Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:51 AM GMT

PDB ID	:	3N82
Title	:	T244A mutant of Human mitochondrial aldehyde dehydrogenase, NADH complex
Authors	:	Gonzalez-Segura, L.; Hurley, T.D.
Deposited on	:	2010-05-27
Resolution	:	2.25 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 ①) were used in the production of this report:

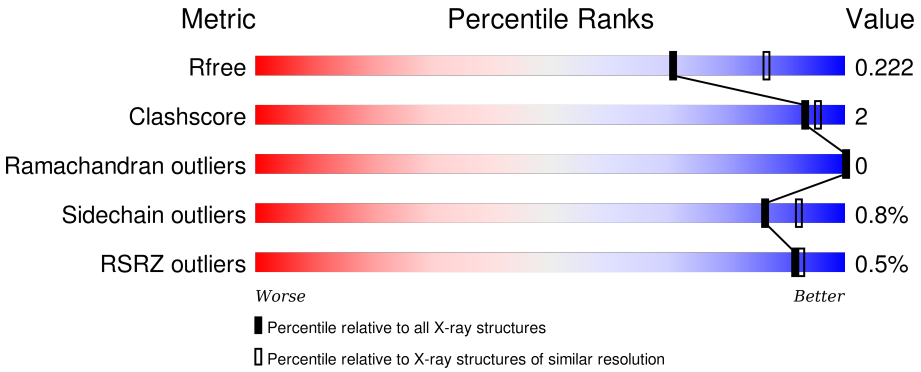
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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 <=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	500	94%
1	B	500	% 94%
1	C	500	92% 7%
1	D	500	93% 6%
1	E	500	94% 5%

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Mol	Chain	Length	Quality of chain
1	F	500	93% 6%
1	G	500	% 94% 5%
1	H	500	% 93% 6%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GAI	B	802	-	-	-	X
4	GAI	B	812	-	-	-	X
4	GAI	D	804	-	-	-	X
4	GAI	D	814	-	-	-	X
4	GAI	E	805	-	-	-	X
4	GAI	E	815	-	-	-	X
4	GAI	F	806	-	-	-	X
4	GAI	G	817	-	-	-	X
4	GAI	H	808	-	-	-	X
5	EDO	C	963	-	-	-	X
5	EDO	D	944	-	-	-	X
5	EDO	F	946	-	-	-	X
5	EDO	F	966	-	-	-	X
6	NAD	A	501	-	-	-	X
6	NAD	G	507	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 33806 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 Aldehyde dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	5	0
			3833	2436	654	722	21			
1	B	494	Total	C	N	O	S	0	4	0
			3828	2432	654	722	20			
1	C	494	Total	C	N	O	S	0	3	0
			3819	2427	652	720	20			
1	D	494	Total	C	N	O	S	0	5	0
			3834	2436	654	724	20			
1	E	494	Total	C	N	O	S	0	4	0
			3828	2432	654	722	20			
1	F	494	Total	C	N	O	S	0	3	0
			3819	2427	652	720	20			
1	G	494	Total	C	N	O	S	0	3	0
			3819	2427	652	720	20			
1	H	494	Total	C	N	O	S	0	5	0
			3834	2435	655	724	20			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	ALA	THR	ENGINEERED MUTATION	UNP P05091
B	244	ALA	THR	ENGINEERED MUTATION	UNP P05091
C	244	ALA	THR	ENGINEERED MUTATION	UNP P05091
D	244	ALA	THR	ENGINEERED MUTATION	UNP P05091
E	244	ALA	THR	ENGINEERED MUTATION	UNP P05091
F	244	ALA	THR	ENGINEERED MUTATION	UNP P05091
G	244	ALA	THR	ENGINEERED MUTATION	UNP P05091
H	244	ALA	THR	ENGINEERED MUTATION	UNP P05091

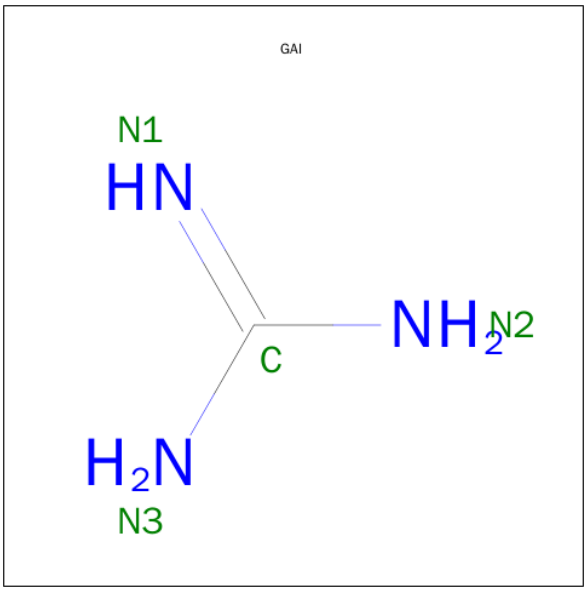
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

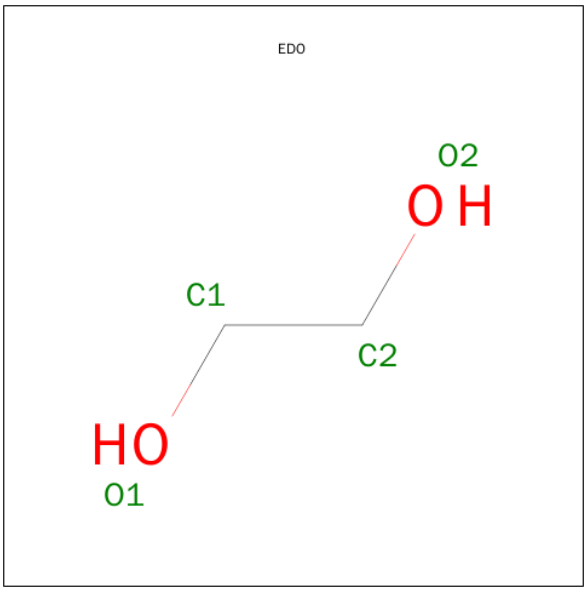
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Na 1 1	0	0
3	D	1	Total Na 1 1	0	0
3	E	1	Total Na 1 1	0	0
3	H	1	Total Na 1 1	0	0
3	B	1	Total Na 1 1	0	0
3	C	1	Total Na 1 1	0	0
3	A	1	Total Na 1 1	0	0
3	F	1	Total Na 1 1	0	0

