Full wwPDB X-ray Structure Validation Report (i)

Aug 26, 2023 – 02:34 PM EDT

PDB ID	:	3F4B
Title	:	Crystal structure of Plasmodium berghei Enoyl-acyl-carrier-protein reductase with TRICLOSAN
Authors	:	Sacchettini, J.C.; Tsai, H.-C.
Deposited on	:	2008-10-31
Resolution	:	2.49 Å(reported)

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

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

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

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

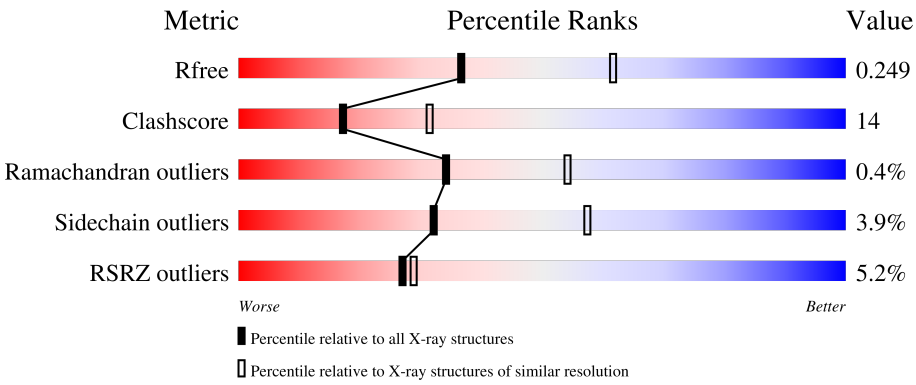
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.49 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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% 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	323	% 69% 18% • 12%
1	B	323	6% 60% 27% • 11%
1	C	323	6% 59% 27% • 13%
1	D	323	6% 63% 24% • 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9407 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 protein reductase.

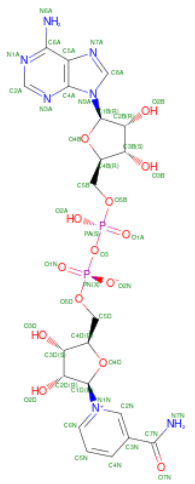
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	284	2208	1406	367	426	9	0	0	0
1	B	289	2250	1430	374	437	9	0	0	0
1	C	282	2191	1396	363	423	9	0	0	0
1	D	289	2250	1430	374	437	9	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	MET	-	expression tag	UNP Q6TEI5
B	74	MET	-	expression tag	UNP Q6TEI5
C	74	MET	-	expression tag	UNP Q6TEI5
D	74	MET	-	expression tag	UNP Q6TEI5

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

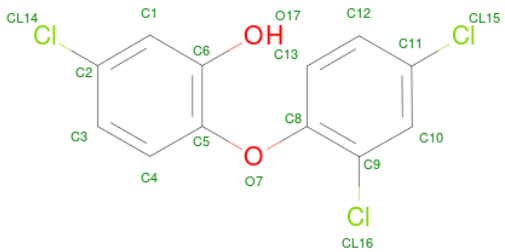
NAD



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

- Molecule 3 is TRICLOSAN (three-letter code: TCL) (formula: $C_{12}H_7Cl_3O_2$).

TCL



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

- Molecule 4 is water.

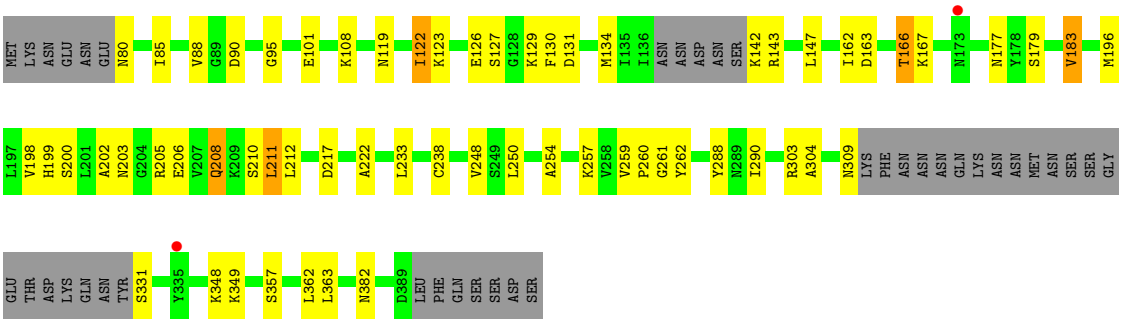
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	79	79	79	0	0
4	B	54	54	54	0	0
4	C	66	66	66	0	0
4	D	65	65	65	0	0

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 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.

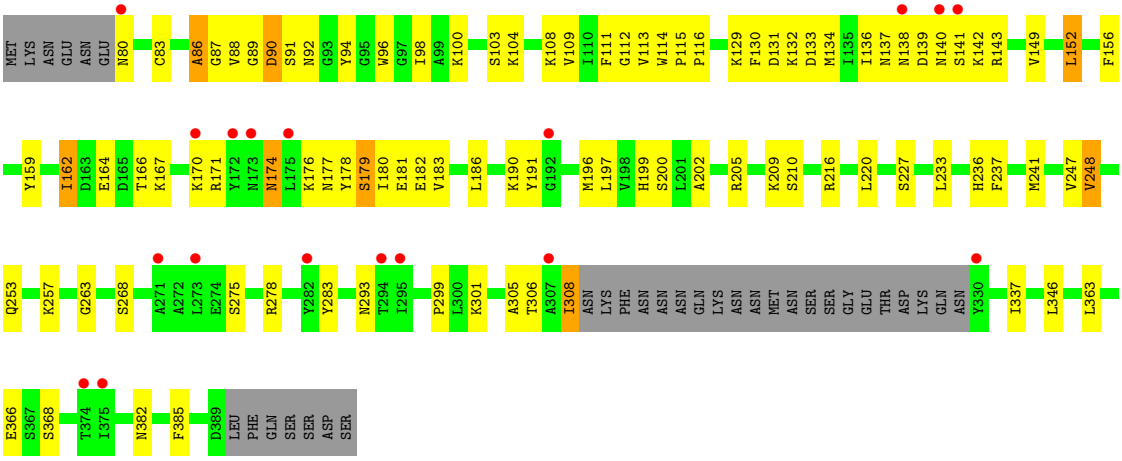
• Molecule 1: Enoyl-acyl carrier protein reductase

Chain A:



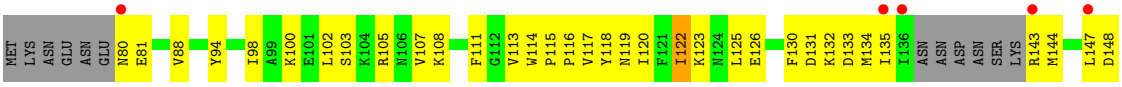
• Molecule 1: Enoyl-acyl carrier protein reductase

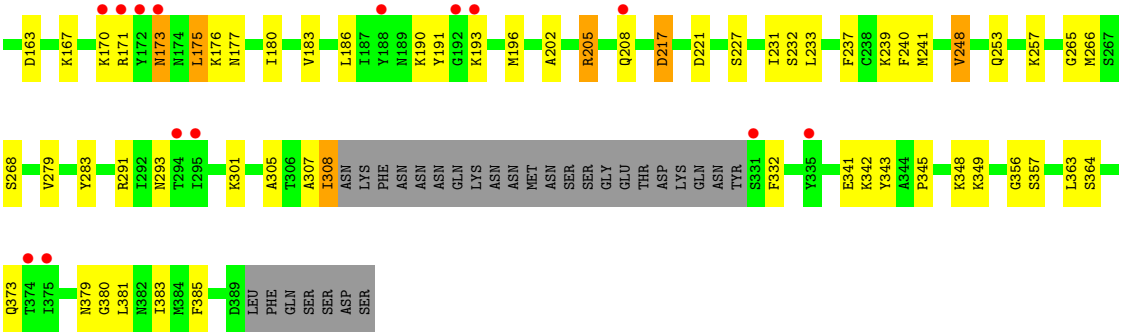
Chain B:



• Molecule 1: Enoyl-acyl carrier protein reductase

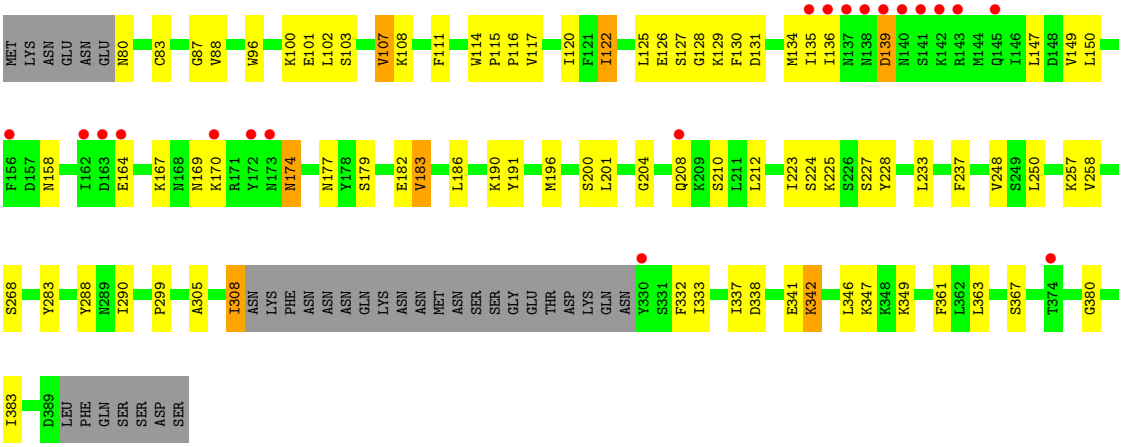
Chain C:





- Molecule 1: Enoyl-acyl carrier protein reductase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.34Å 121.20Å 87.83Å 90.00° 108.97° 90.00°	Depositor
Resolution (Å)	36.33 – 2.49 36.33 – 2.49	Depositor EDS
% Data completeness (in resolution range)	92.2 (36.33-2.49) 92.2 (36.33-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.183 , 0.254 0.180 , 0.249	Depositor DCC
R_{free} test set	2075 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	60.7	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 49.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9407	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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, 0.333 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: TCL, 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	0.41	0/2246	0.56	1/3026 (0.0%)
1	B	0.35	0/2290	0.51	0/3088
1	C	0.37	0/2229	0.51	0/3004
1	D	0.37	0/2290	0.51	0/3088
All	All	0.37	0/9055	0.52	1/12206 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	331	SER	N-CA-C	-5.13	97.15	111.00

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	2208	0	2210	49	0
1	B	2250	0	2241	74	0
1	C	2191	0	2191	81	0
1	D	2250	0	2241	63	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	44	0	26	1	0
2	D	44	0	26	1	0
3	A	17	0	6	1	0
3	B	17	0	6	2	0
3	C	17	0	7	0	0
3	D	17	0	6	1	0
4	A	79	0	0	9	0
4	B	54	0	0	3	0
4	C	66	0	0	8	0
4	D	65	0	0	9	0
All	All	9407	0	9012	252	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 14.

