



Full wwPDB X-ray Structure Validation Report

Nov 6, 2014 – 11:43 PM EST

PDB ID : 2ONP
Title : Arg475Gln Mutant of Human Mitochondrial Aldehyde Dehydrogenase, complexed with NAD+
Authors : Larson, H.N.; Hurley, T.D.
Deposited on : 2007-01-24
Resolution : 2.00 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>

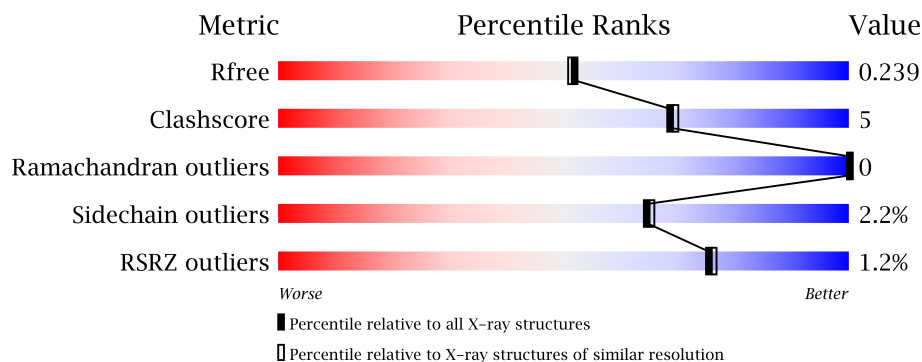
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable24103
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.1.3
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable24103

1 Overall quality at a glance

The reported resolution of this entry is 2.00 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	500	
1	B	500	
1	C	500	
1	D	500	
1	E	500	
1	F	500	
1	G	500	
1	H	500	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	C	603	-	X
2	MG	D	604	-	X
2	MG	G	607	-	X
3	NA	C	703	-	X
3	NA	H	708	-	X
5	EDO	A	6941	-	X
5	EDO	A	6951	-	X
5	EDO	B	6902	-	X
5	EDO	B	6912	-	X
5	EDO	B	6942	-	X
5	EDO	B	6952	-	X
5	EDO	B	6962	-	X
5	EDO	C	6903	-	X
5	EDO	C	6923	-	X
5	EDO	C	6943	-	X
5	EDO	C	6953	-	X
5	EDO	D	6914	-	X
5	EDO	D	6924	-	X
5	EDO	E	6905	-	X
5	EDO	E	6925	-	X
5	EDO	E	6945	-	X
5	EDO	E	6955	-	X
5	EDO	E	6965	-	X
5	EDO	F	6906	-	X
5	EDO	F	6946	-	X
5	EDO	F	6956	-	X
5	EDO	F	6966	-	X
5	EDO	G	6907	-	X
5	EDO	G	6917	-	X
5	EDO	G	6947	-	X
5	EDO	H	6908	-	X
5	EDO	H	6928	-	X
5	EDO	H	6948	-	X
6	GAI	A	6811	-	X
6	GAI	A	6821	-	X
6	GAI	B	6812	-	X
6	GAI	C	6803	-	X
6	GAI	C	6813	-	X
6	GAI	F	6806	-	X
6	GAI	F	6816	-	X
6	GAI	G	6817	-	X
6	GAI	H	6818	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 33651 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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	B	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	C	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	D	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	E	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	F	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	G	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	H	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	475	GLN	ARG	ENGINEERED	UNP P05091
B	475	GLN	ARG	ENGINEERED	UNP P05091
C	475	GLN	ARG	ENGINEERED	UNP P05091
D	475	GLN	ARG	ENGINEERED	UNP P05091
E	475	GLN	ARG	ENGINEERED	UNP P05091
F	475	GLN	ARG	ENGINEERED	UNP P05091
G	475	GLN	ARG	ENGINEERED	UNP P05091
H	475	GLN	ARG	ENGINEERED	UNP P05091

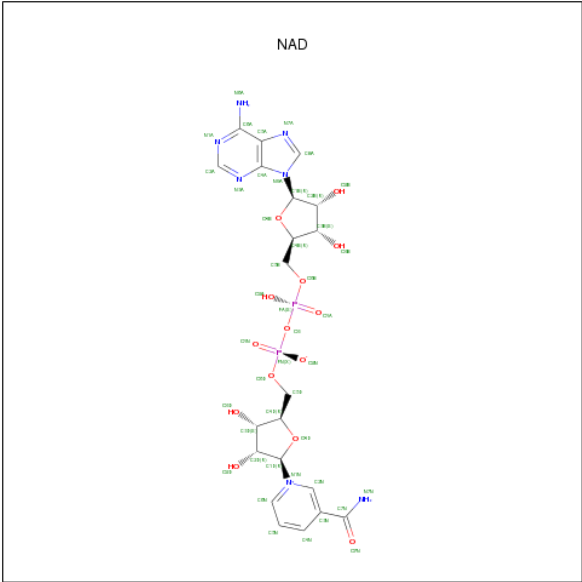
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

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

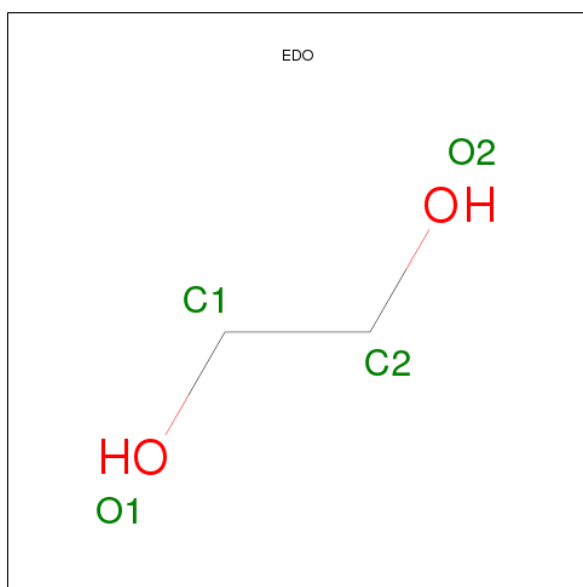
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Na 1 1	0	0
3	D	1	Total Na 1 1	0	0
3	E	1	Total Na 1 1	0	0
3	H	1	Total Na 1 1	0	0
3	B	1	Total Na 1 1	0	0
3	C	1	Total Na 1 1	0	0
3	A	1	Total Na 1 1	0	0
3	F	1	Total Na 1 1	0	0

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0

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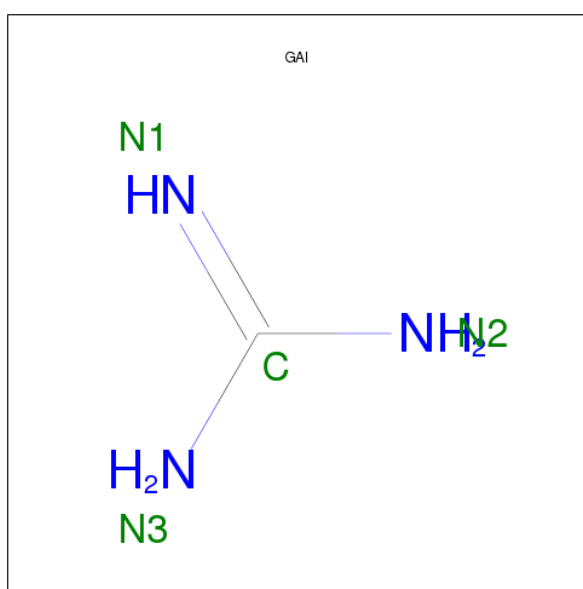
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	G	1	Total 4	C 2	O 2	0	0
5	G	1	Total 4	C 2	O 2	0	0
5	G	1	Total 4	C 2	O 2	0	0
5	G	1	Total 4	C 2	O 2	0	0

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

- Molecule 6 is GUANIDINE (three-letter code: GAI) (formula: CH_5N_3).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total 4	C 1	N 3	0	0
6	D	1	Total 4	C 1	N 3	0	0
6	D	1	Total 4	C 1	N 3	0	0
6	D	1	Total 4	C 1	N 3	0	0
6	E	1	Total 4	C 1	N 3	0	0
6	E	1	Total 4	C 1	N 3	0	0
6	F	1	Total 4	C 1	N 3	0	0
6	F	1	Total 4	C 1	N 3	0	0
6	F	1	Total 4	C 1	N 3	0	0
6	G	1	Total 4	C 1	N 3	0	0
6	G	1	Total 4	C 1	N 3	0	0
6	H	1	Total 4	C 1	N 3	0	0
6	H	1	Total 4	C 1	N 3	0	0
6	B	1	Total 4	C 1	N 3	0	0
6	A	1	Total 4	C 1	N 3	0	0
6	D	1	Total 4	C 1	N 3	0	0
6	C	1	Total 4	C 1	N 3	0	0
6	E	1	Total 4	C 1	N 3	0	0
6	E	1	Total 4	C 1	N 3	0	0
6	H	1	Total 4	C 1	N 3	0	0
6	G	1	Total 4	C 1	N 3	0	0

- Molecule 7 is water.

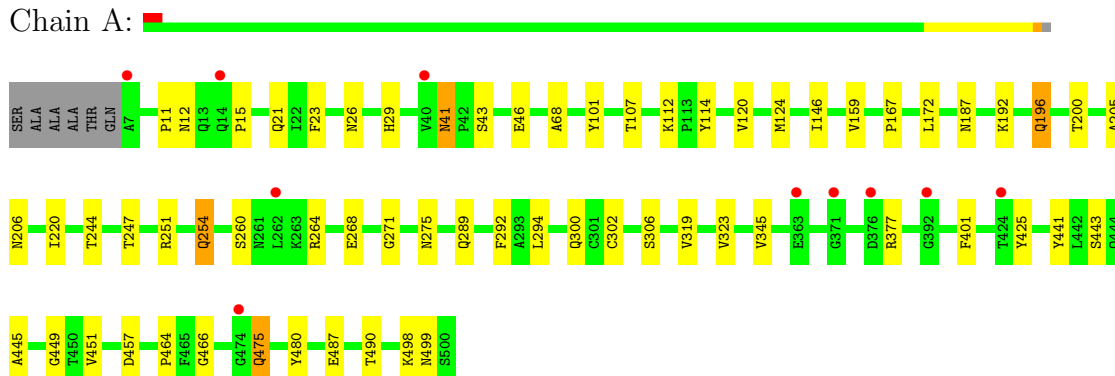
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	292	Total 292	O 292	0	0
7	B	317	Total 317	O 317	0	0
7	C	398	Total 398	O 398	0	0
7	D	333	Total 333	O 333	0	0
7	E	338	Total 338	O 338	0	0
7	F	410	Total 410	O 410	0	0
7	G	292	Total 292	O 292	0	0
7	H	267	Total 267	O 267	0	0

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.

