WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

May 22, 2020 – 04:11 am BST

PDB ID : 2P5U

Title : Crystal structure of Thermus thermophilus HB8 UDP-glucose 4-epimerase complex with NAD

Authors : Fu, Z.-Q.; Chen, L.; Ebihara, A.; Shinkai, A.; Kuramitsu, S.; Yokoyama, S.; Zhao, M.; Dillard, B.; Chrzas, J.; Rose, J.P.; Wang, B.-C.; Southeast Collaboratory for Structural Genomics (SECSG); RIKEN Structural Genomics/Proteomics Initiative (RSGI)

Deposited on : 2007-03-16

Resolution : 2.37 Å(reported)

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

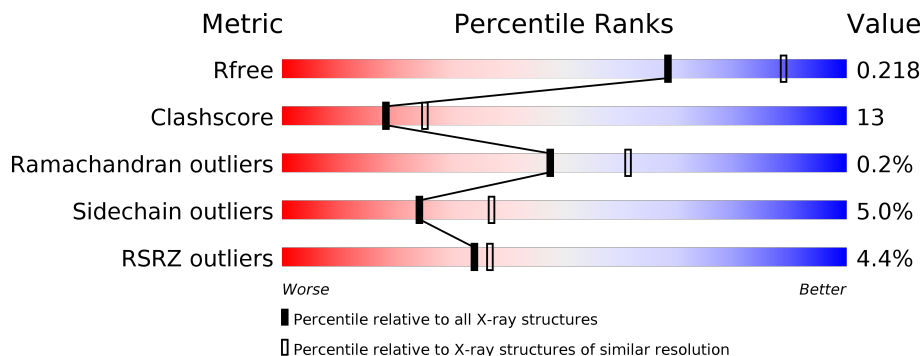|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.37 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		0.218
Clashscore		13
Ramachandran outliers		0.2%
Sidechain outliers		5.0%
RSRZ outliers		4.4%

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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 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	311	5% / 76% / 22% / •
1	B	311	6% / 75% / 23% / •
1	C	311	5% / 72% / 26% / •
1	D	311	2% / 71% / 27% / •

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 crite-

ria:

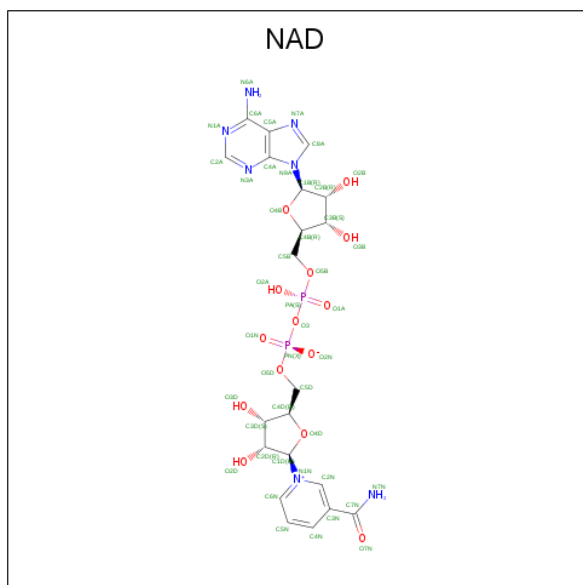| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAD	B	1118	-	-	-	X
2	NAD	C	1118	-	-	-	X
2	NAD	D	1118	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10139 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 UDP-glucose 4-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2388	1520	424	439	5			
1	B	311	Total	C	N	O	S	0	0	0
			2388	1520	424	439	5			
1	C	311	Total	C	N	O	S	0	0	0
			2388	1520	424	439	5			
1	D	311	Total	C	N	O	S	0	0	0
			2388	1520	424	439	5			

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

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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	112	Total 112	O 112	0	0
3	B	99	Total 99	O 99	0	0
3	C	78	Total 78	O 78	0	0
3	D	122	Total 122	O 122	0	0

3 Residue-property plots (i)

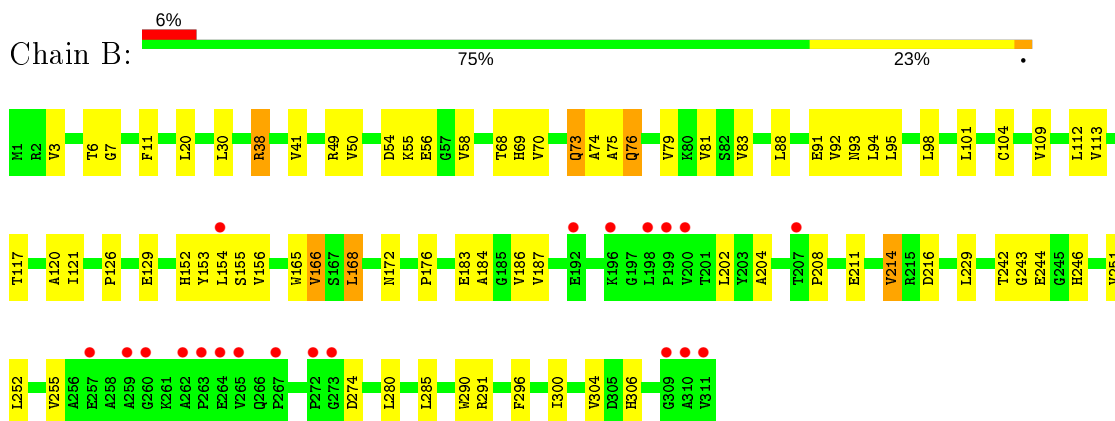These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.
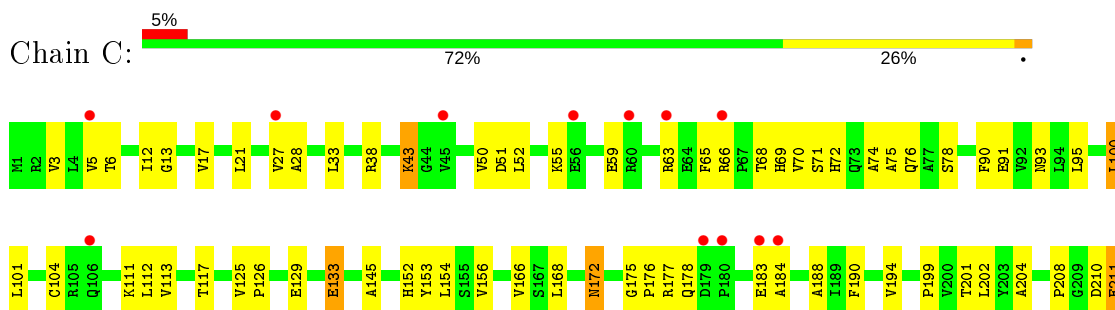
- Molecule 1: UDP-glucose 4-epimerase

- Molecule 1: UDP-glucose 4-epimerase

- Molecule 1: UDP-glucose 4-epimerase

H227 A228 L229 A230 L231 F232 S233 L234 G243 T247 T248 R249 E250 V251 L252 M253 E257 E264 R277 S278 V279 L280 K284 Q297 E298 R301 L302 V311

• Molecule 1: UDP-glucose 4-epimerase

Chain D:

2%

71%   27%

M1 V5 T6 F11 I12 H15 I16 V17 L21 L25 V29 L30 T35 E39 K43 F47 F48 R49 E56 E59 R63 R66 P67 T68 H69 V70 S71 H72 Q73 A74 A75 Q76 A77 S78 V81 L88 D89 F90 E91 V92 N93 L94 L95

L98 L101 C104 R105 V109 E110 K111 L112 T117 I121 Y122 G123 E124 E127 S146 H152 Y153 L154 S155 V156 Y161 V166 S167 L168 R169 N172 P176 R177 Q178 D179 P180 A184 A188 K196 G197 L198 P199 V200 A204 R205 E211 V218

Y219 V220 V223 A224 E225 A226 H227 A228 L229 A230 L234 E235 G241 T242 G243 T247 E250 P270 D274 L275 E276 L280 W290 R291 H306 A310 V311

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	250.92Å 250.92Å 121.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.85 – 2.37 49.85 – 2.37	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.85-2.37) 99.7 (49.85-2.37)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	14.57 (at 2.37Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.261 0.219 , 0.218	Depositor DCC
R_{free} test set	4519 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	25.2	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 45.2	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	0.92	EDS
Total number of atoms	10139	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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: 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	0.38	0/2446	0.60	0/3320
1	B	0.36	0/2446	0.56	0/3320
1	C	0.35	0/2446	0.57	0/3320
1	D	0.39	0/2446	0.60	0/3320
All	All	0.37	0/9784	0.58	0/13280

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	2388	0	2370	65	0
1	B	2388	0	2370	62	0
1	C	2388	0	2370	69	0
1	D	2388	0	2370	68	0
2	A	44	0	26	3	0
2	B	44	0	25	3	0
2	C	44	0	25	1	0
2	D	44	0	25	3	0
3	A	112	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	99	0	0	5	0
3	C	78	0	0	3	0
3	D	122	0	0	7	0
All	All	10139	0	9581	256	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 13.

