



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:34 PM GMT

PDB ID : 1U7T
Title : Crystal Structure of ABAD/HSD10 with a Bound Inhibitor
Authors : Kissinger, C.R.; Rejto, P.A.; Pelletier, L.A.; Showalter, R.E.; Villafranca, J.E.
Deposited on : 2004-08-04
Resolution : 2.00 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

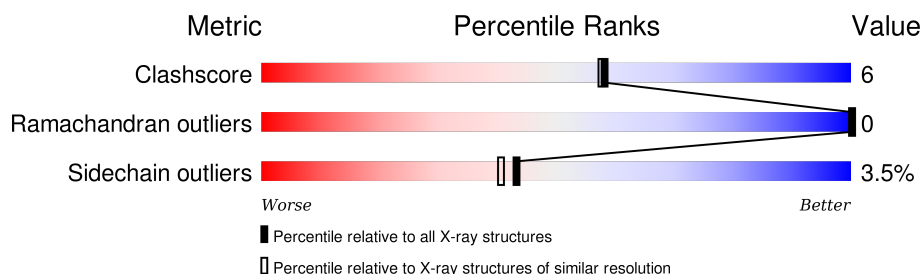
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (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. 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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	261	 88% 8% ..
1	B	261	 83% 14% ..
1	C	261	 84% 13% ..
1	D	261	 85% 11% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7760 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.

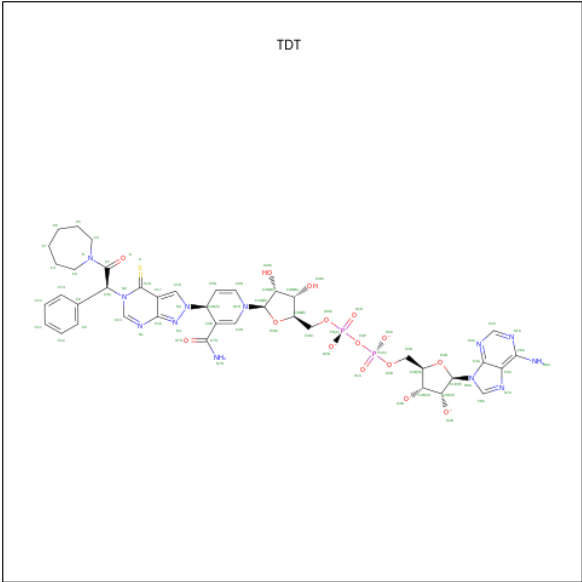
- Molecule 1 is a protein called 3-hydroxyacyl-CoA dehydrogenase type II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			1806	1138	316	345	7			
1	B	255	Total	C	N	O	S	0	0	0
			1806	1138	316	345	7			
1	C	255	Total	C	N	O	S	0	0	0
			1806	1138	316	345	7			
1	D	255	Total	C	N	O	S	0	0	0
			1806	1138	316	345	7			

There are 4 discrepancies between the modelled and reference sequences:

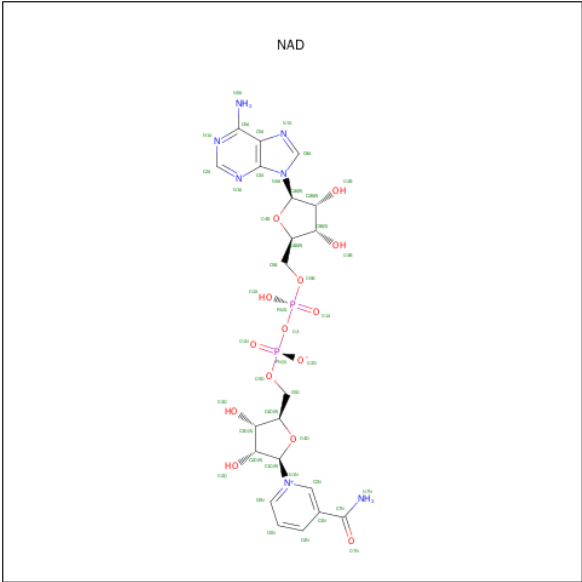
Chain	Residue	Modelled	Actual	Comment	Reference
A	214	ARG	CYS	ENGINEERED	UNP Q99714
B	214	ARG	CYS	ENGINEERED	UNP Q99714
C	214	ARG	CYS	ENGINEERED	UNP Q99714
D	214	ARG	CYS	ENGINEERED	UNP Q99714