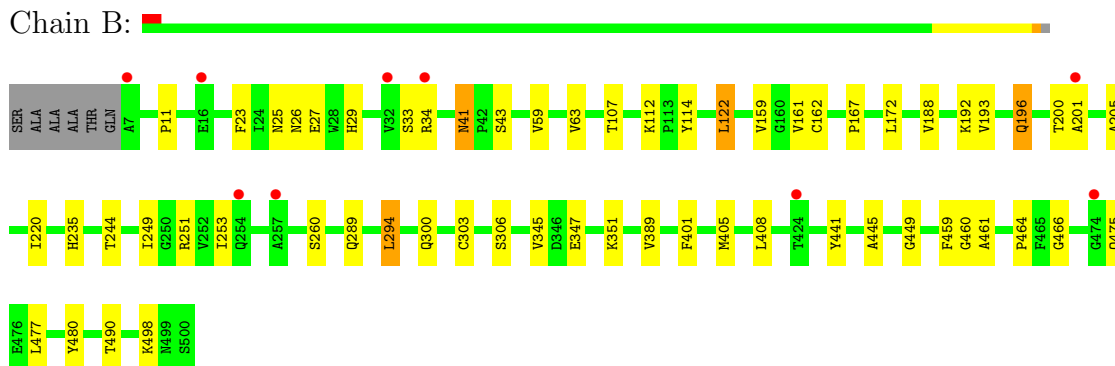
- Molecule 1: Aldehyde dehydrogenase

Chain A:



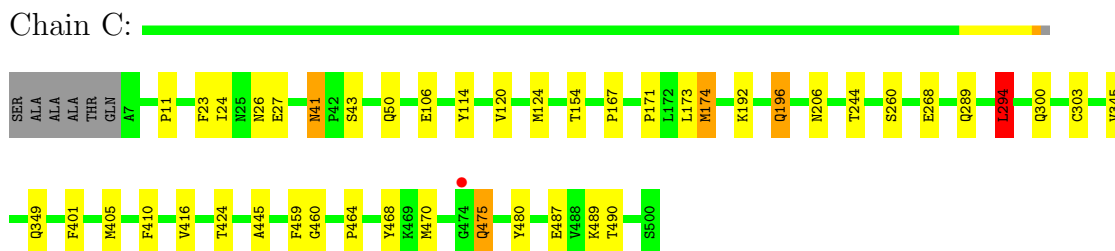
- Molecule 1: Aldehyde dehydrogenase

Chain B:



- Molecule 1: Aldehyde dehydrogenase

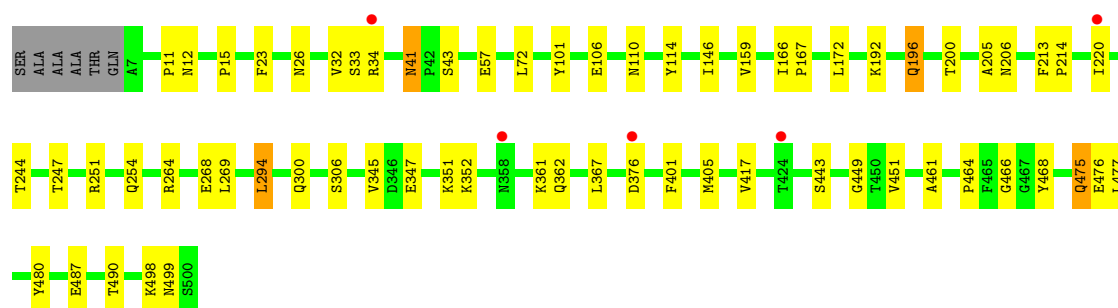
Chain C:



- Molecule 1: Aldehyde dehydrogenase

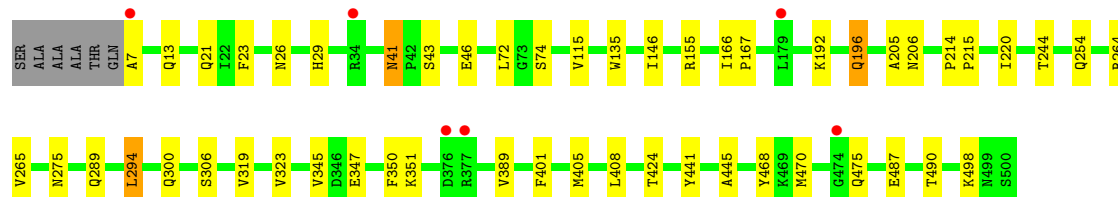
Chain D:





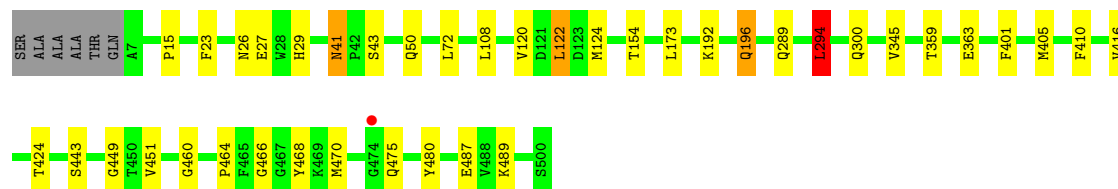
- Molecule 1: Aldehyde dehydrogenase

Chain E:



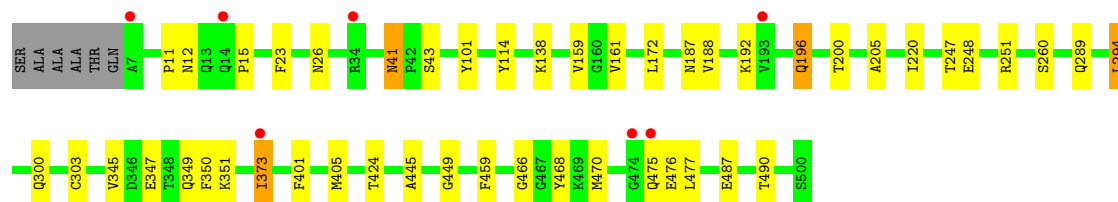
- Molecule 1: Aldehyde dehydrogenase

Chain F:



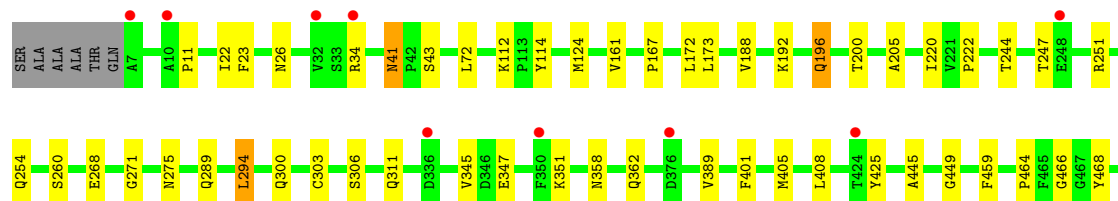
- Molecule 1: Aldehyde dehydrogenase

Chain G:



- Molecule 1: Aldehyde dehydrogenase

Chain H:



Q475	
E487	
Y488	
K498	
Y499	
S500	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	142.85Å 150.84Å 177.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 2.00 29.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (29.97-2.00) 97.5 (29.97-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.26	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.204 , 0.240 0.204 , 0.239	Depositor DCC
R_{free} test set	12682 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.774	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 251560 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	33651	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 67.51 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.0895e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NA, MG, EDO, NAD, GAI

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	0.52	1/3880 (0.0%)	0.64	0/5265
1	B	0.50	0/3880	0.66	1/5265 (0.0%)
1	C	0.51	0/3880	0.67	1/5265 (0.0%)
1	D	0.48	0/3880	0.64	0/5265
1	E	0.47	0/3880	0.63	0/5265
1	F	0.48	0/3880	0.67	2/5265 (0.0%)
1	G	0.44	0/3880	0.63	0/5265
1	H	0.44	0/3880	0.62	0/5265
All	All	0.48	1/31040 (0.0%)	0.64	4/42120 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	487	GLU	CB-CG	-6.58	1.39	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	122	LEU	CA-CB-CG	-7.52	98.01	115.30
1	F	122	LEU	CA-CB-CG	-6.67	99.95	115.30
1	F	294	LEU	CA-CB-CG	-5.57	102.49	115.30
1	C	294	LEU	CA-CB-CG	-5.28	103.16	115.30

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	3796	0	3740	43	0
1	B	3796	0	3740	42	0
1	C	3796	0	3740	33	0
1	D	3796	0	3740	45	0
1	E	3796	0	3740	44	0
1	F	3796	0	3740	26	0
1	G	3796	0	3740	40	0
1	H	3796	0	3740	44	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	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
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	44	0	26	0	0
4	B	44	0	26	0	0
4	C	44	0	26	0	0
4	D	44	0	26	0	0
4	E	44	0	26	0	0
4	F	44	0	26	0	0
4	G	44	0	26	0	0
4	H	44	0	26	0	0
5	A	20	0	30	5	0
5	B	20	0	30	4	0
5	C	24	0	36	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	12	0	18	1	0
5	E	24	0	36	13	0
5	F	24	0	36	1	0
5	G	16	0	24	3	0
5	H	16	0	24	2	0
6	A	16	0	19	0	0
6	B	12	0	15	0	0
6	C	16	0	19	1	0
6	D	16	0	20	0	0
6	E	16	0	18	1	0
6	F	12	0	15	0	0
6	G	12	0	14	0	0
6	H	12	0	14	0	0
7	A	292	0	0	2	0
7	B	317	0	0	3	0
7	C	398	0	0	3	0
7	D	333	0	0	3	0
7	E	338	0	0	4	0
7	F	410	0	0	1	0
7	G	292	0	0	2	0
7	H	267	0	0	4	0
All	All	33651	0	30496	292	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 5.