All (252) 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:C:105:ARG:NH1	1:C:364:SER:HB3	1.71	1.04
1:D:88:VAL:HG11	1:D:111:PHE:CD1	2.07	0.90
1:C:202:ALA:HB1	1:C:266:MET:HE1	1.57	0.86
1:C:105:ARG:HH12	1:C:364:SER:HB3	1.39	0.85
1:B:80:ASN:HD22	1:B:108:LYS:HE2	1.42	0.85
1:B:80:ASN:ND2	1:B:108:LYS:HE2	1.92	0.84
1:C:341:GLU:OE2	1:C:349:LYS:HG3	1.80	0.81
1:A:288:TYR:HB2	1:A:290:ILE:HG13	1.61	0.80
1:D:122:ILE:O	1:D:126:GLU:HG2	1.82	0.79
1:D:135:ILE:HG23	1:D:139:ASP:HA	1.66	0.78
1:A:303:ARG:HD3	4:A:58:HOH:O	1.83	0.78
1:C:88:VAL:HG21	1:C:111:PHE:CD1	2.18	0.77
1:C:196:MET:HG2	1:C:363:LEU:HB3	1.64	0.77
1:A:208:GLN:HG3	4:A:439:HOH:O	1.85	0.76
1:A:199:HIS:HD2	1:A:233:LEU:HD12	1.50	0.76
1:B:382:ASN:HD21	1:C:373:GLN:HE22	1.31	0.75
1:D:108:LYS:HE2	1:D:147:LEU:HD22	1.67	0.75
1:A:257:LYS:HE2	1:B:385:PHE:HA	1.70	0.74
1:C:385:PHE:HA	1:D:257:LYS:HE2	1.69	0.73
1:B:91:SER:HA	1:B:96:TRP:CG	2.23	0.73
1:C:122:ILE:O	1:C:126:GLU:HG2	1.89	0.73
1:C:102:LEU:HB3	1:C:107:VAL:CG1	2.18	0.73
1:A:179:SER:O	1:A:183:VAL:HG13	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:ASN:HA	4:C:445:HOH:O	1.89	0.71
1:D:182:GLU:HG3	4:D:423:HOH:O	1.90	0.70
1:A:127:SER:OG	1:A:129:LYS:HE2	1.92	0.70
1:B:237:PHE:O	1:B:241:MET:HG3	1.92	0.69
1:B:139:ASP:HA	1:B:141:SER:HA	1.73	0.69
1:B:190:LYS:HD3	1:B:191:TYR:CE2	2.28	0.69
1:C:102:LEU:O	1:C:107:VAL:HG12	1.92	0.69
1:D:190:LYS:HD3	1:D:191:TYR:CZ	2.27	0.69
1:C:94:TYR:O	1:C:98:ILE:HG13	1.93	0.68
1:A:80:ASN:ND2	1:A:108:LYS:HG3	2.08	0.68
1:B:197:LEU:HB3	1:B:247:VAL:HG22	1.73	0.68
1:B:170:LYS:HG2	1:B:171:ARG:NH1	2.08	0.67
1:A:163:ASP:OD1	1:A:166:THR:HG23	1.95	0.67
1:D:299:PRO:HB2	1:D:337:ILE:HG13	1.77	0.67
1:C:122:ILE:HB	4:C:445:HOH:O	1.95	0.66
1:A:122:ILE:O	1:A:126:GLU:HG2	1.97	0.65
1:D:341:GLU:O	1:D:347:LYS:HD3	1.97	0.65
1:A:254:ALA:HB2	1:A:259:VAL:HG21	1.79	0.65
1:D:150:LEU:HD13	1:D:186:LEU:HD22	1.78	0.64
1:C:105:ARG:NH1	1:C:364:SER:CB	2.57	0.64
1:C:202:ALA:HB1	1:C:266:MET:CE	2.26	0.64
1:A:248:VAL:HG22	1:A:363:LEU:HD21	1.79	0.64
1:C:108:LYS:HB3	1:C:147:LEU:HG	1.80	0.64
1:C:307:ALA:O	1:C:308:ILE:HG12	1.98	0.64
1:C:102:LEU:HD22	1:C:107:VAL:HG11	1.80	0.63
1:B:299:PRO:HB2	1:B:337:ILE:HG13	1.80	0.63
1:C:190:LYS:HD2	1:C:191:TYR:CE2	2.34	0.63
1:D:164:GLU:HA	1:D:167:LYS:HD2	1.81	0.63
1:C:380:GLY:O	1:C:383:ILE:HG12	1.98	0.63
1:D:83:CYS:HB2	1:D:196:MET:HB2	1.81	0.63
1:B:202:ALA:HB3	3:B:500:TCL:CL16	2.36	0.63
1:B:209:LYS:O	1:B:263:GLY:HA3	1.99	0.62
1:C:131:ASP:O	1:C:135:ILE:HG23	1.99	0.61
1:C:163:ASP:O	1:C:167:LYS:HG3	2.00	0.61
1:A:259:VAL:HG23	1:A:259:VAL:O	2.00	0.61
1:B:220:LEU:HD11	1:D:224:SER:HB2	1.81	0.61
1:D:174:ASN:OD1	1:D:174:ASN:N	2.32	0.61
1:A:108:LYS:HD2	1:A:147:LEU:HD13	1.81	0.61
1:B:89:GLY:O	1:B:90:ASP:HB3	2.00	0.60
1:D:338:ASP:O	1:D:342:LYS:HB2	2.02	0.60
1:A:205:ARG:HG3	4:A:414:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:MET:HG2	1:A:363:LEU:HB3	1.83	0.60
1:B:109:VAL:HG11	1:B:111:PHE:HE1	1.66	0.60
1:D:101:GLU:HB3	4:D:404:HOH:O	2.01	0.59
1:B:111:PHE:HB2	1:B:149:VAL:HG22	1.84	0.59
1:C:180:ILE:HD13	1:C:232:SER:HB3	1.84	0.59
1:B:91:SER:HA	1:B:96:TRP:CB	2.32	0.58
1:B:109:VAL:CG1	1:B:111:PHE:HE1	2.16	0.58
1:D:127:SER:OG	1:D:129:LYS:HG2	2.03	0.58
1:A:205:ARG:NH2	1:A:217:ASP:OD2	2.35	0.57
1:C:102:LEU:HB3	1:C:107:VAL:HG11	1.86	0.57
1:D:177:ASN:HA	1:D:182:GLU:OE1	2.05	0.57
1:D:196:MET:HG2	1:D:363:LEU:HB3	1.86	0.57
1:B:179:SER:HB2	1:B:182:GLU:OE1	2.04	0.56
1:A:238:CYS:HB2	4:A:55:HOH:O	2.05	0.56
1:C:301:LYS:HG3	1:C:301:LYS:O	2.05	0.56
1:D:88:VAL:HG11	1:D:111:PHE:CG	2.39	0.56
1:A:130:PHE:O	1:A:134:MET:HG3	2.06	0.56
1:C:105:ARG:HH11	1:C:364:SER:HB3	1.68	0.56
1:C:115:PRO:HB2	1:C:116:PRO:HD3	1.87	0.56
1:C:265:GLY:O	1:C:268:SER:HB3	2.05	0.56
1:B:181:GLU:HB2	1:B:236:HIS:CE1	2.41	0.56
1:C:108:LYS:HE3	4:C:427:HOH:O	2.06	0.56
1:D:149:VAL:O	1:D:150:LEU:HD23	2.05	0.55
1:D:102:LEU:O	1:D:107:VAL:HG13	2.06	0.55
1:B:131:ASP:CG	1:B:143:ARG:HH12	2.09	0.55
1:A:142:LYS:HA	4:A:446:HOH:O	2.06	0.54
1:D:342:LYS:O	1:D:347:LYS:HE3	2.08	0.54
1:A:80:ASN:HD21	1:A:108:LYS:HG3	1.71	0.54
1:A:211:LEU:HD22	1:C:231:ILE:HD13	1.89	0.53
1:D:179:SER:HB2	4:D:423:HOH:O	2.08	0.53
1:C:305:ALA:O	1:C:308:ILE:HG13	2.09	0.53
1:C:105:ARG:NH2	1:C:196:MET:SD	2.81	0.53
1:D:258:VAL:HA	4:D:429:HOH:O	2.09	0.53
1:A:288:TYR:CB	1:A:290:ILE:HG13	2.38	0.52
1:C:237:PHE:O	1:C:241:MET:HG3	2.09	0.52
1:B:94:TYR:O	1:B:98:ILE:HG13	2.08	0.52
1:C:88:VAL:HG12	4:C:426:HOH:O	2.10	0.52
1:A:162:ILE:HG22	1:A:167:LYS:HG3	1.92	0.51
1:C:193:LYS:HD3	4:C:421:HOH:O	2.09	0.51
1:B:186:LEU:C	1:B:186:LEU:HD23	2.31	0.51
1:D:204:GLY:N	3:D:500:TCL:CL15	2.80	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:LYS:HD3	1:B:191:TYR:CZ	2.45	0.51
1:C:132:LYS:O	1:C:135:ILE:HG12	2.11	0.51
1:B:205:ARG:HD3	4:B:430:HOH:O	2.10	0.51
1:C:125:LEU:HD13	1:C:130:PHE:HD2	1.74	0.51
1:D:257:LYS:HD2	4:D:435:HOH:O	2.10	0.51
1:B:205:ARG:CD	4:B:430:HOH:O	2.59	0.51
1:B:210:SER:HB2	1:D:283:TYR:CZ	2.46	0.50
1:C:98:ILE:HG12	1:C:356:GLY:HA2	1.94	0.50
1:B:104:LYS:HB3	1:B:136:ILE:HG21	1.94	0.50
1:B:156:PHE:CE1	1:B:162:ILE:HA	2.47	0.50
1:B:190:LYS:HG2	1:B:191:TYR:CD2	2.47	0.50
1:B:301:LYS:HE3	1:B:306:THR:OG1	2.12	0.50
1:C:348:LYS:HE3	4:C:430:HOH:O	2.12	0.50
1:D:158:ASN:HA	4:D:423:HOH:O	2.12	0.50
1:C:100:LYS:HD3	1:C:133:ASP:O	2.11	0.50
1:C:170:LYS:O	1:C:170:LYS:HG2	2.11	0.50
1:C:80:ASN:HB2	1:C:108:LYS:NZ	2.28	0.49
1:C:176:LYS:O	1:C:177:ASN:HB2	2.12	0.49
1:D:114:TRP:CD1	1:D:115:PRO:HD2	2.47	0.49
1:D:288:TYR:HB2	1:D:290:ILE:HG13	1.93	0.49
1:A:259:VAL:HG23	1:A:262:TYR:HB3	1.93	0.49
1:B:100:LYS:O	1:B:103:SER:HB2	2.11	0.49
1:D:80:ASN:HB3	1:D:108:LYS:NZ	2.27	0.49
1:D:305:ALA:HB1	1:D:333:ILE:HG12	1.94	0.49
1:D:130:PHE:O	1:D:134:MET:HG3	2.13	0.49
