W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Feb 26, 2014 – 08:08 PM GMT

PDB ID : 1T2F
Title : Human B lactate dehydrogenase complexed with NAD+ and 4-hydroxy-1,2,5
-oxadiazole-3-carboxylicacid
Authors : Cameron, A.; Read, J.; Tranter, R.; Winter, V.J.; Sessions, R.B.; Brady, R.L.;
Vivas, L.; Easton, A.; Kendrick, H.; Croft, S.L.; Barros, D.; Lavandera, J.L.;
Martin, J.J.; Risco, F.; Garcia-Ochoa, S.; Gamo, F.J.; Sanz, L.; Leon, L.;
Ruiz, J.R.; Gabarro, R.; Mallo, A.; De Las Heras, F.G.
Deposited on : 2004-04-21
Resolution : 3.00 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html

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

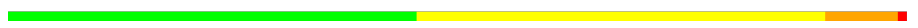|		
MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1   Overall quality at a glance ⓘ

The reported resolution of this entry is 3.00 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	Percentile Ranks	Value
Rfree		0.295
Clashscore		24
Ramachandran outliers		3.8%
Sidechain outliers		16.1%
RSRZ outliers		0

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
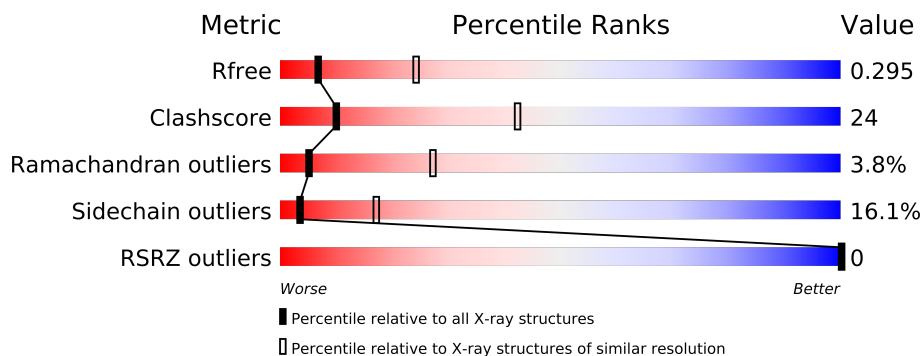
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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	333	
1	B	333	
1	C	333	
1	D	333	

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 10665 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 L-lactate dehydrogenase B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total 2555	C 1627	N 430	O 484	S 14	51	0	0
1	B	332	Total 2555	C 1627	N 430	O 484	S 14	71	0	0
1	C	332	Total 2555	C 1627	N 430	O 484	S 14	65	0	0
1	D	332	Total 2555	C 1627	N 430	O 484	S 14	78	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	PHE	ASP	ENGINEERED	UNP P07195
B	332	PHE	ASP	ENGINEERED	UNP P07195
C	332	PHE	ASP	ENGINEERED	UNP P07195
D	332	PHE	ASP	ENGINEERED	UNP P07195

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).

