Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:08 AM GMT

PDB ID	:	1ZW1
Title	:	Synthesis, Biological Activity, and X-Ray Crystal Structural Analysis of Diaryl Ether Inhibitors of Malarial Enoyl ACP Reductase. Part 1:4'-Substituted Triclosan Derivatives
Authors	:	Freundlich, J.S.; Anderson, J.W.; Sarantakis, D.; Shieh, H.M.; Yu, M.; Lucumi, E.; Kuo, M.; Schiehser, G.A.; Jacobus, D.P.; Jacobs Jr., W.R.; Fidock, D.A.; Sacchettini, J.C.
Deposited on	:	2005-06-03
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

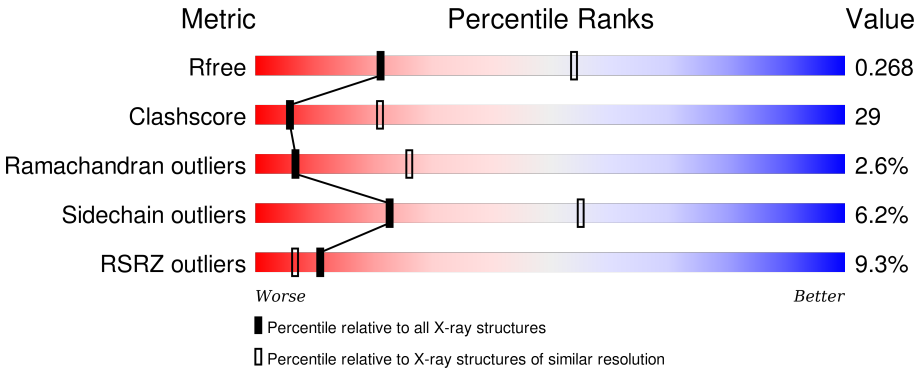
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	336	8% 44% 39% • 14%
1	B	336	8% 45% 36% 6% 14%

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	TN5	A	500	-	X	-	-
3	TN5	B	501	-	X	-	X

2 Entry composition

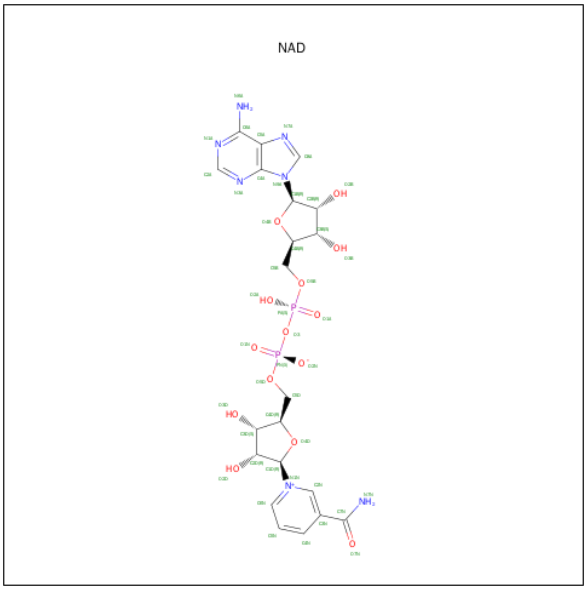
There are 3 unique types of molecules in this entry. The entry contains 4696 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 enoyl-acyl carrier reductase.

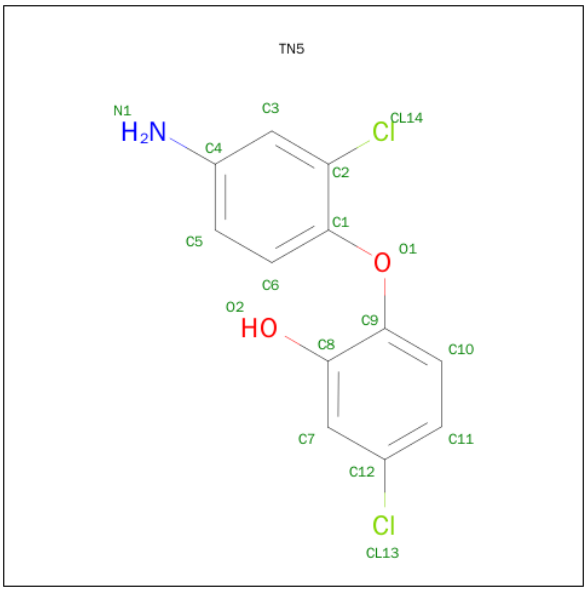
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2287	1458	384	434	11			
1	B	289	Total	C	N	O	S	0	0	0
			2287	1458	384	434	11			

- 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		

- Molecule 3 is 2-(4-AMINO-2-CHLOROPHENOXY)-5-CHLOROPHENOL (three-letter code: TN5) (formula: $C_{12}H_9Cl_2NO_2$).



