



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 02:51 AM GMT

PDB ID : 4F3X
Title : Crystal structure of putative aldehyde dehydrogenase from Sinorhizobium meliloti 1021 complexed with NAD
Authors : Malashkevich, V.N.; Bhosle, R.; Toro, R.; Hillerich, B.; Gizzi, A.; Garforth, S.; Kar, A.; Chan, M.K.; Lafluer, J.; Patel, H.; Matikainen, B.; Chamala, S.; Lim, S.; Celikgil, A.; Villegas, G.; Evans, B.; Zenchek, W.; Love, J.; Fiser, A.; Khafizov, K.; Seidel, R.; Bonanno, J.B.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRC)
Deposited on : 2012-05-09
Resolution : 2.01 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

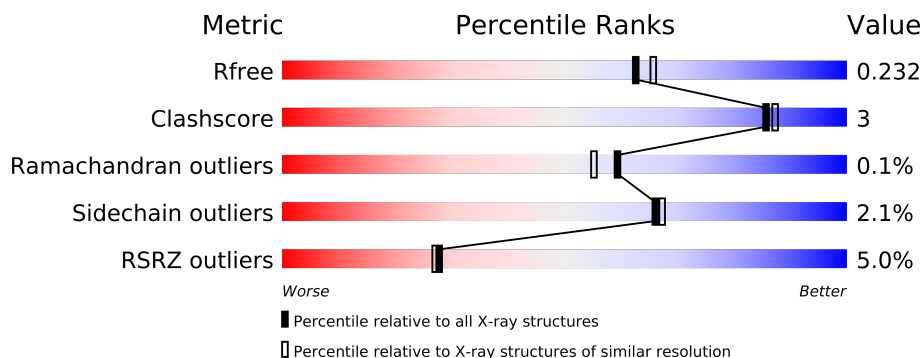
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.01 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}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (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. 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	498	
1	B	498	
1	C	498	
1	D	498	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	GOL	B	501	-	X
3	GOL	C	501	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15314 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 Putative aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	Se	0	2	0
			3621	2276	636	692	5	12			
1	B	476	Total	C	N	O	S	Se	0	4	0
			3628	2281	636	693	5	13			
1	C	476	Total	C	N	O	S	Se	0	2	0
			3618	2274	633	694	5	12			
1	D	475	Total	C	N	O	S	Se	0	0	0
			3599	2262	632	689	5	11			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MSE	-	EXPRESSION TAG	UNP Q92ND9
A	-21	HIS	-	EXPRESSION TAG	UNP Q92ND9
A	-20	HIS	-	EXPRESSION TAG	UNP Q92ND9
A	-19	HIS	-	EXPRESSION TAG	UNP Q92ND9
A	-18	HIS	-	EXPRESSION TAG	UNP Q92ND9
A	-17	HIS	-	EXPRESSION TAG	UNP Q92ND9
A	-16	HIS	-	EXPRESSION TAG	UNP Q92ND9
A	-15	SER	-	EXPRESSION TAG	UNP Q92ND9
A	-14	SER	-	EXPRESSION TAG	UNP Q92ND9
A	-13	GLY	-	EXPRESSION TAG	UNP Q92ND9
A	-12	VAL	-	EXPRESSION TAG	UNP Q92ND9
A	-11	ASP	-	EXPRESSION TAG	UNP Q92ND9
A	-10	LEU	-	EXPRESSION TAG	UNP Q92ND9
A	-9	GLY	-	EXPRESSION TAG	UNP Q92ND9
A	-8	THR	-	EXPRESSION TAG	UNP Q92ND9
A	-7	GLU	-	EXPRESSION TAG	UNP Q92ND9
A	-6	ASN	-	EXPRESSION TAG	UNP Q92ND9
A	-5	LEU	-	EXPRESSION TAG	UNP Q92ND9
A	-4	TYR	-	EXPRESSION TAG	UNP Q92ND9
A	-3	PHE	-	EXPRESSION TAG	UNP Q92ND9
A	-2	GLN	-	EXPRESSION TAG	UNP Q92ND9

