wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:16 PM GMT

PDB ID	:	1O01
Title	:	Human mitochondrial aldehyde dehydrogenase complexed with crotonaldehyde, NAD(H) and Mg2+
Authors	:	Perez-Miller, S.J.; Hurley, T.D.
Deposited on	:	2003-02-20
Resolution	:	2.15 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

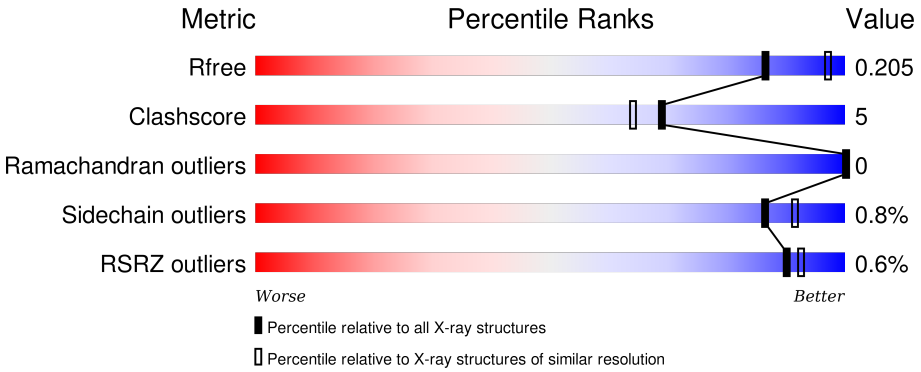
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	91% 8%
1	B	500	89% 10%
1	C	500	87% 12%
1	D	500	88% 10%
1	E	500	91% 8%

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Mol	Chain	Length	Quality of chain
1	F	500	
1	G	500	
1	H	500	

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
3	NA	E	4705	-	-	-	X
3	NA	F	4706	-	-	-	X
4	CRD	B	4512	-	-	X	X
4	CRD	C	4513	-	-	X	X
4	CRD	D	4514	-	-	X	X
4	CRD	E	4515	-	-	X	X
4	CRD	F	4516	-	-	X	X
4	CRD	G	4517	-	-	X	X
5	GAI	A	4801	-	-	-	X
5	GAI	F	4806	-	-	-	X
5	GAI	H	4808	-	-	-	X
6	EDO	C	4902	-	-	-	X
6	EDO	F	4906	-	-	-	X
6	EDO	H	4908	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 34568 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	1	0
			3804	2418	649	718	19			
1	B	494	Total	C	N	O	S	0	1	0
			3804	2418	649	718	19			
1	C	495	Total	C	N	O	S	0	1	0
			3813	2423	651	720	19			
1	D	494	Total	C	N	O	S	0	1	0
			3804	2418	649	718	19			
1	E	494	Total	C	N	O	S	0	1	0
			3804	2418	649	718	19			
1	F	494	Total	C	N	O	S	0	1	0
			3804	2418	649	718	19			
1	G	494	Total	C	N	O	S	0	1	0
			3804	2418	649	718	19			
1	H	494	Total	C	N	O	S	0	1	0
			3804	2418	649	718	19			

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

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

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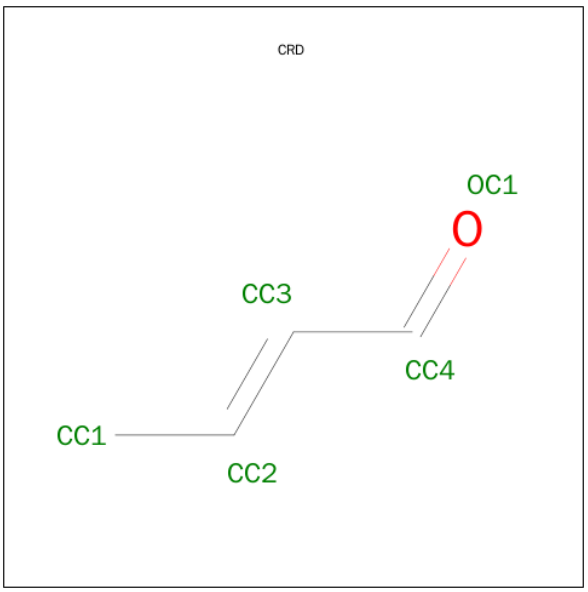
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