- Molecule 4 is GUANIDINE (three-letter code: GAI) (formula: CH_5N_3).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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	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
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0

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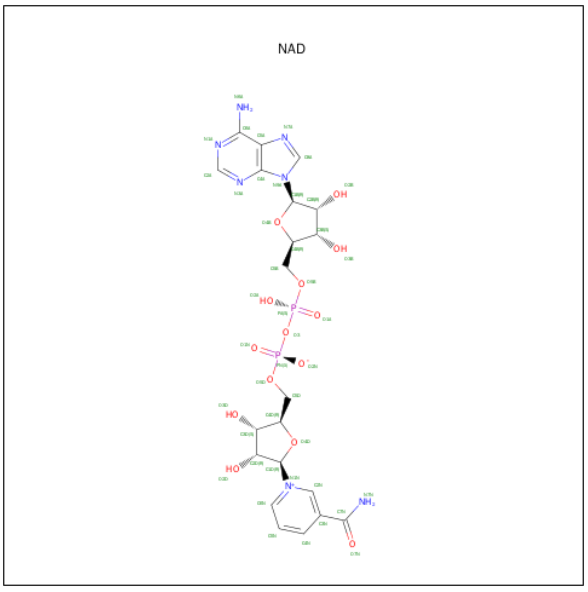
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total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

- Molecule 6 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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

- Molecule 7 is water.

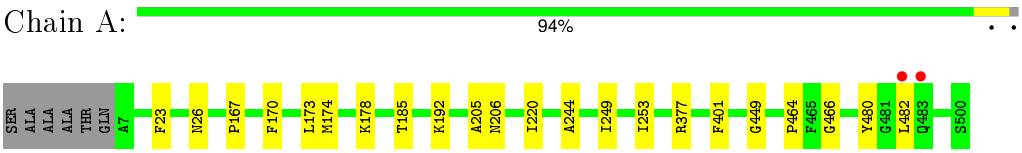
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	332	Total	O	0	0
			332	332		
7	B	355	Total	O	0	0
			355	355		
7	C	346	Total	O	0	0
			346	346		
7	D	342	Total	O	0	0
			342	342		
7	E	349	Total	O	0	0
			349	349		
7	F	343	Total	O	0	0
			343	343		
7	G	301	Total	O	0	0
			301	301		
7	H	308	Total	O	0	0
			308	308		

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.

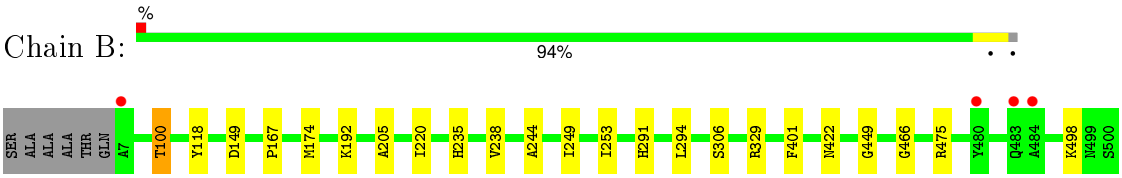
- Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain A:



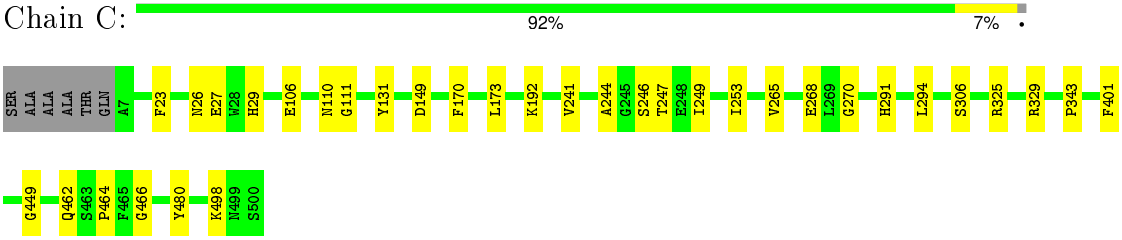
- Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain B:



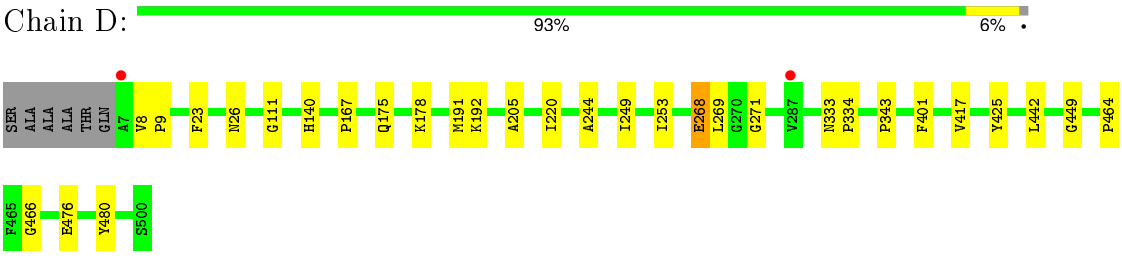
- Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain C:



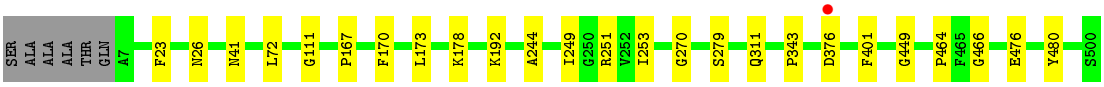
- Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain D:



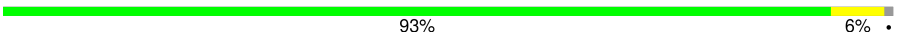
- Molecule 1: Aldehyde dehydrogenase, mitochondrial

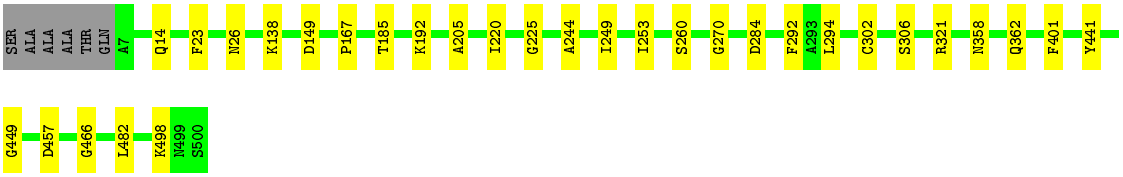
Chain E:



• Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain F:



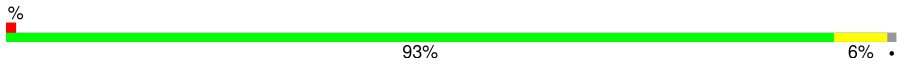


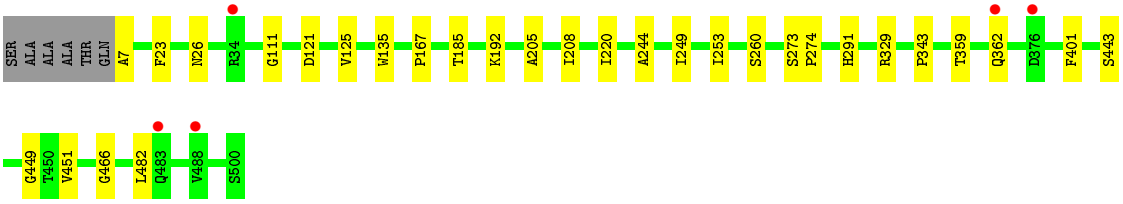
• Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain G:

• Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	142.22Å 150.72Å 177.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.25 49.65 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.25) 99.6 (49.65-2.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.60 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.168 , 0.219 0.171 , 0.222	Depositor DCC
R_{free} test set	8995 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	23.2	Xtriage
Anisotropy	0.857	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 39.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	1 of 179564 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	33806	wwPDB-VP
Average B, all atoms (Å^2)	25.0	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 55.57 % 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 3.1035e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.44	0/3920	0.52	0/5316
1	B	0.45	0/3912	0.51	0/5306
1	C	0.43	0/3903	0.52	0/5294
1	D	0.43	0/3921	0.52	0/5318
1	E	0.43	0/3912	0.51	0/5306
1	F	0.45	0/3903	0.51	0/5294
1	G	0.42	0/3903	0.51	0/5294
1	H	0.43	0/3918	0.51	0/5314
All	All	0.43	0/31292	0.51	0/42442

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3833	0	3778	12	0
1	B	3828	0	3769	11	0
1	C	3819	0	3762	19	0
1	D	3834	0	3775	17	0
1	E	3828	0	3769	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3819	0	3762	17	0
1	G	3819	0	3762	13	0
1	H	3834	0	3773	18	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	4	0	4	0	0
4	B	8	0	8	0	0
4	C	4	0	4	0	0
4	D	8	0	8	0	0
4	E	8	0	8	0	0
4	F	8	0	8	0	0
4	G	8	0	8	0	0
4	H	4	0	4	0	0
5	A	12	0	18	0	0
5	B	8	0	12	0	0
5	C	16	0	24	0	0
5	D	8	0	12	1	0
5	E	12	0	18	1	0
5	F	20	0	30	2	0
5	G	12	0	18	0	0
5	H	8	0	12	0	0
6	A	44	0	26	0	0
6	B	44	0	26	0	0
6	C	44	0	26	1	0
6	D	44	0	26	0	0
6	E	44	0	26	0	0
6	F	44	0	26	1	0
6	G	44	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	44	0	26	0	0
7	A	332	0	0	0	0
7	B	355	0	0	1	0
7	C	346	0	0	2	0
7	D	342	0	0	1	0
7	E	349	0	0	1	0
7	F	343	0	0	2	0
7	G	301	0	0	2	0
7	H	308	0	0	3	0
All	All	33806	0	30554	119	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 2.

