Full wwPDB X-ray Structure Validation Report (i)

Dec 13, 2023 – 01:33 pm GMT

PDB ID	:	2WOV
Title	:	Trypanosoma brucei trypanothione reductase with bound NADP.
Authors	:	Alphey, M.S.; Fairlamb, A.H.
Deposited on	:	2009-07-30
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 (i)) were used in the production of this report:

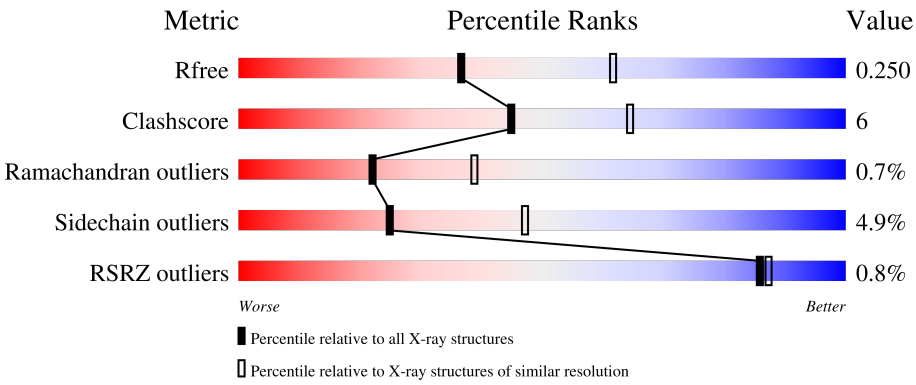
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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))
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	495	% 83% 15% • •
1	B	495	% 81% 16% • •
1	C	495	80% 17% • •
1	D	495	% 80% 16% • •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15706 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 TRYPANOTHIONE REDUCTASE.

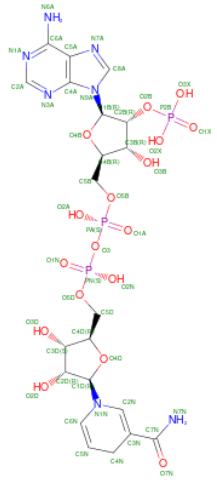
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	490	3735	2375	637	703	20	0	2	0
1	B	486	3691	2348	627	697	19	0	0	0
1	C	490	3733	2374	634	705	20	0	2	0
1	D	487	3696	2351	628	698	19	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q389T8
A	-1	SER	-	expression tag	UNP Q389T8
A	0	HIS	-	expression tag	UNP Q389T8
B	-2	GLY	-	expression tag	UNP Q389T8
B	-1	SER	-	expression tag	UNP Q389T8
B	0	HIS	-	expression tag	UNP Q389T8
C	-2	GLY	-	expression tag	UNP Q389T8
C	-1	SER	-	expression tag	UNP Q389T8
C	0	HIS	-	expression tag	UNP Q389T8
D	-2	GLY	-	expression tag	UNP Q389T8
D	-1	SER	-	expression tag	UNP Q389T8
D	0	HIS	-	expression tag	UNP Q389T8

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

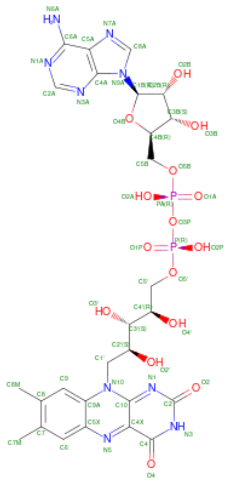
NDP



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
2	B	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
2	C	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
2	D	1	48	21	7	17	3	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

FAD



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	53	27	9	15	2	0	0
3	B	1	53	27	9	15	2	0	0
3	C	1	53	27	9	15	2	0	0
3	D	1	53	27	9	15	2	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
4	A	1	1	1	0	0
4	B	2	2	2	0	0
4	C	2	2	2	0	0
4	D	2	2	2	0	0

- Molecule 5 is water.

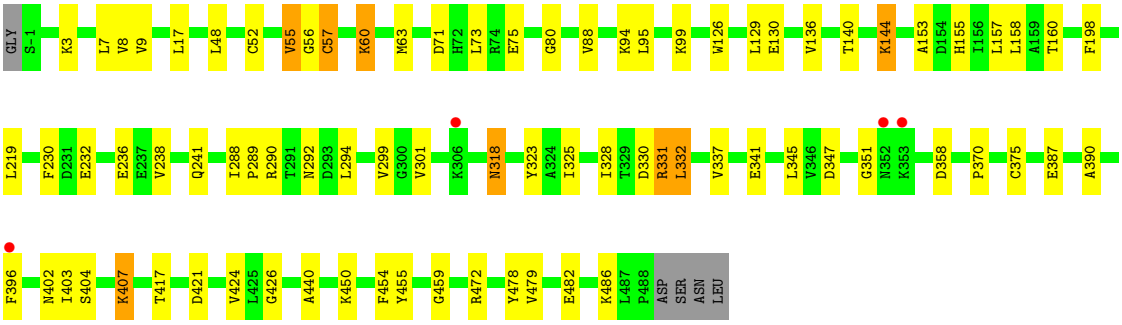
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	121	121	121	0	0
5	B	99	99	99	0	0
5	C	128	128	128	0	0
5	D	92	92	92	0	0

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.

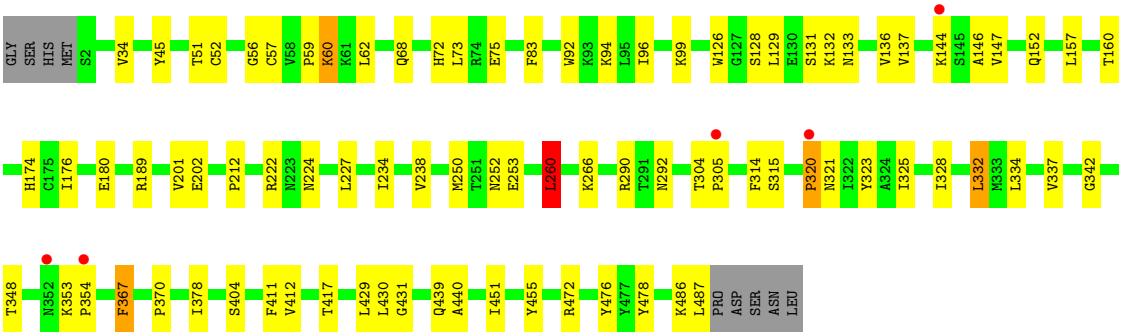
• Molecule 1: TRYPANOTHIONE REDUCTASE

Chain A:



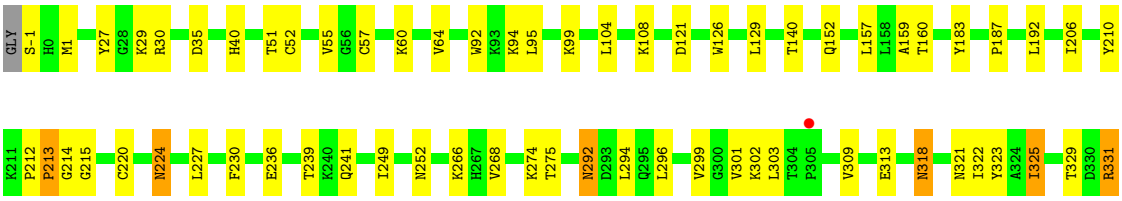
• Molecule 1: TRYPANOTHIONE REDUCTASE

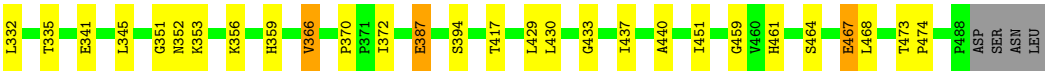
Chain B:



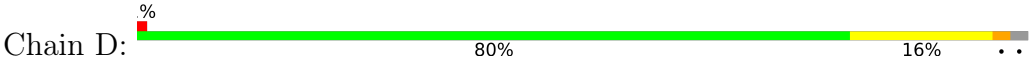
• Molecule 1: TRYPANOTHIONE REDUCTASE

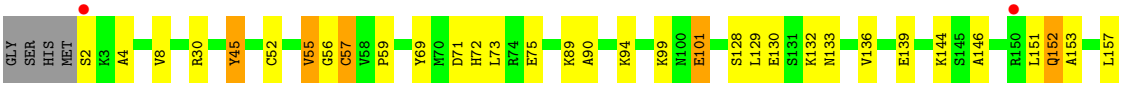
Chain C:

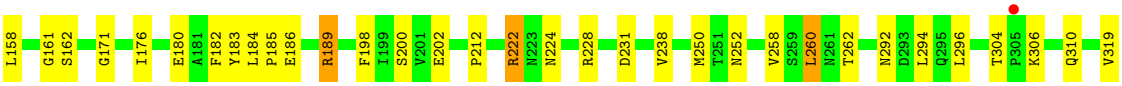


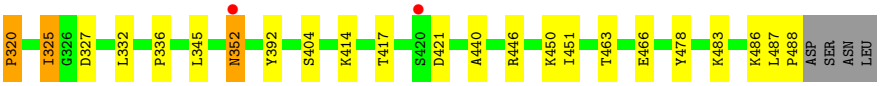


• Molecule 1: TRYPANOTHIONE REDUCTASE









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	100.87Å 63.45Å 169.35Å 90.00° 97.85° 90.00°	Depositor
Resolution (Å)	19.85 – 2.50 19.85 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.85-2.50) 98.1 (19.85-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.36 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.179 , 0.251 0.179 , 0.250	Depositor DCC
R_{free} test set	3628 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	29.4	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 33.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15706	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.96% 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: NDP, FAD, NA

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	0.80	0/3820	0.80	1/5181 (0.0%)
1	B	0.75	0/3768	0.78	2/5111 (0.0%)
1	C	0.83	0/3818	0.82	2/5179 (0.0%)
1	D	0.81	0/3773	0.80	4/5118 (0.1%)
All	All	0.80	0/15179	0.80	9/20589 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	222	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	A	290	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	C	121	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	D	260	LEU	CB-CG-CD2	6.14	121.45	111.00
1	B	260	LEU	CB-CG-CD1	-5.95	100.88	111.00
1	D	488	PRO	N-CA-CB	5.83	110.30	103.30
1	D	222	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	D	260	LEU	CA-CB-CG	5.29	127.48	115.30
1	C	215	GLY	N-CA-C	5.17	126.02	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	214	GLY	Peptide
1	C	352	ASN	Peptide

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	3735	0	3753	54	0
1	B	3691	0	3703	55	0
1	C	3733	0	3746	56	0
1	D	3696	0	3704	44	0
2	A	48	0	26	1	0
2	B	48	0	26	0	0
2	C	48	0	26	0	0
2	D	48	0	26	1	0
3	A	53	0	31	1	0
3	B	53	0	31	2	0
3	C	53	0	31	2	0
3	D	53	0	31	1	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	121	0	0	1	0
5	B	99	0	0	4	0
5	C	128	0	0	2	0
5	D	92	0	0	2	0
All	All	15706	0	15134	196	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 6.

