



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2016 – 02:25 AM EDT

PDB ID : 5KLK
Title : Crystal structure of 2-aminomuconate 6-semialdehyde dehydrogenase N169D
in complex with NAD⁺ and 2-hydroxymuconate-6-semialdehyde
Authors : Yang, Y.; Davis, I.; Ha, U.; Wang, Y.; Shin, I.; Liu, A.
Deposited on : 2016-06-24
Resolution : 2.01 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028320
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : rb-20028320

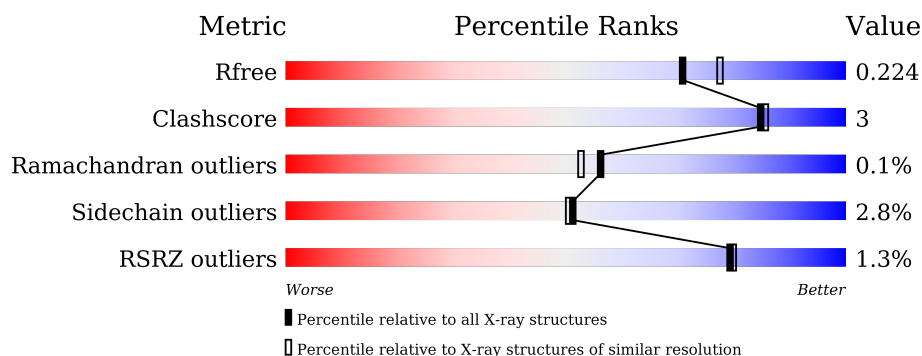
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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>85%</div> <div>7% • 7%</div> </div>
1	B	520	<div> <div>87%</div> <div>6% 7%</div> </div>
1	C	520	<div> <div>86%</div> <div>7% 7%</div> </div>
1	D	520	<div> <div>3%</div> <div>85%</div> <div>8% 7%</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	6OH	B	602	-	-	X	-
4	NA	A	603	-	-	-	X
4	NA	B	603	-	-	-	X
4	NA	C	603	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16006 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	483	Total	C	N	O	S	0	1	0
			3678	2326	638	702	12			
1	B	484	Total	C	N	O	S	0	1	0
			3685	2331	639	703	12			
1	D	483	Total	C	N	O	S	0	0	0
			3671	2321	636	702	12			
1	C	483	Total	C	N	O	S	0	0	0
			3671	2321	636	702	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	ASP	ASN	engineered mutation	UNP Q83V33

Continued on next page...

Continued from previous page...

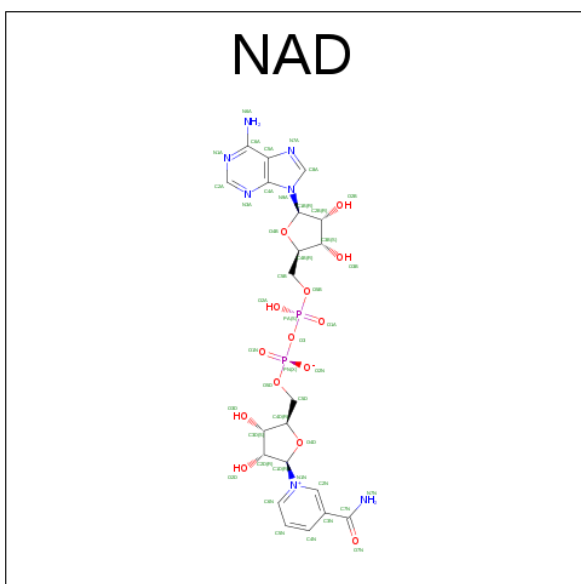
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP Q83V33
B	-18	GLY	-	expression tag	UNP Q83V33
B	-17	SER	-	expression tag	UNP Q83V33
B	-16	SER	-	expression tag	UNP Q83V33
B	-15	HIS	-	expression tag	UNP Q83V33
B	-14	HIS	-	expression tag	UNP Q83V33
B	-13	HIS	-	expression 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	ASP	ASN	engineered mutation	UNP Q83V33
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	ASP	ASN	engineered mutation	UNP Q83V33

Continued on next page...

