Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:09 AM GMT

PDB ID	:	1ZXB
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	:	2005-06-07
Resolution	:	2.68 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:

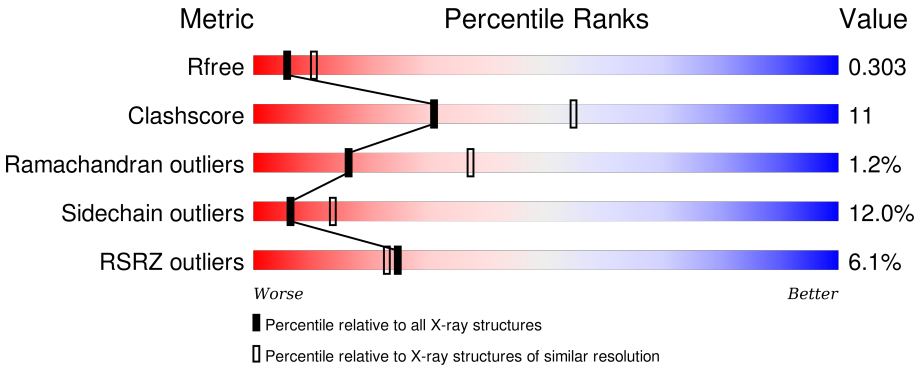
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.68 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	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

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	5% 61% 22% • • 14%
1	B	336	5% 63% 20% • 14%

2 Entry composition

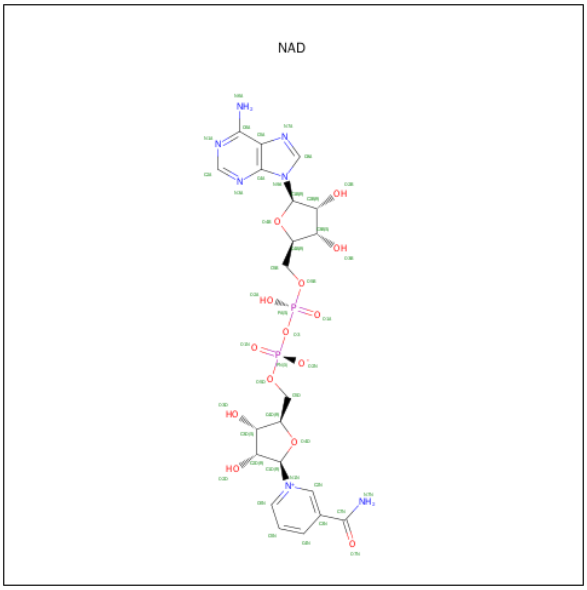
There are 3 unique types of molecules in this entry. The entry contains 4702 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

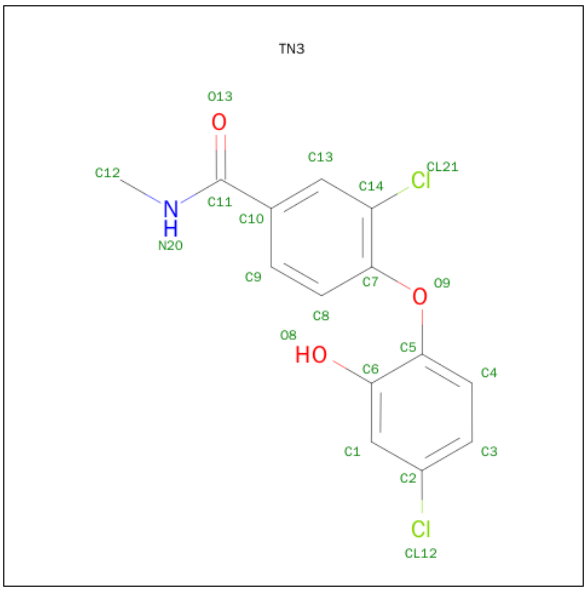
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2287	1458	384	434	11			
1	B	289	Total	C	N	O	S	0	0	0
			2287	1458	384	434	11			

- 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 3-CHLORO-4-(4-CHLORO-2-HYDROXYPHENOXY)-N-METHYLBENZAMIDE (three-letter code: TN3) (formula: $C_{14}H_{11}Cl_2NO_3$).