All (196) 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:486:LYS:O	1:B:487:LEU:HB2	1.54	1.06
1:A:292[B]:ASN:H	1:A:292[B]:ASN:ND2	1.61	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:CYS:HG	1:B:57:CYS:HG	1.03	0.93
1:A:73:LEU:HD23	1:B:73:LEU:HD23	1.58	0.86
1:A:440:ALA:HB3	1:B:440:ALA:HB3	1.57	0.86
1:B:224:ASN:HD22	1:B:252:ASN:HD21	1.23	0.83
1:A:9:VAL:HG13	1:A:157:LEU:HD23	1.60	0.81
1:A:292[B]:ASN:H	1:A:292[B]:ASN:HD22	0.86	0.79
1:C:366:VAL:HG13	1:C:372:ILE:HB	1.65	0.79
1:B:157:LEU:HD11	1:B:325:ILE:HG12	1.64	0.78
1:C:366:VAL:CG1	1:C:372:ILE:HB	2.14	0.77
1:B:332:LEU:HD13	1:B:337:VAL:HG21	1.67	0.76
1:A:73:LEU:HD23	1:B:73:LEU:CD2	2.14	0.75
1:C:440:ALA:HB3	1:D:440:ALA:HB3	1.69	0.75
1:B:304:THR:HB	1:B:305:PRO:HD2	1.68	0.75
1:B:75:GLU:HG2	1:B:404:SER:HB2	1.70	0.73
1:C:433:GLY:O	1:C:437:ILE:HG13	1.87	0.73
1:D:52:CYS:HG	1:D:57:CYS:HG	1.37	0.73
1:A:331:ARG:NH1	1:A:341:GLU:OE2	2.22	0.72
1:C:318:ASN:H	1:C:318:ASN:HD22	1.37	0.72
1:A:358:ASP:O	5:A:2098:HOH:O	2.06	0.72
1:B:486:LYS:O	1:B:487:LEU:CB	2.35	0.72
1:A:71:ASP:O	1:A:75:GLU:HG3	1.92	0.70
1:A:75:GLU:HB3	1:A:404:SER:HB2	1.73	0.69
1:A:129:LEU:HD23	1:A:299:VAL:HG21	1.76	0.67
1:C:160:THR:HG21	1:C:294:LEU:HD21	1.75	0.67
1:D:228:ARG:HD3	2:D:800:NDP:O3X	1.94	0.67
1:C:345:LEU:O	1:C:345:LEU:HG	1.93	0.66
1:B:321:ASN:OD1	1:B:321:ASN:N	2.28	0.65
1:B:250:MET:HE2	1:B:253:GLU:HG3	1.78	0.64
1:A:73:LEU:CD2	1:B:73:LEU:HD23	2.27	0.64
1:A:73:LEU:CD2	1:B:73:LEU:CD2	2.75	0.64
1:C:157:LEU:HD11	1:C:325:ILE:HG12	1.80	0.64
1:A:387:GLU:O	1:A:479:VAL:O	2.16	0.63
1:D:75:GLU:HB3	1:D:404:SER:HB2	1.81	0.63
1:A:241:GLN:OE1	1:A:370:PRO:HG3	1.97	0.63
1:B:160:THR:OG1	1:B:328:ILE:HD12	1.99	0.63
1:C:313:GLU:HB2	1:C:356:LYS:HD3	1.82	0.61
1:D:71:ASP:O	1:D:75:GLU:HG3	2.00	0.61
1:D:162:SER:HB3	1:D:327:ASP:HB3	1.82	0.60
1:D:130:GLU:HB2	1:D:136:VAL:CG2	2.31	0.60
1:A:157:LEU:HD11	1:A:325:ILE:HG12	1.83	0.60
1:B:234:ILE:O	1:B:238:VAL:HG12	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:TYR:CZ	1:B:472:ARG:HD3	2.36	0.60
1:C:341:GLU:OE2	1:C:359:HIS:HE1	1.85	0.60
1:C:299:VAL:HG23	1:C:301:VAL:HG23	1.84	0.60
1:D:189:ARG:HG3	1:D:212:PRO:HG2	1.84	0.59
1:D:8:VAL:HG23	1:D:153:ALA:HB2	1.84	0.59
1:D:89:LYS:HG3	1:D:90:ALA:N	2.16	0.59
1:A:155:HIS:HB3	1:A:323:TYR:HE2	1.66	0.59
1:B:126:TRP:O	1:B:137:VAL:HA	2.03	0.59
1:A:130:GLU:HB2	1:A:136:VAL:HG23	1.83	0.58
1:D:478:TYR:CE1	1:D:483:LYS:HB2	2.39	0.57
1:B:260:LEU:H	1:C:152:GLN:NE2	2.02	0.57
1:C:27:TYR:CE1	1:C:351:GLY:HA2	2.40	0.57
1:D:198:PHE:O	1:D:202:GLU:HG3	2.04	0.57
1:C:302:LYS:H	1:C:318:ASN:ND2	2.03	0.57
1:B:68:GLN:NE2	5:B:2011:HOH:O	2.36	0.57
1:C:292[B]:ASN:H	1:C:292[B]:ASN:ND2	2.01	0.57
1:D:157:LEU:HD13	1:D:345:LEU:HD22	1.86	0.56
1:C:224:ASN:HB2	1:C:252:ASN:HD21	1.70	0.56
1:B:250:MET:CE	1:B:253:GLU:HG3	2.35	0.56
1:A:390:ALA:HB3	1:A:417:THR:OG1	2.04	0.56
5:B:2053:HOH:O	1:C:1:MET:HG2	2.04	0.56
1:A:301:VAL:HA	1:A:318:ASN:HD21	1.71	0.56
1:C:40:HIS:ND1	1:C:183:TYR:OH	2.34	0.55
1:D:176:ILE:HB	1:D:180:GLU:HB2	1.88	0.55
1:A:332:LEU:HD13	1:A:337:VAL:HG21	1.89	0.55
1:B:260:LEU:HD12	1:C:152:GLN:HB3	1.89	0.55
1:C:52:CYS:SG	1:C:57:CYS:SG	3.05	0.55
1:D:130:GLU:HB2	1:D:136:VAL:HG23	1.88	0.55
1:D:101:GLU:O	1:D:101:GLU:HG3	2.06	0.55
1:B:224:ASN:HD22	1:B:252:ASN:ND2	2.00	0.54
1:A:52:CYS:CB	1:A:57:CYS:HG	2.20	0.54
1:B:72:HIS:HD2	5:B:2014:HOH:O	1.91	0.54
1:D:224:ASN:HD22	1:D:252:ASN:HD21	1.55	0.53
1:C:104:LEU:HG	1:C:108:LYS:HE3	1.90	0.53
1:C:239:THR:HG23	1:C:249:ILE:HD12	1.91	0.53
1:A:198:PHE:CZ	1:A:230:PHE:HZ	2.28	0.52
1:B:60:LYS:HE3	1:B:367:PHE:HB2	1.92	0.52
1:C:302:LYS:H	1:C:318:ASN:HD21	1.56	0.52
1:B:348:THR:HA	1:B:354:PRO:HA	1.91	0.52
1:C:461:HIS:HB2	1:D:336:PRO:HG3	1.90	0.52
1:A:421:ASP:O	1:A:450:LYS:HD3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:LEU:HD22	1:B:334:LEU:HG	1.91	0.52
1:B:411:PHE:CD1	1:B:431:GLY:HA3	2.45	0.52
1:C:95:LEU:HD22	1:C:210:TYR:CZ	2.45	0.52
5:C:2016:HOH:O	1:D:72:HIS:HD2	1.91	0.52
1:C:370:PRO:HG2	1:C:430:LEU:HD11	1.91	0.51
1:D:304:THR:HG22	1:D:310:GLN:NE2	2.24	0.51
1:B:131:SER:O	1:B:133:ASN:N	2.43	0.51
1:A:318:ASN:HD22	1:A:318:ASN:H	1.58	0.51
1:A:80:GLY:HA2	1:B:94:LYS:HG2	1.93	0.51
1:D:133:ASN:O	1:D:152:GLN:HA	2.11	0.51
1:A:9:VAL:CG1	1:A:157:LEU:HD23	2.37	0.50
1:A:60:LYS:HD2	1:A:60:LYS:C	2.32	0.50
1:B:224:ASN:ND2	1:B:252:ASN:HD21	2.01	0.50
1:D:69:TYR:O	1:D:73:LEU:HG	2.11	0.50
1:B:325:ILE:HD13	1:B:342:GLY:HA2	1.93	0.50
1:C:92:TRP:HB3	1:C:187:PRO:HD3	1.94	0.50
1:D:59:PRO:HB2	1:D:182:PHE:CE1	2.47	0.49
1:B:176:ILE:HB	1:B:180:GLU:HB2	1.94	0.49
1:B:260:LEU:H	1:C:152:GLN:HE22	1.59	0.49
1:C:429:LEU:HD21	1:C:468:LEU:HD21	1.94	0.49
1:B:34:VAL:HG12	3:B:998:FAD:H2A	1.95	0.49
1:C:417:THR:HG21	1:C:451:ILE:HB	1.95	0.49
1:C:157:LEU:HD13	1:C:345:LEU:HD22	1.94	0.49
1:D:157:LEU:HD11	1:D:325:ILE:HG12	1.95	0.49
1:A:403:ILE:HD12	1:B:62:LEU:HD13	1.95	0.48
1:A:289:PRO:HG3	1:A:330:ASP:HB2	1.95	0.48
1:B:417:THR:HG21	1:B:451:ILE:HB	1.94	0.48
1:C:329:THR:OG1	1:C:331:ARG:HD2	2.14	0.48
1:A:7:LEU:HA	1:A:155:HIS:O	2.14	0.47
1:A:126:TRP:CD1	1:A:140:THR:HA	2.49	0.47
1:C:192:LEU:HD11	1:C:220:CYS:SG	2.54	0.47
1:B:59:PRO:HB3	1:B:99:LYS:HD3	1.97	0.47
1:C:126:TRP:CD1	1:C:140:THR:HA	2.50	0.47
1:C:366:VAL:HG11	1:C:372:ILE:HD12	1.97	0.47
1:C:459:GLY:O	1:D:336:PRO:HG2	2.14	0.47
1:A:459:GLY:HA2	1:B:439:GLN:OE1	2.15	0.47
1:A:17:LEU:HD23	1:A:17:LEU:HA	1.75	0.46
1:B:314:PHE:O	1:B:315:SER:HB2	2.15	0.46
1:D:463:THR:O	1:D:466:GLU:HG2	2.14	0.46
1:B:325:ILE:HD13	1:B:342:GLY:CA	2.45	0.46
1:C:129:LEU:HD23	1:C:299:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:VAL:HA	1:C:318:ASN:HD21	1.80	0.46
1:A:63:MET:HG2	1:A:95:LEU:HD21	1.98	0.46
1:D:56:GLY:O	1:D:59:PRO:HD2	2.16	0.46
1:C:51:THR:O	1:C:52:CYS:C	2.54	0.45
1:C:212:PRO:CB	1:C:213:PRO:HD2	2.46	0.45
1:C:29:LYS:HA	1:C:29:LYS:HD3	1.79	0.45
1:C:268:VAL:O	1:C:275:THR:HA	2.17	0.45
1:A:52:CYS:SG	1:A:57:CYS:SG	3.12	0.45
1:C:64:VAL:HG23	1:C:206:ILE:HD11	1.98	0.45
1:A:330:ASP:O	1:A:330:ASP:CG	2.54	0.45
1:C:52:CYS:CB	1:C:57:CYS:HG	2.29	0.45
1:C:464:SER:O	1:C:467:GLU:HB2	2.17	0.45
1:B:201:VAL:HG21	1:B:227:LEU:HD11	1.99	0.44
1:C:227:LEU:O	1:C:230:PHE:HB2	2.16	0.44
1:A:130:GLU:HB2	1:A:136:VAL:CG2	2.47	0.44
1:A:160:THR:OG1	1:A:328:ILE:HD12	2.17	0.44
1:D:30:ARG:NE	5:D:2001:HOH:O	2.38	0.44
1:B:189:ARG:HA	1:B:212:PRO:HD2	1.99	0.43
1:B:56:GLY:HA2	3:B:998:FAD:C7	2.49	0.43
1:D:8:VAL:CG2	1:D:153:ALA:HB2	2.48	0.43
1:D:352:ASN:HD22	1:D:352:ASN:C	2.21	0.43
1:C:318:ASN:HD22	1:C:318:ASN:N	2.11	0.43
1:C:387:GLU:HG2	5:C:2102:HOH:O	2.18	0.43
1:D:30:ARG:NH1	5:D:2001:HOH:O	2.32	0.43
1:A:424:VAL:HG21	1:A:454:PHE:CE2	2.53	0.43
1:A:88:VAL:HG22	1:B:83:PHE:HB3	2.01	0.43
1:A:455:TYR:CZ	1:A:472:ARG:HD2	2.54	0.43
1:B:412:VAL:O	1:B:429:LEU:HA	2.18	0.43
1:C:129:LEU:HD22	1:C:296:LEU:HD23	2.00	0.43
1:C:394:SER:OG	1:C:467:GLU:HG3	2.18	0.43
1:A:424:VAL:HG21	1:A:454:PHE:HE2	1.83	0.43
1:D:158:LEU:HD22	1:D:294:LEU:HD22	2.01	0.43
1:A:232:GLU:O	1:A:236:GLU:HG3	2.19	0.42
1:D:319:VAL:HA	1:D:320:PRO:HD2	1.71	0.42
1:D:392:TYR:O	1:D:414:LYS:HA	2.18	0.42
1:A:158:LEU:HD22	1:A:294:LEU:HD13	2.00	0.42
1:A:402:ASN:HA	1:A:407:LYS:HE2	2.00	0.42
1:B:56:GLY:O	1:B:59:PRO:HD2	2.19	0.42
1:A:478:TYR:HA	1:A:482:GLU:O	2.20	0.42
1:D:45:TYR:HB3	1:D:55:VAL:HG11	2.00	0.42
1:C:241:GLN:OE1	1:C:370:PRO:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:CYS:O	1:A:426:GLY:HA2	2.20	0.42
1:C:35:ASP:HA	3:C:998:FAD:N3A	2.35	0.42
1:B:60:LYS:HD3	1:B:202:GLU:OE1	2.20	0.41
1:B:476:TYR:HE2	1:B:478:TYR:HE2	1.67	0.41
1:D:171:GLY:HA3	1:D:258:VAL:O	2.19	0.41
1:B:378:ILE:HG12	5:B:2076:HOH:O	2.20	0.41
1:C:473:THR:HA	1:C:474:PRO:HD3	1.91	0.41
1:A:144:LYS:HB2	1:A:144:LYS:HE2	1.46	0.41
1:A:8:VAL:HG23	1:A:153:ALA:HB2	2.02	0.41
1:A:347:ASP:O	1:A:351:GLY:HA3	2.20	0.41
1:A:56:GLY:O	1:A:57:CYS:C	2.59	0.41
1:B:92:TRP:CZ2	1:B:96:ILE:HD11	2.55	0.41
1:B:370:PRO:HG2	1:B:430:LEU:HD11	2.01	0.41
1:D:129:LEU:HD22	1:D:296:LEU:HD23	2.03	0.41
1:D:421:ASP:OD1	1:D:421:ASP:C	2.59	0.41
1:C:303:LEU:HD23	1:C:309:VAL:HA	2.03	0.41
1:C:318:ASN:H	1:C:318:ASN:ND2	2.11	0.41
1:B:51:THR:O	1:B:52:CYS:C	2.58	0.41
1:B:174:HIS:HB3	1:B:266:LYS:HD2	2.03	0.41
1:D:417:THR:HG21	1:D:451:ILE:HB	2.02	0.41
1:D:486:LYS:HA	1:D:486:LYS:HD3	1.83	0.41
3:D:998:FAD:H1'1	3:D:998:FAD:H9	1.80	0.40
1:C:159:ALA:O	3:C:998:FAD:H52A	2.21	0.40
1:D:183:TYR:O	1:D:184:LEU:C	2.57	0.40
1:D:4:ALA:HA	1:D:152:GLN:HG3	2.03	0.40
1:D:139:GLU:HG3	1:D:146:ALA:HB3	2.02	0.40
1:D:161:GLY:HA2	1:D:327:ASP:HB2	2.03	0.40
2:A:800:NDP:H41N	3:A:998:FAD:N5	2.37	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	490/495 (99%)	474 (97%)	14 (3%)	2 (0%)	34	54
1	B	484/495 (98%)	459 (95%)	19 (4%)	6 (1%)	13	24
1	C	490/495 (99%)	470 (96%)	18 (4%)	2 (0%)	34	54
1	D	485/495 (98%)	469 (97%)	12 (2%)	4 (1%)	19	35
All	All	1949/1980 (98%)	1872 (96%)	63 (3%)	14 (1%)	22	39

