Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 12:35 AM EDT

PDB ID	:	1NNU
Title	:	Crystal Structure Analysis of Plasmodium falciparum enoyl-acyl-carrier-protein reductase with Triclosan Analog
Authors	:	Perozzo, R.; Kuo, M.; Sidhu, A.S.; Valiyaveettil, J.T.; Bittman, R.; Jacobs Jr., W.R.; Fidock, D.A.; Sacchettini, J.C.
Deposited on	:	2003-01-14
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

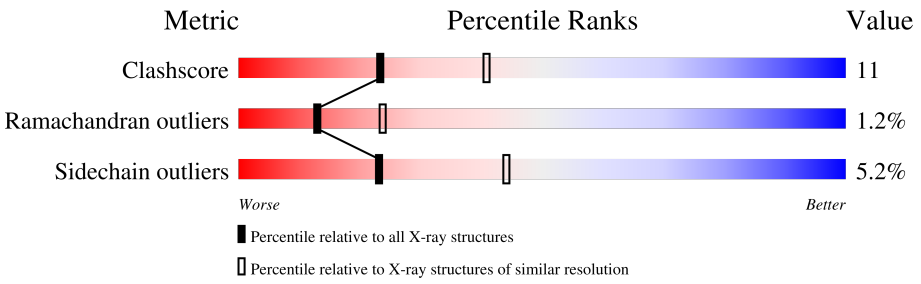
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	229	73% 25% •
1	B	229	72% 25% •
2	C	60	88% 8% •
2	D	60	83% 13% •

2 Entry composition (i)

There are 4 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.

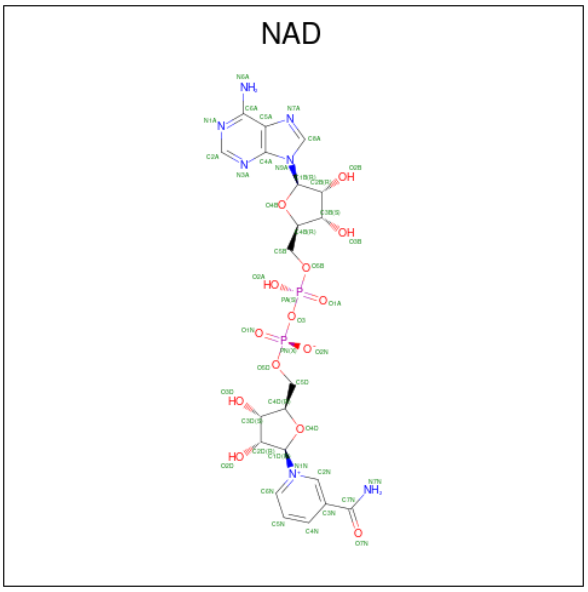
- Molecule 1 is a protein called enoyl-acyl carrier reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	229	1806	1148	309	339	10	0	0	0
1	B	229	1806	1148	309	339	10	0	0	0

- Molecule 2 is a protein called enoyl-acyl carrier reductase.

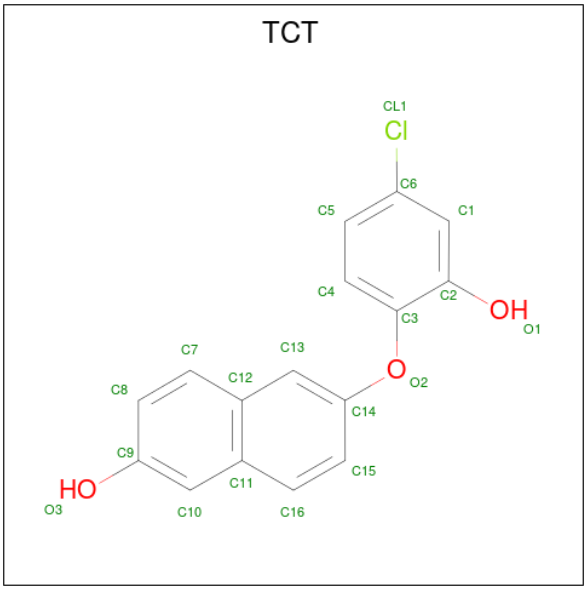
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	60	481	310	75	95	1	0	0	0
2	D	60	481	310	75	95	1	0	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 4 is 6-(4-CHLORO-2-HYDROXY-PHENOXY)-NAPHTHALEN-2-OL (three-letter code: TCT) (formula: $C_{16}H_{11}ClO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	Cl	O		
4	A	1	20	16	1	3	0	0
			Total	C	Cl	O		
4	B	1	20	16	1	3	0	0