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

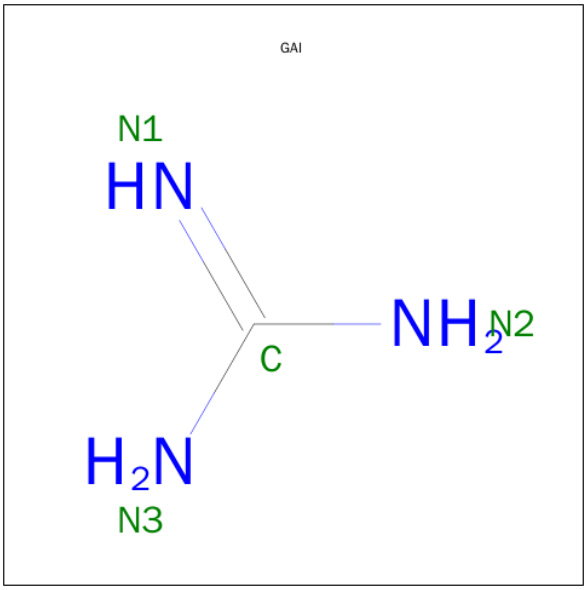
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Na 1 1	0	0
3	D	1	Total Na 1 1	0	0
3	E	1	Total Na 1 1	0	0
3	H	1	Total Na 1 1	0	0
3	B	1	Total Na 1 1	0	0
3	C	1	Total Na 1 1	0	0
3	A	1	Total Na 1 1	0	0
3	F	1	Total Na 1 1	0	0

- Molecule 4 is (2E)-BUT-2-ENAL (three-letter code: CRD) (formula: C_4H_6O).



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

- Molecule 5 is GUANIDINE (three-letter code: GAI) (formula: CH_5N_3).



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

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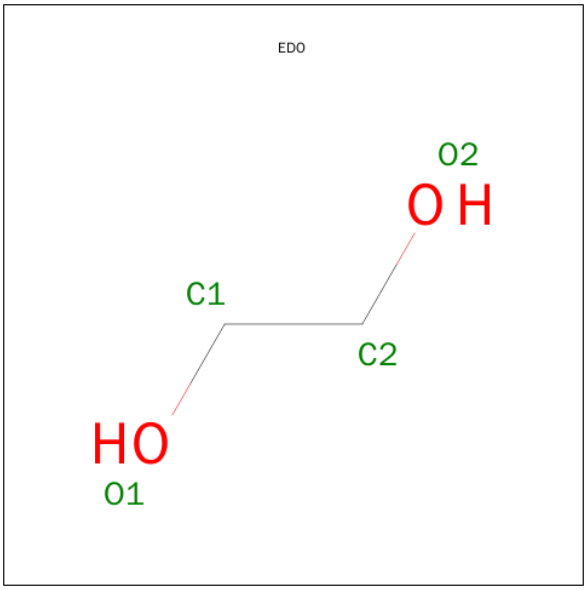
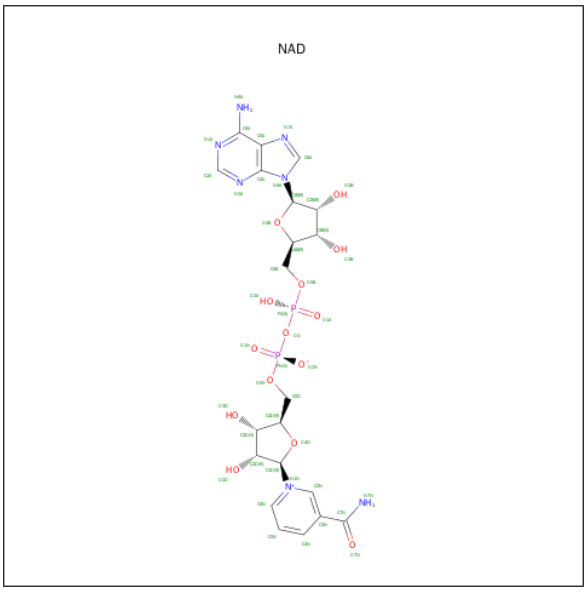
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total C N 4 1 3	0	0
5	H	1	Total C N 4 1 3	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	454	Total	O	0	0
			454	454		
8	B	514	Total	O	0	0
			514	514		
8	C	488	Total	O	0	0
			488	488		
8	D	458	Total	O	0	0
			458	458		