Continued from previous page...

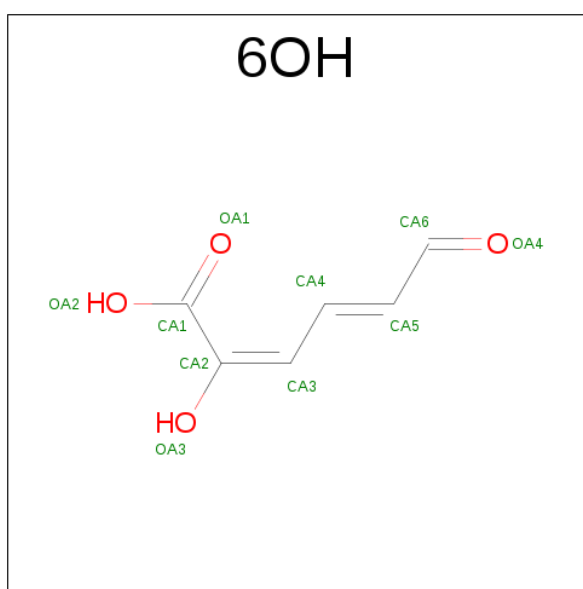
Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	initiating methionine	UNP Q83V33
C	-18	GLY	-	expression tag	UNP Q83V33
C	-17	SER	-	expression tag	UNP Q83V33
C	-16	SER	-	expression tag	UNP Q83V33
C	-15	HIS	-	expression tag	UNP Q83V33
C	-14	HIS	-	expression tag	UNP Q83V33
C	-13	HIS	-	expression 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	ASP	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	B	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	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is (2E,4E)-2-hydroxy-6-oxohexa-2,4-dienoic acid (three-letter code: 6OH) (formula: C₆H₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		
4	A	1	Total	Na	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Na	0	0
			1	1		

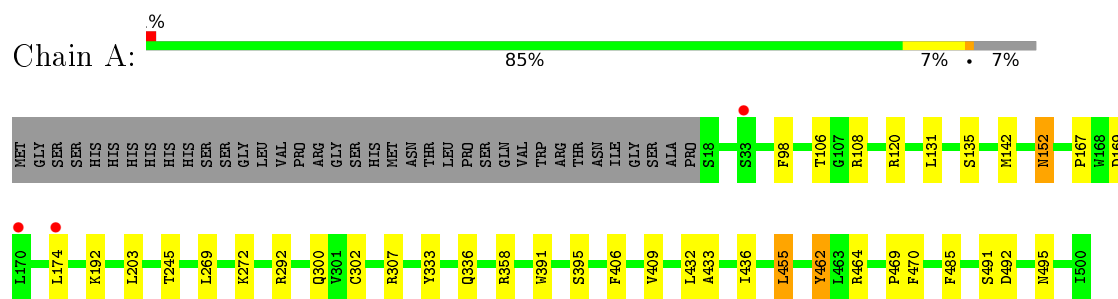
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	306	Total	O	0	0
			306	306		
5	B	293	Total	O	0	0
			293	293		
5	D	239	Total	O	0	0
			239	239		
5	C	254	Total	O	0	0
			254	254		

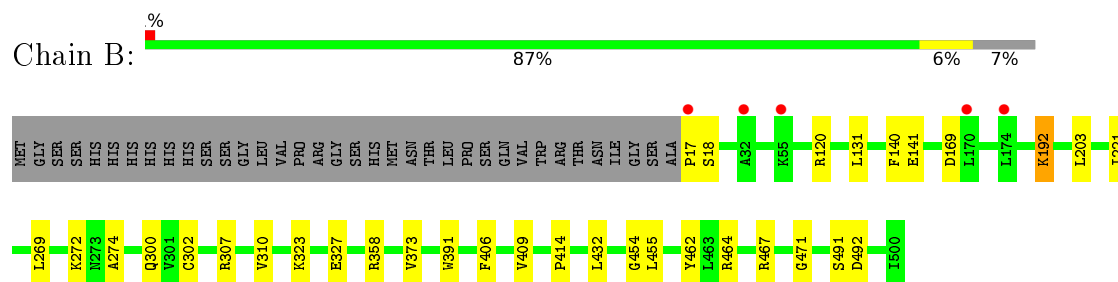
3 Residue-property plots [i](#)

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.