All (256) 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:218:VAL:HG11	1:D:241:GLY:HA2	1.52	0.91
1:C:247:THR:HG22	1:C:250:GLU:H	1.42	0.84
1:B:216:ASP:OD1	1:B:242:THR:HG22	1.76	0.84
1:A:76:GLN:HB2	1:A:92:VAL:HG21	1.59	0.84
1:B:76:GLN:HE22	1:B:81:VAL:HB	1.43	0.84
1:A:183:GLU:HA	1:A:271:ARG:HH12	1.42	0.84
1:A:76:GLN:HE22	1:A:78:SER:HB3	1.44	0.82
1:B:291:ARG:HH21	1:B:291:ARG:HG3	1.46	0.81
1:D:76:GLN:HB2	1:D:92:VAL:HG11	1.64	0.80
1:D:218:VAL:HG12	1:D:242:THR:HG23	1.65	0.79
1:C:230:ALA:HA	1:C:234:LEU:HB2	1.64	0.78
1:A:54:ASP:OD2	1:A:56:GLU:HG2	1.83	0.77
1:B:76:GLN:HB3	1:B:92:VAL:HG11	1.67	0.76
1:A:152:HIS:HE1	1:D:152:HIS:HE1	1.32	0.76
1:B:76:GLN:O	1:B:76:GLN:HG3	1.86	0.75
1:B:242:THR:HG23	1:B:244:GLU:H	1.53	0.73
1:A:152:HIS:CE1	1:D:152:HIS:HE1	2.07	0.71
1:C:297:GLN:HG2	1:C:301:ARG:HH22	1.54	0.71
1:D:63:ARG:HA	1:D:66:ARG:NH2	2.05	0.71
1:A:117:THR:HG23	1:A:121:ILE:HG23	1.73	0.70
1:A:178:GLN:HG3	1:A:188:ALA:HB2	1.72	0.70
1:D:172:ASN:HB3	1:D:184:ALA:HB2	1.75	0.69
1:C:12:ILE:HD11	2:C:1118:NAD:H71N	1.58	0.69
1:D:290:TRP:O	1:D:291:ARG:HG3	1.95	0.67
1:C:297:GLN:HG2	1:C:301:ARG:NH2	2.10	0.66
1:B:290:TRP:O	1:B:291:ARG:HG3	1.95	0.65
1:B:172:ASN:HB3	1:B:184:ALA:HB2	1.78	0.65
1:A:11:PHE:HB3	2:A:1118:NAD:O2N	1.97	0.65
1:A:113:VAL:HA	1:A:166:VAL:HG13	1.77	0.65
1:D:291:ARG:HH11	1:D:291:ARG:HG3	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ARG:NH2	1:B:291:ARG:HG3	2.12	0.63
1:C:43:LYS:HA	1:C:43:LYS:NZ	2.14	0.63
1:B:154:LEU:HD13	1:B:165:TRP:CE3	2.33	0.63
1:C:75:ALA:HB1	1:C:93:ASN:OD1	2.00	0.62
1:C:76:GLN:NE2	1:C:78:SER:H	1.98	0.61
1:A:154:LEU:HD13	1:A:165:TRP:CD2	2.34	0.61
1:C:76:GLN:HE22	1:C:78:SER:HB3	1.65	0.60
1:A:218:VAL:HG21	1:A:241:GLY:HA2	1.83	0.60
1:A:154:LEU:HD13	1:A:165:TRP:CE3	2.36	0.60
1:D:127:GLU:HG3	3:D:1129:HOH:O	2.02	0.59
1:A:102:GLU:OE1	1:A:105:ARG:HD3	2.03	0.59
1:A:183:GLU:HA	1:A:271:ARG:NH1	2.16	0.59
1:C:125:VAL:CG1	1:C:278:SER:HA	2.33	0.59
1:C:91:GLU:O	1:C:95:LEU:HB3	2.02	0.58
1:D:39:GLU:HG3	3:D:1214:HOH:O	2.03	0.58
1:B:242:THR:HG23	1:B:244:GLU:N	2.17	0.58
1:D:218:VAL:CG1	1:D:241:GLY:HA2	2.31	0.58
1:D:88:LEU:O	1:D:92:VAL:HG12	2.04	0.58
1:C:125:VAL:HG12	1:C:277:ARG:O	2.03	0.58
1:D:29:VAL:HG23	1:D:47:PHE:HD1	1.68	0.57
1:B:41:VAL:HB	3:B:1158:HOH:O	2.04	0.57
1:C:126:PRO:HG2	1:C:129:GLU:CD	2.25	0.57
1:C:43:LYS:HA	1:C:43:LYS:HZ3	1.68	0.57
1:A:152:HIS:HE1	1:D:152:HIS:CE1	2.19	0.57
1:C:74:ALA:O	1:C:75:ALA:HB2	2.05	0.57
1:A:218:VAL:CG2	1:A:241:GLY:HA2	2.35	0.57
1:C:211:GLU:O	1:C:247:THR:HG23	2.04	0.57
1:B:154:LEU:HD13	1:B:165:TRP:CD2	2.39	0.57
1:B:211:GLU:H	1:B:211:GLU:CD	2.08	0.56
1:B:176:PRO:HB3	1:B:306:HIS:HB2	1.87	0.56
1:C:6:THR:O	1:C:74:ALA:HB2	2.04	0.56
1:B:300:ILE:O	1:B:304:VAL:HG23	2.05	0.56
1:B:113:VAL:HA	1:B:166:VAL:HG13	1.87	0.56
1:B:75:ALA:HB1	1:B:93:ASN:OD1	2.05	0.56
1:B:76:GLN:HE22	1:B:81:VAL:CB	2.16	0.56
1:C:3:VAL:HB	1:C:27:VAL:HG12	1.88	0.56
1:B:154:LEU:HD12	1:B:155:SER:N	2.21	0.55
1:A:76:GLN:HB2	1:A:92:VAL:CG2	2.35	0.55
1:C:172:ASN:HB3	1:C:184:ALA:HB2	1.87	0.55
1:C:243:GLY:HA2	1:C:280:LEU:O	2.06	0.55
1:D:105:ARG:HD3	1:D:161:TYR:CG	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:VAL:HA	1:C:166:VAL:HG13	1.89	0.54
1:D:15:HIS:HE1	1:D:176:PRO:O	1.91	0.54
1:B:251:VAL:O	1:B:255:VAL:HG23	2.07	0.54
1:D:121:ILE:HD13	1:D:169:ARG:CZ	2.38	0.53
1:A:178:GLN:CG	1:A:188:ALA:HB2	2.39	0.53
1:C:176:PRO:O	1:C:177:ARG:HB2	2.08	0.53
1:D:291:ARG:HG3	1:D:291:ARG:NH1	2.21	0.53
1:C:153:TYR:HA	1:C:156:VAL:HG22	1.91	0.53
1:D:93:ASN:HB2	1:D:146:SER:OG	2.08	0.53
1:C:175:GLY:O	1:C:178:GLN:HG2	2.09	0.53
1:D:243:GLY:HA2	1:D:280:LEU:O	2.09	0.53
1:A:6:THR:OG1	1:A:72:HIS:HD2	1.92	0.53
1:C:70:VAL:HG23	1:C:112:LEU:HG	1.89	0.53
1:A:176:PRO:O	1:A:177:ARG:HB2	2.08	0.53
1:A:175:GLY:H	1:A:178:GLN:NE2	2.07	0.53
1:B:74:ALA:O	1:B:75:ALA:HB2	2.09	0.53
1:C:125:VAL:HG11	1:C:278:SER:HA	1.91	0.53
1:A:246:HIS:HD2	3:A:1128:HOH:O	1.91	0.52
1:D:5:VAL:HG11	1:D:17:VAL:HG22	1.89	0.52
1:B:152:HIS:HE1	1:C:152:HIS:NE2	2.07	0.52
1:D:176:PRO:O	1:D:177:ARG:HB2	2.10	0.52
1:A:291:ARG:HH11	1:A:291:ARG:HG3	1.74	0.52
1:A:205:ARG:HD3	1:A:276:GLU:HB3	1.91	0.52
1:D:70:VAL:HG12	1:D:109:VAL:HG11	1.92	0.52
1:D:71:SER:OG	1:D:227:HIS:HE1	1.93	0.52
1:D:127:GLU:OE1	3:D:1151:HOH:O	2.19	0.51
1:D:71:SER:OG	1:D:227:HIS:CE1	2.63	0.51
1:B:55:LYS:HE2	3:B:1151:HOH:O	2.09	0.51
1:B:38:ARG:CZ	3:B:1158:HOH:O	2.57	0.51
1:B:126:PRO:HG2	1:B:129:GLU:CD	2.31	0.51
1:A:91:GLU:O	1:A:95:LEU:HB3	2.10	0.51
1:A:243:GLY:HA2	1:A:280:LEU:O	2.10	0.51
1:B:113:VAL:HG22	1:B:166:VAL:CG1	2.40	0.51
1:D:91:GLU:O	1:D:95:LEU:HB3	2.10	0.51
1:D:12:ILE:HD11	2:D:1118:NAD:H71N	1.76	0.50
1:D:204:ALA:HB3	1:D:270:PRO:HD3	1.93	0.50
1:C:247:THR:HG23	1:C:249:ARG:H	1.75	0.50
1:C:199:PRO:HB3	1:C:264:GLU:HG3	1.94	0.50
1:C:5:VAL:HG11	1:C:17:VAL:HG22	1.93	0.50
1:D:112:LEU:HD23	1:D:112:LEU:C	2.32	0.50
1:D:124:GLU:HG3	3:D:1189:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ARG:HD3	1:B:49:ARG:NH2	2.27	0.50
1:A:291:ARG:HG3	1:A:291:ARG:NH1	2.27	0.50
1:A:112:LEU:C	1:A:112:LEU:HD23	2.33	0.50
1:A:205:ARG:HD2	1:A:206:LYS:HD2	1.94	0.49
1:C:183:GLU:HB2	3:C:1145:HOH:O	2.13	0.49
1:A:7:GLY:HA2	1:A:31:ASP:OD2	2.12	0.49
1:A:290:TRP:O	1:A:291:ARG:HG3	2.13	0.49
1:D:70:VAL:HG11	1:D:104:CYS:SG	2.53	0.49
1:B:6:THR:HG1	1:B:73:GLN:H	1.61	0.48
1:D:218:VAL:HG11	1:D:241:GLY:CA	2.35	0.48
1:D:153:TYR:HA	1:D:156:VAL:HG22	1.96	0.48
1:A:183:GLU:HG2	1:A:271:ARG:NH1	2.29	0.48
1:D:121:ILE:HD11	1:D:122:TYR:CZ	2.48	0.48
1:D:63:ARG:HA	1:D:66:ARG:HH21	1.77	0.48
1:B:246:HIS:HD2	3:B:1131:HOH:O	1.96	0.48
1:C:68:THR:OG1	1:C:69:HIS:HD2	1.97	0.48
1:A:11:PHE:HB3	2:A:1118:NAD:PN	2.53	0.48
1:B:153:TYR:HA	1:B:156:VAL:HG22	1.96	0.48
1:C:112:LEU:C	1:C:112:LEU:HD23	2.33	0.48
1:A:113:VAL:HG22	1:A:166:VAL:CG1	2.44	0.48