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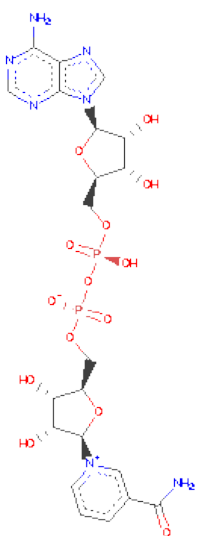
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP Q92ND9
A	0	MSE	-	EXPRESSION TAG	UNP Q92ND9
B	-22	MSE	-	EXPRESSION TAG	UNP Q92ND9
B	-21	HIS	-	EXPRESSION TAG	UNP Q92ND9
B	-20	HIS	-	EXPRESSION TAG	UNP Q92ND9
B	-19	HIS	-	EXPRESSION TAG	UNP Q92ND9
B	-18	HIS	-	EXPRESSION TAG	UNP Q92ND9
B	-17	HIS	-	EXPRESSION TAG	UNP Q92ND9
B	-16	HIS	-	EXPRESSION TAG	UNP Q92ND9
B	-15	SER	-	EXPRESSION TAG	UNP Q92ND9
B	-14	SER	-	EXPRESSION TAG	UNP Q92ND9
B	-13	GLY	-	EXPRESSION TAG	UNP Q92ND9
B	-12	VAL	-	EXPRESSION TAG	UNP Q92ND9
B	-11	ASP	-	EXPRESSION TAG	UNP Q92ND9
B	-10	LEU	-	EXPRESSION TAG	UNP Q92ND9
B	-9	GLY	-	EXPRESSION TAG	UNP Q92ND9
B	-8	THR	-	EXPRESSION TAG	UNP Q92ND9
B	-7	GLU	-	EXPRESSION TAG	UNP Q92ND9
B	-6	ASN	-	EXPRESSION TAG	UNP Q92ND9
B	-5	LEU	-	EXPRESSION TAG	UNP Q92ND9
B	-4	TYR	-	EXPRESSION TAG	UNP Q92ND9
B	-3	PHE	-	EXPRESSION TAG	UNP Q92ND9
B	-2	GLN	-	EXPRESSION TAG	UNP Q92ND9
B	-1	SER	-	EXPRESSION TAG	UNP Q92ND9
B	0	MSE	-	EXPRESSION TAG	UNP Q92ND9
C	-22	MSE	-	EXPRESSION TAG	UNP Q92ND9
C	-21	HIS	-	EXPRESSION TAG	UNP Q92ND9
C	-20	HIS	-	EXPRESSION TAG	UNP Q92ND9
C	-19	HIS	-	EXPRESSION TAG	UNP Q92ND9
C	-18	HIS	-	EXPRESSION TAG	UNP Q92ND9
C	-17	HIS	-	EXPRESSION TAG	UNP Q92ND9
C	-16	HIS	-	EXPRESSION TAG	UNP Q92ND9
C	-15	SER	-	EXPRESSION TAG	UNP Q92ND9
C	-14	SER	-	EXPRESSION TAG	UNP Q92ND9
C	-13	GLY	-	EXPRESSION TAG	UNP Q92ND9
C	-12	VAL	-	EXPRESSION TAG	UNP Q92ND9
C	-11	ASP	-	EXPRESSION TAG	UNP Q92ND9
C	-10	LEU	-	EXPRESSION TAG	UNP Q92ND9
C	-9	GLY	-	EXPRESSION TAG	UNP Q92ND9
C	-8	THR	-	EXPRESSION TAG	UNP Q92ND9
C	-7	GLU	-	EXPRESSION TAG	UNP Q92ND9
C	-6	ASN	-	EXPRESSION TAG	UNP Q92ND9

