



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:59 am GMT

PDB ID : 5KLN
Title : Crystal structure of 2-aminomuconate 6-semialdehyde dehydrogenase N169A
in complex with NAD⁺
Authors : Yang, Y.; Davis, I.; Ha, U.; Wang, Y.; Shin, I.; Liu, A.
Deposited on : 2016-06-24
Resolution : 1.99 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

<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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

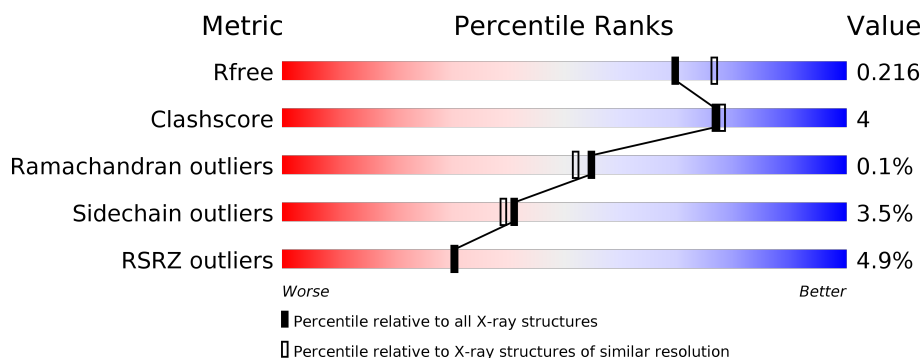
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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.

Mol	Chain	Length	Quality of chain
1	A	520	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>8%</div> <div>7%</div> </div> </div>
1	B	520	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>7%</div> <div>7%</div> </div> </div>
1	C	520	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>7%</div> <div>7%</div> </div> </div>
1	D	520	<div> <div>7%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>7%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NA	A	602	-	-	-	X
3	NA	B	602	-	-	-	X
3	NA	C	602	-	-	-	X
3	NA	D	602	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16060 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 2-aminomuconate 6-semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3675	2325	637	701	12			
1	D	483	Total	C	N	O	S	0	0	0
			3668	2320	636	700	12			
1	B	483	Total	C	N	O	S	0	2	0
			3690	2332	644	702	12			
1	C	483	Total	C	N	O	S	0	0	0
			3668	2320	636	700	12			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q83V33
A	-18	GLY	-	expression tag	UNP Q83V33
A	-17	SER	-	expression tag	UNP Q83V33
A	-16	SER	-	expression tag	UNP Q83V33
A	-15	HIS	-	expression tag	UNP Q83V33
A	-14	HIS	-	expression tag	UNP Q83V33
A	-13	HIS	-	expression tag	UNP Q83V33
A	-12	HIS	-	expression tag	UNP Q83V33
A	-11	HIS	-	expression tag	UNP Q83V33
A	-10	HIS	-	expression tag	UNP Q83V33
A	-9	SER	-	expression tag	UNP Q83V33
A	-8	SER	-	expression tag	UNP Q83V33
A	-7	GLY	-	expression tag	UNP Q83V33
A	-6	LEU	-	expression tag	UNP Q83V33
A	-5	VAL	-	expression tag	UNP Q83V33
A	-4	PRO	-	expression tag	UNP Q83V33
A	-3	ARG	-	expression tag	UNP Q83V33
A	-2	GLY	-	expression tag	UNP Q83V33
A	-1	SER	-	expression tag	UNP Q83V33
A	0	HIS	-	expression tag	UNP Q83V33
A	169	ALA	ASN	engineered mutation	UNP Q83V33

