



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:05 PM GMT

PDB ID : 1KR2
Title : CRYSTAL STRUCTURE OF HUMAN NMN/NAMN ADENYLYL TRANSFERASE COMPLEXED WITH TIAZOFURIN ADENINE DINUCLEOTIDE (TAD)
Authors : Zhou, T.; Kurnasov, O.; Tomchick, D.R.; Binns, D.D.; Grishin, N.V.; Marquez, V.E.; Osterman, A.L.; Zhang, H.
Deposited on : 2002-01-08
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

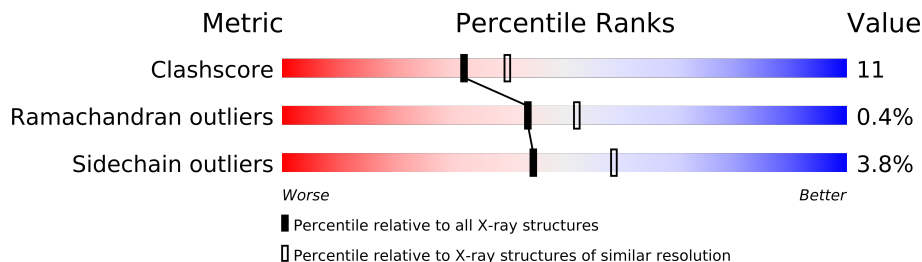
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
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 2.30 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	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	279	
1	B	279	
1	C	279	
1	D	279	
1	E	279	
1	F	279	

2 Entry composition i

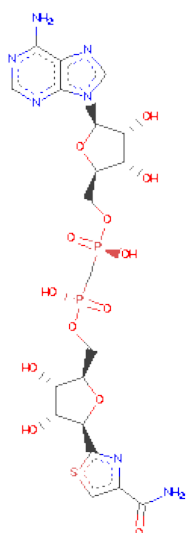
There are 3 unique types of molecules in this entry. The entry contains 12192 atoms, of which 0 are hydrogen and 0 are deuterium.

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 NICOTINAMIDE MONONUCLEOTIDE ADENYLYL TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1875	1195	331	343	6			
1	B	233	Total	C	N	O	S	0	0	0
			1875	1195	331	343	6			
1	C	233	Total	C	N	O	S	0	0	0
			1875	1195	331	343	6			
1	D	233	Total	C	N	O	S	0	0	0
			1875	1195	331	343	6			
1	E	232	Total	C	N	O	S	0	0	0
			1866	1190	330	340	6			
1	F	231	Total	C	N	O	S	0	0	0
			1861	1187	329	339	6			

- Molecule 2 is BETA-METHYLENE-THIAZOLE-4-CARBOXYAMIDE-ADENINEDINUCLEOTIDE (three-letter code: TAD) (formula: C₂₀H₂₇N₇O₁₃P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 43	C 20	N 7	O 13	P 2	S 1	0	0
2	B	1	Total 43	C 20	N 7	O 13	P 2	S 1	0	0
2	C	1	Total 43	C 20	N 7	O 13	P 2	S 1	0	0
2	D	1	Total 43	C 20	N 7	O 13	P 2	S 1	0	0
2	E	1	Total 43	C 20	N 7	O 13	P 2	S 1	0	0
2	F	1	Total 43	C 20	N 7	O 13	P 2	S 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	155	Total 155	O 155	0	0
3	B	128	Total 128	O 128	0	0
3	C	168	Total 168	O 168	0	0
3	D	103	Total 103	O 103	0	0
3	E	83	Total 83	O 83	0	0
3	F	70	Total 70	O 70	0	0

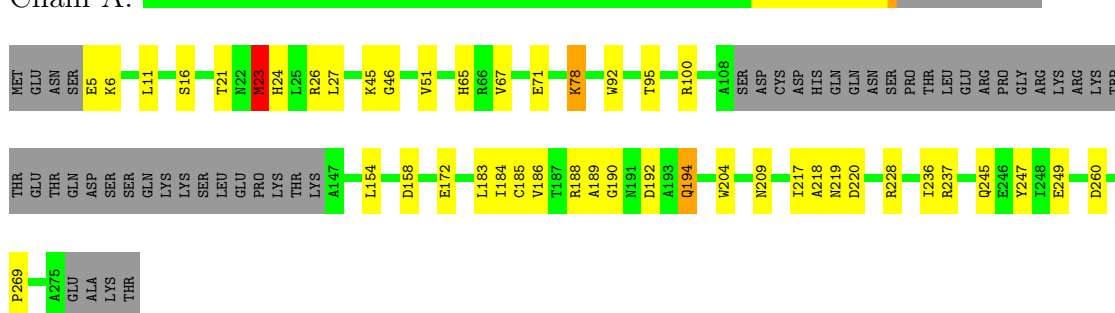
3 Residue-property plots

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.

Note EDS was not executed.

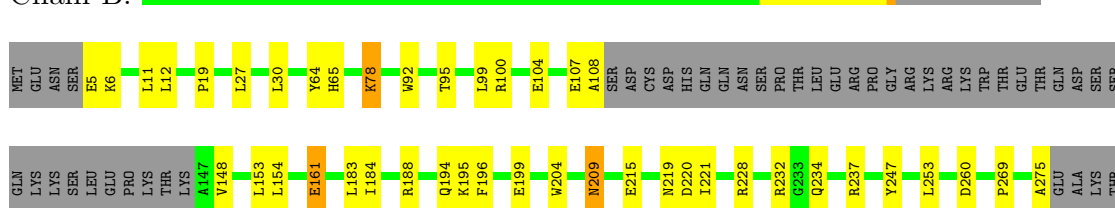
• Molecule 1: NICOTINAMIDE MONONUCLEOTIDE ADENYLYL TRANSFERASE

Chain A:



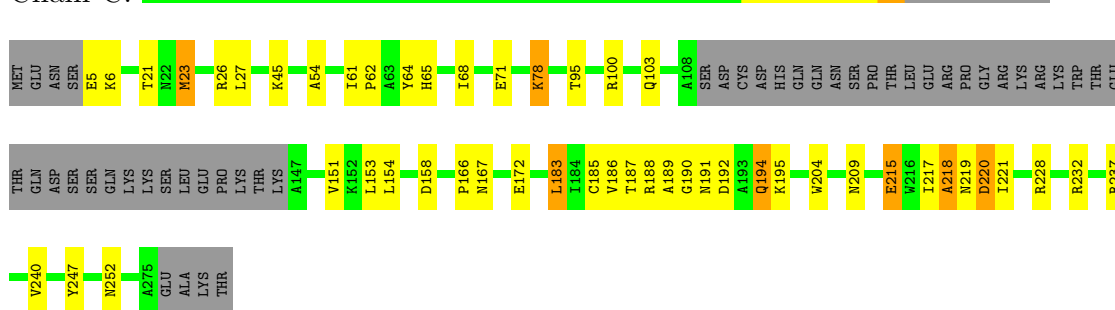
• Molecule 1: NICOTINAMIDE MONONUCLEOTIDE ADENYLYL TRANSFERASE