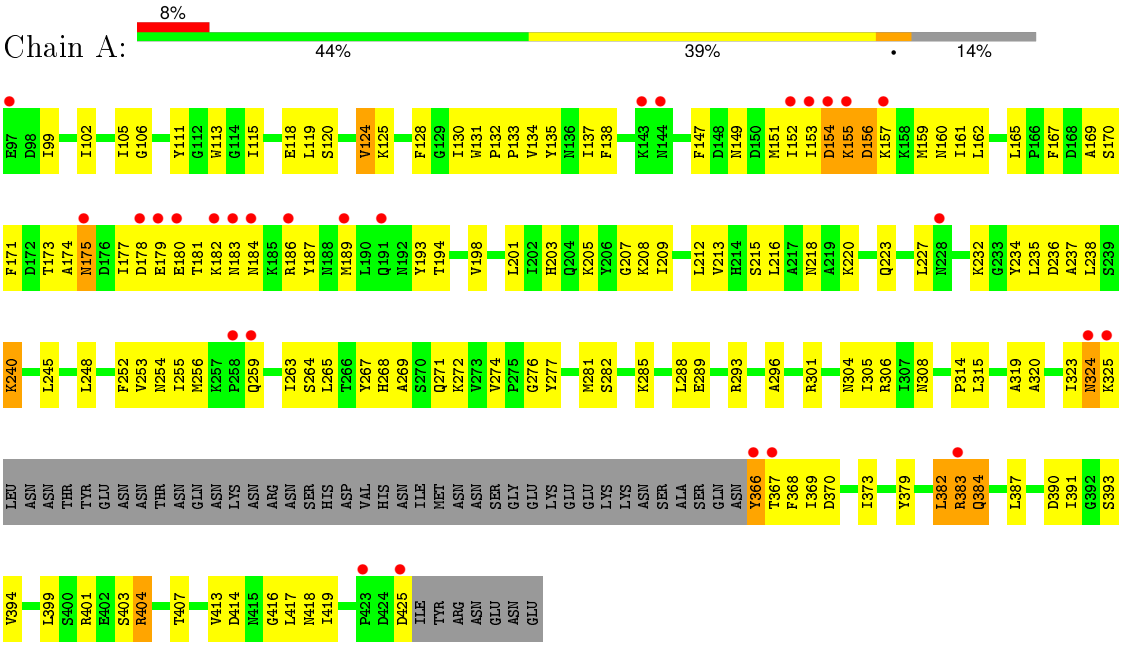
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			17	12	2	1	2		
3	B	1	Total	C	Cl	N	O	0	0
			17	12	2	1	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

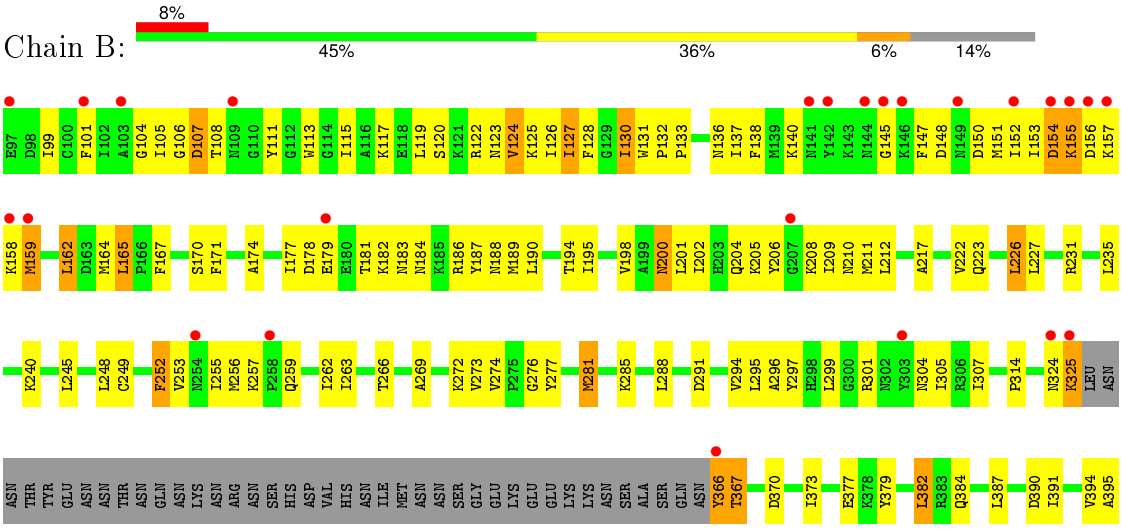
- Molecule 1: enoyl-acyl carrier reductase

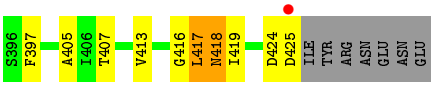
Chain A:



- Molecule 1: enoyl-acyl carrier reductase

Chain B:




S396
F397
A405
I406
T407
V413
G416
L417
N418
I419
D424
D425
ILE
TYR
ARG
ASN
GLU
ASN
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	131.27Å 131.27Å 82.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.72 – 2.90 29.72 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.5 (29.72-2.90) 98.1 (29.72-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.38 (at 2.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.297 0.261 , 0.268	Depositor DCC
R_{free} test set	821 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	39.3	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	1 of 16253 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	4696	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TN5, 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	0.40	0/2329	0.65	0/3141
1	B	0.39	0/2329	0.66	0/3141
All	All	0.40	0/4658	0.65	0/6282

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

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	2287	0	2297	142	0
1	B	2287	0	2297	142	0
2	A	44	0	26	2	0
2	B	44	0	26	2	0
3	A	17	0	8	4	0
3	B	17	0	8	3	0
All	All	4696	0	4662	269	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 29.