- Molecule 2 is 1-AZEPAN-1-YL-2-PHENYL-2-(4-THIOXO-1,4-DIHYDRO-PYRAZOL O[3,4-D]PYRIMIDIN-5-YL)ETHANONE ADDUCT (three-letter code: TDT) (formula: C₄₀H₄₄N₁₂O₁₅P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			70	40	12	15	2	1		
2	C	1	Total	C	N	O	P	S	0	0
			70	40	12	15	2	1		
2	D	1	Total	C	N	O	P	S	0	0
			70	40	12	15	2	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 4 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	66	Total	O	0	0
			66	66		
4	B	63	Total	O	0	0
			63	63		
4	C	75	Total	O	0	0
			75	75		
4	D	78	Total	O	0	0
			78	78		

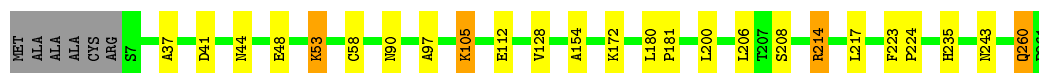
3 Residue-property plots [i](#)

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.


Note EDS was not executed.

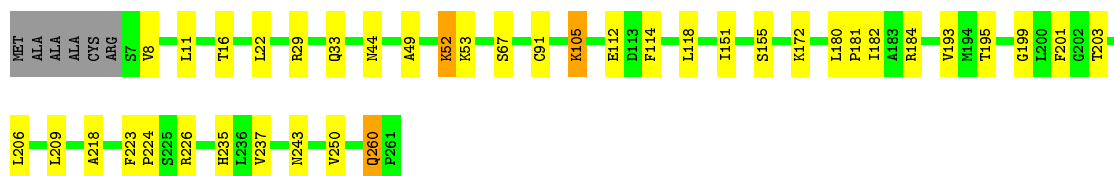
- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase type II

Chain A: 




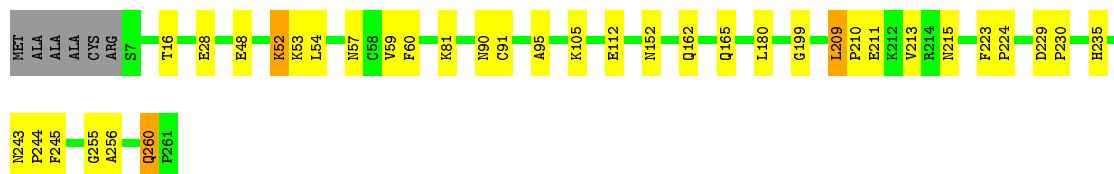
- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase type II

Chain B: 




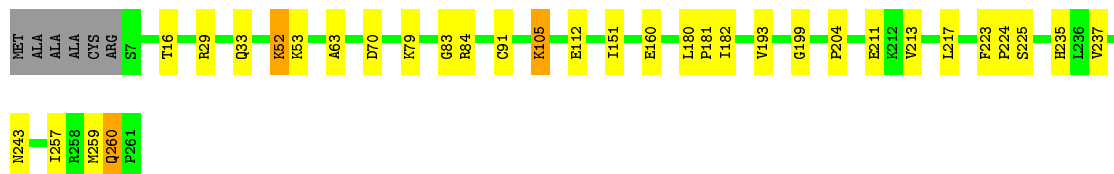
- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase type II

Chain C: 



- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase type II

Chain D: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.00 Å 80.80 Å 110.00 Å 90.00° 105.60° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.215 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7760	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, TDT

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	0.29	0/1832	0.77	1/2495 (0.0%)
1	B	0.31	0/1832	0.77	0/2495
1	C	0.31	0/1832	0.75	0/2495
1	D	0.30	0/1832	0.77	0/2495
All	All	0.30	0/7328	0.76	1/9980 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	ARG	NE-CZ-NH2	-5.09	117.76	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1806	0	1802	17	0
1	B	1806	0	1802	31	0
1	C	1806	0	1802	27	0
1	D	1806	0	1802	24	0
2	A	70	0	44	2	0
2	C	70	0	44	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	70	0	44	2	0
3	B	44	0	26	3	0
4	A	66	0	0	0	0
4	B	63	0	0	0	0
4	C	75	0	0	1	0
4	D	78	0	0	1	0
All	All	7760	0	7366	87	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 6.