All (119) 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:G:174:MET:SD	7:G:2134:HOH:O	2.37	0.81
1:E:279:SER:H	1:E:311[B]:GLN:HE21	1.35	0.73
1:F:270:GLY:HA3	7:F:572:HOH:O	1.96	0.65
1:H:291:HIS:HE1	1:H:329:ARG:HH11	1.47	0.61
1:E:279:SER:H	1:E:311[B]:GLN:NE2	1.98	0.59
1:H:291:HIS:HD2	7:H:503:HOH:O	1.84	0.59
1:E:167:PRO:HD3	1:E:244:ALA:HB3	1.84	0.59
1:F:302:CYS:SG	7:F:2678:HOH:O	2.57	0.57
1:G:279:SER:H	1:G:311[B]:GLN:HE21	1.53	0.57
1:C:291:HIS:HE1	1:C:329:ARG:HH11	1.53	0.56
1:B:205:ALA:HB2	1:B:220:ILE:HD12	1.89	0.55
1:E:23:PHE:CZ	1:E:26:ASN:HA	2.41	0.55
1:G:23:PHE:CZ	1:G:26:ASN:HA	2.42	0.54
1:E:72:LEU:HD21	5:F:946:EDO:H11	1.89	0.54
1:C:23:PHE:CZ	1:C:26:ASN:HA	2.42	0.53
1:E:464:PRO:HG3	1:E:480:TYR:CD1	2.43	0.53
1:G:279:SER:H	1:G:311[B]:GLN:NE2	2.07	0.53
1:G:167:PRO:HD3	1:G:244:ALA:HB3	1.91	0.52
1:F:23:PHE:CZ	1:F:26:ASN:HA	2.43	0.52
1:F:358:ASN:O	1:F:362:GLN:HG2	2.08	0.52
1:E:41:ASN:HD22	5:E:915:EDO:H22	1.75	0.52
1:C:291:HIS:HD2	7:C:1421:HOH:O	1.92	0.51
1:C:270:GLY:HA3	7:C:920:HOH:O	2.11	0.51
1:F:205:ALA:HB2	1:F:220:ILE:HD12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:167:PRO:HD3	1:H:244:ALA:HB3	1.92	0.51
1:H:23:PHE:CZ	1:H:26:ASN:HA	2.46	0.51
1:G:449:GLY:HA3	1:G:466:GLY:O	2.11	0.51
1:B:100:THR:HG22	1:B:118:TYR:HE1	1.76	0.50
1:E:449:GLY:HA3	1:E:466:GLY:O	2.12	0.50
1:D:271:GLY:HA2	1:D:425:TYR:CD2	2.47	0.50
1:B:466:GLY:HA3	1:B:475:ARG:HD3	1.94	0.50
1:E:170:PHE:HB3	1:E:173:LEU:HB3	1.94	0.50
1:D:417:VAL:HG23	1:D:442:LEU:CD2	2.42	0.49
1:A:205:ALA:HB2	1:A:220:ILE:HD12	1.94	0.49
1:E:251:ARG:NH1	1:F:260:SER:O	2.24	0.49
1:F:167:PRO:HD3	1:F:244:ALA:HB3	1.92	0.49
1:D:449:GLY:HA3	1:D:466:GLY:O	2.11	0.49
1:C:464:PRO:HG3	1:C:480:TYR:CD1	2.48	0.49
1:A:449:GLY:HA3	1:A:466:GLY:O	2.13	0.49
1:C:449:GLY:HA3	1:C:466:GLY:O	2.12	0.48
1:G:251:ARG:NH1	1:H:260:SER:O	2.37	0.48
1:D:167:PRO:HD3	1:D:244:ALA:HB3	1.96	0.48
1:C:294:LEU:HD23	1:C:306:SER:HA	1.95	0.47
1:C:291:HIS:CE1	1:C:329:ARG:HD2	2.49	0.47
1:B:449:GLY:HA3	1:B:466:GLY:O	2.15	0.47
1:A:174[B]:MET:HE3	1:A:178:LYS:CE	2.45	0.47
1:F:441:TYR:CD1	5:F:946:EDO:H21	2.50	0.47
1:C:149:ASP:HA	1:C:498:LYS:HB2	1.97	0.47
1:A:174[B]:MET:CE	1:A:178:LYS:CE	2.92	0.47
1:F:149:ASP:HA	1:F:498:LYS:HB2	1.98	0.46
1:C:106:GLU:O	1:C:110:ASN:HB3	2.15	0.46
1:A:249:ILE:O	1:A:253:ILE:HG12	2.16	0.46
1:G:483:GLN:HG2	7:H:2552:HOH:O	2.16	0.46
1:D:417:VAL:HG23	1:D:442:LEU:HD23	1.98	0.45
1:F:185:THR:HG23	1:F:482:LEU:HD22	1.97	0.45
1:D:140:HIS:HE1	7:D:509:HOH:O	2.00	0.45
1:F:449:GLY:HA3	1:F:466:GLY:O	2.16	0.45
1:C:246:SER:HB3	6:C:503:NAD:O4D	2.16	0.45
1:B:294:LEU:HD23	1:B:306:SER:HA	1.97	0.45
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.51	0.45
1:F:249:ILE:O	1:F:253:ILE:HG12	2.16	0.45
1:G:111:GLY:O	1:G:343:PRO:HD2	2.16	0.45
1:B:174:MET:SD	7:B:826:HOH:O	2.61	0.45
1:A:170:PHE:O	1:A:174[A]:MET:HG2	2.16	0.45
1:B:149:ASP:HA	1:B:498:LYS:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:PRO:HD3	1:B:244:ALA:HB3	1.99	0.45
1:B:249:ILE:O	1:B:253:ILE:HG12	2.16	0.45
1:F:284:ASP:OD1	1:F:321:ARG:NH1	2.50	0.45
1:H:443:SER:HA	1:H:451:VAL:HG11	1.99	0.45
