WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2024 – 08:46 am BST

PDB ID	:	2VOJ
Title	:	Ternary complex of M. tuberculosis Rv2780 with NAD and pyruvate
Authors	:	Tripathi, S.M.; Ramachandran, R.
Deposited on	:	2008-02-18
Resolution	:	2.60 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

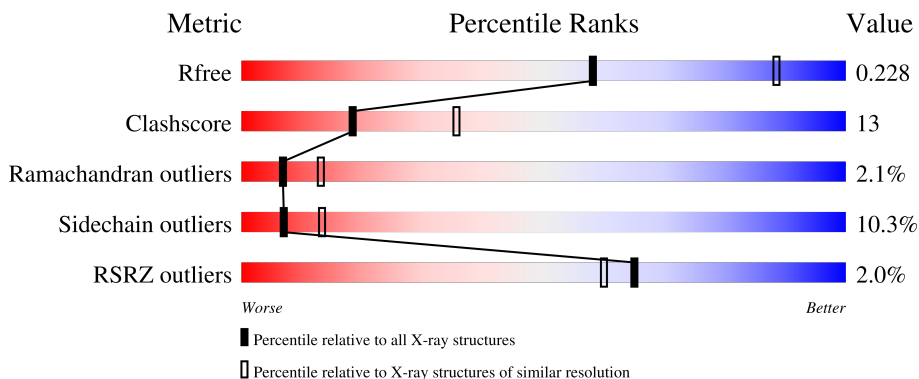|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance ⓘ

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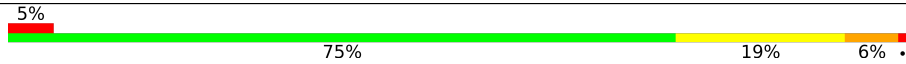*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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		0.228
Clashscore		13
Ramachandran outliers		2.1%
Sidechain outliers		10.3%
RSRZ outliers		2.0%

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	371	75% 17% 7% ·
1	C	371	.% 75% 18% 7%
1	E	371	5% 75% 19% 6% ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

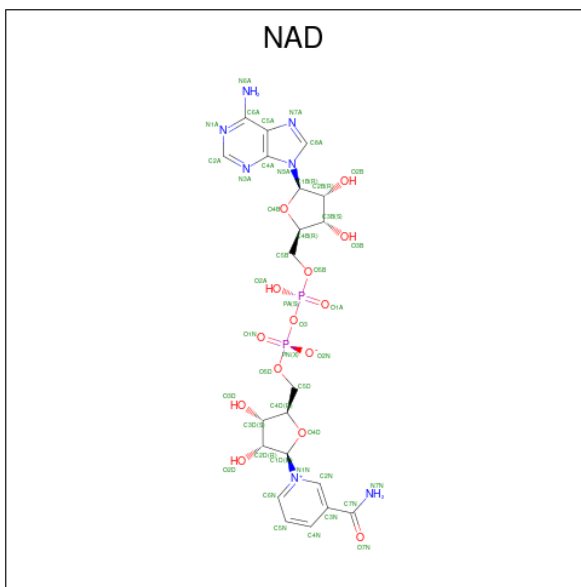| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	2OP	A	501	X	X	-	-
3	2OP	C	501	X	X	-	-
3	2OP	E	501	X	X	-	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 8412 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 ALANINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2708	1699	479	517	13			
1	C	371	Total	C	N	O	S	0	0	0
			2696	1692	476	515	13			
1	E	371	Total	C	N	O	S	0	0	0
			2699	1695	476	515	13			

- 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	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is (2S)-2-HYDROXYPROPANOIC ACID (three-letter code: 2OP) (formula: $C_3H_6O_3$).
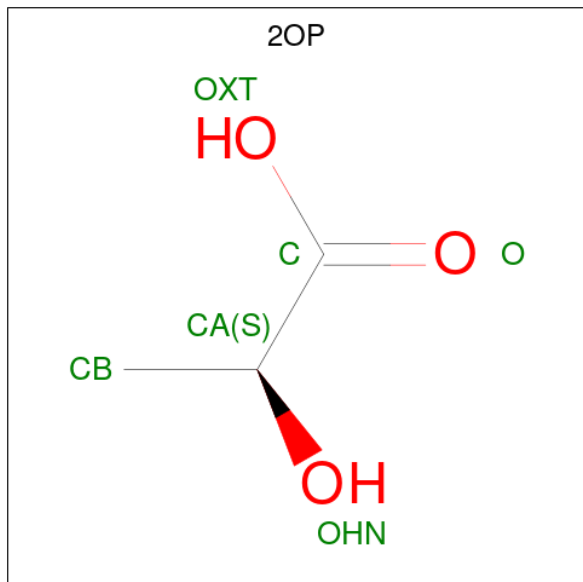
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	E	1	Total 6	C 3	O 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	65	Total 65	O 65	0	0
4	C	49	Total 49	O 49	0	0
4	E	45	Total 45	O 45	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.
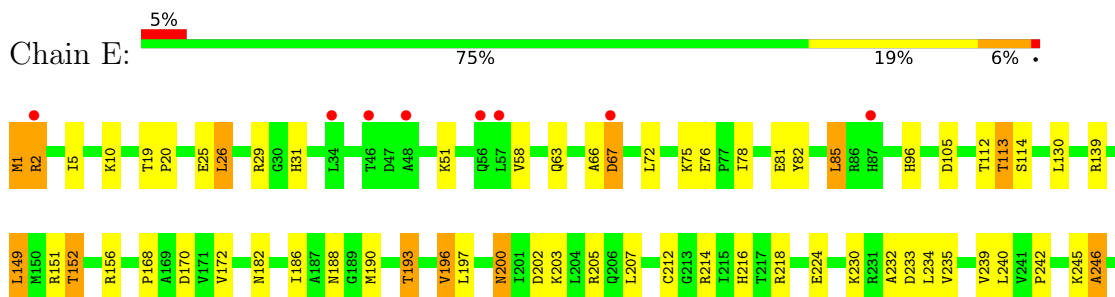
- Molecule 1: ALANINE DEHYDROGENASE

Chain A:

- Molecule 1: ALANINE DEHYDROGENASE

Chain C:
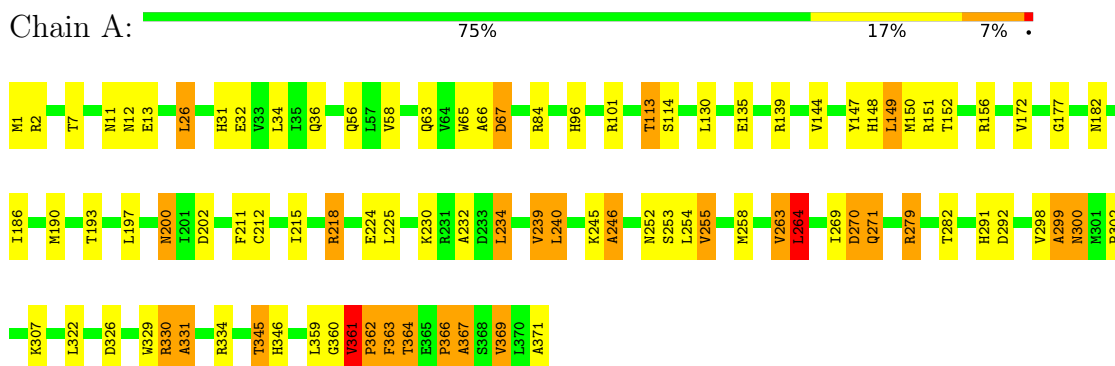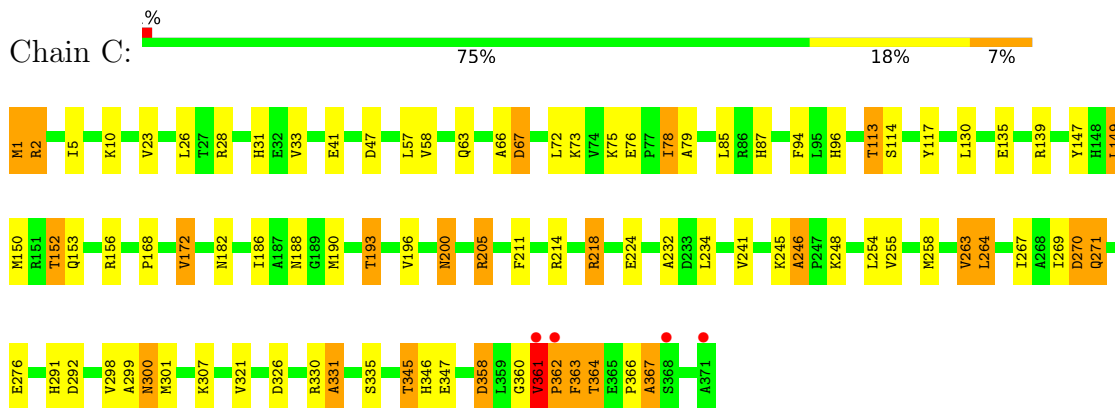
- Molecule 1: ALANINE DEHYDROGENASE

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	88.99Å 88.99Å 373.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	377.96 – 2.60 39.80 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.9 (377.96-2.60) 98.1 (39.80-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.18 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.187 , 0.230 0.186 , 0.228	Depositor DCC
R_{free} test set	2358 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	32.4	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 37.8	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8412	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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: 2OP, 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	0.67	0/2757	0.85	5/3757 (0.1%)
1	C	0.70	0/2745	0.85	5/3742 (0.1%)
1	E	0.72	0/2748	0.82	3/3746 (0.1%)
All	All	0.70	0/8250	0.84	13/11245 (0.1%)

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	0	2
1	C	0	2
1	E	0	1
All	All	0	5

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	240	LEU	N-CA-C	7.51	131.29	111.00
1	C	264	LEU	CA-CB-CG	7.38	132.28	115.30
1	A	264	LEU	CA-CB-CG	6.53	130.31	115.30
1	E	264	LEU	CA-CB-CG	6.36	129.92	115.30
1	C	300	ASN	N-CA-CB	-6.04	99.73	110.60
1	A	270	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	270	ASP	N-CA-C	-5.57	95.97	111.00
1	C	73	LYS	CD-CE-NZ	5.39	124.10	111.70
1	E	270	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	299	ALA	N-CA-C	-5.32	96.64	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	270	ASP	N-CA-C	-5.30	96.68	111.00
1	C	205	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	E	270	ASP	N-CA-C	-5.18	97.01	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	361	VAL	Peptide
1	A	364	THR	Peptide
1	C	361	VAL	Peptide
1	C	364	THR	Peptide
1	E	361	VAL	Peptide

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	2708	0	2709	78	1
1	C	2696	0	2687	70	0
1	E	2699	0	2696	73	1
2	A	44	0	26	4	0
2	C	44	0	26	0	0
2	E	44	0	26	2	0
3	A	6	0	3	1	0
3	C	6	0	3	2	0
3	E	6	0	3	1	0
4	A	65	0	0	0	0
4	C	49	0	0	2	0
4	E	45	0	0	6	0
All	All	8412	0	8179	219	1

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 13.