All (292) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:196:GLN:HE21	1:H:196:GLN:H	1.02	0.98
1:D:475:GLN:NE2	1:D:480:TYR:HB3	1.84	0.93
1:G:196:GLN:H	1:G:196:GLN:HE21	1.16	0.92
1:D:475:GLN:HE21	1:D:480:TYR:HB3	1.34	0.92
1:F:196:GLN:H	1:F:196:GLN:HE21	1.24	0.84
1:G:294:LEU:HD22	1:G:405:MET:HB2	1.59	0.82
1:C:196:GLN:H	1:C:196:GLN:HE21	1.28	0.81
1:H:311:GLN:HG3	7:H:2748:HOH:O	1.82	0.78
1:D:300:GLN:HE22	1:D:345:VAL:H	1.33	0.76
1:G:347:GLU:HG2	1:G:351:LYS:HE2	1.67	0.76
1:G:300:GLN:HE22	1:G:345:VAL:H	1.34	0.76
1:H:445:ALA:HB2	5:H:6948:EDO:H11	1.68	0.76
1:B:196:GLN:H	1:B:196:GLN:HE21	1.33	0.74
1:C:475:GLN:HE21	1:C:480:TYR:HB3	1.50	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:196:GLN:H	1:H:196:GLN:NE2	1.83	0.73
1:E:347:GLU:HG2	1:E:351:LYS:HE2	1.69	0.73
1:H:294:LEU:HD22	1:H:405:MET:HB2	1.70	0.73
1:H:300:GLN:HE22	1:H:345:VAL:H	1.35	0.72
1:E:300:GLN:HE22	1:E:345:VAL:H	1.37	0.71
1:A:300:GLN:HE22	1:A:345:VAL:H	1.39	0.70
1:C:300:GLN:HE22	1:C:345:VAL:H	1.38	0.70
1:F:300:GLN:HE22	1:F:345:VAL:H	1.40	0.68
1:G:445:ALA:HB2	5:G:6947:EDO:H11	1.75	0.68
1:H:41:ASN:HD22	1:H:43:SER:H	1.40	0.67
1:B:300:GLN:HE22	1:B:345:VAL:H	1.42	0.67
1:D:196:GLN:H	1:D:196:GLN:HE21	1.43	0.67
1:A:475:GLN:HG3	1:A:480:TYR:HB3	1.76	0.66
1:H:196:GLN:HE21	1:H:196:GLN:N	1.84	0.65
1:F:294:LEU:HD22	1:F:405:MET:HB2	1.77	0.65
1:C:294:LEU:HD22	1:C:405:MET:HB2	1.79	0.63
1:D:294:LEU:HD22	1:D:405:MET:HB2	1.80	0.63
1:G:196:GLN:H	1:G:196:GLN:NE2	1.94	0.63
1:H:358:ASN:O	1:H:362:GLN:HG2	1.99	0.62
1:H:41:ASN:ND2	1:H:43:SER:H	1.96	0.62
1:E:441:TYR:CE1	5:E:6945:EDO:H22	2.35	0.62
1:B:445:ALA:HB2	5:B:6942:EDO:H11	1.83	0.61
1:D:41:ASN:HD22	1:D:41:ASN:C	2.03	0.61
1:E:196:GLN:H	1:E:196:GLN:HE21	1.47	0.61
1:A:196:GLN:HE21	1:A:196:GLN:H	1.48	0.61
1:E:487:GLU:HG3	1:F:468:TYR:CE1	2.36	0.61
1:A:41:ASN:HD22	1:A:41:ASN:C	2.03	0.61
1:H:124:MET:HE3	1:H:173:LEU:HD22	1.83	0.60
1:G:251:ARG:NH2	1:H:260:SER:O	2.34	0.60
1:F:41:ASN:C	1:F:41:ASN:HD22	2.04	0.60
1:G:172:LEU:HD21	1:G:200:THR:HB	1.82	0.60
1:B:172:LEU:HD21	1:B:200:THR:HB	1.83	0.59
1:F:289:GLN:NE2	7:F:3289:HOH:O	2.33	0.59
1:F:475:GLN:OE1	1:F:480:TYR:HB3	2.03	0.59
1:G:41:ASN:C	1:G:41:ASN:HD22	2.04	0.59
1:B:196:GLN:H	1:B:196:GLN:NE2	1.98	0.59
1:A:260:SER:O	1:B:251:ARG:NH2	2.34	0.59
1:B:294:LEU:HD22	1:B:405:MET:HB2	1.84	0.59
1:B:347:GLU:HG3	5:B:6962:EDO:H12	1.84	0.59
1:B:41:ASN:HD22	1:B:41:ASN:C	2.06	0.59
1:C:445:ALA:HB2	5:C:6943:EDO:H11	1.85	0.58
1:C:424:THR:CG2	1:C:470:MET:SD	2.92	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:155:ARG:HD2	5:E:6905:EDO:H22	1.85	0.58
1:F:41:ASN:ND2	1:F:43:SER:H	2.01	0.58
1:D:41:ASN:ND2	1:D:43:SER:H	2.02	0.57
1:D:475:GLN:HE21	1:D:480:TYR:CB	2.14	0.57
1:E:74:SER:HA	5:E:6955:EDO:H22	1.85	0.57
1:E:264:ARG:HD2	6:E:6835:GAI:N1	2.20	0.57
1:B:41:ASN:HD22	1:B:43:SER:H	1.53	0.57
1:B:347:GLU:HG2	1:B:351:LYS:HE2	1.87	0.56
1:H:41:ASN:C	1:H:41:ASN:HD22	2.08	0.56
1:A:41:ASN:ND2	1:A:43:SER:H	2.03	0.56
1:C:41:ASN:HD22	1:C:41:ASN:C	2.08	0.56
1:C:487:GLU:HG3	1:D:468:TYR:CE1	2.41	0.56
1:E:41:ASN:HB2	5:E:6915:EDO:H11	1.87	0.56
1:E:72:LEU:HD21	5:F:6946:EDO:H11	1.86	0.56
1:E:347:GLU:O	1:E:351:LYS:HG2	2.05	0.56
1:C:475:GLN:NE2	1:C:480:TYR:HB3	2.18	0.55
1:A:445:ALA:HB2	5:A:6941:EDO:H11	1.88	0.55
1:A:196:GLN:NE2	1:A:196:GLN:H	2.04	0.55
1:G:196:GLN:N	1:G:196:GLN:HE21	1.97	0.55
1:A:475:GLN:HG3	1:A:480:TYR:CB	2.36	0.55
1:C:260:SER:O	1:D:251:ARG:NH2	2.40	0.55
1:E:468:TYR:CE1	1:F:487:GLU:HG3	2.42	0.55
1:E:424:THR:CG2	1:E:470:MET:SD	2.95	0.55
1:G:101:TYR:CG	5:G:6927:EDO:H11	2.42	0.55
1:E:46:GLU:HB2	5:E:6915:EDO:H21	1.88	0.54
1:F:196:GLN:H	1:F:196:GLN:NE2	1.99	0.54
1:B:41:ASN:ND2	1:B:43:SER:H	2.05	0.54
1:E:289:GLN:NE2	7:E:3288:HOH:O	2.39	0.54
1:D:172:LEU:HD21	1:D:200:THR:HB	1.89	0.54
1:D:294:LEU:HD12	1:D:306:SER:HA	1.90	0.54
1:G:468:TYR:CE1	1:H:487:GLU:HG3	2.43	0.53
1:A:205:ALA:HB2	1:A:220:ILE:HD12	1.90	0.53
1:A:11:PRO:HB3	1:A:114:TYR:CZ	2.43	0.53
1:A:498:LYS:HG2	1:A:499:ASN:N	2.24	0.53
1:A:251:ARG:NH2	1:B:260:SER:O	2.41	0.53
1:F:424:THR:CG2	1:F:470:MET:SD	2.96	0.53
1:G:475:GLN:HE21	1:H:488:VAL:HG21	1.74	0.53
1:B:11:PRO:HB3	1:B:114:TYR:CZ	2.45	0.52
1:A:302:CYS:SG	7:A:3143:HOH:O	2.58	0.52
1:G:23:PHE:CZ	1:G:26:ASN:HA	2.44	0.52
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.43	0.52
1:B:289:GLN:NE2	7:B:3301:HOH:O	2.29	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:349:GLN:HG3	7:G:3432:HOH:O	2.09	0.52
1:B:205:ALA:HB2	1:B:220:ILE:HD12	1.92	0.52
1:G:487:GLU:HG3	1:H:468:TYR:CE1	2.45	0.52
1:A:247:THR:O	1:A:251:ARG:HG3	2.09	0.52
1:H:172:LEU:HD21	1:H:200:THR:HB	1.92	0.52
1:D:347:GLU:O	1:D:351:LYS:HG2	2.10	0.52
1:H:205:ALA:HB2	1:H:220:ILE:HD12	1.92	0.52
1:C:468:TYR:CE1	1:D:487:GLU:HG3	2.45	0.51
1:A:441:TYR:CD1	5:A:6941:EDO:H12	2.45	0.51
1:C:41:ASN:ND2	1:C:43:SER:H	2.09	0.51
1:E:41:ASN:ND2	1:E:43:SER:H	2.08	0.51
1:G:289:GLN:NE2	7:G:3261:HOH:O	2.34	0.51
1:H:449:GLY:HA3	1:H:466:GLY:O	2.10	0.51
1:E:41:ASN:CB	5:E:6915:EDO:H11	2.41	0.51
1:G:260:SER:O	1:H:251:ARG:NH2	2.43	0.51
1:G:41:ASN:ND2	1:G:43:SER:H	2.08	0.51
1:D:205:ALA:HB2	1:D:220:ILE:HD12	1.92	0.50
1:G:294:LEU:HD22	1:G:405:MET:CB	2.38	0.50
1:D:196:GLN:H	1:D:196:GLN:NE2	2.08	0.50
1:A:41:ASN:HD22	1:A:43:SER:H	1.60	0.50
1:G:424:THR:CG2	1:G:470:MET:SD	3.00	0.50
1:E:294:LEU:HD22	1:E:405:MET:HB2	1.94	0.49
1:C:23:PHE:CZ	1:C:26:ASN:HA	2.48	0.49
1:F:124:MET:HE3	1:F:173:LEU:HD22	1.93	0.49
1:F:41:ASN:HD22	1:F:43:SER:H	1.60	0.49
1:B:33:SER:O	1:B:34:ARG:HB2	2.11	0.49
5:E:6945:EDO:H11	1:F:72:LEU:HD21	1.95	0.49
1:D:167:PRO:HD3	1:D:244:THR:HB	1.95	0.49
1:F:15:PRO:HD2	1:F:108:LEU:HD22	1.93	0.49
1:E:350:PHE:CE2	5:E:6965:EDO:H12	2.46	0.49
1:D:41:ASN:HD22	1:D:43:SER:H	1.61	0.48
1:F:23:PHE:CZ	1:F:26:ASN:HA	2.48	0.48
1:B:23:PHE:CZ	1:B:26:ASN:HA	2.48	0.48
5:C:6943:EDO:H11	1:D:72:LEU:HD21	1.94	0.48
1:G:205:ALA:HB2	1:G:220:ILE:HD12	1.96	0.48
1:H:23:PHE:CZ	1:H:26:ASN:HA	2.48	0.48
1:H:271:GLY:HA2	1:H:425:TYR:CG	2.48	0.48
1:A:172:LEU:HD21	1:A:200:THR:HB	1.96	0.48
1:G:449:GLY:HA3	1:G:466:GLY:O	2.13	0.48
1:E:41:ASN:C	1:E:41:ASN:HD22	2.17	0.48
1:B:449:GLY:HA3	1:B:466:GLY:O	2.13	0.48
1:E:115:VAL:HG23	7:E:1458:HOH:O	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:167:PRO:HD3	1:E:244:THR:HB	1.96	0.48
1:B:475:GLN:OE1	1:B:480:TYR:HB3	2.14	0.48
1:G:161:VAL:HA	1:G:188:VAL:HG23	1.96	0.47
1:C:196:GLN:H	1:C:196:GLN:NE2	2.04	0.47
1:D:294:LEU:HD13	7:D:1077:HOH:O	2.14	0.47
1:E:135:TRP:CE2	1:G:138:LYS:HD3	2.49	0.47
1:A:289:GLN:NE2	7:A:3151:HOH:O	2.37	0.47
1:A:490:THR:OG1	1:B:464:PRO:HG2	2.15	0.47
1:B:441:TYR:CD1	5:B:6942:EDO:H12	2.50	0.47
1:H:167:PRO:HD3	1:H:244:THR:HB	1.96	0.47
1:E:490:THR:OG1	1:F:464:PRO:HG2	2.15	0.47
1:G:11:PRO:HB3	1:G:114:TYR:CZ	2.50	0.47
1:A:449:GLY:HA3	1:A:466:GLY:O	2.14	0.47
1:B:27:GLU:HB2	1:B:29:HIS:CE1	2.49	0.47
1:H:389:VAL:HB	1:H:408:LEU:HG	1.97	0.47
1:E:21:GLN:HB3	1:E:29:HIS:O	2.14	0.47