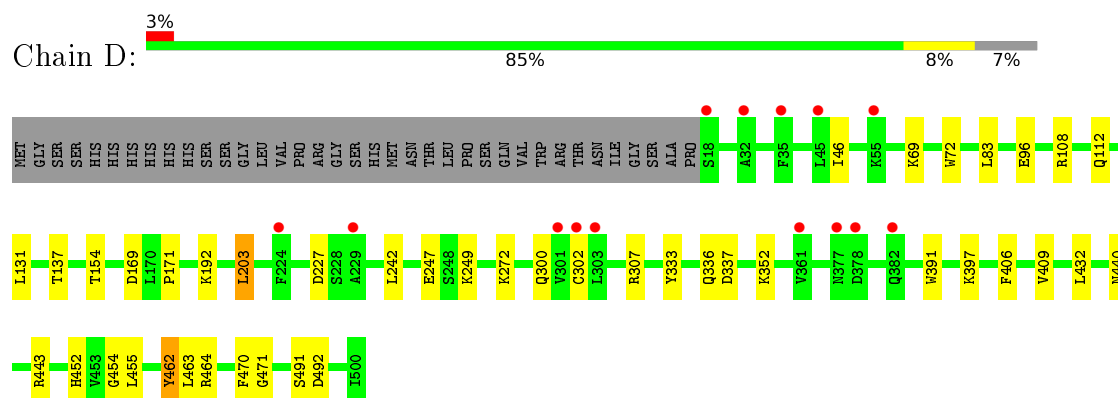
- Molecule 1: 2-aminomuconate 6-semialdehyde dehydrogenase



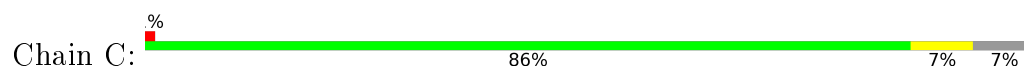
- Molecule 1: 2-aminomuconate 6-semialdehyde dehydrogenase

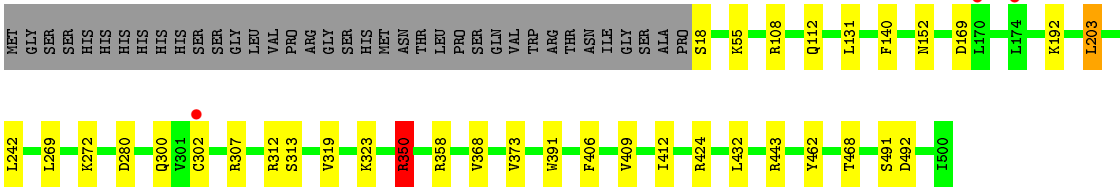


- Molecule 1: 2-aminomuconate 6-semialdehyde dehydrogenase



- 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	88.25Å 142.95Å 174.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.70 – 2.01 37.95 – 2.01	Depositor EDS
% Data completeness (in resolution range)	98.4 (36.70-2.01) 95.6 (37.95-2.01)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.187 , 0.231 0.182 , 0.224	Depositor DCC
R_{free} test set	1946 reflections (1.38%)	DCC
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.0	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	0.96	EDS
Total number of atoms	16006	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% 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, 6OH, 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	0/3761	0.57	0/5113
1	B	0.39	0/3769	0.55	0/5124
1	C	0.40	0/3750	0.59	2/5098 (0.0%)
1	D	0.36	0/3750	0.53	0/5098
All	All	0.38	0/15030	0.56	2/20433 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	350	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	C	350	ARG	NE-CZ-NH2	-5.59	117.50	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	3678	0	3610	25	0
1	B	3685	0	3618	18	0
1	C	3671	0	3603	21	0
1	D	3671	0	3603	19	0
2	A	44	0	26	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	44	0	26	3	0
2	C	44	0	26	3	0
2	D	44	0	26	1	0
3	A	10	0	4	3	0
3	B	10	0	4	4	0
3	C	10	0	4	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	306	0	0	5	0
5	B	293	0	0	3	0
5	C	254	0	0	3	0
5	D	239	0	0	3	0
All	All	16006	0	14550	85	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 3.