All (219) 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:E:255:VAL:HA	1:E:258:MET:HE2	1.42	1.01
1:A:96:HIS:HD2	1:A:271:GLN:NE2	1.58	0.99
1:C:299:ALA:O	1:C:300:ASN:HB3	1.60	0.98
1:A:255:VAL:HB	1:A:258:MET:CE	1.96	0.94
1:A:66:ALA:O	1:A:67:ASP:HB2	1.68	0.91
1:A:361:VAL:O	1:A:363:PHE:N	2.05	0.89
1:C:361:VAL:O	1:C:363:PHE:N	2.07	0.88
1:E:361:VAL:O	1:E:363:PHE:N	2.06	0.87
1:E:66:ALA:O	1:E:67:ASP:HB2	1.76	0.84
1:E:291:HIS:O	1:E:292:ASP:HB2	1.75	0.84
1:E:245:LYS:O	1:E:246:ALA:HB3	1.76	0.84
1:A:96:HIS:HD2	1:A:271:GLN:HE21	1.26	0.83
1:C:66:ALA:O	1:C:67:ASP:HB2	1.77	0.83
1:C:245:LYS:O	1:C:246:ALA:HB3	1.78	0.82
1:A:330:ARG:O	1:A:331:ALA:CB	2.28	0.81
1:C:139:ARG:HE	1:C:182:ASN:ND2	1.78	0.81
1:E:139:ARG:HE	1:E:182:ASN:HD22	1.30	0.80
1:E:361:VAL:HA	4:E:2044:HOH:O	1.81	0.80
1:C:291:HIS:O	1:C:292:ASP:HB2	1.82	0.79
1:A:255:VAL:HB	1:A:258:MET:HE2	1.62	0.79
1:C:58:VAL:HG11	1:C:63:GLN:HB2	1.66	0.78
1:C:218:ARG:HG2	1:C:224:GLU:HG3	1.64	0.77
1:C:362:PRO:O	1:C:363:PHE:CB	2.32	0.77
1:E:245:LYS:O	1:E:246:ALA:CB	2.29	0.77
1:E:218:ARG:HE	1:E:224:GLU:HG3	1.50	0.76
1:A:218:ARG:NH1	1:A:224:GLU:OE1	2.19	0.76
1:E:96:HIS:HD2	1:E:271:GLN:NE2	1.83	0.76
1:A:245:LYS:O	1:A:271:GLN:O	2.04	0.75
1:E:245:LYS:O	1:E:271:GLN:O	2.04	0.75
1:C:96:HIS:HD2	1:C:271:GLN:NE2	1.85	0.74
1:A:96:HIS:CD2	1:A:271:GLN:NE2	2.49	0.74
1:C:152:THR:HG22	1:C:153:GLN:HE21	1.52	0.74
1:C:245:LYS:O	1:C:246:ALA:CB	2.34	0.74
1:C:10:LYS:HE3	1:C:76:GLU:OE2	1.89	0.73
1:C:139:ARG:HE	1:C:182:ASN:HD22	1.33	0.73
1:E:362:PRO:O	1:E:363:PHE:CB	2.36	0.72
1:C:28:ARG:HH11	1:C:28:ARG:HG3	1.55	0.72
1:A:362:PRO:O	1:A:363:PHE:CB	2.39	0.71
1:A:245:LYS:O	1:A:246:ALA:HB3	1.91	0.71
1:E:58:VAL:HG11	1:E:63:GLN:HB3	1.72	0.70
1:A:139:ARG:HE	1:A:182:ASN:ND2	1.90	0.69
1:C:245:LYS:O	1:C:271:GLN:O	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:VAL:HG12	1:A:299:ALA:O	1.92	0.68
1:A:149:LEU:HD13	1:A:263:VAL:HG13	1.75	0.68
1:A:255:VAL:HB	1:A:258:MET:HE3	1.75	0.68
1:E:139:ARG:HE	1:E:182:ASN:ND2	1.91	0.67
1:C:96:HIS:HE1	3:C:501:2OP:OHN	1.77	0.67
1:E:298:VAL:HG12	1:E:299:ALA:O	1.95	0.67
1:C:31:HIS:HE1	1:C:326:ASP:OD1	1.78	0.67
1:A:139:ARG:HE	1:A:182:ASN:HD22	1.44	0.66
1:A:96:HIS:CD2	1:A:271:GLN:HE21	2.13	0.66
1:A:113:THR:HB	1:A:346:HIS:HD2	1.59	0.65
1:A:270:ASP:O	1:A:271:GLN:HB2	1.95	0.65
1:C:298:VAL:HG12	1:C:299:ALA:O	1.97	0.65
1:A:2:ARG:HG2	1:A:32:GLU:HB2	1.78	0.64
1:A:258:MET:HE1	1:A:264:LEU:HD21	1.79	0.64
1:A:291:HIS:O	1:A:292:ASP:HB2	1.98	0.64
1:A:245:LYS:O	1:A:246:ALA:CB	2.43	0.64
1:C:299:ALA:O	1:C:300:ASN:CB	2.35	0.64
1:C:75:LYS:HE2	1:C:75:LYS:HA	1.79	0.64
1:A:330:ARG:O	1:A:331:ALA:HB3	1.98	0.63
1:C:330:ARG:O	1:C:331:ALA:CB	2.46	0.63
1:A:11:ASN:ND2	1:A:282:THR:HB	2.13	0.62
1:A:270:ASP:O	1:A:271:GLN:CB	2.42	0.62
1:E:96:HIS:HE1	3:E:501:2OP:OHN	1.82	0.62
1:C:78:ILE:CD1	1:C:79:ALA:H	2.13	0.61
1:A:66:ALA:O	1:A:67:ASP:CB	2.42	0.61
1:A:113:THR:HB	1:A:346:HIS:CD2	2.35	0.60
1:A:172:VAL:HG13	1:A:232:ALA:HB2	1.84	0.60
1:E:360:GLY:O	1:E:361:VAL:C	2.39	0.59
1:C:78:ILE:HD13	1:C:79:ALA:H	1.66	0.59
1:E:330:ARG:O	1:E:331:ALA:CB	2.50	0.59
1:C:245:LYS:HB2	1:C:358:ASP:OD1	2.03	0.59
1:A:58:VAL:HG11	1:A:63:GLN:HB3	1.85	0.59
1:C:113:THR:HB	1:C:346:HIS:HD2	1.68	0.59
1:E:203:LYS:HE3	2:E:500:NAD:O3B	2.03	0.59
1:C:360:GLY:O	1:C:361:VAL:C	2.42	0.58
1:C:330:ARG:O	1:C:331:ALA:HB3	2.04	0.58
1:E:200:ASN:C	1:E:200:ASN:HD22	2.07	0.57
1:A:31:HIS:HE1	1:A:326:ASP:OD1	1.87	0.57
1:C:114:SER:OG	1:C:345:THR:HB	2.03	0.57
1:E:113:THR:HB	1:E:346:HIS:HD2	1.69	0.57
1:A:360:GLY:O	1:A:361:VAL:C	2.42	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:291:HIS:O	1:E:292:ASP:CB	2.43	0.57
1:C:96:HIS:HD2	1:C:271:GLN:HE21	1.50	0.57
1:E:10:LYS:HE3	1:E:76:GLU:OE2	2.04	0.57
1:C:255:VAL:HA	1:C:258:MET:HG3	1.86	0.57
1:C:113:THR:HB	1:C:346:HIS:CD2	2.40	0.56
1:E:168:PRO:HG2	1:E:193:THR:HG22	1.87	0.56
1:A:11:ASN:HD22	1:A:282:THR:HB	1.68	0.56
1:C:58:VAL:CG1	1:C:63:GLN:HB2	2.36	0.56
1:E:270:ASP:O	1:E:271:GLN:CB	2.51	0.56
1:A:13:GLU:OE1	1:A:300:ASN:ND2	2.30	0.56
1:A:298:VAL:C	1:A:299:ALA:O	2.42	0.56
1:A:114:SER:OG	1:A:345:THR:HB	2.05	0.56
1:E:66:ALA:O	1:E:67:ASP:CB	2.51	0.55
1:E:26:LEU:HD13	1:E:322:LEU:HD23	1.89	0.55
1:C:270:ASP:O	1:C:271:GLN:CB	2.46	0.55
1:E:113:THR:HB	1:E:346:HIS:CD2	2.42	0.55
1:C:361:VAL:O	1:C:362:PRO:C	2.45	0.54
1:C:218:ARG:HG2	1:C:224:GLU:CG	2.37	0.54
1:A:299:ALA:O	1:A:300:ASN:CB	2.53	0.54
1:E:172:VAL:HG13	1:E:232:ALA:HB2	1.89	0.53
1:E:255:VAL:HB	1:E:258:MET:HE3	1.88	0.53
1:E:364:THR:HG21	4:E:2045:HOH:O	2.09	0.53
1:C:255:VAL:HB	1:C:258:MET:HE3	1.91	0.53
1:A:258:MET:HE1	1:A:264:LEU:HD11	1.90	0.53
1:E:172:VAL:CG1	1:E:232:ALA:HB2	2.39	0.53
1:A:200:ASN:C	1:A:200:ASN:HD22	2.11	0.53
1:A:361:VAL:O	1:A:362:PRO:C	2.46	0.53