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	132	LYS
1	D	132	LYS
1	B	320	PRO
1	A	48	LEU
1	B	45	TYR
1	C	213	PRO
1	D	45	TYR
1	B	367	PHE
1	B	146	ALA
1	B	147	VAL
1	C	55	VAL
1	D	55	VAL
1	A	55	VAL
1	D	320	PRO

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	405/407 (100%)	388 (96%)	17 (4%)	30	54
1	B	399/407 (98%)	386 (97%)	13 (3%)	38	64
1	C	405/407 (100%)	382 (94%)	23 (6%)	20	39
1	D	399/407 (98%)	372 (93%)	27 (7%)	16	30
All	All	1608/1628 (99%)	1528 (95%)	80 (5%)	25	46

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	55	VAL
1	A	57	CYS
1	A	60	LYS
1	A	94	LYS
1	A	99	LYS
1	A	144	LYS
1	A	219	LEU
1	A	238	VAL
1	A	288	ILE
1	A	318	ASN
1	A	331	ARG
1	A	332	LEU
1	A	345	LEU
1	A	396	PHE
1	A	407	LYS
1	A	486	LYS
1	B	60	LYS
1	B	128	SER
1	B	129	LEU
1	B	136	VAL
1	B	144	LYS
1	B	152	GLN
1	B	260	LEU
1	B	290	ARG
1	B	292	ASN
1	B	320	PRO
1	B	323	TYR
1	B	332	LEU
1	B	353	LYS
1	C	-1	SER
1	C	30	ARG
1	C	60	LYS
1	C	94	LYS
1	C	99	LYS
1	C	224	ASN
1	C	236	GLU
1	C	266	LYS
1	C	274	LYS
1	C	292[A]	ASN
1	C	292[B]	ASN
1	C	318	ASN

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Mol	Chain	Res	Type
1	C	321	ASN
1	C	322	ILE
1	C	323	TYR
1	C	325	ILE
1	C	331	ARG
1	C	332	LEU
1	C	335	THR
1	C	353	LYS
1	C	366	VAL
1	C	387	GLU
1	C	467	GLU
1	D	2	SER
1	D	57	CYS
1	D	94	LYS
1	D	99	LYS
1	D	101	GLU
1	D	128	SER
1	D	144	LYS
1	D	151	LEU
1	D	152	GLN
1	D	185	PRO
1	D	186	GLU
1	D	189	ARG
1	D	200	SER
1	D	222	ARG
1	D	231	ASP
1	D	238	VAL
1	D	250	MET
1	D	260	LEU
1	D	262	THR
1	D	292	ASN
1	D	306	LYS
1	D	325	ILE
1	D	332	LEU
1	D	352	ASN
1	D	446	ARG
1	D	450	LYS
1	D	487	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	A	224	ASN
1	A	318	ASN
1	A	402	ASN
1	B	72	HIS
1	B	107	ASN
1	B	133	ASN
1	B	174	HIS
1	B	252	ASN
1	B	359	HIS
1	C	68	GLN
1	C	115	ASN
1	C	152	GLN
1	C	252	ASN
1	C	318	ASN
1	C	321	ASN
1	C	359	HIS
1	D	72	HIS
1	D	107	ASN
1	D	224	ASN
1	D	310	GLN
1	D	352	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)

Of 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 for Mogul analysis.

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	NDP	C	800	-	45,52,52	1.68	8 (17%)	53,80,80	1.38	6 (11%)
3	FAD	C	998	-	53,58,58	1.46	7 (13%)	68,89,89	1.66	13 (19%)
3	FAD	D	998	-	53,58,58	1.30	8 (15%)	68,89,89	1.46	9 (13%)
3	FAD	A	998	-	53,58,58	1.11	4 (7%)	68,89,89	1.50	11 (16%)
3	FAD	B	998	-	53,58,58	1.36	6 (11%)	68,89,89	1.48	14 (20%)
2	NDP	A	800	-	45,52,52	1.74	12 (26%)	53,80,80	1.30	5 (9%)
2	NDP	D	800	-	45,52,52	1.55	7 (15%)	53,80,80	1.47	7 (13%)
2	NDP	B	800	-	45,52,52	1.65	11 (24%)	53,80,80	1.47	7 (13%)

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	NDP	C	800	-	-	5/30/77/77	0/5/5/5
3	FAD	C	998	-	-	2/30/50/50	0/6/6/6
3	FAD	D	998	-	-	5/30/50/50	0/6/6/6
3	FAD	A	998	-	-	5/30/50/50	0/6/6/6
3	FAD	B	998	-	-	8/30/50/50	0/6/6/6
2	NDP	A	800	-	-	5/30/77/77	0/5/5/5
2	NDP	D	800	-	-	4/30/77/77	0/5/5/5
2	NDP	B	800	-	-	6/30/77/77	0/5/5/5

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	800	NDP	PN-O1N	5.17	1.69	1.50
3	C	998	FAD	C2A-N3A	4.99	1.40	1.32
2	A	800	NDP	C6N-C5N	4.88	1.42	1.33
2	C	800	NDP	P2B-O1X	4.57	1.65	1.50
3	B	998	FAD	C2A-N3A	4.55	1.39	1.32
3	C	998	FAD	C4X-N5	4.51	1.39	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	NDP	PN-O1N	4.04	1.65	1.50
2	B	800	NDP	C6N-C5N	4.00	1.40	1.33
2	D	800	NDP	PA-O1A	3.99	1.65	1.50
2	D	800	NDP	C6N-C5N	3.95	1.40	1.33
3	D	998	FAD	C4X-N5	3.88	1.38	1.30
2	A	800	NDP	O4D-C1D	3.83	1.51	1.42
3	D	998	FAD	C2A-N3A	3.69	1.38	1.32
2	C	800	NDP	C6N-C5N	3.65	1.39	1.33
3	B	998	FAD	C4X-N5	3.60	1.37	1.30
2	B	800	NDP	C4N-C3N	3.50	1.56	1.49
3	B	998	FAD	C10-N1	3.48	1.40	1.33
2	A	800	NDP	PA-O1A	3.37	1.62	1.50
2	C	800	NDP	C4N-C5N	-3.29	1.40	1.48
2	C	800	NDP	PA-O1A	3.21	1.62	1.50
3	A	998	FAD	C2A-N3A	3.18	1.37	1.32
2	B	800	NDP	P2B-O2B	3.17	1.65	1.59
2	B	800	NDP	C4N-C5N	-3.06	1.40	1.48
2	A	800	NDP	C4N-C5N	-3.03	1.41	1.48
2	B	800	NDP	PN-O1N	2.95	1.61	1.50
2	B	800	NDP	P2B-O3X	-2.92	1.43	1.54
3	B	998	FAD	C5'-C4'	2.88	1.55	1.51
2	A	800	NDP	C4N-C3N	2.84	1.55	1.49
2	B	800	NDP	C7N-C3N	2.82	1.54	1.48
2	D	800	NDP	C4N-C5N	-2.81	1.41	1.48
3	D	998	FAD	C2A-N1A	2.77	1.39	1.33
3	A	998	FAD	C2B-C1B	-2.77	1.49	1.53
3	C	998	FAD	C2A-N1A	2.69	1.38	1.33
3	D	998	FAD	C10-N1	2.67	1.38	1.33
2	B	800	NDP	O4D-C1D	2.66	1.48	1.42
2	C	800	NDP	O4D-C1D	2.65	1.48	1.42
3	C	998	FAD	C10-N1	2.64	1.38	1.33
2	D	800	NDP	O4D-C4D	2.58	1.50	1.45
3	D	998	FAD	C5'-C4'	2.58	1.55	1.51
2	D	800	NDP	PN-O1N	2.55	1.60	1.50
3	A	998	FAD	C10-N1	2.53	1.38	1.33
2	D	800	NDP	P2B-O3X	-2.53	1.45	1.54
2	B	800	NDP	O4D-C4D	2.52	1.50	1.45
2	A	800	NDP	P2B-O1X	2.49	1.58	1.50
2	D	800	NDP	C7N-C3N	2.42	1.53	1.48
2	A	800	NDP	P2B-O3X	-2.41	1.45	1.54
3	A	998	FAD	C2A-N1A	2.39	1.38	1.33
3	C	998	FAD	O4B-C4B	-2.37	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	998	FAD	C2A-N1A	2.37	1.38	1.33
3	C	998	FAD	C2B-C1B	-2.37	1.50	1.53
3	C	998	FAD	C4X-C10	-2.31	1.37	1.44
3	B	998	FAD	C4X-C10	-2.22	1.37	1.44
2	C	800	NDP	P2B-O3X	-2.21	1.46	1.54
2	A	800	NDP	O4B-C1B	2.18	1.44	1.41
3	D	998	FAD	C4X-C10	-2.16	1.37	1.44
2	B	800	NDP	PA-O1A	2.14	1.58	1.50
2	C	800	NDP	PN-O5D	2.10	1.67	1.59
3	D	998	FAD	C1'-N10	2.10	1.53	1.48
2	A	800	NDP	C2N-C3N	2.07	1.40	1.34
3	D	998	FAD	O4-C4	2.07	1.27	1.23
2	A	800	NDP	C5A-N7A	-2.06	1.32	1.39
2	A	800	NDP	P2B-O2B	2.06	1.63	1.59
2	B	800	NDP	C6N-N1N	2.03	1.42	1.37