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

- Molecule 3 is 4-HYDROXY-1,2,5-OXADIAZOLE-3-CARBOXYLICACID (three-letter code: OXQ) (formula: $C_3H_2N_2O_4$).
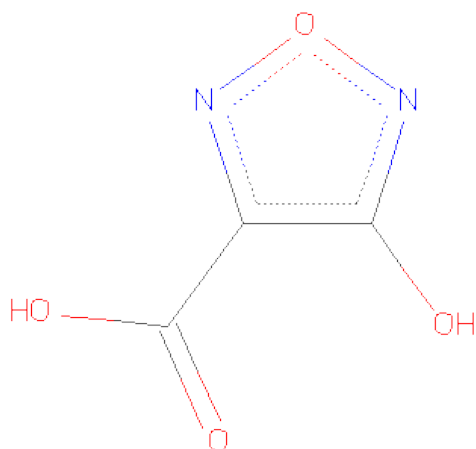
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 9	C 3	N 2	O 4	0	0
3	B	1	Total 9	C 3	N 2	O 4	0	0
3	C	1	Total 9	C 3	N 2	O 4	0	0
3	D	1	Total 9	C 3	N 2	O 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	66	Total 66	O 66	0	0
4	B	76	Total 76	O 76	0	0
4	C	48	Total 48	O 48	0	0
4	D	43	Total 43	O 43	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.
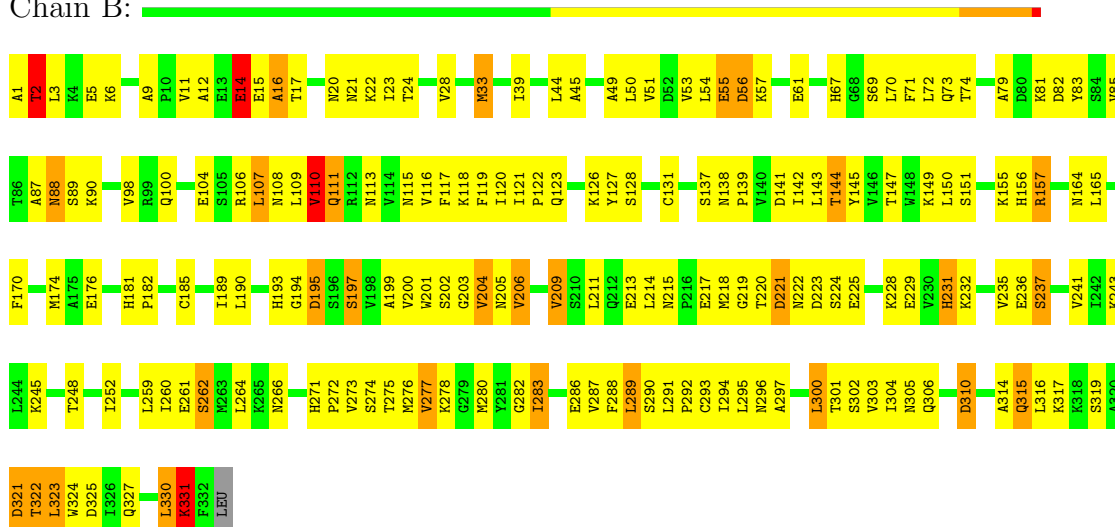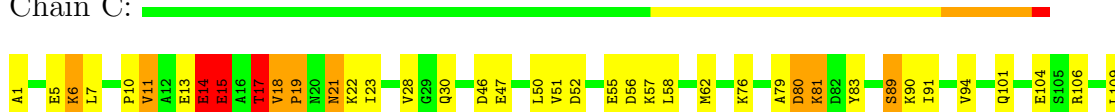
• Molecule 1: L-lactate dehydrogenase B chain