All (269) 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)
3:A:500:TN5:C4	3:A:500:TN5:N1	1.69	1.52
3:B:501:TN5:N1	3:B:501:TN5:C4	1.69	1.52
1:A:212:LEU:HD21	1:A:248:LEU:HD22	1.46	0.98
1:B:366:TYR:O	1:B:370:ASP:HB2	1.71	0.90
1:B:155:LYS:HE3	1:B:157:LYS:HE3	1.55	0.88
1:B:155:LYS:HD3	1:B:157:LYS:HZ1	1.42	0.83
1:A:259:GLN:HG2	1:A:304:ASN:ND2	1.93	0.83
1:B:212:LEU:HB3	1:B:262:ILE:HG12	1.61	0.81
1:A:170:SER:HB3	1:A:240:LYS:HD2	1.61	0.81
1:A:301:ARG:NH2	1:B:379:TYR:HA	1.96	0.81
1:B:248:LEU:O	1:B:252:PHE:HB2	1.84	0.77
1:A:325:LYS:HB3	1:A:368:PHE:HB2	1.65	0.77
1:B:201:LEU:HD21	1:B:205:LYS:HE3	1.67	0.75
1:A:111:TYR:O	1:A:115:ILE:HG13	1.87	0.73
1:B:170:SER:OG	1:B:240:LYS:HE2	1.90	0.72
1:B:155:LYS:CD	1:B:157:LYS:HZ1	2.04	0.71
1:A:174:ALA:O	1:A:177:ILE:HG22	1.90	0.70
1:A:167:PHE:HD1	1:A:198:VAL:HG11	1.56	0.70
1:A:128:PHE:HB3	1:A:130:ILE:HD11	1.74	0.70
1:A:132:PRO:HB2	1:A:133:PRO:HD3	1.73	0.70
1:A:281:MET:CE	1:A:285:LYS:HE2	2.22	0.69
1:B:99:ILE:HD13	1:B:125:LYS:HB2	1.74	0.69
1:B:106:GLY:O	1:B:107:ASP:HB3	1.92	0.69
1:A:301:ARG:HH21	1:B:379:TYR:HA	1.55	0.69
1:A:155:LYS:O	1:A:157:LYS:HG3	1.93	0.69
1:B:108:THR:HG22	1:B:113:TRP:CE3	2.28	0.68
1:A:178:ASP:OD2	1:A:180:GLU:HB3	1.93	0.68
1:A:154:ASP:O	1:A:156:ASP:N	2.27	0.68
1:A:177:ILE:HG23	1:A:177:ILE:O	1.94	0.68
1:B:177:ILE:HG13	1:B:177:ILE:O	1.93	0.67
1:A:379:TYR:OH	1:A:425:ASP:HB3	1.93	0.67
1:B:210:ASN:HD22	1:B:257:LYS:NZ	1.93	0.67
1:A:281:MET:HE1	1:A:285:LYS:HE2	1.75	0.67
1:B:194:THR:O	1:B:198:VAL:HG13	1.95	0.67
1:B:259:GLN:HG2	1:B:304:ASN:HD21	1.60	0.67
1:A:314:PRO:HB2	1:A:373:ILE:HG12	1.77	0.65
1:B:418:ASN:HD22	1:B:418:ASN:H	1.43	0.65
1:A:175:ASN:H	1:A:175:ASN:ND2	1.95	0.65
1:A:125:LYS:N	1:A:125:LYS:HD2	2.12	0.64
1:A:252:PHE:O	1:A:256:MET:HG3	1.96	0.64
1:B:195:ILE:HG23	1:B:248:LEU:HD23	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLU:HG3	1:A:393:SER:N	2.13	0.64
1:A:99:ILE:HB	1:A:209:ILE:HG22	1.81	0.63
1:A:387:LEU:O	1:A:390:ASP:HB2	1.99	0.63
1:B:259:GLN:HG2	1:B:304:ASN:ND2	2.14	0.62
1:B:183:ASN:HA	1:B:188:ASN:HD21	1.63	0.62
1:A:179:GLU:O	1:A:182:LYS:HB3	2.01	0.61
1:B:301:ARG:HH11	1:B:301:ARG:HG3	1.65	0.61
1:A:366:TYR:O	1:A:370:ASP:HB2	2.00	0.61
1:B:210:ASN:O	1:B:211:MET:HG3	1.99	0.61
1:B:274:VAL:O	1:B:274:VAL:CG2	2.49	0.61
1:A:147:PHE:O	1:A:151:MET:HG3	2.00	0.60
1:B:174:ALA:HA	1:B:194:THR:HG21	1.84	0.60
1:B:154:ASP:O	1:B:156:ASP:N	2.26	0.60
1:A:212:LEU:HB2	1:A:256:MET:CE	2.32	0.60
1:A:120:SER:HB2	1:A:153:ILE:HG12	1.83	0.60
1:B:105:ILE:HD12	1:B:128:PHE:CD1	2.37	0.60
1:B:301:ARG:HG3	1:B:301:ARG:NH1	2.16	0.59
1:B:105:ILE:HD12	1:B:128:PHE:CE1	2.37	0.59
1:A:301:ARG:HH21	1:B:379:TYR:C	2.06	0.59
1:A:277:TYR:CE2	1:A:281:MET:HB3	2.37	0.59
1:A:212:LEU:HD21	1:A:248:LEU:CD2	2.28	0.59
1:A:149:ASN:O	1:A:152:ILE:HG12	2.01	0.59
1:A:215:SER:HA	1:A:265:LEU:HD23	1.84	0.59
1:B:274:VAL:O	1:B:274:VAL:HG23	2.01	0.59
1:B:200:ASN:HD22	1:B:200:ASN:N	2.00	0.59
1:A:414:ASP:CG	1:A:418:ASN:HD22	2.06	0.59
1:B:155:LYS:HB2	1:B:157:LYS:NZ	2.18	0.59
1:A:125:LYS:HE3	1:A:160:ASN:HD22	1.68	0.59
1:A:379:TYR:HA	1:B:301:ARG:NH2	2.18	0.58
1:A:223:GLN:NE2	1:A:324:ASN:HB3	2.18	0.58
1:B:252:PHE:O	1:B:256:MET:HG3	2.03	0.58
1:A:125:LYS:HE3	1:A:160:ASN:ND2	2.19	0.58
1:A:306:ARG:HG2	1:B:382:LEU:HD21	1.85	0.57
1:A:301:ARG:HH21	1:B:379:TYR:CA	2.18	0.56
1:B:148:ASP:HA	1:B:151:MET:HE3	1.87	0.56
1:B:130:ILE:O	1:B:167:PHE:N	2.36	0.56
1:B:113:TRP:CH2	1:B:151:MET:HG2	2.41	0.56
1:A:265:LEU:HD22	1:A:265:LEU:N	2.21	0.56
1:A:179:GLU:OE1	1:A:182:LYS:HD3	2.06	0.56
1:B:126:ILE:HG22	1:B:127:ILE:H	1.71	0.56
1:A:276:GLY:HA2	1:A:325:LYS:HE3	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ILE:HG23	1:A:399:LEU:HD21	1.87	0.56
1:A:391:ILE:HD12	1:A:391:ILE:N	2.22	0.55
1:A:404:ARG:HH21	1:B:384:GLN:CD	2.10	0.55
1:B:165:LEU:HD13	1:B:201:LEU:HD12	1.88	0.55
1:B:126:ILE:HG21	1:B:128:PHE:HE1	1.72	0.55
1:A:128:PHE:HB3	1:A:130:ILE:CD1	2.36	0.54
1:B:147:PHE:O	1:B:151:MET:HG3	2.07	0.54
1:A:379:TYR:HA	1:B:301:ARG:HH21	1.73	0.54