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.52	0.44
1:H:7:ALA:N	7:H:1819:HOH:O	2.49	0.44
1:H:449:GLY:HA3	1:H:466:GLY:O	2.18	0.44
1:B:291:HIS:NE2	1:B:329:ARG:HD2	2.32	0.44
1:A:170:PHE:HB3	1:A:173:LEU:HB3	2.00	0.44
1:C:249:ILE:O	1:C:253:ILE:HG12	2.17	0.44
1:H:121:ASP:O	1:H:125:VAL:HG23	2.18	0.44
1:A:185:THR:HG23	1:A:482:LEU:HD22	2.00	0.43
1:C:27:GLU:HB2	1:C:29:HIS:CE1	2.53	0.43
1:C:291:HIS:CD2	1:C:325:ARG:HG3	2.53	0.43
1:B:235:HIS:HB3	1:B:238:VAL:HG23	2.00	0.43
1:F:292:PHE:HE1	1:F:457:ASP:HB2	1.83	0.43
1:C:131:TYR:CE1	1:C:462:GLN:HG3	2.53	0.43
1:D:249:ILE:O	1:D:253:ILE:HG12	2.18	0.43
1:G:121:ASP:O	1:G:125:VAL:HG23	2.19	0.43
1:A:167:PRO:HD3	1:A:244:ALA:HB3	2.00	0.43
1:F:294:LEU:HD23	1:F:306:SER:HA	2.00	0.43
1:H:205:ALA:HA	1:H:208:ILE:HD12	2.01	0.42
1:H:359:THR:HA	1:H:362:GLN:HG2	2.01	0.42
1:E:178:LYS:NZ	1:E:476:GLU:OE2	2.53	0.42
1:F:225:GLY:HA3	6:F:506:NAD:C8A	2.49	0.42
1:G:358:ASN:ND2	7:G:2498:HOH:O	2.52	0.42
1:D:205:ALA:HB2	1:D:220:ILE:HD12	2.02	0.42
1:C:111:GLY:O	1:C:343:PRO:HD2	2.20	0.42
1:C:244:ALA:HA	1:C:268:GLU:O	2.20	0.42
1:H:291:HIS:CE1	1:H:329:ARG:HH11	2.33	0.41
1:D:417:VAL:HG12	5:D:944:EDO:H12	2.02	0.41
1:H:205:ALA:HB2	1:H:220:ILE:HD12	2.01	0.41
1:A:464:PRO:HG3	1:A:480:TYR:CD1	2.55	0.41
1:E:270:GLY:HA3	7:E:2564:HOH:O	2.19	0.41
1:E:249:ILE:O	1:E:253:ILE:HG12	2.21	0.41
1:H:111:GLY:O	1:H:343:PRO:HD2	2.19	0.41
1:H:185:THR:HG23	1:H:482:LEU:HD22	2.02	0.41
1:D:333:ASN:HA	1:D:334:PRO:HD2	1.93	0.41
1:F:138:LYS:HD3	1:H:135:TRP:CE2	2.56	0.41
1:D:268:GLU:OE2	1:D:269:LEU:O	2.38	0.41
1:H:273:SER:HA	1:H:274:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:279:SER:N	1:E:311[B]:GLN:HE21	2.10	0.41
1:G:166:ILE:HD11	1:G:193:VAL:HG12	2.02	0.41
1:C:170:PHE:HB3	1:C:173:LEU:HB3	2.02	0.41
1:D:178:LYS:NZ	1:D:476:GLU:OE2	2.50	0.41
1:C:241:VAL:CG1	1:C:265:VAL:HG22	2.51	0.41
1:D:464:PRO:HG3	1:D:480:TYR:CD1	2.56	0.41
1:H:249:ILE:O	1:H:253:ILE:HG12	2.21	0.40
1:D:111:GLY:O	1:D:343:PRO:HD2	2.21	0.40
1:G:294:LEU:HD23	1:G:306:SER:HA	2.04	0.40
1:D:175:GLN:HG3	1:D:191:MET:SD	2.62	0.40
1:D:8:VAL:HA	1:D:9:PRO:HD3	1.91	0.40
1:E:111:GLY:O	1:E:343:PRO:HD2	2.21	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	497/500 (99%)	483 (97%)	14 (3%)	0	100	100
1	B	496/500 (99%)	484 (98%)	12 (2%)	0	100	100
1	C	495/500 (99%)	483 (98%)	12 (2%)	0	100	100
1	D	497/500 (99%)	479 (96%)	18 (4%)	0	100	100
1	E	496/500 (99%)	483 (97%)	13 (3%)	0	100	100
1	F	495/500 (99%)	482 (97%)	13 (3%)	0	100	100
1	G	495/500 (99%)	483 (98%)	12 (2%)	0	100	100
1	H	497/500 (99%)	482 (97%)	15 (3%)	0	100	100
All	All	3968/4000 (99%)	3859 (97%)	109 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	403/401 (100%)	399 (99%)	4 (1%)	82	89
1	B	402/401 (100%)	398 (99%)	4 (1%)	82	89
1	C	401/401 (100%)	398 (99%)	3 (1%)	88	93
1	D	403/401 (100%)	400 (99%)	3 (1%)	88	93
1	E	402/401 (100%)	399 (99%)	3 (1%)	88	93
1	F	401/401 (100%)	398 (99%)	3 (1%)	88	93
1	G	401/401 (100%)	396 (99%)	5 (1%)	78	87
1	H	403/401 (100%)	401 (100%)	2 (0%)	92	95
All	All	3216/3208 (100%)	3189 (99%)	27 (1%)	86	92

