 (1%)	18	17
1	G	308/310 (99%)	296 (96%)	10 (3%)	2 (1%)	33	39
1	H	304/310 (98%)	294 (97%)	8 (3%)	2 (1%)	30	34
All	All	2424/2480 (98%)	2306 (95%)	102 (4%)	16 (1%)	30	34

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	264	GLU
1	F	80	ARG
1	F	81	PRO
1	H	228	TYR
1	C	52	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	231/229 (101%)	224 (97%)	7 (3%)	53	70
1	B	227/229 (99%)	215 (95%)	12 (5%)	32	41
1	C	232/229 (101%)	219 (94%)	13 (6%)	30	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	226/229 (99%)	214 (95%)	12 (5%)	32	41
1	E	229/229 (100%)	221 (96%)	8 (4%)	48	63
1	F	231/229 (101%)	216 (94%)	15 (6%)	24	30
1	G	232/229 (101%)	218 (94%)	14 (6%)	27	35
1	H	231/229 (101%)	221 (96%)	10 (4%)	40	52
All	All	1839/1832 (100%)	1748 (95%)	91 (5%)	35	45

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	296	ARG
1	E	292	GLU
1	H	104	LEU
1	D	303	GLU
1	E	178	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	41	HIS
1	E	47	HIS
1	F	79	GLN
1	D	172	HIS
1	E	117	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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

6 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	$\# Z > 2$
3	NAD	A	1401	-	48,48,48	2.54	17 (35%)	73,73,73	2.50	19 (26%)
2	SO4	B	1501	-	4,4,4	1.55	1 (25%)	6,6,6	1.35	1 (16%)
3	NAD	C	1402	-	48,48,48	2.51	17 (35%)	73,73,73	2.47	18 (24%)
3	NAD	E	1403	-	48,48,48	2.56	17 (35%)	73,73,73	2.47	19 (26%)
3	NAD	G	1404	-	48,48,48	2.56	17 (35%)	73,73,73	2.50	18 (24%)
2	SO4	H	1502	-	4,4,4	0.31	0	6,6,6	0.07	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	1401	-	-	0/30/62/62	0/3/5/5
2	SO4	B	1501	-	-	0/0/0/0	0/0/0/0
3	NAD	C	1402	-	-	0/30/62/62	0/3/5/5
3	NAD	E	1403	-	-	0/30/62/62	0/3/5/5
3	NAD	G	1404	-	-	0/30/62/62	0/3/5/5
2	SO4	H	1502	-	-	0/0/0/0	0/0/0/0

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1403	NAD	C2N-N1N	8.03	1.45	1.35
3	G	1404	NAD	C2N-N1N	7.89	1.45	1.35
3	A	1401	NAD	C2N-N1N	7.79	1.45	1.35
3	C	1402	NAD	C2N-N1N	7.54	1.45	1.35
3	A	1401	NAD	C4N-C3N	5.86	1.49	1.39

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1402	NAD	N3A-C2A-N1A	-12.17	118.54	128.71
3	A	1401	NAD	N3A-C2A-N1A	-12.14	118.56	128.71
3	G	1404	NAD	N3A-C2A-N1A	-12.13	118.57	128.71
3	E	1403	NAD	N3A-C2A-N1A	-12.13	118.57	128.71
3	A	1401	NAD	C4B-O4B-C1B	-9.60	99.32	109.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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	308/310 (99%)	0.03	6 (1%) 64 73	31, 43, 61, 91	0
1	B	304/310 (98%)	0.23	9 (2%) 48 58	28, 47, 72, 98	0
1	C	310/310 (100%)	-0.13	2 (0%) 86 92	26, 40, 52, 69	0
1	D	302/310 (97%)	0.47	21 (6%) 16 23	32, 55, 82, 99	0
1	E	304/310 (98%)	0.29	12 (3%) 37 48	32, 46, 67, 93	0
1	F	308/310 (99%)	0.21	9 (2%) 49 59	31, 44, 73, 103	0
1	G	310/310 (100%)	-0.12	3 (0%) 79 87	27, 39, 55, 68	0
1	H	308/310 (99%)	-0.02	2 (0%) 86 92	24, 38, 64, 80	0
All	All	2454/2480 (98%)	0.12	64 (2%) 53 63	24, 43, 70, 103	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	191	LEU	5.5
1	D	306	PHE	4.9
1	D	86	LEU	4.8
1	D	263	LEU	4.8
1	D	296	ARG	4.8

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	B	1501	5/5	0.30	4.12	112,112,112,113	0
3	NAD	A	1401	44/44	0.15	1.02	48,56,69,70	0
3	NAD	G	1404	44/44	0.16	0.99	50,56,67,68	0
2	SO4	H	1502	5/5	0.15	0.72	100,101,102,102	0
3	NAD	C	1402	44/44	0.15	0.66	59,64,71,72	0
3	NAD	E	1403	44/44	0.15	0.64	50,63,80,81	0

6.5 Other polymers

There are no such residues in this entry.