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	998	FAD	N3A-C2A-N1A	-6.32	118.80	128.68
3	A	998	FAD	N3A-C2A-N1A	-5.19	120.56	128.68
2	C	800	NDP	O4D-C1D-N1N	5.08	117.99	108.06
2	B	800	NDP	O4D-C1D-N1N	4.75	117.35	108.06
2	D	800	NDP	N3A-C2A-N1A	-4.69	121.35	128.68
3	B	998	FAD	N3A-C2A-N1A	-4.60	121.48	128.68
2	A	800	NDP	O4D-C1D-N1N	4.26	116.38	108.06
2	D	800	NDP	C2D-C1D-N1N	-4.17	102.86	113.30
2	A	800	NDP	N3A-C2A-N1A	-4.11	122.26	128.68
2	B	800	NDP	N3A-C2A-N1A	-4.09	122.28	128.68
3	C	998	FAD	O4B-C1B-C2B	-4.03	101.03	106.93
3	C	998	FAD	C4A-C5A-N7A	-3.98	105.25	109.40
3	C	998	FAD	O3B-C3B-C4B	-3.84	99.94	111.05
3	C	998	FAD	C9A-C5X-N5	-3.79	118.31	122.43
3	C	998	FAD	N3A-C2A-N1A	-3.64	123.00	128.68
3	C	998	FAD	C4-N3-C2	-3.53	119.12	125.64
3	D	998	FAD	P-O3P-PA	-3.52	120.76	132.83
3	B	998	FAD	C9A-C5X-N5	-3.46	118.68	122.43
3	D	998	FAD	C4X-C10-N10	3.45	121.53	116.48
3	A	998	FAD	C4-N3-C2	-3.45	119.27	125.64
3	C	998	FAD	C10-C4X-N5	-3.34	117.76	124.86
2	B	800	NDP	C3N-C7N-N7N	-3.15	112.06	117.67
2	D	800	NDP	O4D-C1D-N1N	3.14	114.19	108.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	998	FAD	C9A-C5X-N5	-3.09	119.07	122.43
3	C	998	FAD	C4X-C10-N10	3.08	120.99	116.48
3	A	998	FAD	C4X-C10-N10	2.98	120.84	116.48
2	C	800	NDP	N3A-C2A-N1A	-2.92	124.12	128.68
2	C	800	NDP	O3B-C3B-C4B	-2.89	102.71	111.05
3	C	998	FAD	C4-C4X-N5	2.80	122.22	118.23
2	C	800	NDP	O5D-PN-O1N	-2.76	98.28	109.07
3	C	998	FAD	C5X-N5-C4X	2.75	122.65	118.07
3	B	998	FAD	P-O3P-PA	-2.73	123.47	132.83
3	A	998	FAD	C1B-N9A-C4A	-2.72	121.86	126.64
3	D	998	FAD	C4-N3-C2	-2.66	120.72	125.64
3	B	998	FAD	C4A-C5A-N7A	-2.66	106.63	109.40
3	A	998	FAD	C4X-C10-N1	-2.65	118.59	124.73
3	B	998	FAD	C4X-C10-N10	2.61	120.30	116.48
3	D	998	FAD	C10-C4X-N5	-2.60	119.35	124.86
3	C	998	FAD	C4X-C4-N3	2.60	119.78	113.19
3	A	998	FAD	C4X-C4-N3	2.59	119.78	113.19
2	B	800	NDP	C2D-C1D-N1N	-2.54	106.94	113.30
2	D	800	NDP	C4A-C5A-N7A	-2.51	106.79	109.40
2	B	800	NDP	C3N-C2N-N1N	-2.49	119.54	123.10
3	B	998	FAD	C4-N3-C2	-2.45	121.11	125.64
2	D	800	NDP	C5D-C4D-C3D	-2.45	106.00	115.18
3	B	998	FAD	C10-C4X-N5	-2.42	119.72	124.86
3	A	998	FAD	C4-C4X-C10	2.42	120.85	116.79
2	C	800	NDP	O2B-C2B-C1B	-2.41	101.44	110.10
3	A	998	FAD	C10-C4X-N5	-2.40	119.76	124.86
3	D	998	FAD	C4X-C4-N3	2.38	119.24	113.19
3	C	998	FAD	C4X-C10-N1	-2.36	119.25	124.73
2	A	800	NDP	O3X-P2B-O2B	2.34	116.48	105.99
3	A	998	FAD	O3B-C3B-C4B	-2.31	104.36	111.05
3	B	998	FAD	C4X-C4-N3	2.30	119.02	113.19
3	A	998	FAD	C5X-C9A-N10	2.28	120.31	117.95
3	D	998	FAD	C4X-C10-N1	-2.27	119.47	124.73
2	C	800	NDP	C2D-C1D-N1N	-2.25	107.66	113.30
3	B	998	FAD	C5X-N5-C4X	2.25	121.81	118.07
3	B	998	FAD	O3'-C3'-C4'	2.22	114.17	108.81
3	B	998	FAD	C5X-C9A-N10	2.19	120.21	117.95
2	A	800	NDP	O2B-P2B-O1X	-2.14	101.14	109.39
3	B	998	FAD	C4-C4X-C10	2.11	120.34	116.79
2	B	800	NDP	C4A-C5A-N7A	-2.11	107.20	109.40
3	D	998	FAD	C1B-N9A-C4A	-2.09	122.96	126.64
3	B	998	FAD	C4X-C10-N1	-2.08	119.89	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	998	FAD	C4-C4X-C10	2.08	120.29	116.79
2	D	800	NDP	C5A-C6A-N6A	2.04	123.45	120.35
3	C	998	FAD	C10-N1-C2	2.04	120.97	116.90
3	B	998	FAD	O4B-C1B-C2B	-2.03	103.96	106.93
2	B	800	NDP	PN-O3-PA	-2.02	125.89	132.83
2	D	800	NDP	O3X-P2B-O2X	2.01	115.31	107.64
2	A	800	NDP	C3N-C2N-N1N	-2.01	120.23	123.10