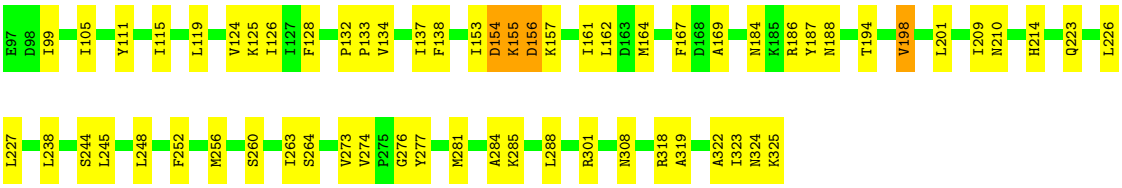
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

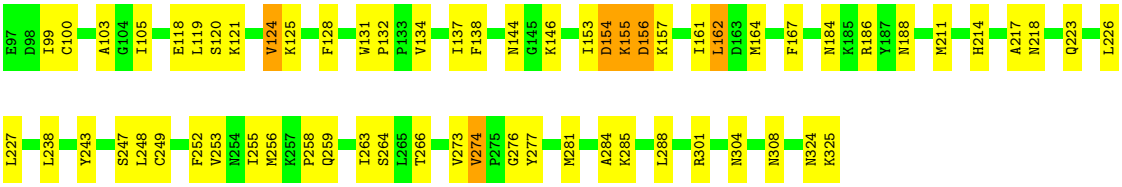
• Molecule 1: enoyl-acyl carrier reductase

Chain A:



• Molecule 1: enoyl-acyl carrier reductase

Chain B:

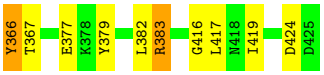


• Molecule 2: enoyl-acyl carrier reductase

Chain C:

• Molecule 2: enoyl-acyl carrier reductase

Chain D:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	133.10Å 133.10Å 83.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.176 , 0.227	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4702	wwPDB-VP
Average B, all atoms ($Å^2$)	34.0	wwPDB-VP