1:C:174:MET:HE3	1:C:174:MET:HA	1.97	0.47
1:C:490:THR:OG1	1:D:464:PRO:HG2	2.15	0.46
1:E:23:PHE:CZ	1:E:26:ASN:HA	2.50	0.46
1:C:349:GLN:HB3	7:C:2406:HOH:O	2.14	0.46
1:D:268:GLU:HB3	7:D:1339:HOH:O	2.15	0.46
1:H:294:LEU:HD13	7:H:1076:HOH:O	2.15	0.46
1:E:146:ILE:HG13	1:F:460:GLY:HA3	1.97	0.46
1:G:350:PHE:HZ	1:G:373:ILE:CG2	2.28	0.46
1:D:352:LYS:HD3	7:D:1766:HOH:O	2.14	0.46
1:H:112:LYS:HB2	7:H:1922:HOH:O	2.16	0.46
1:D:247:THR:HA	1:D:269:LEU:HD13	1.97	0.46
1:A:46:GLU:HB2	5:A:6911:EDO:H21	1.97	0.46
1:B:59:VAL:O	1:B:63:VAL:HG23	2.15	0.46
1:D:361:LYS:HD3	1:D:367:LEU:HD22	1.98	0.46
1:A:464:PRO:HG2	1:B:490:THR:OG1	2.17	0.45
1:C:464:PRO:HG2	1:D:490:THR:OG1	2.16	0.45
1:C:124:MET:HE3	1:C:173:LEU:CD2	2.46	0.45
1:B:161:VAL:HA	1:B:188:VAL:HG23	1.99	0.45
1:E:441:TYR:CD1	5:E:6945:EDO:H12	2.52	0.45
1:C:24:ILE:O	1:C:27:GLU:HG2	2.17	0.45
1:D:294:LEU:HD13	1:D:405:MET:HA	1.99	0.45
1:H:445:ALA:HB2	5:H:6948:EDO:C1	2.43	0.45
1:H:289:GLN:NE2	7:H:3279:HOH:O	2.48	0.45
1:C:268:GLU:HB3	7:C:1687:HOH:O	2.17	0.44
1:B:167:PRO:HD3	1:B:244:THR:HB	1.99	0.44
1:E:445:ALA:HB2	5:E:6945:EDO:H11	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:303:CYS:SG	1:G:459:PHE:HZ	2.41	0.44
1:A:159:VAL:HG12	1:A:187:ASN:OD1	2.17	0.44
1:B:193:VAL:HG11	1:B:201:ALA:CB	2.47	0.44
1:B:347:GLU:HG3	5:B:6962:EDO:C1	2.47	0.44
1:C:424:THR:HG22	1:C:470:MET:HB2	1.99	0.44
1:E:389:VAL:HB	1:E:408:LEU:HG	2.00	0.44
1:H:11:PRO:HB3	1:H:114:TYR:CZ	2.52	0.44
1:C:120:VAL:O	1:C:124:MET:HG3	2.18	0.44
1:D:461:ALA:HA	1:D:477:LEU:HD22	2.00	0.44
1:C:124:MET:HE3	1:C:173:LEU:HD22	1.98	0.44
1:D:498:LYS:HG2	1:D:499:ASN:N	2.33	0.44
1:F:196:GLN:N	1:F:196:GLN:HE21	2.04	0.44
1:E:13:GLN:NE2	7:E:3330:HOH:O	2.50	0.44
1:E:254:GLN:NE2	1:E:265:VAL:HG11	2.32	0.44
1:H:294:LEU:HD12	1:H:306:SER:HA	1.99	0.43
1:G:490:THR:OG1	1:H:464:PRO:HG2	2.19	0.43
1:A:101:TYR:CD2	5:A:6921:EDO:H11	2.52	0.43
1:C:460:GLY:HA3	1:D:146:ILE:HG13	2.00	0.43
6:C:6834:GAI:N1	1:D:264:ARG:HD2	2.33	0.43
1:E:350:PHE:HE2	5:E:6965:EDO:H12	1.83	0.43
1:G:41:ASN:HD22	1:G:43:SER:H	1.65	0.43
1:A:21:GLN:HB3	1:A:29:HIS:O	2.18	0.43
1:B:461:ALA:HA	1:B:477:LEU:HD22	2.00	0.43
1:E:196:GLN:H	1:E:196:GLN:NE2	2.15	0.43
1:F:410:PHE:CD1	1:F:416:VAL:HB	2.52	0.43
1:A:120:VAL:O	1:A:124:MET:HG3	2.18	0.43
1:D:33:SER:O	1:D:34:ARG:HB2	2.19	0.43
1:F:154:THR:HA	1:F:489:LYS:O	2.19	0.43
1:A:146:ILE:HG13	1:B:460:GLY:HA3	2.00	0.43
1:H:41:ASN:HD21	1:H:43:SER:HB2	1.84	0.43
1:D:449:GLY:HA3	1:D:466:GLY:O	2.18	0.43
1:C:289:GLN:NE2	7:C:3194:HOH:O	2.40	0.43
1:D:11:PRO:HB3	1:D:114:TYR:CZ	2.53	0.43
1:F:27:GLU:HB2	1:F:29:HIS:CE1	2.54	0.43
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.53	0.42
1:E:498:LYS:HE2	1:E:498:LYS:HB3	1.91	0.42
1:E:74:SER:N	5:E:6955:EDO:H12	2.33	0.42
1:F:120:VAL:HG12	1:F:124:MET:HE1	2.00	0.42
1:H:498:LYS:HG2	1:H:499:ASN:N	2.34	0.42
1:C:11:PRO:HB3	1:C:114:TYR:CZ	2.54	0.42
1:H:347:GLU:HG2	1:H:351:LYS:HE3	2.01	0.42
1:B:249:ILE:O	1:B:253:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:27:GLU:HG3	7:B:1707:HOH:O	2.19	0.42
1:C:106:GLU:OE2	1:C:171:PRO:HB2	2.19	0.42
1:G:350:PHE:CZ	1:G:373:ILE:CG2	3.02	0.42
1:A:443:SER:HA	1:A:451:VAL:HG11	2.01	0.42
1:B:63:VAL:HG11	1:B:235:HIS:CE1	2.54	0.42
1:G:12:ASN:O	1:G:15:PRO:HD3	2.18	0.42
1:E:214:PRO:HA	1:E:215:PRO:HD3	1.94	0.42
1:E:294:LEU:HD12	1:E:306:SER:HA	2.02	0.42
1:H:124:MET:HE3	1:H:173:LEU:CD2	2.50	0.42
1:D:166:ILE:HB	1:D:167:PRO:HD2	2.01	0.42
1:H:303:CYS:SG	1:H:459:PHE:HZ	2.43	0.42
1:A:271:GLY:HA2	1:A:425:TYR:CG	2.55	0.41
1:B:172:LEU:CD2	1:B:200:THR:HB	2.50	0.41
1:B:303:CYS:SG	1:B:459:PHE:HZ	2.43	0.41
1:C:154:THR:HA	1:C:489:LYS:O	2.20	0.41
1:D:12:ASN:O	1:D:15:PRO:HD3	2.20	0.41
1:E:166:ILE:HB	1:E:167:PRO:HD2	2.02	0.41
1:H:22:ILE:HG12	1:H:222:PRO:HD2	2.02	0.41
1:C:167:PRO:HD3	1:C:244:THR:HB	2.01	0.41
1:E:205:ALA:HB2	1:E:220:ILE:HD12	2.02	0.41
1:H:161:VAL:HA	1:H:188:VAL:HG23	2.03	0.41
1:A:11:PRO:HB3	1:A:114:TYR:CE1	2.56	0.41
1:A:475:GLN:CG	1:A:480:TYR:HB3	2.48	0.41
1:C:303:CYS:SG	1:C:459:PHE:HZ	2.43	0.41
1:D:498:LYS:HB3	1:D:498:LYS:HE2	1.91	0.41
1:D:32:VAL:HG11	1:D:57:GLU:OE2	2.20	0.41
1:D:106:GLU:O	1:D:110:ASN:HB3	2.21	0.41
1:A:244:THR:HG23	1:A:268:GLU:HG3	2.03	0.41
1:A:319:VAL:O	1:A:323:VAL:HG23	2.20	0.41
1:A:498:LYS:HB3	1:A:498:LYS:HE2	1.86	0.41
1:D:11:PRO:HB3	1:D:114:TYR:CE2	2.55	0.41
1:F:449:GLY:HA3	1:F:466:GLY:O	2.20	0.41
1:A:292:PHE:HE1	1:A:457:ASP:HB2	1.85	0.41
1:C:410:PHE:CD1	1:C:416:VAL:HB	2.55	0.41
1:A:294:LEU:HD23	1:A:306:SER:HA	2.02	0.41
1:D:101:TYR:CB	5:D:6924:EDO:H11	2.50	0.41
1:E:319:VAL:O	1:E:323:VAL:HG23	2.21	0.41
1:F:443:SER:HA	1:F:451:VAL:HG11	2.03	0.41
1:H:247:THR:O	1:H:251:ARG:HG3	2.21	0.41
1:A:107:THR:HG23	1:A:112:LYS:O	2.20	0.41
1:B:389:VAL:HB	1:B:408:LEU:HG	2.01	0.41
1:G:159:VAL:HG12	1:G:187:ASN:OD1	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:254:GLN:HE21	1:A:254:GLN:HB2	1.64	0.41
1:B:294:LEU:HD12	1:B:306:SER:HA	2.02	0.41
1:C:196:GLN:HE21	1:C:196:GLN:N	2.06	0.41
1:D:213:PHE:HA	1:D:214:PRO:HD3	1.95	0.41
1:D:476:GLU:O	1:D:477:LEU:HB2	2.21	0.41
1:E:347:GLU:CG	1:E:351:LYS:HE2	2.46	0.41
1:E:7:ALA:HA	7:E:2509:HOH:O	2.21	0.41
1:G:475:GLN:NE2	1:H:488:VAL:CG2	2.84	0.41
1:A:167:PRO:HD3	1:A:244:THR:HB	2.02	0.40
5:G:6947:EDO:H11	1:H:72:LEU:HD21	2.03	0.40
1:A:12:ASN:O	1:A:15:PRO:HD3	2.21	0.40
1:A:68:ALA:HB1	5:A:6951:EDO:H21	2.03	0.40
1:D:443:SER:HA	1:D:451:VAL:HG11	2.04	0.40
1:F:359:THR:O	1:F:363:GLU:HG2	2.22	0.40
1:G:247:THR:O	1:G:251:ARG:HG3	2.20	0.40
1:G:350:PHE:HZ	1:G:373:ILE:HG21	1.87	0.40
1:G:475:GLN:HE21	1:H:488:VAL:CG2	2.34	0.40
1:E:155:ARG:HH11	5:E:6905:EDO:H22	1.86	0.40
1:G:41:ASN:ND2	1:G:41:ASN:C	2.74	0.40
1:B:107:THR:HG23	1:B:112:LYS:O	2.21	0.40
1:B:159:VAL:HG13	1:B:162:CYS:SG	2.62	0.40
1:B:25:ASN:O	1:B:27:GLU:HG2	2.21	0.40
1:B:294:LEU:HD13	7:B:1013:HOH:O	2.21	0.40
1:G:476:GLU:O	1:G:477:LEU:HB2	2.21	0.40
1:H:34:ARG:HD3	1:H:34:ARG:HA	1.89	0.40
1:G:475:GLN:NE2	1:H:488:VAL:HG21	2.37	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	492/500 (98%)	478 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	492/500 (98%)	477 (97%)	15 (3%)	0	100	100
1	C	492/500 (98%)	478 (97%)	14 (3%)	0	100	100
1	D	492/500 (98%)	473 (96%)	19 (4%)	0	100	100
1	E	492/500 (98%)	478 (97%)	14 (3%)	0	100	100
1	F	492/500 (98%)	478 (97%)	14 (3%)	0	100	100
1	G	492/500 (98%)	473 (96%)	19 (4%)	0	100	100
1	H	492/500 (98%)	477 (97%)	15 (3%)	0	100	100
All	All	3936/4000 (98%)	3812 (97%)	124 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	399/402 (99%)	389 (98%)	10 (2%)	60	59
1	B	399/402 (99%)	392 (98%)	7 (2%)	71	73
1	C	399/402 (99%)	390 (98%)	9 (2%)	63	63
1	D	399/402 (99%)	387 (97%)	12 (3%)	53	50
1	E	399/402 (99%)	391 (98%)	8 (2%)	68	69
1	F	399/402 (99%)	392 (98%)	7 (2%)	71	73
1	G	399/402 (99%)	392 (98%)	7 (2%)	71	73
1	H	399/402 (99%)	390 (98%)	9 (2%)	63	63
All	All	3192/3216 (99%)	3123 (98%)	69 (2%)	64	65