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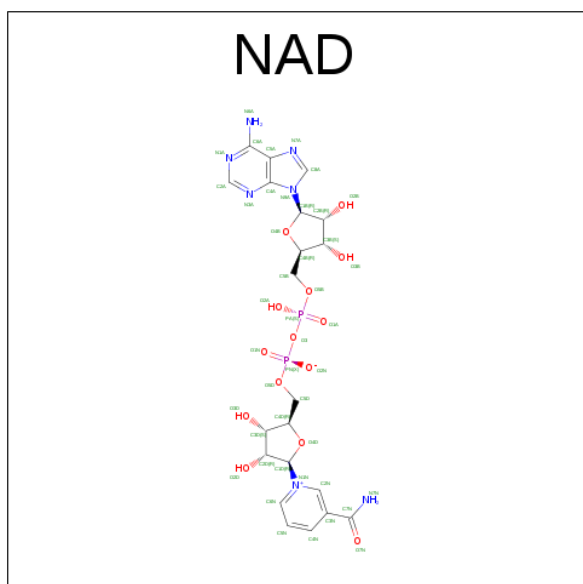
Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	initiating methionine	UNP Q83V33
D	-18	GLY	-	expression tag	UNP Q83V33
D	-17	SER	-	expression tag	UNP Q83V33
D	-16	SER	-	expression tag	UNP Q83V33
D	-15	HIS	-	expression tag	UNP Q83V33
D	-14	HIS	-	expression tag	UNP Q83V33
D	-13	HIS	-	expression tag	UNP Q83V33
D	-12	HIS	-	expression tag	UNP Q83V33
D	-11	HIS	-	expression tag	UNP Q83V33
D	-10	HIS	-	expression tag	UNP Q83V33
D	-9	SER	-	expression tag	UNP Q83V33
D	-8	SER	-	expression tag	UNP Q83V33
D	-7	GLY	-	expression tag	UNP Q83V33
D	-6	LEU	-	expression tag	UNP Q83V33
D	-5	VAL	-	expression tag	UNP Q83V33
D	-4	PRO	-	expression tag	UNP Q83V33
D	-3	ARG	-	expression tag	UNP Q83V33
D	-2	GLY	-	expression tag	UNP Q83V33
D	-1	SER	-	expression tag	UNP Q83V33
D	0	HIS	-	expression tag	UNP Q83V33
D	169	ALA	ASN	engineered mutation	UNP Q83V33
B	-19	MET	-	initiating methionine	UNP Q83V33
B	-18	GLY	-	expression tag	UNP Q83V33
B	-17	SER	-	expression tag	UNP Q83V33
B	-16	SER	-	expression tag	UNP Q83V33
B	-15	HIS	-	expression tag	UNP Q83V33
B	-14	HIS	-	expression tag	UNP Q83V33
B	-13	HIS	-	expression tag	UNP Q83V33
B	-12	HIS	-	expression tag	UNP Q83V33
B	-11	HIS	-	expression tag	UNP Q83V33
B	-10	HIS	-	expression tag	UNP Q83V33
B	-9	SER	-	expression tag	UNP Q83V33
B	-8	SER	-	expression tag	UNP Q83V33
B	-7	GLY	-	expression tag	UNP Q83V33
B	-6	LEU	-	expression tag	UNP Q83V33
B	-5	VAL	-	expression tag	UNP Q83V33
B	-4	PRO	-	expression tag	UNP Q83V33
B	-3	ARG	-	expression tag	UNP Q83V33
B	-2	GLY	-	expression tag	UNP Q83V33
B	-1	SER	-	expression tag	UNP Q83V33
B	0	HIS	-	expression tag	UNP Q83V33
B	169	ALA	ASN	engineered mutation	UNP Q83V33

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	initiating methionine	UNP Q83V33
C	-18	GLY	-	expression tag	UNP Q83V33
C	-17	SER	-	expression tag	UNP Q83V33
C	-16	SER	-	expression tag	UNP Q83V33
C	-15	HIS	-	expression tag	UNP Q83V33
C	-14	HIS	-	expression tag	UNP Q83V33
C	-13	HIS	-	expression tag	UNP Q83V33
C	-12	HIS	-	expression tag	UNP Q83V33
C	-11	HIS	-	expression tag	UNP Q83V33
C	-10	HIS	-	expression tag	UNP Q83V33
C	-9	SER	-	expression tag	UNP Q83V33
C	-8	SER	-	expression tag	UNP Q83V33
C	-7	GLY	-	expression tag	UNP Q83V33
C	-6	LEU	-	expression tag	UNP Q83V33
C	-5	VAL	-	expression tag	UNP Q83V33
C	-4	PRO	-	expression tag	UNP Q83V33
C	-3	ARG	-	expression tag	UNP Q83V33
C	-2	GLY	-	expression tag	UNP Q83V33
C	-1	SER	-	expression tag	UNP Q83V33
C	0	HIS	-	expression tag	UNP Q83V33
C	169	ALA	ASN	engineered mutation	UNP Q83V33