1:B:137:ILE:HD12	1:B:140:LYS:HD3	1.88	0.54
1:B:295:LEU:O	1:B:299:LEU:HG	2.07	0.54
1:A:259:GLN:HE21	1:A:304:ASN:HD21	1.55	0.54
1:B:132:PRO:HG2	1:B:187:TYR:CE2	2.43	0.54
1:B:108:THR:HG22	1:B:113:TRP:CD2	2.43	0.53
1:A:212:LEU:HB2	1:A:256:MET:HE1	1.89	0.53
1:B:249:CYS:O	1:B:253:VAL:HB	2.09	0.53
1:A:232:LYS:O	1:A:236:ASP:HB2	2.08	0.53
1:B:155:LYS:HD3	1:B:157:LYS:NZ	2.18	0.53
1:A:125:LYS:HB3	1:A:162:LEU:HG	1.91	0.53
1:B:126:ILE:HG22	1:B:127:ILE:N	2.23	0.53
1:A:267:TYR:CD2	1:A:269:ALA:HB2	2.44	0.53
1:B:119:LEU:O	1:B:124:VAL:HG13	2.09	0.53
1:B:145:GLY:HA2	1:B:148:ASP:OD1	2.08	0.53
1:B:148:ASP:O	1:B:158:LYS:NZ	2.42	0.53
1:B:131:TRP:CG	1:B:133:PRO:HD2	2.44	0.53
1:A:187:TYR:HD2	1:A:193:TYR:OH	1.92	0.52
1:A:178:ASP:O	1:A:182:LYS:HB2	2.08	0.52
1:A:99:ILE:HG23	1:A:162:LEU:HD12	1.91	0.52
1:B:263:ILE:CD1	1:B:395:ALA:HB1	2.39	0.52
1:A:177:ILE:HD11	1:A:193:TYR:OH	2.09	0.52
1:A:245:LEU:HD22	1:A:288:LEU:CD1	2.39	0.52
1:A:234:TYR:O	1:A:237:ALA:HB3	2.09	0.52
1:B:416:GLY:O	1:B:419:ILE:HG12	2.10	0.52
1:A:175:ASN:HD22	1:A:175:ASN:H	1.56	0.52
1:A:212:LEU:HD11	1:A:248:LEU:HD21	1.92	0.51
1:A:245:LEU:HD22	1:A:288:LEU:HD12	1.93	0.51
1:A:404:ARG:HH12	1:B:387:LEU:HD12	1.74	0.51
1:A:175:ASN:N	1:A:175:ASN:HD22	2.06	0.51
1:A:175:ASN:N	1:A:175:ASN:ND2	2.57	0.51
1:A:105:ILE:CG2	1:A:130:ILE:HD12	2.41	0.51
1:A:153:ILE:CD1	1:A:159:MET:HB2	2.41	0.51
1:A:391:ILE:CD1	1:A:391:ILE:N	2.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ALA:HB1	1:B:281:MET:CE	2.41	0.51
1:B:209:ILE:O	1:B:256:MET:HA	2.11	0.50
1:B:178:ASP:O	1:B:182:LYS:HB2	2.10	0.50
1:B:138:PHE:CE2	1:B:164:MET:HE3	2.47	0.50
1:B:269:ALA:HA	1:B:272:LYS:O	2.12	0.50
1:A:263:ILE:HA	1:A:308:ASN:O	2.10	0.50
1:B:153:ILE:HB	1:B:157:LYS:HB2	1.92	0.50
1:A:271:GLN:NE2	1:A:289:GLU:OE1	2.45	0.50
1:B:155:LYS:HB2	1:B:157:LYS:HZ1	1.76	0.50
1:A:120:SER:CB	1:A:153:ILE:HG12	2.42	0.50
1:A:308:ASN:OD1	1:A:407:THR:HA	2.12	0.50
1:B:171:PHE:O	1:B:195:ILE:HG13	2.12	0.50
1:B:202:ILE:HD12	1:B:252:PHE:HZ	1.77	0.50
1:A:383:ARG:HE	1:B:301:ARG:HD2	1.76	0.50
1:B:104:GLY:O	2:B:451:NAD:H4B	2.12	0.50
1:B:184:ASN:ND2	1:B:186:ARG:H	2.09	0.50
1:A:131:TRP:CG	1:A:133:PRO:HD2	2.47	0.49
1:A:259:GLN:HG2	1:A:304:ASN:HD21	1.74	0.49
1:A:366:TYR:N	1:A:366:TYR:CD2	2.79	0.49
1:B:117:LYS:HE3	1:B:150:ASP:O	2.12	0.49
1:B:113:TRP:HH2	1:B:151:MET:HG2	1.78	0.49
1:A:379:TYR:C	1:B:301:ARG:HH21	2.16	0.49
1:B:277:TYR:CE2	1:B:281:MET:HB3	2.48	0.48
1:B:155:LYS:HE3	1:B:157:LYS:CE	2.38	0.48
1:B:132:PRO:HB2	1:B:133:PRO:HD3	1.96	0.48
1:A:134:VAL:O	1:A:137:ILE:HG22	2.13	0.48
1:A:102:ILE:HA	1:A:213:VAL:HB	1.96	0.48
1:A:99:ILE:HD12	1:A:162:LEU:HD11	1.96	0.47
1:A:201:LEU:HD21	1:A:205:LYS:HE3	1.95	0.47
1:A:151:MET:O	1:A:153:ILE:HD12	2.14	0.47
1:A:159:MET:HE2	1:A:161:ILE:HG12	1.97	0.47
1:A:264:SER:C	1:A:265:LEU:HD22	2.33	0.47
1:A:404:ARG:HH21	1:B:384:GLN:NE2	2.12	0.47
1:B:120:SER:O	1:B:123:ASN:N	2.31	0.47
1:B:106:GLY:O	1:B:107:ASP:CB	2.62	0.47
1:B:183:ASN:CA	1:B:188:ASN:HD21	2.26	0.47
1:B:223:GLN:HE21	1:B:324:ASN:HB3	1.77	0.47
1:A:212:LEU:HB2	1:A:256:MET:HE3	1.96	0.47
1:B:183:ASN:C	1:B:188:ASN:HD21	2.17	0.47
1:B:294:VAL:O	1:B:297:TYR:HB3	2.14	0.47
1:B:165:LEU:CD1	1:B:201:LEU:HD12	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:TYR:CZ	1:A:281:MET:HB3	2.50	0.47
1:B:291:ASP:O	1:B:295:LEU:HG	2.15	0.47
1:B:390:ASP:O	1:B:394:VAL:HG23	2.15	0.47
1:A:269:ALA:HA	1:A:274:VAL:HG12	1.97	0.47
1:A:382:LEU:HD22	1:B:407:THR:HG21	1.97	0.47
1:B:266:THR:HA	1:B:285:LYS:HD2	1.96	0.47
1:B:108:THR:HA	1:B:113:TRP:HB2	1.97	0.47
1:A:203:HIS:HB2	1:A:255:ILE:HG21	1.97	0.47
1:A:208:LYS:HA	1:A:255:ILE:O	2.15	0.46
1:B:210:ASN:HB3	1:B:257:LYS:HE3	1.96	0.46
1:B:245:LEU:HD22	1:B:288:LEU:HD11	1.96	0.46
1:A:413:VAL:HG13	1:B:405:ALA:HB3	1.97	0.46
1:B:179:GLU:O	1:B:182:LYS:HB3	2.16	0.46
1:B:276:GLY:HA2	1:B:325:LYS:NZ	2.31	0.46
1:B:373:ILE:O	1:B:377:GLU:HG3	2.15	0.46
1:B:252:PHE:CD1	1:B:255:ILE:HD11	2.50	0.46
1:A:218:ASN:HA	3:A:500:TN5:HN12	1.81	0.46
1:B:150:ASP:C	1:B:152:ILE:H	2.20	0.46