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	LYS
1	A	206	ASN
1	A	377	ARG
1	A	401	PHE
1	B	100	THR
1	B	192	LYS
1	B	401	PHE
1	B	422	ASN
1	C	192	LYS
1	C	247	THR
1	C	401	PHE
1	D	192	LYS
1	D	268	GLU
1	D	401	PHE
1	E	192	LYS
1	E	376	ASP
1	E	401	PHE
1	F	14	GLN
1	F	192	LYS

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Mol	Chain	Res	Type
1	F	401	PHE
1	G	27	GLU
1	G	192	LYS
1	G	338	LYS
1	G	401	PHE
1	G	483	GLN
1	H	192	LYS
1	H	401	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	440	ASN
1	B	14	GLN
1	B	422	ASN
1	B	440	ASN
1	C	29	HIS
1	C	291	HIS
1	D	140	HIS
1	D	390	GLN
1	F	14	GLN
1	F	358	ASN
1	G	254	GLN
1	G	358	ASN
1	G	362	GLN
1	G	390	GLN
1	H	291	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 61 ligands modelled in this entry, 16 are monoatomic - leaving 45 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	$\#\|Z\| > 2$
6	NAD	A	501	2	38,48,48	1.63	3 (7%)	47,73,73	2.12	4 (8%)
4	GAI	A	801	-	0,3,3	0.00	-	0,3,3	0.00	-
5	EDO	A	901	-	3,3,3	0.44	0	2,2,2	0.22	0
5	EDO	A	911	-	3,3,3	0.41	0	2,2,2	0.32	0
5	EDO	A	921	-	3,3,3	0.37	0	2,2,2	0.51	0
6	NAD	B	502	2	38,48,48	1.64	3 (7%)	47,73,73	1.96	4 (8%)
4	GAI	B	802	-	0,3,3	0.00	-	0,3,3	0.00	-
4	GAI	B	812	-	0,3,3	0.00	-	0,3,3	0.00	-
5	EDO	B	902	-	3,3,3	0.41	0	2,2,2	0.33	0
5	EDO	B	912	-	3,3,3	0.41	0	2,2,2	0.42	0
6	NAD	C	503	2	38,48,48	1.61	3 (7%)	47,73,73	1.95	5 (10%)
4	GAI	C	803	-	0,3,3	0.00	-	0,3,3	0.00	-
5	EDO	C	903	-	3,3,3	0.42	0	2,2,2	0.23	0
5	EDO	C	913	-	3,3,3	0.37	0	2,2,2	0.47	0
5	EDO	C	923	-	3,3,3	0.35	0	2,2,2	0.57	0
5	EDO	C	963	-	3,3,3	0.41	0	2,2,2	0.40	0
6	NAD	D	504	2	38,48,48	1.62	3 (7%)	47,73,73	2.04	5 (10%)
4	GAI	D	804	-	0,3,3	0.00	-	0,3,3	0.00	-
4	GAI	D	814	-	0,3,3	0.00	-	0,3,3	0.00	-
5	EDO	D	904	-	3,3,3	0.39	0	2,2,2	0.46	0
5	EDO	D	944	-	3,3,3	0.38	0	2,2,2	0.51	0
6	NAD	E	505	2	38,48,48	1.63	3 (7%)	47,73,73	2.06	5 (10%)
4	GAI	E	805	-	0,3,3	0.00	-	0,3,3	0.00	-
4	GAI	E	815	-	0,3,3	0.00	-	0,3,3	0.00	-
5	EDO	E	905	-	3,3,3	0.42	0	2,2,2	0.34	0
5	EDO	E	915	-	3,3,3	0.39	0	2,2,2	0.57	0
5	EDO	E	925	-	3,3,3	0.42	0	2,2,2	0.33	0
6	NAD	F	506	2	38,48,48	1.63	3 (7%)	47,73,73	1.87	4 (8%)
4	GAI	F	806	-	0,3,3	0.00	-	0,3,3	0.00	-
4	GAI	F	826	-	0,3,3	0.00	-	0,3,3	0.00	-
5	EDO	F	906	-	3,3,3	0.41	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	F	916	-	3,3,3	0.41	0	2,2,2	0.44	0
5	EDO	F	926	-	3,3,3	0.41	0	2,2,2	0.43	0
5	EDO	F	946	-	3,3,3	0.41	0	2,2,2	0.41	0
5	EDO	F	966	-	3,3,3	0.45	0	2,2,2	0.24	0
6	NAD	G	507	2	38,48,48	1.63	3 (7%)	47,73,73	1.86	4 (8%)
4	GAI	G	807	-	0,3,3	0.00	-	0,3,3	0.00	-
4	GAI	G	817	-	0,3,3	0.00	-	0,3,3	0.00	-
5	EDO	G	907	-	3,3,3	0.39	0	2,2,2	0.47	0
5	EDO	G	917	-	3,3,3	0.43	0	2,2,2	0.37	0
5	EDO	G	927	-	3,3,3	0.38	0	2,2,2	0.49	0
6	NAD	H	508	2	38,48,48	1.64	3 (7%)	47,73,73	1.98	3 (6%)
4	GAI	H	808	-	0,3,3	0.00	-	0,3,3	0.00	-
5	EDO	H	908	-	3,3,3	0.37	0	2,2,2	0.56	0
5	EDO	H	928	-	3,3,3	0.38	0	2,2,2	0.48	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
6	NAD	A	501	2	-	0/22/62/62	0/5/5/5
4	GAI	A	801	-	-	0/0/0/0	0/0/0/0
5	EDO	A	901	-	-	0/1/1/1	0/0/0/0
5	EDO	A	911	-	-	0/1/1/1	0/0/0/0
5	EDO	A	921	-	-	0/1/1/1	0/0/0/0
6	NAD	B	502	2	-	0/22/62/62	0/5/5/5
4	GAI	B	802	-	-	0/0/0/0	0/0/0/0
4	GAI	B	812	-	-	0/0/0/0	0/0/0/0
5	EDO	B	902	-	-	0/1/1/1	0/0/0/0
5	EDO	B	912	-	-	0/1/1/1	0/0/0/0
6	NAD	C	503	2	-	0/22/62/62	0/5/5/5
4	GAI	C	803	-	-	0/0/0/0	0/0/0/0
5	EDO	C	903	-	-	0/1/1/1	0/0/0/0
5	EDO	C	913	-	-	0/1/1/1	0/0/0/0
5	EDO	C	923	-	-	0/1/1/1	0/0/0/0
5	EDO	C	963	-	-	0/1/1/1	0/0/0/0
6	NAD	D	504	2	-	0/22/62/62	0/5/5/5
4	GAI	D	804	-	-	0/0/0/0	0/0/0/0
4	GAI	D	814	-	-	0/0/0/0	0/0/0/0
5	EDO	D	904	-	-	0/1/1/1	0/0/0/0
5	EDO	D	944	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAD	E	505	2	-	0/22/62/62	0/5/5/5
4	GAI	E	805	-	-	0/0/0/0	0/0/0/0
4	GAI	E	815	-	-	0/0/0/0	0/0/0/0
5	EDO	E	905	-	-	0/1/1/1	0/0/0/0
5	EDO	E	915	-	-	0/1/1/1	0/0/0/0
5	EDO	E	925	-	-	0/1/1/1	0/0/0/0
6	NAD	F	506	2	-	0/22/62/62	0/5/5/5
4	GAI	F	806	-	-	0/0/0/0	0/0/0/0
4	GAI	F	826	-	-	0/0/0/0	0/0/0/0
5	EDO	F	906	-	-	0/1/1/1	0/0/0/0
5	EDO	F	916	-	-	0/1/1/1	0/0/0/0
5	EDO	F	926	-	-	0/1/1/1	0/0/0/0
5	EDO	F	946	-	-	0/1/1/1	0/0/0/0
5	EDO	F	966	-	-	0/1/1/1	0/0/0/0
6	NAD	G	507	2	-	0/22/62/62	0/5/5/5
4	GAI	G	807	-	-	0/0/0/0	0/0/0/0
4	GAI	G	817	-	-	0/0/0/0	0/0/0/0
5	EDO	G	907	-	-	0/1/1/1	0/0/0/0
5	EDO	G	917	-	-	0/1/1/1	0/0/0/0
5	EDO	G	927	-	-	0/1/1/1	0/0/0/0
6	NAD	H	508	2	-	0/22/62/62	0/5/5/5
4	GAI	H	808	-	-	0/0/0/0	0/0/0/0
5	EDO	H	908	-	-	0/1/1/1	0/0/0/0
5	EDO	H	928	-	-	0/1/1/1	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	504	NAD	C2A-N1A	2.36	1.38	1.33
6	F	506	NAD	C2A-N1A	2.38	1.38	1.33
6	A	501	NAD	C2A-N1A	2.39	1.38	1.33
6	B	502	NAD	C2A-N1A	2.40	1.38	1.33
6	G	507	NAD	C2A-N1A	2.40	1.38	1.33
6	E	505	NAD	C2A-N1A	2.41	1.38	1.33
6	H	508	NAD	C2A-N1A	2.45	1.38	1.33
6	C	503	NAD	C2A-N1A	2.51	1.38	1.33
6	D	504	NAD	C2A-N3A	3.52	1.38	1.32
6	A	501	NAD	C2A-N3A	3.53	1.38	1.32
6	G	507	NAD	C2A-N3A	3.54	1.38	1.32
6	E	505	NAD	C2A-N3A	3.55	1.38	1.32
6	B	502	NAD	C2A-N3A	3.61	1.38	1.32
6	H	508	NAD	C2A-N3A	3.64	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	503	NAD	C2A-N3A	3.64	1.38	1.32
6	F	506	NAD	C2A-N3A	3.66	1.38	1.32
6	C	503	NAD	O7N-C7N	7.97	1.41	1.24
6	D	504	NAD	O7N-C7N	8.15	1.41	1.24
6	F	506	NAD	O7N-C7N	8.16	1.41	1.24
6	A	501	NAD	O7N-C7N	8.19	1.41	1.24
6	G	507	NAD	O7N-C7N	8.19	1.41	1.24
6	B	502	NAD	O7N-C7N	8.25	1.41	1.24
6	E	505	NAD	O7N-C7N	8.25	1.41	1.24
6	H	508	NAD	O7N-C7N	8.25	1.41	1.24