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	192	LYS
1	A	196	GLN
1	A	206	ASN

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Mol	Chain	Res	Type
1	A	254	GLN
1	A	264	ARG
1	A	275	ASN
1	A	377	ARG
1	A	401	PHE
1	A	475	GLN
1	B	41	ASN
1	B	122	LEU
1	B	192	LYS
1	B	196	GLN
1	B	294	LEU
1	B	401	PHE
1	B	498	LYS
1	C	41	ASN
1	C	50	GLN
1	C	174	MET
1	C	192	LYS
1	C	196	GLN
1	C	206	ASN
1	C	294	LEU
1	C	401	PHE
1	C	475	GLN
1	D	41	ASN
1	D	159	VAL
1	D	192	LYS
1	D	196	GLN
1	D	206	ASN
1	D	254	GLN
1	D	294	LEU
1	D	362	GLN
1	D	376	ASP
1	D	401	PHE
1	D	417	VAL
1	D	475	GLN
1	E	41	ASN
1	E	192	LYS
1	E	196	GLN
1	E	206	ASN
1	E	275	ASN
1	E	294	LEU
1	E	401	PHE
1	E	475	GLN

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Mol	Chain	Res	Type
1	F	41	ASN
1	F	50	GLN
1	F	122	LEU
1	F	192	LYS
1	F	196	GLN
1	F	294	LEU
1	F	401	PHE
1	G	41	ASN
1	G	192	LYS
1	G	196	GLN
1	G	248	GLU
1	G	294	LEU
1	G	373	ILE
1	G	401	PHE
1	H	41	ASN
1	H	192	LYS
1	H	196	GLN
1	H	254	GLN
1	H	268	GLU
1	H	275	ASN
1	H	294	LEU
1	H	401	PHE
1	H	475	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	41	ASN
1	A	175	GLN
1	A	196	GLN
1	A	254	GLN
1	A	275	ASN
1	A	300	GLN
1	A	475	GLN
1	B	26	ASN
1	B	29	HIS
1	B	41	ASN
1	B	50	GLN
1	B	175	GLN
1	B	196	GLN
1	B	275	ASN

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Mol	Chain	Res	Type
1	B	300	GLN
1	B	349	GLN
1	C	14	GLN
1	C	26	ASN
1	C	41	ASN
1	C	50	GLN
1	C	175	GLN
1	C	196	GLN
1	C	254	GLN
1	C	300	GLN
1	C	475	GLN
1	D	13	GLN
1	D	26	ASN
1	D	41	ASN
1	D	50	GLN
1	D	175	GLN
1	D	196	GLN
1	D	254	GLN
1	D	289	GLN
1	D	300	GLN
1	D	475	GLN
1	E	13	GLN
1	E	26	ASN
1	E	41	ASN
1	E	175	GLN
1	E	196	GLN
1	E	254	GLN
1	E	275	ASN
1	E	289	GLN
1	E	300	GLN
1	E	475	GLN
1	F	14	GLN
1	F	26	ASN
1	F	29	HIS
1	F	41	ASN
1	F	50	GLN
1	F	175	GLN
1	F	196	GLN
1	F	254	GLN
1	F	275	ASN
1	F	300	GLN
1	G	13	GLN

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Mol	Chain	Res	Type
1	G	26	ASN
1	G	41	ASN
1	G	175	GLN
1	G	196	GLN
1	G	275	ASN
1	G	300	GLN
1	H	26	ASN
1	H	41	ASN
1	H	175	GLN
1	H	196	GLN
1	H	275	ASN
1	H	300	GLN

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 ⓘ

Of 91 ligands modelled in this entry, 16 are monoatomic - leaving 75 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	$\# Z > 2$
4	NAD	A	501	2	48,48,48	2.09	10 (20%)	73,73,73	1.72	15 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GAI	A	6801	-	3,3,3	1.18	0	3,3,3	1.38	1 (33%)
6	GAI	A	6811	-	3,3,3	1.47	1 (33%)	3,3,3	1.29	0
6	GAI	A	6821	-	3,3,3	1.62	1 (33%)	3,3,3	1.35	1 (33%)
6	GAI	A	6832	-	3,3,3	1.52	1 (33%)	3,3,3	1.26	0
5	EDO	A	6901	-	3,3,3	0.62	0	2,2,2	0.39	0
5	EDO	A	6911	-	3,3,3	0.68	0	2,2,2	0.30	0
5	EDO	A	6921	-	3,3,3	0.48	0	2,2,2	0.43	0
5	EDO	A	6941	-	3,3,3	0.71	0	2,2,2	0.31	0
5	EDO	A	6951	-	3,3,3	0.64	0	2,2,2	0.34	0
4	NAD	B	502	2	48,48,48	1.92	11 (22%)	73,73,73	1.56	13 (17%)
6	GAI	B	6802	-	3,3,3	1.44	1 (33%)	3,3,3	1.28	0
6	GAI	B	6812	-	3,3,3	1.55	1 (33%)	3,3,3	1.28	0
6	GAI	B	6831	-	3,3,3	1.84	1 (33%)	3,3,3	1.34	0
5	EDO	B	6902	-	3,3,3	0.59	0	2,2,2	0.36	0
5	EDO	B	6912	-	3,3,3	0.61	0	2,2,2	0.36	0
5	EDO	B	6942	-	3,3,3	0.57	0	2,2,2	0.44	0
5	EDO	B	6952	-	3,3,3	0.63	0	2,2,2	0.34	0
5	EDO	B	6962	-	3,3,3	0.58	0	2,2,2	0.29	0
4	NAD	C	503	2	48,48,48	1.89	10 (20%)	73,73,73	1.77	18 (24%)
6	GAI	C	6803	-	3,3,3	1.09	0	3,3,3	1.34	1 (33%)
6	GAI	C	6813	-	3,3,3	1.48	1 (33%)	3,3,3	1.32	1 (33%)
6	GAI	C	6823	-	3,3,3	1.48	1 (33%)	3,3,3	1.24	0
6	GAI	C	6834	-	3,3,3	1.92	1 (33%)	3,3,3	1.37	1 (33%)
5	EDO	C	6903	-	3,3,3	0.52	0	2,2,2	0.32	0
5	EDO	C	6913	-	3,3,3	0.59	0	2,2,2	0.43	0
5	EDO	C	6923	-	3,3,3	0.40	0	2,2,2	0.52	0
5	EDO	C	6943	-	3,3,3	0.63	0	2,2,2	0.37	0
5	EDO	C	6953	-	3,3,3	0.70	0	2,2,2	0.35	0
5	EDO	C	6963	-	3,3,3	0.53	0	2,2,2	0.48	0
4	NAD	D	504	2	48,48,48	1.95	12 (25%)	73,73,73	1.83	17 (23%)
6	GAI	D	6804	-	3,3,3	1.76	1 (33%)	3,3,3	1.24	0
6	GAI	D	6814	-	3,3,3	1.72	1 (33%)	3,3,3	1.34	1 (33%)
6	GAI	D	6824	-	3,3,3	1.58	1 (33%)	3,3,3	1.34	1 (33%)
6	GAI	D	6833	-	3,3,3	1.47	1 (33%)	3,3,3	1.33	1 (33%)
5	EDO	D	6904	-	3,3,3	0.58	0	2,2,2	0.42	0
5	EDO	D	6914	-	3,3,3	0.63	0	2,2,2	0.37	0
5	EDO	D	6924	-	3,3,3	0.49	0	2,2,2	0.44	0
4	NAD	E	505	2	48,48,48	1.91	9 (18%)	73,73,73	1.76	20 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GAI	E	6805	-	3,3,3	1.44	1 (33%)	3,3,3	1.54	1 (33%)
6	GAI	E	6815	-	3,3,3	1.60	1 (33%)	3,3,3	1.32	1 (33%)
6	GAI	E	6835	-	3,3,3	1.52	0	3,3,3	1.50	1 (33%)
6	GAI	E	6836	-	3,3,3	1.27	1 (33%)	3,3,3	1.45	1 (33%)
5	EDO	E	6905	-	3,3,3	0.51	0	2,2,2	0.50	0
5	EDO	E	6915	-	3,3,3	0.51	0	2,2,2	0.33	0
5	EDO	E	6925	-	3,3,3	0.44	0	2,2,2	0.48	0
5	EDO	E	6945	-	3,3,3	0.89	0	2,2,2	0.11	0
5	EDO	E	6955	-	3,3,3	0.57	0	2,2,2	0.35	0
5	EDO	E	6965	-	3,3,3	0.57	0	2,2,2	0.42	0
4	NAD	F	506	2	48,48,48	1.87	9 (18%)	73,73,73	1.76	15 (20%)
6	GAI	F	6806	-	3,3,3	1.39	1 (33%)	3,3,3	1.35	1 (33%)
6	GAI	F	6816	-	3,3,3	1.41	1 (33%)	3,3,3	1.26	0
6	GAI	F	6826	-	3,3,3	1.51	1 (33%)	3,3,3	1.34	1 (33%)
5	EDO	F	6906	-	3,3,3	0.65	0	2,2,2	0.31	0
5	EDO	F	6916	-	3,3,3	0.50	0	2,2,2	0.46	0
5	EDO	F	6926	-	3,3,3	0.59	0	2,2,2	0.38	0
5	EDO	F	6946	-	3,3,3	0.69	0	2,2,2	0.38	0
5	EDO	F	6956	-	3,3,3	0.58	0	2,2,2	0.39	0
5	EDO	F	6966	-	3,3,3	0.69	0	2,2,2	0.39	0
4	NAD	G	507	2	48,48,48	1.68	8 (16%)	73,73,73	1.69	13 (17%)
6	GAI	G	6807	-	3,3,3	1.44	1 (33%)	3,3,3	1.48	1 (33%)
6	GAI	G	6817	-	3,3,3	1.32	1 (33%)	3,3,3	1.26	0
6	GAI	G	6838	-	3,3,3	1.47	1 (33%)	3,3,3	1.17	0
5	EDO	G	6907	-	3,3,3	0.50	0	2,2,2	0.43	0
5	EDO	G	6917	-	3,3,3	0.57	0	2,2,2	0.39	0
5	EDO	G	6927	-	3,3,3	0.45	0	2,2,2	0.45	0
5	EDO	G	6947	-	3,3,3	0.70	0	2,2,2	0.32	0
4	NAD	H	508	2	48,48,48	1.88	11 (22%)	73,73,73	1.83	15 (20%)
6	GAI	H	6808	-	3,3,3	1.49	1 (33%)	3,3,3	1.45	1 (33%)
6	GAI	H	6818	-	3,3,3	1.49	1 (33%)	3,3,3	1.25	0
6	GAI	H	6837	-	3,3,3	1.28	1 (33%)	3,3,3	1.29	1 (33%)
5	EDO	H	6908	-	3,3,3	0.61	0	2,2,2	0.47	0
5	EDO	H	6918	-	3,3,3	0.62	0	2,2,2	0.33	0
5	EDO	H	6928	-	3,3,3	0.42	0	2,2,2	0.52	0
5	EDO	H	6948	-	3,3,3	0.54	0	2,2,2	0.37	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
4	NAD	A	501	2	-	0/30/62/62	0/5/5/5
6	GAI	A	6801	-	-	0/0/0/0	0/0/0/0
6	GAI	A	6811	-	-	0/0/0/0	0/0/0/0
6	GAI	A	6821	-	-	0/0/0/0	0/0/0/0
6	GAI	A	6832	-	-	0/0/0/0	0/0/0/0
5	EDO	A	6901	-	-	0/1/1/1	0/0/0/0
5	EDO	A	6911	-	-	0/1/1/1	0/0/0/0
5	EDO	A	6921	-	-	0/1/1/1	0/0/0/0
5	EDO	A	6941	-	-	0/1/1/1	0/0/0/0
5	EDO	A	6951	-	-	0/1/1/1	0/0/0/0
4	NAD	B	502	2	-	0/30/62/62	0/5/5/5
6	GAI	B	6802	-	-	0/0/0/0	0/0/0/0
6	GAI	B	6812	-	-	0/0/0/0	0/0/0/0
6	GAI	B	6831	-	-	0/0/0/0	0/0/0/0
5	EDO	B	6902	-	-	0/1/1/1	0/0/0/0
5	EDO	B	6912	-	-	0/1/1/1	0/0/0/0
5	EDO	B	6942	-	-	0/1/1/1	0/0/0/0
5	EDO	B	6952	-	-	0/1/1/1	0/0/0/0
5	EDO	B	6962	-	-	0/1/1/1	0/0/0/0
4	NAD	C	503	2	-	0/30/62/62	0/5/5/5
6	GAI	C	6803	-	-	0/0/0/0	0/0/0/0
6	GAI	C	6813	-	-	0/0/0/0	0/0/0/0
6	GAI	C	6823	-	-	0/0/0/0	0/0/0/0
6	GAI	C	6834	-	-	0/0/0/0	0/0/0/0
5	EDO	C	6903	-	-	0/1/1/1	0/0/0/0
5	EDO	C	6913	-	-	0/1/1/1	0/0/0/0
5	EDO	C	6923	-	-	0/1/1/1	0/0/0/0
5	EDO	C	6943	-	-	0/1/1/1	0/0/0/0
5	EDO	C	6953	-	-	0/1/1/1	0/0/0/0
5	EDO	C	6963	-	-	0/1/1/1	0/0/0/0
4	NAD	D	504	2	-	0/30/62/62	0/5/5/5
6	GAI	D	6804	-	-	0/0/0/0	0/0/0/0
6	GAI	D	6814	-	-	0/0/0/0	0/0/0/0
6	GAI	D	6824	-	-	0/0/0/0	0/0/0/0
6	GAI	D	6833	-	-	0/0/0/0	0/0/0/0
5	EDO	D	6904	-	-	0/1/1/1	0/0/0/0
5	EDO	D	6914	-	-	0/1/1/1	0/0/0/0
5	EDO	D	6924	-	-	0/1/1/1	0/0/0/0
4	NAD	E	505	2	-	0/30/62/62	0/5/5/5
6	GAI	E	6805	-	-	0/0/0/0	0/0/0/0
6	GAI	E	6815	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GAI	E	6835	-	-	0/0/0/0	0/0/0/0
6	GAI	E	6836	-	-	0/0/0/0	0/0/0/0
5	EDO	E	6905	-	-	0/1/1/1	0/0/0/0
5	EDO	E	6915	-	-	0/1/1/1	0/0/0/0
5	EDO	E	6925	-	-	0/1/1/1	0/0/0/0
5	EDO	E	6945	-	-	0/1/1/1	0/0/0/0
5	EDO	E	6955	-	-	0/1/1/1	0/0/0/0
5	EDO	E	6965	-	-	0/1/1/1	0/0/0/0
4	NAD	F	506	2	-	0/30/62/62	0/5/5/5
6	GAI	F	6806	-	-	0/0/0/0	0/0/0/0
6	GAI	F	6816	-	-	0/0/0/0	0/0/0/0
6	GAI	F	6826	-	-	0/0/0/0	0/0/0/0
5	EDO	F	6906	-	-	0/1/1/1	0/0/0/0
5	EDO	F	6916	-	-	0/1/1/1	0/0/0/0
5	EDO	F	6926	-	-	0/1/1/1	0/0/0/0
5	EDO	F	6946	-	-	0/1/1/1	0/0/0/0
5	EDO	F	6956	-	-	0/1/1/1	0/0/0/0
5	EDO	F	6966	-	-	0/1/1/1	0/0/0/0
4	NAD	G	507	2	-	0/30/62/62	0/5/5/5
6	GAI	G	6807	-	-	0/0/0/0	0/0/0/0
6	GAI	G	6817	-	-	0/0/0/0	0/0/0/0
6	GAI	G	6838	-	-	0/0/0/0	0/0/0/0
5	EDO	G	6907	-	-	0/1/1/1	0/0/0/0
5	EDO	G	6917	-	-	0/1/1/1	0/0/0/0
5	EDO	G	6927	-	-	0/1/1/1	0/0/0/0
5	EDO	G	6947	-	-	0/1/1/1	0/0/0/0
4	NAD	H	508	2	-	0/30/62/62	0/5/5/5
6	GAI	H	6808	-	-	0/0/0/0	0/0/0/0
6	GAI	H	6818	-	-	0/0/0/0	0/0/0/0
6	GAI	H	6837	-	-	0/0/0/0	0/0/0/0
5	EDO	H	6908	-	-	0/1/1/1	0/0/0/0
5	EDO	H	6918	-	-	0/1/1/1	0/0/0/0
5	EDO	H	6928	-	-	0/1/1/1	0/0/0/0
5	EDO	H	6948	-	-	0/1/1/1	0/0/0/0