Chain A:
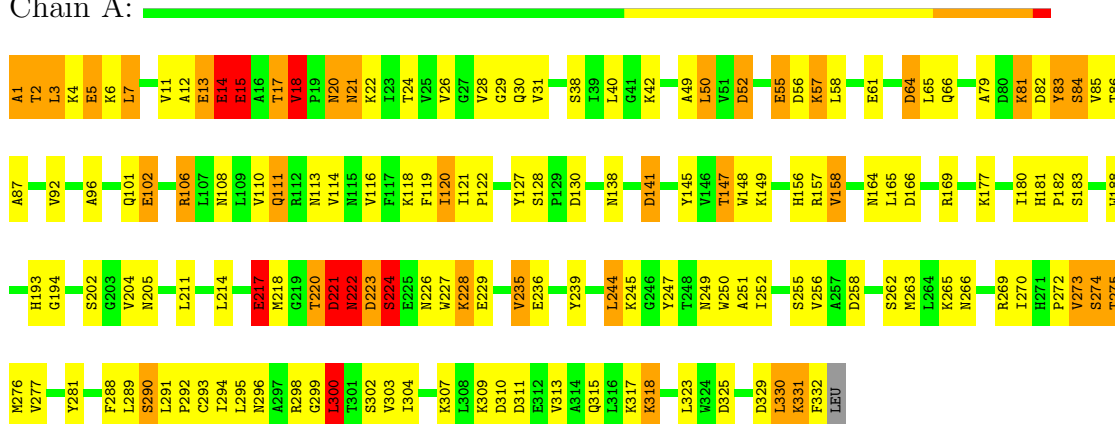
• Molecule 1: L-lactate dehydrogenase B chain
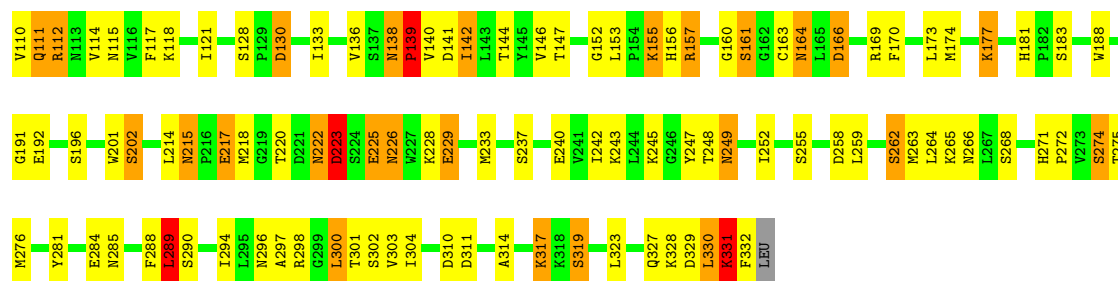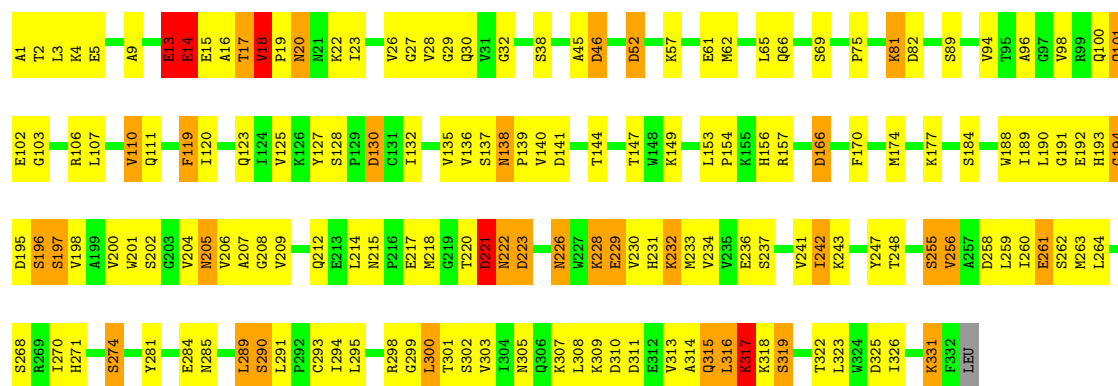
Chain B:

• Molecule 1: L-lactate dehydrogenase B chain

Chain C:

• Molecule 1: L-lactate dehydrogenase B chain

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	137.40Å 160.44Å 59.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 3.00 28.90 – 2.99	Depositor EDS
% Data completeness (in resolution range)	90.5 (29.88-3.00) 90.3 (28.90-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.215 , 0.321 0.201 , 0.295	Depositor DCC
R_{free} test set	1242 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	37.1	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 43.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.42, < L^2 > = 0.24$	Xtriage
Outliers	1 of 24666 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10665	wwPDB-VP
Average B, all atoms (Å^2)	56.0	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 46.79 % 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 1.0889e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities 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: OXQ, NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	1.26	8/2597 (0.3%)	1.28	18/3520 (0.5%)
1	B	1.19	6/2597 (0.2%)	1.19	24/3520 (0.7%)
1	C	1.24	8/2597 (0.3%)	1.28	29/3520 (0.8%)
1	D	1.49	13/2597 (0.5%)	1.52	36/3520 (1.0%)
All	All	1.30	35/10388 (0.3%)	1.32	107/14080 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2
1	B	1	3
1	C	2	2
1	D	4	0
All	All	8	7