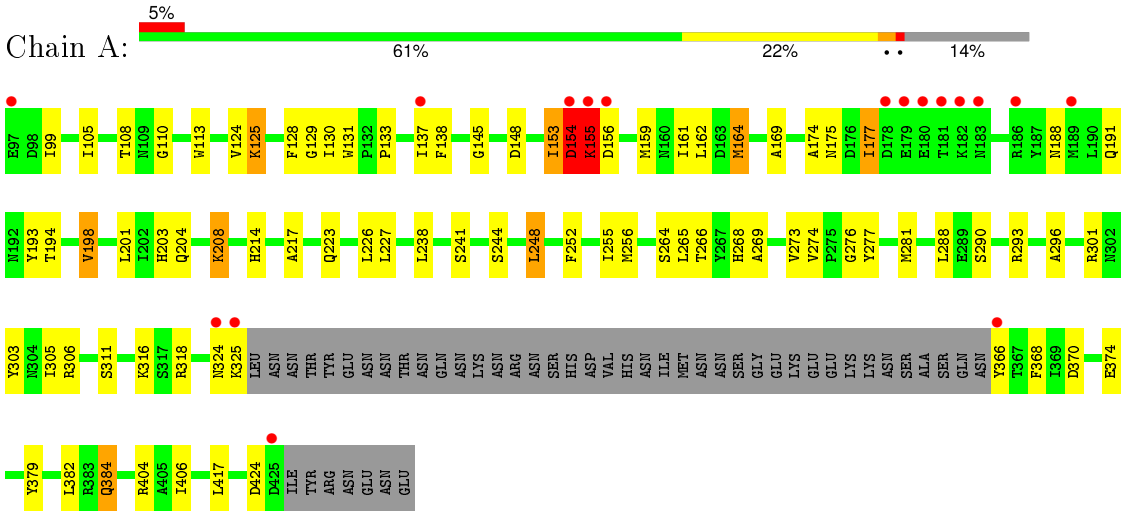
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			20	14	2	1	3		
3	B	1	Total	C	Cl	N	O	0	0
			20	14	2	1	3		

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.

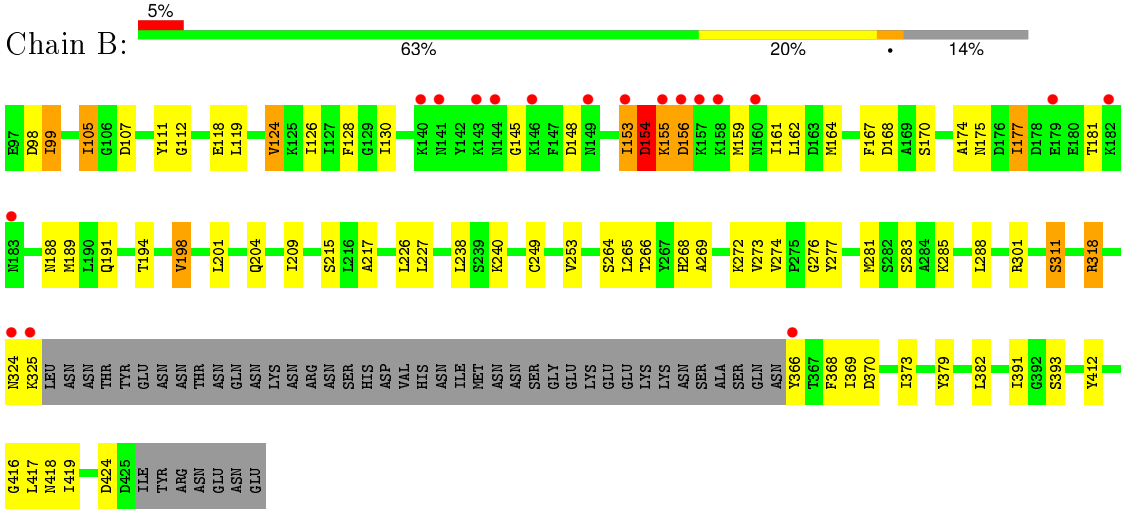
- Molecule 1: enoyl-acyl carrier reductase

Chain A:



- Molecule 1: enoyl-acyl carrier reductase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	131.43Å 131.43Å 82.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.68 29.75 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.68) 99.9 (29.75-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.53 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.233 , 0.301 0.234 , 0.303	Depositor DCC
R_{free} test set	1068 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	32.7	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	2 of 20884 reflections (0.010%)	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	4702	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: NAD, TN3

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	0.54	0/2329	0.65	0/3141
1	B	0.55	0/2329	0.67	0/3141
All	All	0.55	0/4658	0.66	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	53	0
1	B	2287	0	2297	52	0
2	A	44	0	26	2	0
2	B	44	0	26	0	0
3	A	20	0	10	1	0
3	B	20	0	11	1	0
All	All	4702	0	4667	102	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 11.

