



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:15 AM UTC

PDB ID : 4JDC / pdb_00004jdc
Title : Crystal structure of the Delta-pyrroline-5-carboxylate dehydrogenase from Mycobacterium tuberculosis
Authors : Lagautriere, T.; Bashiri, G.; Baker, E.N.
Deposited on : 2013-02-24
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

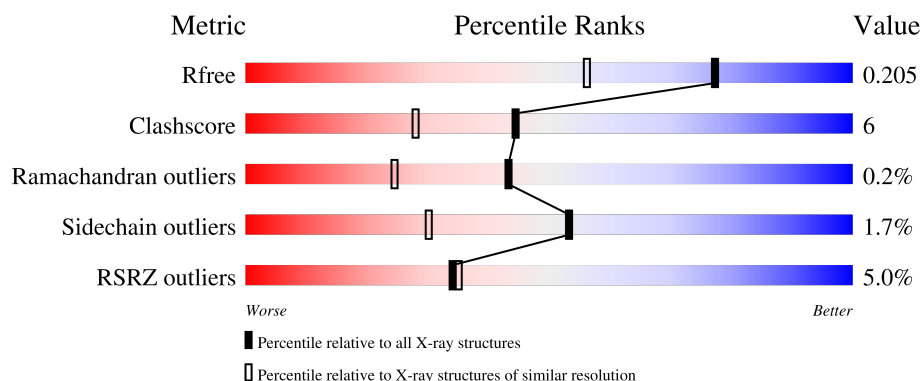
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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))
R_{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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.

Mol	Chain	Length	Quality of chain
1	A	563	5% 70% 23% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4528 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 1-pyrroline-5-carboxylate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	536	4112	2604	729	768	11	0	1	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP I6X0K4
A	-18	GLY	-	expression tag	UNP I6X0K4
A	-17	SER	-	expression tag	UNP I6X0K4
A	-16	SER	-	expression tag	UNP I6X0K4
A	-15	HIS	-	expression tag	UNP I6X0K4
A	-14	HIS	-	expression tag	UNP I6X0K4
A	-13	HIS	-	expression tag	UNP I6X0K4
A	-12	HIS	-	expression tag	UNP I6X0K4
A	-11	HIS	-	expression tag	UNP I6X0K4
A	-10	HIS	-	expression tag	UNP I6X0K4
A	-9	SER	-	expression tag	UNP I6X0K4
A	-8	SER	-	expression tag	UNP I6X0K4
A	-7	GLY	-	expression tag	UNP I6X0K4
A	-6	LEU	-	expression tag	UNP I6X0K4
A	-5	VAL	-	expression tag	UNP I6X0K4
A	-4	PRO	-	expression tag	UNP I6X0K4
A	-3	ARG	-	expression tag	UNP I6X0K4
A	-2	GLY	-	expression tag	UNP I6X0K4
A	-1	SER	-	expression tag	UNP I6X0K4
A	0	HIS	-	expression tag	UNP I6X0K4
A	505	ASP	GLY	engineered mutation	UNP I6X0K4