1:E:75:LYS:HE2	1:E:75:LYS:HA	1.91	0.53
1:E:1:MET:HG3	1:E:2:ARG:N	2.23	0.53
1:E:96:HIS:CD2	1:E:271:GLN:NE2	2.73	0.52
1:A:7:THR:H	1:A:36:GLN:NE2	2.06	0.52
1:C:96:HIS:CE1	3:C:501:2OP:OHN	2.62	0.52
1:C:188:ASN:HD21	1:C:214:ARG:HD3	1.74	0.52
1:E:269:ILE:HD13	1:E:278:SER:HB3	1.92	0.52
1:A:96:HIS:HE1	3:A:501:2OP:OHN	1.92	0.52
1:C:152:THR:CG2	1:C:153:GLN:HE21	2.22	0.52
1:C:23:VAL:HG22	1:C:33:VAL:HG11	1.91	0.51
1:C:186:ILE:HG22	1:C:190:MET:HE1	1.91	0.51
1:E:19:THR:HB	1:E:20:PRO:CD	2.40	0.51
1:A:330:ARG:O	1:A:331:ALA:HB2	2.08	0.51
1:A:240:LEU:CB	2:A:500:NAD:H51A	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:ILE:HG13	1:E:72:LEU:HB2	1.92	0.51
1:C:72:LEU:HD21	1:C:321:VAL:HG22	1.92	0.50
1:C:66:ALA:O	1:C:67:ASP:CB	2.48	0.50
1:E:186:ILE:HG22	1:E:190:MET:CE	2.41	0.50
1:A:211:PHE:CD1	1:A:215:ILE:HD12	2.45	0.50
1:C:291:HIS:O	1:C:292:ASP:CB	2.53	0.50
1:E:269:ILE:C	1:E:270:ASP:O	2.46	0.50
1:C:28:ARG:HH11	1:C:28:ARG:CG	2.24	0.50
1:A:252:ASN:HA	1:A:255:VAL:HG13	1.94	0.50
1:C:168:PRO:HG2	1:C:193:THR:HG22	1.94	0.50
1:E:19:THR:HB	1:E:20:PRO:HD2	1.93	0.50
1:A:258:MET:CE	1:A:264:LEU:HD11	2.41	0.49
1:A:11:ASN:ND2	1:A:12:ASN:HD22	2.09	0.49
1:C:267:ILE:HG23	1:C:301:MET:HE1	1.95	0.49
1:E:10:LYS:HE2	1:E:78:ILE:HD12	1.94	0.49
1:A:334:ARG:HH21	1:A:371:ALA:HB3	1.78	0.49
1:C:366:PRO:O	1:C:367:ALA:HB2	2.13	0.49
1:C:139:ARG:HH21	1:C:182:ASN:HD21	1.59	0.48
1:A:11:ASN:HD21	1:A:12:ASN:HD22	1.61	0.48
1:A:101:ARG:NH2	1:A:359:LEU:O	2.46	0.48
1:C:269:ILE:C	1:C:270:ASP:O	2.45	0.48
1:C:248:LYS:HD2	1:C:276:GLU:HA	1.96	0.48
1:A:135:GLU:OE2	1:C:205:ARG:HD3	2.13	0.48
1:C:149:LEU:HD13	1:C:263:VAL:HG13	1.95	0.48
1:A:96:HIS:HD2	1:A:271:GLN:HE22	1.51	0.48
1:A:291:HIS:O	1:A:292:ASP:CB	2.62	0.48
1:A:26:LEU:HD13	1:A:322:LEU:HD23	1.96	0.48
1:E:330:ARG:O	1:E:331:ALA:HB3	2.14	0.48
1:C:200:ASN:C	1:C:200:ASN:HD22	2.16	0.47
1:C:300:ASN:HB2	4:C:2004:HOH:O	2.13	0.47
1:A:186:ILE:HG22	1:A:190:MET:HE2	1.96	0.47
1:A:139:ARG:HH21	1:A:182:ASN:HD21	1.60	0.47
1:A:200:ASN:HD21	1:A:202:ASP:HB2	1.79	0.47
1:E:255:VAL:HB	1:E:258:MET:CE	2.45	0.47
1:E:26:LEU:HD13	1:E:322:LEU:CD2	2.44	0.46
1:E:31:HIS:HE1	1:E:326:ASP:OD1	1.99	0.46
1:E:149:LEU:HD13	1:E:263:VAL:HG13	1.97	0.46
1:A:239:VAL:HG22	2:A:500:NAD:C4A	2.46	0.46
1:E:75:LYS:HE2	4:E:2007:HOH:O	2.16	0.45
1:E:255:VAL:CA	1:E:258:MET:HE2	2.31	0.45
1:E:186:ILE:HG22	1:E:190:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:TRP:CD1	1:A:84:ARG:HD3	2.52	0.45
1:E:96:HIS:HD2	1:E:271:GLN:HE21	1.59	0.45
1:E:96:HIS:HD2	1:E:271:GLN:HE22	1.61	0.45
1:E:205:ARG:NH2	4:E:2023:HOH:O	2.49	0.45
1:E:235:VAL:HB	1:E:264:LEU:HD13	1.99	0.45
1:A:269:ILE:C	1:A:270:ASP:O	2.49	0.44
1:C:139:ARG:NE	1:C:182:ASN:HD22	2.09	0.44
1:E:240:LEU:HB2	2:E:500:NAD:H3D	2.00	0.44
1:C:186:ILE:HG22	1:C:190:MET:CE	2.48	0.44
1:C:298:VAL:C	1:C:299:ALA:O	2.51	0.44
1:A:255:VAL:HA	1:A:258:MET:HG3	2.00	0.44
1:A:329:TRP:HH2	1:A:369:VAL:HG13	1.82	0.44
1:E:364:THR:CB	4:E:2045:HOH:O	2.66	0.44
1:A:255:VAL:CB	1:A:258:MET:HE3	2.45	0.43
1:E:25:GLU:OE2	1:E:29:ARG:NH1	2.49	0.43
1:A:144:VAL:O	1:A:148:HIS:HD2	2.00	0.43
1:A:149:LEU:HD13	1:A:263:VAL:CG1	2.44	0.43
1:C:211:PHE:HB2	4:C:2026:HOH:O	2.18	0.43
1:C:87:HIS:HE2	1:C:347:GLU:CG	2.31	0.43
1:A:366:PRO:O	1:A:367:ALA:HB2	2.19	0.43
1:E:188:ASN:HD21	1:E:214:ARG:HD3	1.83	0.43
1:E:216:HIS:CD2	1:E:216:HIS:N	2.87	0.43
1:C:172:VAL:HG13	1:C:232:ALA:HB2	2.01	0.43
1:E:78:ILE:HG22	1:E:81:GLU:OE1	2.18	0.43
1:E:172:VAL:HG13	1:E:232:ALA:CB	2.49	0.43
1:C:1:MET:HG3	1:C:2:ARG:N	2.34	0.42
1:A:234:LEU:HD23	1:A:263:VAL:HG22	2.01	0.42
1:C:147:TYR:CE1	1:C:150:MET:HE1	2.54	0.42
1:E:264:LEU:HB3	1:E:275:PHE:CE1	2.54	0.42
1:E:156:ARG:HD3	1:E:233:ASP:OD1	2.19	0.42
1:A:177:GLY:HA3	2:A:500:NAD:O5B	2.19	0.42
1:A:34:LEU:HD23	1:A:56:GLN:HB2	2.02	0.42
1:C:135:GLU:OE2	1:E:205:ARG:HD3	2.19	0.42
1:E:196:VAL:HG11	1:E:207:LEU:HD23	2.02	0.42
1:E:197:LEU:HA	1:E:218:ARG:O	2.20	0.42
1:A:255:VAL:HA	1:A:258:MET:CE	2.49	0.41
1:E:112:THR:O	1:E:345:THR:CG2	2.68	0.41
1:A:1:MET:CG	1:A:2:ARG:N	2.84	0.41
1:E:114:SER:OG	1:E:345:THR:HB	2.20	0.41
1:C:94:PHE:CD2	1:C:117:TYR:HB2	2.55	0.41
1:E:82:TYR:HA	1:E:85:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ILE:HG22	1:A:190:MET:CE	2.50	0.41
1:A:200:ASN:HD22	1:A:202:ASP:N	2.19	0.41
1:E:345:THR:HG23	4:E:2009:HOH:O	2.21	0.41
1:E:366:PRO:O	1:E:367:ALA:HB2	2.20	0.41
1:A:147:TYR:O	1:A:150:MET:HG3	2.21	0.41
1:A:197:LEU:HG	1:A:218:ARG:HB3	2.03	0.40
1:A:302:PRO:HD3	2:A:500:NAD:O7N	2.21	0.40
1:C:47:ASP:HB3	1:C:57:LEU:HD11	2.03	0.40
1:E:361:VAL:C	1:E:363:PHE:N	2.72	0.40
1:C:218:ARG:NH1	1:C:224:GLU:OE1	2.52	0.40
1:C:147:TYR:CD1	1:C:150:MET:HE2	2.56	0.40
1:C:5:ILE:HG13	1:C:72:LEU:HB2	2.02	0.40
1:E:200:ASN:HD21	1:E:202:ASP:HB2	1.86	0.40