All (102) 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:B:170:SER:HB3	1:B:240:LYS:HE2	1.46	0.97
1:B:281:MET:HE1	1:B:285:LYS:HE2	1.63	0.80
1:A:223:GLN:NE2	1:A:324:ASN:HB3	1.99	0.78
1:A:203:HIS:HE1	1:A:208:LYS:NZ	1.93	0.67
1:B:119:LEU:O	1:B:124:VAL:HG13	1.95	0.67
1:A:276:GLY:HA2	1:A:325:LYS:HE3	1.77	0.67
1:B:170:SER:CB	1:B:240:LYS:HE2	2.23	0.66
1:A:203:HIS:HB2	1:A:255:ILE:HG21	1.78	0.66
1:B:274:VAL:O	1:B:274:VAL:HG23	1.96	0.66
1:A:203:HIS:HE1	1:A:208:LYS:HZ1	1.42	0.65
1:B:111:TYR:CE1	1:B:391:ILE:HD13	2.35	0.61
1:A:277:TYR:CE2	1:A:281:MET:HB3	2.36	0.61
1:B:168:ASP:OD1	1:B:170:SER:OG	2.18	0.60
1:A:161:ILE:HD13	1:A:164:MET:HE1	1.83	0.60
1:B:105:ILE:HG22	1:B:112:GLY:HA3	1.84	0.60
1:A:223:GLN:HE21	1:A:324:ASN:HB3	1.67	0.59
1:B:276:GLY:HA2	1:B:325:LYS:HE3	1.83	0.59
1:B:154:ASP:OD1	1:B:154:ASP:N	2.34	0.59
1:B:118:GLU:HG3	1:B:393:SER:N	2.18	0.59
1:A:301:ARG:NH2	1:B:379:TYR:HA	2.18	0.58
1:B:128:PHE:HB3	1:B:130:ILE:HD11	1.85	0.58
1:A:269:ALA:HB2	1:A:274:VAL:CG2	2.35	0.56
1:A:203:HIS:CE1	1:A:208:LYS:NZ	2.73	0.56
1:A:269:ALA:CB	1:A:274:VAL:HG22	2.35	0.56
1:A:194:THR:O	1:A:198:VAL:HG13	2.06	0.56
1:B:194:THR:O	1:B:198:VAL:HG13	2.06	0.56
1:B:274:VAL:HG23	1:B:277:TYR:HB2	1.89	0.55
1:B:153:ILE:HD11	1:B:159:MET:HA	1.89	0.54
1:B:366:TYR:O	1:B:370:ASP:HB2	2.07	0.54
1:A:274:VAL:HG23	1:A:277:TYR:CB	2.38	0.54
1:A:325:LYS:HB3	1:A:368:PHE:HB2	1.90	0.53
1:A:125:LYS:H	1:A:125:LYS:HD2	1.74	0.52
1:A:161:ILE:HD13	1:A:164:MET:CE	2.40	0.52
1:A:269:ALA:HB2	1:A:274:VAL:HG21	1.92	0.51
1:B:111:TYR:HE1	1:B:391:ILE:HD13	1.75	0.51
1:B:416:GLY:O	1:B:419:ILE:HG12	2.11	0.51
1:A:290:SER:HA	1:A:293:ARG:NH2	2.26	0.51
1:A:379:TYR:HA	1:B:301:ARG:NH2	2.25	0.50
1:B:281:MET:CE	1:B:285:LYS:HE2	2.38	0.50
1:A:269:ALA:CB	1:A:274:VAL:CG2	2.90	0.50
1:A:153:ILE:O	1:A:154:ASP:C	2.49	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ASP:O	1:B:156:ASP:N	2.38	0.50
1:B:177:ILE:HG22	1:B:177:ILE:O	2.12	0.49
1:A:301:ARG:HH21	1:B:379:TYR:C	2.15	0.49
1:A:290:SER:HA	1:A:293:ARG:HH21	1.78	0.49
1:A:293:ARG:O	1:A:296:ALA:HB3	2.12	0.49
1:B:266:THR:HA	1:B:285:LYS:HD2	1.94	0.49
1:B:119:LEU:HB2	1:B:126:ILE:HD11	1.95	0.48
1:B:145:GLY:CA	1:B:148:ASP:OD2	2.61	0.48
1:A:217:ALA:HB3	3:A:500:TN3:CL21	2.50	0.48
1:A:145:GLY:HA2	1:A:148:ASP:OD2	2.14	0.48
1:B:269:ALA:CB	1:B:274:VAL:HG22	2.44	0.48