1:B:418:ASN:ND2	1:B:418:ASN:H	2.10	0.46
1:A:274:VAL:O	1:A:274:VAL:HG13	2.16	0.45
1:A:384:GLN:NE2	1:A:384:GLN:H	2.14	0.45
1:B:217:ALA:HB1	1:B:281:MET:HE1	1.98	0.45
1:B:117:LYS:HE2	1:B:152:ILE:O	2.17	0.45
1:B:128:PHE:HB3	1:B:130:ILE:CD1	2.47	0.45
1:A:384:GLN:HE21	1:A:384:GLN:H	1.64	0.45
1:B:153:ILE:O	1:B:154:ASP:C	2.55	0.45
1:A:216:LEU:HD12	1:A:216:LEU:O	2.16	0.45
1:B:208:LYS:HA	1:B:255:ILE:O	2.16	0.45
1:A:304:ASN:CG	1:A:304:ASN:O	2.54	0.45
1:B:391:ILE:HA	1:B:413:VAL:HG11	1.99	0.45
1:B:108:THR:HG22	1:B:113:TRP:CZ3	2.51	0.45
1:A:153:ILE:O	1:A:154:ASP:C	2.55	0.45
1:B:231:ARG:O	1:B:235:LEU:HG	2.17	0.45
1:B:296:ALA:HA	1:B:307:ILE:HG22	1.99	0.44
1:A:173:THR:OG1	1:A:175:ASN:ND2	2.51	0.44
1:A:183:ASN:O	1:A:184:ASN:C	2.55	0.44
1:A:137:ILE:HA	1:A:137:ILE:HD12	1.81	0.44
1:A:223:GLN:HE21	1:A:324:ASN:HB3	1.82	0.44
1:B:245:LEU:HD22	1:B:288:LEU:CD1	2.47	0.44
1:A:320:ALA:HB1	1:A:369:ILE:HD13	1.99	0.44
1:B:314:PRO:HA	2:B:451:NAD:O7N	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:TYR:O	1:A:138:PHE:HB3	2.17	0.44
1:A:301:ARG:NH2	1:B:424:ASP:OD2	2.49	0.44
1:B:252:PHE:CE1	1:B:255:ILE:HD11	2.52	0.44
1:B:177:ILE:HD11	1:B:182:LYS:HE3	2.00	0.44
1:A:253:VAL:HG13	1:A:254:ASN:N	2.33	0.44
1:B:366:TYR:CD2	1:B:366:TYR:N	2.86	0.44
1:B:122:ARG:O	1:B:123:ASN:HB2	2.18	0.44
1:B:217:ALA:HB3	3:B:501:TN5:CL14	2.54	0.44
1:A:263:ILE:HG23	1:A:399:LEU:CD2	2.48	0.44
1:B:222:VAL:HG21	3:B:501:TN5:H5	1.99	0.43
1:A:181:THR:HB	1:A:187:TYR:CD2	2.52	0.43
1:A:253:VAL:CG1	1:A:254:ASN:N	2.80	0.43
1:B:151:MET:HB3	1:B:159:MET:HB2	2.00	0.43
1:B:131:TRP:CD1	1:B:132:PRO:HD2	2.53	0.43
1:A:293:ARG:O	1:A:296:ALA:HB3	2.17	0.43
1:A:269:ALA:CB	1:A:277:TYR:CD2	3.01	0.43
1:A:253:VAL:HG23	1:A:305:ILE:HD12	2.01	0.43
1:A:404:ARG:NH1	1:B:387:LEU:HD12	2.34	0.43
1:A:234:TYR:HD1	1:A:235:LEU:HD23	1.84	0.43
1:A:416:GLY:O	1:A:419:ILE:HG12	2.18	0.43
1:A:306:ARG:NH1	1:A:403:SER:O	2.52	0.43
1:A:186:ARG:NH2	1:A:189:MET:SD	2.91	0.43
1:B:101:PHE:CD1	1:B:252:PHE:CZ	3.07	0.43
1:B:162:LEU:HD21	1:B:206:TYR:CE1	2.53	0.43
1:A:414:ASP:OD1	1:A:418:ASN:ND2	2.51	0.43
1:B:189:MET:HG3	1:B:190:LEU:HD23	2.00	0.43
1:A:319:ALA:HB1	3:A:500:TN5:C2	2.49	0.43
1:B:418:ASN:N	1:B:418:ASN:ND2	2.66	0.43
1:A:218:ASN:HA	3:A:500:TN5:N1	2.34	0.42
1:A:177:ILE:CG2	1:A:177:ILE:O	2.65	0.42
1:A:132:PRO:CB	1:A:133:PRO:HD3	2.46	0.42
1:B:263:ILE:HD11	1:B:395:ALA:HB1	2.00	0.42
1:A:315:LEU:N	2:A:450:NAD:O7N	2.52	0.42
1:A:171:PHE:HZ	1:A:181:THR:HG21	1.84	0.42
1:A:401:ARG:C	1:A:403:SER:H	2.22	0.42
1:B:111:TYR:O	1:B:115:ILE:HG13	2.19	0.42
1:A:153:ILE:HD11	1:A:159:MET:HB2	2.02	0.42
1:A:201:LEU:CD1	1:A:205:LYS:HD2	2.49	0.42
1:A:105:ILE:HD11	1:A:113:TRP:HE3	1.85	0.42
1:A:113:TRP:CZ2	1:A:151:MET:HG2	2.55	0.42
1:B:183:ASN:HA	1:B:188:ASN:ND2	2.32	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LEU:O	1:A:124:VAL:HG13	2.20	0.42
1:B:117:LYS:O	1:B:120:SER:HB2	2.20	0.42
1:B:148:ASP:HA	1:B:151:MET:CE	2.48	0.42
1:B:391:ILE:HD12	1:B:391:ILE:N	2.35	0.41
1:A:105:ILE:HD12	1:A:128:PHE:CE1	2.56	0.41
1:B:158:LYS:O	1:B:159:MET:C	2.59	0.41
1:A:271:GLN:O	1:A:272:LYS:HD3	2.20	0.41
1:A:174:ALA:HA	1:A:194:THR:HG21	2.00	0.41
1:B:301:ARG:HH11	1:B:301:ARG:CG	2.32	0.41
1:A:169:ALA:H	2:A:450:NAD:C2A	2.30	0.41
1:B:253:VAL:CG2	1:B:305:ILE:HD12	2.51	0.41
1:B:417:LEU:HD23	1:B:417:LEU:HA	1.90	0.41
1:B:136:ASN:OD1	1:B:189:MET:SD	2.79	0.41
1:A:267:TYR:C	1:A:269:ALA:H	2.25	0.41
1:B:178:ASP:C	1:B:178:ASP:OD2	2.59	0.41
1:A:323:ILE:O	1:A:324:ASN:HB3	2.21	0.41
1:A:394:VAL:HG22	1:B:397:PHE:HZ	1.85	0.41
1:A:203:HIS:O	1:A:207:GLY:HA2	2.22	0.40
1:B:325:LYS:HA	1:B:325:LYS:HD3	1.92	0.40
1:B:126:ILE:O	1:B:162:LEU:HB3	2.21	0.40
1:B:120:SER:HB2	1:B:153:ILE:HD11	2.02	0.40
1:A:220:LYS:HE3	1:A:240:LYS:HZ1	1.86	0.40
1:B:137:ILE:CD1	1:B:140:LYS:HD3	2.51	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	285/336 (85%)	247 (87%)	30 (10%)	8 (3%)	6 24
1	B	285/336 (85%)	250 (88%)	28 (10%)	7 (2%)	7 27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	570/672 (85%)	497 (87%)	58 (10%)	15 (3%)	7 26