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	14	GLU	CA-CB	-33.15	0.81	1.53
1	D	119	PHE	CB-CG	29.10	2.00	1.51
1	A	222	ASN	CA-CB	27.49	2.24	1.53
1	D	318	LYS	CA-CB	-27.04	0.94	1.53
1	D	217	GLU	CB-CG	-26.53	1.01	1.52

The worst 5 of 107 bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	221	ASP	CA-CB-CG	27.37	173.62	113.40
1	D	318	LYS	CA-CB-CG	27.25	173.35	113.40
1	D	119	PHE	CB-CG-CD2	20.86	135.40	120.80
1	A	221	ASP	N-CA-CB	20.71	147.88	110.60
1	D	331	LYS	N-CA-CB	20.29	147.12	110.60

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	221	ASP	CA
1	B	222	ASN	CA
1	C	6	LYS	CA
1	C	284	GLU	CA
1	D	221	ASP	CA

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	ALA	Peptide
1	A	15	GLU	Peptide
1	B	1	ALA	Peptide
1	B	139	PRO	Peptide
1	B	222	ASN	Peptide

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	2555	0	2627	126	4
1	B	2555	0	2627	149	4
1	C	2555	0	2627	113	3
1	D	2555	0	2627	109	3
2	A	44	0	26	1	0
2	B	44	0	26	4	0
2	C	44	0	26	4	0
2	D	44	0	26	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	9	0	0	1	0
3	B	9	0	0	1	0
3	C	9	0	0	3	0
3	D	9	0	0	2	0
4	A	66	0	0	17	0
4	B	76	0	0	34	0
4	C	48	0	0	27	0
4	D	43	0	0	13	0
All	All	10665	0	10612	485	7

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 24.

The worst 5 of 485 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:294:ILE:HB	4:C:452:HOH:O	1.29	1.24
1:B:324:TRP:HB3	4:B:456:HOH:O	1.38	1.23
1:C:152:GLY:HA3	4:C:454:HOH:O	1.42	1.18
1:C:302:SER:HB2	4:C:452:HOH:O	1.49	1.12
1:A:229:GLU:HG3	4:A:456:HOH:O	1.48	1.10

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:149:LYS:CA	1:B:14:GLU:OE2[1_554]	1.19	1.01
1:C:14:GLU:OE1	1:D:149:LYS:NZ[1_554]	1.69	0.51
1:A:148:TRP:O	1:B:14:GLU:OE1[1_554]	1.75	0.45
1:A:149:LYS:C	1:B:14:GLU:OE2[1_554]	1.78	0.42
1:C:14:GLU:OE2	1:D:149:LYS:NZ[1_554]	1.82	0.38

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	330/333 (99%)	272 (82%)	45 (14%)	13 (4%)	5	26
1	B	330/333 (99%)	264 (80%)	51 (16%)	15 (4%)	4	22
1	C	330/333 (99%)	275 (83%)	45 (14%)	10 (3%)	7	34
1	D	330/333 (99%)	269 (82%)	49 (15%)	12 (4%)	5	29
All	All	1320/1332 (99%)	1080 (82%)	190 (14%)	50 (4%)	5	27

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	221	ASP
1	A	222	ASN
1	A	224	SER
1	A	226	ASN

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	288/289 (100%)	236 (82%)	52 (18%)	2	13
1	B	288/289 (100%)	248 (86%)	40 (14%)	5	23
1	C	288/289 (100%)	241 (84%)	47 (16%)	3	17
1	D	288/289 (100%)	241 (84%)	47 (16%)	3	17
All	All	1152/1156 (100%)	966 (84%)	186 (16%)	3	17