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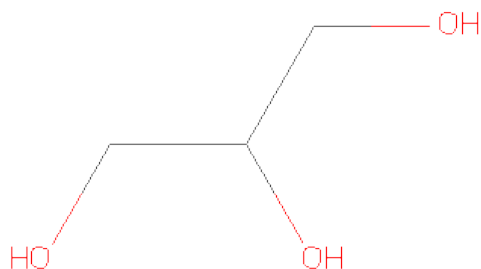
Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	LEU	-	EXPRESSION TAG	UNP Q92ND9
C	-4	TYR	-	EXPRESSION TAG	UNP Q92ND9
C	-3	PHE	-	EXPRESSION TAG	UNP Q92ND9
C	-2	GLN	-	EXPRESSION TAG	UNP Q92ND9
C	-1	SER	-	EXPRESSION TAG	UNP Q92ND9
C	0	MSE	-	EXPRESSION TAG	UNP Q92ND9
D	-22	MSE	-	EXPRESSION TAG	UNP Q92ND9
D	-21	HIS	-	EXPRESSION TAG	UNP Q92ND9
D	-20	HIS	-	EXPRESSION TAG	UNP Q92ND9
D	-19	HIS	-	EXPRESSION TAG	UNP Q92ND9
D	-18	HIS	-	EXPRESSION TAG	UNP Q92ND9
D	-17	HIS	-	EXPRESSION TAG	UNP Q92ND9
D	-16	HIS	-	EXPRESSION TAG	UNP Q92ND9
D	-15	SER	-	EXPRESSION TAG	UNP Q92ND9
D	-14	SER	-	EXPRESSION TAG	UNP Q92ND9
D	-13	GLY	-	EXPRESSION TAG	UNP Q92ND9
D	-12	VAL	-	EXPRESSION TAG	UNP Q92ND9
D	-11	ASP	-	EXPRESSION TAG	UNP Q92ND9
D	-10	LEU	-	EXPRESSION TAG	UNP Q92ND9
D	-9	GLY	-	EXPRESSION TAG	UNP Q92ND9
D	-8	THR	-	EXPRESSION TAG	UNP Q92ND9
D	-7	GLU	-	EXPRESSION TAG	UNP Q92ND9
D	-6	ASN	-	EXPRESSION TAG	UNP Q92ND9
D	-5	LEU	-	EXPRESSION TAG	UNP Q92ND9
D	-4	TYR	-	EXPRESSION TAG	UNP Q92ND9
D	-3	PHE	-	EXPRESSION TAG	UNP Q92ND9
D	-2	GLN	-	EXPRESSION TAG	UNP Q92ND9
D	-1	SER	-	EXPRESSION TAG	UNP Q92ND9
D	0	MSE	-	EXPRESSION TAG	UNP Q92ND9

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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	C	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		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is water.

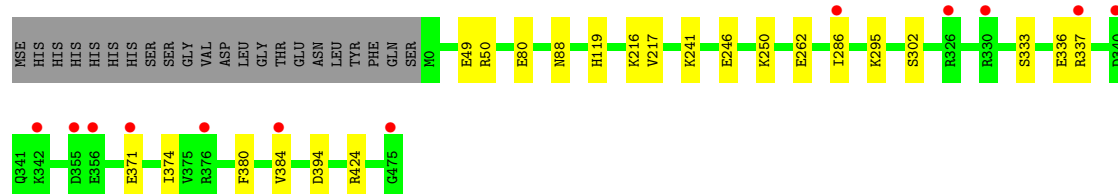
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	187	Total	O	0	0
			187	187		
4	B	170	Total	O	0	0
			170	170		
4	C	165	Total	O	0	0
			165	165		
4	D	120	Total	O	0	0
			120	120		

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.