Chain B:



• Molecule 1: NICOTINAMIDE MONONUCLEOTIDE ADENYLYL TRANSFERASE

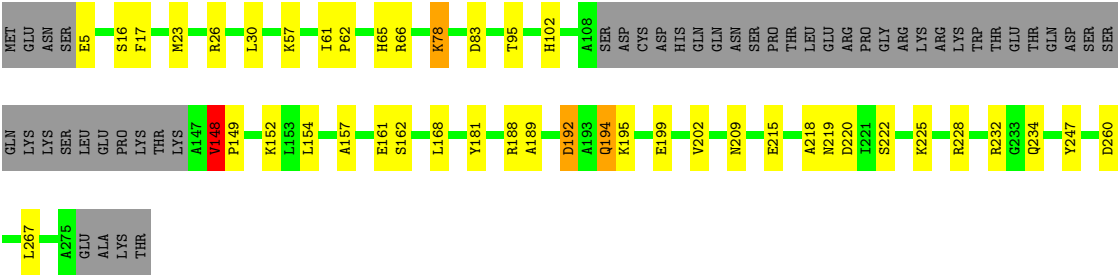
Chain C:



• Molecule 1: NICOTINAMIDE MONONUCLEOTIDE ADENYLYL TRANSFERASE

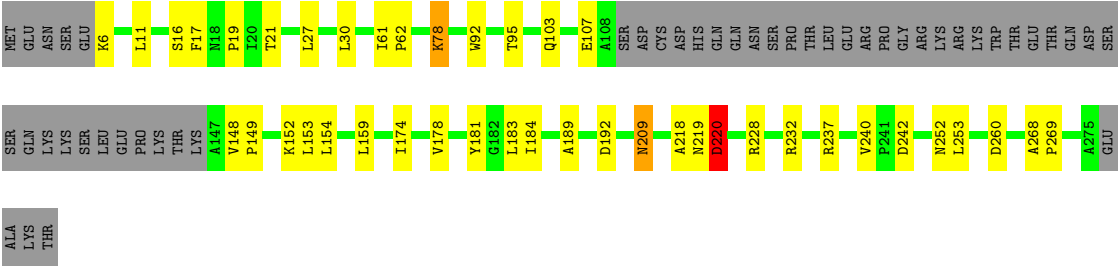
Chain D:





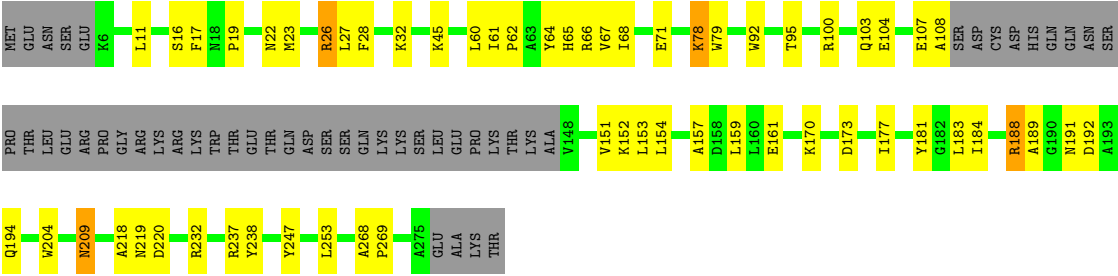
• Molecule 1: NICOTINAMIDE MONONUCLEOTIDE ADENYLYL TRANSFERASE

Chain E:



• Molecule 1: NICOTINAMIDE MONONUCLEOTIDE ADENYLYL TRANSFERASE

Chain F:



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	131.48Å 89.39Å 137.75Å 90.00° 117.42° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.30)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.203 , 0.231	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12192	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.68	1/1912 (0.1%)	0.76	0/2588
1	B	0.70	0/1912	0.78	1/2588 (0.0%)
1	C	0.70	0/1912	0.81	1/2588 (0.0%)
1	D	0.66	0/1912	0.77	1/2588 (0.0%)
1	E	0.57	0/1903	0.73	2/2576 (0.1%)
1	F	0.57	0/1898	0.74	1/2569 (0.0%)
All	All	0.65	1/11449 (0.0%)	0.76	6/15497 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	MET	CG-SD	5.10	1.94	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	183	LEU	CA-CB-CG	6.54	130.35	115.30
1	B	253	LEU	N-CA-C	6.07	127.38	111.00
1	D	148	VAL	N-CA-C	5.89	126.90	111.00
1	F	26	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	E	220	ASP	N-CA-C	5.47	125.78	111.00
1	E	253	LEU	N-CA-C	5.30	125.32	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1875	0	1903	55	0
1	B	1875	0	1903	42	0
1	C	1875	0	1903	61	0
1	D	1875	0	1903	39	0
1	E	1866	0	1897	33	0
1	F	1861	0	1892	43	0
2	A	43	0	25	1	0
2	B	43	0	25	1	0
2	C	43	0	25	1	0
2	D	43	0	25	5	0
2	E	43	0	25	2	0
2	F	43	0	25	2	0
3	A	155	0	0	13	0
3	B	128	0	0	11	0
3	C	168	0	0	18	0
3	D	103	0	0	6	0
3	E	83	0	0	4	0
3	F	70	0	0	4	0
All	All	12192	0	11551	263	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (263) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:23:MET:HB3	3:C:941:HOH:O	1.29	1.27
1:D:78:LYS:HD2	1:D:78:LYS:H	1.11	1.10
1:B:78:LYS:HD2	1:B:78:LYS:H	0.98	1.09
1:B:78:LYS:CD	1:B:78:LYS:H	1.69	1.03
1:E:219:ASN:HA	1:F:219:ASN:OD1	1.60	1.00
1:D:78:LYS:H	1:D:78:LYS:CD	1.76	0.97
1:C:183:LEU:HB3	3:C:977:HOH:O	1.64	0.96
1:B:78:LYS:HD2	1:B:78:LYS:N	1.80	0.95
1:C:78:LYS:HD2	1:C:78:LYS:H	1.28	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:192:ASP:HA	3:C:939:HOH:O	1.67	0.92
1:A:183:LEU:HB3	3:A:891:HOH:O	1.70	0.91
1:C:158:ASP:HB2	3:C:933:HOH:O	1.70	0.90
1:F:78:LYS:H	1:F:78:LYS:HD2	1.35	0.89
1:A:23:MET:HE2	1:A:23:MET:HA	1.56	0.88
1:D:78:LYS:HD2	1:D:78:LYS:N	1.88	0.88
1:F:78:LYS:CD	1:F:78:LYS:H	1.87	0.86
1:A:78:LYS:H	1:A:78:LYS:HD2	1.38	0.85
1:A:236:ILE:HG12	3:A:959:HOH:O	1.76	0.84
1:A:78:LYS:CD	1:A:78:LYS:H	1.90	0.83
1:A:194:GLN:HA	1:A:194:GLN:HE21	1.43	0.82
2:F:814:TAD:H31	3:F:881:HOH:O	1.80	0.81
1:A:23:MET:HE3	1:A:219:ASN:HB3	1.61	0.81
1:A:21:THR:H	1:A:24:HIS:HD2	1.27	0.81
1:C:78:LYS:CD	1:C:78:LYS:H	1.83	0.79
1:C:194:GLN:HA	1:C:194:GLN:HE21	1.48	0.79
1:D:23:MET:HG2	3:D:901:HOH:O	1.82	0.79
1:C:95:THR:H	2:C:811:TAD:H61N	1.30	0.78
1:C:5:GLU:HG3	1:C:6:LYS:H	1.48	0.78
1:F:78:LYS:N	1:F:78:LYS:HD2	1.98	0.77
1:C:189:ALA:HB1	1:C:192:ASP:HB2	1.67	0.77
1:C:188:ARG:HD2	1:C:218:ALA:HA	1.65	0.76
1:F:189:ALA:HB1	1:F:192:ASP:HB2	1.68	0.76
1:B:219:ASN:HB3	3:B:853:HOH:O	1.87	0.75
1:B:234:GLN:HG2	3:B:922:HOH:O	1.84	0.75
1:C:78:LYS:N	1:C:78:LYS:HD2	2.00	0.74
1:C:5:GLU:HB2	3:C:972:HOH:O	1.87	0.74
1:C:219:ASN:OD1	1:C:220:ASP:N	2.19	0.74
1:A:95:THR:H	2:A:809:TAD:H61N	1.36	0.74
1:C:5:GLU:HG2	3:C:966:HOH:O	1.87	0.73
1:A:245:GLN:O	1:A:249:GLU:HG2	1.89	0.73
1:C:217:ILE:HD12	3:C:935:HOH:O	1.89	0.73
1:B:188:ARG:HD3	3:B:916:HOH:O	1.90	0.71
1:A:78:LYS:N	1:A:78:LYS:HD2	2.06	0.71
1:F:65:HIS:HD2	1:F:247:TYR:OH	1.73	0.71
1:B:65:HIS:HD2	1:B:247:TYR:OH	1.75	0.70
1:F:157:ALA:O	1:F:161:GLU:HG3	1.90	0.70
1:B:215:GLU:OE2	3:B:908:HOH:O	2.09	0.70
1:D:95:THR:H	2:D:812:TAD:H61N	1.40	0.69
1:D:202:VAL:HG23	3:D:845:HOH:O	1.92	0.69
1:F:268:ALA:HB3	1:F:269:PRO:HD3	1.74	0.69
1:F:92:TRP:CH2	1:F:269:PRO:HG3	2.26	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:78:LYS:HD2	1:E:78:LYS:H	1.57	0.69
1:C:5:GLU:HG3	1:C:6:LYS:N	2.07	0.69
1:A:172:GLU:HB3	3:A:962:HOH:O	1.92	0.68
1:D:234:GLN:HG2	3:D:891:HOH:O	1.93	0.68
1:A:23:MET:HE1	1:A:219:ASN:OD1	1.94	0.68
1:F:95:THR:H	2:F:814:TAD:H61N	1.42	0.68
1:E:11:LEU:HD22	1:E:184:ILE:HD12	1.75	0.68
1:D:30:LEU:HD11	1:D:215:GLU:CD	2.15	0.67
1:C:228:ARG:HD2	1:C:232:ARG:NH2	2.10	0.67
1:E:153:LEU:HB3	1:E:183:LEU:HD23	1.77	0.66
1:A:23:MET:HG3	3:A:932:HOH:O	1.94	0.66
1:C:219:ASN:O	1:C:220:ASP:CB	2.43	0.66
1:A:186:VAL:HG12	3:A:951:HOH:O	1.96	0.66
1:E:78:LYS:CD	1:E:78:LYS:H	2.07	0.66
1:B:95:THR:H	2:B:810:TAD:H61N	1.43	0.65
1:F:64:TYR:O	1:F:68:ILE:HG12	1.96	0.65
1:C:219:ASN:O	1:C:220:ASP:HB3	1.96	0.65