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: TCT, 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	0.33	0/1839	0.56	0/2477
1	B	0.32	0/1839	0.57	0/2477
2	C	0.35	0/490	0.61	0/664
2	D	0.36	0/490	0.59	0/664
All	All	0.33	0/4658	0.57	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 (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	1806	0	1824	46	0
1	B	1806	0	1824	52	0
2	C	481	0	473	8	0
2	D	481	0	473	8	0
3	A	44	0	26	0	0
3	B	44	0	26	0	0
4	A	20	0	11	0	0
4	B	20	0	10	0	0
All	All	4702	0	4667	106	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 (106) 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:276:GLY:HA2	1:B:325:LYS:HG2	1.63	0.79
1:B:301:ARG:CD	2:C:383:ARG:HD2	2.19	0.73
1:A:99:ILE:HD13	1:A:125:LYS:HB2	1.72	0.71
1:B:184:ASN:ND2	1:B:186:ARG:H	1.88	0.70
1:B:155:LYS:HD3	1:B:157:LYS:HZ1	1.57	0.68
1:B:252:PHE:O	1:B:256:MET:HG3	1.94	0.68
1:A:276:GLY:HA2	1:A:325:LYS:HG2	1.75	0.67
1:B:144:ASN:O	1:B:146:LYS:HE3	1.93	0.67
1:A:119:LEU:HB3	1:A:124:VAL:CG2	2.26	0.65
2:C:407:THR:HG21	2:D:382:LEU:HD13	1.77	0.65
1:A:184:ASN:HD22	1:A:187:TYR:HD1	1.44	0.64
1:A:184:ASN:HD21	1:A:186:ARG:HG2	1.62	0.64
1:B:155:LYS:HD3	1:B:157:LYS:NZ	2.13	0.63
1:A:161:ILE:HG21	1:A:164:MET:HE3	1.80	0.62
1:B:252:PHE:CD1	1:B:255:ILE:HD11	2.35	0.61
1:B:223:GLN:HE21	1:B:324:ASN:HB3	1.68	0.59
1:A:153:ILE:HB	1:A:157:LYS:HB2	1.84	0.59
1:A:119:LEU:HB3	1:A:124:VAL:HG22	1.85	0.59
1:B:99:ILE:HD13	1:B:125:LYS:HB2	1.85	0.59
2:D:416:GLY:O	2:D:419:ILE:HG12	2.02	0.59
1:A:132:PRO:HB2	1:A:133:PRO:HD3	1.84	0.59
1:A:263:ILE:HA	1:A:308:ASN:O	2.02	0.58
1:A:194:THR:O	1:A:198:VAL:HG13	2.03	0.58
1:B:154:ASP:O	1:B:156:ASP:N	2.32	0.58
1:B:153:ILE:HB	1:B:157:LYS:HB2	1.86	0.58
1:B:155:LYS:HB2	1:B:157:LYS:NZ	2.19	0.57
1:A:274:VAL:HG23	1:A:274:VAL:O	2.04	0.56
1:B:134:VAL:O	1:B:137:ILE:HG22	2.05	0.56
1:B:138:PHE:HE2	1:B:164:MET:CE	2.18	0.56
1:A:169:ALA:HB1	1:A:244:SER:HB2	1.87	0.55
1:B:155:LYS:HB2	1:B:157:LYS:HZ2	1.70	0.55
1:A:105:ILE:HD12	1:A:128:PHE:CD1	2.42	0.55
2:C:366:TYR:N	2:C:366:TYR:CD2	2.77	0.53
1:A:223:GLN:NE2	1:A:324:ASN:HB3	2.24	0.53
1:A:301:ARG:NH2	2:D:379:TYR:HA	2.24	0.52
1:B:301:ARG:HD2	2:C:383:ARG:HD2	1.90	0.52
1:A:276:GLY:CA	1:A:325:LYS:HG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ARG:HH11	1:A:318:ARG:HG2	1.75	0.52
1:B:217:ALA:HB1	1:B:281:MET:HE1	1.92	0.51
1:B:138:PHE:HE2	1:B:164:MET:HE2	1.77	0.49
1:A:161:ILE:HD13	1:A:164:MET:HE3	1.94	0.49
1:B:118:GLU:O	1:B:121:LYS:HB2	2.13	0.49
1:A:119:LEU:HB3	1:A:124:VAL:HG21	1.93	0.49
1:A:138:PHE:HE2	1:A:164:MET:HE2	1.77	0.49
1:A:238:LEU:HD23	1:A:284:ALA:HA	1.95	0.49
1:A:277:TYR:CE2	1:A:281:MET:HB3	2.47	0.48
1:A:301:ARG:HH21	2:D:379:TYR:C	2.17	0.48
1:B:184:ASN:HD21	1:B:186:ARG:HG2	1.78	0.48
1:B:99:ILE:CD1	1:B:125:LYS:HB2	2.44	0.48
2:C:366:TYR:N	2:C:366:TYR:HD2	2.11	0.48
1:A:214:HIS:O	1:A:264:SER:HA	2.14	0.47
1:A:184:ASN:ND2	1:A:186:ARG:HG2	2.29	0.47
1:A:318:ARG:HG2	1:A:318:ARG:NH1	2.31	0.46
1:B:161:ILE:HG21	1:B:164:MET:HE3	1.97	0.46
1:B:153:ILE:O	1:B:155:LYS:N	2.48	0.46
1:B:277:TYR:CE2	1:B:281:MET:HB3	2.51	0.46
1:B:301:ARG:HH21	2:C:379:TYR:C	2.19	0.46
1:A:281:MET:CE	1:A:285:LYS:HE2	2.46	0.46
1:A:209:ILE:O	1:A:256:MET:HA	2.16	0.46
1:B:184:ASN:HD22	1:B:186:ARG:H	1.60	0.46
1:B:266:THR:HA	1:B:285:LYS:HD2	1.98	0.46
1:A:126:ILE:HG21	1:A:128:PHE:CE1	2.51	0.46
1:B:274:VAL:O	1:B:274:VAL:CG2	2.63	0.46
1:B:131:TRP:CD1	1:B:132:PRO:HD2	2.51	0.46
1:A:134:VAL:O	1:A:137:ILE:HG23	2.16	0.45
1:A:252:PHE:O	1:A:256:MET:HG3	2.15	0.45
2:D:366:TYR:O	2:D:367:THR:OG1	2.32	0.45
1:B:128:PHE:HD2	1:B:164:MET:HE2	1.82	0.45
1:A:210:ASN:HA	1:A:260:SER:OG	2.16	0.45
1:B:274:VAL:CG2	1:B:277:TYR:HB2	2.47	0.45
1:B:125:LYS:HB3	1:B:162:LEU:HD12	1.98	0.45
1:B:105:ILE:HD12	1:B:128:PHE:CD1	2.52	0.44
1:B:249:CYS:O	1:B:253:VAL:HB	2.17	0.44
1:B:301:ARG:HD3	2:C:383:ARG:HD2	1.97	0.44
2:D:377:GLU:O	2:D:383:ARG:HG3	2.18	0.44
1:A:111:TYR:O	1:A:115:ILE:HG13	2.18	0.44
1:B:155:LYS:C	1:B:157:LYS:H	2.20	0.44
1:A:167:PHE:HD1	1:A:198:VAL:HG11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ALA:HB1	1:B:167:PHE:CE2	2.53	0.43
2:D:366:TYR:N	2:D:366:TYR:CD2	2.86	0.43
1:A:156:ASP:OD1	1:A:156:ASP:O	2.35	0.43
1:A:248:LEU:O	1:A:252:PHE:HB2	2.19	0.43
1:A:245:LEU:HD22	1:A:288:LEU:HD11	2.01	0.43
1:B:100:CYS:HA	1:B:211:MET:O	2.19	0.42
1:A:153:ILE:O	1:A:154:ASP:C	2.57	0.42
1:A:156:ASP:O	1:A:156:ASP:CG	2.56	0.42
1:A:319:ALA:O	1:A:322:ALA:HB3	2.19	0.42
1:A:155:LYS:O	1:A:156:ASP:HB3	2.20	0.42
1:B:146:LYS:HA	1:B:146:LYS:HD3	1.93	0.42
1:A:325:LYS:HB3	2:C:368:PHE:HB2	2.02	0.42
1:B:243:TYR:CE2	1:B:247:SER:HB2	2.55	0.42
1:B:154:ASP:OD2	1:B:154:ASP:N	2.53	0.42
1:B:238:LEU:HD23	1:B:284:ALA:HA	2.02	0.42
1:A:281:MET:HE1	1:A:285:LYS:HE2	2.01	0.42
1:B:161:ILE:HD13	1:B:164:MET:HE3	2.02	0.41
1:B:137:ILE:HG23	1:B:138:PHE:N	2.34	0.41
1:B:119:LEU:HB3	1:B:124:VAL:HG22	2.03	0.41
1:B:155:LYS:CB	1:B:157:LYS:HZ2	2.34	0.41
1:B:214:HIS:O	1:B:264:SER:HA	2.20	0.41
1:B:248:LEU:O	1:B:252:PHE:HB2	2.21	0.41
1:B:263:ILE:HA	1:B:308:ASN:O	2.21	0.41
1:A:134:VAL:HA	1:A:137:ILE:CG2	2.51	0.41
1:A:138:PHE:HE2	1:A:164:MET:CE	2.34	0.40
1:B:258:PRO:O	1:B:259:GLN:HB2	2.22	0.40
1:B:154:ASP:C	1:B:156:ASP:H	2.22	0.40
2:D:366:TYR:N	2:D:366:TYR:HD2	2.19	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	227/229 (99%)	213 (94%)	11 (5%)	3 (1%)	12	21
1	B	227/229 (99%)	209 (92%)	16 (7%)	2 (1%)	17	31
2	C	58/60 (97%)	53 (91%)	4 (7%)	1 (2%)	9	16
2	D	58/60 (97%)	52 (90%)	5 (9%)	1 (2%)	9	16
All	All	570/578 (99%)	527 (92%)	36 (6%)	7 (1%)	13	24