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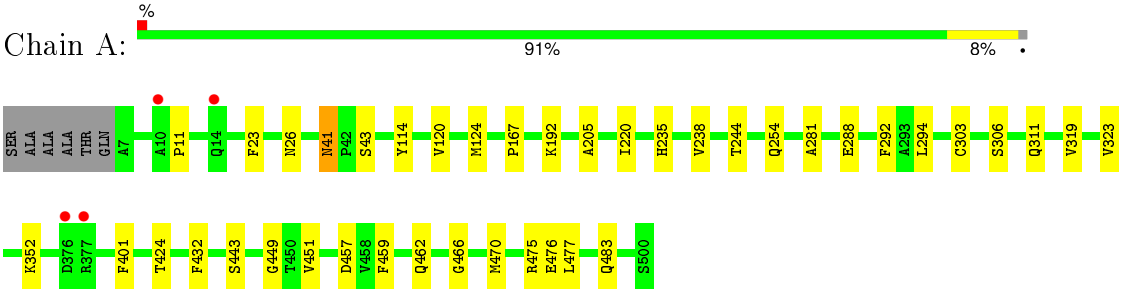
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	449	Total O 449 449	0	0
8	F	480	Total O 480 480	0	0
8	G	440	Total O 440 440	0	0
8	H	382	Total O 382 382	0	0

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.

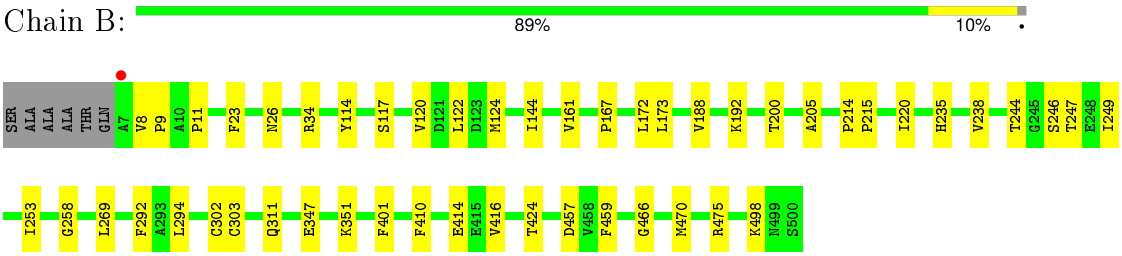
- Molecule 1: Aldehyde dehydrogenase

Chain A:



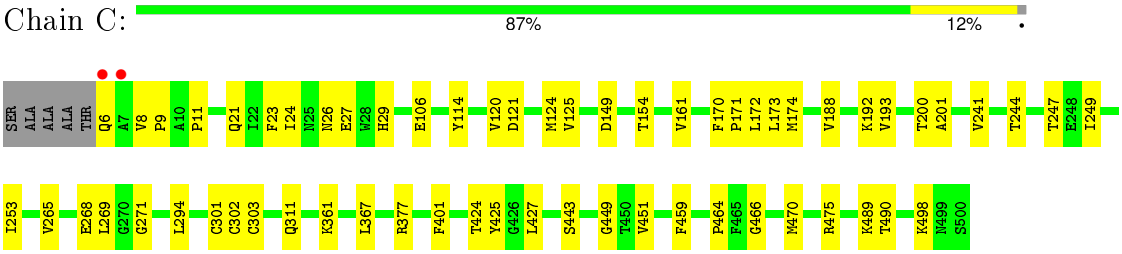
- Molecule 1: Aldehyde dehydrogenase

Chain B:



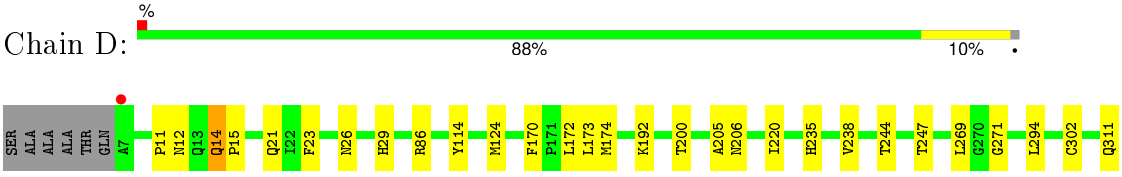
- Molecule 1: Aldehyde dehydrogenase

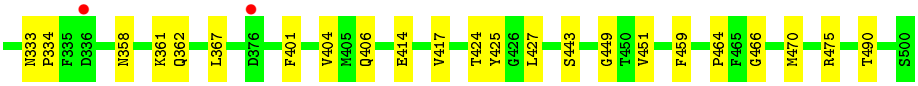
Chain C:



- Molecule 1: Aldehyde dehydrogenase

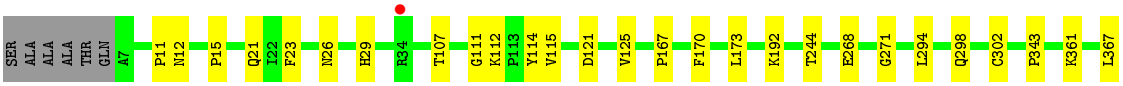
Chain D:

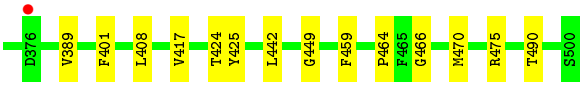




• Molecule 1: Aldehyde dehydrogenase

Chain E:



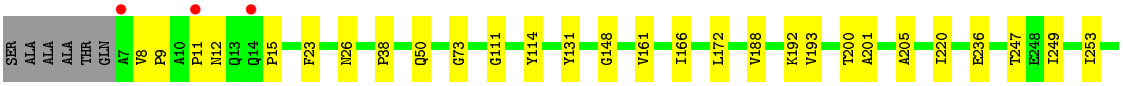


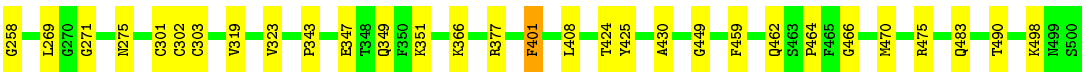
• Molecule 1: Aldehyde dehydrogenase

Chain F:

• Molecule 1: Aldehyde dehydrogenase

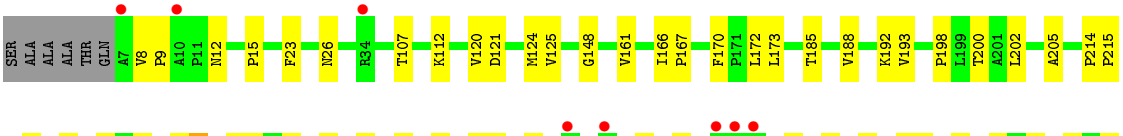
Chain G:

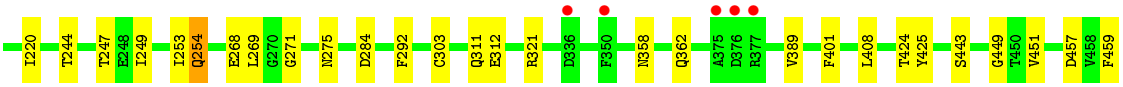




• Molecule 1: Aldehyde dehydrogenase

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	142.13Å 150.57Å 176.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.84 – 2.15 40.24 – 2.14	Depositor EDS
% Data completeness (in resolution range)	91.1 (34.84-2.15) 90.4 (40.24-2.14)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.79 (at 2.14Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.170 , 0.206 0.170 , 0.205	Depositor DCC
R_{free} test set	9407 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	13.6	Xtriage
Anisotropy	1.212	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	7 of 188580 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	34568	wwPDB-VP
Average B, all atoms (Å^2)	19.0	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 54.54 % 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 3.6010e-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: MG, CRD, NAD, NA, EDO, 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	0.33	0/3888	0.58	0/5275
1	B	0.34	0/3888	0.58	0/5275
1	C	0.34	0/3897	0.59	0/5287
1	D	0.33	0/3888	0.59	0/5275
1	E	0.34	0/3888	0.58	0/5275
1	F	0.33	0/3888	0.59	0/5275
1	G	0.33	0/3888	0.57	0/5275
1	H	0.33	0/3888	0.57	0/5275
All	All	0.33	0/31113	0.58	0/42212