1:D:16:SER:H	2:D:812:TAD:H32	1.62	0.65
1:C:252:ASN:HB3	3:C:968:HOH:O	1.95	0.65
1:A:71:GLU:CD	3:A:934:HOH:O	2.35	0.64
1:A:204:TRP:CD1	1:D:232:ARG:HD3	2.33	0.64
1:A:194:GLN:HA	1:A:194:GLN:NE2	2.13	0.64
1:E:220:ASP:HB3	3:E:837:HOH:O	1.96	0.64
1:B:194:GLN:HE21	1:B:194:GLN:HA	1.63	0.64
1:A:65:HIS:HD2	1:A:247:TYR:OH	1.81	0.64
1:A:185:CYS:HB2	3:A:891:HOH:O	1.98	0.63
1:F:188:ARG:HD3	3:F:838:HOH:O	1.97	0.63
1:B:275:ALA:HB2	3:B:917:HOH:O	1.97	0.63
1:B:64:TYR:HE1	3:B:926:HOH:O	1.82	0.63
1:C:183:LEU:HD13	3:C:977:HOH:O	1.98	0.63
1:D:194:GLN:HE21	1:D:194:GLN:HA	1.62	0.62
1:C:23:MET:SD	3:C:958:HOH:O	2.56	0.62
1:E:95:THR:H	2:E:813:TAD:H61N	1.46	0.62
1:E:228:ARG:HD2	1:E:232:ARG:NH2	2.14	0.62
1:A:92:TRP:CH2	1:A:269:PRO:HG3	2.35	0.62
1:E:92:TRP:CH2	1:E:269:PRO:HG3	2.35	0.62
1:C:189:ALA:CB	1:C:192:ASP:HB2	2.31	0.61
1:B:100:ARG:O	1:B:104:GLU:HG3	2.01	0.61
1:C:54:ALA:HB3	3:C:945:HOH:O	2.00	0.60
1:A:23:MET:CE	1:A:23:MET:HA	2.27	0.60
1:C:5:GLU:CG	1:C:6:LYS:H	2.13	0.60
1:F:60:LEU:HD11	1:F:66:ARG:CZ	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:107:GLU:O	1:B:108:ALA:HB2	2.03	0.59
1:B:92:TRP:CH2	1:B:269:PRO:HB3	2.37	0.59
1:F:173:ASP:O	1:F:177:ILE:HG13	2.02	0.59
1:A:23:MET:HB3	3:A:932:HOH:O	2.02	0.59
1:C:194:GLN:HA	1:C:194:GLN:NE2	2.18	0.59
1:D:78:LYS:HD3	3:D:886:HOH:O	2.02	0.59
1:A:5:GLU:HG3	1:A:6:LYS:HG3	1.85	0.58
1:C:65:HIS:HD2	1:C:247:TYR:OH	1.85	0.58
1:B:5:GLU:HG3	1:B:6:LYS:N	2.18	0.58
1:F:100:ARG:O	1:F:104:GLU:HG3	2.04	0.58
1:A:217:ILE:HG22	1:A:219:ASN:ND2	2.18	0.58
1:F:92:TRP:CZ2	1:F:269:PRO:HG3	2.39	0.57
1:F:247:TYR:CE2	1:F:253:LEU:HD11	2.39	0.57
1:F:189:ALA:CB	1:F:192:ASP:HB2	2.34	0.57
1:E:237:ARG:NE	3:E:890:HOH:O	2.37	0.57
1:F:11:LEU:CD2	1:F:184:ILE:HD12	2.33	0.57
1:C:189:ALA:O	1:C:192:ASP:HB3	2.05	0.57
1:B:209:ASN:ND2	3:B:936:HOH:O	2.36	0.56
1:B:78:LYS:CD	1:B:78:LYS:N	2.49	0.56
1:D:23:MET:HE1	2:D:812:TAD:N7A	2.21	0.56
1:C:219:ASN:HA	1:D:219:ASN:OD1	2.06	0.56
1:F:170:LYS:O	1:F:173:ASP:HB2	2.05	0.56
1:E:6:LYS:HE2	3:E:893:HOH:O	2.06	0.56
1:C:192:ASP:CA	3:C:939:HOH:O	2.38	0.56
1:E:78:LYS:HD2	1:E:78:LYS:N	2.21	0.56
1:A:23:MET:HE3	1:A:219:ASN:CB	2.35	0.56
1:B:153:LEU:HD23	1:B:183:LEU:CD2	2.36	0.55
1:B:194:GLN:NE2	1:B:194:GLN:HA	2.21	0.55
1:B:78:LYS:HD3	3:B:894:HOH:O	2.06	0.55
1:D:189:ALA:HB1	1:D:192:ASP:HB2	1.88	0.55
1:D:26:ARG:HG2	3:D:895:HOH:O	2.06	0.55
1:C:221:ILE:O	1:C:221:ILE:HG22	2.06	0.55
1:E:92:TRP:CZ2	1:E:269:PRO:HG3	2.42	0.55
1:A:189:ALA:O	1:A:192:ASP:HB3	2.06	0.55
1:A:71:GLU:CG	3:A:934:HOH:O	2.55	0.55
1:A:23:MET:CE	1:A:219:ASN:CB	2.85	0.55
1:D:228:ARG:HD2	1:D:232:ARG:NH2	2.22	0.55
1:B:65:HIS:CD2	1:B:247:TYR:OH	2.58	0.54
1:E:218:ALA:HB3	1:F:220:ASP:OD1	2.07	0.54
1:C:221:ILE:HD11	1:D:219:ASN:ND2	2.23	0.54
1:E:152:LYS:HD3	1:E:181:TYR:O	2.07	0.54
1:B:107:GLU:HG2	1:B:148:VAL:HG11	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:5:GLU:HG3	1:B:6:LYS:H	1.71	0.53
1:B:12:LEU:HD23	1:B:99:LEU:HD23	1.90	0.53
1:C:153:LEU:HD23	1:C:183:LEU:CD2	2.38	0.53
1:A:21:THR:N	1:A:24:HIS:HD2	2.02	0.53
1:A:67:VAL:O	1:A:71:GLU:HG3	2.08	0.53
1:B:204:TRP:CD1	1:F:232:ARG:HD3	2.42	0.53
1:D:157:ALA:O	1:D:161:GLU:HG3	2.08	0.53
1:C:190:GLY:O	1:C:194:GLN:HG2	2.08	0.53
1:B:194:GLN:CA	1:B:194:GLN:HE21	2.21	0.53
1:A:23:MET:CE	1:A:219:ASN:HB3	2.33	0.52
1:C:194:GLN:CA	1:C:194:GLN:HE21	2.16	0.52
1:F:61:ILE:HB	1:F:62:PRO:CD	2.39	0.52
1:C:64:TYR:CE2	1:C:68:ILE:HD11	2.44	0.52
1:F:65:HIS:CD2	1:F:247:TYR:OH	2.57	0.52
1:A:158:ASP:HB2	3:A:824:HOH:O	2.10	0.51
1:D:16:SER:O	1:D:66:ARG:HD2	2.09	0.51
1:F:11:LEU:HD22	1:F:184:ILE:HD12	1.92	0.51
1:C:232:ARG:HD3	1:F:204:TRP:CD1	2.45	0.51
1:D:23:MET:CE	2:D:812:TAD:N7A	2.73	0.51
1:A:65:HIS:CD2	1:A:247:TYR:OH	2.64	0.51
1:C:188:ARG:HD3	3:C:970:HOH:O	2.11	0.51
1:A:21:THR:H	1:A:24:HIS:CD2	2.18	0.50
1:B:11:LEU:CD2	1:B:184:ILE:HD12	2.41	0.50
1:A:5:GLU:HG3	1:A:6:LYS:N	2.26	0.50
1:E:61:ILE:HB	1:E:62:PRO:HD2	1.93	0.50
1:D:195:LYS:O	1:D:199:GLU:HG3	2.12	0.50
1:A:45:LYS:HG2	1:A:46:GLY:N	2.26	0.50
1:C:153:LEU:HD11	3:C:956:HOH:O	2.11	0.49
1:A:188:ARG:NH1	1:A:220:ASP:OD2	2.40	0.49
1:D:152:LYS:HD3	1:D:181:TYR:O	2.13	0.49
2:D:812:TAD:H4B	3:D:904:HOH:O	2.11	0.49
1:D:194:GLN:HE21	1:D:194:GLN:CA	2.24	0.49
1:A:237:ARG:NH1	1:B:78:LYS:HE3	2.28	0.49
1:B:219:ASN:HD21	1:B:221:ILE:HD11	1.77	0.49
1:B:30:LEU:HD11	1:B:215:GLU:OE2	2.13	0.49
1:F:61:ILE:HB	1:F:62:PRO:HD2	1.95	0.49