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	154	ASP
1	B	155	LYS
2	D	424	ASP
1	A	154	ASP
1	A	323	ILE
1	A	155	LYS
2	C	367	THR

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	197/197 (100%)	189 (96%)	8 (4%)	30	55
1	B	197/197 (100%)	185 (94%)	12 (6%)	18	36
2	C	53/53 (100%)	50 (94%)	3 (6%)	20	39
2	D	53/53 (100%)	50 (94%)	3 (6%)	20	39
All	All	500/500 (100%)	474 (95%)	26 (5%)	23	44

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	ASP
1	A	162	LEU
1	A	188	ASN
1	A	198	VAL

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Mol	Chain	Res	Type
1	A	201	LEU
1	A	226	LEU
1	A	227	LEU
1	A	273	VAL
1	B	120	SER
1	B	124	VAL
1	B	156	ASP
1	B	162	LEU
1	B	188	ASN
1	B	218	ASN
1	B	226	LEU
1	B	227	LEU
1	B	273	VAL
1	B	274	VAL
1	B	288	LEU
1	B	304	ASN
2	C	366	TYR
2	C	383	ARG
2	C	417	LEU
2	D	366	TYR
2	D	383	ARG
2	D	417	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	141	ASN
1	A	183	ASN
1	A	184	ASN
1	A	188	ASN
1	A	200	ASN
1	A	204	GLN
1	A	223	GLN
1	A	302	ASN
1	A	304	ASN
1	B	141	ASN
1	B	184	ASN
1	B	188	ASN
1	B	200	ASN
1	B	218	ASN
1	B	223	GLN

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Mol	Chain	Res	Type
1	B	259	GLN
1	B	302	ASN
1	B	324	ASN
2	C	384	GLN
2	D	384	GLN