All (85) 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:108:ARG:NH1	1:D:112:GLN:OE1	2.14	0.80
1:C:350:ARG:HH11	1:C:350:ARG:HG2	1.46	0.80
1:C:280:ASP:OD2	1:C:443:ARG:NH1	2.19	0.75
1:A:491:SER:O	5:A:702:HOH:O	2.07	0.73
1:A:272:LYS:HG3	1:A:307:ARG:HD2	1.71	0.71
1:A:142:MET:SD	5:A:705:HOH:O	2.49	0.69
1:D:272:LYS:HG3	1:D:307:ARG:HD2	1.75	0.68
2:C:601:NAD:H4N	3:C:602:6OH:H1	1.76	0.67
1:D:108:ARG:NH2	1:D:169:ASP:O	2.28	0.66
1:C:491:SER:O	5:C:701:HOH:O	2.13	0.66
1:A:152:ASN:OD1	1:A:495:ASN:ND2	2.29	0.65
1:D:491:SER:O	5:D:701:HOH:O	2.13	0.65
1:B:120:ARG:NH1	3:B:602:6OH:OA3	2.25	0.64
1:B:272:LYS:HG3	1:B:307:ARG:HD2	1.79	0.64
1:C:108:ARG:NH1	1:C:112:GLN:OE1	2.32	0.63
1:C:462:TYR:OH	3:C:602:6OH:H6	2.00	0.62
1:A:302:CYS:SG	2:A:601:NAD:C4N	2.90	0.60
1:C:302:CYS:SG	2:C:601:NAD:C4N	2.90	0.59
3:B:602:6OH:OA2	3:B:602:6OH:OA4	2.20	0.59
1:B:302:CYS:SG	2:B:601:NAD:C4N	2.92	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:LEU:O	2:C:601:NAD:H2N	2.04	0.57
1:C:350:ARG:HH11	1:C:350:ARG:CG	2.17	0.56
1:D:302:CYS:SG	2:D:601:NAD:C4N	2.94	0.56
1:A:462:TYR:CE1	1:A:464:ARG:HG3	2.42	0.55
1:C:272:LYS:HG3	1:C:307:ARG:HD2	1.88	0.55
1:D:96:GLU:OE1	5:D:702:HOH:O	2.19	0.54
1:A:462:TYR:HE1	1:A:464:ARG:HG3	1.73	0.53
1:B:491:SER:O	5:B:701:HOH:O	2.19	0.52
1:A:106:THR:HG21	1:A:108:ARG:HH21	1.75	0.52
1:A:358:ARG:NH2	5:A:704:HOH:O	2.27	0.52
1:A:169:ASP:HB2	1:A:300:GLN:O	2.10	0.51
1:B:391:TRP:CH2	1:B:409:VAL:HG21	2.46	0.51
1:B:141:GLU:OE1	5:B:702:HOH:O	2.19	0.50
1:C:350:ARG:NH1	1:C:350:ARG:HG2	2.20	0.50
1:A:391:TRP:CH2	1:A:409:VAL:HG21	2.48	0.49
1:B:323:LYS:NZ	1:B:327:GLU:OE2	2.46	0.49
1:B:358:ARG:NH2	5:B:714:HOH:O	2.45	0.48
1:B:192:LYS:HG2	1:B:221:ILE:HG13	1.96	0.47
1:D:462:TYR:CE1	1:D:464:ARG:HG3	2.48	0.47
1:A:120:ARG:NH1	3:A:602:6OH:OA3	2.30	0.47
1:A:464:ARG:HD3	3:A:602:6OH:CA2	2.45	0.46
1:B:464:ARG:HE	3:B:602:6OH:CA2	2.29	0.46
1:A:469:PRO:HB3	1:A:485:PHE:CE2	2.51	0.46
1:D:247:GLU:OE1	1:D:249:LYS:HE2	2.16	0.45
1:D:391:TRP:CH2	1:D:409:VAL:HG21	2.51	0.45
1:A:269:LEU:O	2:A:601:NAD:H2N	2.17	0.45