1:F:22:ASN:O	1:F:26:ARG:HB2	2.13	0.49
1:C:45:LYS:NZ	3:C:900:HOH:O	2.36	0.49
1:C:188:ARG:HD2	1:C:218:ALA:CA	2.41	0.49
1:A:194:GLN:CA	1:A:194:GLN:HE21	2.11	0.48
1:A:100:ARG:HD2	3:A:882:HOH:O	2.13	0.48
1:A:71:GLU:CB	3:A:934:HOH:O	2.61	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:186:VAL:O	1:C:187:THR:HB	2.14	0.48
1:E:11:LEU:CD2	1:E:184:ILE:HD12	2.44	0.48
1:A:23:MET:CA	1:A:23:MET:HE2	2.38	0.47
1:D:65:HIS:HD2	1:D:247:TYR:OH	1.96	0.47
1:C:185:CYS:HB2	3:C:977:HOH:O	2.13	0.47
1:C:219:ASN:HA	1:D:219:ASN:HA	1.96	0.47
1:B:30:LEU:HD11	1:B:215:GLU:CD	2.34	0.47
1:F:45:LYS:NZ	3:F:878:HOH:O	2.47	0.47
1:C:103:GLN:OE1	1:C:151:VAL:HG12	2.14	0.47
1:B:219:ASN:ND2	3:B:823:HOH:O	2.47	0.47
1:A:16:SER:HA	1:A:51:VAL:HG12	1.97	0.47
1:A:228:ARG:NH2	3:A:960:HOH:O	2.45	0.47
1:D:188:ARG:HD3	1:D:220:ASP:OD2	2.15	0.47
1:E:107:GLU:HG2	1:E:148:VAL:HG11	1.96	0.47
1:F:152:LYS:NZ	1:F:209:ASN:HD21	2.13	0.47
1:C:153:LEU:CD1	3:C:956:HOH:O	2.62	0.46
1:A:189:ALA:HB1	1:A:192:ASP:HB2	1.96	0.46
1:F:107:GLU:O	1:F:108:ALA:HB2	2.15	0.46
1:A:23:MET:SD	1:A:219:ASN:HB2	2.55	0.46
1:D:5:GLU:CD	1:D:5:GLU:N	2.68	0.46
1:A:217:ILE:HG22	1:A:219:ASN:HD21	1.81	0.46
1:F:28:PHE:HB3	1:F:79:TRP:CH2	2.50	0.46
1:E:209:ASN:HA	1:E:209:ASN:HD22	1.56	0.46
1:C:64:TYR:O	1:C:68:ILE:HG13	2.15	0.46
1:B:107:GLU:O	1:B:108:ALA:CB	2.63	0.46
1:D:148:VAL:HA	1:D:149:PRO:HD3	1.70	0.45
1:B:161:GLU:HG3	1:B:196:PHE:CD1	2.51	0.45
1:A:190:GLY:O	1:A:194:GLN:HG2	2.16	0.45
1:E:61:ILE:HB	1:E:62:PRO:CD	2.46	0.45
1:C:21:THR:HA	1:C:240:VAL:HG12	1.98	0.45
1:C:61:ILE:HB	1:C:62:PRO:CD	2.45	0.45
1:C:166:PRO:O	1:C:167:ASN:HB2	2.17	0.45
1:A:11:LEU:CD2	1:A:184:ILE:HD12	2.47	0.45
1:B:228:ARG:HD2	1:B:232:ARG:NH2	2.32	0.44
1:D:61:ILE:HB	1:D:62:PRO:CD	2.47	0.44
1:C:220:ASP:O	1:C:220:ASP:CG	2.56	0.44
1:A:5:GLU:HG3	1:A:6:LYS:H	1.82	0.44
1:C:100:ARG:HD2	3:C:929:HOH:O	2.17	0.44
1:F:16:SER:O	1:F:17:PHE:C	2.56	0.44
1:D:16:SER:O	1:D:17:PHE:C	2.56	0.44
1:E:152:LYS:NZ	1:E:209:ASN:HD21	2.16	0.44
1:E:103:GLN:O	1:E:107:GLU:HG3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:152:LYS:HD3	1:F:181:TYR:O	2.18	0.43
1:D:222:SER:OG	1:D:225:LYS:HG3	2.18	0.43
1:C:188:ARG:CD	1:C:218:ALA:HA	2.44	0.43
1:F:247:TYR:HE2	1:F:253:LEU:HD11	1.81	0.43
1:A:78:LYS:HE3	1:B:237:ARG:HH12	1.84	0.43
1:C:189:ALA:O	1:C:192:ASP:CB	2.67	0.43
1:F:26:ARG:HD2	1:F:26:ARG:HA	1.74	0.43
1:E:189:ALA:O	1:E:192:ASP:HB2	2.19	0.43
1:D:30:LEU:HD11	1:D:215:GLU:OE2	2.18	0.42
1:E:242:ASP:HB3	3:E:890:HOH:O	2.19	0.42
1:C:191:ASN:HA	1:C:194:GLN:HB2	2.01	0.42
1:E:153:LEU:HD23	1:E:183:LEU:HD21	2.01	0.42
1:E:159:LEU:C	1:E:159:LEU:HD23	2.40	0.42
1:E:27:LEU:HD11	2:E:813:TAD:C2A	2.49	0.42
1:F:151:VAL:HG13	1:F:151:VAL:O	2.19	0.42
1:F:153:LEU:HB3	1:F:183:LEU:HD23	2.00	0.42
1:F:237:ARG:O	1:F:238:TYR:HB2	2.19	0.42
1:E:16:SER:O	1:E:17:PHE:C	2.57	0.42
1:E:148:VAL:HA	1:E:149:PRO:HD3	1.78	0.42
1:C:215:GLU:HG3	1:C:215:GLU:O	2.20	0.42
1:F:23:MET:HG2	3:F:821:HOH:O	2.19	0.42
1:E:268:ALA:HB3	1:E:269:PRO:HD3	2.02	0.41
1:D:57:LYS:HA	1:D:267:LEU:CD1	2.50	0.41
1:A:188:ARG:HD2	1:A:218:ALA:HA	2.02	0.41
1:A:26:ARG:HA	1:A:26:ARG:HD2	1.81	0.41
1:D:83:ASP:CG	1:D:102:HIS:HE1	2.24	0.41
1:C:191:ASN:O	1:C:195:LYS:HB2	2.20	0.41
1:B:228:ARG:HD3	3:B:824:HOH:O	2.20	0.41
1:E:174:ILE:O	1:E:178:VAL:HG22	2.21	0.41
1:B:219:ASN:ND2	1:B:221:ILE:HD11	2.36	0.41
1:D:188:ARG:HD2	1:D:218:ALA:HB1	2.03	0.41
1:F:67:VAL:O	1:F:71:GLU:HG3	2.20	0.41
1:B:232:ARG:HD3	1:C:204:TRP:CD1	2.56	0.41
1:F:103:GLN:OE1	1:F:151:VAL:HG12	2.21	0.41
1:C:26:ARG:HA	1:C:26:ARG:HD2	1.77	0.41
1:C:237:ARG:NH1	1:D:78:LYS:HE3	2.35	0.41
1:D:162:SER:HB2	1:D:168:LEU:HD23	2.03	0.41
1:F:32:LYS:HD2	1:F:79:TRP:CE2	2.57	0.40
1:A:189:ALA:HB1	1:A:192:ASP:CB	2.51	0.40
1:E:30:LEU:HA	1:E:30:LEU:HD23	1.92	0.40
1:E:21:THR:HA	1:E:240:VAL:HG12	2.03	0.40
1:B:188:ARG:NH1	3:B:916:HOH:O	2.53	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:194:GLN:NE2	1:D:194:GLN:HA	2.34	0.40
1:B:195:LYS:O	1:B:199:GLU:HG3	2.21	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	229/279 (82%)	223 (97%)	6 (3%)	0	100	100
1	B	229/279 (82%)	221 (96%)	8 (4%)	0	100	100
1	C	229/279 (82%)	219 (96%)	8 (4%)	2 (1%)	25	26
1	D	229/279 (82%)	218 (95%)	10 (4%)	1 (0%)	43	52
1	E	228/279 (82%)	221 (97%)	6 (3%)	1 (0%)	43	52
1	F	227/279 (81%)	220 (97%)	6 (3%)	1 (0%)	43	52
All	All	1371/1674 (82%)	1322 (96%)	44 (3%)	5 (0%)	43	52