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 monosaccharides 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	$\#\|Z\| > 2$
4	TCT	B	600	-	22,22,22	1.97	9 (40%)	31,31,31	1.12	2 (6%)
3	NAD	B	550	-	42,48,48	2.39	9 (21%)	50,73,73	2.88	12 (24%)
3	NAD	A	450	-	42,48,48	2.46	9 (21%)	50,73,73	2.86	11 (22%)
4	TCT	A	500	-	22,22,22	1.99	9 (40%)	31,31,31	1.09	2 (6%)

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
4	TCT	B	600	-	-	0/4/4/4	0/3/3/3
3	NAD	B	550	-	-	9/26/62/62	0/5/5/5
3	NAD	A	450	-	-	8/26/62/62	0/5/5/5
4	TCT	A	500	-	-	0/4/4/4	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	450	NAD	PN-O3	-9.28	1.49	1.59
3	B	550	NAD	PN-O3	-8.32	1.50	1.59
3	B	550	NAD	C2N-N1N	6.78	1.42	1.35
3	A	450	NAD	C2N-N1N	6.49	1.42	1.35
3	A	450	NAD	PA-O3	-6.40	1.52	1.59
3	B	550	NAD	PA-O3	-6.17	1.52	1.59
3	A	450	NAD	O7N-C7N	5.57	1.34	1.24
3	B	550	NAD	O7N-C7N	5.26	1.33	1.24
4	A	500	TCT	C13-C14	3.88	1.43	1.37
4	B	600	TCT	C13-C14	3.77	1.43	1.37
4	A	500	TCT	C1-C2	3.63	1.44	1.38
4	B	600	TCT	C1-C6	3.21	1.43	1.38
4	B	600	TCT	C1-C2	3.16	1.43	1.38
3	A	450	NAD	C6N-C5N	3.10	1.45	1.38
4	A	500	TCT	C1-C6	3.09	1.43	1.38
4	A	500	TCT	C11-C12	3.02	1.49	1.42
3	B	550	NAD	C5N-C4N	2.97	1.44	1.38
3	A	450	NAD	C5N-C4N	2.96	1.44	1.38
4	B	600	TCT	C11-C12	2.96	1.49	1.42
3	B	550	NAD	C6N-C5N	2.80	1.44	1.38
4	B	600	TCT	C7-C8	2.71	1.42	1.36
4	A	500	TCT	C7-C8	2.52	1.42	1.36
3	B	550	NAD	C3N-C7N	-2.31	1.47	1.50
4	A	500	TCT	C5-C4	2.26	1.42	1.38
4	B	600	TCT	C5-C4	2.25	1.42	1.38
3	B	550	NAD	O4D-C1D	2.24	1.43	1.40
4	B	600	TCT	C10-C9	2.24	1.41	1.37
3	A	450	NAD	O4D-C1D	2.11	1.43	1.40
4	B	600	TCT	C4-C3	2.07	1.43	1.39
3	A	450	NAD	C4A-N3A	2.05	1.38	1.35
4	A	500	TCT	C10-C9	2.05	1.41	1.37
4	B	600	TCT	C15-C14	2.03	1.42	1.38
4	A	500	TCT	C8-C9	2.03	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	450	NAD	C3N-C7N	-2.01	1.47	1.50
3	B	550	NAD	O4B-C1B	2.01	1.43	1.40
4	A	500	TCT	C16-C15	2.01	1.41	1.36

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	550	NAD	C5N-C4N-C3N	8.39	128.62	120.36
3	B	550	NAD	C2N-C3N-C4N	-8.15	108.78	118.26
3	A	450	NAD	C5N-C4N-C3N	8.12	128.35	120.36
3	A	450	NAD	C2N-C3N-C4N	-8.06	108.88	118.26
3	B	550	NAD	C1B-N9A-C4A	-7.53	113.41	126.64
3	A	450	NAD	C1B-N9A-C4A	-7.44	113.58	126.64
3	B	550	NAD	O7N-C7N-N7N	-7.42	111.90	122.62
3	A	450	NAD	O7N-C7N-N7N	-7.38	111.95	122.62
3	A	450	NAD	C4D-O4D-C1D	-5.92	104.50	109.92
3	B	550	NAD	C3N-C7N-N7N	5.78	124.86	117.74
3	B	550	NAD	C4D-O4D-C1D	-5.58	104.81	109.92
3	A	450	NAD	C3N-C7N-N7N	5.57	124.60	117.74
4	B	600	TCT	C3-O2-C14	4.16	128.03	117.95
3	A	450	NAD	O2A-PA-O3	-4.15	96.04	107.27
3	B	550	NAD	O2A-PA-O3	-3.71	97.24	107.27
3	B	550	NAD	O3-PA-O1A	3.54	121.35	110.70
4	A	500	TCT	C3-O2-C14	3.46	126.32	117.95
3	A	450	NAD	O3-PA-O1A	3.36	120.80	110.70
4	A	500	TCT	O2-C3-C2	3.33	122.22	116.59
3	A	450	NAD	O7N-C7N-C3N	3.10	123.39	119.60
3	B	550	NAD	C2N-C3N-C7N	3.07	128.33	119.46
4	B	600	TCT	O2-C3-C2	2.97	121.61	116.59
3	B	550	NAD	O7N-C7N-C3N	2.97	123.23	119.60
3	A	450	NAD	C2N-C3N-C7N	2.95	127.98	119.46
3	B	550	NAD	C5N-C6N-N1N	-2.74	116.65	120.38
3	A	450	NAD	C5N-C6N-N1N	-2.67	116.74	120.38
3	B	550	NAD	O3B-C3B-C4B	-2.18	104.82	111.08