1:B:199:HIS:HD2	1:B:233:LEU:HD12	1.78	0.49
1:B:170:LYS:HG2	1:B:171:ARG:HH12	1.77	0.49
1:B:346:LEU:HD11	1:C:291:ARG:HG2	1.94	0.49
1:B:174:ASN:OD1	1:B:174:ASN:N	2.45	0.49
1:C:248:VAL:HA	1:C:293:ASN:O	2.13	0.49
1:C:81:GLU:HB3	1:C:196:MET:HE1	1.95	0.48
1:C:147:LEU:HD13	1:C:191:TYR:CE1	2.48	0.48
1:B:115:PRO:HB2	1:B:116:PRO:HD3	1.94	0.48
1:C:123:LYS:HB3	1:C:123:LYS:HE2	1.65	0.48
1:B:87:GLY:HA3	1:B:200:SER:O	2.14	0.48
1:B:159:TYR:O	1:B:162:ILE:HG23	2.13	0.48
1:C:117:VAL:HA	1:C:120:ILE:HD12	1.95	0.48
1:A:382:ASN:CG	4:A:429:HOH:O	2.52	0.48
1:B:90:ASP:OD1	1:B:92:ASN:HB2	2.14	0.48
1:B:114:TRP:CE2	1:B:116:PRO:HG2	2.49	0.48
1:C:130:PHE:O	1:C:134:MET:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:GLU:OE2	1:D:349:LYS:HG3	2.13	0.48
1:D:341:GLU:HA	4:D:422:HOH:O	2.13	0.47
1:A:163:ASP:CG	1:A:166:THR:HG23	2.35	0.47
1:C:135:ILE:HG22	1:C:143:ARG:HH11	1.79	0.47
1:B:205:ARG:HB2	4:B:430:HOH:O	2.14	0.47
1:A:131:ASP:HB3	1:A:143:ARG:HH12	1.80	0.47
1:C:118:TYR:CD2	1:C:175:LEU:HD22	2.50	0.47
1:C:123:LYS:O	1:C:126:GLU:HB2	2.15	0.47
1:C:170:LYS:HA	1:C:173:ASN:ND2	2.30	0.47
1:D:208:GLN:HE21	1:D:308:ILE:HA	1.80	0.47
1:B:109:VAL:CG1	1:B:111:PHE:CE1	2.96	0.46
1:D:170:LYS:HE2	1:D:170:LYS:HB3	1.73	0.46
1:A:382:ASN:OD1	4:A:429:HOH:O	2.20	0.46
1:A:203:ASN:O	1:A:222:ALA:HA	2.14	0.46
1:B:152:LEU:HD23	1:B:178:TYR:O	2.15	0.46
1:C:342:LYS:HG2	1:C:343:TYR:CZ	2.50	0.46
1:D:179:SER:O	1:D:183:VAL:HG13	2.15	0.46
1:B:283:TYR:CZ	1:D:210:SER:HB2	2.51	0.46
1:B:368:SER:HB2	1:C:348:LYS:NZ	2.31	0.46
1:B:139:ASP:HB2	1:B:140:ASN:OD1	2.15	0.46
1:A:348:LYS:HG2	1:A:349:LYS:N	2.31	0.46
1:C:134:MET:HE3	1:C:144:MET:HB3	1.97	0.46
1:C:381:LEU:HD23	4:C:444:HOH:O	2.15	0.46
1:D:200:SER:O	2:D:550:NAD:H52N	2.16	0.46
1:A:206:GLU:HA	1:A:208:GLN:HE21	1.81	0.45
1:A:261:GLY:N	4:A:427:HOH:O	2.23	0.45
1:D:115:PRO:HB2	1:D:116:PRO:HD3	1.97	0.45
1:A:257:LYS:HE3	1:B:257:LYS:HZ3	1.80	0.45
1:D:233:LEU:O	1:D:237:PHE:HB2	2.16	0.45
1:A:254:ALA:CB	1:A:259:VAL:CG2	2.94	0.45
1:B:162:ILE:HG13	1:B:166:THR:CG2	2.47	0.45
1:B:308:ILE:H	1:B:308:ILE:HG13	1.33	0.45
1:A:208:GLN:HG3	1:A:208:GLN:H	1.49	0.44
1:D:380:GLY:O	1:D:383:ILE:HG12	2.16	0.44
1:C:88:VAL:O	1:C:113:VAL:HG22	2.17	0.44
1:A:210:SER:HB2	1:C:283:TYR:CZ	2.52	0.44
1:A:260:PRO:HA	4:A:427:HOH:O	2.17	0.44
1:B:164:GLU:OE1	1:B:167:LYS:HD2	2.18	0.44
1:B:132:LYS:HG3	1:B:133:ASP:OD1	2.17	0.44
1:B:248:VAL:HA	1:B:293:ASN:O	2.18	0.44
1:B:83:CYS:HB2	1:B:196:MET:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:PHE:O	1:B:134:MET:HG3	2.18	0.43
1:D:87:GLY:HA3	1:D:201:LEU:HB3	2.00	0.43
1:A:202:ALA:HB3	3:A:400:TCL:CL16	2.55	0.43
1:C:205:ARG:NH2	1:C:217:ASP:OD2	2.50	0.43
1:D:288:TYR:CB	1:D:290:ILE:HG13	2.48	0.43
1:C:103:SER:OG	1:C:144:MET:HG3	2.18	0.43
1:A:119:ASN:O	1:A:123:LYS:HG3	2.18	0.43
1:D:117:VAL:HA	1:D:120:ILE:HD12	2.01	0.43
1:D:204:GLY:HA2	4:D:426:HOH:O	2.19	0.43
1:B:142:LYS:O	1:B:142:LYS:HG3	2.19	0.43
1:D:128:GLY:HA2	1:D:131:ASP:OD1	2.18	0.43
1:A:85:ILE:HG12	1:A:198:VAL:HB	1.99	0.43
1:A:88:VAL:HG22	1:A:95:GLY:HA3	2.01	0.43
1:B:366:GLU:O	1:C:357:SER:OG	2.37	0.43
1:D:83:CYS:HB2	1:D:196:MET:CB	2.48	0.43
1:C:107:VAL:O	1:C:107:VAL:HG13	2.17	0.43
1:C:345:PRO:HD2	1:C:379:ASN:O	2.19	0.43
1:D:96:TRP:O	1:D:100:LYS:HG3	2.19	0.43
1:B:275:SER:HA	1:B:278:ARG:NH2	2.33	0.42
1:C:253:GLN:HG2	1:C:253:GLN:O	2.20	0.42
1:C:81:GLU:HB3	1:C:196:MET:CE	2.48	0.42
1:A:177:ASN:O	1:A:183:VAL:HG12	2.19	0.42
1:C:193:LYS:HA	1:C:240:PHE:O	2.20	0.42
1:C:308:ILE:HB	1:C:332:PHE:HB3	2.01	0.42
1:C:186:LEU:C	1:C:186:LEU:HD23	2.40	0.42
2:C:450:NAD:O2N	2:C:450:NAD:N7N	2.48	0.42
1:C:257:LYS:CE	4:D:408:HOH:O	2.67	0.42
1:D:201:LEU:C	1:D:201:LEU:HD12	2.39	0.42
1:D:223:ILE:O	1:D:227:SER:HB2	2.20	0.42
1:B:196:MET:HG2	1:B:363:LEU:HB3	2.02	0.42
1:A:362:LEU:HD23	1:A:362:LEU:HA	1.88	0.42
1:B:382:ASN:ND2	1:C:373:GLN:HE22	2.07	0.42
1:A:257:LYS:NZ	1:B:257:LYS:NZ	2.67	0.42
1:B:86:ALA:O	1:B:112:GLY:O	2.37	0.42
1:B:216:ARG:HB2	1:D:228:TYR:CE2	2.55	0.42
1:C:239:LYS:HG2	4:C:67:HOH:O	2.20	0.42
1:A:200:SER:CB	1:A:250:LEU:HD23	2.50	0.41
1:B:88:VAL:O	1:B:113:VAL:HG22	2.20	0.41
1:B:171:ARG:HA	1:B:171:ARG:HD3	1.96	0.41
1:D:248:VAL:HG23	1:D:363:LEU:HD21	2.02	0.41
1:C:114:TRP:CG	1:C:116:PRO:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:PHE:CZ	1:D:367:SER:HB3	2.55	0.41
1:C:205:ARG:HD3	1:C:221:ASP:OD2	2.20	0.41
1:D:169:ASN:OD1	1:D:170:LYS:N	2.52	0.41
1:D:248:VAL:HG23	1:D:363:LEU:CD2	2.50	0.41
1:A:101:GLU:HG3	1:A:357:SER:N	2.36	0.41
1:B:180:ILE:O	1:B:183:VAL:HG22	2.20	0.41
1:D:117:VAL:HG12	1:D:120:ILE:HD12	2.02	0.41
1:B:137:ASN:HA	1:B:138:ASN:C	2.40	0.41
1:B:114:TRP:CG	1:B:116:PRO:HD2	2.56	0.41
1:B:176:LYS:O	1:B:177:ASN:HB2	2.21	0.41
1:B:253:GLN:OE1	1:B:257:LYS:HE3	2.21	0.41
1:C:170:LYS:HE3	1:C:171:ARG:HD2	2.03	0.41
1:C:233:LEU:HD23	1:C:233:LEU:HA	1.84	0.41
1:D:125:LEU:CD1	1:D:134:MET:HE1	2.51	0.41
1:A:211:LEU:HD12	1:C:279:VAL:HB	2.03	0.41
1:C:307:ALA:C	1:C:308:ILE:HG12	2.41	0.41
1:A:303:ARG:HG3	1:A:304:ALA:N	2.36	0.40
1:B:301:LYS:O	1:B:301:LYS:HG3	2.21	0.40
1:C:114:TRP:CD1	1:C:116:PRO:HD2	2.56	0.40
1:D:100:LYS:O	1:D:103:SER:HB2	2.20	0.40
1:B:305:ALA:HB2	3:B:500:TCL:H41	2.03	0.40
1:B:139:ASP:HA	1:B:140:ASN:HA	1.64	0.40
1:D:103:SER:HB3	1:D:136:ILE:HD13	2.03	0.40
1:D:200:SER:HA	1:D:250:LEU:HD23	2.04	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	278/323 (86%)	266 (96%)	11 (4%)	1 (0%)	34 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	285/323 (88%)	270 (95%)	13 (5%)	2 (1%)	22	39
1	C	276/323 (85%)	258 (94%)	17 (6%)	1 (0%)	34	54
1	D	285/323 (88%)	266 (93%)	19 (7%)	0	100	100
All	All	1124/1292 (87%)	1060 (94%)	60 (5%)	4 (0%)	34	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	90	ASP
1	A	90	ASP
1	C	173	ASN
1	B	86	ALA