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	220	ASP
1	D	148	VAL
1	E	220	ASP
1	F	218	ALA
1	C	218	ALA

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	204/248 (82%)	197 (97%)	7 (3%)	49	64
1	B	204/248 (82%)	196 (96%)	8 (4%)	43	57
1	C	204/248 (82%)	195 (96%)	9 (4%)	39	51
1	D	204/248 (82%)	197 (97%)	7 (3%)	49	64
1	E	203/248 (82%)	197 (97%)	6 (3%)	53	70
1	F	203/248 (82%)	194 (96%)	9 (4%)	39	51
All	All	1222/1488 (82%)	1176 (96%)	46 (4%)	44	59

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	MET
1	A	27	LEU
1	A	78	LYS
1	A	154	LEU
1	A	194	GLN
1	A	209	ASN
1	A	260	ASP
1	B	19	PRO
1	B	27	LEU
1	B	78	LYS
1	B	154	LEU
1	B	161	GLU
1	B	209	ASN
1	B	220	ASP
1	B	260	ASP
1	C	23	MET
1	C	27	LEU
1	C	71	GLU
1	C	78	LYS
1	C	154	LEU
1	C	172	GLU
1	C	194	GLN
1	C	209	ASN
1	C	215	GLU
1	D	78	LYS
1	D	148	VAL
1	D	154	LEU
1	D	192	ASP
1	D	194	GLN
1	D	209	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	260	ASP
1	E	19	PRO
1	E	78	LYS
1	E	154	LEU
1	E	209	ASN
1	E	252	ASN
1	E	260	ASP
1	F	19	PRO
1	F	27	LEU
1	F	78	LYS
1	F	154	LEU
1	F	159	LEU
1	F	188	ARG
1	F	191	ASN
1	F	194	GLN
1	F	209	ASN

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	24	HIS
1	A	65	HIS
1	A	194	GLN
1	A	206	HIS
1	A	209	ASN
1	A	211	HIS
1	B	65	HIS
1	B	76	ASN
1	B	194	GLN
1	B	209	ASN
1	C	65	HIS
1	C	194	GLN
1	C	209	ASN
1	D	65	HIS
1	D	76	ASN
1	D	102	HIS
1	D	194	GLN
1	D	209	ASN
1	E	76	ASN
1	E	102	HIS
1	E	194	GLN
1	E	209	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	219	ASN
1	F	65	HIS
1	F	102	HIS
1	F	194	GLN
1	F	206	HIS
1	F	209	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 ⓘ

6 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	TAD	A	809	-	47,47,47	1.45	8 (17%)	68,72,72	2.41	18 (26%)
2	TAD	B	810	-	47,47,47	1.39	8 (17%)	68,72,72	2.60	23 (33%)
2	TAD	C	811	-	47,47,47	1.50	6 (12%)	68,72,72	2.42	19 (27%)
2	TAD	D	812	-	47,47,47	1.52	9 (19%)	68,72,72	2.59	24 (35%)
2	TAD	E	813	-	47,47,47	1.48	8 (17%)	68,72,72	2.57	22 (32%)
2	TAD	F	814	-	47,47,47	1.46	7 (14%)	68,72,72	2.51	20 (29%)

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	TAD	A	809	-	-	0/24/62/62	0/3/5/5
2	TAD	B	810	-	-	0/24/62/62	0/3/5/5
2	TAD	C	811	-	-	0/24/62/62	0/3/5/5
2	TAD	D	812	-	-	0/24/62/62	0/3/5/5
2	TAD	E	813	-	-	0/24/62/62	0/3/5/5
2	TAD	F	814	-	-	0/24/62/62	0/3/5/5