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	800	NDP	C2B-O2B-P2B-O1X
2	B	800	NDP	C5D-O5D-PN-O3
2	C	800	NDP	C2B-O2B-P2B-O1X
2	D	800	NDP	C2B-O2B-P2B-O1X
3	A	998	FAD	PA-O3P-P-O5'
3	B	998	FAD	O4'-C4'-C5'-O5'
3	B	998	FAD	C5'-O5'-P-O2P
2	A	800	NDP	O4D-C1D-N1N-C2N
2	B	800	NDP	O4D-C1D-N1N-C2N
2	C	800	NDP	O4D-C1D-N1N-C2N
2	D	800	NDP	O4D-C1D-N1N-C2N
3	A	998	FAD	O4B-C4B-C5B-O5B
3	A	998	FAD	C3B-C4B-C5B-O5B
3	B	998	FAD	PA-O3P-P-O5'
3	C	998	FAD	PA-O3P-P-O5'
2	A	800	NDP	C5D-O5D-PN-O3
2	C	800	NDP	C2B-O2B-P2B-O3X
2	D	800	NDP	C5D-O5D-PN-O3
3	B	998	FAD	C5'-O5'-P-O3P
3	A	998	FAD	P-O3P-PA-O1A
2	B	800	NDP	C5D-O5D-PN-O1N
2	B	800	NDP	C5D-O5D-PN-O2N
3	B	998	FAD	C5'-O5'-P-O1P
3	D	998	FAD	P-O3P-PA-O2A
3	D	998	FAD	O4B-C4B-C5B-O5B
3	A	998	FAD	P-O3P-PA-O2A
3	D	998	FAD	PA-O3P-P-O5'
3	D	998	FAD	C3B-C4B-C5B-O5B
2	B	800	NDP	C2B-O2B-P2B-O1X
2	A	800	NDP	C2B-O2B-P2B-O3X

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Mol	Chain	Res	Type	Atoms
2	A	800	NDP	O4B-C4B-C5B-O5B
2	C	800	NDP	PA-O3-PN-O1N
3	B	998	FAD	P-O3P-PA-O1A
3	B	998	FAD	P-O3P-PA-O2A
3	D	998	FAD	P-O3P-PA-O1A
2	B	800	NDP	O4B-C4B-C5B-O5B
2	C	800	NDP	O4B-C4B-C5B-O5B
2	D	800	NDP	O4B-C4B-C5B-O5B
3	B	998	FAD	O4B-C4B-C5B-O5B
3	C	998	FAD	O4B-C4B-C5B-O5B

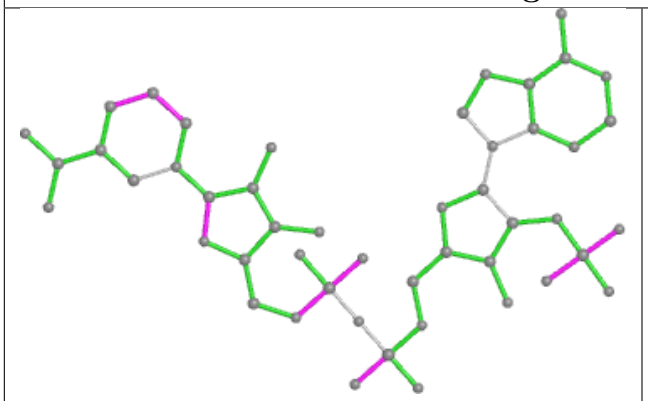
There are no ring outliers.

6 monomers are involved in 7 short contacts:

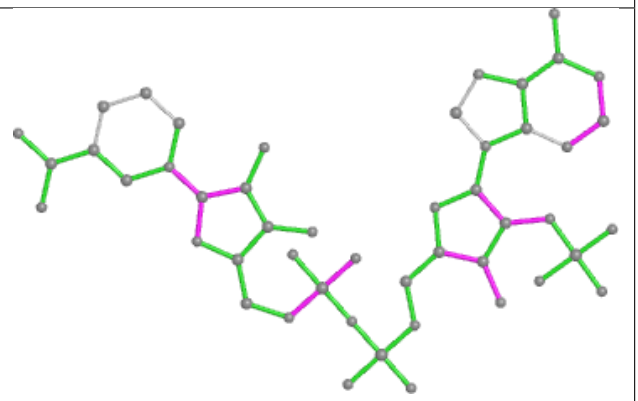
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	998	FAD	2	0
3	D	998	FAD	1	0
3	A	998	FAD	1	0
3	B	998	FAD	2	0
2	A	800	NDP	1	0
2	D	800	NDP	1	0

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 NDP C 800



Bond lengths



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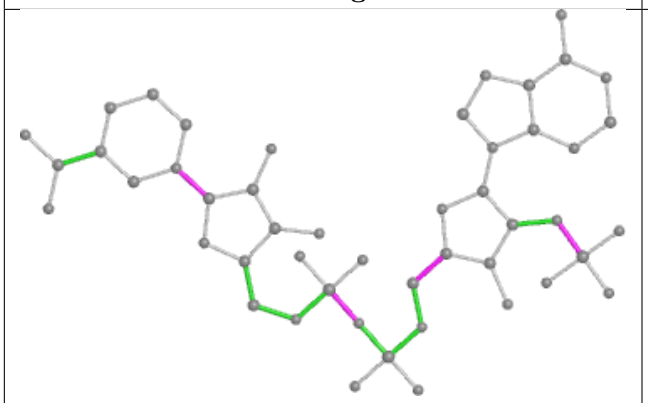
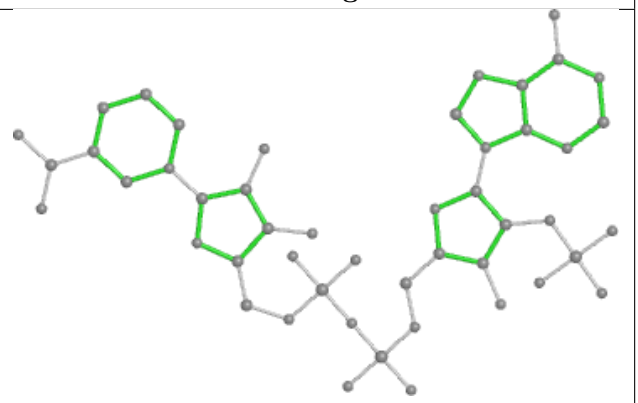
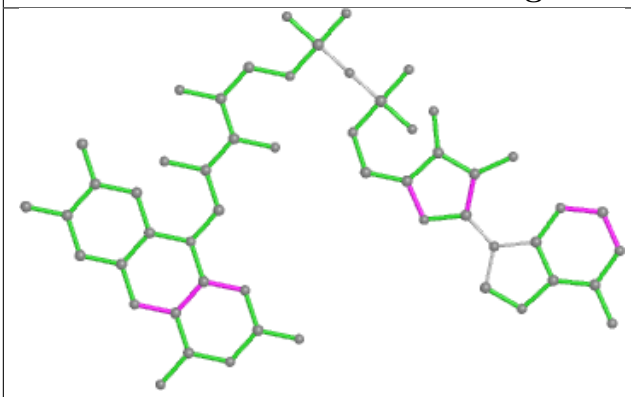


Torsions



Rings

Ligand FAD C 998



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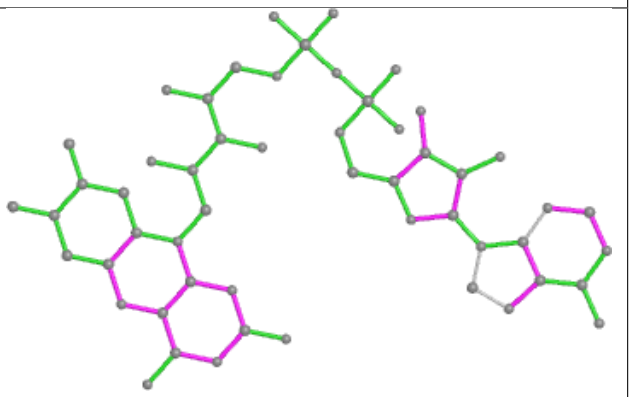

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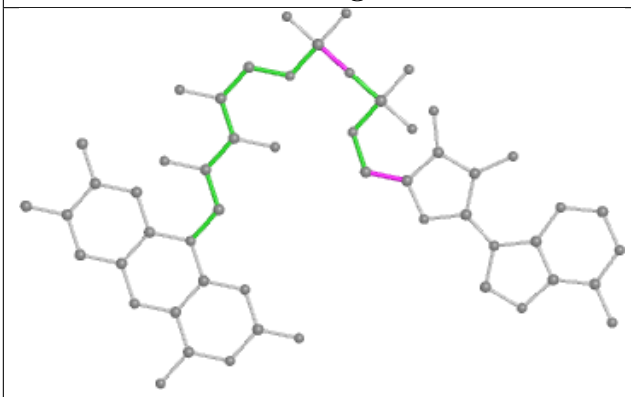

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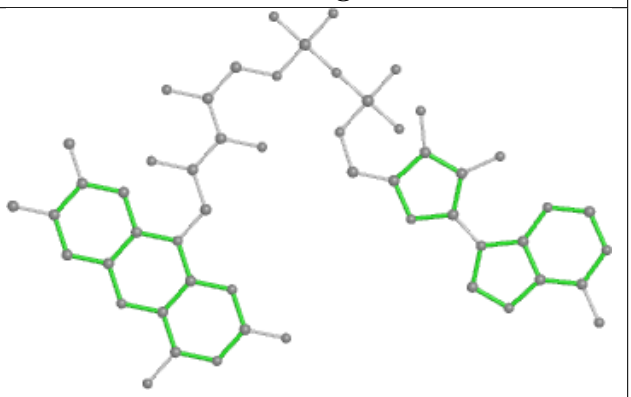