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	3804	0	3749	27	0
1	B	3804	0	3749	35	0
1	C	3813	0	3757	45	0
1	D	3804	0	3749	38	0
1	E	3804	0	3749	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3804	0	3749	35	0
1	G	3804	0	3749	43	0
1	H	3804	0	3749	40	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	B	5	0	6	4	0
4	C	5	0	6	6	0
4	D	5	0	6	5	0
4	E	5	0	6	4	0
4	F	5	0	6	8	0
4	G	5	0	6	9	0
5	A	4	0	5	0	0
5	B	4	0	5	0	0
5	C	4	0	4	0	0
5	D	4	0	5	0	0
5	E	4	0	4	0	0
5	F	4	0	5	0	0
5	G	4	0	4	0	0
5	H	4	0	5	0	0
6	C	8	0	12	0	0
6	D	8	0	12	0	0
6	E	4	0	6	0	0
6	F	4	0	6	0	0
6	G	4	0	6	0	0
6	H	4	0	6	0	0
7	A	44	0	26	0	0
7	B	44	0	26	1	0
7	C	44	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	44	0	26	0	0
7	E	44	0	26	0	0
7	F	44	0	26	0	0
7	G	44	0	26	0	0
7	H	44	0	26	0	0
8	A	454	0	0	4	0
8	B	514	0	0	2	0
8	C	488	0	0	2	0
8	D	458	0	0	3	0
8	E	449	0	0	3	0
8	F	480	0	0	0	0
8	G	440	0	0	3	0
8	H	382	0	0	0	0
All	All	34568	0	30329	284	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 5.

The worst 5 of 284 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:C:302:CYS:SG	4:C:4513:CRD:HC4	1.38	1.64
1:G:302:CYS:SG	4:G:4517:CRD:HC4	1.50	1.52
1:F:302:CYS:SG	4:F:4516:CRD:HC4	1.56	1.46
1:C:302:CYS:SG	4:C:4513:CRD:CC4	2.13	1.37
1:G:302:CYS:SG	4:G:4517:CRD:CC4	2.17	1.32

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	493/500 (99%)	477 (97%)	16 (3%)	0	100	100
1	B	493/500 (99%)	476 (97%)	17 (3%)	0	100	100
1	C	494/500 (99%)	477 (97%)	17 (3%)	0	100	100
1	D	493/500 (99%)	475 (96%)	18 (4%)	0	100	100
1	E	493/500 (99%)	476 (97%)	17 (3%)	0	100	100
1	F	493/500 (99%)	476 (97%)	17 (3%)	0	100	100
1	G	493/500 (99%)	471 (96%)	22 (4%)	0	100	100
1	H	493/500 (99%)	474 (96%)	19 (4%)	0	100	100
All	All	3945/4000 (99%)	3802 (96%)	143 (4%)	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	400/402 (100%)	397 (99%)	3 (1%)	86	91
1	B	400/402 (100%)	396 (99%)	4 (1%)	82	87
1	C	401/402 (100%)	397 (99%)	4 (1%)	82	87
1	D	400/402 (100%)	396 (99%)	4 (1%)	82	87
1	E	400/402 (100%)	398 (100%)	2 (0%)	92	95
1	F	400/402 (100%)	396 (99%)	4 (1%)	82	87
1	G	400/402 (100%)	398 (100%)	2 (0%)	92	95
1	H	400/402 (100%)	396 (99%)	4 (1%)	82	87
All	All	3201/3216 (100%)	3174 (99%)	27 (1%)	86	91