5 of 186 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	295	LEU
1	C	81	LYS
1	D	261	GLU
1	B	310	ASP
1	C	11	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	315	GLN
1	C	181	HIS
1	D	266	ASN
1	C	21	ASN
1	C	108	ASN

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 ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	NAD	A	401	-	48,48,48	1.61	5 (10%)	73,73,73	2.03	16 (21%)
3	OXQ	A	402	-	7,9,9	1.93	3 (42%)	6,12,12	1.68	2 (33%)
2	NAD	B	403	-	48,48,48	1.66	3 (6%)	73,73,73	2.73	18 (24%)
3	OXQ	B	404	-	7,9,9	2.26	3 (42%)	6,12,12	1.95	2 (33%)
2	NAD	C	405	-	48,48,48	1.58	7 (14%)	73,73,73	2.17	12 (16%)
3	OXQ	C	406	-	7,9,9	1.88	2 (28%)	6,12,12	0.99	0
2	NAD	D	407	-	48,48,48	1.71	5 (10%)	73,73,73	2.06	14 (19%)
3	OXQ	D	408	-	7,9,9	2.16	4 (57%)	6,12,12	2.30	2 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	401	-	-	0/30/62/62	0/3/5/5
3	OXQ	A	402	-	-	1/3/4/4	0/0/1/1
2	NAD	B	403	-	-	0/30/62/62	0/3/5/5
3	OXQ	B	404	-	-	1/3/4/4	0/0/1/1
2	NAD	C	405	-	-	0/30/62/62	0/3/5/5
3	OXQ	C	406	-	-	1/3/4/4	0/0/1/1
2	NAD	D	407	-	-	0/30/62/62	0/3/5/5
3	OXQ	D	408	-	-	1/3/4/4	0/0/1/1

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	403	NAD	O7N-C7N	8.36	1.43	1.24
2	D	407	NAD	O7N-C7N	7.99	1.42	1.24
2	A	401	NAD	O7N-C7N	7.52	1.41	1.24
2	C	405	NAD	O7N-C7N	5.94	1.38	1.24
2	D	407	NAD	C2A-N3A	5.09	1.42	1.32

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	403	NAD	N3A-C2A-N1A	-14.48	116.60	128.71
2	B	403	NAD	O4B-C1B-N9A	10.08	117.81	108.44
2	C	405	NAD	N3A-C2A-N1A	-8.94	121.23	128.71
2	D	407	NAD	O4B-C1B-N9A	8.85	116.67	108.44
2	A	401	NAD	N3A-C2A-N1A	-8.38	121.70	128.71

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	404	OXQ	O9-C6-C2-C1
3	C	406	OXQ	O9-C6-C2-C1
3	A	402	OXQ	O9-C6-C2-C1
3	D	408	OXQ	O9-C6-C2-C1

There are no ring outliers.

5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	332/333 (99%)	-0.46	0	100	100	37, 50, 82, 93	11 (3%)
1	B	332/333 (99%)	-0.36	0	100	100	38, 61, 85, 90	15 (4%)
1	C	332/333 (99%)	-0.44	0	100	100	37, 54, 84, 92	14 (4%)
1	D	332/333 (99%)	-0.44	0	100	100	37, 53, 85, 93	18 (5%)
All	All	1328/1332 (99%)	-0.42	0	100	100	37, 54, 84, 93	58 (4%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	OXQ	A	402	9/9	0.16	1.02	63,64,65,65	0
3	OXQ	D	408	9/9	0.17	0.81	63,65,67,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å²)	Q<0.9
3	OXQ	C	406	9/9	0.17	0.70	56,58,59,59	0
3	OXQ	B	404	9/9	0.18	0.33	53,56,60,62	0
2	NAD	A	401	44/44	0.14	0.12	29,40,50,51	0
2	NAD	C	405	44/44	0.14	-0.38	33,43,52,57	0
2	NAD	B	403	44/44	0.16	-0.40	46,61,84,87	0
2	NAD	D	407	44/44	0.12	-0.93	33,42,47,49	0

6.5 Other polymers ⓘ

There are no such residues in this entry.