1:A:184:ALA:C	1:A:186:VAL:H	2.18	0.48
1:B:70:VAL:HG11	1:B:104:CYS:SG	2.54	0.47
1:C:190:PHE:O	1:C:194:VAL:HG23	2.14	0.47
1:C:63:ARG:HG3	1:C:66:ARG:NH2	2.29	0.47
1:C:6:THR:OG1	1:C:72:HIS:HA	2.15	0.47
1:C:125:VAL:HG11	1:C:279:VAL:H	1.80	0.47
1:D:117:THR:O	1:D:121:ILE:HG12	2.14	0.47
1:A:70:VAL:HG12	1:A:109:VAL:HG11	1.96	0.47
1:C:247:THR:CG2	1:C:249:ARG:H	2.28	0.47
1:C:55:LYS:O	1:C:59:GLU:HG2	2.15	0.47
1:C:71:SER:OG	1:C:227:HIS:CE1	2.68	0.47
1:D:59:GLU:O	1:D:63:ARG:HG3	2.14	0.47
1:A:154:LEU:HD12	1:A:155:SER:N	2.31	0.46
1:B:38:ARG:CG	1:B:38:ARG:HH11	2.29	0.46
1:A:30:LEU:C	1:A:30:LEU:HD23	2.35	0.46
1:B:30:LEU:HG	1:B:50:VAL:HG22	1.97	0.46
1:B:79:VAL:O	1:B:83:VAL:HG23	2.15	0.46
1:D:205:ARG:HD2	3:D:1145:HOH:O	2.15	0.46
1:D:166:VAL:HG22	1:D:235:GLU:HA	1.97	0.46
1:D:68:THR:OG1	1:D:69:HIS:HD2	1.97	0.46
1:D:74:ALA:O	1:D:75:ALA:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:VAL:HA	1:B:69:HIS:O	2.15	0.46
1:D:247:THR:OG1	1:D:250:GLU:HG2	2.16	0.46
1:A:283:LEU:CD1	1:A:286:MET:HE3	2.46	0.46
1:B:68:THR:OG1	1:B:69:HIS:HD2	1.98	0.46
1:C:6:THR:HG21	1:C:100:LEU:HD11	1.96	0.46
1:A:70:VAL:HG13	1:A:112:LEU:HG	1.98	0.46
1:B:166:VAL:HG22	1:B:168:LEU:HD13	1.97	0.45
1:C:13:GLY:O	1:C:17:VAL:HG23	2.16	0.45
1:D:230:ALA:HA	1:D:234:LEU:HB2	1.98	0.45
1:C:21:LEU:HD13	1:C:27:VAL:HG22	1.98	0.45
1:D:196:LYS:HB3	1:D:198:LEU:HD13	1.98	0.45
1:A:74:ALA:O	1:A:75:ALA:HB2	2.16	0.45
1:A:92:VAL:HG23	1:A:93:ASN:N	2.31	0.45
1:B:3:VAL:HG11	1:B:20:LEU:HD13	1.99	0.45
1:A:205:ARG:HG3	1:A:206:LYS:HG3	1.99	0.45
1:B:183:GLU:HB2	2:B:1118:NAD:H71N	1.81	0.45
1:A:75:ALA:HB1	1:A:93:ASN:OD1	2.16	0.45
1:C:168:LEU:N	1:C:168:LEU:HD22	2.32	0.45
1:A:205:ARG:HG3	1:A:206:LYS:N	2.32	0.45
1:D:112:LEU:HD22	1:D:154:LEU:HD21	1.98	0.45
1:D:30:LEU:HD23	1:D:30:LEU:C	2.37	0.45
1:C:76:GLN:HE22	1:C:78:SER:H	1.61	0.44
1:A:98:LEU:HD22	1:D:90:PHE:CG	2.52	0.44
1:D:43:LYS:N	1:D:43:LYS:HD2	2.32	0.44
1:B:243:GLY:HA2	1:B:280:LEU:O	2.17	0.44
1:B:94:LEU:HA	1:B:94:LEU:HD23	1.77	0.44
1:D:179:ASP:HB2	1:D:180:PRO:HD2	1.99	0.44
1:D:78:SER:HB3	1:D:81:VAL:HB	1.99	0.44
1:A:11:PHE:CE2	1:A:178:GLN:HB3	2.53	0.44
1:D:220:VAL:O	1:D:223:VAL:HG22	2.18	0.44
1:B:70:VAL:HG12	1:B:109:VAL:HG11	2.00	0.44
1:B:296:PHE:O	1:B:300:ILE:HD13	2.17	0.44
1:A:113:VAL:HG22	1:A:166:VAL:HG11	2.00	0.44
1:B:117:THR:HG23	1:B:121:ILE:HG23	2.00	0.44
1:B:202:LEU:HA	3:B:1198:HOH:O	2.17	0.44
1:A:283:LEU:HD13	1:A:286:MET:CE	2.48	0.43
1:A:60:ARG:HG3	1:A:61:ALA:N	2.32	0.43
1:D:176:PRO:HB3	1:D:306:HIS:HB2	2.00	0.43
1:D:166:VAL:HG11	1:D:230:ALA:HB1	2.01	0.43
1:D:205:ARG:NH2	1:D:276:GLU:OE2	2.51	0.43
1:B:98:LEU:HD22	1:C:90:PHE:CG	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ALA:HB2	1:B:208:PRO:HA	2.01	0.43
1:A:23:ARG:HB2	1:A:25:LEU:HD23	2.01	0.43
1:C:38:ARG:HA	1:C:38:ARG:HD2	1.91	0.43
1:D:35:THR:HG22	2:D:1118:NAD:H2B	2.00	0.43
1:A:87:VAL:HG22	1:D:98:LEU:HD11	2.01	0.43
1:A:49:ARG:HG2	1:A:49:ARG:HH11	1.84	0.43
1:B:88:LEU:O	1:B:92:VAL:HG12	2.18	0.43
1:D:111:LYS:HG2	1:D:112:LEU:N	2.34	0.43
1:B:75:ALA:HB3	2:B:1118:NAD:O3D	2.19	0.42
1:B:7:GLY:N	1:B:74:ALA:HB2	2.35	0.42
1:B:117:THR:CG2	1:B:120:ALA:HB3	2.49	0.42
1:C:133:GLU:HG3	1:C:284:LYS:HD2	2.01	0.42
1:C:50:VAL:HG12	1:C:51:ASP:N	2.34	0.42
1:A:214:VAL:HA	1:A:246:HIS:O	2.19	0.42
1:A:296:PHE:O	1:A:300:ILE:HD13	2.20	0.42
1:C:211:GLU:OE2	1:C:249:ARG:HD2	2.20	0.42
1:C:252:LEU:HD13	1:C:253:MET:CE	2.49	0.42
1:A:176:PRO:HB3	1:A:306:HIS:HB2	2.02	0.42
1:C:227:HIS:HD2	3:C:1126:HOH:O	2.02	0.42
1:D:1:MET:HG3	1:D:69:HIS:CD2	2.55	0.42
1:D:6:THR:OG1	1:D:72:HIS:HD2	2.03	0.42
1:B:54:ASP:O	1:B:58:VAL:HG23	2.19	0.42
1:C:101:LEU:HD21	1:C:154:LEU:CD1	2.50	0.42
1:C:113:VAL:HG22	1:C:166:VAL:CG1	2.50	0.42
1:C:33:LEU:HD12	1:C:33:LEU:N	2.34	0.42
1:A:121:ILE:HD11	1:A:122:TYR:CE2	2.55	0.42
1:A:105:ARG:HD2	1:A:157:TYR:CE1	2.54	0.42
1:A:214:VAL:HG13	1:A:277:ARG:HA	2.02	0.42
1:A:283:LEU:HD12	1:A:286:MET:HE3	2.02	0.42
1:C:298:GLU:O	1:C:302:LEU:HD13	2.20	0.42
1:C:210:ASP:HB2	3:C:1175:HOH:O	2.18	0.41
1:C:71:SER:OG	1:C:227:HIS:HE1	2.02	0.41
1:A:282:PRO:HG2	1:A:286:MET:CE	2.49	0.41
1:D:105:ARG:NH2	3:D:1187:HOH:O	2.53	0.41
1:D:227:HIS:HD2	3:D:1121:HOH:O	2.03	0.41
1:D:75:ALA:HB3	2:D:1118:NAD:O3D	2.20	0.41
1:B:112:LEU:HD23	1:B:112:LEU:C	2.40	0.41
1:B:91:GLU:O	1:B:95:LEU:HB3	2.20	0.41
1:C:204:ALA:HB2	1:C:208:PRO:HA	2.01	0.41
1:A:75:ALA:HB3	2:A:1118:NAD:H3D	2.02	0.41
1:C:111:LYS:HG2	1:C:112:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:VAL:HG13	1:D:93:ASN:N	2.35	0.41
1:D:178:GLN:HG3	1:D:188:ALA:HB2	2.03	0.41
1:B:11:PHE:HB3	2:B:1118:NAD:PN	2.61	0.41
1:B:166:VAL:CG2	1:B:168:LEU:HD13	2.51	0.41
1:C:178:GLN:HG3	1:C:188:ALA:HB2	2.02	0.41
1:B:252:LEU:C	1:B:252:LEU:HD13	2.41	0.40
1:B:76:GLN:HB3	1:B:92:VAL:CG1	2.43	0.40
1:C:70:VAL:HG21	1:C:104:CYS:SG	2.61	0.40
1:B:156:VAL:HG11	1:C:145:ALA:HB2	2.03	0.40
1:C:172:ASN:CB	1:C:184:ALA:HB2	2.50	0.40
1:C:21:LEU:HA	1:C:21:LEU:HD12	1.91	0.40
1:A:230:ALA:HA	1:A:234:LEU:HB2	2.03	0.40
1:B:186:VAL:HG13	1:B:187:VAL:N	2.36	0.40
1:B:214:VAL:HG23	1:B:246:HIS:H	1.86	0.40
1:C:100:LEU:O	1:C:100:LEU:HD23	2.21	0.40
1:C:5:VAL:O	1:C:5:VAL:HG13	2.21	0.40
1:D:49:ARG:HH11	1:D:49:ARG:HG2	1.86	0.40
1:D:29:VAL:CG2	1:D:47:PHE:HD1	2.34	0.40
1:C:117:THR:O	1:C:117:THR:HG23	2.21	0.40
1:A:233:SER:HB2	3:A:1222:HOH:O	2.22	0.40
1:C:28:ALA:HB2	1:C:65:PHE:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	309/311 (99%)	297 (96%)	11 (4%)	1 (0%)	41	53
1	B	309/311 (99%)	300 (97%)	9 (3%)	0	100	100
1	C	309/311 (99%)	298 (96%)	11 (4%)	0	100	100
1	D	309/311 (99%)	299 (97%)	9 (3%)	1 (0%)	41	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1236/1244 (99%)	1194 (97%)	40 (3%)	2 (0%)	47 61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	11	PHE
1	A	11	PHE