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

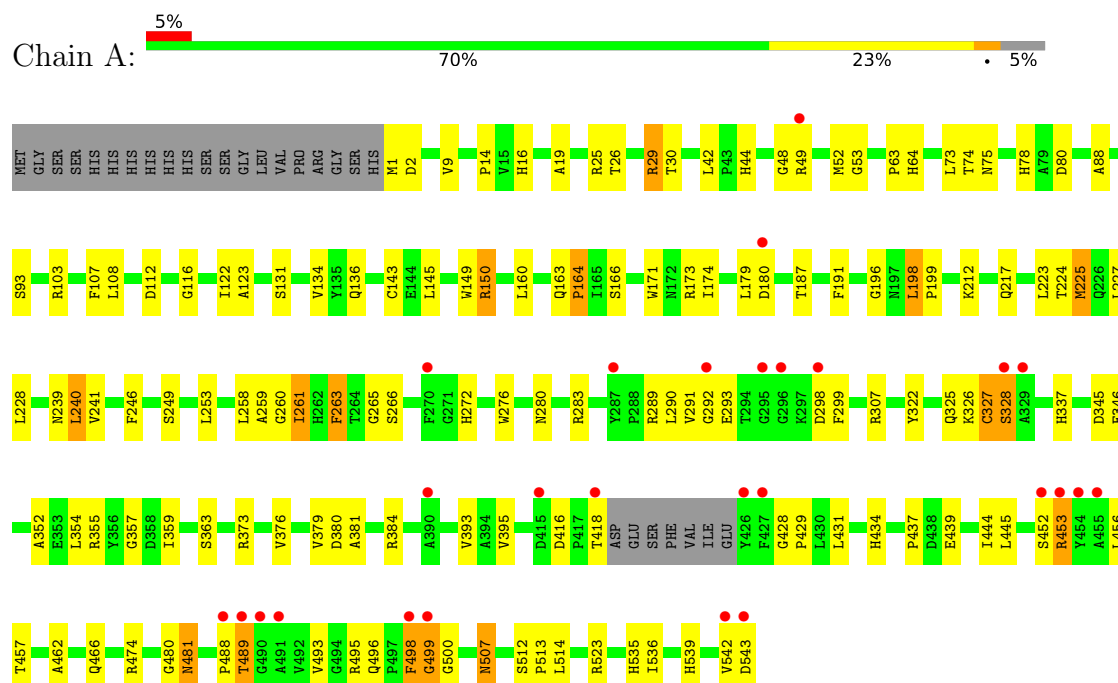
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	389	Total	O	0	0
			389	389		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 1-pyrroline-5-carboxylate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 6 2 2	Depositor
Cell constants a, b, c, α , β , γ	163.13Å 163.13Å 96.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.80 – 1.60 29.80 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.80-1.60) 99.7 (29.80-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.170 , 0.202 0.179 , 0.205	Depositor DCC
R_{free} test set	4908 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4528	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, CME

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	1.86	93/4201 (2.2%)	1.49	29/5728 (0.5%)