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: 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
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

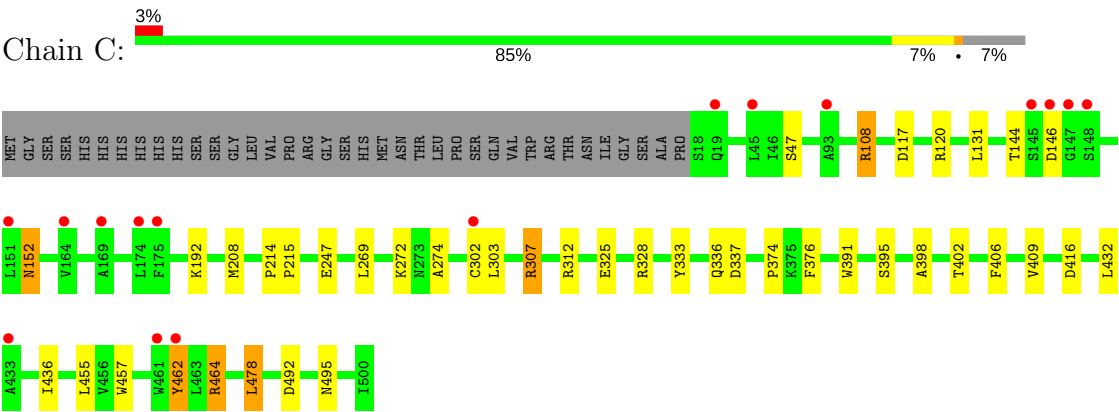
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	313	Total	O	0	0
			313	313		
4	D	241	Total	O	0	0
			241	241		
4	B	327	Total	O	0	0
			327	327		
4	C	298	Total	O	0	0
			298	298		



● Molecule 1: 2-aminomuconate 6-semialdehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.70Å 140.99Å 173.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.54 – 1.99 34.54 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.54-1.99) 96.4 (34.54-1.99)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.187 , 0.222 0.182 , 0.216	Depositor DCC
R_{free} test set	2002 reflections (1.35%)	DCC
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16060	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 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	0.41	0/3755	0.57	1/5105 (0.0%)
1	B	0.42	0/3769	0.58	1/5122 (0.0%)
1	C	0.42	0/3747	0.58	3/5094 (0.1%)
1	D	0.37	0/3747	0.54	1/5094 (0.0%)
All	All	0.40	0/15018	0.57	6/20415 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	478	LEU	CA-CB-CG	7.93	133.55	115.30
1	D	478	LEU	CA-CB-CG	7.04	131.50	115.30
1	C	478	LEU	CA-CB-CG	6.85	131.06	115.30
1	C	307	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	478	LEU	CA-CB-CG	6.26	129.71	115.30
1	C	307	ARG	NE-CZ-NH1	5.16	122.88	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3675	0	3612	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3690	0	3628	25	0
1	C	3668	0	3604	19	0
1	D	3668	0	3604	29	0
2	A	44	0	26	3	0
2	B	44	0	26	2	0
2	C	44	0	26	3	0
2	D	44	0	26	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	313	0	0	6	0
4	B	327	0	0	1	0
4	C	298	0	0	1	0
4	D	241	0	0	4	0
All	All	16060	0	14552	103	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 4.