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	242/280 (86%)	235 (97%)	7 (3%)	42	69
1	B	247/280 (88%)	238 (96%)	9 (4%)	35	61
1	C	240/280 (86%)	230 (96%)	10 (4%)	30	54
1	D	247/280 (88%)	235 (95%)	12 (5%)	25	47
All	All	976/1120 (87%)	938 (96%)	38 (4%)	32	57

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	ILE
1	A	166	THR
1	A	183	VAL
1	A	208	GLN
1	A	211	LEU
1	A	212	LEU
1	A	309	ASN

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Mol	Chain	Res	Type
1	B	129	LYS
1	B	152	LEU
1	B	162	ILE
1	B	174	ASN
1	B	179	SER
1	B	227	SER
1	B	248	VAL
1	B	268	SER
1	B	308	ILE
1	C	122	ILE
1	C	148	ASP
1	C	175	LEU
1	C	183	VAL
1	C	205	ARG
1	C	208	GLN
1	C	217	ASP
1	C	227	SER
1	C	248	VAL
1	C	308	ILE
1	D	107	VAL
1	D	122	ILE
1	D	139	ASP
1	D	174	ASN
1	D	183	VAL
1	D	212	LEU
1	D	225	LYS
1	D	268	SER
1	D	308	ILE
1	D	332	PHE
1	D	342	LYS
1	D	346	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	208	GLN
1	B	169	ASN
1	B	236	HIS
1	B	253	GLN
1	C	119	ASN
1	C	174	ASN

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Mol	Chain	Res	Type
1	C	253	GLN
1	C	373	GLN
1	D	208	GLN
1	D	242	ASN
1	D	382	ASN

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)

8 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	-	42,48,48	0.73	2 (4%)	50,73,73	1.33	6 (12%)
3	TCL	C	400	-	18,18,18	1.05	3 (16%)	25,25,25	0.81	0
2	NAD	D	550	-	42,48,48	0.72	1 (2%)	50,73,73	1.23	4 (8%)
3	TCL	D	500	-	18,18,18	1.14	3 (16%)	25,25,25	0.82	1 (4%)
2	NAD	B	550	-	42,48,48	0.76	1 (2%)	50,73,73	1.22	4 (8%)
3	TCL	B	500	-	18,18,18	1.20	3 (16%)	25,25,25	1.03	2 (8%)
3	TCL	A	400	-	18,18,18	1.08	2 (11%)	25,25,25	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAD	C	450	-	42,48,48	0.73	1 (2%)	50,73,73	1.26	4 (8%)

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	-	-	5/26/62/62	0/5/5/5
3	TCL	C	400	-	-	0/4/4/4	0/2/2/2
2	NAD	D	550	-	-	6/26/62/62	0/5/5/5
3	TCL	D	500	-	-	0/4/4/4	0/2/2/2
2	NAD	B	550	-	-	7/26/62/62	0/5/5/5
3	TCL	B	500	-	-	0/4/4/4	0/2/2/2
3	TCL	A	400	-	-	0/4/4/4	0/2/2/2
2	NAD	C	450	-	-	8/26/62/62	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	TCL	C9-CL16	3.34	1.81	1.73
3	D	500	TCL	C9-CL16	3.01	1.80	1.73
2	B	550	NAD	O4D-C1D	2.58	1.44	1.41
3	D	500	TCL	C11-CL15	2.40	1.79	1.74
3	A	400	TCL	C9-CL16	2.37	1.79	1.73
3	C	400	TCL	C9-CL16	2.36	1.79	1.73
3	B	500	TCL	C11-CL15	2.29	1.79	1.74
2	A	450	NAD	O4B-C1B	2.19	1.44	1.41
2	C	450	NAD	O4D-C1D	2.12	1.44	1.41
3	B	500	TCL	C2-CL14	2.10	1.79	1.74
2	D	550	NAD	O4B-C1B	2.08	1.44	1.41
2	A	450	NAD	O4D-C1D	2.05	1.43	1.41
3	D	500	TCL	C2-CL14	2.02	1.78	1.74
3	A	400	TCL	C11-CL15	2.02	1.78	1.74
3	C	400	TCL	C2-CL14	2.02	1.78	1.74
3	C	400	TCL	C11-CL15	2.01	1.78	1.74

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	450	NAD	N3A-C2A-N1A	-5.28	120.42	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	550	NAD	N3A-C2A-N1A	-4.85	121.10	128.68
2	B	550	NAD	N3A-C2A-N1A	-4.75	121.25	128.68
2	C	450	NAD	N3A-C2A-N1A	-4.68	121.37	128.68
2	B	550	NAD	O4B-C1B-C2B	-3.02	102.51	106.93
2	B	550	NAD	PN-O3-PA	-2.90	122.87	132.83
2	D	550	NAD	C3B-C2B-C1B	2.81	105.21	100.98
2	C	450	NAD	PN-O3-PA	-2.80	123.21	132.83
2	C	450	NAD	C1B-N9A-C4A	-2.70	121.89	126.64
2	D	550	NAD	O4D-C1D-C2D	-2.56	103.18	106.93
3	D	500	TCL	O7-C5-C6	2.50	120.89	116.22
2	A	450	NAD	O4B-C1B-C2B	-2.48	103.30	106.93
3	B	500	TCL	C8-C9-CL16	2.45	122.31	119.43
3	B	500	TCL	O7-C5-C6	2.31	120.54	116.22
2	B	550	NAD	C4A-C5A-N7A	-2.20	107.11	109.40
2	A	450	NAD	C3N-C7N-N7N	2.18	120.36	117.75
2	A	450	NAD	C4A-C5A-N7A	-2.18	107.13	109.40
2	A	450	NAD	O7N-C7N-C3N	-2.09	117.13	119.63
2	A	450	NAD	O4D-C1D-C2D	-2.09	103.88	106.93
2	C	450	NAD	C5B-C4B-C3B	-2.02	107.62	115.18
2	D	550	NAD	O2N-PN-O1N	2.00	122.13	112.24

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	450	NAD	C5D-O5D-PN-O1N
2	A	450	NAD	C5D-O5D-PN-O2N
2	A	450	NAD	O4D-C1D-N1N-C2N
2	B	550	NAD	C5D-O5D-PN-O1N
2	B	550	NAD	C5D-O5D-PN-O2N
2	B	550	NAD	O4D-C1D-N1N-C2N
2	B	550	NAD	O4D-C1D-N1N-C6N
2	C	450	NAD	C5D-O5D-PN-O1N
2	C	450	NAD	C5D-O5D-PN-O2N
2	C	450	NAD	O4D-C1D-N1N-C2N
2	D	550	NAD	O4B-C4B-C5B-O5B
2	D	550	NAD	C5D-O5D-PN-O1N
2	D	550	NAD	O4D-C1D-N1N-C2N
2	C	450	NAD	O4B-C4B-C5B-O5B
2	C	450	NAD	C3B-C4B-C5B-O5B
2	D	550	NAD	C3B-C4B-C5B-O5B
2	A	450	NAD	C5D-O5D-PN-O3

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Mol	Chain	Res	Type	Atoms
2	D	550	NAD	C5D-O5D-PN-O3
2	D	550	NAD	C5D-O5D-PN-O2N
2	A	450	NAD	O4B-C4B-C5B-O5B
2	B	550	NAD	C5D-O5D-PN-O3
2	B	550	NAD	C2D-C1D-N1N-C6N
2	C	450	NAD	C5D-O5D-PN-O3
2	B	550	NAD	O4B-C4B-C5B-O5B
2	C	450	NAD	C5B-O5B-PA-O1A
2	C	450	NAD	C5B-O5B-PA-O2A