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	NAD	C3N-C7N	-9.89	1.34	1.50
4	D	504	NAD	C3N-C7N	-8.78	1.36	1.50
4	E	505	NAD	C3N-C7N	-8.73	1.36	1.50
4	C	503	NAD	C3N-C7N	-8.42	1.36	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	502	NAD	C3N-C7N	-8.40	1.36	1.50
4	H	508	NAD	C3N-C7N	-8.37	1.36	1.50
4	F	506	NAD	C3N-C7N	-8.35	1.36	1.50
4	G	507	NAD	C3N-C7N	-7.10	1.38	1.50
4	B	502	NAD	C2A-N3A	5.23	1.41	1.32
4	E	505	NAD	C2A-N3A	4.79	1.40	1.32
4	C	503	NAD	C2A-N3A	4.74	1.40	1.32
4	H	508	NAD	C2A-N3A	4.61	1.40	1.32
4	F	506	NAD	C2A-N3A	4.54	1.40	1.32
4	G	507	NAD	C2A-N3A	4.03	1.39	1.32
4	A	501	NAD	C2A-N3A	3.80	1.38	1.32
4	D	504	NAD	C8A-N7A	3.79	1.41	1.34
4	A	501	NAD	O4D-C1D	3.61	1.45	1.41
4	D	504	NAD	C2N-C3N	-3.36	1.33	1.39
4	A	501	NAD	C2N-C3N	-3.35	1.33	1.39
6	B	6831	GAI	C-N1	3.18	1.37	1.30
4	C	503	NAD	C2A-N1A	3.13	1.40	1.33
4	G	507	NAD	C2A-N1A	3.11	1.40	1.33
6	C	6834	GAI	C-N1	3.08	1.37	1.30
4	G	507	NAD	C8A-N7A	3.03	1.40	1.34
4	E	505	NAD	C4N-C3N	-3.00	1.34	1.39
6	D	6804	GAI	C-N1	2.99	1.36	1.30
4	B	502	NAD	C2A-N1A	2.95	1.39	1.33
4	D	504	NAD	C8A-N9A	2.94	1.41	1.36
4	D	504	NAD	C2A-N1A	2.93	1.39	1.33
4	C	503	NAD	C2D-C1D	2.88	1.57	1.53
4	F	506	NAD	C4N-C3N	-2.88	1.34	1.39
6	D	6814	GAI	C-N1	2.88	1.36	1.30
4	A	501	NAD	C2A-N1A	2.87	1.39	1.33
4	H	508	NAD	O4D-C1D	2.83	1.44	1.41
4	H	508	NAD	C5N-C4N	-2.82	1.33	1.38
4	D	504	NAD	C5N-C4N	-2.80	1.33	1.38
4	H	508	NAD	C8A-N9A	2.80	1.40	1.36
6	A	6821	GAI	C-N1	2.79	1.36	1.30
4	F	506	NAD	C2A-N1A	2.79	1.39	1.33
4	B	502	NAD	C8A-N7A	2.79	1.40	1.34
4	H	508	NAD	C2A-N1A	2.78	1.39	1.33
6	E	6815	GAI	C-N1	2.76	1.36	1.30
4	F	506	NAD	C2D-C1D	2.76	1.57	1.53
4	G	507	NAD	C8A-N9A	2.75	1.40	1.36
4	A	501	NAD	O4B-C1B	2.73	1.44	1.41
4	E	505	NAD	C2N-C3N	-2.71	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	NAD	C8A-N7A	2.70	1.39	1.34
4	D	504	NAD	C2A-N3A	2.69	1.36	1.32
4	A	501	NAD	C8A-N9A	2.68	1.40	1.36
4	A	501	NAD	PN-O3	2.66	1.65	1.60
6	D	6824	GAI	C-N1	2.65	1.36	1.30
4	B	502	NAD	PN-O3	2.63	1.65	1.60
6	B	6812	GAI	C-N1	2.63	1.36	1.30
6	C	6813	GAI	C-N1	2.56	1.36	1.30
6	G	6838	GAI	C-N1	2.55	1.36	1.30
4	E	505	NAD	C8A-N9A	2.54	1.40	1.36
6	D	6833	GAI	C-N1	2.53	1.35	1.30
4	E	505	NAD	C2A-N1A	2.53	1.38	1.33
6	H	6818	GAI	C-N1	2.53	1.35	1.30
6	A	6811	GAI	C-N1	2.52	1.35	1.30
4	B	502	NAD	C4A-N3A	2.51	1.39	1.35
6	C	6823	GAI	C-N1	2.49	1.35	1.30
4	C	503	NAD	PN-O3	2.49	1.65	1.60
6	B	6802	GAI	C-N1	2.49	1.35	1.30
4	C	503	NAD	C8A-N7A	2.48	1.39	1.34
4	D	504	NAD	C2N-N1N	-2.46	1.32	1.35
4	F	506	NAD	PA-O3	-2.46	1.55	1.59
6	H	6808	GAI	C-N1	2.45	1.35	1.30
6	F	6826	GAI	C-N1	2.44	1.35	1.30
4	D	504	NAD	C2D-C1D	2.42	1.57	1.53
4	F	506	NAD	C2N-C3N	-2.42	1.35	1.39
6	G	6807	GAI	C-N1	2.39	1.35	1.30
4	C	503	NAD	PN-O5D	2.39	1.67	1.59
4	B	502	NAD	C4N-C3N	-2.38	1.35	1.39
4	E	505	NAD	C2D-C1D	2.37	1.56	1.53
4	E	505	NAD	C8A-N7A	2.37	1.39	1.34
6	E	6805	GAI	C-N1	2.36	1.35	1.30
4	F	506	NAD	C8A-N7A	2.35	1.39	1.34
4	H	508	NAD	C2N-C3N	-2.34	1.35	1.39
4	H	508	NAD	PN-O3	2.34	1.65	1.60
6	F	6806	GAI	C-N1	2.34	1.35	1.30
4	D	504	NAD	O4D-C1D	2.32	1.44	1.41
6	F	6816	GAI	C-N1	2.28	1.35	1.30
4	B	502	NAD	C8A-N9A	2.27	1.40	1.36
6	A	6832	GAI	C-N1	2.24	1.35	1.30
4	B	502	NAD	O4B-C1B	2.24	1.44	1.41
4	G	507	NAD	C4A-N3A	2.23	1.39	1.35
4	D	504	NAD	C4N-C3N	-2.22	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	503	NAD	O4D-C1D	2.21	1.44	1.41
6	G	6817	GAI	C-N1	2.20	1.35	1.30
4	E	505	NAD	O4D-C1D	2.19	1.44	1.41
4	G	507	NAD	O4B-C1B	2.18	1.44	1.41
6	H	6837	GAI	C-N1	2.16	1.35	1.30
4	C	503	NAD	C4N-C3N	-2.15	1.35	1.39
6	E	6836	GAI	C-N1	2.15	1.35	1.30
4	B	502	NAD	C5N-C4N	-2.14	1.34	1.38
4	H	508	NAD	C8A-N7A	2.12	1.38	1.34
4	D	504	NAD	PA-O2A	-2.11	1.45	1.55
4	F	506	NAD	O4D-C1D	2.11	1.43	1.41
4	G	507	NAD	C4N-C3N	-2.05	1.35	1.39
4	H	508	NAD	C2D-C1D	2.04	1.56	1.53
4	C	503	NAD	C2N-C3N	-2.04	1.35	1.39
4	H	508	NAD	C4N-C3N	-2.02	1.35	1.39
4	B	502	NAD	C2N-C3N	-2.02	1.35	1.39
4	A	501	NAD	C5N-C4N	-2.01	1.34	1.38