All (103) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:ASP:OD2	1:D:443:ARG:NH1	2.16	0.77
1:C:152:ASN:OD1	1:C:495:ASN:ND2	2.18	0.77
1:B:152:ASN:OD1	1:B:495:ASN:ND2	2.21	0.73
1:C:272:LYS:HG3	1:C:307:ARG:HD2	1.72	0.72
1:A:449:ARG:NH2	1:B:141:GLU:OE2	2.24	0.71
1:A:247:GLU:OE2	4:A:701:HOH:O	2.08	0.71
1:C:302:CYS:SG	2:C:601:NAD:C4N	2.79	0.70
1:A:350:ARG:NH1	1:A:351:ASP:OD1	2.26	0.69
1:A:288:GLU:OE1	1:A:292:ARG:NH2	2.27	0.67
1:A:302:CYS:SG	2:A:601:NAD:C4N	2.83	0.67
1:B:302:CYS:SG	2:B:601:NAD:C4N	2.84	0.66
1:A:18:SER:HB3	1:A:47:SER:HB3	1.76	0.66
1:D:272:LYS:HG3	1:D:307:ARG:HD2	1.78	0.66
1:B:350[B]:ARG:HG2	1:B:350[B]:ARG:HH11	1.62	0.64
1:D:462:TYR:HE1	1:D:464:ARG:HG3	1.62	0.64
1:A:152:ASN:OD1	1:A:495:ASN:ND2	2.30	0.64
1:D:302:CYS:SG	2:D:601:NAD:C4N	2.86	0.64
1:B:247:GLU:OE2	4:B:701:HOH:O	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:462:TYR:CE1	1:D:464:ARG:HG3	2.35	0.61
1:A:292:ARG:HG2	1:A:292:ARG:HH11	1.66	0.61
1:A:491:SER:O	4:A:702:HOH:O	2.16	0.60
1:C:247:GLU:OE2	4:C:701:HOH:O	2.17	0.60
1:A:226:LYS:HE2	2:A:601:NAD:N7A	2.17	0.60
1:A:449:ARG:HH22	1:B:141:GLU:CD	2.05	0.60
1:B:272:LYS:HG3	1:B:307:ARG:HD2	1.82	0.60
1:A:292:ARG:NH1	4:A:703:HOH:O	2.24	0.59
1:C:108:ARG:HD3	1:C:117:ASP:OD2	2.03	0.59
1:C:312:ARG:HD2	1:C:416:ASP:OD1	2.03	0.59
1:B:152:ASN:ND2	1:B:495:ASN:OD1	2.26	0.58
1:A:495:ASN:HD22	1:D:455:LEU:HD13	1.69	0.57
1:A:272:LYS:HG3	1:A:307:ARG:HD2	1.87	0.57
1:A:397:LYS:NZ	4:A:712:HOH:O	2.38	0.55
1:D:464:ARG:NH2	4:D:701:HOH:O	2.19	0.55
1:D:333:TYR:HB2	1:D:336:GLN:HB2	1.89	0.55
1:D:18:SER:HB3	1:D:47:SER:HB3	1.88	0.55
1:B:117:ASP:OD1	1:B:117:ASP:N	2.38	0.54
1:B:108:ARG:HD3	1:B:117:ASP:OD2	2.07	0.54
1:C:269:LEU:O	2:C:601:NAD:H2N	2.09	0.53
1:D:55:LYS:O	1:D:59:GLU:HG3	2.09	0.53
1:A:269:LEU:O	2:A:601:NAD:H2N	2.10	0.52
1:B:350[B]:ARG:HH11	1:B:350[B]:ARG:CG	2.22	0.52
1:A:333:TYR:HB2	1:A:336:GLN:HB2	1.91	0.52
1:C:303:LEU:HD13	1:C:457:TRP:HH2	1.75	0.51
1:D:37:ASN:O	1:D:46:ILE:HG13	2.10	0.51
1:D:151:LEU:HG	1:D:500:ILE:HD11	1.94	0.50
1:B:55:LYS:HE3	1:B:59:GLU:OE1	2.11	0.50
1:C:333:TYR:HB2	1:C:336:GLN:HB2	1.95	0.49
1:B:391:TRP:CH2	1:B:409:VAL:HG21	2.48	0.48
1:A:449:ARG:HG3	1:A:449:ARG:HH21	1.78	0.48
1:D:98:PHE:CE1	1:D:203:LEU:HB3	2.49	0.48
1:D:288:GLU:OE2	1:D:292:ARG:NE	2.47	0.48
1:A:117:ASP:OD1	1:A:117:ASP:N	2.44	0.48
1:D:391:TRP:CH2	1:D:409:VAL:HG21	2.49	0.48
1:D:117:ASP:N	1:D:117:ASP:OD1	2.47	0.48
1:D:20:LEU:HD12	1:D:198:PRO:HG2	1.97	0.47