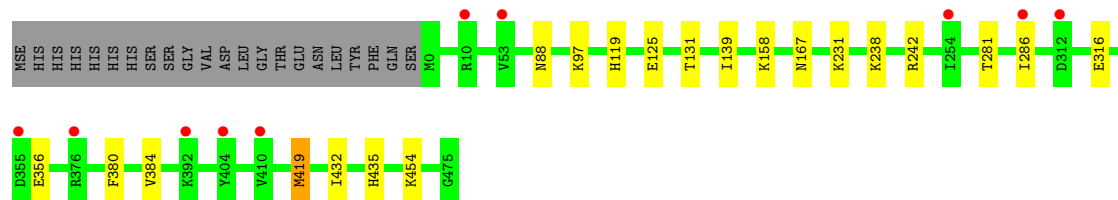
- Molecule 1: Putative aldehyde dehydrogenase

Chain A: 



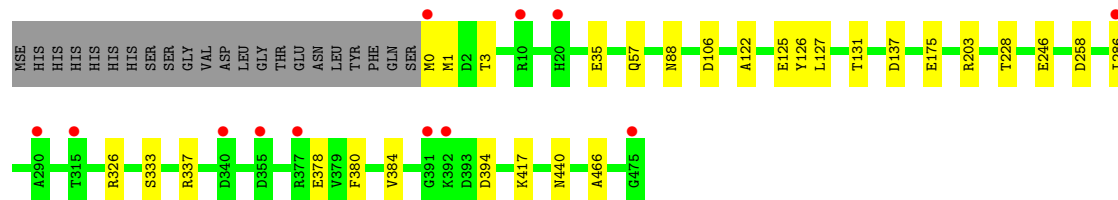
- Molecule 1: Putative aldehyde dehydrogenase

Chain B: 



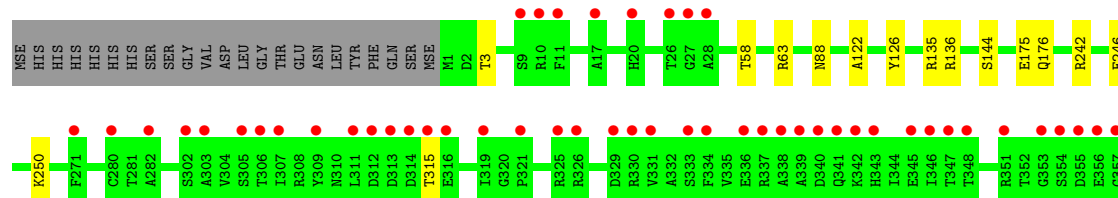
- Molecule 1: Putative aldehyde dehydrogenase

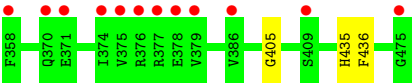
Chain C: 



- Molecule 1: Putative aldehyde dehydrogenase

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.44Å 96.91Å 121.81Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	19.91 – 2.01 19.87 – 2.01	Depositor EDS
% Data completeness (in resolution range)	95.5 (19.91-2.01) 95.7 (19.87-2.01)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.7.0025	Depositor
R, R_{free}	0.180 , 0.233 0.180 , 0.232	Depositor DCC
R_{free} test set	6378 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 55.2	EDS
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 126673 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15314	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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: GOL, 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	0.48	0/3686	0.65	0/4987
1	B	0.46	0/3698	0.66	1/5001 (0.0%)
1	C	0.45	0/3683	0.64	0/4984
1	D	0.44	0/3659	0.61	0/4954
All	All	0.46	0/14726	0.64	1/19926 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	419	MSE	CG-SE-CE	6.73	113.70	98.90

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	3621	0	0	9	0
1	B	3628	0	0	9	0
1	C	3618	0	0	12	0
1	D	3599	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	44	0	0	1	0
2	B	44	0	0	0	0
2	C	44	0	0	3	0
2	D	44	0	0	1	0
3	A	6	0	0	0	0
3	B	12	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
4	A	187	0	0	2	0
4	B	170	0	0	3	0
4	C	165	0	0	1	0
4	D	120	0	0	3	0
All	All	15314	0	0	40	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 3.