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	462	ALA	N-CA	8.19	1.56	1.46
1	A	64	HIS	CE1-NE2	7.91	1.40	1.32
1	A	9	VAL	CA-C	7.47	1.59	1.53
1	A	291	VAL	C-O	-7.37	1.16	1.24
1	A	163	GLN	C-O	-7.27	1.16	1.24
1	A	198	LEU	C-O	-7.14	1.17	1.24
1	A	507	ASN	CG-ND2	7.02	1.48	1.33
1	A	191	PHE	C-O	-6.74	1.16	1.23
1	A	239	ASN	C-O	-6.62	1.16	1.24
1	A	73	LEU	CA-CB	6.57	1.63	1.53
1	A	261	ILE	C-O	-6.57	1.17	1.24
1	A	507	ASN	N-CA	6.47	1.54	1.46
1	A	143	CYS	C-O	-6.46	1.16	1.24
1	A	145	LEU	C-O	-6.42	1.16	1.24
1	A	64	HIS	CG-CD2	6.36	1.42	1.35
1	A	535	HIS	ND1-CE1	6.34	1.38	1.32
1	A	16	HIS	C-O	-6.26	1.16	1.23
1	A	29	ARG	N-CA	6.25	1.53	1.46
1	A	116	GLY	N-CA	6.05	1.53	1.44
1	A	493	VAL	N-CA	6.01	1.53	1.46
1	A	434	HIS	ND1-CE1	5.99	1.38	1.32
1	A	381	ALA	CA-C	-5.99	1.45	1.52
1	A	507	ASN	CA-C	5.99	1.60	1.52
1	A	289	ARG	C-O	-5.98	1.16	1.24
1	A	393	VAL	CA-C	-5.96	1.46	1.53
1	A	439	GLU	CD-OE1	5.95	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	PRO	N-CD	5.94	1.56	1.47
1	A	272	HIS	CG-CD2	5.93	1.42	1.35
1	A	78	HIS	CG-CD2	5.90	1.42	1.35
1	A	512	SER	N-CA	-5.90	1.40	1.46
1	A	380	ASP	N-CA	5.87	1.53	1.46
1	A	357	GLY	N-CA	5.87	1.52	1.45
1	A	536	ILE	CA-CB	5.77	1.60	1.54
1	A	513	PRO	N-CD	5.76	1.55	1.47
1	A	75	ASN	CA-C	-5.71	1.45	1.52
1	A	429	PRO	N-CD	5.67	1.55	1.47
1	A	437	PRO	CA-CB	5.67	1.61	1.53
1	A	431	LEU	C-O	-5.67	1.17	1.24
1	A	48	GLY	C-O	-5.66	1.16	1.24
1	A	379	VAL	C-O	5.63	1.30	1.24
1	A	376	VAL	N-CA	5.62	1.53	1.46
1	A	171	TRP	N-CA	5.61	1.53	1.46
1	A	196	GLY	C-O	-5.59	1.17	1.24
1	A	434	HIS	CE1-NE2	5.58	1.38	1.32
1	A	293	GLU	C-O	-5.58	1.17	1.23
1	A	2	ASP	C-O	-5.57	1.17	1.23
1	A	173	ARG	N-CA	5.57	1.53	1.45
1	A	498	PHE	N-CA	5.53	1.53	1.46
1	A	445	LEU	C-O	-5.53	1.17	1.24
1	A	150	ARG	C-O	-5.52	1.17	1.24
1	A	325	GLN	CA-CB	5.51	1.61	1.53
1	A	337	HIS	CA-C	-5.50	1.45	1.52
1	A	363	SER	CA-CB	5.50	1.62	1.53
1	A	428	GLY	C-O	-5.49	1.16	1.24
1	A	263	PHE	C-O	-5.44	1.17	1.23
1	A	166	SER	C-O	-5.44	1.17	1.24
1	A	14	PRO	C-O	-5.43	1.17	1.23
1	A	258	LEU	C-O	-5.42	1.17	1.24
1	A	225	MET	C-O	-5.40	1.17	1.24
1	A	123	ALA	N-CA	5.39	1.52	1.46
1	A	466	GLN	C-O	-5.37	1.17	1.24
1	A	134	VAL	C-O	-5.37	1.17	1.24
1	A	149	TRP	C-O	-5.36	1.17	1.24
1	A	246	PHE	C-O	5.36	1.30	1.24
1	A	228	LEU	C-O	-5.34	1.17	1.24
1	A	539	HIS	CE1-NE2	5.34	1.37	1.32
1	A	103	ARG	CD-NE	5.32	1.53	1.46
1	A	260	GLY	C-O	-5.31	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	PRO	N-CD	5.27	1.55	1.47
1	A	53	GLY	C-O	5.25	1.29	1.23
1	A	63	PRO	CA-CB	5.25	1.61	1.53
1	A	539	HIS	CG-CD2	5.21	1.41	1.35
1	A	488	PRO	N-CD	5.17	1.54	1.47
1	A	500	GLY	C-O	5.17	1.28	1.23
1	A	240	LEU	C-O	-5.16	1.17	1.24
1	A	49	ARG	C-O	-5.16	1.17	1.24
1	A	345	ASP	N-CA	5.14	1.52	1.46
1	A	112	ASP	C-O	5.14	1.30	1.24
1	A	523	ARG	N-CA	5.11	1.52	1.46
1	A	179	LEU	C-O	-5.10	1.16	1.23
1	A	481	ASN	C-O	-5.10	1.17	1.23
1	A	272	HIS	ND1-CE1	5.09	1.37	1.32
1	A	42	LEU	CA-CB	5.09	1.60	1.53
1	A	322	TYR	CA-CB	5.09	1.61	1.53
1	A	357	GLY	C-O	5.09	1.28	1.23
1	A	512	SER	C-O	-5.09	1.19	1.24
1	A	224	THR	C-O	-5.06	1.18	1.24
1	A	539	HIS	ND1-CE1	5.06	1.37	1.32
1	A	354	LEU	C-O	-5.02	1.18	1.23
1	A	266	SER	C-O	-5.02	1.17	1.23
1	A	44	HIS	CG-CD2	5.00	1.41	1.35
1	A	217	GLN	CA-CB	5.00	1.61	1.53
1	A	265	GLY	C-O	-5.00	1.17	1.23