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	ASP
1	A	155	LYS
1	B	107	ASP
1	B	155	LYS
1	A	156	ASP
1	A	404	ARG
1	B	154	ASP
1	B	159	MET
1	B	226	LEU
1	B	367	THR
1	A	324	ASN
1	A	367	THR
1	A	268	HIS
1	A	106	GLY
1	B	127	ILE

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	250/295 (85%)	238 (95%)	12 (5%)	31 67
1	B	250/295 (85%)	231 (92%)	19 (8%)	16 43
All	All	500/590 (85%)	469 (94%)	31 (6%)	23 55

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	VAL
1	A	165	LEU
1	A	175	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	227	LEU
1	A	238	LEU
1	A	240	LYS
1	A	282	SER
1	A	366	TYR
1	A	382	LEU
1	A	383	ARG
1	A	384	GLN
1	A	417	LEU
1	B	124	VAL
1	B	130	ILE
1	B	162	LEU
1	B	165	LEU
1	B	181	THR
1	B	200	ASN
1	B	204	GLN
1	B	226	LEU
1	B	227	LEU
1	B	252	PHE
1	B	273	VAL
1	B	281	MET
1	B	325	LYS
1	B	366	TYR
1	B	367	THR
1	B	382	LEU
1	B	417	LEU
1	B	418	ASN
1	B	425	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	144	ASN
1	A	160	ASN
1	A	175	ASN
1	A	183	ASN
1	A	188	ASN
1	A	200	ASN
1	A	203	HIS
1	A	218	ASN
1	A	223	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	228	ASN
1	A	254	ASN
1	A	302	ASN
1	A	304	ASN
1	A	384	GLN
1	A	409	GLN
1	B	109	ASN
1	B	144	ASN
1	B	184	ASN
1	B	188	ASN
1	B	200	ASN
1	B	210	ASN
1	B	223	GLN
1	B	254	ASN
1	B	302	ASN
1	B	304	ASN
1	B	384	GLN
1	B	415	ASN
1	B	418	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAD	A	450	-	38,48,48	1.65	5 (13%)	47,73,73	3.09	13 (27%)
3	TN5	A	500	-	18,18,18	6.74	15 (83%)	25,25,25	1.56	7 (28%)
2	NAD	B	451	-	38,48,48	1.55	5 (13%)	47,73,73	3.00	11 (23%)
3	TN5	B	501	-	18,18,18	6.49	15 (83%)	25,25,25	1.71	7 (28%)