Rings

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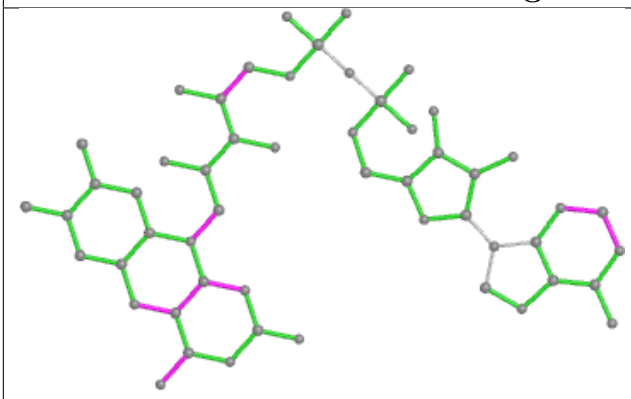
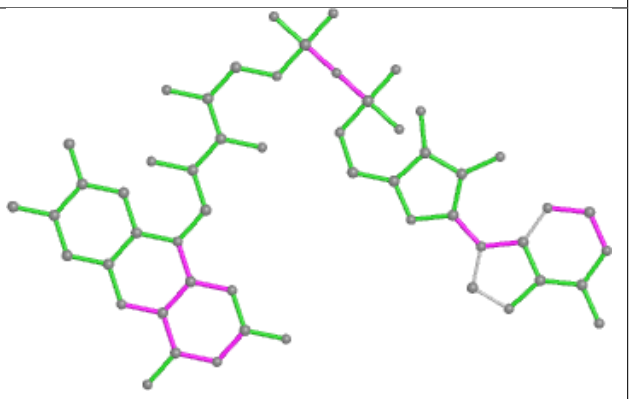
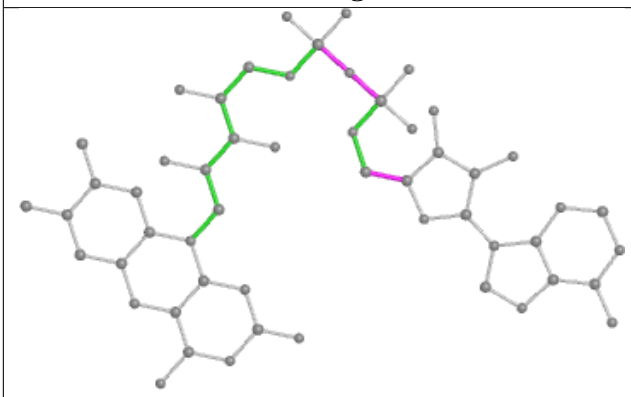
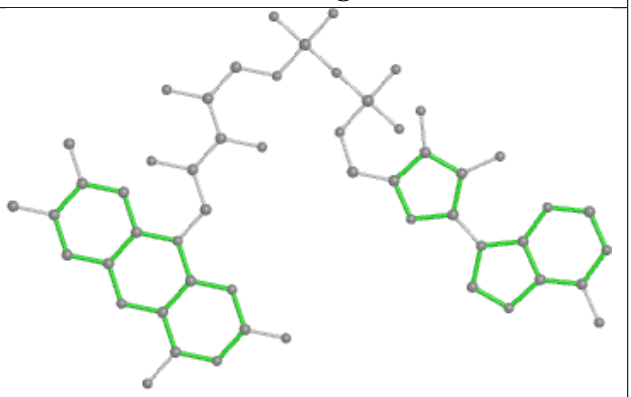
 Bond lengths	 Bond angles
 Torsions	 Rings

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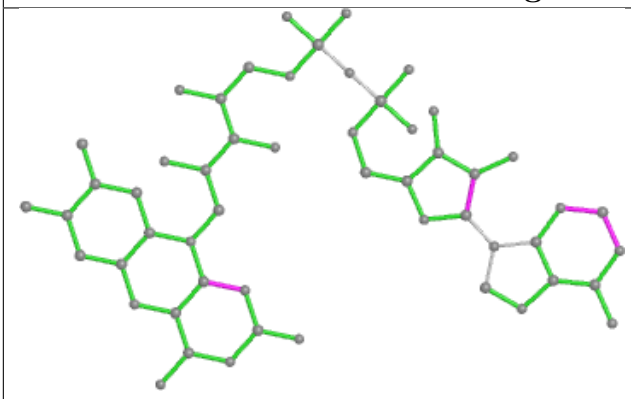

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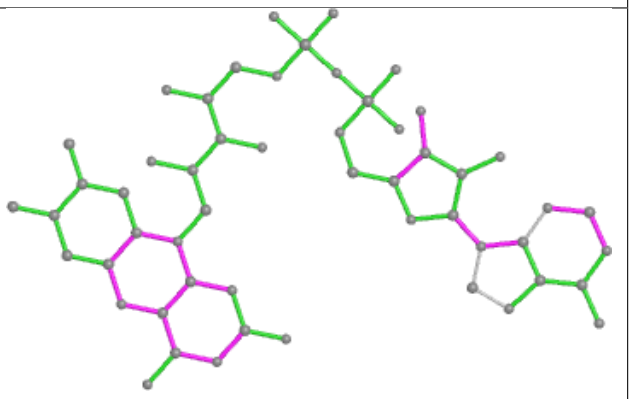
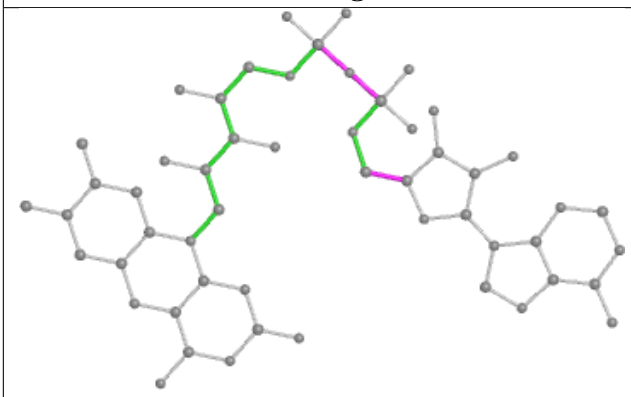


Bond angles



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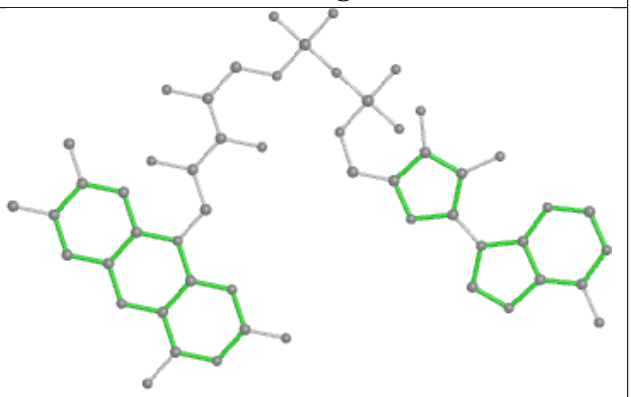
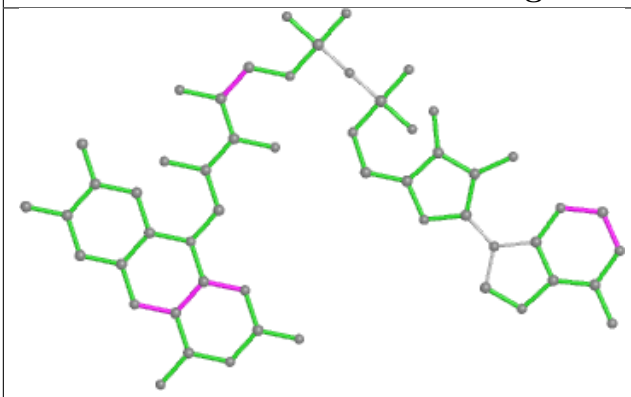


Rings

Ligand FAD B 998



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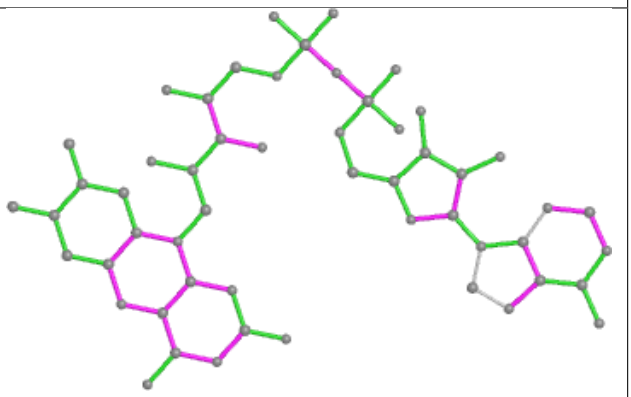
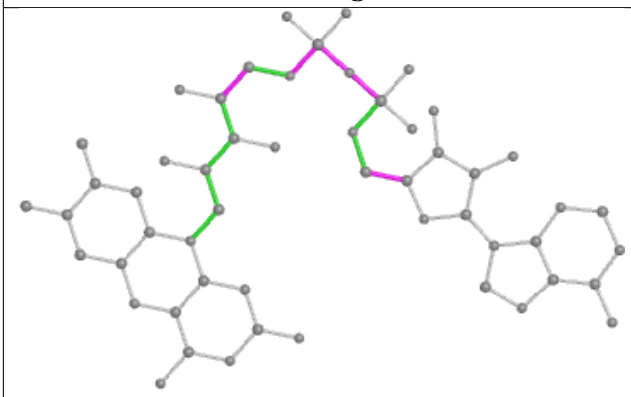