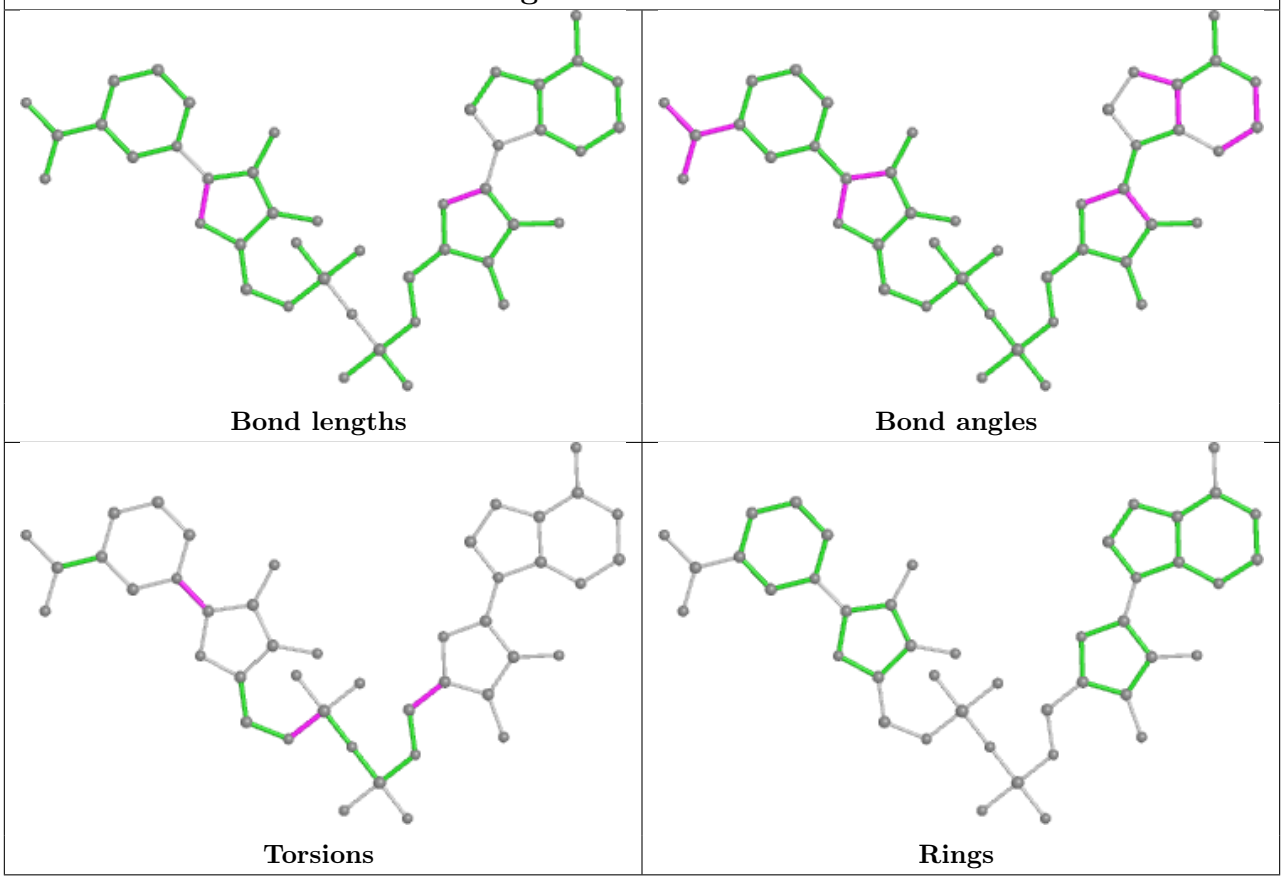
There are no ring outliers.

5 monomers are involved in 6 short contacts:

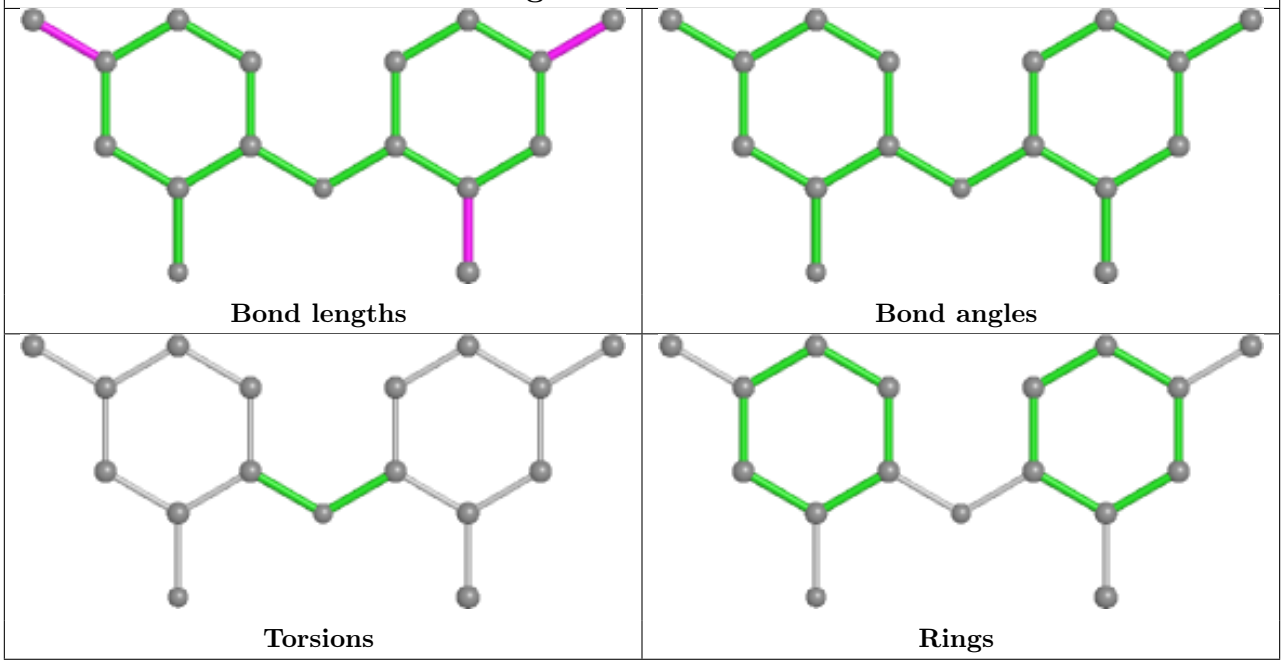
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	550	NAD	1	0
3	D	500	TCL	1	0
3	B	500	TCL	2	0
3	A	400	TCL	1	0
2	C	450	NAD	1	0

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.