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ARG:NH1	1:E:105:ASP:OD2[7_545]	2.14	0.06

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	369/371 (100%)	348 (94%)	13 (4%)	8 (2%)	6	12
1	C	369/371 (100%)	350 (95%)	12 (3%)	7 (2%)	8	15
1	E	369/371 (100%)	345 (94%)	16 (4%)	8 (2%)	6	12
All	All	1107/1113 (100%)	1043 (94%)	41 (4%)	23 (2%)	7	13

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	331	ALA
1	A	362	PRO
1	A	363	PHE
1	A	367	ALA
1	C	331	ALA
1	C	362	PRO
1	C	363	PHE
1	C	367	ALA
1	E	67	ASP
1	E	331	ALA
1	E	362	PRO
1	E	363	PHE
1	E	367	ALA
1	A	67	ASP
1	A	361	VAL
1	C	67	ASP
1	E	246	ALA
1	A	246	ALA
1	C	246	ALA
1	E	152	THR
1	E	361	VAL
1	C	361	VAL
1	A	366	PRO

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	273/276 (99%)	245 (90%)	28 (10%)	7	13
1	C	270/276 (98%)	243 (90%)	27 (10%)	7	14
1	E	271/276 (98%)	242 (89%)	29 (11%)	6	12
All	All	814/828 (98%)	730 (90%)	84 (10%)	7	13

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	113	THR
1	A	130	LEU
1	A	149	LEU
1	A	151	ARG
1	A	152	THR
1	A	156	ARG
1	A	193	THR
1	A	200	ASN
1	A	212	CYS
1	A	218	ARG
1	A	225	LEU
1	A	230	LYS
1	A	234	LEU
1	A	239	VAL
1	A	253	SER
1	A	254	LEU
1	A	255	VAL
1	A	263	VAL
1	A	264	LEU
1	A	271	GLN
1	A	279	ARG
1	A	300	ASN
1	A	307	LYS
1	A	330	ARG
1	A	345	THR
1	A	364	THR
1	A	369	VAL
1	C	1	MET
1	C	2	ARG
1	C	26	LEU
1	C	41	GLU
1	C	78	ILE
1	C	85	LEU
1	C	113	THR
1	C	130	LEU
1	C	149	LEU
1	C	152	THR
1	C	156	ARG
1	C	172	VAL
1	C	193	THR
1	C	196	VAL
1	C	200	ASN

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Mol	Chain	Res	Type
1	C	218	ARG
1	C	234	LEU
1	C	241	VAL
1	C	254	LEU
1	C	263	VAL
1	C	264	LEU
1	C	271	GLN
1	C	307	LYS
1	C	335	SER
1	C	345	THR
1	C	358	ASP
1	C	364	THR
1	E	1	MET
1	E	2	ARG
1	E	26	LEU
1	E	51	LYS
1	E	85	LEU
1	E	113	THR
1	E	130	LEU
1	E	149	LEU
1	E	151	ARG
1	E	152	THR
1	E	170	ASP
1	E	193	THR
1	E	196	VAL
1	E	200	ASN
1	E	212	CYS
1	E	230	LYS
1	E	234	LEU
1	E	239	VAL
1	E	242	PRO
1	E	254	LEU
1	E	255	VAL
1	E	263	VAL
1	E	264	LEU
1	E	271	GLN
1	E	300	ASN
1	E	307	LYS
1	E	339	LEU
1	E	345	THR
1	E	364	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	31	HIS
1	A	36	GLN
1	A	63	GLN
1	A	96	HIS
1	A	148	HIS
1	A	153	GLN
1	A	182	ASN
1	A	200	ASN
1	A	271	GLN
1	A	346	HIS
1	C	31	HIS
1	C	36	GLN
1	C	89	GLN
1	C	96	HIS
1	C	148	HIS
1	C	153	GLN
1	C	182	ASN
1	C	188	ASN
1	C	200	ASN
1	C	257	HIS
1	C	271	GLN
1	C	327	HIS
1	C	346	HIS
1	E	31	HIS
1	E	36	GLN
1	E	63	GLN
1	E	89	GLN
1	E	96	HIS
1	E	148	HIS
1	E	153	GLN
1	E	182	ASN
1	E	200	ASN
1	E	216	HIS
1	E	257	HIS
1	E	271	GLN
1	E	300	ASN
1	E	346	HIS

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides 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	$\#|Z| > 2$
3	2OP	C	501	-	5,5,5	2.74	3 (60%)	4,6,6	2.60	3 (75%)
2	NAD	C	500	-	42,48,48	1.80	3 (7%)	50,73,73	1.21	4 (8%)
3	2OP	E	501	-	5,5,5	2.79	3 (60%)	4,6,6	3.25	3 (75%)
2	NAD	E	500	-	42,48,48	1.70	3 (7%)	50,73,73	1.45	7 (14%)
3	2OP	A	501	-	5,5,5	2.81	3 (60%)	4,6,6	2.62	3 (75%)
2	NAD	A	500	-	42,48,48	1.70	5 (11%)	50,73,73	1.43	5 (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
3	2OP	C	501	-	1/1/2/2	2/4/4/4	-
3	2OP	E	501	-	1/1/2/2	2/4/4/4	-
3	2OP	A	501	-	1/1/2/2	2/4/4/4	-
2	NAD	E	500	-	-	9/26/62/62	0/5/5/5
2	NAD	C	500	-	-	7/26/62/62	0/5/5/5
2	NAD	A	500	-	-	6/26/62/62	0/5/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	NAD	O7N-C7N	9.02	1.41	1.24
2	E	500	NAD	O7N-C7N	8.10	1.39	1.24
2	A	500	NAD	O7N-C7N	8.03	1.39	1.24
3	A	501	2OP	CA-C	-4.72	1.39	1.51
3	C	501	2OP	CA-C	-4.71	1.39	1.51
2	E	500	NAD	C2A-N3A	4.71	1.39	1.32
2	C	500	NAD	C2A-N3A	4.48	1.39	1.32
3	E	501	2OP	CA-C	-4.12	1.40	1.51
2	A	500	NAD	C2A-N3A	3.53	1.37	1.32
3	E	501	2OP	OHN-CA	-3.50	1.30	1.42
3	E	501	2OP	O-C	3.10	1.31	1.22
3	A	501	2OP	O-C	3.09	1.31	1.22
2	C	500	NAD	C2A-N1A	2.92	1.39	1.33
3	C	501	2OP	O-C	2.87	1.30	1.22
3	A	501	2OP	OHN-CA	-2.78	1.33	1.42
2	E	500	NAD	C2A-N1A	2.67	1.38	1.33
3	C	501	2OP	OHN-CA	-2.64	1.33	1.42
2	A	500	NAD	C2A-N1A	2.50	1.38	1.33
2	A	500	NAD	O4B-C4B	-2.32	1.39	1.45
2	A	500	NAD	C2N-N1N	2.18	1.37	1.35