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	450	NAD	C5B-O5B-PA-O2A
3	A	450	NAD	C5D-O5D-PN-O3
3	A	450	NAD	C5D-O5D-PN-O1N

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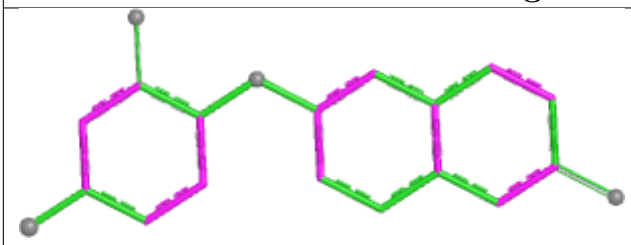
Mol	Chain	Res	Type	Atoms
3	B	550	NAD	C5B-O5B-PA-O1A
3	B	550	NAD	C5B-O5B-PA-O2A
3	B	550	NAD	C5B-O5B-PA-O3
3	B	550	NAD	C5D-O5D-PN-O3
3	B	550	NAD	C5D-O5D-PN-O1N
3	B	550	NAD	O4B-C4B-C5B-O5B
3	B	550	NAD	C3B-C4B-C5B-O5B
3	A	450	NAD	O4B-C4B-C5B-O5B
3	A	450	NAD	C3B-C4B-C5B-O5B
3	A	450	NAD	C5B-O5B-PA-O1A
3	A	450	NAD	C5D-O5D-PN-O2N
3	B	550	NAD	C5D-O5D-PN-O2N
3	A	450	NAD	O4D-C1D-N1N-C6N
3	B	550	NAD	C4B-C5B-O5B-PA

There are no ring outliers.

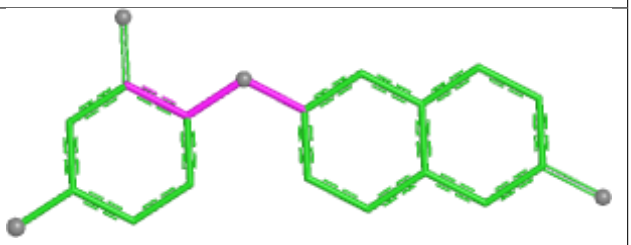
No monomer is involved in short contacts.

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.