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	450	-	-	0/22/62/62	0/5/5/5
3	TN5	A	500	-	-	0/4/4/4	0/2/2/2
2	NAD	B	451	-	-	0/22/62/62	0/5/5/5
3	TN5	B	501	-	-	0/4/4/4	0/2/2/2

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	TN5	C12-CL13	-5.33	1.62	1.74
3	B	501	TN5	C12-CL13	-4.84	1.63	1.74
3	B	501	TN5	C2-CL14	-2.62	1.67	1.73
3	A	500	TN5	C2-CL14	-2.03	1.68	1.73
2	A	450	NAD	O4D-C1D	2.11	1.43	1.41
3	A	500	TN5	C5-C4	2.23	1.45	1.39
2	B	451	NAD	O4D-C1D	2.32	1.44	1.41
3	B	501	TN5	C5-C4	2.39	1.45	1.39
2	A	450	NAD	C6N-C5N	3.12	1.45	1.38
2	B	451	NAD	C6N-C5N	3.23	1.45	1.38
2	B	451	NAD	C5N-C4N	3.23	1.45	1.38
2	A	450	NAD	C5N-C4N	3.63	1.46	1.38
3	B	501	TN5	O1-C1	3.67	1.47	1.39
3	A	500	TN5	O1-C1	3.78	1.47	1.39
2	B	451	NAD	C4A-N3A	3.82	1.41	1.35
2	A	450	NAD	C4A-N3A	3.87	1.41	1.35
2	B	451	NAD	O7N-C7N	4.40	1.33	1.24
2	A	450	NAD	O7N-C7N	4.59	1.34	1.24
3	B	501	TN5	C11-C12	5.11	1.48	1.38
3	B	501	TN5	C10-C9	5.35	1.51	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	TN5	C10-C9	5.38	1.51	1.39
3	A	500	TN5	C11-C12	5.44	1.48	1.38
3	A	500	TN5	C8-C9	5.53	1.49	1.40
3	B	501	TN5	C8-C9	5.58	1.49	1.40
3	A	500	TN5	C7-C12	6.12	1.48	1.38
3	B	501	TN5	C7-C12	6.57	1.49	1.38
3	B	501	TN5	C3-C2	7.16	1.50	1.38
3	B	501	TN5	C10-C11	7.38	1.52	1.38
3	A	500	TN5	C3-C2	7.57	1.51	1.38
3	B	501	TN5	C6-C1	7.69	1.56	1.39
3	A	500	TN5	C10-C11	7.97	1.53	1.38
3	A	500	TN5	C4-N1	8.30	1.69	1.38
3	B	501	TN5	C4-N1	8.32	1.69	1.38
3	A	500	TN5	C6-C1	8.47	1.57	1.39
3	B	501	TN5	C1-C2	9.99	1.57	1.39
3	A	500	TN5	C1-C2	10.41	1.58	1.39
3	A	500	TN5	C7-C8	10.50	1.53	1.38
3	B	501	TN5	C7-C8	10.66	1.53	1.38
3	B	501	TN5	C3-C4	11.30	1.56	1.39
3	A	500	TN5	C3-C4	12.53	1.58	1.39