1:A:274:VAL:HG23	1:A:277:TYR:HB3	1.95	0.48
1:B:269:ALA:HA	1:B:272:LYS:O	2.13	0.47
2:A:450:NAD:H2N	2:A:450:NAD:O2N	2.14	0.47
1:B:217:ALA:HB3	3:B:501:TN3:CL21	2.51	0.47
1:B:177:ILE:CG2	1:B:177:ILE:O	2.61	0.47
1:A:129:GLY:C	1:A:130:ILE:HD13	2.34	0.47
1:B:369:ILE:O	1:B:373:ILE:HG13	2.14	0.47
1:A:105:ILE:HG13	1:A:130:ILE:HD12	1.97	0.47
1:A:252:PHE:O	1:A:256:MET:HG3	2.15	0.46
1:B:174:ALA:O	1:B:177:ILE:HB	2.16	0.46
1:B:269:ALA:HB1	1:B:274:VAL:HG22	1.96	0.46
1:B:161:ILE:HD13	1:B:164:MET:CE	2.46	0.45
1:B:161:ILE:HD13	1:B:164:MET:HE3	1.99	0.45
1:A:131:TRP:CZ2	1:A:133:PRO:HG2	2.53	0.44
1:B:288:LEU:O	1:B:288:LEU:HD23	2.17	0.44
1:B:264:SER:OG	1:B:288:LEU:HD21	2.18	0.44
1:B:215:SER:HA	1:B:265:LEU:HD23	2.00	0.44
1:A:177:ILE:HD11	1:A:193:TYR:CE2	2.52	0.44
1:A:384:GLN:HB3	1:A:384:GLN:HE21	1.56	0.44
1:B:99:ILE:HB	1:B:209:ILE:HG22	1.99	0.44
1:A:203:HIS:CE1	1:A:208:LYS:HZ2	2.36	0.44
1:B:418:ASN:H	1:B:418:ASN:HD22	1.66	0.43
1:A:266:THR:O	1:A:311:SER:HA	2.18	0.43
1:A:108:THR:HG22	1:A:113:TRP:CE2	2.53	0.43
1:A:153:ILE:HD11	1:A:159:MET:HA	2.00	0.43
1:A:174:ALA:O	1:A:177:ILE:HB	2.19	0.42
1:B:274:VAL:O	1:B:274:VAL:CG2	2.65	0.42
1:A:306:ARG:HD2	1:A:406:ILE:O	2.20	0.42
1:A:110:GLY:HA3	2:A:450:NAD:O2A	2.18	0.42
1:A:248:LEU:HD22	1:A:252:PHE:CD2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:ARG:HB3	1:B:318:ARG:HH11	1.85	0.42
1:A:155:LYS:HD3	1:A:155:LYS:O	2.20	0.42
1:B:98:ASP:HB3	1:B:124:VAL:HB	2.01	0.42
1:B:325:LYS:HB3	1:B:368:PHE:HB2	2.02	0.42
1:A:128:PHE:HZ	1:A:159:MET:HE1	1.85	0.41
1:A:379:TYR:C	1:B:301:ARG:HH21	2.17	0.41
1:A:223:GLN:HE22	1:A:324:ASN:HB3	1.80	0.41
1:A:169:ALA:HB1	1:A:244:SER:HB2	2.02	0.41
1:A:138:PHE:HE2	1:A:164:MET:HE2	1.86	0.41
1:B:311:SER:HB3	1:B:412:TYR:CD1	2.56	0.41
1:A:303:TYR:HB3	1:A:305:ILE:HD12	2.02	0.41
1:A:214:HIS:O	1:A:264:SER:HA	2.21	0.41
1:A:274:VAL:HG23	1:A:277:TYR:HB2	2.02	0.41
1:B:268:HIS:HB2	1:B:412:TYR:HE1	1.85	0.41
1:B:130:ILE:O	1:B:167:PHE:N	2.54	0.41
1:A:154:ASP:O	1:A:156:ASP:N	2.53	0.41
1:A:316:LYS:NZ	1:A:370:ASP:OD1	2.53	0.41
1:B:153:ILE:HG13	1:B:153:ILE:H	1.77	0.40
1:B:249:CYS:O	1:B:253:VAL:HB	2.20	0.40
1:B:145:GLY:HA3	1:B:148:ASP:OD2	2.22	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%)	259 (91%)	22 (8%)	4 (1%)	14	32
1	B	285/336 (85%)	266 (93%)	16 (6%)	3 (1%)	17	40
All	All	570/672 (85%)	525 (92%)	38 (7%)	7 (1%)	16	37