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	ARG	NE-CZ-NH1	-10.82	110.67	121.50
1	A	307	ARG	NE-CZ-NH2	9.87	128.08	119.20
1	A	452	SER	N-CA-C	9.38	122.91	112.97
1	A	500	GLY	N-CA-C	-8.60	96.94	111.20
1	A	495	ARG	CA-C-N	-6.45	115.23	123.16
1	A	495	ARG	C-N-CA	-6.45	115.23	123.16
1	A	163	GLN	CA-C-N	-6.44	114.09	120.98
1	A	163	GLN	C-N-CA	-6.44	114.09	120.98
1	A	30	THR	N-CA-C	6.31	117.83	111.07
1	A	507	ASN	N-CA-CB	6.29	120.08	110.14
1	A	108	LEU	N-CA-C	-5.92	104.90	111.36
1	A	26	THR	N-CA-C	5.80	118.35	111.33
1	A	507	ASN	N-CA-C	-5.77	104.36	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	LEU	CA-C-O	-5.66	113.71	120.10
1	A	93	SER	CA-C-O	-5.64	114.44	120.42
1	A	453	ARG	N-CA-C	5.58	117.44	111.36
1	A	416	ASP	CA-C-N	-5.48	112.99	119.84
1	A	416	ASP	C-N-CA	-5.48	112.99	119.84
1	A	107	PHE	CA-CB-CG	-5.47	108.33	113.80
1	A	163	GLN	O-C-N	5.47	125.81	121.55
1	A	512	SER	CA-C-N	-5.46	113.99	119.56
1	A	512	SER	C-N-CA	-5.46	113.99	119.56
1	A	379	VAL	CA-C-O	-5.44	115.40	121.17
1	A	19	ALA	CA-C-N	-5.35	114.27	119.78
1	A	19	ALA	C-N-CA	-5.35	114.27	119.78
1	A	496	GLN	O-C-N	5.28	126.12	121.37
1	A	80	ASP	N-CA-C	-5.25	105.46	111.07
1	A	88	ALA	N-CA-C	-5.15	105.67	111.28
1	A	122	ILE	O-C-N	5.12	127.11	121.83

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	4112	0	4023	49	0
2	A	27	0	12	1	0
3	A	389	0	0	12	0
All	All	4528	0	4035	49	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 6.

All (49) 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:542:VAL:HA	1:A:543:ASP:C	2.00	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ARG:HG2	1:A:474:ARG:HH11	1.50	0.76
1:A:298:ASP:C	3:A:1084:HOH:O	2.29	0.75
1:A:299:PHE:HB3	3:A:1084:HOH:O	1.90	0.71
1:A:542:VAL:CA	1:A:543:ASP:C	2.66	0.67
1:A:298:ASP:OD2	1:A:328:SER:HB3	1.94	0.66
1:A:164:PRO:HD3	1:A:174:ILE:HG13	1.77	0.66
1:A:418:THR:HG22	1:A:418:THR:O	1.98	0.62
1:A:52:MET:HE3	1:A:74:THR:HG23	1.82	0.62
1:A:480:GLY:O	1:A:481:ASN:ND2	2.28	0.62
1:A:240:LEU:C	1:A:240:LEU:HD23	2.26	0.61
1:A:373:ARG:NH1	3:A:809:HOH:O	2.34	0.60
1:A:355:ARG:HD2	3:A:893:HOH:O	2.03	0.57
1:A:489:THR:CG2	3:A:1038:HOH:O	2.51	0.57
1:A:136:GLN:OE1	1:A:326:LYS:HE3	2.05	0.57
1:A:474:ARG:HG2	1:A:474:ARG:NH1	2.14	0.57
1:A:299:PHE:N	3:A:1084:HOH:O	2.39	0.54
1:A:489:THR:HG23	3:A:1038:HOH:O	2.08	0.53
1:A:481:ASN:ND2	1:A:499[B]:GLY:HA3	2.24	0.53
1:A:298:ASP:CG	1:A:457:THR:OG1	2.52	0.52
1:A:261:ILE:HB	1:A:290:LEU:HD23	1.91	0.52
1:A:328:SER:O	1:A:489:THR:HG23	2.10	0.51
1:A:326:LYS:O	1:A:328:SER:N	2.44	0.51
1:A:253:LEU:HD23	1:A:276:TRP:CG	2.47	0.49
1:A:227:LEU:C	1:A:227:LEU:HD23	2.37	0.49
1:A:384:ARG:NH2	3:A:946:HOH:O	2.46	0.48
1:A:346:GLU:HG3	3:A:932:HOH:O	2.14	0.47
1:A:498:PHE:O	1:A:499[B]:GLY:O	2.31	0.47
1:A:180:ASP:O	1:A:259:ALA:HB2	2.15	0.47
1:A:249:SER:OG	2:A:601:NAD:N1A	2.46	0.47
1:A:489:THR:HG22	3:A:1038:HOH:O	2.14	0.46
1:A:25:ARG:O	1:A:29:ARG:HG2	2.16	0.46
1:A:352:ALA:HB2	1:A:395:VAL:HG21	1.98	0.46
1:A:514:LEU:HD22	1:A:514:LEU:N	2.31	0.45
1:A:480:GLY:C	1:A:481:ASN:HD22	2.20	0.44
1:A:150:ARG:HD2	3:A:728:HOH:O	2.16	0.44
1:A:326:LYS:C	1:A:328:SER:N	2.72	0.44
1:A:507:ASN:HA	3:A:888:HOH:O	2.18	0.43
1:A:240:LEU:HD23	1:A:241:VAL:N	2.34	0.43
1:A:187:THR:HG22	1:A:198:LEU:HD12	2.00	0.43
1:A:240:LEU:C	1:A:240:LEU:CD2	2.92	0.42
1:A:263:PHE:O	1:A:292:GLY:HA3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ASN:O	1:A:283:ARG:HG2	2.18	0.42
1:A:456:LEU:HG	1:A:457:THR:HG23	2.02	0.41
1:A:223:LEU:HD23	1:A:223:LEU:HA	1.95	0.41
1:A:225:MET:HG3	1:A:240:LEU:HD12	2.01	0.41
1:A:298:ASP:OD2	1:A:457:THR:OG1	2.38	0.40
1:A:326:LYS:O	1:A:327:CME:C	2.69	0.40
1:A:444:ILE:HD13	1:A:444:ILE:HA	1.98	0.40