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	501	NAD	N3A-C2A-N1A	-11.92	119.77	128.89
6	H	508	NAD	N3A-C2A-N1A	-11.76	119.89	128.89
6	D	504	NAD	N3A-C2A-N1A	-11.35	120.20	128.89
6	C	503	NAD	N3A-C2A-N1A	-11.33	120.22	128.89
6	B	502	NAD	N3A-C2A-N1A	-11.20	120.32	128.89
6	E	505	NAD	N3A-C2A-N1A	-10.99	120.48	128.89
6	F	506	NAD	N3A-C2A-N1A	-10.68	120.72	128.89
6	G	507	NAD	N3A-C2A-N1A	-10.59	120.78	128.89
6	E	505	NAD	PN-O3-PA	-3.57	122.72	132.73
6	G	507	NAD	PN-O3-PA	-3.41	123.17	132.73
6	D	504	NAD	PN-O3-PA	-3.36	123.29	132.73
6	C	503	NAD	PN-O3-PA	-3.21	123.71	132.73
6	B	502	NAD	PN-O3-PA	-3.01	124.29	132.73
6	F	506	NAD	PN-O3-PA	-2.93	124.50	132.73
6	A	501	NAD	PN-O3-PA	-2.90	124.58	132.73
6	H	508	NAD	PN-O3-PA	-2.52	125.66	132.73
6	E	505	NAD	C4A-C5A-N7A	-2.36	107.31	109.48
6	D	504	NAD	C4A-C5A-N7A	-2.13	107.52	109.48
6	C	503	NAD	C4A-C5A-N7A	-2.06	107.58	109.48
6	F	506	NAD	C1B-N9A-C4A	-2.04	123.86	126.94
6	C	503	NAD	O4B-C1B-N9A	2.12	112.54	108.10
6	G	507	NAD	C4B-O4B-C1B	2.18	112.12	109.72
6	E	505	NAD	C4B-O4B-C1B	2.28	112.22	109.72
6	B	502	NAD	O4B-C1B-N9A	2.33	112.98	108.10
6	A	501	NAD	O4B-C1B-N9A	2.44	113.20	108.10
6	D	504	NAD	C4B-O4B-C1B	2.50	112.47	109.72
6	G	507	NAD	O4D-C1D-N1N	2.52	110.90	108.13
6	C	503	NAD	O4D-C1D-N1N	3.11	111.55	108.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	508	NAD	O4D-C1D-N1N	3.27	111.72	108.13
6	F	506	NAD	O4D-C1D-N1N	3.34	111.80	108.13
6	B	502	NAD	O4D-C1D-N1N	4.15	112.69	108.13
6	D	504	NAD	O4D-C1D-N1N	4.42	112.98	108.13
6	A	501	NAD	O4D-C1D-N1N	4.72	113.32	108.13
6	E	505	NAD	O4D-C1D-N1N	5.46	114.13	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	503	NAD	1	0
5	D	944	EDO	1	0
5	E	915	EDO	1	0
6	F	506	NAD	1	0
5	F	946	EDO	2	0