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	244/244 (100%)	232 (95%)	12 (5%)	25 38
1	B	244/244 (100%)	233 (96%)	11 (4%)	27 41
1	C	244/244 (100%)	233 (96%)	11 (4%)	27 41
1	D	244/244 (100%)	229 (94%)	15 (6%)	18 27
All	All	976/976 (100%)	927 (95%)	49 (5%)	24 37

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	37	LYS
1	A	38	ARG
1	A	60	ARG
1	A	66	ARG
1	A	94	LEU
1	A	168	LEU
1	A	183	GLU
1	A	205	ARG
1	A	214	VAL
1	A	229	LEU
1	A	283	LEU
1	B	38	ARG

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Mol	Chain	Res	Type
1	B	56	GLU
1	B	73	GLN
1	B	76	GLN
1	B	101	LEU
1	B	166	VAL
1	B	168	LEU
1	B	214	VAL
1	B	229	LEU
1	B	274	ASP
1	B	285	LEU
1	C	43	LYS
1	C	52	LEU
1	C	100	LEU
1	C	133	GLU
1	C	172	ASN
1	C	201	THR
1	C	202	LEU
1	C	211	GLU
1	C	229	LEU
1	C	247	THR
1	C	252	LEU
1	D	21	LEU
1	D	25	LEU
1	D	43	LYS
1	D	76	GLN
1	D	101	LEU
1	D	105	ARG
1	D	117	THR
1	D	121	ILE
1	D	168	LEU
1	D	172	ASN
1	D	200	VAL
1	D	211	GLU
1	D	225	GLU
1	D	229	LEU
1	D	274	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	72	HIS

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Mol	Chain	Res	Type
1	A	76	GLN
1	A	106	GLN
1	A	152	HIS
1	A	172	ASN
1	A	178	GLN
1	A	239	ASN
1	A	246	HIS
1	B	15	HIS
1	B	69	HIS
1	B	72	HIS
1	B	76	GLN
1	B	152	HIS
1	B	239	ASN
1	B	246	HIS
1	B	266	GLN
1	C	69	HIS
1	C	76	GLN
1	C	172	ASN
1	C	227	HIS
1	C	239	ASN
1	C	297	GLN
1	D	15	HIS
1	D	69	HIS
1	D	72	HIS
1	D	106	GLN
1	D	152	HIS
1	D	172	ASN
1	D	227	HIS
1	D	239	ASN
1	D	288	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	NAD	A	1118	-	42,48,48	1.64	6 (14%)	50,73,73	2.07	12 (24%)
2	NAD	D	1118	-	42,48,48	1.57	4 (9%)	50,73,73	1.98	15 (30%)
2	NAD	B	1118	-	42,48,48	1.64	5 (11%)	50,73,73	2.16	16 (32%)
2	NAD	C	1118	-	42,48,48	1.62	5 (11%)	50,73,73	2.00	16 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	1118	-	-	10/26/62/62	0/5/5/5
2	NAD	D	1118	-	-	12/26/62/62	0/5/5/5
2	NAD	B	1118	-	-	12/26/62/62	0/5/5/5
2	NAD	C	1118	-	-	9/26/62/62	0/5/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1118	NAD	C2N-N1N	7.43	1.44	1.35
2	B	1118	NAD	C2N-N1N	7.34	1.43	1.35
2	D	1118	NAD	C2N-N1N	7.20	1.43	1.35
2	A	1118	NAD	C2N-N1N	7.13	1.43	1.35
2	A	1118	NAD	O4B-C1B	3.71	1.46	1.41
2	D	1118	NAD	O4B-C1B	3.25	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1118	NAD	C6N-N1N	2.91	1.42	1.35
2	C	1118	NAD	C6N-N1N	2.81	1.42	1.35
2	B	1118	NAD	O4D-C1D	2.74	1.44	1.41
2	B	1118	NAD	O4B-C1B	2.68	1.44	1.41
2	A	1118	NAD	C6N-N1N	2.64	1.41	1.35
2	D	1118	NAD	C6N-N1N	2.62	1.41	1.35
2	C	1118	NAD	C3N-C7N	2.60	1.54	1.50
2	A	1118	NAD	O4D-C1D	2.42	1.44	1.41
2	C	1118	NAD	O4B-C1B	2.40	1.44	1.41
2	A	1118	NAD	C3N-C7N	2.27	1.54	1.50
2	C	1118	NAD	O4D-C1D	2.26	1.44	1.41
2	B	1118	NAD	C5D-C4D	2.23	1.58	1.51
2	D	1118	NAD	C3N-C7N	2.08	1.53	1.50
2	A	1118	NAD	C5D-C4D	2.04	1.58	1.51