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	532/563 (94%)	517 (97%)	13 (2%)	2 (0%)	30 14

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	499[A]	GLY
1	A	499[B]	GLY

5.3.2 Protein sidechains [i](#)

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	415/439 (94%)	408 (98%)	7 (2%)	53 30

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	131	SER
1	A	212	LYS
1	A	328	SER
1	A	359	ILE
1	A	453	ARG
1	A	489	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	272	HIS
1	A	372	GLN
1	A	481	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	CME	A	327	1	8,9,10	0.91	0	6,9,11	2.71	2 (33%)

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
1	CME	A	327	1	-	3/5/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	327	CME	CB-SG-SD	5.96	119.29	103.86
1	A	327	CME	CB-CA-C	-2.24	104.73	110.80

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	327	CME	SD-CE-CZ-OH
1	A	327	CME	CE-SD-SG-CB
1	A	327	CME	CZ-CE-SD-SG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	327	CME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAD	A	601	-	28,29,48	1.90	6 (21%)	43,45,73	2.45	17 (39%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	601	-	-	0/16/32/62	0/3/3/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	NAD	PA-O3	5.34	1.65	1.59
2	A	601	NAD	O4B-C1B	3.71	1.50	1.42
2	A	601	NAD	C5A-C4A	3.43	1.45	1.39
2	A	601	NAD	C5A-N7A	-2.52	1.34	1.39
2	A	601	NAD	C8A-N7A	2.46	1.36	1.31
2	A	601	NAD	PN-O5D	2.37	1.63	1.54

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	NAD	C5A-C4A-N3A	-6.58	117.66	126.72
2	A	601	NAD	N3A-C4A-N9A	6.04	137.44	127.17
2	A	601	NAD	N9A-C8A-N7A	-4.40	107.69	113.94
2	A	601	NAD	C4A-N9A-C8A	4.23	110.18	105.74
2	A	601	NAD	C2A-N3A-C4A	3.87	121.28	111.83
2	A	601	NAD	C5A-N7A-C8A	3.56	109.04	103.45
2	A	601	NAD	C2B-C1B-N9A	3.55	122.11	113.30
2	A	601	NAD	N3A-C2A-N1A	-3.49	123.30	128.58
2	A	601	NAD	O3-PA-O1A	-3.08	101.42	110.70
2	A	601	NAD	O2N-PN-O3	3.05	114.88	104.64
2	A	601	NAD	O2A-PA-O1A	2.90	125.94	112.44
2	A	601	NAD	O2A-PA-O3	2.73	114.66	107.27
2	A	601	NAD	O5B-C5B-C4B	-2.71	99.76	108.99
2	A	601	NAD	O2N-PN-O1N	2.63	121.06	110.83
2	A	601	NAD	C5A-C6A-N6A	-2.44	117.26	123.29
2	A	601	NAD	O4B-C1B-C2B	-2.41	101.45	106.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	NAD	C4A-C5A-N7A	-2.16	108.11	110.58