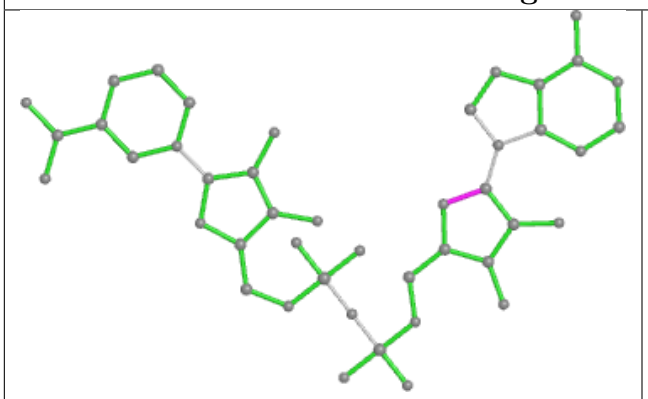
Ligand NAD A 450



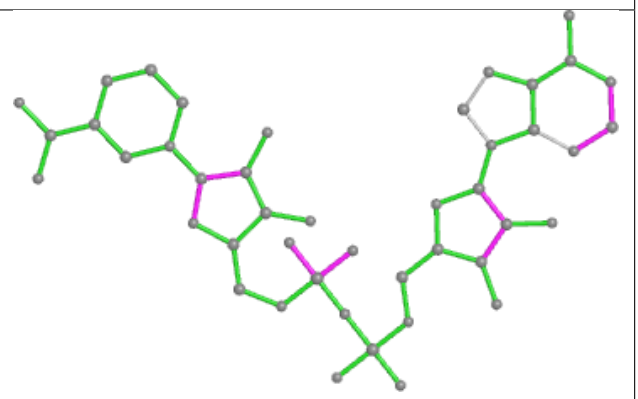
Ligand TCL C 400



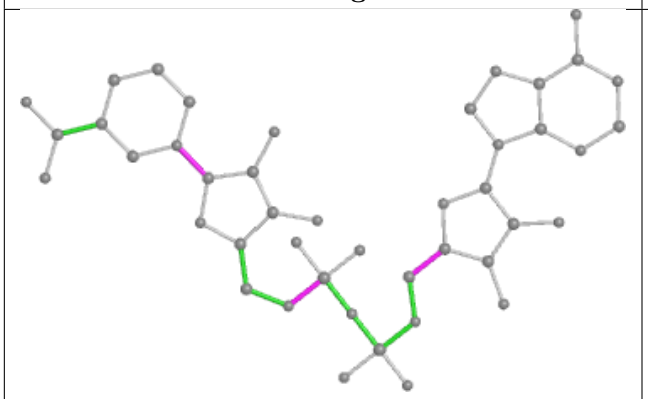
Ligand NAD D 550



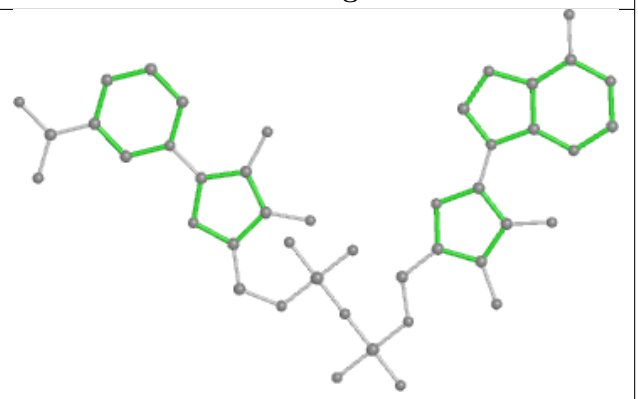
Bond lengths



Bond angles

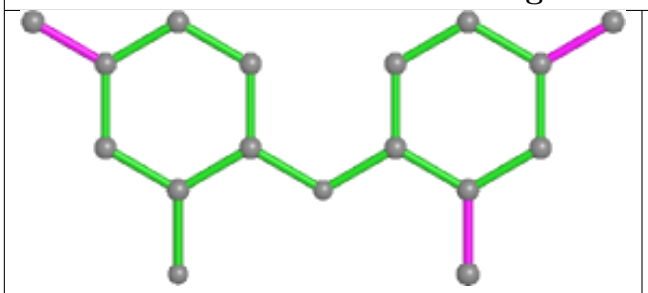


Torsions

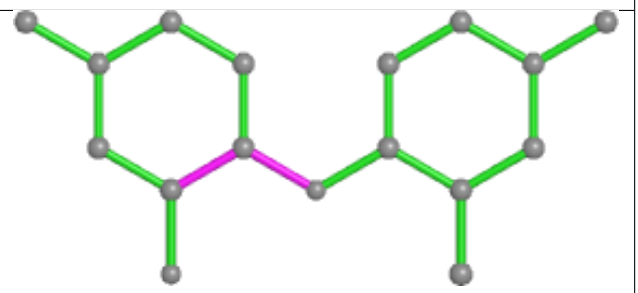


Rings

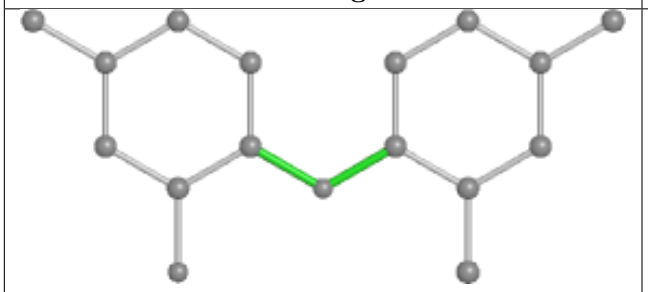
Ligand TCL D 500



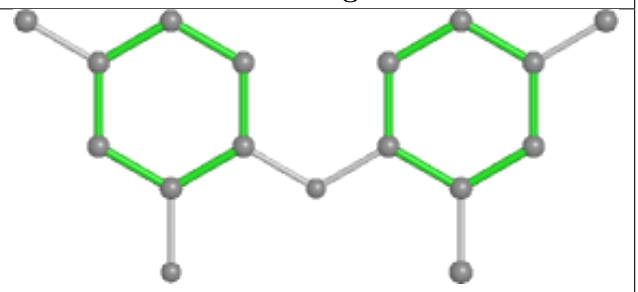
Bond lengths



Bond angles

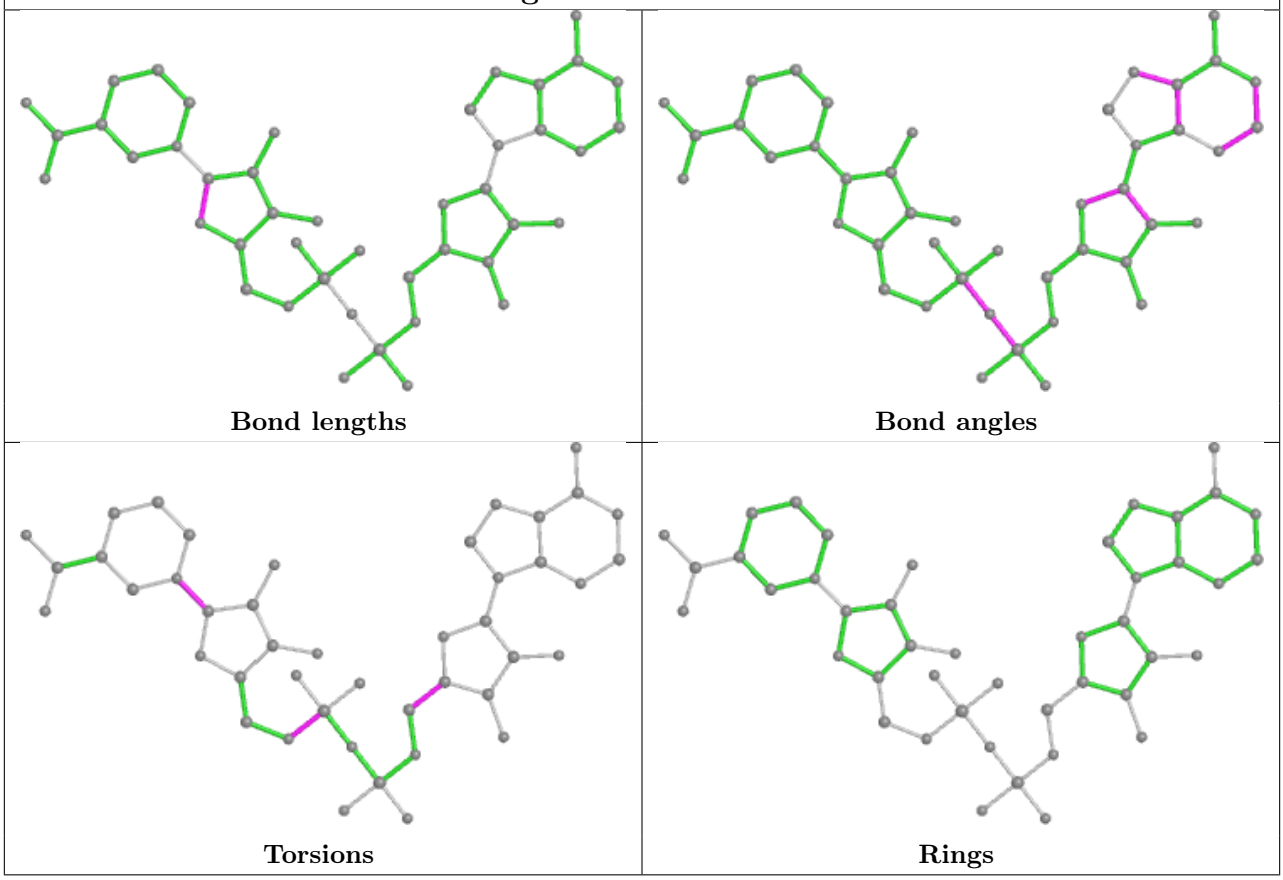


Torsions

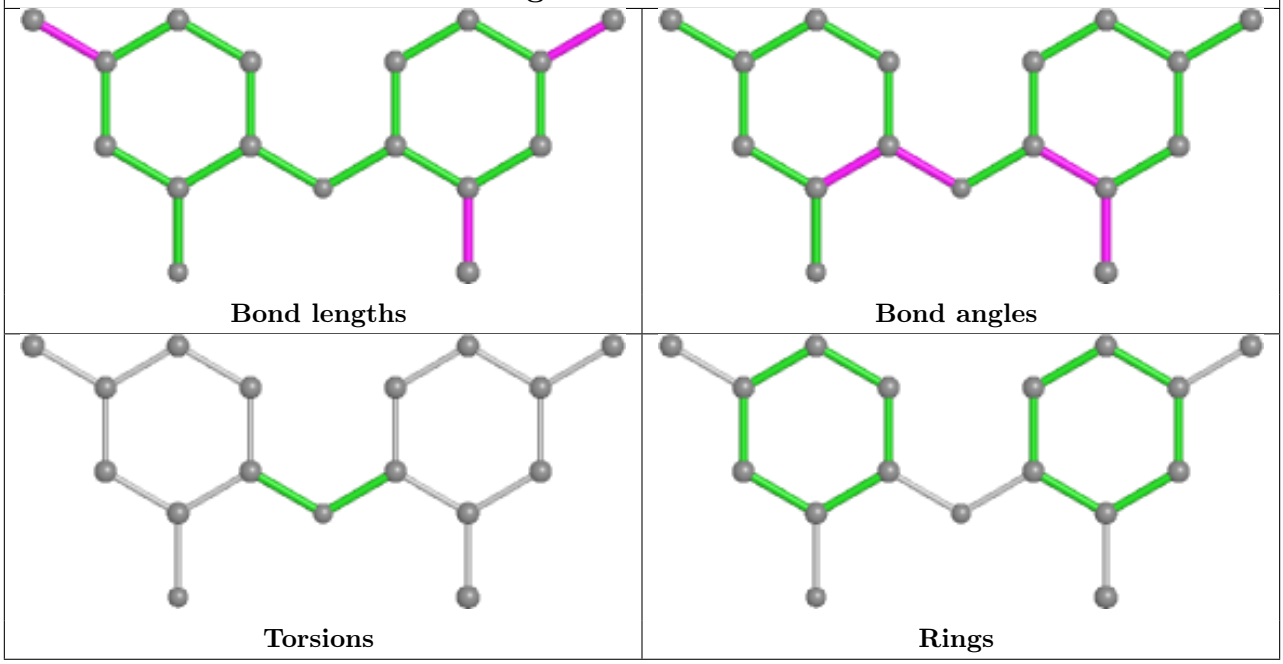


Rings

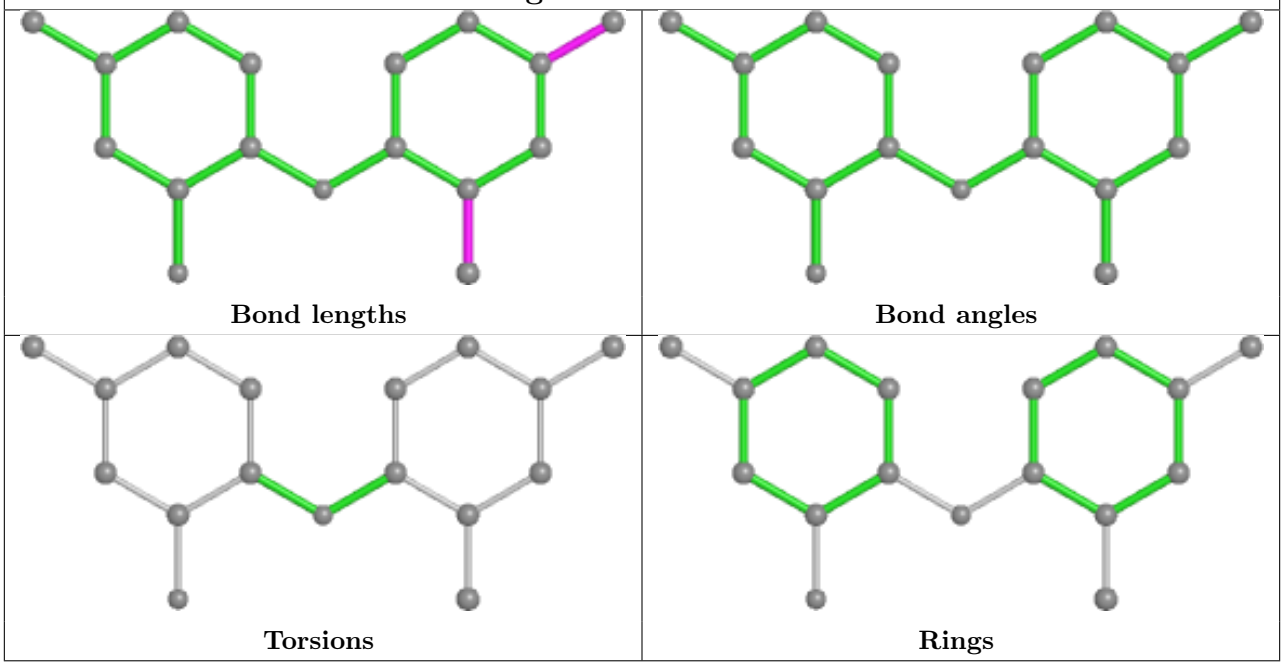
Ligand NAD B 550



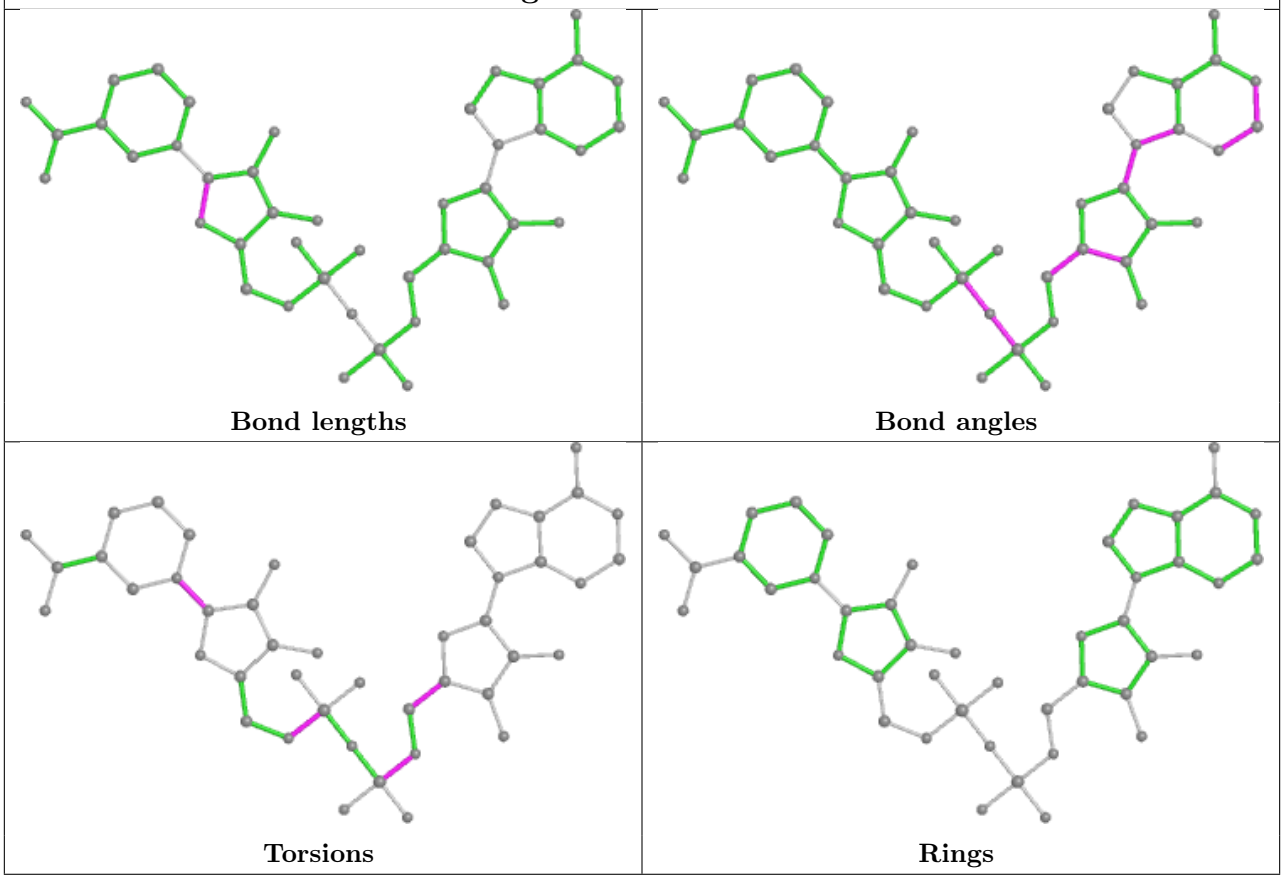
Ligand TCL B 500



Ligand TCL A 400



Ligand NAD C 450



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)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	284/323 (87%)	-0.13	2 (0%)	87	89	43, 58, 78, 93	0
1	B	289/323 (89%)	0.33	18 (6%)	20	21	47, 68, 110, 140	0
1	C	282/323 (87%)	0.14	19 (6%)	17	18	46, 66, 90, 109	0
1	D	289/323 (89%)	0.27	20 (6%)	16	17	46, 67, 109, 138	0
All	All	1144/1292 (88%)	0.15	59 (5%)	27	29	43, 64, 98, 140	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	136	ILE	6.4
1	D	330	TYR	5.8
1	B	140	ASN	5.6
1	B	141	SER	5.0
1	D	172	TYR	4.7
1	D	135	ILE	4.5
1	B	330	TYR	4.4
1	D	140	ASN	4.2
1	D	142	LYS	3.9
1	D	139	ASP	3.8
1	D	141	SER	3.8
1	D	208	GLN	3.5
1	C	335	TYR	3.5
1	D	143	ARG	3.4
1	D	162	ILE	3.3
1	C	143	ARG	3.3
1	B	170	LYS	3.2
1	D	137	ASN	3.2
1	B	295	ILE	3.1
1	B	80	ASN	3.0
1	C	172	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	335	TYR	2.9