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	814	TAD	O4B-C1B	4.59	1.48	1.41
2	C	811	TAD	PA-C3	4.24	1.83	1.79
2	D	812	TAD	C2N-C1D	-4.10	1.46	1.51
2	E	813	TAD	PA-C3	4.08	1.83	1.79
2	C	811	TAD	C2N-S1N	-4.00	1.68	1.73
2	E	813	TAD	O4B-C1B	3.79	1.47	1.41
2	D	812	TAD	C2D-C1D	-3.70	1.50	1.53
2	B	810	TAD	O4B-C1B	3.43	1.46	1.41
2	E	813	TAD	PN-O2N	-3.40	1.48	1.56
2	A	809	TAD	PN-O2N	-3.38	1.48	1.56
2	C	811	TAD	PN-O2N	-3.37	1.48	1.56
2	B	810	TAD	C2D-C1D	-3.32	1.50	1.53
2	A	809	TAD	O4B-C1B	3.30	1.46	1.41
2	A	809	TAD	PN-C3	3.24	1.82	1.79
2	D	812	TAD	O4B-C1B	3.22	1.46	1.41
2	A	809	TAD	C2B-C1B	-3.13	1.49	1.53
2	F	814	TAD	C2D-C1D	-3.08	1.50	1.53
2	A	809	TAD	C2N-S1N	-3.07	1.69	1.73
2	F	814	TAD	C2B-C1B	-3.04	1.49	1.53
2	F	814	TAD	PN-O2N	-2.92	1.49	1.56
2	E	813	TAD	PN-C3	2.78	1.82	1.79
2	C	811	TAD	C2B-C1B	-2.64	1.49	1.53
2	C	811	TAD	C2N-C1D	-2.62	1.48	1.51
2	B	810	TAD	PA-O1A	-2.57	1.45	1.51
2	B	810	TAD	PA-C3	2.56	1.82	1.79
2	D	812	TAD	C2A-N3A	2.55	1.37	1.32
2	B	810	TAD	PN-O2N	-2.54	1.50	1.56
2	D	812	TAD	PA-O2A	-2.50	1.50	1.56
2	A	809	TAD	PA-C3	2.50	1.82	1.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	812	TAD	PN-C3	2.42	1.81	1.79
2	D	812	TAD	PN-O2N	-2.37	1.50	1.56
2	F	814	TAD	C2N-C1D	-2.36	1.48	1.51
2	B	810	TAD	C2B-C1B	-2.34	1.50	1.53
2	C	811	TAD	PA-O2A	-2.33	1.50	1.56
2	A	809	TAD	PN-O1N	-2.30	1.45	1.51
2	B	810	TAD	PN-C3	2.29	1.81	1.79
2	E	813	TAD	PN-O1N	-2.29	1.45	1.51
2	E	813	TAD	C2N-S1N	-2.24	1.70	1.73
2	E	813	TAD	C2D-C1D	-2.17	1.51	1.53
2	F	814	TAD	PN-O1N	-2.16	1.46	1.51
2	F	814	TAD	PA-O1A	-2.16	1.46	1.51
2	A	809	TAD	C4N-N3N	-2.16	1.33	1.38
2	E	813	TAD	C2A-N3A	2.12	1.36	1.32
2	B	810	TAD	PN-O1N	-2.08	1.46	1.51
2	D	812	TAD	PN-O1N	-2.05	1.46	1.51
2	D	812	TAD	C2B-C1B	-2.01	1.50	1.53