There are no chirality outliers.

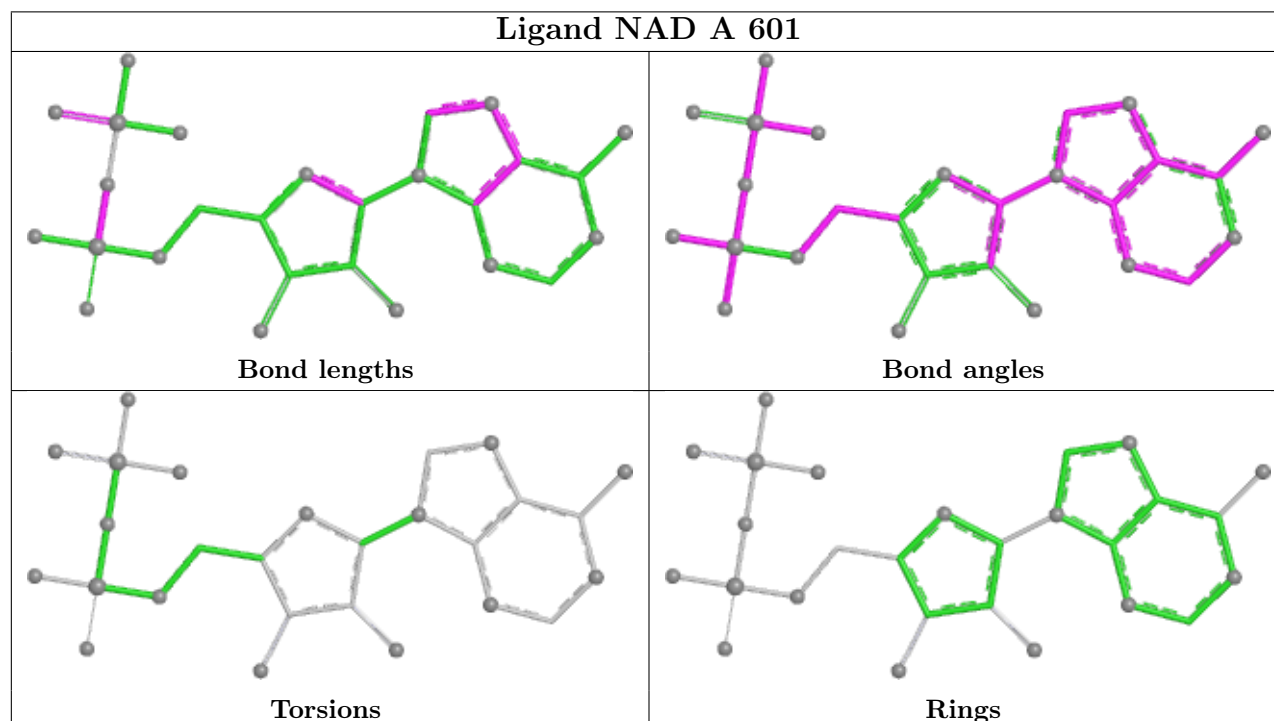
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NAD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 ⓘ