All (87) 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:D:213:VAL:HG12	1:D:217:LEU:HD11	1.61	0.81
1:B:8:VAL:HA	1:B:11:LEU:HD12	1.70	0.73
1:B:199:GLY:O	3:B:502:NAD:H4N	1.92	0.69
1:A:206:LEU:O	1:A:214:ARG:HD2	1.97	0.64
1:C:211:GLU:HG3	1:C:215:ASN:ND2	2.12	0.64
1:B:235:HIS:HD2	1:C:243:ASN:HD22	1.45	0.63
1:C:16:THR:O	1:C:91:CYS:HB2	1.99	0.62
1:D:213:VAL:HG12	1:D:217:LEU:CD1	2.27	0.62
1:A:243:ASN:HD22	1:D:235:HIS:HD2	1.45	0.62
1:B:243:ASN:HD22	1:C:235:HIS:HD2	1.45	0.62
1:B:16:THR:O	1:B:91:CYS:HB2	2.00	0.61
1:D:199:GLY:O	2:D:504:TDT:H4N	2.00	0.61
1:C:52:LYS:HE2	1:C:53:LYS:N	2.15	0.60
1:D:29:ARG:O	1:D:33:GLN:HG2	2.02	0.59
1:B:235:HIS:CD2	1:C:243:ASN:HD22	2.21	0.59
1:B:49:ALA:O	1:B:52:LYS:HE2	2.03	0.59
1:C:52:LYS:HE2	1:C:53:LYS:CA	2.34	0.58
1:A:260:GLN:NE2	1:A:260:GLN:HA	2.18	0.57
1:C:48:GLU:OE2	1:C:60:PHE:HD2	1.88	0.57
1:B:203:THR:HG21	3:B:502:NAD:O1N	2.06	0.56
1:B:218:ALA:HB1	1:B:226:ARG:HA	1.87	0.56
1:D:182:ILE:HG22	1:D:193:VAL:HG21	1.90	0.54
1:C:223:PHE:CD1	1:C:224:PRO:HA	2.42	0.54
1:A:223:PHE:CD1	1:A:224:PRO:HA	2.43	0.53
1:B:29:ARG:O	1:B:33:GLN:HG2	2.09	0.52
1:D:63:ALA:HB1	1:D:70:ASP:HB3	1.91	0.52
1:D:223:PHE:CD1	1:D:224:PRO:HA	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:LEU:HA	1:B:209:LEU:HD12	1.92	0.52
1:C:210:PRO:HB2	1:C:213:VAL:HG23	1.91	0.51
1:C:209:LEU:HD21	2:C:503:TDT:C9	2.40	0.51
1:B:260:GLN:HA	1:B:260:GLN:NE2	2.25	0.51
1:B:180:LEU:HG	1:B:184:ARG:HD2	1.93	0.51
1:D:151:ILE:HD12	1:D:237:VAL:HG13	1.94	0.50
1:B:260:GLN:HG2	1:D:260:GLN:HG2	1.92	0.50
1:B:223:PHE:CD1	1:B:224:PRO:HA	2.47	0.50
1:A:243:ASN:HD22	1:D:235:HIS:CD2	2.27	0.50
1:A:154:ALA:HA	1:A:172:LYS:HD2	1.94	0.50
1:A:235:HIS:CD2	1:D:243:ASN:HB2	2.47	0.50
1:B:151:ILE:HD12	1:B:237:VAL:HG13	1.94	0.49
1:B:201:PHE:O	1:B:206:LEU:HD12	2.13	0.49
1:B:22:LEU:HD12	3:B:502:NAD:O4D	2.13	0.48
1:D:52:LYS:HE2	1:D:53:LYS:N	2.29	0.48
1:B:8:VAL:HA	1:B:11:LEU:CD1	2.39	0.47
1:A:105:LYS:HB3	1:A:105:LYS:HE3	1.42	0.47
1:D:16:THR:O	1:D:91:CYS:HB2	2.14	0.47
1:A:243:ASN:HB2	1:D:235:HIS:CD2	2.50	0.47
1:C:180:LEU:HD23	1:D:160:GLU:HA	1.97	0.47
1:B:243:ASN:HD22	1:C:235:HIS:CD2	2.31	0.46
1:B:114:PHE:CE1	1:B:118:LEU:HD11	2.50	0.46