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1118	NAD	O4D-C4D-C5D	6.29	130.08	109.37
2	D	1118	NAD	N3A-C2A-N1A	-5.39	120.25	128.68
2	A	1118	NAD	N3A-C2A-N1A	-5.33	120.34	128.68
2	B	1118	NAD	N3A-C2A-N1A	-5.28	120.42	128.68
2	C	1118	NAD	N3A-C2A-N1A	-5.22	120.52	128.68
2	A	1118	NAD	O4D-C1D-C2D	-5.08	99.50	106.93
2	A	1118	NAD	O5D-C5D-C4D	4.93	125.95	108.99
2	C	1118	NAD	O4D-C4D-C5D	4.49	124.13	109.37
2	D	1118	NAD	C3D-C2D-C1D	4.24	107.36	100.98
2	D	1118	NAD	O4D-C4D-C5D	4.19	123.15	109.37
2	B	1118	NAD	O4D-C1D-C2D	-4.18	100.81	106.93
2	A	1118	NAD	O4D-C4D-C5D	4.12	122.93	109.37
2	A	1118	NAD	O4D-C4D-C3D	-4.12	96.96	105.11
2	C	1118	NAD	O4D-C1D-C2D	-3.91	101.21	106.93
2	D	1118	NAD	O4D-C1D-C2D	-3.90	101.22	106.93
2	B	1118	NAD	O4D-C4D-C3D	-3.86	97.48	105.11
2	B	1118	NAD	C6N-N1N-C2N	-3.64	118.65	121.97
2	B	1118	NAD	C3D-C2D-C1D	3.64	106.46	100.98
2	B	1118	NAD	O5D-C5D-C4D	3.58	121.31	108.99
2	A	1118	NAD	O4B-C1B-C2B	-3.54	101.76	106.93
2	C	1118	NAD	C3D-C2D-C1D	3.31	105.96	100.98
2	C	1118	NAD	C4A-C5A-N7A	3.30	112.83	109.40
2	A	1118	NAD	C6N-N1N-C2N	-3.22	119.03	121.97
2	C	1118	NAD	O4B-C1B-C2B	-3.18	102.27	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1118	NAD	C3N-C7N-N7N	-3.14	113.99	117.75
2	B	1118	NAD	C4A-C5A-N7A	3.11	112.64	109.40
2	A	1118	NAD	C4A-C5A-N7A	3.08	112.61	109.40
2	C	1118	NAD	O5D-C5D-C4D	3.07	119.56	108.99
2	C	1118	NAD	C6N-N1N-C2N	-3.00	119.23	121.97
2	B	1118	NAD	C2N-N1N-C1D	3.00	125.81	119.14
2	D	1118	NAD	O4B-C1B-C2B	-2.99	102.56	106.93
2	C	1118	NAD	O4B-C4B-C5B	2.79	118.54	109.37
2	C	1118	NAD	C2N-N1N-C1D	2.75	125.27	119.14
2	B	1118	NAD	O4B-C1B-C2B	-2.65	103.05	106.93
2	D	1118	NAD	C2N-N1N-C1D	2.65	125.04	119.14
2	B	1118	NAD	O4B-C4B-C5B	2.64	118.06	109.37
2	D	1118	NAD	C4A-C5A-N7A	2.60	112.11	109.40
2	C	1118	NAD	O4D-C4D-C3D	-2.58	100.00	105.11
2	A	1118	NAD	C2N-N1N-C1D	2.56	124.83	119.14
2	C	1118	NAD	C3N-C7N-N7N	-2.52	114.73	117.75
2	C	1118	NAD	O7N-C7N-C3N	2.49	122.61	119.63
2	C	1118	NAD	PN-O3-PA	2.37	140.97	132.83
2	D	1118	NAD	PN-O5D-C5D	2.36	135.51	121.68
2	D	1118	NAD	PN-O3-PA	2.34	140.85	132.83
2	D	1118	NAD	C6N-N1N-C2N	-2.32	119.86	121.97
2	D	1118	NAD	C5A-C6A-N6A	2.32	123.87	120.35
2	A	1118	NAD	C3D-C2D-C1D	2.28	104.41	100.98
2	B	1118	NAD	PN-O5D-C5D	2.24	134.81	121.68
2	A	1118	NAD	O4B-C4B-C3B	-2.14	100.88	105.11
2	A	1118	NAD	C2A-N1A-C6A	2.09	122.34	118.75
2	B	1118	NAD	C2A-N1A-C6A	2.09	122.33	118.75
2	D	1118	NAD	C2A-N1A-C6A	2.09	122.33	118.75
2	D	1118	NAD	O7N-C7N-C3N	2.07	122.11	119.63
2	D	1118	NAD	C3N-C2N-N1N	-2.03	118.44	120.43
2	B	1118	NAD	C2N-C3N-C4N	2.02	120.55	118.26
2	C	1118	NAD	C1B-N9A-C4A	-2.02	123.10	126.64
2	B	1118	NAD	C3B-C2B-C1B	2.01	104.00	100.98
2	B	1118	NAD	C1B-N9A-C4A	-2.00	123.12	126.64
2	C	1118	NAD	C2A-N1A-C6A	2.00	122.18	118.75

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1118	NAD	PN-O3-PA-O5B
2	A	1118	NAD	C5D-O5D-PN-O3

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Mol	Chain	Res	Type	Atoms
2	A	1118	NAD	O4D-C1D-N1N-C2N
2	A	1118	NAD	O4D-C1D-N1N-C6N
2	A	1118	NAD	C2D-C1D-N1N-C6N
2	D	1118	NAD	C5D-O5D-PN-O3
2	D	1118	NAD	O4D-C1D-N1N-C2N
2	D	1118	NAD	O4D-C1D-N1N-C6N
2	D	1118	NAD	C2D-C1D-N1N-C6N
2	B	1118	NAD	O4D-C1D-N1N-C2N
2	B	1118	NAD	O4D-C1D-N1N-C6N
2	B	1118	NAD	C2D-C1D-N1N-C6N
2	B	1118	NAD	C2N-C3N-C7N-O7N
2	C	1118	NAD	O4D-C1D-N1N-C2N
2	C	1118	NAD	O4D-C1D-N1N-C6N
2	B	1118	NAD	C4N-C3N-C7N-O7N
2	B	1118	NAD	C4N-C3N-C7N-N7N
2	B	1118	NAD	C2N-C3N-C7N-N7N
2	C	1118	NAD	C3D-C4D-C5D-O5D
2	D	1118	NAD	C4N-C3N-C7N-O7N
2	D	1118	NAD	C4N-C3N-C7N-N7N
2	C	1118	NAD	C4N-C3N-C7N-O7N
2	C	1118	NAD	C4N-C3N-C7N-N7N
2	D	1118	NAD	PA-O3-PN-O1N
2	D	1118	NAD	PN-O3-PA-O5B
2	B	1118	NAD	PN-O3-PA-O5B
2	A	1118	NAD	PA-O3-PN-O2N
2	A	1118	NAD	C5D-O5D-PN-O1N
2	A	1118	NAD	C5D-O5D-PN-O2N
2	D	1118	NAD	C5D-O5D-PN-O1N
2	C	1118	NAD	O4D-C4D-C5D-O5D
2	D	1118	NAD	PA-O3-PN-O2N
2	B	1118	NAD	PA-O3-PN-O2N
2	B	1118	NAD	C3D-C4D-C5D-O5D
2	D	1118	NAD	O4B-C4B-C5B-O5B
2	C	1118	NAD	C2N-C3N-C7N-O7N
2	C	1118	NAD	O4B-C4B-C5B-O5B
2	D	1118	NAD	C2D-C1D-N1N-C2N
2	B	1118	NAD	C5B-O5B-PA-O3
2	C	1118	NAD	C2N-C3N-C7N-N7N
2	A	1118	NAD	O4B-C4B-C5B-O5B
2	B	1118	NAD	O4B-C4B-C5B-O5B
2	A	1118	NAD	PA-O3-PN-O1N