1:A:455:LEU:HD11	1:A:470:PHE:CE2	2.52	0.44
1:D:169:ASP:HB2	1:D:300:GLN:O	2.17	0.44
1:C:307:ARG:NH2	1:C:424:ARG:O	2.50	0.44
1:A:333:TYR:HB2	1:A:336:GLN:HB2	1.99	0.44
1:C:312:ARG:HG3	1:C:313:SER:N	2.32	0.44
1:C:319:VAL:HG22	1:C:412:ILE:HD12	1.98	0.44
1:C:323:LYS:HE2	1:C:368:VAL:O	2.17	0.44
1:A:135:SER:O	1:B:467:ARG:NH1	2.51	0.43
1:C:169:ASP:HB2	1:C:300:GLN:O	2.17	0.43
1:B:169:ASP:HB2	1:B:300:GLN:O	2.18	0.43
1:A:292:ARG:HD2	5:A:944:HOH:O	2.17	0.43
1:A:108:ARG:NH2	5:A:715:HOH:O	2.52	0.43
2:B:601:NAD:O7N	3:B:602:6OH:H1	2.19	0.42
3:A:602:6OH:OA4	3:A:602:6OH:OA1	2.38	0.42
1:D:452:HIS:HD2	5:D:747:HOH:O	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LYS:HG3	1:A:307:ARG:CD	2.46	0.42
1:D:333:TYR:HB2	1:D:336:GLN:HB2	2.00	0.42
1:D:454:GLY:HA3	1:D:471:GLY:O	2.19	0.42
1:B:310:VAL:O	1:B:414:PRO:HA	2.19	0.42
1:A:433:ALA:HB2	1:A:455:LEU:HD12	2.02	0.42
1:C:391:TRP:CH2	1:C:409:VAL:HG21	2.54	0.41
1:B:140:PHE:CD1	1:C:468:THR:HG22	2.56	0.41
1:B:269:LEU:O	2:B:601:NAD:H2N	2.21	0.41
1:D:72:TRP:HZ3	1:D:83:LEU:HD23	1.84	0.41
1:C:203:LEU:HA	1:C:203:LEU:HD12	1.97	0.41
1:C:443:ARG:NE	5:C:704:HOH:O	2.32	0.41
1:D:463:LEU:HA	1:D:463:LEU:HD23	1.85	0.41
1:D:455:LEU:HD21	1:D:470:PHE:HD2	1.85	0.41
1:A:167:PRO:HG3	1:A:245:THR:HG22	2.02	0.40
1:C:358:ARG:NH2	5:C:721:HOH:O	2.53	0.40
1:D:440:ASN:HB3	1:D:443:ARG:HB3	2.03	0.40
1:A:174:LEU:HA	1:A:174:LEU:HD23	1.90	0.40
1:A:98:PHE:CZ	1:A:203:LEU:HB3	2.57	0.40
1:D:137:THR:HB	1:D:154:THR:OG1	2.21	0.40
1:B:274:ALA:HA	1:B:307:ARG:O	2.22	0.40
1:B:454:GLY:HA3	1:B:471:GLY:O	2.20	0.40
1:C:140:PHE:HB2	1:C:152:ASN:HB2	2.03	0.40
1:D:203:LEU:HD12	1:D:203:LEU:HA	1.88	0.40
1:B:17:PRO:HB2	1:B:18:SER:H	1.62	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%)	468 (97%)	14 (3%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	483/520 (93%)	465 (96%)	18 (4%)	0	100	100
1	C	481/520 (92%)	466 (97%)	15 (3%)	0	100	100
1	D	481/520 (92%)	466 (97%)	14 (3%)	1 (0%)	52	48
All	All	1927/2080 (93%)	1865 (97%)	61 (3%)	1 (0%)	56	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	171	PRO