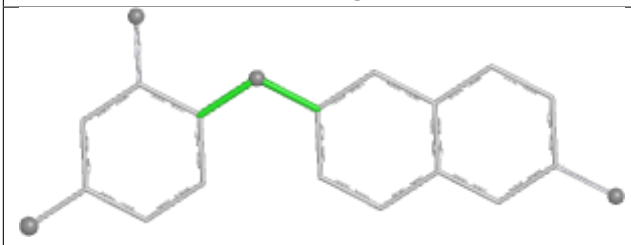
Ligand TCT B 600



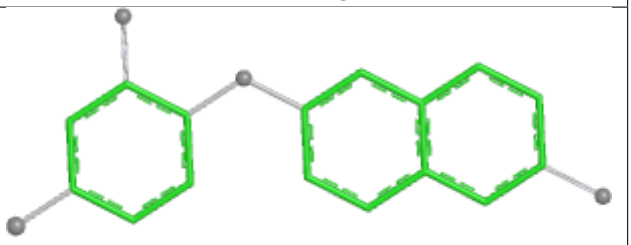
Bond lengths



Bond angles

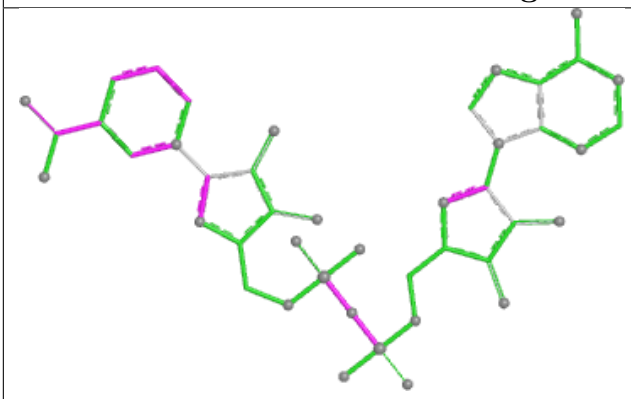


Torsions

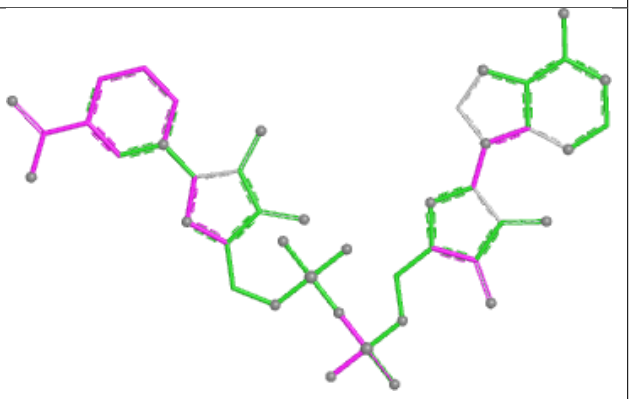


Rings

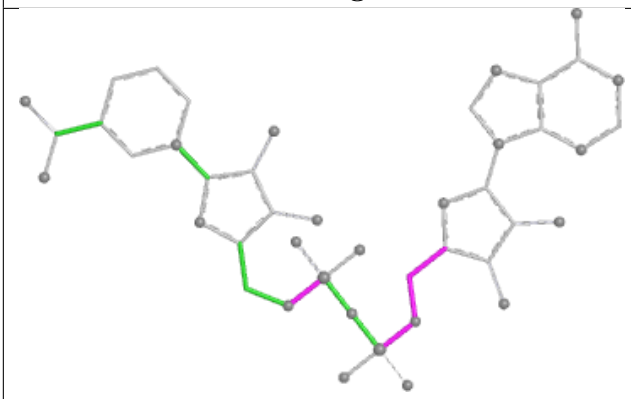
Ligand NAD B 550