There are no ring outliers.
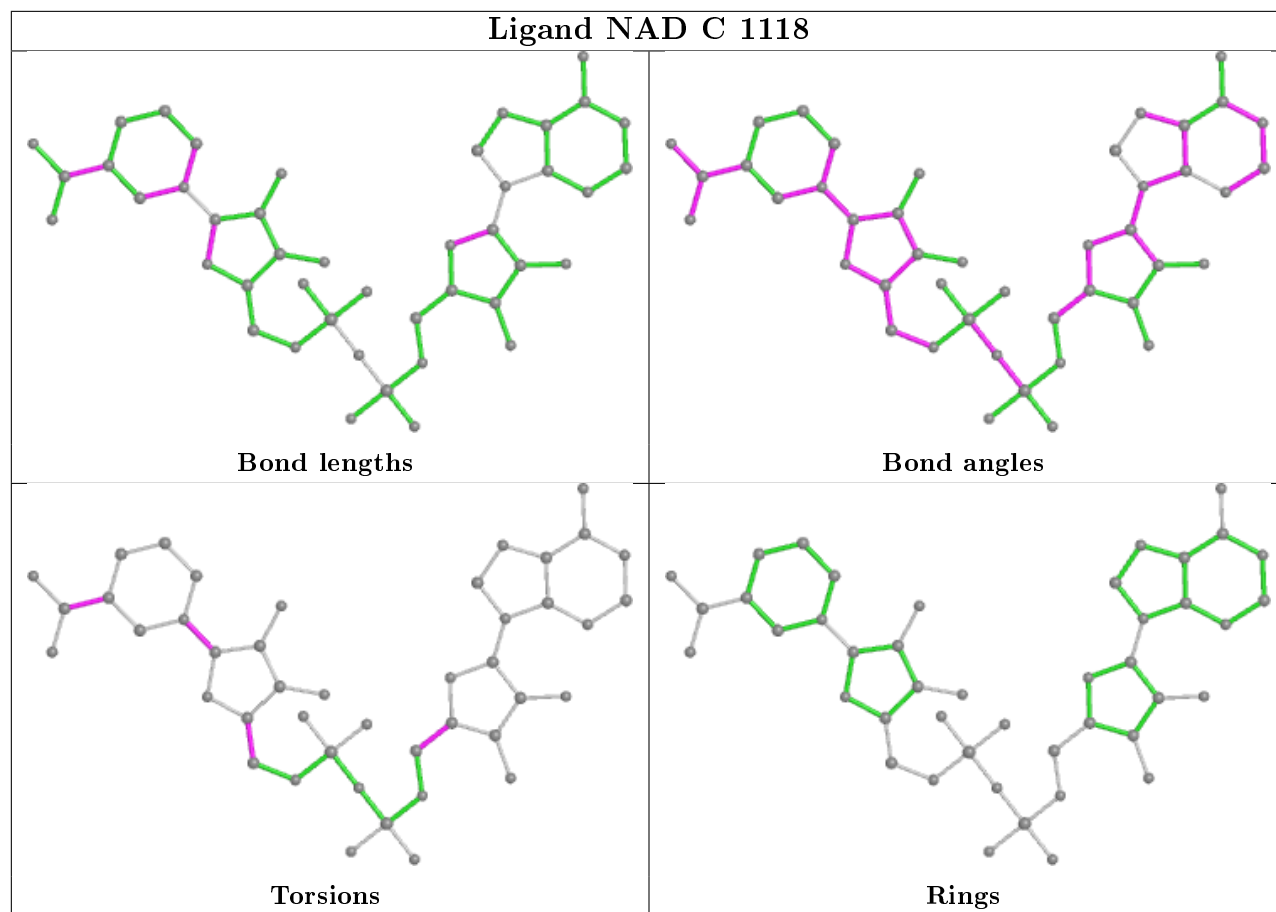
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1118	NAD	3	0
2	D	1118	NAD	3	0
2	B	1118	NAD	3	0
2	C	1118	NAD	1	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 A 1118

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD D 1118

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD B 1118

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD C 1118

Bond lengths

Bond angles

Torsions

Rings
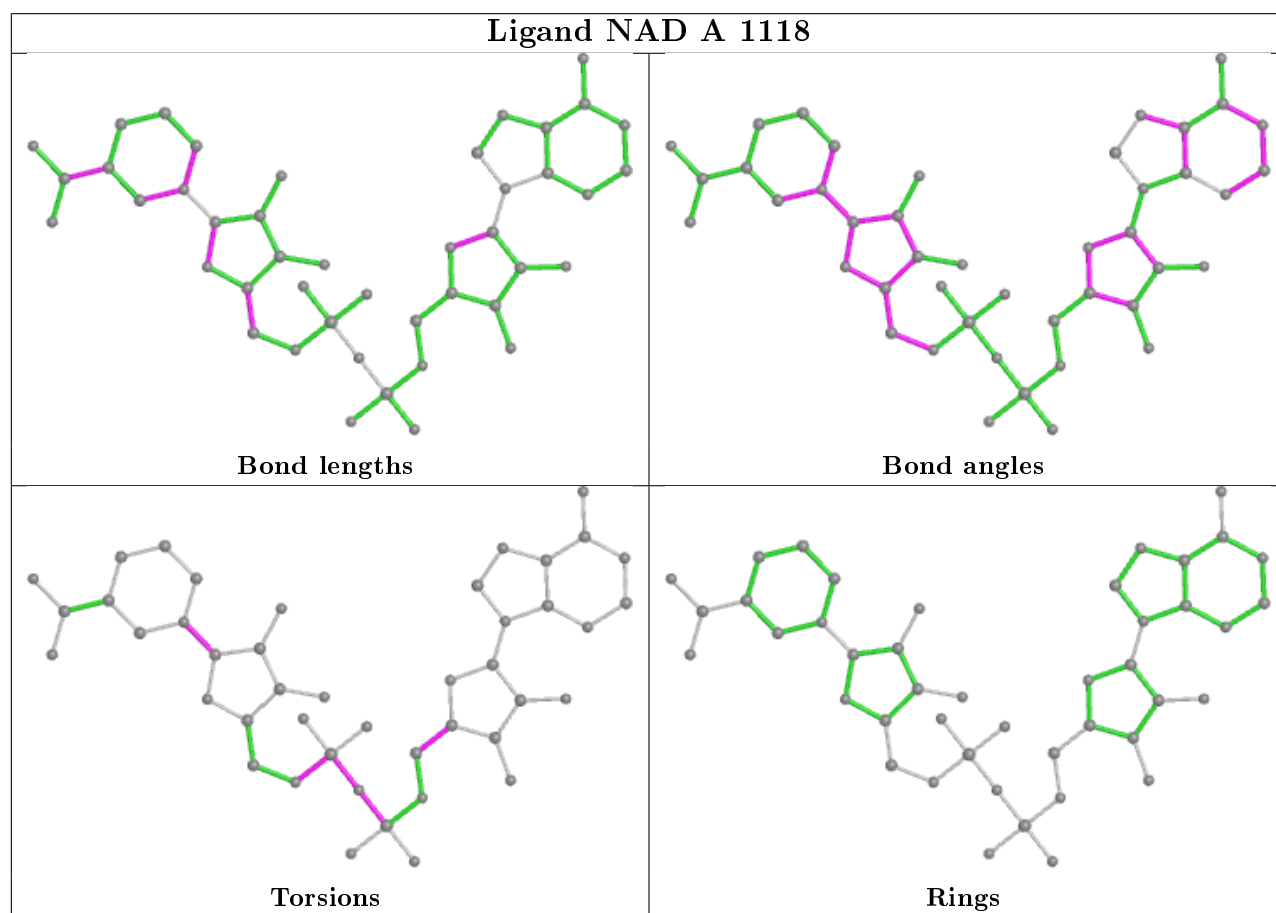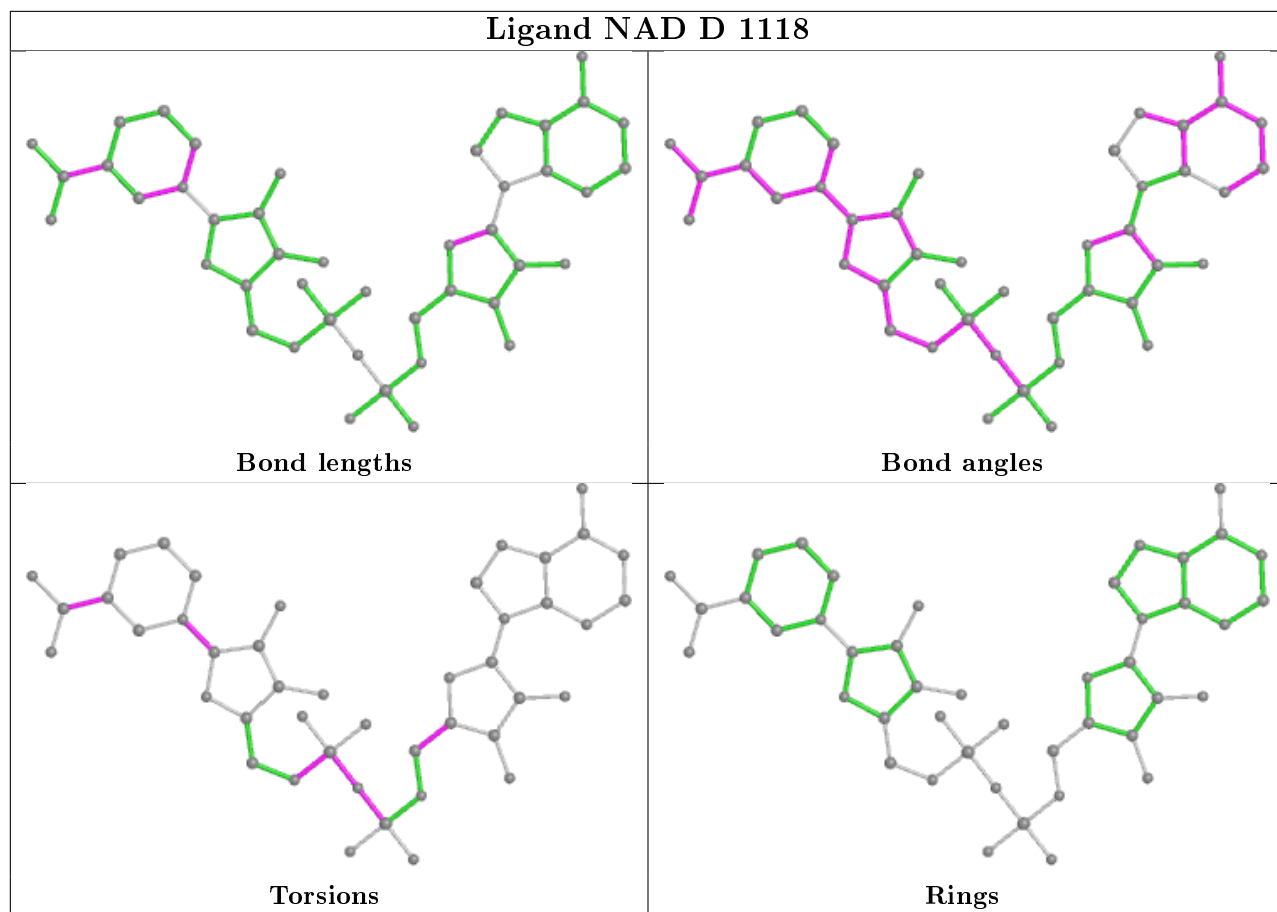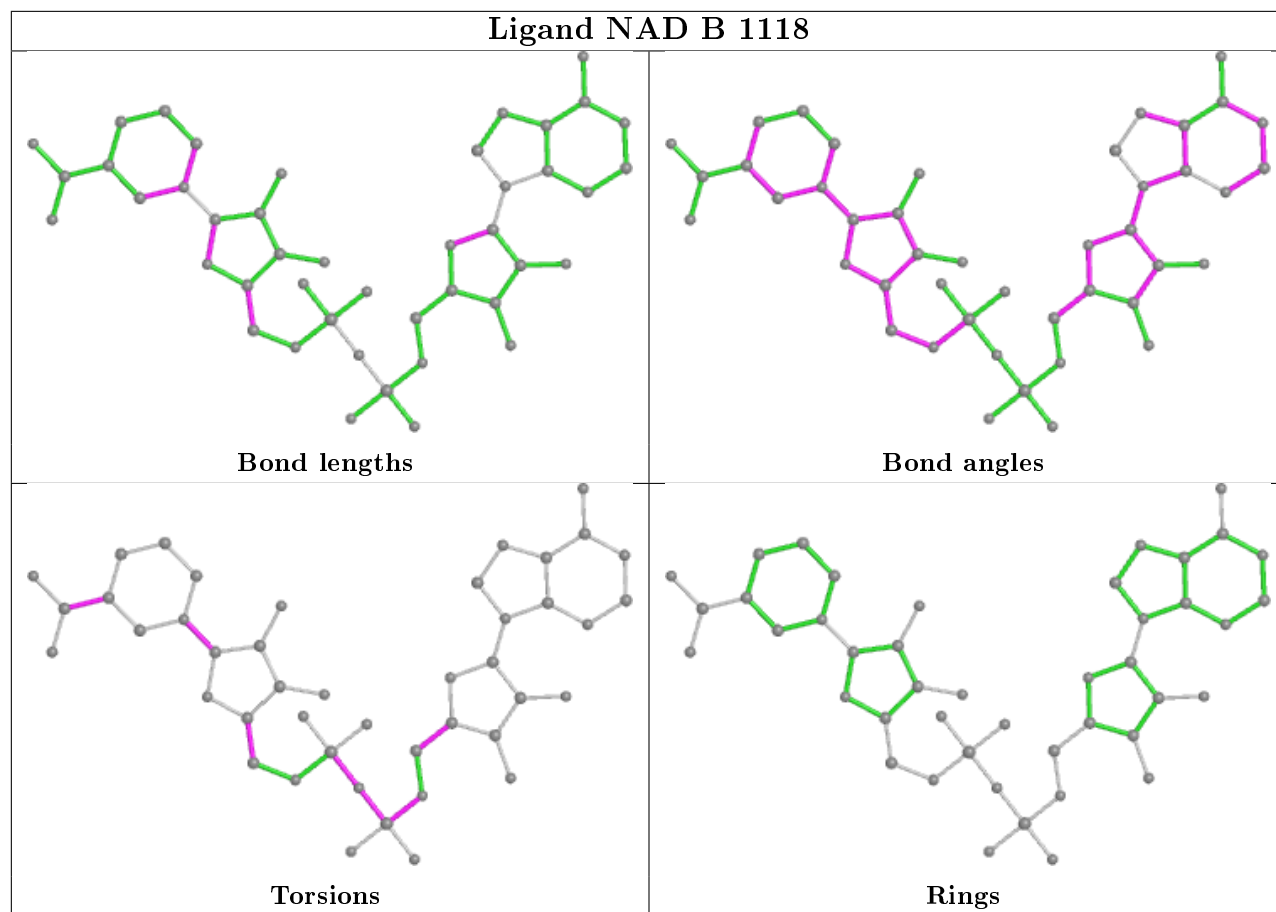
5.7 Other polymers ⓘ