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	192	LYS
1	E	192	LYS

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Mol	Chain	Res	Type
1	H	254	GLN
1	D	206	ASN
1	B	192	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	362	GLN
1	F	499	ASN
1	H	358	ASN
1	F	14	GLN
1	F	89	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 46 ligands modelled in this entry, 16 are monoatomic - leaving 30 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	$\#\|Z\| > 2$
5	GAI	A	4801	-	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAD	A	5501	2	38,48,48	2.18	8 (21%)	47,73,73	1.83	9 (19%)
4	CRD	B	4512	-	4,4,4	0.55	0	3,3,3	2.28	2 (66%)
5	GAI	B	4802	-	0,3,3	0.00	-	0,3,3	0.00	-
7	NAD	B	5502	2	38,48,48	2.29	9 (23%)	47,73,73	1.68	10 (21%)
4	CRD	C	4513	-	4,4,4	0.52	0	3,3,3	2.10	1 (33%)
5	GAI	C	4803	-	0,3,3	0.00	-	0,3,3	0.00	-
6	EDO	C	4902	-	3,3,3	0.50	0	2,2,2	0.41	0
6	EDO	C	4903	-	3,3,3	0.51	0	2,2,2	0.38	0
7	NAD	C	5503	2	38,48,48	2.15	9 (23%)	47,73,73	1.70	7 (14%)
4	CRD	D	4514	-	4,4,4	0.55	0	3,3,3	2.58	2 (66%)
5	GAI	D	4804	-	0,3,3	0.00	-	0,3,3	0.00	-
6	EDO	D	4901	-	3,3,3	0.45	0	2,2,2	0.47	0
6	EDO	D	4904	-	3,3,3	0.46	0	2,2,2	0.39	0
7	NAD	D	5504	2	38,48,48	2.08	8 (21%)	47,73,73	1.99	9 (19%)
4	CRD	E	4515	-	4,4,4	0.57	0	3,3,3	2.34	2 (66%)
5	GAI	E	4805	-	0,3,3	0.00	-	0,3,3	0.00	-
6	EDO	E	4905	-	3,3,3	0.49	0	2,2,2	0.40	0
7	NAD	E	5505	2	38,48,48	2.10	9 (23%)	47,73,73	2.04	8 (17%)
4	CRD	F	4516	-	4,4,4	0.42	0	3,3,3	2.38	2 (66%)
5	GAI	F	4806	-	0,3,3	0.00	-	0,3,3	0.00	-
6	EDO	F	4906	-	3,3,3	0.48	0	2,2,2	0.46	0
7	NAD	F	5506	2	38,48,48	2.14	9 (23%)	47,73,73	1.77	7 (14%)
4	CRD	G	4517	-	4,4,4	0.52	0	3,3,3	2.70	2 (66%)
5	GAI	G	4807	-	0,3,3	0.00	-	0,3,3	0.00	-
6	EDO	G	4907	-	3,3,3	0.52	0	2,2,2	0.41	0
7	NAD	G	5507	2	38,48,48	2.22	8 (21%)	47,73,73	1.62	7 (14%)
5	GAI	H	4808	-	0,3,3	0.00	-	0,3,3	0.00	-
6	EDO	H	4908	-	3,3,3	0.44	0	2,2,2	0.47	0
7	NAD	H	5508	2	38,48,48	2.19	9 (23%)	47,73,73	1.95	9 (19%)