1:B:206:LEU:HA	1:B:209:LEU:CD1	2.45	0.46
1:C:162:GLN:O	1:C:165:GLN:HB2	2.15	0.46
1:B:52:LYS:HE2	1:B:53:LYS:N	2.31	0.45
1:B:182:ILE:HG22	1:B:193:VAL:HG21	1.98	0.45
1:C:52:LYS:HE2	1:C:53:LYS:HA	1.98	0.45
1:C:255:GLY:O	1:C:256:ALA:HB3	2.17	0.45
1:C:210:PRO:O	1:C:213:VAL:HB	2.16	0.45
1:C:210:PRO:O	1:C:213:VAL:N	2.50	0.45
1:A:97:ALA:HB2	2:A:501:TDT:H13	1.99	0.45
1:B:260:GLN:HG2	1:D:260:GLN:CG	2.47	0.45
1:C:90:ASN:OD1	1:C:152:ASN:ND2	2.50	0.45
1:A:37:ALA:O	1:A:58:CYS:HA	2.17	0.45
1:D:257:ILE:HD13	1:D:259:MET:SD	2.58	0.44
1:A:200:LEU:HD13	1:A:217:LEU:HB3	2.00	0.44
1:B:105:LYS:HE2	1:B:105:LYS:HB3	1.33	0.44
1:A:53:LYS:HE2	1:A:53:LYS:HB3	1.30	0.43
1:D:204:PRO:HD2	2:D:504:TDT:O2A	2.18	0.42
1:D:180:LEU:N	1:D:181:PRO:HD2	2.33	0.42
1:C:199:GLY:O	2:C:503:TDT:H4N	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:THR:HB	1:B:250:VAL:HG22	2.00	0.42
1:A:90:ASN:HD21	1:A:128:VAL:HB	1.85	0.42
2:C:503:TDT:H15	4:C:538:HOH:O	2.19	0.42
1:D:105:LYS:HE2	1:D:105:LYS:HB3	1.22	0.42
1:B:155:SER:HB3	1:B:172:LYS:HG3	2.01	0.42
1:B:180:LEU:N	1:B:181:PRO:HD2	2.35	0.42
1:C:229:ASP:OD2	1:C:230:PRO:HD2	2.20	0.42
1:A:180:LEU:N	1:A:181:PRO:HD2	2.34	0.41
1:A:260:GLN:HG2	1:C:260:GLN:CD	2.40	0.41
1:C:57:ASN:HA	1:C:57:ASN:HD22	1.70	0.41
1:C:95:ALA:HB1	2:C:503:TDT:H15	2.03	0.41
1:C:28:GLU:HG2	1:C:54:LEU:HD21	2.03	0.41
1:A:41:ASP:OD2	2:A:501:TDT:O3B	2.39	0.41
1:B:260:GLN:NE2	1:D:260:GLN:NE2	2.69	0.41
1:B:114:PHE:HE1	1:B:118:LEU:HD11	1.85	0.40
1:D:79:LYS:O	1:D:83:GLY:N	2.50	0.40
1:C:59:VAL:HG11	1:C:81:LYS:HE2	2.04	0.40
1:C:243:ASN:HA	1:C:244:PRO:HD3	1.86	0.40
1:D:84:ARG:HD2	4:D:579:HOH:O	2.22	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	253/261 (97%)	242 (96%)	11 (4%)	0	100	100
1	B	253/261 (97%)	244 (96%)	9 (4%)	0	100	100
1	C	253/261 (97%)	241 (95%)	12 (5%)	0	100	100
1	D	253/261 (97%)	241 (95%)	12 (5%)	0	100	100
All	All	1012/1044 (97%)	968 (96%)	44 (4%)	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	180/195 (92%)	173 (96%)	7 (4%)	39	35
1	B	180/195 (92%)	174 (97%)	6 (3%)	45	43
1	C	180/195 (92%)	174 (97%)	6 (3%)	45	43
1	D	180/195 (92%)	174 (97%)	6 (3%)	45	43
All	All	720/780 (92%)	695 (96%)	25 (4%)	43	40