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9
1	A	311/311 (100%)	0.12	15 (4%)	30 33	9, 21, 42, 80	0
1	B	311/311 (100%)	0.23	20 (6%)	19 21	13, 24, 65, 89	0
1	C	311/311 (100%)	0.25	15 (4%)	30 33	14, 28, 50, 67	0
1	D	311/311 (100%)	-0.07	5 (1%)	72 73	8, 21, 40, 60	0
All	All	1244/1244 (100%)	0.13	55 (4%)	34 37	8, 23, 51, 89	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	311	VAL	13.4
1	A	184	ALA	12.0
1	C	311	VAL	11.9
1	A	311	VAL	10.8
1	D	311	VAL	9.9
1	A	310	ALA	8.6
1	B	310	ALA	6.3
1	B	262	ALA	6.2
1	A	180	PRO	5.1
1	C	180	PRO	4.8
1	A	181	HIS	4.8
1	A	44	GLY	4.3
1	B	265	VAL	4.0
1	B	259	ALA	3.9
1	B	267	PRO	3.5
1	B	198	LEU	3.4
1	C	184	ALA	3.2
1	C	63	ARG	3.2
1	D	310	ALA	3.2
1	B	260	GLY	3.2
1	A	179	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	273	GLY	2.9
1	B	200	VAL	2.9
1	A	77	ALA	2.9
1	C	66	ARG	2.8
1	A	183	GLU	2.7
1	D	56	GLU	2.6
1	A	257	GLU	2.6
1	B	272	PRO	2.6
1	B	257	GLU	2.5
1	B	264	GLU	2.5
1	A	182	GLY	2.4
1	B	154	LEU	2.4
1	C	183	GLU	2.4
1	C	257	GLU	2.4
1	A	56	GLU	2.4
1	A	211	GLU	2.3
1	A	63	ARG	2.3
1	D	35	THR	2.3
1	B	263	PRO	2.3
1	B	199	PRO	2.2
1	C	5	VAL	2.2
1	B	196	LYS	2.2
1	B	309	GLY	2.2
1	B	192	GLU	2.2
1	A	43	LYS	2.2
1	B	207	THR	2.2
1	D	43	LYS	2.2
1	C	45	VAL	2.2
1	C	232	PHE	2.1
1	C	60	ARG	2.1
1	C	179	ASP	2.1
1	C	27	VAL	2.0
1	C	56	GLU	2.0
1	C	106	GLN	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 (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	D	1118	44/44	0.72	0.48	52,98,136,140	0
2	NAD	B	1118	44/44	0.75	0.48	51,102,136,141	0
2	NAD	C	1118	44/44	0.75	0.45	80,112,144,149	0
2	NAD	A	1118	44/44	0.76	0.40	56,96,130,134	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 D 1118:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
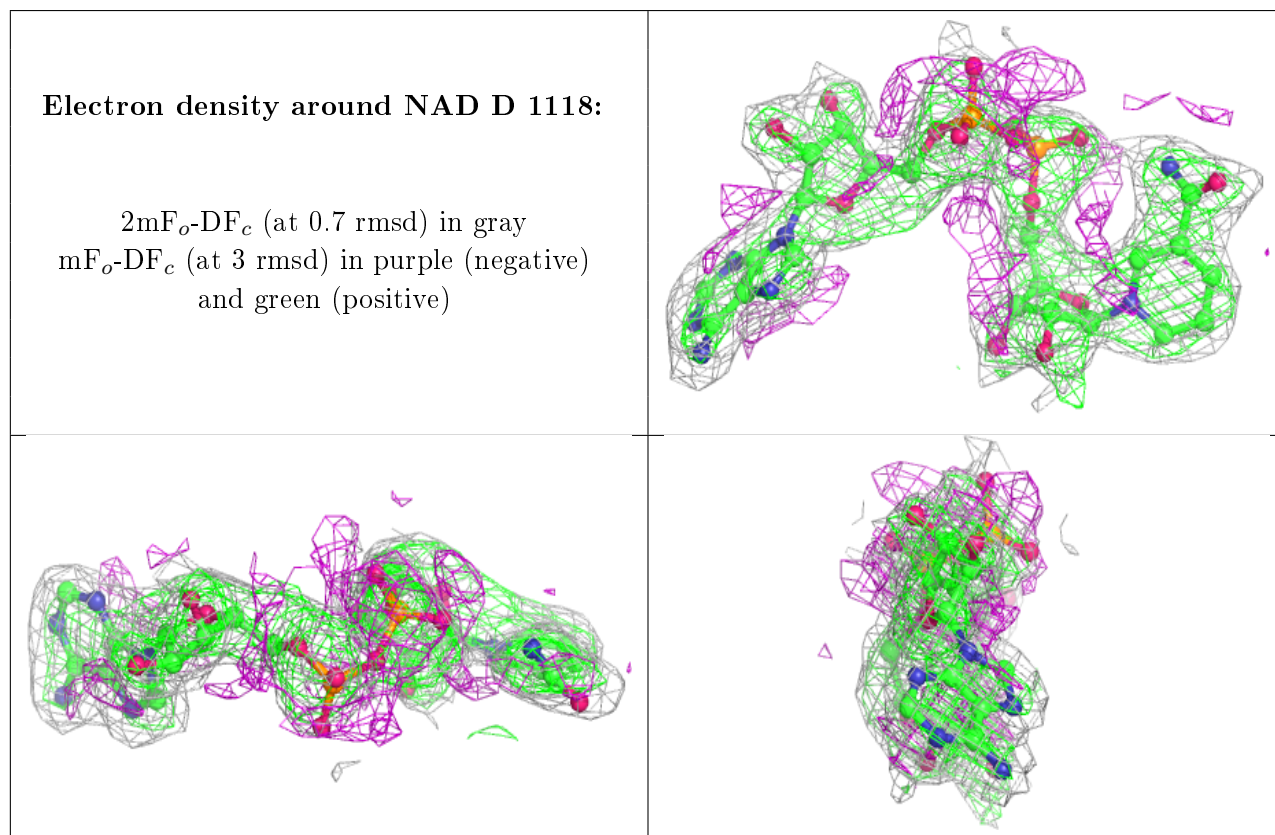
Electron density around NAD B 1118:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
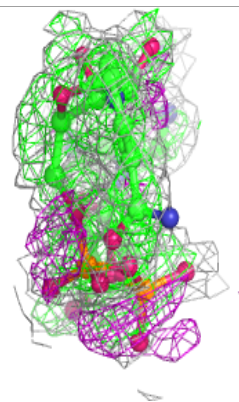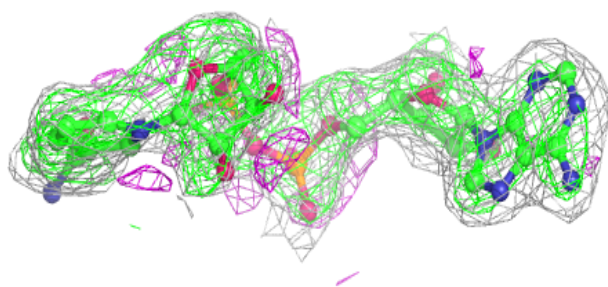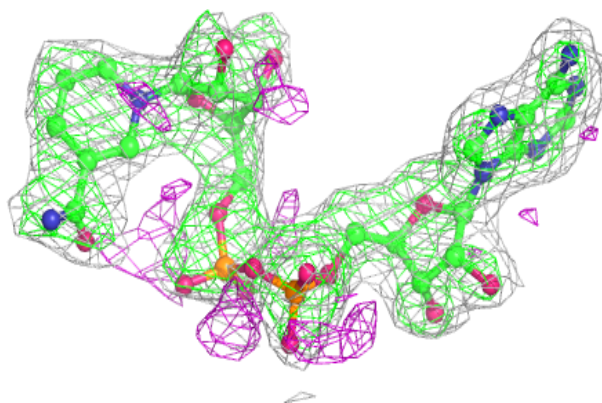
Electron density around NAD C 1118:

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

Electron density around NAD A 1118:

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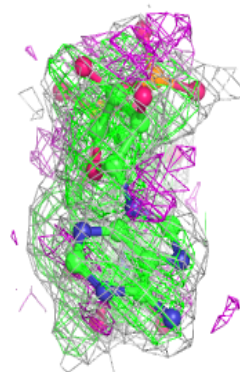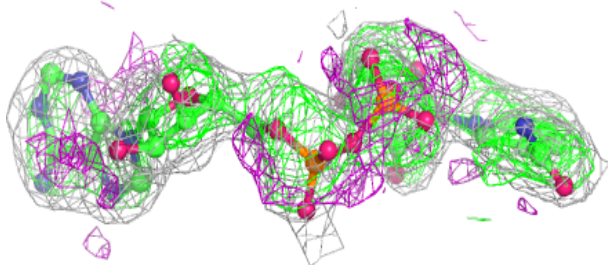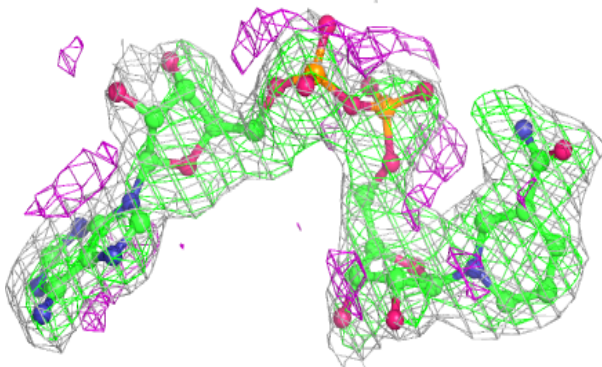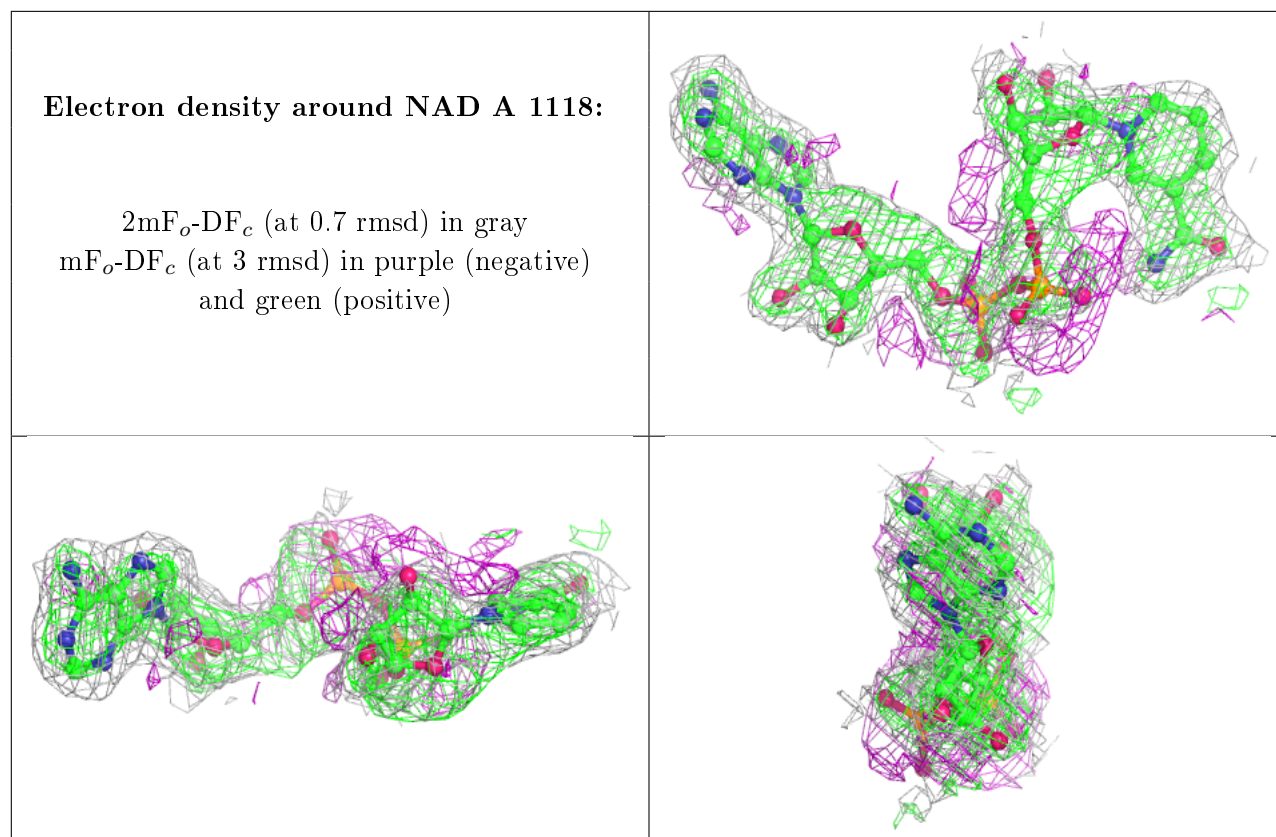
6.5 Other polymers (i)

There are no such residues in this entry.