1	B	374	THR	2.9
1	D	170	LYS	2.9
1	B	138	ASN	2.8
1	C	294	THR	2.8
1	A	173	ASN	2.8
1	C	170	LYS	2.8
1	B	173	ASN	2.7
1	D	173	ASN	2.7
1	C	374	THR	2.7
1	C	375	ILE	2.7
1	C	295	ILE	2.7
1	C	135	ILE	2.6
1	B	273	LEU	2.6
1	D	138	ASN	2.5
1	B	375	ILE	2.5
1	B	307	ALA	2.5
1	B	172	TYR	2.5
1	C	136	ILE	2.4
1	C	192	GLY	2.4
1	C	80	ASN	2.4
1	C	331	SER	2.4
1	B	294	THR	2.3
1	C	208	GLN	2.3
1	C	188	TYR	2.2
1	D	156	PHE	2.2
1	C	173	ASN	2.2
1	C	193	LYS	2.1
1	C	171	ARG	2.1
1	D	374	THR	2.1
1	B	192	GLY	2.1
1	C	147	LEU	2.1
1	B	282	TYR	2.1
1	D	164	GLU	2.1
1	D	145	GLN	2.1
1	B	271	ALA	2.0
1	D	163	ASP	2.0
1	B	175	LEU	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 monosaccharides in this entry.

6.4 Ligands (i)

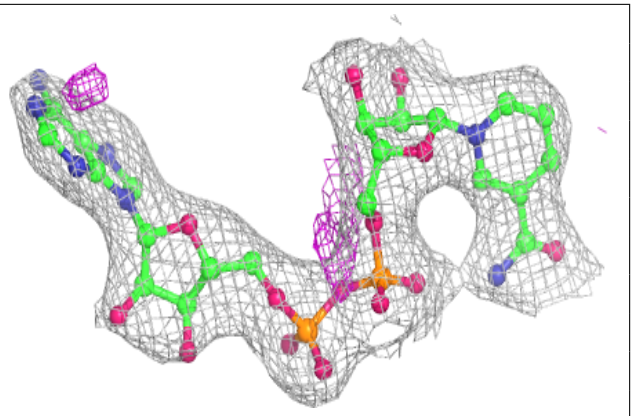
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

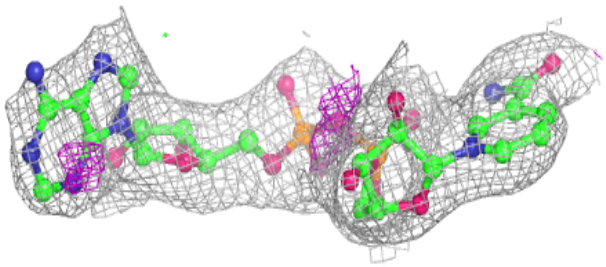
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	D	550	44/44	0.92	0.15	53,71,85,88	0
3	TCL	D	500	17/17	0.92	0.17	57,68,79,86	0
3	TCL	C	400	17/17	0.93	0.16	57,65,80,90	0
3	TCL	B	500	17/17	0.93	0.17	57,67,84,90	0
2	NAD	B	550	44/44	0.96	0.13	56,72,79,82	0
2	NAD	C	450	44/44	0.96	0.14	59,69,77,82	0
3	TCL	A	400	17/17	0.97	0.12	49,58,74,86	0
2	NAD	A	450	44/44	0.97	0.13	44,56,64,68	0

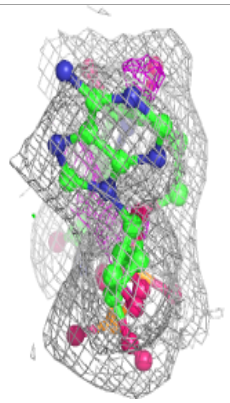
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD D 550:

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

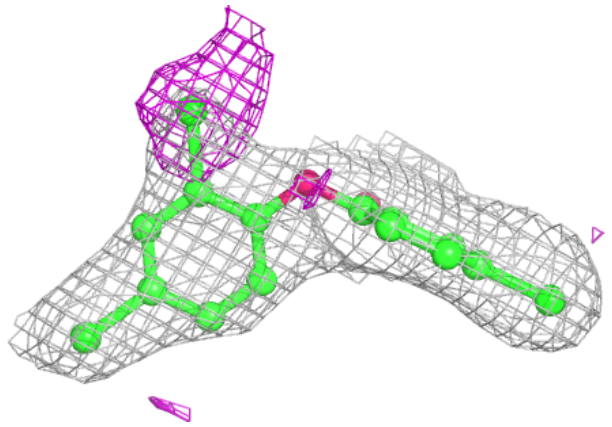


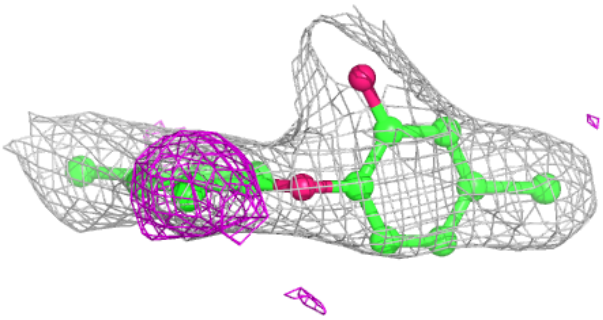


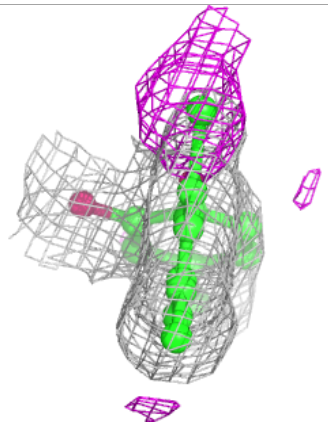


Electron density around TCL D 500:

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

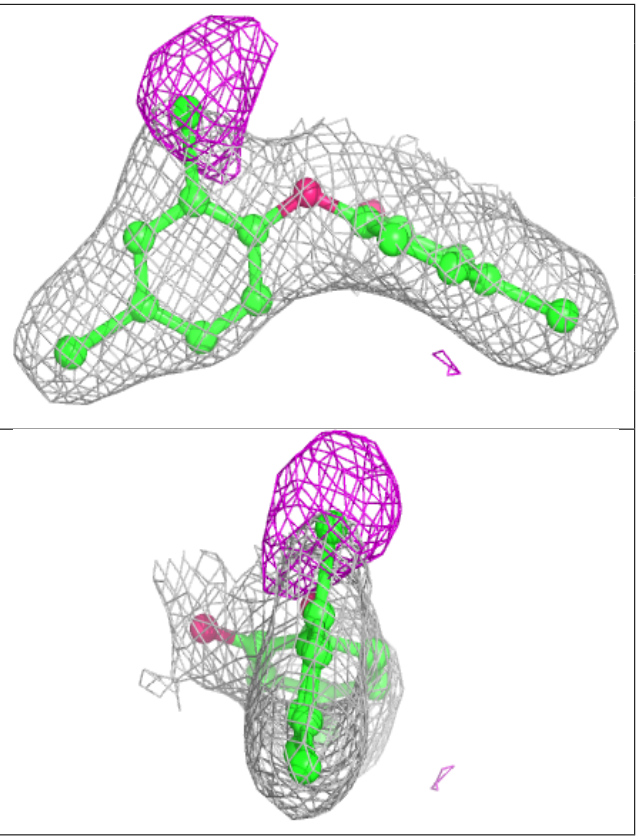






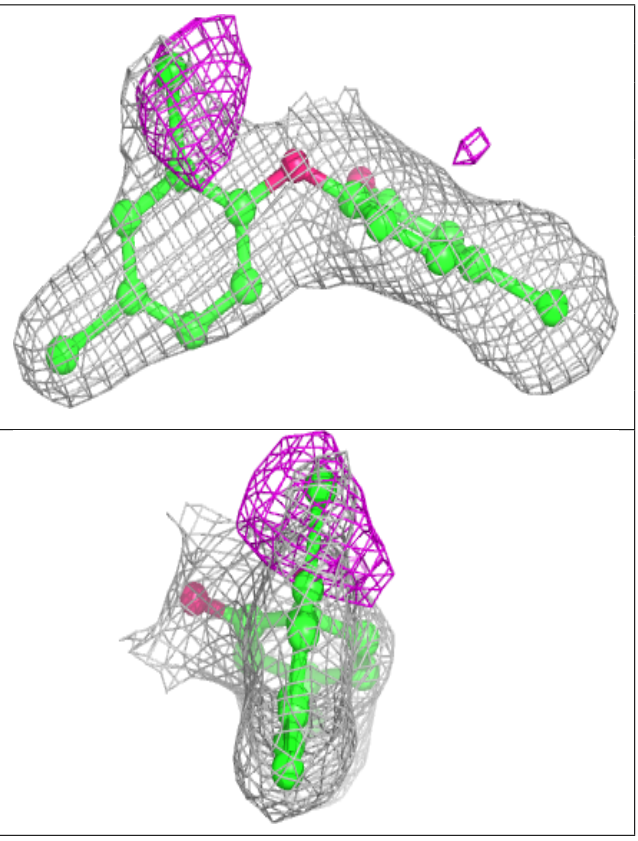
Electron density around TCL C 400:

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



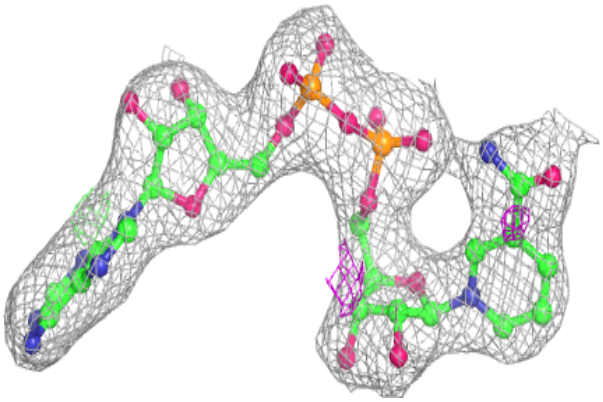
Electron density around TCL B 500:

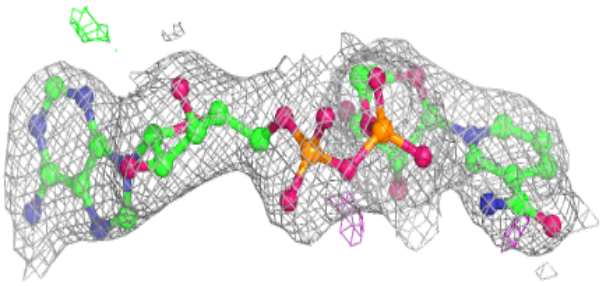
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

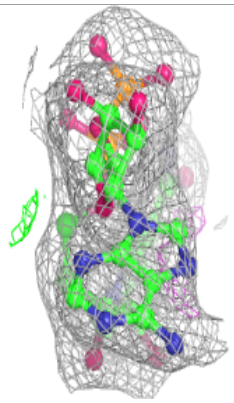


Electron density around NAD B 550:

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







Electron density around NAD C 450:

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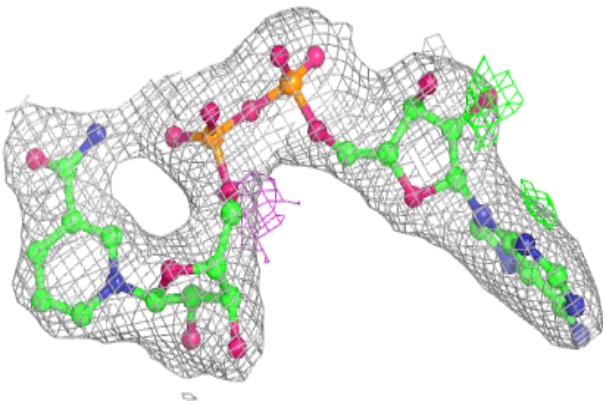
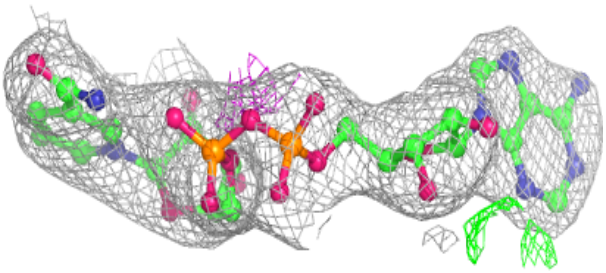
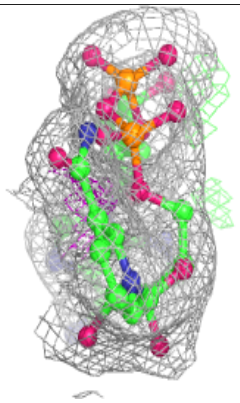
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

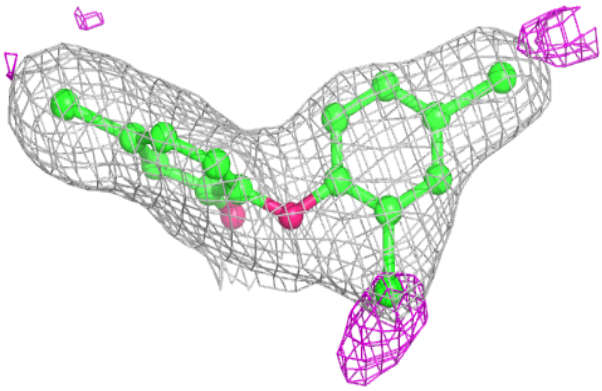


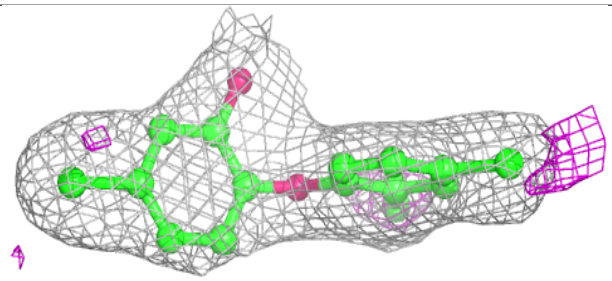


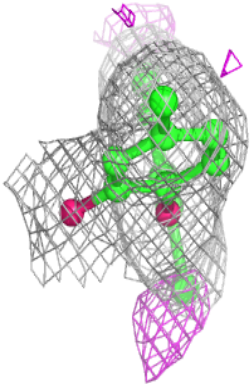


Electron density around TCL A 400:

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

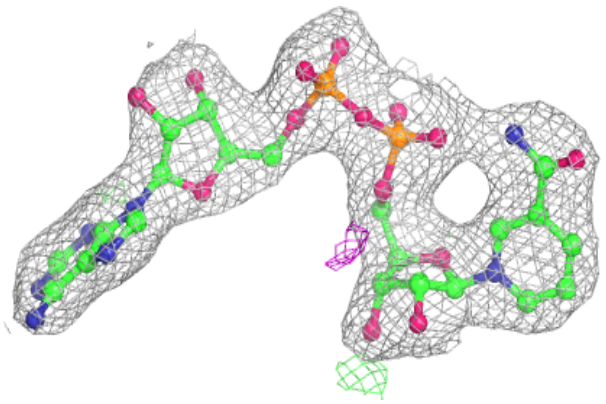


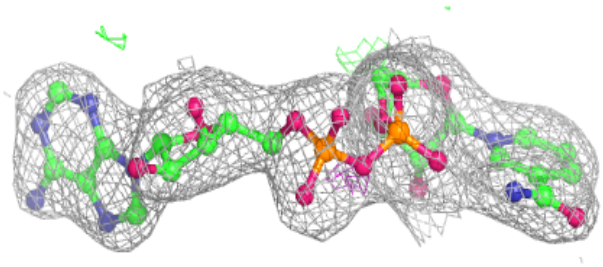


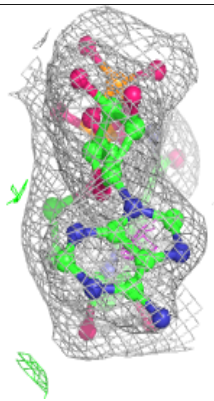


Electron density around NAD A 450:

$2mF_o$-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.