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	48	GLU
1	A	53	LYS
1	A	105	LYS
1	A	112	GLU
1	A	208	SER
1	A	260	GLN
1	B	44	ASN
1	B	52	LYS
1	B	67	SER
1	B	105	LYS
1	B	112	GLU
1	B	260	GLN
1	C	52	LYS
1	C	105	LYS
1	C	112	GLU
1	C	209	LEU
1	C	245	PHE
1	C	260	GLN
1	D	52	LYS
1	D	105	LYS
1	D	112	GLU

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Mol	Chain	Res	Type
1	D	211	GLU
1	D	225	SER
1	D	260	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	56	ASN
1	A	90	ASN
1	A	152	ASN
1	A	235	HIS
1	A	260	GLN
1	B	50	GLN
1	B	56	ASN
1	B	57	ASN
1	B	90	ASN
1	B	152	ASN
1	B	235	HIS
1	C	50	GLN
1	C	56	ASN
1	C	57	ASN
1	C	90	ASN
1	C	152	ASN
1	C	215	ASN
1	C	235	HIS
1	C	260	GLN
1	D	50	GLN
1	D	56	ASN
1	D	57	ASN
1	D	90	ASN
1	D	152	ASN
1	D	215	ASN
1	D	235	HIS
1	D	260	GLN

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 ⓘ

4 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	TDT	A	501	-	64,78,78	2.32	13 (20%)	65,117,117	1.24	7 (10%)
3	NAD	B	502	-	38,48,48	1.89	3 (7%)	47,73,73	2.08	8 (17%)
2	TDT	C	503	-	64,78,78	2.34	13 (20%)	65,117,117	1.47	7 (10%)
2	TDT	D	504	-	64,78,78	2.29	13 (20%)	65,117,117	1.36	7 (10%)

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	TDT	A	501	-	-	0/36/104/104	0/9/9/9
3	NAD	B	502	-	-	0/22/62/62	0/5/5/5
2	TDT	C	503	-	-	0/36/104/104	0/9/9/9
2	TDT	D	504	-	-	0/36/104/104	0/9/9/9