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	NAD	N3A-C2A-N1A	-6.51	118.50	128.68
2	E	500	NAD	N3A-C2A-N1A	-5.90	119.46	128.68
3	E	501	2OP	CB-CA-C	5.00	121.96	110.63
2	C	500	NAD	N3A-C2A-N1A	-4.94	120.96	128.68
3	A	501	2OP	CB-CA-C	3.60	118.79	110.63
2	A	500	NAD	O4D-C1D-C2D	-3.23	102.20	106.93
3	C	501	2OP	CB-CA-C	3.20	117.88	110.63
3	A	501	2OP	OHN-CA-CB	3.07	123.59	110.54
2	E	500	NAD	PN-O3-PA	-3.00	122.54	132.83
3	C	501	2OP	OHN-CA-CB	2.84	122.60	110.54
2	E	500	NAD	C1B-N9A-C4A	-2.82	121.68	126.64
3	E	501	2OP	OHN-CA-C	2.74	119.80	109.75
3	C	501	2OP	OHN-CA-C	2.66	119.52	109.75
3	E	501	2OP	OXT-C-O	-2.54	118.32	124.09
2	E	500	NAD	O4D-C1D-C2D	-2.45	103.34	106.93
2	E	500	NAD	C3N-C7N-N7N	2.44	120.67	117.75
2	E	500	NAD	O4B-C4B-C3B	2.42	109.90	105.11
2	A	500	NAD	O2N-PN-O1N	2.22	123.20	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	NAD	O3D-C3D-C2D	-2.13	104.94	111.82
3	A	501	2OP	OHN-CA-C	2.12	117.53	109.75
2	E	500	NAD	O2N-PN-O1N	2.08	122.53	112.24
2	A	500	NAD	O4B-C1B-C2B	-2.05	103.92	106.93
2	C	500	NAD	O4D-C1D-C2D	-2.05	103.93	106.93
2	C	500	NAD	O2N-PN-O1N	2.04	122.35	112.24
2	C	500	NAD	C3D-C2D-C1D	-2.02	97.94	100.98

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	501	2OP	CA
3	C	501	2OP	CA
3	E	501	2OP	CA

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	NAD	O4D-C1D-N1N-C6N
2	C	500	NAD	O4D-C1D-N1N-C6N
2	E	500	NAD	O4B-C4B-C5B-O5B
2	E	500	NAD	O4D-C1D-N1N-C6N
3	A	501	2OP	O-C-CA-CB
3	A	501	2OP	OXT-C-CA-CB
3	C	501	2OP	O-C-CA-CB
3	C	501	2OP	OXT-C-CA-CB
3	E	501	2OP	O-C-CA-CB
3	E	501	2OP	OXT-C-CA-CB
2	A	500	NAD	C4N-C3N-C7N-N7N
2	E	500	NAD	C4N-C3N-C7N-O7N
2	E	500	NAD	C4N-C3N-C7N-N7N
2	A	500	NAD	C4N-C3N-C7N-O7N
2	C	500	NAD	C4N-C3N-C7N-N7N
2	E	500	NAD	C2N-C3N-C7N-O7N
2	E	500	NAD	C2N-C3N-C7N-N7N
2	C	500	NAD	C4N-C3N-C7N-O7N
2	A	500	NAD	C2N-C3N-C7N-O7N
2	A	500	NAD	C2N-C3N-C7N-N7N
2	C	500	NAD	C2N-C3N-C7N-O7N
2	C	500	NAD	C2N-C3N-C7N-N7N
2	E	500	NAD	C3B-C4B-C5B-O5B
2	E	500	NAD	PN-O3-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	C	500	NAD	PN-O3-PA-O1A
2	E	500	NAD	PN-O3-PA-O2A
2	A	500	NAD	O4B-C4B-C5B-O5B
2	C	500	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	2OP	2	0
3	E	501	2OP	1	0
2	E	500	NAD	2	0
3	A	501	2OP	1	0
2	A	500	NAD	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand NAD C 500