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	393/424 (93%)	383 (98%)	10 (2%)	55	55
1	B	394/424 (93%)	385 (98%)	9 (2%)	58	60
1	C	392/424 (92%)	381 (97%)	11 (3%)	51	50
1	D	392/424 (92%)	378 (96%)	14 (4%)	42	39
All	All	1571/1696 (93%)	1527 (97%)	44 (3%)	51	50

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	LEU
1	A	152	ASN
1	A	192	LYS
1	A	395	SER
1	A	406	PHE
1	A	432	LEU
1	A	436	ILE
1	A	455	LEU
1	A	462	TYR
1	A	492	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	131	LEU
1	B	192	LYS
1	B	203	LEU
1	B	373	VAL
1	B	406	PHE
1	B	432	LEU
1	B	455	LEU
1	B	462	TYR
1	B	492	ASP
1	D	46	ILE
1	D	69	LYS
1	D	131	LEU
1	D	192	LYS
1	D	203	LEU
1	D	227	ASP
1	D	242	LEU
1	D	337	ASP
1	D	352	LYS
1	D	397	LYS
1	D	406	PHE
1	D	432	LEU
1	D	462	TYR
1	D	492	ASP
1	C	18	SER
1	C	55	LYS
1	C	131	LEU
1	C	192	LYS
1	C	203	LEU
1	C	242	LEU
1	C	350	ARG
1	C	373	VAL
1	C	406	PHE
1	C	432	LEU
1	C	492	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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	-	42,48,48	1.67	10 (23%)	46,73,73	1.89	5 (10%)
3	6OH	A	602	-	5,9,9	3.86	4 (80%)	4,10,10	5.33	3 (75%)
2	NAD	B	601	-	42,48,48	1.73	10 (23%)	46,73,73	1.89	5 (10%)
3	6OH	B	602	-	5,9,9	3.90	4 (80%)	4,10,10	3.08	4 (100%)
2	NAD	C	601	-	42,48,48	1.70	9 (21%)	46,73,73	1.86	5 (10%)
3	6OH	C	602	-	5,9,9	3.87	3 (60%)	4,10,10	5.32	4 (100%)
2	NAD	D	601	-	42,48,48	1.75	10 (23%)	46,73,73	1.71	4 (8%)

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
3	6OH	A	602	-	-	1/3/9/9	0/0/0/0
2	NAD	B	601	-	-	0/22/62/62	0/5/5/5
3	6OH	B	602	-	-	1/3/9/9	0/0/0/0
2	NAD	C	601	-	-	0/22/62/62	0/5/5/5
3	6OH	C	602	-	-	2/3/9/9	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	D	601	-	-	0/22/62/62	0/5/5/5