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	503	TDT	C4N-C5N	2.03	1.55	1.49
2	A	501	TDT	C16-N4	2.08	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	504	TDT	C-N2	2.09	1.54	1.49
2	D	504	TDT	C16-N4	2.12	1.38	1.34
2	A	501	TDT	C-N2	2.22	1.54	1.49
2	C	503	TDT	C-N2	2.22	1.54	1.49
2	D	504	TDT	C5A-C4A	2.37	1.45	1.40
2	A	501	TDT	C5A-C4A	2.42	1.46	1.40
2	C	503	TDT	C5A-C4A	2.77	1.46	1.40
2	D	504	TDT	O4B-C1B	2.89	1.44	1.41
2	D	504	TDT	C1-N	3.11	1.39	1.34
2	C	503	TDT	C6N-N1N	3.16	1.46	1.37
2	A	501	TDT	C6N-N1N	3.19	1.46	1.37
2	C	503	TDT	C1-N	3.24	1.39	1.34
2	D	504	TDT	C6N-N1N	3.27	1.47	1.37
2	A	501	TDT	C1-N	3.27	1.39	1.34
2	A	501	TDT	O4B-C1B	3.33	1.45	1.41
3	B	502	NAD	O4D-C1D	3.62	1.45	1.41
2	C	503	TDT	C19-N3	3.74	1.39	1.35
2	A	501	TDT	C19-N3	3.88	1.40	1.35
2	C	503	TDT	O4B-C1B	4.05	1.46	1.41
2	D	504	TDT	C19-N3	4.16	1.40	1.35
2	D	504	TDT	C16-N1	4.73	1.45	1.37
2	A	501	TDT	C16-N1	4.74	1.45	1.37
2	C	503	TDT	C16-N1	4.80	1.45	1.37
2	D	504	TDT	C8-C	5.18	1.57	1.52
2	D	504	TDT	C18-S	5.23	1.77	1.67
2	C	503	TDT	C18-S	5.49	1.78	1.67
2	D	504	TDT	C-C1	5.51	1.60	1.54
2	A	501	TDT	C8-C	5.52	1.57	1.52
2	C	503	TDT	C8-C	5.53	1.57	1.52
2	A	501	TDT	C18-S	5.60	1.78	1.67
2	C	503	TDT	C-C1	5.60	1.60	1.54
2	A	501	TDT	C-C1	5.86	1.60	1.54
3	B	502	NAD	C5N-C4N	6.04	1.51	1.38
2	A	501	TDT	C4A-N3A	7.26	1.46	1.35
2	C	503	TDT	C4A-N3A	7.32	1.46	1.35
2	D	504	TDT	C4A-N3A	7.39	1.46	1.35
3	B	502	NAD	C4N-C3N	7.53	1.52	1.39
2	D	504	TDT	C18-C17	8.20	1.55	1.41
2	C	503	TDT	C18-C17	8.26	1.55	1.41
2	A	501	TDT	C18-C17	8.27	1.55	1.41

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	NAD	N3A-C2A-N1A	-8.81	122.15	128.89
3	B	502	NAD	C5N-C4N-C3N	-5.80	113.04	120.33
2	C	503	TDT	C4B-O4B-C1B	-4.36	104.93	109.72
2	C	503	TDT	C3N-C2N-N1N	-4.28	119.41	122.84
2	D	504	TDT	C3N-C2N-N1N	-4.07	119.58	122.84
2	A	501	TDT	C3N-C2N-N1N	-3.83	119.77	122.84
3	B	502	NAD	C4D-O4D-C1D	-3.51	105.86	109.72
3	B	502	NAD	C4B-O4B-C1B	-2.90	106.53	109.72
2	D	504	TDT	PA-O3P-PN	-2.78	124.93	132.73
2	D	504	TDT	C4B-O4B-C1B	-2.59	106.87	109.72
2	A	501	TDT	C4B-O4B-C1B	-2.16	107.34	109.72
3	B	502	NAD	O5B-C5B-C4B	-2.01	101.70	109.12
2	C	503	TDT	C4A-C5A-N7A	2.27	111.57	109.48
2	C	503	TDT	O4M-C1M-N1N	2.37	113.06	108.07
2	A	501	TDT	C4A-C5A-N7A	2.40	111.69	109.48
2	D	504	TDT	O3P-PA-O5B	2.40	109.31	102.94
2	D	504	TDT	C4A-C5A-N7A	2.51	111.79	109.48
3	B	502	NAD	O2A-PA-O1A	2.55	126.33	112.53
2	A	501	TDT	O4M-C1M-N1N	2.75	113.88	108.07
2	A	501	TDT	C19-N3-C4N	2.84	128.66	125.57
2	A	501	TDT	C4-N-C2	2.85	121.18	116.29
3	B	502	NAD	C4A-C5A-N7A	2.91	112.16	109.48
2	D	504	TDT	C4-N-C2	2.92	121.29	116.29
2	C	503	TDT	C4-N-C2	2.95	121.35	116.29
2	C	503	TDT	O3P-PA-O5B	3.01	110.93	102.94
2	A	501	TDT	O3P-PA-O5B	3.19	111.40	102.94
3	B	502	NAD	C2N-C3N-C4N	3.55	122.24	118.29
2	D	504	TDT	C19-N3-C4N	4.82	130.82	125.57
2	C	503	TDT	C19-N3-C4N	4.96	130.97	125.57

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	TDT	2	0
3	B	502	NAD	3	0
2	C	503	TDT	4	0
2	D	504	TDT	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.