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
5	GAI	A	4801	-	-	0/0/0/0	0/0/0/0
7	NAD	A	5501	2	-	0/22/62/62	0/5/5/5
4	CRD	B	4512	-	-	1/2/2/2	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GAI	B	4802	-	-	0/0/0/0	0/0/0/0
7	NAD	B	5502	2	-	0/22/62/62	0/5/5/5
4	CRD	C	4513	-	-	0/2/2/2	0/0/0/0
5	GAI	C	4803	-	-	0/0/0/0	0/0/0/0
6	EDO	C	4902	-	-	0/1/1/1	0/0/0/0
6	EDO	C	4903	-	-	0/1/1/1	0/0/0/0
7	NAD	C	5503	2	-	0/22/62/62	0/5/5/5
4	CRD	D	4514	-	-	0/2/2/2	0/0/0/0
5	GAI	D	4804	-	-	0/0/0/0	0/0/0/0
6	EDO	D	4901	-	-	0/1/1/1	0/0/0/0
6	EDO	D	4904	-	-	0/1/1/1	0/0/0/0
7	NAD	D	5504	2	-	0/22/62/62	0/5/5/5
4	CRD	E	4515	-	-	1/2/2/2	0/0/0/0
5	GAI	E	4805	-	-	0/0/0/0	0/0/0/0
6	EDO	E	4905	-	-	0/1/1/1	0/0/0/0
7	NAD	E	5505	2	-	0/22/62/62	0/5/5/5
4	CRD	F	4516	-	-	1/2/2/2	0/0/0/0
5	GAI	F	4806	-	-	0/0/0/0	0/0/0/0
6	EDO	F	4906	-	-	0/1/1/1	0/0/0/0
7	NAD	F	5506	2	-	0/22/62/62	0/5/5/5
4	CRD	G	4517	-	-	1/2/2/2	0/0/0/0
5	GAI	G	4807	-	-	0/0/0/0	0/0/0/0
6	EDO	G	4907	-	-	0/1/1/1	0/0/0/0
7	NAD	G	5507	2	-	0/22/62/62	0/5/5/5
5	GAI	H	4808	-	-	0/0/0/0	0/0/0/0
6	EDO	H	4908	-	-	0/1/1/1	0/0/0/0
7	NAD	H	5508	2	-	0/22/62/62	0/5/5/5

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	5507	NAD	C3N-C7N	-10.28	1.34	1.50
7	B	5502	NAD	C3N-C7N	-10.12	1.34	1.50
7	A	5501	NAD	C3N-C7N	-9.66	1.35	1.50
7	C	5503	NAD	C3N-C7N	-9.64	1.35	1.50
7	H	5508	NAD	C3N-C7N	-9.55	1.35	1.50

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	E	5505	NAD	N3A-C2A-N1A	-8.81	122.15	128.89
7	H	5508	NAD	N3A-C2A-N1A	-8.59	122.32	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	5504	NAD	N3A-C2A-N1A	-8.17	122.64	128.89
7	A	5501	NAD	N3A-C2A-N1A	-7.78	122.94	128.89
7	F	5506	NAD	N3A-C2A-N1A	-7.68	123.01	128.89

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	4515	CRD	OC1-CC4-CC3-CC2
4	B	4512	CRD	OC1-CC4-CC3-CC2
4	F	4516	CRD	OC1-CC4-CC3-CC2
4	G	4517	CRD	OC1-CC4-CC3-CC2

There are no ring outliers.

7 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	4512	CRD	4	0
7	B	5502	NAD	1	0
4	C	4513	CRD	6	0
4	D	4514	CRD	5	0
4	E	4515	CRD	4	0
4	F	4516	CRD	8	0
4	G	4517	CRD	9	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.30	4 (0%) 87 90	8, 18, 31, 47	0
1	B	494/500 (98%)	-0.48	1 (0%) 95 96	9, 15, 24, 39	0
1	C	495/500 (99%)	-0.49	2 (0%) 93 94	9, 15, 24, 42	1 (0%)
1	D	494/500 (98%)	-0.41	3 (0%) 90 92	9, 16, 28, 48	0
1	E	494/500 (98%)	-0.40	2 (0%) 93 94	9, 16, 28, 51	0
1	F	494/500 (98%)	-0.53	0 100 100	8, 15, 25, 36	0
1	G	494/500 (98%)	-0.32	3 (0%) 90 92	12, 18, 31, 53	0
1	H	494/500 (98%)	-0.10	8 (1%) 74 81	11, 21, 36, 53	0
All	All	3953/4000 (98%)	-0.38	23 (0%) 90 92	8, 17, 30, 53	1 (0%)

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	376	ASP	5.5
1	G	7	ALA	4.8
1	B	7	ALA	4.4
1	H	7	ALA	4.1
1	H	10	ALA	3.8