1:D:247:GLU:OE2	4:D:702:HOH:O	2.20	0.47
1:C:144:THR:OG1	1:C:146:ASP:OD1	2.28	0.46
1:B:269:LEU:O	2:B:601:NAD:H2N	2.15	0.46
1:C:391:TRP:CH2	1:C:409:VAL:HG21	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:VAL:O	1:B:414:PRO:HA	2.16	0.46
1:B:249:LYS:HE2	1:B:249:LYS:HB3	1.74	0.46
1:D:168:TRP:O	1:D:171:PRO:HD3	2.16	0.46
1:B:289:GLY:HA3	1:B:437:TRP:CZ2	2.50	0.45
1:D:461:TRP:CE3	1:D:462:TYR:HB2	2.51	0.45
1:B:350[B]:ARG:HG2	1:B:350[B]:ARG:NH1	2.29	0.45
1:C:398:ALA:O	1:C:402:THR:HG23	2.16	0.45
1:A:397:LYS:NZ	1:A:427:ASP:OD2	2.49	0.45
1:B:274:ALA:HA	1:B:307:ARG:O	2.17	0.45
1:B:203:LEU:HD12	1:B:203:LEU:HA	1.86	0.45
1:C:462:TYR:CE1	1:C:464:ARG:HG3	2.52	0.44
1:D:289:GLY:HA3	1:D:437:TRP:CZ2	2.53	0.44
1:A:111:HIS:HB3	4:A:921:HOH:O	2.17	0.44
1:D:301:VAL:HG12	1:D:303:LEU:H	1.82	0.44
1:C:302:CYS:SG	2:C:601:NAD:C3N	3.06	0.44
1:A:18:SER:CB	1:A:47:SER:HB3	2.47	0.43
1:C:117:ASP:N	1:C:117:ASP:OD1	2.49	0.43
1:D:288:GLU:OE1	4:D:703:HOH:O	2.21	0.43
1:A:397:LYS:HD3	1:A:397:LYS:HA	1.77	0.43
1:A:263:LYS:O	1:D:478:LEU:HD12	2.18	0.43
1:A:142:MET:HG3	1:A:150:ALA:HB3	2.00	0.43
1:B:272:LYS:HG3	1:B:307:ARG:CD	2.49	0.43
1:B:324:VAL:O	1:B:328:ARG:HG3	2.19	0.42
1:A:391:TRP:CH2	1:A:409:VAL:HG21	2.54	0.42
1:D:102:GLU:OE2	1:D:171:PRO:HG2	2.18	0.42
1:D:454:GLY:HA3	1:D:471:GLY:O	2.19	0.42
1:A:310:VAL:O	1:A:414:PRO:HA	2.20	0.42
1:D:89:ASP:OD1	1:D:126:ARG:NH2	2.44	0.42
1:C:214:PRO:HA	1:C:215:PRO:HD3	1.91	0.42
1:A:469:PRO:HB3	1:A:485:PHE:CD2	2.54	0.42
1:A:499:LYS:HB2	1:D:460:THR:HB	2.02	0.42
1:A:98:PHE:CE1	1:A:203:LEU:HB3	2.55	0.42
1:B:322:LEU:HD23	1:B:412:ILE:HD11	2.02	0.42
1:C:374:PRO:HG2	1:C:376:PHE:CE2	2.55	0.41
1:C:325:GLU:OE2	1:C:328:ARG:NH1	2.53	0.41
1:A:214:PRO:HA	1:A:215:PRO:HD3	1.91	0.41
1:B:374:PRO:HG2	1:B:376:PHE:CZ	2.55	0.41
2:D:601:NAD:O2N	4:D:702:HOH:O	2.22	0.41
1:A:464:ARG:NH1	4:A:708:HOH:O	2.34	0.41
1:A:108:ARG:HD3	1:A:117:ASP:OD2	2.21	0.41
1:C:274:ALA:HA	1:C:307:ARG:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LEU:HA	1:A:203:LEU:HD12	1.87	0.40
1:D:302:CYS:SG	2:D:601:NAD:C3N	3.10	0.40
1:B:462:TYR:CE1	1:B:464:ARG:HG3	2.57	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	482/520 (93%)	467 (97%)	15 (3%)	0	100	100
1	B	483/520 (93%)	469 (97%)	14 (3%)	0	100	100
1	C	481/520 (92%)	467 (97%)	14 (3%)	0	100	100
1	D	481/520 (92%)	466 (97%)	14 (3%)	1 (0%)	51	48
All	All	1927/2080 (93%)	1869 (97%)	57 (3%)	1 (0%)	55	52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	167	PRO