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	809	TAD	N3A-C2A-N1A	-10.30	120.09	128.71
2	F	814	TAD	N3A-C2A-N1A	-10.24	120.14	128.71
2	C	811	TAD	N3A-C2A-N1A	-10.21	120.17	128.71
2	E	813	TAD	N3A-C2A-N1A	-10.16	120.22	128.71
2	B	810	TAD	N3A-C2A-N1A	-9.88	120.45	128.71
2	D	812	TAD	N3A-C2A-N1A	-9.71	120.59	128.71
2	E	813	TAD	N3A-C4A-N9A	8.09	140.04	125.43
2	F	814	TAD	N3A-C4A-N9A	8.04	139.94	125.43
2	D	812	TAD	N3A-C4A-N9A	7.88	139.66	125.43
2	C	811	TAD	N3A-C4A-N9A	7.70	139.33	125.43
2	B	810	TAD	N3A-C4A-N9A	7.65	139.24	125.43
2	A	809	TAD	N3A-C4A-N9A	7.27	138.55	125.43
2	D	812	TAD	C5N-S1N-C2N	-6.29	86.12	95.29
2	B	810	TAD	C5N-S1N-C2N	-5.80	86.84	95.29
2	A	809	TAD	C5N-S1N-C2N	-5.77	86.88	95.29
2	E	813	TAD	O6N-C6N-C4N	5.54	125.20	119.65
2	C	811	TAD	C5N-S1N-C2N	-5.39	87.43	95.29
2	E	813	TAD	C5N-S1N-C2N	-5.06	87.91	95.29
2	C	811	TAD	C4A-C5A-N7A	5.06	113.86	109.52
2	F	814	TAD	C5N-S1N-C2N	-5.05	87.92	95.29
2	B	810	TAD	O6N-C6N-C4N	5.03	124.68	119.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	812	TAD	PN-C3-PA	5.02	124.84	117.62
2	D	812	TAD	C4A-C5A-N7A	4.98	113.79	109.52
2	E	813	TAD	C4N-C6N-N6N	-4.85	111.73	115.96
2	B	810	TAD	C4A-C5A-N7A	4.82	113.65	109.52
2	A	809	TAD	C4A-C5A-N7A	4.81	113.64	109.52
2	C	811	TAD	O5B-PA-C3	-4.61	92.53	103.97
2	E	813	TAD	C4A-C5A-N7A	4.56	113.43	109.52
2	B	810	TAD	C5N-C4N-N3N	4.53	116.61	109.74
2	B	810	TAD	O5B-PA-C3	-4.46	92.91	103.97
2	D	812	TAD	O6N-C6N-C4N	4.45	124.11	119.65
2	F	814	TAD	O6N-C6N-C4N	4.45	124.10	119.65
2	F	814	TAD	C4N-C6N-N6N	-4.42	112.11	115.96
2	F	814	TAD	C5N-C4N-N3N	4.31	116.27	109.74
2	A	809	TAD	O6N-C6N-C4N	4.30	123.95	119.65
2	D	812	TAD	O5D-PN-C3	-4.24	93.45	103.97
2	E	813	TAD	C5N-C4N-N3N	4.23	116.15	109.74
2	F	814	TAD	C4A-C5A-N7A	4.22	113.14	109.52
2	D	812	TAD	C5N-C4N-N3N	4.16	116.05	109.74
2	C	811	TAD	C5N-C4N-N3N	4.15	116.04	109.74
2	E	813	TAD	C5A-C4A-N3A	-4.15	116.67	125.70
2	A	809	TAD	O5B-PA-C3	-4.05	93.93	103.97
2	F	814	TAD	C5A-C4A-N3A	-4.01	116.98	125.70
2	B	810	TAD	C4N-C6N-N6N	-3.97	112.50	115.96
2	C	811	TAD	C5A-C4A-N3A	-3.88	117.26	125.70
2	D	812	TAD	C5A-C4A-N3A	-3.88	117.26	125.70
2	B	810	TAD	C3D-C2D-C1D	3.79	106.30	101.85
2	F	814	TAD	O5B-PA-C3	-3.70	94.80	103.97
2	B	810	TAD	C5A-C4A-N3A	-3.67	117.71	125.70
2	D	812	TAD	O4D-C4D-C5D	3.66	122.42	109.36
2	A	809	TAD	C5N-C4N-N3N	3.63	115.24	109.74
2	A	809	TAD	C5A-C4A-N3A	-3.57	117.93	125.70
2	F	814	TAD	PN-C3-PA	3.31	122.38	117.62
2	C	811	TAD	O5B-PA-O1A	-3.22	106.16	114.21
2	D	812	TAD	C4N-C6N-N6N	-3.19	113.17	115.96
2	D	812	TAD	C6A-C5A-C4A	3.16	123.05	117.25
2	A	809	TAD	PN-C3-PA	3.14	122.14	117.62
2	C	811	TAD	O2A-PA-O1A	3.11	120.62	110.93
2	B	810	TAD	PN-C3-PA	3.08	122.05	117.62
2	B	810	TAD	O4D-C4D-C5D	3.05	120.25	109.36
2	C	811	TAD	C6A-C5A-C4A	3.05	122.84	117.25
2	E	813	TAD	O2B-C2B-C1B	2.97	120.22	111.23
2	E	813	TAD	C2A-N3A-C4A	2.93	122.36	114.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	810	TAD	O2A-PA-O5B	2.92	115.15	105.82
2	E	813	TAD	C6A-C5A-C4A	2.91	122.60	117.25
2	B	810	TAD	C6A-C5A-C4A	2.88	122.53	117.25
2	F	814	TAD	C2A-N3A-C4A	2.87	122.19	114.01
2	B	810	TAD	C5A-C4A-N9A	-2.86	103.04	107.16
2	E	813	TAD	O5B-PA-C3	-2.85	96.91	103.97
2	F	814	TAD	C6A-C5A-C4A	2.83	122.44	117.25
2	F	814	TAD	C5A-C4A-N9A	-2.83	103.08	107.16
2	D	812	TAD	C5A-C4A-N9A	-2.83	103.08	107.16
2	E	813	TAD	O5B-PA-O1A	-2.83	107.15	114.21
2	D	812	TAD	O2B-C2B-C1B	2.82	119.75	111.23
2	C	811	TAD	PN-C3-PA	2.81	121.67	117.62
2	E	813	TAD	O4B-C4B-C5B	2.75	119.18	109.36
2	F	814	TAD	O2A-PA-O5B	2.73	114.53	105.82
2	E	813	TAD	PN-C3-PA	2.71	121.51	117.62
2	B	810	TAD	O5B-PA-O1A	-2.70	107.46	114.21
2	E	813	TAD	C5A-C4A-N9A	-2.69	103.28	107.16
2	D	812	TAD	O5B-PA-C3	-2.68	97.32	103.97
2	A	809	TAD	O2A-PA-O5B	2.66	114.33	105.82
2	F	814	TAD	O5B-PA-O1A	-2.65	107.58	114.21
2	A	809	TAD	C6A-C5A-C4A	2.65	122.12	117.25
2	F	814	TAD	O2B-C2B-C1B	2.64	119.21	111.23
2	C	811	TAD	O6N-C6N-C4N	2.61	122.26	119.65
2	C	811	TAD	C5A-C4A-N9A	-2.60	103.41	107.16
2	B	810	TAD	O2B-C2B-C1B	2.59	119.08	111.23
2	A	809	TAD	O5B-PA-O1A	-2.58	107.77	114.21
2	A	809	TAD	C2A-N3A-C4A	2.58	121.35	114.01
2	B	810	TAD	C2A-N3A-C4A	2.58	121.35	114.01
2	A	809	TAD	O4B-C1B-N9A	2.53	110.79	108.44
2	C	811	TAD	O2A-PA-O5B	2.53	113.89	105.82
2	C	811	TAD	C2A-N3A-C4A	2.53	121.20	114.01
2	A	809	TAD	C5A-C4A-N9A	-2.53	103.52	107.16
2	D	812	TAD	C2A-N3A-C4A	2.52	121.18	114.01
2	E	813	TAD	O2A-PA-O5B	2.52	113.86	105.82
2	D	812	TAD	O2A-PA-O1A	2.46	118.58	110.93
2	A	809	TAD	C4N-C6N-N6N	-2.44	113.83	115.96
2	F	814	TAD	O4B-C4B-C5B	2.41	117.98	109.36
2	B	810	TAD	C4B-O4B-C1B	2.40	112.36	109.75
2	E	813	TAD	O2A-PA-O1A	2.40	118.38	110.93
2	D	812	TAD	C3D-C2D-C1D	2.33	104.59	101.85
2	E	813	TAD	C3D-C2D-C1D	2.32	104.57	101.85
2	A	809	TAD	O2B-C2B-C1B	2.31	118.22	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	812	TAD	O4B-C4B-C5B	2.31	117.60	109.36
2	F	814	TAD	O2A-PA-O1A	2.31	118.10	110.93
2	B	810	TAD	PA-O5B-C5B	2.31	129.07	122.43
2	C	811	TAD	N6A-C6A-N1A	2.31	123.89	119.36
2	D	812	TAD	N6A-C6A-N1A	2.28	123.84	119.36
2	A	809	TAD	O2A-PA-O1A	2.24	117.88	110.93
2	C	811	TAD	O2B-C2B-C1B	2.15	117.72	111.23
2	D	812	TAD	C6A-C5A-N7A	-2.14	123.17	131.34
2	E	813	TAD	O4B-C1B-C2B	-2.13	103.51	106.77
2	B	810	TAD	C2B-C1B-N9A	2.13	118.73	113.27
2	F	814	TAD	C3D-C2D-C1D	2.12	104.34	101.85
2	D	812	TAD	C1B-N9A-C4A	2.12	130.30	126.64
2	B	810	TAD	N6A-C6A-N1A	2.11	123.52	119.36
2	B	810	TAD	O2A-PA-O1A	2.11	117.49	110.93
2	C	811	TAD	C6A-C5A-N7A	-2.10	123.30	131.34
2	F	814	TAD	N6A-C6A-N1A	2.08	123.46	119.36
2	D	812	TAD	O4D-C1D-C2D	2.08	107.94	104.37
2	E	813	TAD	C1B-N9A-C4A	2.05	130.18	126.64
2	E	813	TAD	C2B-C1B-N9A	2.02	118.46	113.27
2	D	812	TAD	C8A-N9A-C1B	-2.01	122.42	126.38
2	C	811	TAD	C2A-N1A-C6A	2.00	122.38	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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