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 (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
4	CRD	G	4517	5/5	0.65	0.40	22.67	41,42,46,48	0
4	CRD	E	4515	5/5	0.81	0.41	19.91	48,49,50,53	0
4	CRD	C	4513	5/5	0.74	0.47	19.74	44,46,47,49	0
4	CRD	D	4514	5/5	0.69	0.43	13.28	47,47,48,48	0
4	CRD	B	4512	5/5	0.76	0.44	12.46	44,46,47,48	0
4	CRD	F	4516	5/5	0.87	0.35	9.17	44,44,46,47	0
3	NA	E	4705	1/1	0.87	0.13	4.73	27,27,27,27	0
6	EDO	C	4902	4/4	0.96	0.10	4.36	18,22,24,24	0
5	GAI	H	4808	4/4	0.89	0.14	2.89	22,23,25,25	0
5	GAI	A	4801	4/4	0.90	0.13	2.80	15,16,18,20	0
6	EDO	H	4908	4/4	0.89	0.14	2.62	24,27,27,27	0
5	GAI	F	4806	4/4	0.92	0.11	2.48	18,18,19,20	0
3	NA	F	4706	1/1	0.98	0.14	2.29	21,21,21,21	0
6	EDO	F	4906	4/4	0.95	0.11	2.25	20,23,23,23	0
6	EDO	D	4901	4/4	0.96	0.12	1.94	20,21,24,24	0
5	GAI	D	4804	4/4	0.91	0.13	1.92	13,18,20,21	0
5	GAI	B	4802	4/4	0.94	0.10	1.34	17,19,20,21	0
6	EDO	E	4905	4/4	0.97	0.12	1.10	18,22,22,23	0
5	GAI	E	4805	4/4	0.93	0.11	0.93	20,20,22,23	0
7	NAD	D	5504	44/44	0.93	0.12	0.59	11,22,35,36	0
7	NAD	H	5508	44/44	0.90	0.13	0.57	19,34,43,44	0
7	NAD	E	5505	44/44	0.94	0.11	0.49	13,23,34,34	0
3	NA	B	4702	1/1	0.97	0.10	0.45	18,18,18,18	0
5	GAI	G	4807	4/4	0.96	0.10	0.42	21,22,23,24	0
6	EDO	D	4904	4/4	0.96	0.11	0.32	14,16,17,18	0
6	EDO	G	4907	4/4	0.97	0.09	0.26	22,22,23,24	0
7	NAD	G	5507	44/44	0.94	0.12	0.23	16,30,39,40	0
5	GAI	C	4803	4/4	0.95	0.08	0.04	17,18,19,20	0
7	NAD	A	5501	44/44	0.94	0.11	0.04	14,24,37,37	0
7	NAD	C	5503	44/44	0.95	0.11	-0.03	9,23,31,32	0
3	NA	D	4704	1/1	0.93	0.10	-0.28	24,24,24,24	0
7	NAD	B	5502	44/44	0.95	0.09	-0.43	15,26,33,34	0
7	NAD	F	5506	44/44	0.97	0.09	-0.54	8,19,29,30	0
6	EDO	C	4903	4/4	0.97	0.07	-0.62	16,16,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NA	C	4703	1/1	0.96	0.07	-0.92	18,18,18,18	0
3	NA	A	4701	1/1	0.88	0.08	-1.04	31,31,31,31	0
3	NA	H	4708	1/1	0.95	0.09	-1.62	27,27,27,27	0
3	NA	G	4707	1/1	0.97	0.06	-3.16	19,19,19,19	0
2	MG	E	4605	1/1	0.75	0.18	-	48,48,48,48	0
2	MG	C	4603	1/1	0.84	0.27	-	39,39,39,39	0
2	MG	D	4604	1/1	0.85	0.25	-	43,43,43,43	0
2	MG	A	4601	1/1	0.74	0.10	-	47,47,47,47	0
2	MG	F	4606	1/1	0.80	0.31	-	40,40,40,40	0
2	MG	H	4608	1/1	0.93	0.09	-	32,32,32,32	0
2	MG	B	4602	1/1	0.77	0.18	-	37,37,37,37	0
2	MG	G	4607	1/1	0.91	0.23	-	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.