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	392/423 (93%)	381 (97%)	11 (3%)	49	49
1	B	393/423 (93%)	379 (96%)	14 (4%)	40	38
1	C	391/423 (92%)	374 (96%)	17 (4%)	33	29
1	D	391/423 (92%)	379 (97%)	12 (3%)	45	44
All	All	1567/1692 (93%)	1513 (97%)	54 (3%)	41	40

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ARG
1	A	117	ASP
1	A	131	LEU
1	A	152	ASN
1	A	192	LYS
1	A	226	LYS
1	A	401	VAL
1	A	406	PHE
1	A	432	LEU
1	A	462	TYR
1	A	478	LEU
1	D	33	SER
1	D	46	ILE
1	D	48	ASP
1	D	108	ARG
1	D	117	ASP
1	D	131	LEU
1	D	192	LYS
1	D	395	SER
1	D	432	LEU
1	D	462	TYR
1	D	478	LEU
1	D	492	ASP
1	B	45	LEU
1	B	108	ARG
1	B	117	ASP
1	B	131	LEU
1	B	192	LYS
1	B	203	LEU
1	B	337	ASP
1	B	406	PHE
1	B	432	LEU
1	B	455	LEU

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Mol	Chain	Res	Type
1	B	462	TYR
1	B	478	LEU
1	B	492	ASP
1	B	500	ILE
1	C	47	SER
1	C	108	ARG
1	C	120	ARG
1	C	131	LEU
1	C	152	ASN
1	C	192	LYS
1	C	208	MET
1	C	337	ASP
1	C	395	SER
1	C	406	PHE
1	C	432	LEU
1	C	436	ILE
1	C	455	LEU
1	C	462	TYR
1	C	464	ARG
1	C	478	LEU
1	C	492	ASP

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

Mol	Chain	Res	Type
1	A	152	ASN
1	A	495	ASN
1	C	111	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
2	NAD	A	601	-	41,48,48	1.88	6 (14%)	43,73,73	1.77	6 (13%)
2	NAD	B	601	-	41,48,48	1.93	9 (21%)	43,73,73	1.56	6 (13%)
2	NAD	C	601	-	41,48,48	1.90	8 (19%)	43,73,73	1.64	5 (11%)
2	NAD	D	601	-	41,48,48	1.99	10 (24%)	43,73,73	1.70	6 (13%)