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, 95^{th} 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%)	-0.22	2 (0%) 93 93	17, 25, 35, 42	0
1	B	494/500 (98%)	-0.37	4 (0%) 87 88	17, 22, 30, 37	0
1	C	494/500 (98%)	-0.50	0 100 100	16, 22, 30, 36	0
1	D	494/500 (98%)	-0.42	2 (0%) 93 93	17, 24, 36, 43	0
1	E	494/500 (98%)	-0.45	1 (0%) 95 96	19, 24, 34, 43	0
1	F	494/500 (98%)	-0.52	0 100 100	17, 22, 29, 35	0
1	G	494/500 (98%)	-0.20	6 (1%) 81 83	20, 26, 35, 51	0
1	H	494/500 (98%)	-0.12	5 (1%) 84 85	19, 28, 39, 48	0
All	All	3952/4000 (98%)	-0.35	20 (0%) 91 92	16, 24, 34, 51	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	483[A]	GLN	4.5
1	D	7	ALA	4.1
1	A	483[A]	GLN	3.4
1	B	483[A]	GLN	3.1
1	H	362	GLN	2.7
1	H	488	VAL	2.6
1	G	14	GLN	2.6
1	G	482	LEU	2.4
1	B	7	ALA	2.4
1	D	287	VAL	2.4
1	G	480	TYR	2.3
1	E	376	ASP	2.2
1	H	376	ASP	2.2
1	B	480	TYR	2.2
1	H	34	ARG	2.1
1	G	11	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	482	LEU	2.1
1	G	466	GLY	2.0
1	B	484	ALA	2.0
1	G	47	VAL	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	EDO	F	946	4/4	0.73	0.31	17.24	40,42,43,45	0
5	EDO	D	944	4/4	0.93	0.15	6.55	42,43,44,44	0
4	GAI	F	806	4/4	0.92	0.17	6.41	25,26,26,26	0
4	GAI	B	812	4/4	0.86	0.21	5.74	55,55,55,55	0
4	GAI	D	804	4/4	0.83	0.17	4.68	34,35,35,35	0
5	EDO	F	966	4/4	0.85	0.21	4.42	46,46,47,47	0
4	GAI	D	814	4/4	0.85	0.18	4.37	57,57,57,58	0
4	GAI	H	808	4/4	0.84	0.21	3.38	32,32,32,32	0
4	GAI	E	805	4/4	0.94	0.14	3.11	32,32,32,33	0
5	EDO	C	963	4/4	0.90	0.17	2.73	36,36,37,37	0
6	NAD	A	501	44/44	0.92	0.20	2.70	33,36,43,44	0
4	GAI	E	815	4/4	0.92	0.16	2.55	48,48,48,48	0
4	GAI	G	817	4/4	0.95	0.15	2.15	38,38,39,39	0
4	GAI	B	802	4/4	0.93	0.15	2.03	32,33,33,33	0
6	NAD	G	507	44/44	0.91	0.17	2.01	40,44,46,46	0
5	EDO	C	903	4/4	0.94	0.13	1.92	26,26,27,28	0
4	GAI	C	803	4/4	0.93	0.12	1.78	24,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	NAD	H	508	44/44	0.89	0.19	1.77	35,40,46,47	0
5	EDO	F	906	4/4	0.96	0.11	1.50	26,27,27,27	0
5	EDO	F	916	4/4	0.92	0.13	1.43	33,35,36,37	0
5	EDO	A	901	4/4	0.95	0.17	1.41	22,23,23,23	0
3	NA	D	704	1/1	0.81	0.13	1.25	33,33,33,33	0
5	EDO	B	902	4/4	0.95	0.13	1.19	26,26,28,28	0
5	EDO	F	926	4/4	0.87	0.15	1.18	36,37,38,40	0
3	NA	G	707	1/1	0.78	0.18	1.14	33,33,33,33	0
6	NAD	D	504	44/44	0.93	0.13	1.02	30,36,43,43	0
6	NAD	B	502	44/44	0.93	0.13	0.84	36,40,43,44	0
5	EDO	H	908	4/4	0.95	0.15	0.76	33,33,33,33	0
6	NAD	C	503	44/44	0.94	0.12	0.71	29,33,40,40	0
5	EDO	G	907	4/4	0.93	0.13	0.71	35,35,35,35	0
6	NAD	E	505	44/44	0.93	0.12	0.63	31,34,42,43	0
6	NAD	F	506	44/44	0.94	0.12	0.44	26,33,41,42	0
5	EDO	B	912	4/4	0.95	0.15	0.07	31,31,31,31	0
5	EDO	G	917	4/4	0.94	0.17	0.03	44,44,44,45	0
5	EDO	C	913	4/4	0.98	0.11	-0.09	29,29,30,32	0
5	EDO	E	905	4/4	0.96	0.10	-0.15	26,30,31,32	0
5	EDO	E	915	4/4	0.93	0.14	-0.17	38,39,40,40	0
5	EDO	D	904	4/4	0.98	0.11	-0.17	22,23,24,25	0
4	GAI	G	807	4/4	0.93	0.11	-0.19	38,38,39,39	0
4	GAI	A	801	4/4	0.94	0.10	-0.74	26,27,27,27	0
4	GAI	F	826	4/4	0.94	0.11	-0.86	43,43,43,43	0
5	EDO	A	911	4/4	0.95	0.11	-0.95	47,47,48,48	0
3	NA	H	708	1/1	0.91	0.11	-1.08	38,38,38,38	0
3	NA	E	705	1/1	0.97	0.07	-1.29	33,33,33,33	0
3	NA	A	701	1/1	0.96	0.07	-1.70	34,34,34,34	0
3	NA	B	702	1/1	0.97	0.06	-2.15	25,25,25,25	0
3	NA	F	706	1/1	0.98	0.08	-2.35	27,27,27,27	0
3	NA	C	703	1/1	0.97	0.05	-4.10	23,23,23,23	0
2	MG	F	606	1/1	0.66	0.23	-	45,45,45,45	0
2	MG	D	604	1/1	0.64	0.27	-	50,50,50,50	0
2	MG	A	601	1/1	0.70	0.08	-	51,51,51,51	0
5	EDO	C	923	4/4	0.93	0.21	-	52,52,52,53	0
2	MG	C	603	1/1	0.57	0.14	-	47,47,47,47	0
2	MG	E	605	1/1	0.87	0.28	-	53,53,53,53	0
2	MG	H	608	1/1	0.94	0.09	-	46,46,46,46	0
5	EDO	G	927	4/4	0.83	0.18	-	53,54,54,55	0
5	EDO	A	921	4/4	0.93	0.15	-	54,54,55,55	0
5	EDO	E	925	4/4	0.82	0.16	-	45,45,46,46	0
2	MG	G	607	1/1	0.76	0.13	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	EDO	H	928	4/4	0.92	0.17	-	52,52,53,54	0
2	MG	B	602	1/1	0.82	0.17	-	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.