All (40) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:333:SER:OG	1:C:337:ARG:NH1	2.27	0.67
1:D:58:THR:O	1:D:63:ARG:NH2	2.36	0.58
1:B:286:ILE:CD1	1:B:384:VAL:CG1	2.87	0.53
1:C:378:GLU:OE1	2:C:500:NAD:C5N	2.57	0.52
1:B:125:GLU:OE1	1:D:135:ARG:NH2	2.44	0.50
1:B:419:MSE:CE	1:B:432:ILE:CD1	2.89	0.50
1:C:35:GLU:OE2	1:C:203:ARG:N	2.45	0.49
1:A:333:SER:OG	1:A:337:ARG:NH1	2.46	0.49
1:B:125:GLU:OE2	1:B:131:THR:OG1	2.31	0.49
1:B:242:ARG:NE	4:B:673:HOH:O	2.46	0.49
1:D:435:HIS:O	1:D:436:PHE:CB	2.62	0.48
1:D:242:ARG:NE	4:D:693:HOH:O	2.47	0.47
1:B:119:HIS:CE1	4:B:627:HOH:O	2.67	0.47
1:A:217:VAL:O	1:A:241:LYS:NZ	2.48	0.46
1:C:137:ASP:O	1:C:466:ALA:N	2.48	0.46
2:C:500:NAD:N7N	2:C:500:NAD:O1N	2.49	0.46
1:A:49:GLU:OE1	1:A:216:LYS:NZ	2.49	0.45
1:C:175:GLU:N	1:C:175:GLU:OE1	2.48	0.45
1:D:122:ALA:O	1:D:126:TYR:OH	2.36	0.44
1:C:394:ASP:N	4:C:700:HOH:O	2.51	0.44
1:C:106:ASP:OD2	1:C:440:ASN:ND2	2.52	0.43
1:D:136:ARG:NH1	4:D:701:HOH:O	2.51	0.42
1:C:122:ALA:O	1:C:126:TYR:OH	2.37	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:500:NAD:N7N	2:A:500:NAD:O1N	2.52	0.42
1:D:175:GLU:OE1	1:D:175:GLU:N	2.53	0.42
1:C:258:ASP:OD2	1:C:417:LYS:NZ	2.53	0.42
1:B:139:ILE:N	1:B:167:ASN:OD1	2.53	0.42
1:C:228:THR:OG1	2:C:500:NAD:O1A	2.37	0.42
1:A:250:LYS:NZ	1:A:374:ILE:O	2.54	0.41
1:A:286:ILE:CD1	1:A:384:VAL:CG1	2.98	0.41
1:D:3:THR:N	4:D:689:HOH:O	2.52	0.41
1:D:175:GLU:OE1	2:D:500:NAD:O2B	2.38	0.41
1:B:454:LYS:NZ	4:B:607:HOH:O	2.54	0.41
1:A:119:HIS:NE2	4:A:627:HOH:O	2.37	0.41
1:B:281:THR:O	1:B:435:HIS:NE2	2.54	0.41
1:A:80:GLU:OE1	1:A:80:GLU:N	2.54	0.41
1:A:50:ARG:NH2	4:A:764:HOH:O	2.54	0.41
1:C:125:GLU:OE2	1:C:131:THR:OG1	2.39	0.40
1:A:394:ASP:OD2	1:A:424:ARG:NH2	2.55	0.40
1:C:286:ILE:CD1	1:C:384:VAL:CG1	2.99	0.40

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	476/498 (96%)	463 (97%)	13 (3%)	0	100	100
1	B	478/498 (96%)	463 (97%)	15 (3%)	0	100	100
1	C	476/498 (96%)	461 (97%)	15 (3%)	0	100	100
1	D	473/498 (95%)	458 (97%)	14 (3%)	1 (0%)	56	51
All	All	1903/1992 (96%)	1845 (97%)	57 (3%)	1 (0%)	59	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	405	GLY