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	-	-	0/22/62/62	0/5/5/5
2	NAD	B	601	-	-	0/22/62/62	0/5/5/5
2	NAD	C	601	-	-	0/22/62/62	0/5/5/5
2	NAD	D	601	-	-	0/22/62/62	0/5/5/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	NAD	C2B-C3B	-4.56	1.41	1.53
2	B	601	NAD	C2B-C3B	-4.38	1.41	1.53
2	D	601	NAD	C2B-C3B	-4.24	1.42	1.53
2	A	601	NAD	C2B-C3B	-4.14	1.42	1.53
2	C	601	NAD	C2D-C1D	-3.84	1.47	1.53
2	D	601	NAD	C2D-C1D	-3.74	1.47	1.53
2	A	601	NAD	C2D-C1D	-3.52	1.48	1.53
2	B	601	NAD	C2D-C1D	-3.47	1.48	1.53
2	B	601	NAD	C2B-C1B	-2.56	1.49	1.53
2	D	601	NAD	O2B-C2B	-2.56	1.37	1.43
2	C	601	NAD	C2B-C1B	-2.47	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	NAD	O2B-C2B	-2.47	1.37	1.43
2	D	601	NAD	C2D-C3D	-2.42	1.47	1.53
2	D	601	NAD	O4B-C4B	-2.40	1.39	1.45
2	C	601	NAD	O2B-C2B	-2.39	1.37	1.43
2	A	601	NAD	C2B-C1B	-2.37	1.49	1.53
2	D	601	NAD	C3D-C4D	-2.23	1.47	1.53
2	B	601	NAD	C2D-C3D	-2.22	1.47	1.53
2	C	601	NAD	O4B-C4B	-2.22	1.40	1.45
2	D	601	NAD	O2D-C2D	-2.20	1.37	1.43
2	A	601	NAD	C2D-C3D	-2.17	1.47	1.53
2	D	601	NAD	C2B-C1B	-2.07	1.50	1.53
2	B	601	NAD	C3N-C7N	-2.06	1.47	1.50
2	C	601	NAD	C2D-C3D	-2.04	1.48	1.53
2	B	601	NAD	O7N-C7N	2.02	1.28	1.24
2	C	601	NAD	C6A-N6A	3.19	1.47	1.34
2	B	601	NAD	C6A-N6A	3.20	1.47	1.34
2	A	601	NAD	C6A-N6A	3.25	1.47	1.34
2	D	601	NAD	C6A-N6A	3.34	1.47	1.34
2	C	601	NAD	C7N-N7N	7.42	1.47	1.33
2	B	601	NAD	C7N-N7N	7.64	1.47	1.33
2	A	601	NAD	C7N-N7N	7.75	1.48	1.33
2	D	601	NAD	C7N-N7N	7.92	1.48	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	NAD	N3A-C2A-N1A	-7.89	121.98	128.86
2	B	601	NAD	N3A-C2A-N1A	-7.44	122.38	128.86
2	A	601	NAD	N3A-C2A-N1A	-6.99	122.77	128.86
2	C	601	NAD	N3A-C2A-N1A	-6.99	122.77	128.86
2	A	601	NAD	O7N-C7N-N7N	-3.93	116.99	122.58
2	A	601	NAD	C4D-O4D-C1D	-3.77	105.76	109.77
2	C	601	NAD	O7N-C7N-N7N	-3.53	117.56	122.58
2	D	601	NAD	O7N-C7N-N7N	-3.32	117.86	122.58
2	C	601	NAD	C4D-O4D-C1D	-3.18	106.39	109.77
2	D	601	NAD	C4D-O4D-C1D	-2.57	107.04	109.77
2	B	601	NAD	O7N-C7N-N7N	-2.45	119.10	122.58
2	B	601	NAD	C4D-O4D-C1D	-2.39	107.23	109.77
2	D	601	NAD	C4A-C5A-N7A	-2.09	107.39	109.41
2	A	601	NAD	O5B-C5B-C4B	2.18	116.73	109.00
2	B	601	NAD	O5B-C5B-C4B	2.21	116.84	109.00
2	D	601	NAD	O5B-C5B-C4B	2.26	117.00	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	NAD	C3N-C7N-N7N	2.41	120.53	117.77
2	A	601	NAD	O5D-C5D-C4D	2.55	118.04	109.00
2	B	601	NAD	O5D-C5D-C4D	2.64	118.36	109.00
2	C	601	NAD	O5D-C5D-C4D	3.14	120.14	109.00
2	C	601	NAD	C3N-C7N-N7N	3.49	121.76	117.77
2	D	601	NAD	C3N-C7N-N7N	3.98	122.31	117.77
2	A	601	NAD	C3N-C7N-N7N	4.77	123.22	117.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NAD	3	0
2	B	601	NAD	2	0
2	C	601	NAD	3	0
2	D	601	NAD	3	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