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	NAD	C2B-C3B	-4.39	1.41	1.53
2	B	601	NAD	C2B-C3B	-4.32	1.41	1.53
2	A	601	NAD	C2B-C3B	-4.22	1.42	1.53
2	C	601	NAD	C2B-C3B	-4.16	1.42	1.53
3	A	602	6OH	OA3-CA2	-3.91	1.23	1.32
3	C	602	6OH	OA3-CA2	-3.82	1.23	1.32
3	B	602	6OH	OA3-CA2	-3.65	1.24	1.32
2	C	601	NAD	C2B-C1B	-3.45	1.48	1.53
2	B	601	NAD	C2B-C1B	-3.35	1.48	1.53
2	A	601	NAD	C2D-C1D	-2.99	1.48	1.53
2	D	601	NAD	C2B-C1B	-2.98	1.48	1.53
2	D	601	NAD	C2D-C1D	-2.89	1.49	1.53
2	C	601	NAD	C2D-C1D	-2.75	1.49	1.53
2	B	601	NAD	C2D-C1D	-2.59	1.49	1.53
2	A	601	NAD	C2B-C1B	-2.53	1.49	1.53
2	B	601	NAD	C2D-C3D	-2.49	1.46	1.53
2	C	601	NAD	O3D-C3D	-2.47	1.37	1.43
2	D	601	NAD	O2D-C2D	-2.46	1.37	1.43
2	B	601	NAD	O3D-C3D	-2.40	1.37	1.43
2	B	601	NAD	O2D-C2D	-2.40	1.37	1.43
2	A	601	NAD	O3D-C3D	-2.31	1.37	1.43
2	A	601	NAD	O2D-C2D	-2.29	1.37	1.43
2	D	601	NAD	C2D-C3D	-2.28	1.47	1.53
2	B	601	NAD	O4B-C4B	-2.23	1.39	1.45
2	A	601	NAD	C5D-C4D	-2.20	1.44	1.51
2	B	601	NAD	C5D-C4D	-2.16	1.44	1.51
2	C	601	NAD	C2D-C3D	-2.13	1.47	1.53
2	D	601	NAD	C5D-C4D	-2.13	1.44	1.51
2	D	601	NAD	O3D-C3D	-2.12	1.38	1.43
2	A	601	NAD	O4B-C4B	-2.10	1.40	1.45
2	C	601	NAD	O4B-C4B	-2.10	1.40	1.45
2	A	601	NAD	C2D-C3D	-2.10	1.47	1.53
2	C	601	NAD	C5D-C4D	-2.06	1.45	1.51
2	D	601	NAD	O4B-C4B	-2.06	1.40	1.45
3	B	602	6OH	CA4-CA3	2.05	1.49	1.43
3	A	602	6OH	CA4-CA3	2.09	1.49	1.43
2	A	601	NAD	C6A-N6A	2.98	1.46	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	NAD	C6A-N6A	2.98	1.46	1.34
2	C	601	NAD	C6A-N6A	3.01	1.46	1.34
2	B	601	NAD	C6A-N6A	3.05	1.46	1.34
3	A	602	6OH	CA4-CA5	4.74	1.48	1.35
3	C	602	6OH	CA4-CA5	4.92	1.48	1.35
3	B	602	6OH	CA4-CA5	4.95	1.49	1.35
3	A	602	6OH	OA4-CA6	5.48	1.39	1.22
3	B	602	6OH	OA4-CA6	5.55	1.39	1.22
3	C	602	6OH	OA4-CA6	5.55	1.39	1.22
2	C	601	NAD	C7N-N7N	5.75	1.44	1.33
2	B	601	NAD	C7N-N7N	5.81	1.44	1.33
2	A	601	NAD	C7N-N7N	5.88	1.44	1.33
2	D	601	NAD	C7N-N7N	6.17	1.45	1.33

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	6OH	CA4-CA5-CA6	-8.70	112.50	121.45
2	D	601	NAD	N3A-C2A-N1A	-8.54	122.17	128.87
2	A	601	NAD	N3A-C2A-N1A	-8.37	122.29	128.87
2	B	601	NAD	N3A-C2A-N1A	-7.92	122.65	128.87
3	C	602	6OH	CA4-CA5-CA6	-7.64	113.58	121.45
2	C	601	NAD	N3A-C2A-N1A	-7.57	122.92	128.87
3	C	602	6OH	OA4-CA6-CA5	-5.81	116.11	125.77
3	A	602	6OH	OA4-CA6-CA5	-4.96	117.52	125.77
2	B	601	NAD	O7N-C7N-N7N	-4.22	116.57	122.58
3	B	602	6OH	CA4-CA5-CA6	-4.06	117.27	121.45
3	C	602	6OH	CA5-CA4-CA3	-3.69	115.28	123.23
3	A	602	6OH	CA5-CA4-CA3	-3.37	115.97	123.23
2	C	601	NAD	O7N-C7N-N7N	-3.24	117.96	122.58
3	B	602	6OH	OA4-CA6-CA5	-3.19	120.46	125.77
2	A	601	NAD	O7N-C7N-N7N	-3.18	118.05	122.58
3	C	602	6OH	OA3-CA2-CA3	-2.71	117.58	122.70
3	B	602	6OH	CA5-CA4-CA3	-2.48	117.88	123.23
2	B	601	NAD	C4D-O4D-C1D	-2.36	107.14	109.64
3	B	602	6OH	OA3-CA2-CA3	-2.27	118.42	122.70
2	A	601	NAD	C4D-O4D-C1D	-2.24	107.27	109.64
2	D	601	NAD	O7N-C7N-N7N	-2.05	119.67	122.58
2	C	601	NAD	O2N-PN-O3	2.02	113.93	105.27
2	D	601	NAD	C3N-C7N-N7N	2.21	120.32	117.82
2	A	601	NAD	C3N-C7N-N7N	3.01	121.22	117.82
2	C	601	NAD	C3N-C7N-N7N	4.14	122.50	117.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	NAD	C3N-C7N-N7N	4.36	122.75	117.82
2	D	601	NAD	O4D-C1D-N1N	4.61	113.08	108.10
2	B	601	NAD	O4D-C1D-N1N	6.02	114.60	108.10
2	C	601	NAD	O4D-C1D-N1N	6.34	114.95	108.10
2	A	601	NAD	O4D-C1D-N1N	6.43	115.04	108.10