Bond lengths



Bond angles



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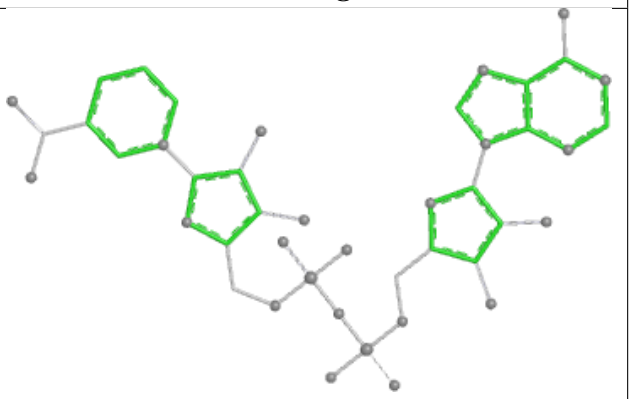
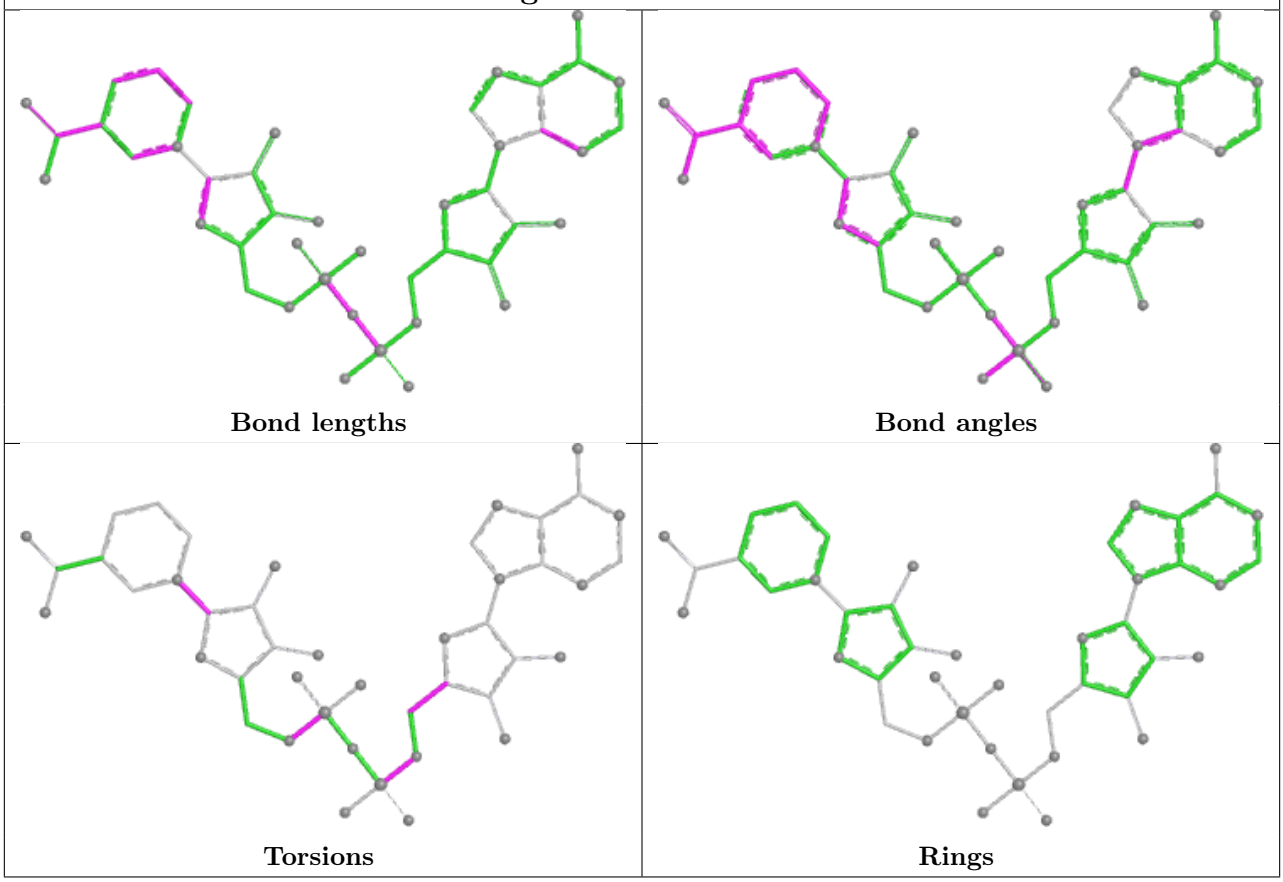
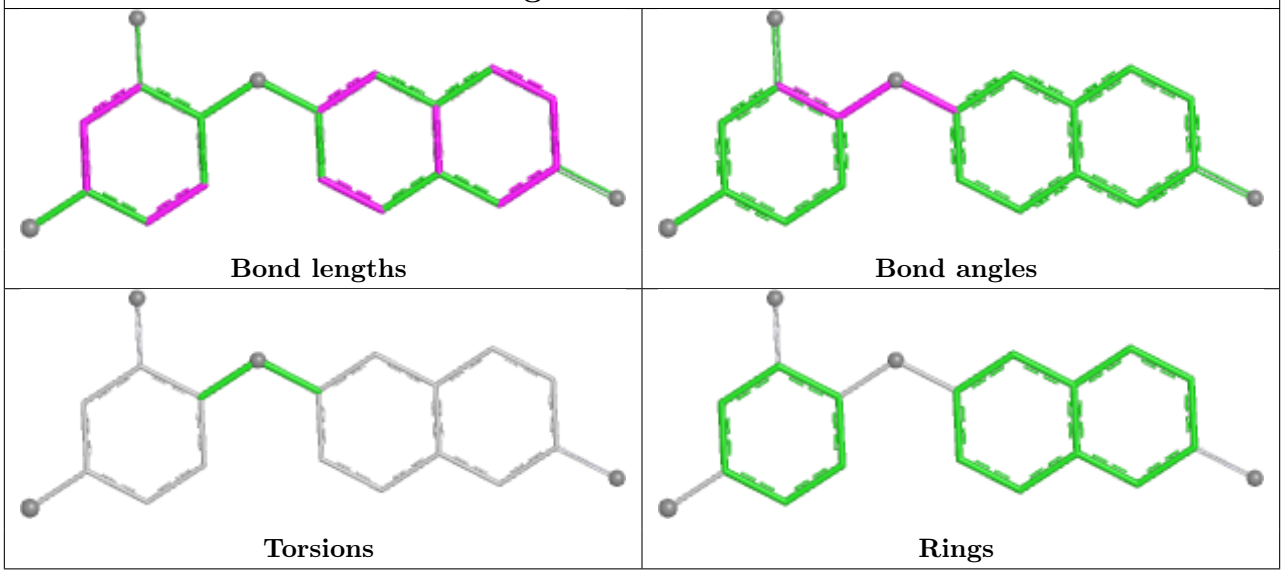


Rings

Ligand NAD A 450



Ligand TCT A 500



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.