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	508	NAD	N3A-C2A-N1A	-8.75	121.19	128.89
4	A	501	NAD	N3A-C2A-N1A	-7.86	121.97	128.89
4	F	506	NAD	N3A-C2A-N1A	-7.47	122.32	128.89
4	E	505	NAD	N3A-C2A-N1A	-6.96	122.76	128.89
4	D	504	NAD	C8A-N9A-C4A	-6.09	102.01	106.96
4	B	502	NAD	N3A-C2A-N1A	-5.81	123.78	128.89
4	G	507	NAD	N3A-C2A-N1A	-5.58	123.98	128.89
4	C	503	NAD	O4B-C1B-C2B	-5.49	98.70	106.69
4	D	504	NAD	N3A-C2A-N1A	-5.43	124.11	128.89
4	C	503	NAD	N3A-C2A-N1A	-5.26	124.27	128.89
4	G	507	NAD	C8A-N9A-C4A	-5.21	102.72	106.96
4	E	505	NAD	C8A-N9A-C4A	-4.93	102.95	106.96
4	F	506	NAD	O7N-C7N-C3N	4.57	124.70	119.59
4	C	503	NAD	O7N-C7N-N7N	-4.45	116.23	122.59
4	A	501	NAD	C8A-N9A-C4A	-4.44	103.35	106.96
4	G	507	NAD	O3-PA-O5B	4.10	113.79	102.91
4	G	507	NAD	O7N-C7N-N7N	-4.06	116.79	122.59
4	E	505	NAD	O7N-C7N-N7N	-4.03	116.83	122.59
4	D	504	NAD	PN-O3-PA	-4.02	117.00	133.17
4	C	503	NAD	O7N-C7N-C3N	3.91	123.96	119.59
4	A	501	NAD	O7N-C7N-C3N	-3.91	115.22	119.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	503	NAD	C8A-N9A-C4A	-3.91	103.78	106.96
4	B	502	NAD	O4D-C4D-C3D	-3.87	97.30	105.16
4	A	501	NAD	O2N-PN-O1N	-3.82	107.28	118.70
4	G	507	NAD	O4B-C1B-C2B	-3.71	101.28	106.69
4	F	506	NAD	O3-PN-O1N	3.69	117.69	108.77
4	H	508	NAD	O7N-C7N-N7N	-3.56	117.50	122.59
4	D	504	NAD	O7N-C7N-N7N	-3.52	117.56	122.59
4	B	502	NAD	C3N-C7N-N7N	3.48	121.66	117.78
4	H	508	NAD	C6N-C5N-C4N	-3.48	114.05	119.44
4	F	506	NAD	C8A-N9A-C4A	-3.42	104.17	106.96
4	D	504	NAD	C5A-C4A-N9A	3.42	111.83	107.09
4	H	508	NAD	C8A-N9A-C4A	-3.41	104.19	106.96
4	H	508	NAD	O2N-PN-O1N	-3.39	108.59	118.70
4	F	506	NAD	O4B-C1B-C2B	-3.37	101.79	106.69
4	F	506	NAD	O7N-C7N-N7N	-3.34	117.81	122.59
4	B	502	NAD	C8A-N9A-C4A	-3.21	104.35	106.96
4	C	503	NAD	O4D-C4D-C3D	-3.20	98.66	105.16
4	F	506	NAD	O4D-C4D-C3D	-3.17	98.71	105.16
4	C	503	NAD	C4B-O4B-C1B	3.14	113.17	109.72
4	D	504	NAD	C6A-C5A-C4A	3.12	121.05	117.55
4	C	503	NAD	C2B-C3B-C4B	-3.11	96.42	102.64
4	E	505	NAD	O7N-C7N-C3N	3.09	123.05	119.59
4	B	502	NAD	O7N-C7N-N7N	-3.09	118.18	122.59
4	E	505	NAD	C8A-N9A-C1B	3.07	131.94	126.15
4	E	505	NAD	C2D-C3D-C4D	-3.04	96.57	102.64
4	D	504	NAD	C6N-C5N-C4N	-2.99	114.80	119.44
4	B	502	NAD	C5A-C4A-N3A	-2.99	123.07	125.98
4	G	507	NAD	C3N-C7N-N7N	2.99	121.11	117.78
4	E	505	NAD	C5A-C4A-N9A	2.98	111.22	107.09
4	E	505	NAD	O4D-C4D-C3D	-2.98	99.10	105.16
4	D	504	NAD	O3-PN-O1N	2.95	115.89	108.77
4	B	502	NAD	C4B-O4B-C1B	-2.95	106.48	109.72
4	C	503	NAD	C6N-C5N-C4N	-2.93	114.89	119.44
4	E	505	NAD	C5N-C4N-C3N	2.90	123.97	120.34
4	G	507	NAD	C5N-C4N-C3N	2.87	123.93	120.34
4	A	501	NAD	O7N-C7N-N7N	2.87	126.70	122.59
4	D	504	NAD	O2N-PN-O1N	-2.86	110.17	118.70
4	D	504	NAD	C5N-C4N-C3N	2.84	123.89	120.34
4	H	508	NAD	C6A-C5A-C4A	2.84	120.73	117.55
4	D	504	NAD	O2A-PA-O3	2.81	118.49	105.14
4	G	507	NAD	C6A-C5A-C4A	2.81	120.70	117.55
4	H	508	NAD	O7N-C7N-C3N	2.74	122.65	119.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	503	NAD	C6A-C5A-C4A	2.73	120.61	117.55
4	D	504	NAD	C8A-N9A-C1B	2.68	131.19	126.15
4	B	502	NAD	C8A-N9A-C1B	2.66	131.17	126.15
4	B	502	NAD	C3D-C2D-C1D	-2.63	96.79	100.92
4	B	502	NAD	C6A-C5A-C4A	2.60	120.47	117.55
4	A	501	NAD	C5A-C4A-N9A	2.59	110.68	107.09
4	H	508	NAD	O4D-C4D-C3D	-2.58	99.91	105.16
4	E	505	NAD	O4B-C1B-C2B	-2.55	102.98	106.69
4	H	508	NAD	C5N-C4N-C3N	2.54	123.51	120.34
4	F	506	NAD	C2B-C3B-C4B	-2.53	97.58	102.64
4	B	502	NAD	O2N-PN-O1N	-2.53	111.15	118.70
4	F	506	NAD	O2N-PN-O1N	-2.50	111.24	118.70
4	F	506	NAD	C6N-C5N-C4N	-2.49	115.58	119.44
4	H	508	NAD	C2B-C3B-C4B	-2.49	97.68	102.64
4	E	505	NAD	C6A-C5A-C4A	2.48	120.34	117.55
4	G	507	NAD	O2N-PN-O1N	-2.48	111.31	118.70
4	C	503	NAD	C8A-N9A-C1B	2.47	130.79	126.15
4	F	506	NAD	C4D-O4D-C1D	2.46	112.42	109.72
4	A	501	NAD	C6A-C5A-C4A	2.43	120.28	117.55
4	E	505	NAD	O4B-C1B-N9A	2.41	113.35	108.10
4	A	501	NAD	C6N-C5N-C4N	-2.41	115.71	119.44
4	E	505	NAD	PN-O5D-C5D	2.39	128.64	120.35
6	E	6805	GAI	N3-C-N2	2.38	120.54	115.83
4	G	507	NAD	C5A-C4A-N9A	2.38	110.39	107.09
4	F	506	NAD	C6A-C5A-C4A	2.37	120.21	117.55
4	H	508	NAD	PN-O3-PA	-2.37	123.63	133.17
4	A	501	NAD	C8A-N9A-C1B	2.37	130.60	126.15
4	D	504	NAD	O7N-C7N-C3N	2.36	122.23	119.59
4	H	508	NAD	O3-PA-O5B	2.35	109.13	102.91
4	F	506	NAD	C8A-N9A-C1B	2.34	130.56	126.15
4	F	506	NAD	C5N-C4N-C3N	2.33	123.26	120.34
4	A	501	NAD	C3D-C2D-C1D	-2.33	97.27	100.92
6	E	6835	GAI	N3-C-N2	2.32	120.42	115.83
4	A	501	NAD	C4D-O4D-C1D	-2.32	107.17	109.72
4	A	501	NAD	C5N-C4N-C3N	2.30	123.22	120.34
4	H	508	NAD	C5A-C4A-N3A	-2.30	123.74	125.98
6	G	6807	GAI	N3-C-N2	2.30	120.38	115.83
4	A	501	NAD	C5A-C4A-N3A	-2.27	123.77	125.98
4	C	503	NAD	C5A-C4A-N9A	2.26	110.22	107.09
4	G	507	NAD	C2B-C3B-C4B	-2.26	98.13	102.64
4	E	505	NAD	O2N-PN-O1N	-2.26	111.96	118.70
6	E	6836	GAI	N3-C-N2	2.26	120.28	115.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	505	NAD	C6N-C5N-C4N	-2.25	115.95	119.44
6	H	6808	GAI	N3-C-N2	2.25	120.27	115.83
4	G	507	NAD	O7N-C7N-C3N	2.24	122.10	119.59
4	D	504	NAD	O4D-C4D-C3D	-2.24	100.61	105.16
4	E	505	NAD	C2B-C3B-C4B	-2.23	98.20	102.64
4	A	501	NAD	O4B-C1B-C2B	-2.21	103.47	106.69
4	G	507	NAD	C5A-C4A-N3A	-2.20	123.83	125.98
4	D	504	NAD	C5A-C6A-N6A	2.18	125.64	120.72
4	C	503	NAD	O2N-PN-O1N	-2.16	112.24	118.70
4	D	504	NAD	C3N-C7N-N7N	2.15	120.17	117.78
6	A	6801	GAI	N3-C-N2	2.15	120.08	115.83
4	H	508	NAD	C4A-C5A-N7A	2.14	111.48	109.41
4	C	503	NAD	C2N-C3N-C4N	2.14	120.71	118.31
4	C	503	NAD	O3-PA-O5B	2.13	108.57	102.91
6	C	6834	GAI	N3-C-N2	2.13	120.03	115.83
4	H	508	NAD	C2N-C3N-C4N	2.13	120.70	118.31
4	B	502	NAD	O4B-C4B-C3B	2.12	109.48	105.16
4	E	505	NAD	C5A-C4A-N3A	-2.12	123.92	125.98
4	A	501	NAD	C2B-C3B-C4B	-2.10	98.45	102.64
4	E	505	NAD	C3N-C7N-N7N	2.10	120.12	117.78
4	E	505	NAD	PN-O3-PA	-2.10	124.75	133.17
6	A	6821	GAI	N3-C-N2	2.09	119.96	115.83
4	E	505	NAD	O3-PN-O1N	2.09	113.82	108.77
6	F	6806	GAI	N3-C-N2	2.09	119.96	115.83
6	D	6814	GAI	N3-C-N2	2.09	119.95	115.83
6	D	6824	GAI	N3-C-N2	2.08	119.94	115.83
6	F	6826	GAI	N3-C-N2	2.07	119.92	115.83
6	C	6803	GAI	N3-C-N2	2.07	119.92	115.83
4	C	503	NAD	C3B-C2B-C1B	2.07	104.17	100.92
4	F	506	NAD	O4D-C1D-C2D	-2.06	103.69	106.69
6	D	6833	GAI	N3-C-N2	2.06	119.89	115.83
4	B	502	NAD	C5N-C4N-C3N	2.05	122.91	120.34
6	E	6815	GAI	N3-C-N2	2.05	119.88	115.83
6	C	6813	GAI	N3-C-N2	2.04	119.87	115.83
4	D	504	NAD	O4B-C1B-N9A	2.04	112.54	108.10
4	C	503	NAD	C5N-C4N-C3N	2.04	122.89	120.34
4	C	503	NAD	O3-PN-O1N	2.03	113.68	108.77
6	H	6837	GAI	N3-C-N2	2.01	119.80	115.83