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	372/377 (99%)	363 (98%)	9 (2%)	61	61
1	B	374/377 (99%)	366 (98%)	8 (2%)	66	67
1	C	372/377 (99%)	362 (97%)	10 (3%)	57	56
1	D	369/377 (98%)	363 (98%)	6 (2%)	75	77
All	All	1487/1508 (99%)	1454 (98%)	33 (2%)	66	65

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	246[A]	GLU
1	A	246[B]	GLU
1	A	262	GLU
1	A	295	LYS
1	A	302	SER
1	A	336	GLU
1	A	371	GLU
1	A	380	PHE
1	B	88	ASN
1	B	97	LYS
1	B	158	LYS
1	B	231	LYS
1	B	238	LYS
1	B	316	GLU
1	B	356	GLU
1	B	380	PHE
1	C	0	MSE
1	C	1	MSE
1	C	3	THR
1	C	57	GLN
1	C	88	ASN
1	C	127	LEU
1	C	246[A]	GLU
1	C	246[B]	GLU
1	C	326	ARG

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Mol	Chain	Res	Type
1	C	380	PHE
1	D	88	ASN
1	D	144	SER
1	D	176	GLN
1	D	246	GLU
1	D	250	LYS
1	D	315	THR

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 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 ⓘ

9 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	$\# Z > 2$
2	NAD	A	500	-	48,48,48	0.92	2 (4%)	73,73,73	1.53	10 (13%)
3	GOL	A	501	-	5,5,5	0.25	0	5,5,5	0.62	0
3	GOL	B	501	-	5,5,5	0.20	0	5,5,5	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	B	502	-	48,48,48	1.01	3 (6%)	73,73,73	1.56	9 (12%)
3	GOL	B	503	-	5,5,5	0.20	0	5,5,5	0.16	0
2	NAD	C	500	-	48,48,48	0.96	2 (4%)	73,73,73	1.56	9 (12%)
3	GOL	C	501	-	5,5,5	0.32	0	5,5,5	0.42	0
2	NAD	D	500	-	48,48,48	0.94	2 (4%)	73,73,73	1.60	10 (13%)
3	GOL	D	501	-	5,5,5	0.28	0	5,5,5	0.31	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
2	NAD	A	500	-	-	0/30/62/62	0/3/5/5
3	GOL	A	501	-	-	0/4/4/4	0/0/0/0
3	GOL	B	501	-	-	0/4/4/4	0/0/0/0
2	NAD	B	502	-	-	0/30/62/62	0/3/5/5
3	GOL	B	503	-	-	0/4/4/4	0/0/0/0
2	NAD	C	500	-	-	0/30/62/62	0/3/5/5
3	GOL	C	501	-	-	0/4/4/4	0/0/0/0
2	NAD	D	500	-	-	0/30/62/62	0/3/5/5
3	GOL	D	501	-	-	0/4/4/4	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	NAD	C5A-C4A	3.14	1.47	1.40
2	B	502	NAD	C5A-C4A	3.08	1.47	1.40
2	D	500	NAD	C4A-N9A	-2.98	1.33	1.37
2	B	502	NAD	C4A-N9A	-2.92	1.33	1.37
2	D	500	NAD	C5A-C4A	2.78	1.46	1.40
2	A	500	NAD	C5A-C4A	2.78	1.46	1.40
2	B	502	NAD	O4B-C1B	2.75	1.45	1.41
2	C	500	NAD	C4A-N9A	-2.66	1.33	1.37
2	A	500	NAD	C4A-N9A	-2.16	1.34	1.37