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	484/520 (93%)	0.22	20 (4%) 38 38	25, 36, 49, 70	0
1	B	483/520 (92%)	0.06	23 (4%) 31 31	25, 33, 46, 62	0
1	C	483/520 (92%)	0.11	16 (3%) 47 47	24, 34, 47, 58	0
1	D	483/520 (92%)	0.35	35 (7%) 16 16	27, 41, 57, 71	0
All	All	1933/2080 (92%)	0.19	94 (4%) 30 30	24, 36, 52, 71	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	338	GLY	4.7
1	A	17	PRO	4.3
1	A	45	LEU	4.2
1	B	174	LEU	3.9
1	D	45	LEU	3.8
1	D	361	VAL	3.5
1	D	337	ASP	3.5
1	C	461	TRP	3.3
1	D	462	TYR	3.3
1	C	93	ALA	3.3
1	A	55	LYS	3.2
1	D	378	ASP	3.2
1	D	111	HIS	3.2
1	D	333	TYR	3.1
1	D	382	GLN	3.1
1	D	28	PHE	3.1
1	B	337	ASP	3.0
1	A	164	VAL	3.0
1	D	376	PHE	3.0
1	D	328	ARG	3.0
1	D	383	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	147	GLY	2.9
1	B	338	GLY	2.9
1	A	174	LEU	2.9
1	D	44	LYS	2.9
1	C	174	LEU	2.9
1	D	174	LEU	2.9
1	C	462	TYR	2.8
1	A	170	LEU	2.8
1	D	18	SER	2.8
1	A	111	HIS	2.8
1	A	462	TYR	2.8
1	A	175	PHE	2.8
1	A	18	SER	2.7
1	A	145	SER	2.7
1	C	302	CYS	2.7
1	D	330	VAL	2.7
1	B	170	LEU	2.6
1	C	145	SER	2.6
1	C	148	SER	2.6
1	B	175	PHE	2.5
1	B	172	LEU	2.5
1	D	32	ALA	2.5
1	B	169	ALA	2.5
1	B	245	THR	2.5
1	D	461	TRP	2.5
1	D	339	VAL	2.5
1	C	146	ASP	2.5
1	B	32	ALA	2.4
1	B	173	LEU	2.4
1	B	166	SER	2.4
1	D	19	GLN	2.4
1	A	167	PRO	2.4
1	D	148	SER	2.3
1	D	177	TRP	2.3
1	B	55	LYS	2.3
1	D	302	CYS	2.3
1	D	377	ASN	2.3
1	B	179	VAL	2.3
1	B	177	TRP	2.3
1	A	165	ILE	2.3
1	C	164	VAL	2.2
1	D	397	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	169	ALA	2.2
1	B	462	TYR	2.2
1	D	175	PHE	2.2
1	C	433	ALA	2.2
1	A	146	ASP	2.2
1	D	170	LEU	2.2
1	C	147	GLY	2.2
1	A	19	GLN	2.2
1	B	165	ILE	2.1
1	D	30	THR	2.1
1	A	62	VAL	2.1
1	D	48	ASP	2.1
1	A	337	ASP	2.1
1	D	147	GLY	2.1
1	D	283	LEU	2.1
1	A	44	LYS	2.1
1	B	176	THR	2.1
1	D	324	VAL	2.1
1	C	175	PHE	2.1
1	A	169	ALA	2.1
1	D	323	LYS	2.1
1	D	358	ARG	2.0
1	B	435	ALA	2.0
1	B	193	PRO	2.0
1	C	45	LEU	2.0
1	B	302	CYS	2.0
1	B	19	GLN	2.0
1	B	120[A]	ARG	2.0
1	C	19	GLN	2.0
1	C	151	LEU	2.0
1	B	148	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NA	D	602	1/1	0.39	0.38	10.65	60,60,60,60	0
3	NA	C	602	1/1	0.98	0.22	3.85	30,30,30,30	0
3	NA	A	602	1/1	0.97	0.22	3.34	32,32,32,32	0
3	NA	B	602	1/1	0.97	0.21	3.10	27,27,27,27	0
2	NAD	D	601	44/44	0.95	0.12	-0.26	34,39,43,46	0
2	NAD	A	601	44/44	0.96	0.11	-0.53	28,34,39,42	0
2	NAD	C	601	44/44	0.97	0.12	-0.53	26,30,34,35	0
2	NAD	B	601	44/44	0.97	0.11	-0.56	26,31,33,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.