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	ASP
1	A	155	LYS
1	B	154	ASP
1	B	155	LYS
1	A	404	ARG
1	A	268	HIS
1	B	156	ASP

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%)	218 (87%)	32 (13%)	5 12
1	B	250/295 (85%)	222 (89%)	28 (11%)	7 16
All	All	500/590 (85%)	440 (88%)	60 (12%)	6 13

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ILE
1	A	124	VAL
1	A	125	LYS
1	A	137	ILE
1	A	153	ILE
1	A	154	ASP
1	A	155	LYS
1	A	162	LEU
1	A	164	MET
1	A	175	ASN
1	A	177	ILE
1	A	188	ASN
1	A	191	GLN
1	A	198	VAL
1	A	201	LEU
1	A	204	GLN
1	A	208	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	226	LEU
1	A	227	LEU
1	A	238	LEU
1	A	241	SER
1	A	248	LEU
1	A	265	LEU
1	A	273	VAL
1	A	288	LEU
1	A	318	ARG
1	A	366	TYR
1	A	374	GLU
1	A	382	LEU
1	A	384	GLN
1	A	417	LEU
1	A	424	ASP
1	B	99	ILE
1	B	105	ILE
1	B	107	ASP
1	B	124	VAL
1	B	153	ILE
1	B	154	ASP
1	B	155	LYS
1	B	162	LEU
1	B	175	ASN
1	B	177	ILE
1	B	181	THR
1	B	188	ASN
1	B	189	MET
1	B	191	GLN
1	B	198	VAL
1	B	201	LEU
1	B	204	GLN
1	B	226	LEU
1	B	227	LEU
1	B	238	LEU
1	B	273	VAL
1	B	283	SER
1	B	311	SER
1	B	318	ARG
1	B	324	ASN
1	B	382	LEU
1	B	417	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	424	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	175	ASN
1	A	184	ASN
1	A	200	ASN
1	A	203	HIS
1	A	204	GLN
1	A	223	GLN
1	A	302	ASN
1	A	384	GLN
1	B	141	ASN
1	B	175	ASN
1	B	184	ASN
1	B	188	ASN
1	B	200	ASN
1	B	223	GLN
1	B	254	ASN
1	B	302	ASN
1	B	384	GLN
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 (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	450	-	38,48,48	1.31	4 (10%)	47,73,73	2.31	8 (17%)
3	TN3	A	500	-	21,21,21	0.93	2 (9%)	29,29,29	1.51	4 (13%)
2	NAD	B	451	-	38,48,48	1.27	4 (10%)	47,73,73	1.71	7 (14%)
3	TN3	B	501	-	21,21,21	1.09	3 (14%)	29,29,29	1.41	3 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	450	-	-	0/22/62/62	0/5/5/5
3	TN3	A	500	-	-	0/10/10/10	0/2/2/2
2	NAD	B	451	-	-	0/22/62/62	0/5/5/5
3	TN3	B	501	-	-	0/10/10/10	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	450	NAD	C7N-N7N	-3.42	1.26	1.33
2	B	451	NAD	C7N-N7N	-3.41	1.26	1.33
3	B	501	TN3	C11-N20	-2.41	1.30	1.33
3	A	500	TN3	C2-CL12	2.02	1.79	1.74
3	A	500	TN3	C14-CL21	2.13	1.78	1.73
2	A	450	NAD	O4D-C1D	2.19	1.44	1.41
3	B	501	TN3	C2-CL12	2.35	1.79	1.74
3	B	501	TN3	C14-CL21	2.41	1.79	1.73
2	B	451	NAD	O4D-C1D	2.46	1.44	1.41
2	B	451	NAD	C5A-C4A	3.18	1.47	1.40
2	A	450	NAD	C5A-C4A	3.42	1.48	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	451	NAD	O7N-C7N	4.22	1.33	1.24
2	A	450	NAD	O7N-C7N	4.47	1.33	1.24