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	NAD	N3A-C2A-N1A	-6.67	123.13	128.71
2	B	502	NAD	N3A-C2A-N1A	-5.80	123.86	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	NAD	N3A-C2A-N1A	-5.59	124.03	128.71
2	C	500	NAD	N3A-C4A-N9A	5.56	135.48	125.43
2	A	500	NAD	N3A-C4A-N9A	5.42	135.22	125.43
2	A	500	NAD	N3A-C2A-N1A	-5.32	124.26	128.71
2	B	502	NAD	O4B-C1B-N9A	5.11	113.19	108.44
2	D	500	NAD	N3A-C4A-N9A	4.95	134.38	125.43
2	B	502	NAD	N3A-C4A-N9A	4.95	134.36	125.43
2	D	500	NAD	O4D-C1D-N1N	4.39	112.45	107.95
2	C	500	NAD	O4D-C1D-N1N	3.98	112.03	107.95
2	D	500	NAD	C4A-C5A-N7A	-3.97	106.12	109.52
2	C	500	NAD	O4B-C1B-N9A	3.93	112.10	108.44
2	A	500	NAD	O4B-C1B-C2B	-3.81	100.94	106.77
2	A	500	NAD	O4D-C1D-N1N	3.55	111.58	107.95
2	A	500	NAD	C4A-C5A-N7A	-3.26	106.73	109.52
2	B	502	NAD	C4A-C5A-N7A	-3.23	106.75	109.52
2	C	500	NAD	C5A-C4A-N3A	-3.23	118.67	125.70
2	A	500	NAD	C5A-C4A-N3A	-3.22	118.69	125.70
2	C	500	NAD	C4A-C5A-N7A	-3.18	106.80	109.52
2	D	500	NAD	C5A-C4A-N3A	-3.11	118.93	125.70
2	B	502	NAD	O4D-C1D-N1N	3.05	111.07	107.95
2	B	502	NAD	C5A-C4A-N3A	-2.90	119.38	125.70
2	D	500	NAD	PN-O3-PA	-2.77	121.07	132.95
2	D	500	NAD	O4B-C1B-N9A	2.64	110.90	108.44
2	D	500	NAD	C3D-C2D-C1D	2.60	104.98	100.91
2	D	500	NAD	C2A-N3A-C4A	2.51	121.14	114.01
2	A	500	NAD	C8A-N9A-C4A	2.40	108.73	106.90
2	C	500	NAD	C8A-N9A-C4A	2.35	108.70	106.90
2	B	502	NAD	C8A-N9A-C4A	2.32	108.67	106.90
2	C	500	NAD	C2A-N3A-C4A	2.30	120.55	114.01
2	A	500	NAD	PN-O3-PA	-2.24	123.32	132.95
2	D	500	NAD	C8A-N9A-C4A	2.24	108.61	106.90
2	C	500	NAD	C3D-C2D-C1D	2.18	104.31	100.91
2	B	502	NAD	C2A-N3A-C4A	2.16	120.15	114.01
2	A	500	NAD	C3D-C2D-C1D	2.07	104.15	100.91
2	A	500	NAD	C2A-N3A-C4A	2.07	119.90	114.01
2	B	502	NAD	PN-O3-PA	-2.02	124.29	132.95