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	494/500 (98%)	0.19	10 (2%) 62 62	17, 32, 47, 62	0
1	B	494/500 (98%)	-0.03	9 (1%) 65 66	16, 28, 42, 61	0
1	C	494/500 (98%)	-0.36	1 (0%) 93 94	15, 22, 33, 54	0
1	D	494/500 (98%)	-0.05	5 (1%) 79 80	15, 30, 45, 60	0
1	E	494/500 (98%)	-0.23	6 (1%) 75 76	18, 28, 42, 59	0
1	F	494/500 (98%)	-0.37	1 (0%) 93 94	16, 22, 33, 55	0
1	G	494/500 (98%)	0.02	7 (1%) 72 72	21, 31, 45, 61	0
1	H	494/500 (98%)	0.25	9 (1%) 65 66	20, 35, 52, 72	0
All	All	3952/4000 (98%)	-0.07	48 (1%) 75 76	15, 29, 45, 72	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	376	ASP	6.8
1	A	474	GLY	5.9
1	H	7	ALA	3.9
1	D	376	ASP	3.8
1	A	7	ALA	3.7
1	E	377	ARG	3.3
1	E	7	ALA	3.2
1	G	7	ALA	3.1
1	A	262	LEU	3.0
1	B	257	ALA	3.0
1	G	474	GLY	3.0
1	H	424	THR	2.9
1	B	7	ALA	2.9
1	E	376	ASP	2.8
1	G	14	GLN	2.8
1	A	376	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	32	VAL	2.7
1	H	34	ARG	2.7
1	H	10	ALA	2.7
1	A	363	GLU	2.7
1	F	474	GLY	2.7
1	E	474	GLY	2.6
1	D	358	ASN	2.6
1	A	40	VAL	2.5
1	B	34	ARG	2.4
1	A	392	GLY	2.4
1	H	32	VAL	2.4
1	D	424	THR	2.3
1	B	254	GLN	2.3
1	H	350	PHE	2.3
1	B	474	GLY	2.3
1	B	424	THR	2.3
1	E	34	ARG	2.3
1	B	16	GLU	2.3
1	G	193	VAL	2.2
1	C	474	GLY	2.2
1	A	424	THR	2.2
1	H	336	ASP	2.2
1	A	14	GLN	2.2
1	D	34	ARG	2.2
1	G	475	GLN	2.2
1	A	371	GLY	2.1
1	G	34	ARG	2.1
1	E	179	LEU	2.1
1	B	201	ALA	2.0
1	H	248	GLU	2.0
1	D	220	ILE	2.0
1	G	373	ILE	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
2	MG	D	604	1/1	0.18	13.67	52,52,52,52	0
5	EDO	B	6962	4/4	0.32	13.48	71,71,72,72	0
5	EDO	C	6943	4/4	0.27	12.93	30,36,37,37	0
2	MG	G	607	1/1	0.15	10.83	59,59,59,59	0
5	EDO	E	6945	4/4	0.27	10.24	34,40,40,41	0
5	EDO	F	6946	4/4	0.28	9.39	29,37,39,39	0
5	EDO	E	6955	4/4	0.34	9.33	52,53,55,55	0
5	EDO	B	6952	4/4	0.42	8.84	60,60,61,61	0
6	GAI	H	6818	4/4	0.33	8.32	57,57,57,57	0
6	GAI	B	6812	4/4	0.34	6.85	51,52,53,53	0
6	GAI	G	6817	4/4	0.38	6.20	52,52,52,53	0
5	EDO	B	6942	4/4	0.20	6.18	36,39,40,40	0
5	EDO	G	6947	4/4	0.22	6.17	34,42,42,43	0
5	EDO	E	6905	4/4	0.17	6.02	37,39,40,40	0
6	GAI	A	6811	4/4	0.24	5.36	56,57,57,58	0
5	EDO	F	6956	4/4	0.23	4.80	49,51,52,52	0
6	GAI	F	6806	4/4	0.16	4.78	31,32,32,33	0
5	EDO	A	6951	4/4	0.27	4.40	54,55,56,56	0
5	EDO	C	6903	4/4	0.15	4.40	37,38,39,39	0
5	EDO	G	6907	4/4	0.19	4.19	38,40,40,41	0
5	EDO	H	6908	4/4	0.15	4.08	36,37,38,38	0
3	NA	H	708	1/1	0.26	4.06	55,55,55,55	0
5	EDO	C	6923	4/4	0.16	3.70	51,52,52,54	0
5	EDO	A	6941	4/4	0.26	3.62	38,43,44,44	0
6	GAI	F	6816	4/4	0.19	3.61	50,50,50,51	0
5	EDO	D	6924	4/4	0.20	3.48	56,57,57,58	0
5	EDO	H	6928	4/4	0.21	3.40	66,66,66,68	0
5	EDO	E	6965	4/4	0.37	3.31	69,70,70,71	0
6	GAI	C	6803	4/4	0.16	3.24	32,34,34,36	0
5	EDO	D	6914	4/4	0.29	3.18	59,59,61,61	0
6	GAI	A	6821	4/4	0.38	3.11	55,56,56,56	0
2	MG	C	603	1/1	0.12	2.90	41,41,41,41	0
5	EDO	F	6966	4/4	0.17	2.88	47,49,49,51	0
5	EDO	G	6917	4/4	0.21	2.86	50,51,52,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	EDO	C	6953	4/4	0.23	2.65	54,54,55,56	0
5	EDO	H	6948	4/4	0.23	2.64	45,47,47,49	0
6	GAI	C	6813	4/4	0.19	2.47	53,53,54,56	0
3	NA	C	703	1/1	0.15	2.41	24,24,24,24	0
5	EDO	F	6906	4/4	0.14	2.37	37,38,38,40	0
5	EDO	B	6902	4/4	0.16	2.25	38,42,42,42	0
5	EDO	B	6912	4/4	0.24	2.11	46,46,47,48	0
5	EDO	E	6925	4/4	0.18	2.02	48,49,49,49	0
6	GAI	A	6801	4/4	0.15	1.97	35,36,37,37	0
6	GAI	D	6824	4/4	0.37	1.92	65,66,66,67	0
5	EDO	H	6918	4/4	0.21	1.91	60,61,61,61	0
5	EDO	C	6913	4/4	0.12	1.86	27,29,30,31	0
5	EDO	A	6901	4/4	0.13	1.54	33,36,36,36	0
6	GAI	E	6836	4/4	0.14	1.42	37,39,40,41	0
6	GAI	D	6814	4/4	0.13	1.38	43,44,45,45	0
5	EDO	F	6926	4/4	0.17	1.32	46,47,47,50	0
5	EDO	F	6916	4/4	0.12	1.16	31,33,33,35	0
6	GAI	F	6826	4/4	0.14	1.09	44,44,44,45	0
5	EDO	D	6904	4/4	0.12	1.09	30,35,35,35	0
5	EDO	A	6921	4/4	0.12	0.98	53,53,54,54	0
6	GAI	G	6838	4/4	0.20	0.97	47,47,49,50	0
5	EDO	G	6927	4/4	0.18	0.97	54,54,54,54	0
6	GAI	B	6831	4/4	0.18	0.74	59,59,59,60	0
6	GAI	H	6808	4/4	0.12	0.71	30,32,32,32	0
6	GAI	H	6837	4/4	0.16	0.64	51,52,53,53	0
5	EDO	A	6911	4/4	0.18	0.49	56,57,58,59	0
6	GAI	G	6807	4/4	0.13	0.49	41,41,42,43	0
6	GAI	D	6833	4/4	0.12	0.38	54,55,55,55	0
6	GAI	A	6832	4/4	0.14	0.37	48,48,48,50	0
6	GAI	E	6835	4/4	0.13	0.24	37,38,38,40	0
6	GAI	B	6802	4/4	0.12	0.20	37,38,39,39	0
6	GAI	C	6834	4/4	0.13	0.19	42,42,43,45	0
4	NAD	D	504	44/44	0.12	0.18	24,36,42,43	0
6	GAI	E	6815	4/4	0.12	0.17	45,46,46,46	0
4	NAD	A	501	44/44	0.15	0.16	32,44,50,50	0
6	GAI	C	6823	4/4	0.13	0.14	35,35,36,36	0
4	NAD	E	505	44/44	0.10	0.08	23,33,41,42	0
3	NA	G	707	1/1	0.12	0.07	35,35,35,35	0
4	NAD	G	507	44/44	0.13	0.06	30,40,44,45	0
5	EDO	C	6963	4/4	0.10	0.02	35,35,36,38	0
2	MG	F	606	1/1	0.12	-0.04	41,41,41,41	0
5	EDO	E	6915	4/4	0.15	-0.10	42,44,45,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAD	B	502	44/44	0.12	-0.21	35,41,44,47	0
6	GAI	E	6805	4/4	0.10	-0.21	27,27,28,29	0
4	NAD	H	508	44/44	0.13	-0.29	35,46,50,51	0
3	NA	F	706	1/1	0.09	-0.43	26,26,26,26	0
2	MG	H	608	1/1	0.09	-0.58	59,59,59,59	0
4	NAD	C	503	44/44	0.08	-0.83	16,26,30,32	0
4	NAD	F	506	44/44	0.09	-0.83	16,25,30,31	0
3	NA	D	704	1/1	0.09	-0.87	41,41,41,41	0
3	NA	A	701	1/1	0.10	-1.10	40,40,40,40	0
2	MG	B	602	1/1	0.07	-1.11	47,47,47,47	0
3	NA	B	702	1/1	0.10	-1.16	34,34,34,34	0
3	NA	E	705	1/1	0.08	-1.16	40,40,40,40	0
6	GAI	D	6804	4/4	0.08	-1.38	25,26,27,29	0
2	MG	A	601	1/1	0.08	-8.25	49,49,49,49	0
2	MG	E	605	1/1	0.10	-	50,50,50,50	0

6.5 Other polymers ⓘ

There are no such residues in this entry.