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD E 500

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD A 500

Bond lengths

Bond angles

Torsions

Rings
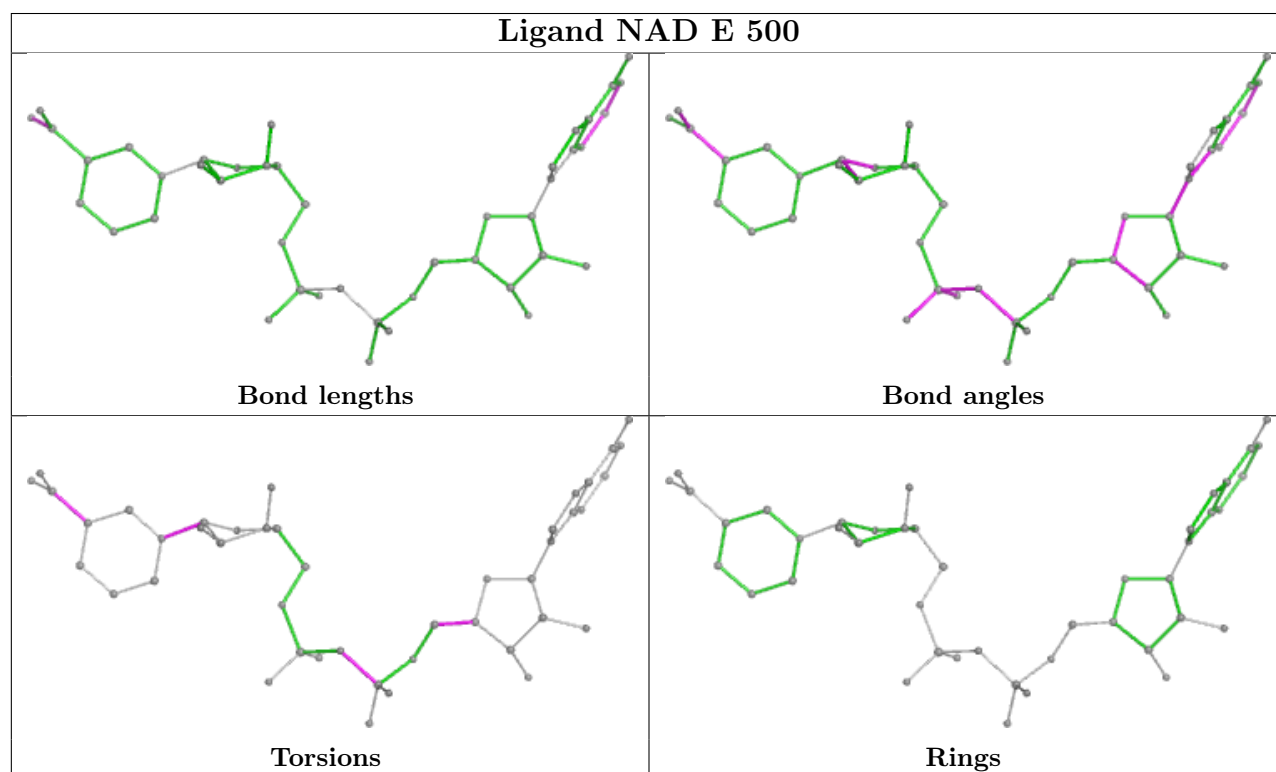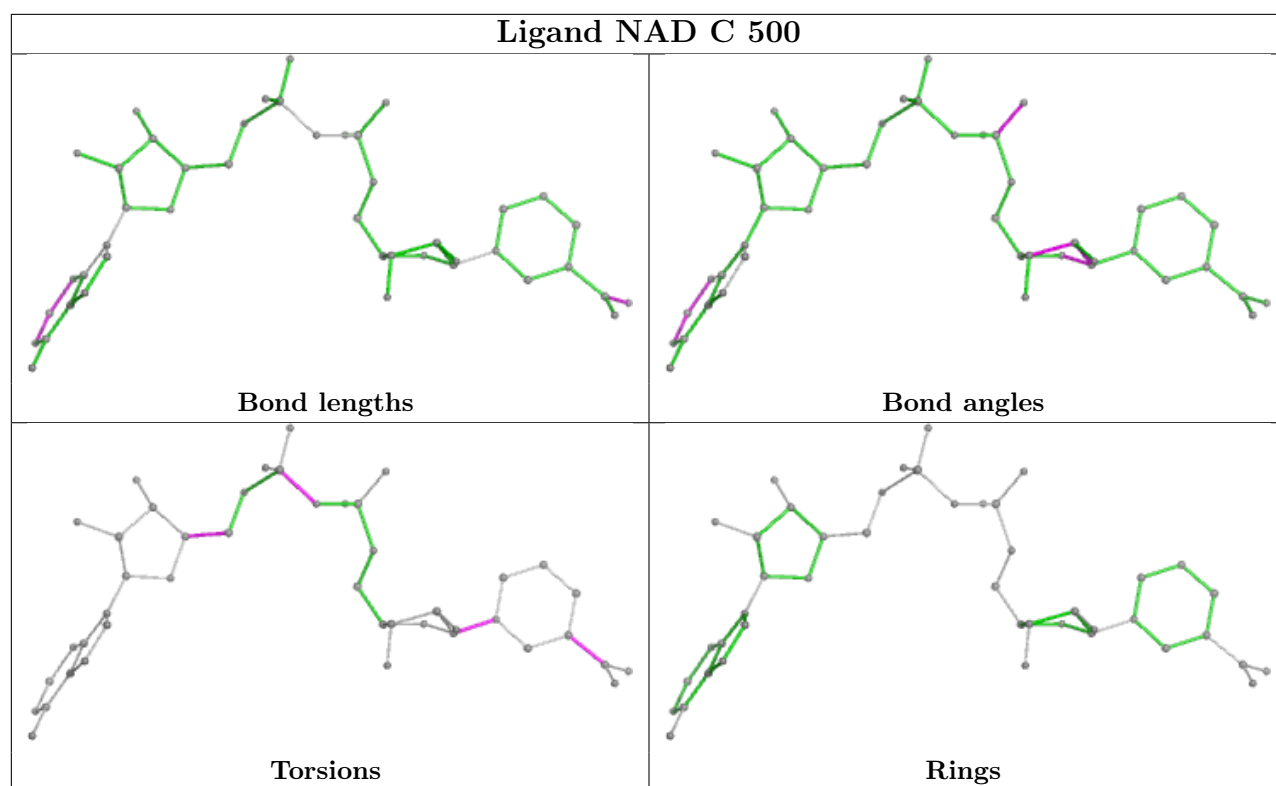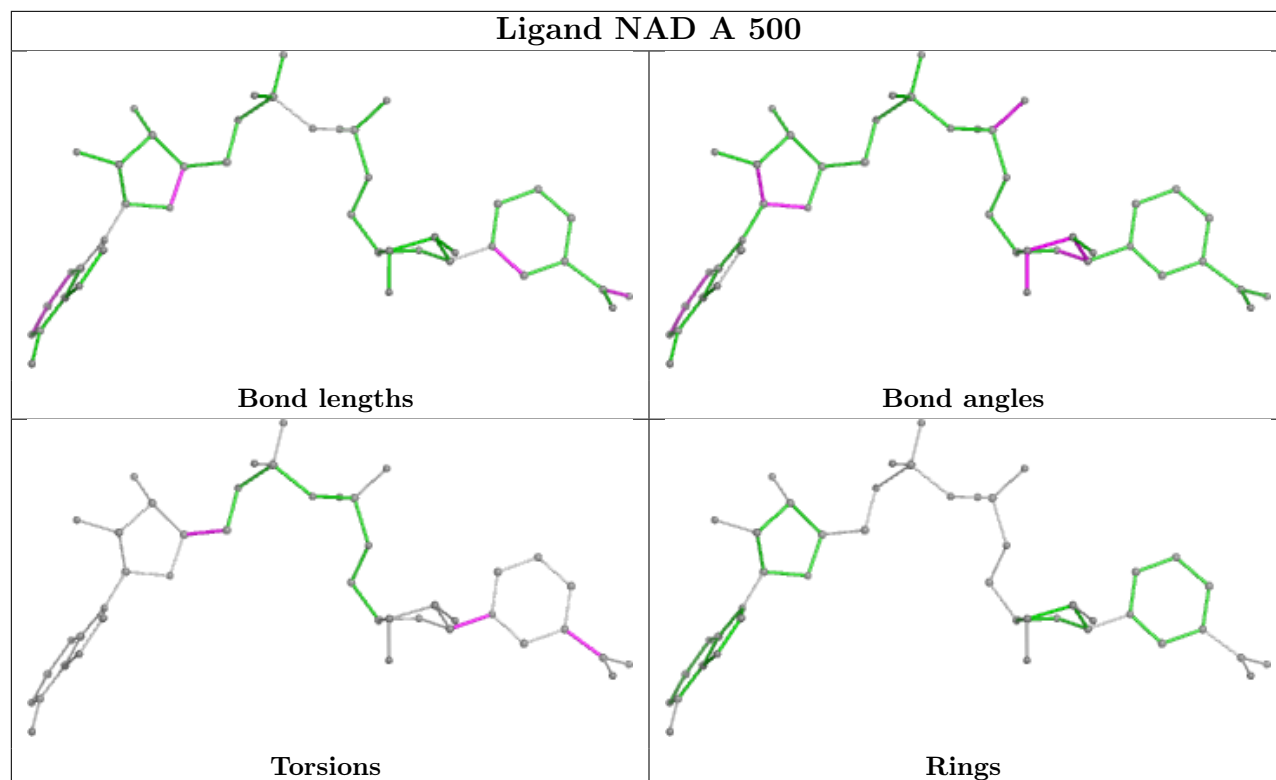
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	371/371 (100%)	-0.48	0	100	100	13, 29, 49, 57	0
1	C	371/371 (100%)	-0.42	4 (1%)	80	78	13, 29, 49, 57	0
1	E	371/371 (100%)	-0.14	18 (4%)	29	23	13, 29, 49, 58	0
All	All	1113/1113 (100%)	-0.35	22 (1%)	65	60	13, 29, 49, 58	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	361	VAL	5.8
1	C	371	ALA	4.3
1	E	371	ALA	4.2
1	E	56	GLN	4.0
1	E	57	LEU	3.3
1	E	347	GLU	3.3
1	E	370	LEU	3.2
1	C	362	PRO	3.1
1	E	48	ALA	3.1
1	E	329	TRP	2.8
1	E	365	GLU	2.8
1	E	334	ARG	2.7
1	E	330	ARG	2.6
1	C	361	VAL	2.5
1	E	34	LEU	2.4
1	E	368	SER	2.3
1	E	2	ARG	2.3
1	C	368	SER	2.3
1	E	87	HIS	2.2
1	E	46	THR	2.2
1	E	360	GLY	2.1
1	E	67	ASP	2.0

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 monosaccharides in this entry.