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	602	6OH	CA3-CA4-CA5-CA6
3	A	602	6OH	OA4-CA6-CA5-CA4
3	C	602	6OH	OA4-CA6-CA5-CA4
3	B	602	6OH	OA4-CA6-CA5-CA4

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NAD	2	0
3	A	602	6OH	3	0
2	B	601	NAD	3	0
3	B	602	6OH	4	0
2	C	601	NAD	3	0
3	C	602	6OH	2	0
2	D	601	NAD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	483/520 (92%)	-0.09	3 (0%) 90 90	25, 37, 48, 57	0
1	B	484/520 (93%)	-0.11	5 (1%) 84 84	25, 37, 49, 70	0
1	C	483/520 (92%)	-0.12	3 (0%) 90 90	25, 37, 48, 64	0
1	D	483/520 (92%)	0.10	14 (2%) 55 56	26, 42, 56, 68	0
All	All	1933/2080 (92%)	-0.05	25 (1%) 79 80	25, 38, 52, 70	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	17	PRO	3.7
1	D	18	SER	3.6
1	D	361	VAL	2.9
1	A	170	LEU	2.9
1	A	174	LEU	2.9
1	D	303	LEU	2.8
1	D	45	LEU	2.7
1	D	35	PHE	2.6
1	D	302	CYS	2.4
1	D	32	ALA	2.4
1	B	170	LEU	2.4
1	B	32	ALA	2.2
1	D	382	GLN	2.2
1	A	33	SER	2.2
1	C	170	LEU	2.2
1	D	301	VAL	2.2
1	B	55	LYS	2.2
1	D	377	ASN	2.2
1	D	378	ASP	2.1
1	D	55	LYS	2.1
1	C	302	CYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	174	LEU	2.0
1	D	229	ALA	2.0
1	D	224	PHE	2.0
1	C	174	LEU	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(\AA^2)	Q<0.9
4	NA	C	603	1/1	0.81	0.22	6.43	52,52,52,52	0
4	NA	A	603	1/1	0.63	0.21	5.15	52,52,52,52	0
4	NA	B	603	1/1	0.82	0.26	5.00	49,49,49,49	0
3	6OH	C	602	10/10	0.88	0.23	1.42	45,50,57,59	0
3	6OH	B	602	10/10	0.90	0.23	1.18	47,52,57,57	0
3	6OH	A	602	10/10	0.92	0.19	0.22	44,50,54,58	0
2	NAD	D	601	44/44	0.94	0.11	-0.55	38,48,57,61	0
2	NAD	A	601	44/44	0.94	0.10	-0.78	37,42,48,51	0
2	NAD	C	601	44/44	0.95	0.10	-0.86	33,38,42,44	0
2	NAD	B	601	44/44	0.96	0.10	-0.92	30,40,45,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.