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	476/498 (95%)	0.00	12 (2%) 54 54	27, 43, 69, 95	0
1	B	476/498 (95%)	-0.07	10 (2%) 60 61	28, 45, 66, 105	0
1	C	476/498 (95%)	-0.00	12 (2%) 54 54	31, 47, 67, 148	0
1	D	475/498 (95%)	0.54	62 (13%) 4 4	31, 50, 104, 122	0
All	All	1903/1992 (95%)	0.12	96 (5%) 28 27	27, 47, 82, 148	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	315	THR	6.5
1	D	355	ASP	6.4
1	D	271	PHE	6.3
1	D	377	ARG	6.0
1	D	340	ASP	5.9
1	D	311	LEU	5.8
1	C	0	MSE	5.7
1	D	316	GLU	5.5
1	D	342	LYS	5.5
1	D	313	ASP	5.4
1	D	20	HIS	5.3
1	D	326	ARG	5.3
1	D	312	ASP	5.0
1	D	371	GLU	4.8
1	D	351	ARG	4.6
1	D	305	SER	4.5
1	D	343	HIS	4.5
1	D	376	ARG	4.4
1	D	339	ALA	4.3
1	D	282	ALA	4.2
1	D	341	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	354	SER	4.1
1	D	17	ALA	4.1
1	D	475	GLY	4.1
1	D	345	GLU	4.0
1	A	355	ASP	3.9
1	D	353	GLY	3.8
1	A	376	ARG	3.8
1	D	378	GLU	3.7
1	C	475	GLY	3.7
1	D	325	ARG	3.6
1	D	337	ARG	3.6
1	D	374	ILE	3.6
1	D	314	ASP	3.6
1	D	356	GLU	3.5
1	D	307	ILE	3.5
1	C	10	ARG	3.5
1	A	475	GLY	3.4
1	D	280	CYS	3.3
1	C	20	HIS	3.3
1	D	375	VAL	3.3
1	D	309	TYR	3.3
1	D	329	ASP	3.2
1	B	312	ASP	3.1
1	D	348	THR	3.1
1	D	346	ILE	3.1
1	D	336	GLU	3.0
1	D	379	VAL	3.0
1	B	404	TYR	3.0
1	D	27	GLY	2.9
1	D	303	ALA	2.8
1	A	286	ILE	2.8
1	A	326	ARG	2.8
1	D	302	SER	2.8
1	A	356	GLU	2.8
1	C	392	LYS	2.8
1	D	338	ALA	2.7
1	D	319	ILE	2.7
1	D	334	PHE	2.7
1	B	10	ARG	2.7
1	D	28	ALA	2.6
1	B	376	ARG	2.6
1	D	333	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	10	ARG	2.6
1	A	337	ARG	2.5
1	D	26	THR	2.5
1	B	286	ILE	2.5
1	C	286	ILE	2.5
1	C	340	ASP	2.5
1	D	370	GLN	2.5
1	D	358	PHE	2.4
1	A	384	VAL	2.4
1	B	53	VAL	2.4
1	D	347	THR	2.4
1	D	330	ARG	2.4
1	A	340	ASP	2.4
1	D	9	SER	2.4
1	C	315	THR	2.4
1	D	11	PHE	2.3
1	D	357	GLY	2.3
1	C	290	ALA	2.3
1	D	306	THR	2.3
1	C	355	ASP	2.2
1	D	331	VAL	2.2
1	B	355	ASP	2.2
1	D	386	VAL	2.2
1	B	410	VAL	2.1
1	B	392	LYS	2.1
1	C	377	ARG	2.1
1	A	330	ARG	2.1
1	D	409	SER	2.1
1	C	391	GLY	2.1
1	A	342	LYS	2.1
1	A	371	GLU	2.1
1	B	254	ILE	2.1
1	D	321	PRO	2.0

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
3	GOL	C	501	6/6	0.17	3.16	55,57,61,70	0
3	GOL	B	501	6/6	0.12	2.54	56,63,73,76	0
3	GOL	B	503	6/6	0.17	1.75	59,68,69,73	0
3	GOL	A	501	6/6	0.13	0.63	53,61,62,79	0
2	NAD	B	502	44/44	0.14	0.30	37,52,99,104	0
2	NAD	A	500	44/44	0.13	0.11	35,49,114,121	0
3	GOL	D	501	6/6	0.16	-0.00	59,62,66,67	0
2	NAD	D	500	44/44	0.14	-0.09	43,58,119,121	0
2	NAD	C	500	44/44	0.12	-0.17	45,60,111,124	0

6.5 Other polymers

There are no such residues in this entry.