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	451	NAD	C1B-N9A-C4A	-8.85	113.60	126.94
2	A	450	NAD	C2N-C3N-C4N	-8.55	108.77	118.29
2	A	450	NAD	C1B-N9A-C4A	-8.52	114.09	126.94
2	B	451	NAD	C2N-C3N-C4N	-8.22	109.13	118.29
2	B	451	NAD	O7N-C7N-N7N	-7.73	111.71	122.59
2	A	450	NAD	O7N-C7N-N7N	-7.62	111.88	122.59
2	A	450	NAD	C4D-O4D-C1D	-5.25	103.95	109.72
2	B	451	NAD	C4D-O4D-C1D	-4.17	105.13	109.72
2	B	451	NAD	N3A-C2A-N1A	-2.72	126.81	128.89
2	A	450	NAD	N3A-C2A-N1A	-2.51	126.97	128.89
3	A	500	TN5	C3-C2-C1	-2.28	117.66	120.99
2	A	450	NAD	C4B-O4B-C1B	-2.26	107.23	109.72
3	B	501	TN5	C3-C4-N1	-2.24	116.89	120.53
3	B	501	TN5	O1-C1-C2	-2.24	114.61	119.84
3	A	500	TN5	O1-C1-C2	-2.16	114.80	119.84
2	A	450	NAD	C5N-C6N-N1N	-2.13	116.78	120.47
3	A	500	TN5	C3-C4-N1	-2.10	117.12	120.53
2	B	451	NAD	O3B-C3B-C4B	-2.00	105.05	111.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	500	TN5	C6-C5-C4	2.12	123.58	120.66
3	B	501	TN5	C7-C12-CL13	2.38	122.10	119.14
3	B	501	TN5	C6-C5-C4	2.39	123.94	120.66
3	A	500	TN5	C1-O1-C9	2.46	123.72	117.75
3	A	500	TN5	O1-C1-C6	2.54	127.38	120.82
3	B	501	TN5	O1-C1-C6	2.72	127.83	120.82
3	B	501	TN5	C1-O1-C9	2.79	124.52	117.75
2	A	450	NAD	O7N-C7N-C3N	2.93	122.78	119.59
2	B	451	NAD	O7N-C7N-C3N	2.95	122.81	119.59
2	A	450	NAD	C2N-C3N-C7N	3.03	128.11	119.31
2	A	450	NAD	O4D-C1D-N1N	3.05	111.48	108.13
2	B	451	NAD	C2N-C3N-C7N	3.16	128.49	119.31
3	A	500	TN5	O1-C9-C8	3.53	123.05	116.12
3	B	501	TN5	O1-C9-C8	4.37	124.72	116.12
2	B	451	NAD	C3N-C2N-N1N	5.62	126.84	120.36
2	A	450	NAD	C3N-C2N-N1N	6.00	127.27	120.36
2	A	450	NAD	C3N-C7N-N7N	6.87	125.33	117.82
2	B	451	NAD	C5N-C4N-C3N	6.96	129.09	120.33
2	B	451	NAD	C3N-C7N-N7N	7.00	125.48	117.82
2	A	450	NAD	C5N-C4N-C3N	7.09	129.26	120.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	450	NAD	2	0
3	A	500	TN5	4	0
2	B	451	NAD	2	0
3	B	501	TN5	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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, 95^{th} 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	289/336 (86%)	0.53	28 (9%)	10	6	7, 25, 62, 76	0
1	B	289/336 (86%)	0.52	26 (8%)	12	7	7, 26, 67, 85	0
All	All	578/672 (86%)	0.53	54 (9%)	11	7	7, 26, 66, 85	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	366	TYR	7.9
1	A	154	ASP	7.7
1	B	324	ASN	7.1
1	B	155	LYS	5.8
1	A	324	ASN	5.5
1	A	144	ASN	4.4
1	A	179	GLU	4.3
1	B	154	ASP	4.3
1	B	146	LYS	4.2
1	A	183	ASN	4.1
1	B	141	ASN	4.1
1	B	152	ILE	4.1
1	A	175	ASN	4.0
1	B	325	LYS	3.9
1	A	425	ASP	3.8
1	A	325	LYS	3.7
1	A	258	PRO	3.6
1	B	109	ASN	3.6
1	B	144	ASN	3.5
1	B	254	ASN	3.4
1	A	157	LYS	3.4
1	B	142	TYR	3.3
1	B	97	GLU	3.3
1	B	145	GLY	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	149	ASN	3.2
1	B	366	TYR	3.2
1	A	259	GLN	3.1
1	B	207	GLY	3.1
1	A	423	PRO	3.0
1	A	180	GLU	3.0
1	B	158	LYS	2.9
1	A	189	MET	2.8
1	A	155	LYS	2.8
1	A	367	THR	2.7
1	A	191	GLN	2.6
1	B	179	GLU	2.5
1	A	97	GLU	2.5
1	B	425	ASP	2.5
1	A	178	ASP	2.4
1	B	156	ASP	2.4
1	B	159	MET	2.4
1	B	303	TYR	2.4
1	A	186	ARG	2.4
1	A	228	ASN	2.3
1	A	153	ILE	2.3
1	B	101	PHE	2.2
1	A	182	LYS	2.2
1	B	157	LYS	2.2
1	A	152	ILE	2.1
1	A	383	ARG	2.1
1	B	103	ALA	2.1
1	A	143	LYS	2.1
1	A	184	ASN	2.1
1	B	258	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	TN5	B	501	17/17	0.81	0.31	2.21	25,30,33,34	0
2	NAD	A	450	44/44	0.88	0.24	0.64	29,38,58,58	0
3	TN5	A	500	17/17	0.84	0.23	0.17	9,19,20,21	0
2	NAD	B	451	44/44	0.93	0.19	-0.25	20,27,31,35	0

6.5 Other polymers

There are no such residues in this entry.