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	535/563 (95%)	-0.02	27 (5%) 34 35	14, 22, 41, 90	1 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	426	TYR	5.7
1	A	490	GLY	5.5
1	A	418	THR	4.8
1	A	454	TYR	4.7
1	A	543	ASP	4.5
1	A	328	SER	4.2
1	A	292	GLY	4.0
1	A	270	PHE	3.5
1	A	542	VAL	3.5
1	A	298	ASP	3.3
1	A	489	THR	3.2
1	A	452	SER	3.0
1	A	295	GLY	3.0
1	A	499[A]	GLY	2.9
1	A	427	PHE	2.9
1	A	296	GLY	2.6
1	A	49	ARG	2.5
1	A	455	ALA	2.5
1	A	415	ASP	2.5
1	A	498	PHE	2.5
1	A	329	ALA	2.4
1	A	390	ALA	2.3
1	A	488	PRO	2.3
1	A	491	ALA	2.3
1	A	287	TYR	2.2
1	A	180	ASP	2.2
1	A	453	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CME	A	327	10/11	0.79	0.19	45,60,78,85	0

6.3 Carbohydrates [i](#)

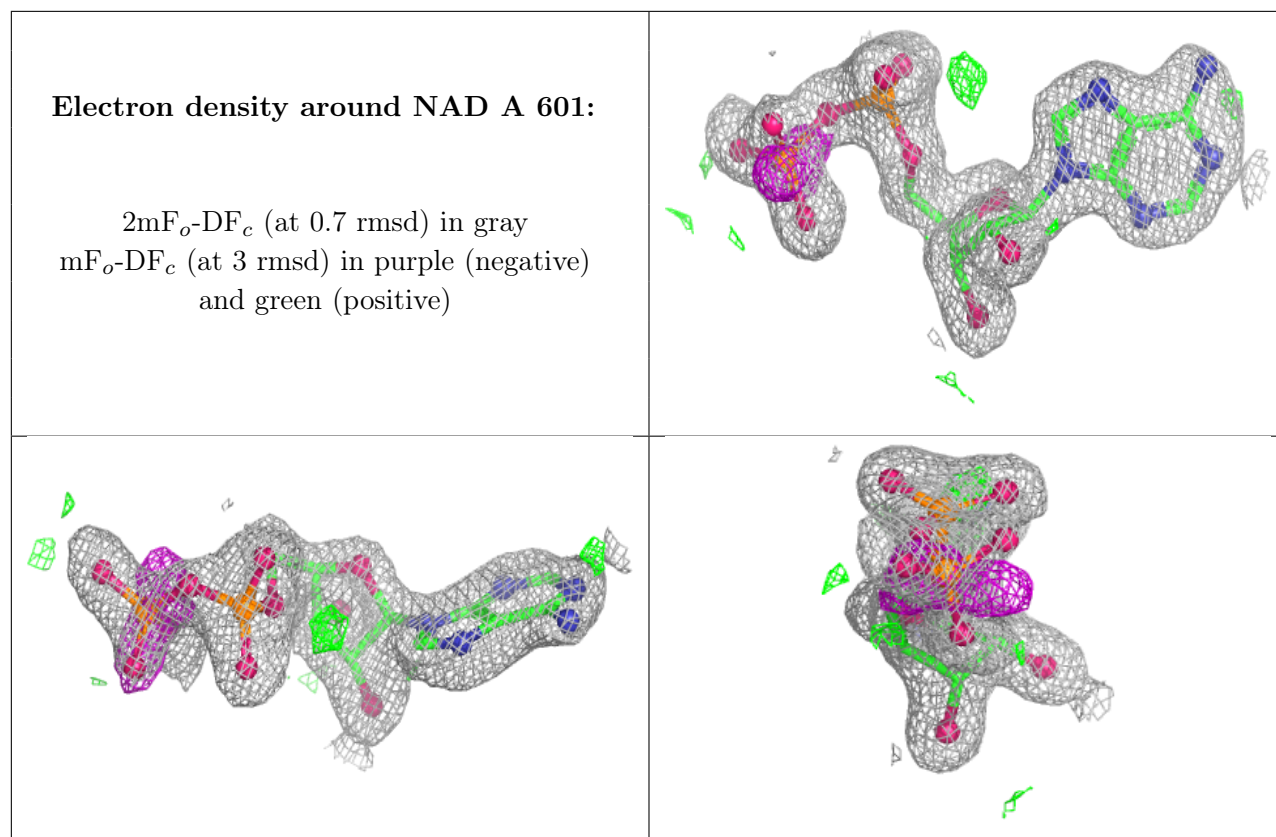
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAD	A	601	27/44	0.90	0.11	20,29,37,45	27

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.