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	450	NAD	N3A-C2A-N1A	-9.28	121.78	128.89
2	A	450	NAD	C4B-O4B-C1B	-8.72	100.13	109.72
2	B	451	NAD	N3A-C2A-N1A	-7.49	123.16	128.89
2	B	451	NAD	C4A-C5A-N7A	-4.03	105.77	109.48
2	A	450	NAD	C1B-N9A-C4A	-3.36	121.87	126.94
3	A	500	TN3	O13-C11-N20	-2.70	118.00	122.47
2	B	451	NAD	C1B-N9A-C4A	-2.70	122.87	126.94
3	B	501	TN3	O13-C11-N20	-2.60	118.17	122.47
2	A	450	NAD	O7N-C7N-N7N	-2.49	119.10	122.59
2	A	450	NAD	C4A-C5A-N7A	-2.44	107.23	109.48
3	A	500	TN3	C8-C9-C10	-2.39	117.99	120.76
2	B	451	NAD	O7N-C7N-N7N	-2.30	119.36	122.59
2	B	451	NAD	C2B-C1B-N9A	-2.21	110.91	114.29
2	A	450	NAD	PN-O3-PA	-2.21	126.53	132.73
3	A	500	TN3	O13-C11-C10	-2.19	117.23	120.97
2	A	450	NAD	C3N-C7N-N7N	2.35	120.39	117.82
2	B	451	NAD	O4D-C1D-N1N	2.43	110.81	108.13
2	B	451	NAD	C3N-C7N-N7N	2.67	120.73	117.82
3	B	501	TN3	C5-O9-C7	3.65	126.61	117.75
3	B	501	TN3	C10-C11-N20	4.01	122.60	116.91
2	A	450	NAD	O4B-C1B-N9A	4.83	118.20	108.10
3	A	500	TN3	C10-C11-N20	5.53	124.77	116.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	450	NAD	2	0
3	A	500	TN3	1	0
3	B	501	TN3	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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%)	0.04	17 (5%)	26	24	14, 27, 67, 84	0
1	B	289/336 (86%)	0.16	18 (6%)	24	22	15, 28, 66, 83	0
All	All	578/672 (86%)	0.10	35 (6%)	25	23	14, 27, 67, 84	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	155	LYS	6.0
1	A	154	ASP	5.7
1	B	182	LYS	5.3
1	A	366	TYR	5.0
1	B	144	ASN	4.8
1	B	324	ASN	4.5
1	B	157	LYS	4.4
1	B	155	LYS	4.4
1	A	180	GLU	4.2
1	B	325	LYS	4.2
1	B	156	ASP	4.2
1	B	366	TYR	4.0
1	A	425	ASP	3.9
1	A	182	LYS	3.8
1	A	181	THR	3.6
1	A	186	ARG	3.6
1	A	183	ASN	3.6
1	B	183	ASN	3.5
1	B	141	ASN	3.1
1	A	179	GLU	3.1
1	A	325	LYS	3.0
1	A	178	ASP	3.0
1	B	146	LYS	2.9
1	B	158	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	97	GLU	2.6
1	B	149	ASN	2.5
1	A	189	MET	2.5
1	B	179	GLU	2.5
1	B	143	LYS	2.3
1	A	156	ASP	2.3
1	A	324	ASN	2.3
1	B	160	ASN	2.2
1	A	137	ILE	2.1
1	B	140	LYS	2.1
1	B	153	ILE	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 (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. 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
2	NAD	B	451	44/44	0.96	0.17	0.37	18,31,43,46	0
3	TN3	A	500	20/20	0.94	0.15	-0.12	22,29,33,39	0
2	NAD	A	450	44/44	0.95	0.15	-0.31	20,32,45,48	0
3	TN3	B	501	20/20	0.94	0.15	-0.44	23,28,33,39	0

6.5 Other polymers (i)

There are no such residues in this entry.