6.4 Ligands ⓘ

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. 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.

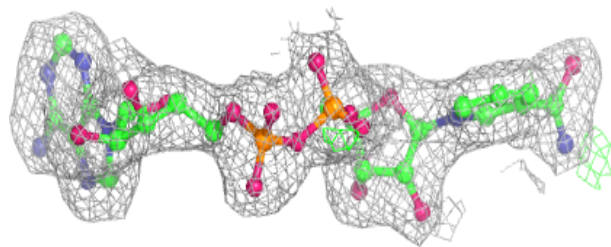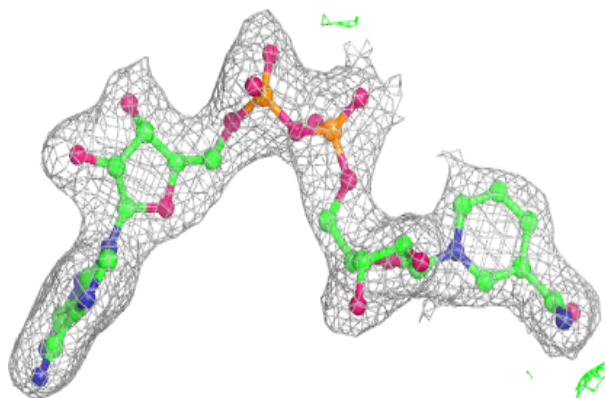| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	C	500	44/44	0.98	0.10	15,21,25,28	0
2	NAD	E	500	44/44	0.98	0.09	19,23,25,26	0
3	2OP	A	501	6/6	0.98	0.10	15,20,21,22	0
3	2OP	C	501	6/6	0.98	0.12	18,20,21,22	0
3	2OP	E	501	6/6	0.98	0.12	25,28,28,29	0
2	NAD	A	500	44/44	0.99	0.10	9,15,20,26	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.
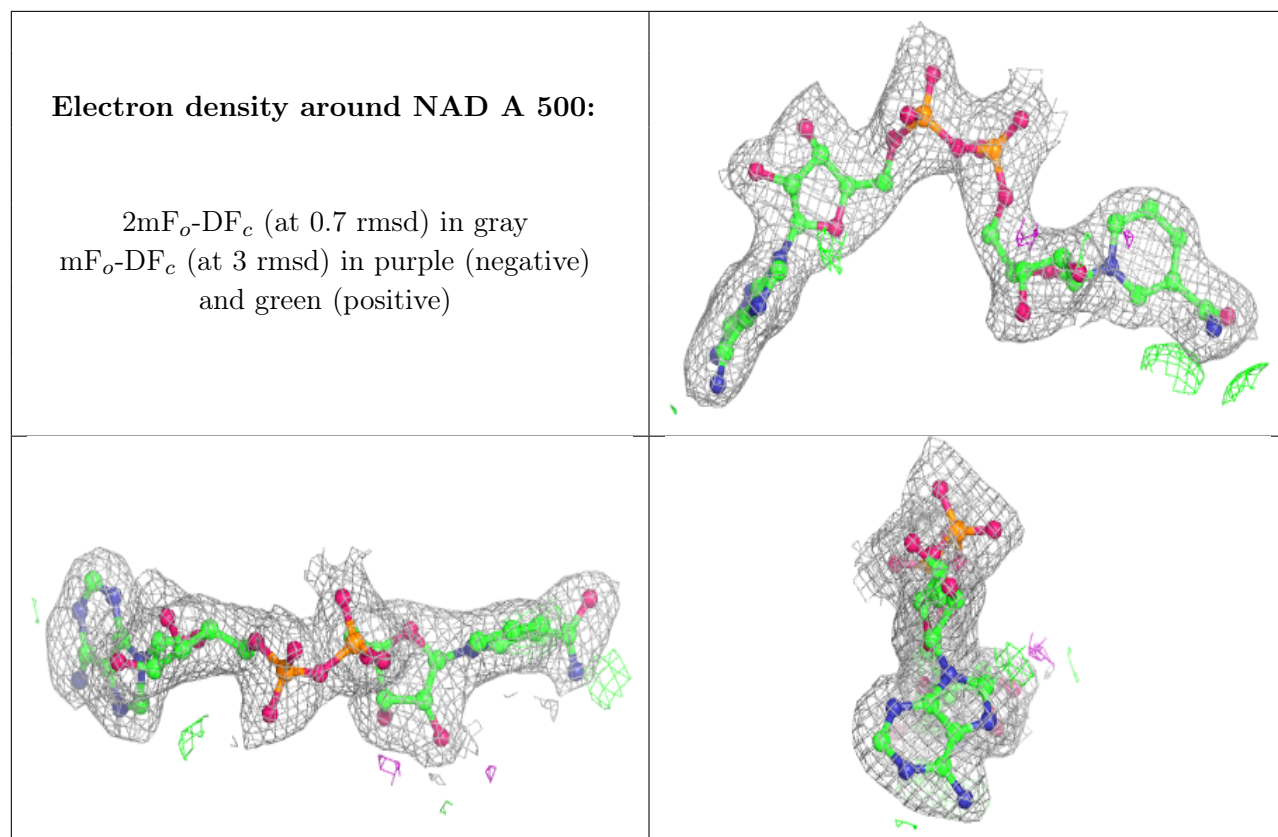
Electron density around NAD C 500:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
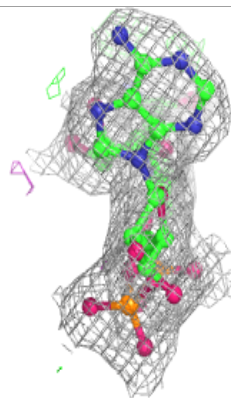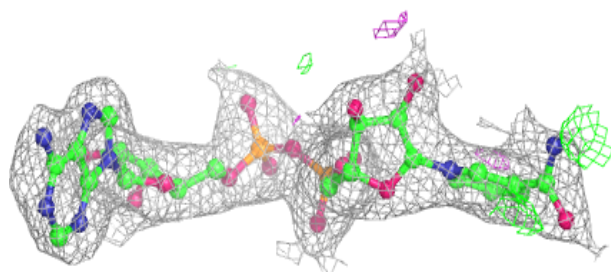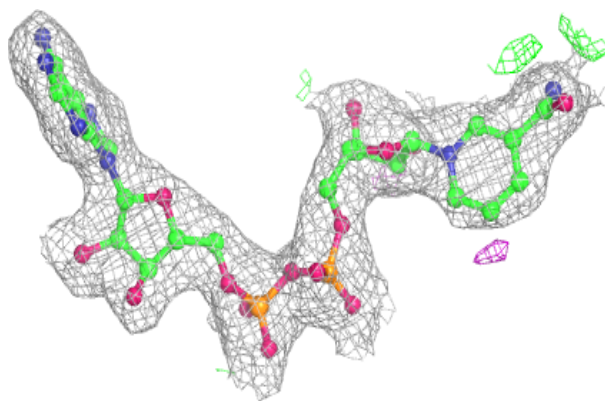
Electron density around NAD E 500:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around NAD A 500:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.