Bond angles



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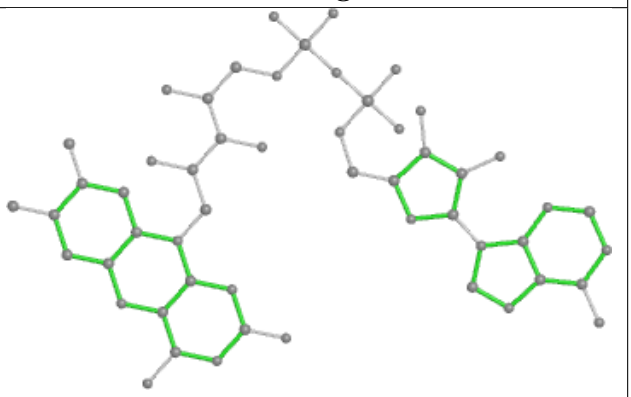
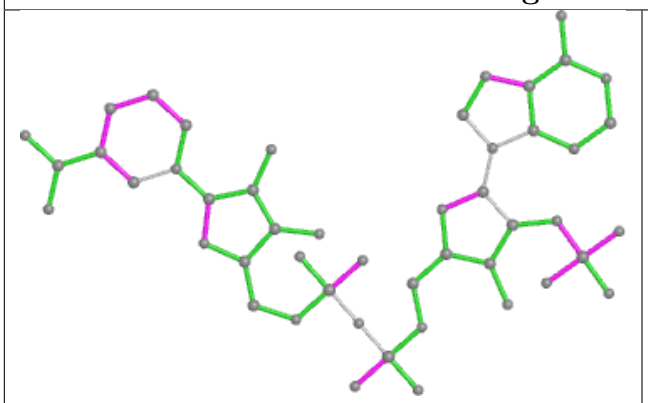


Rings

Ligand NDP A 800



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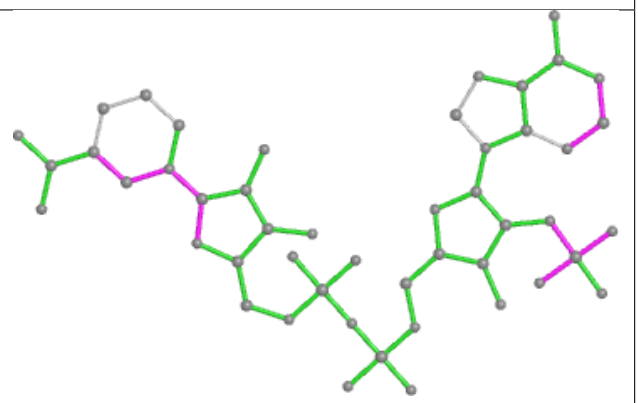
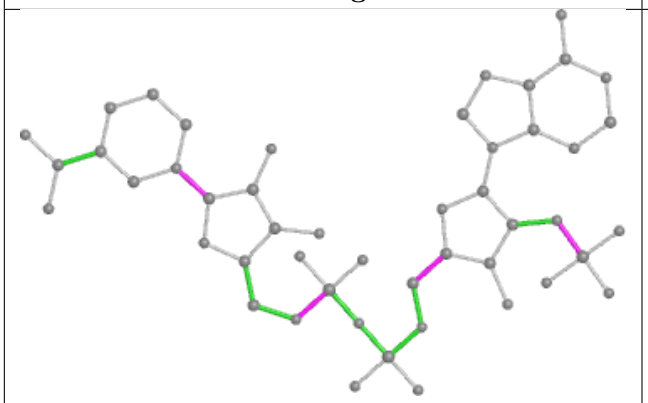
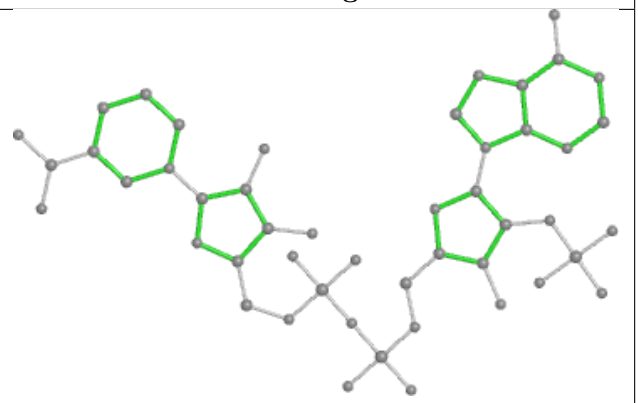


Bond angles

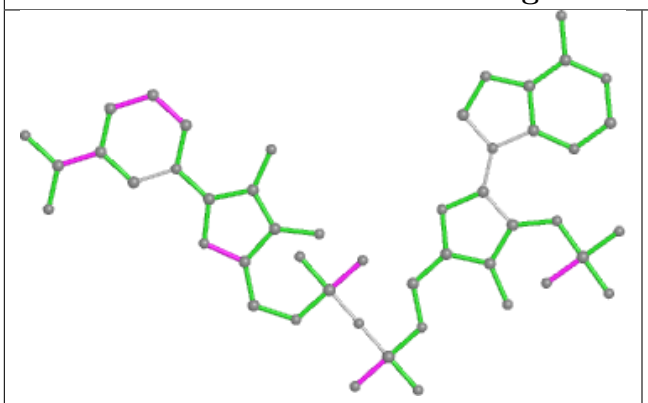


Torsions

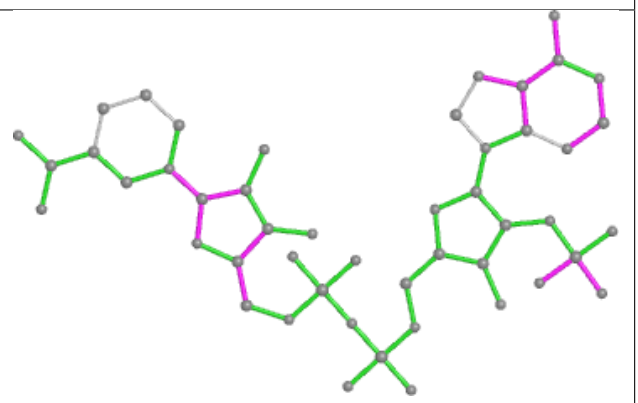


Rings

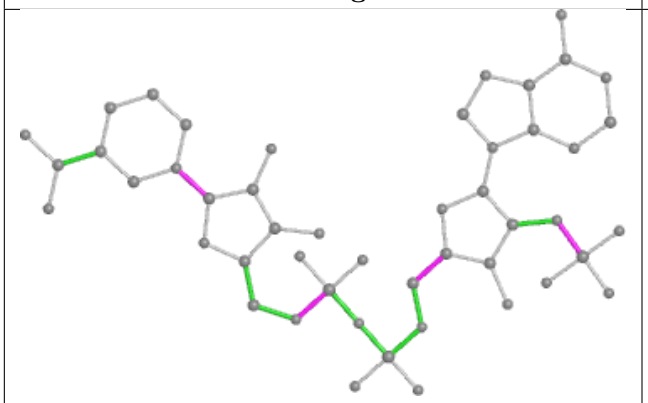
Ligand NDP D 800



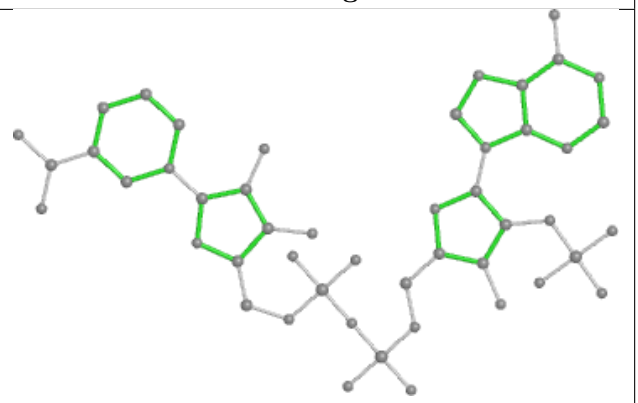
Bond lengths



Bond angles

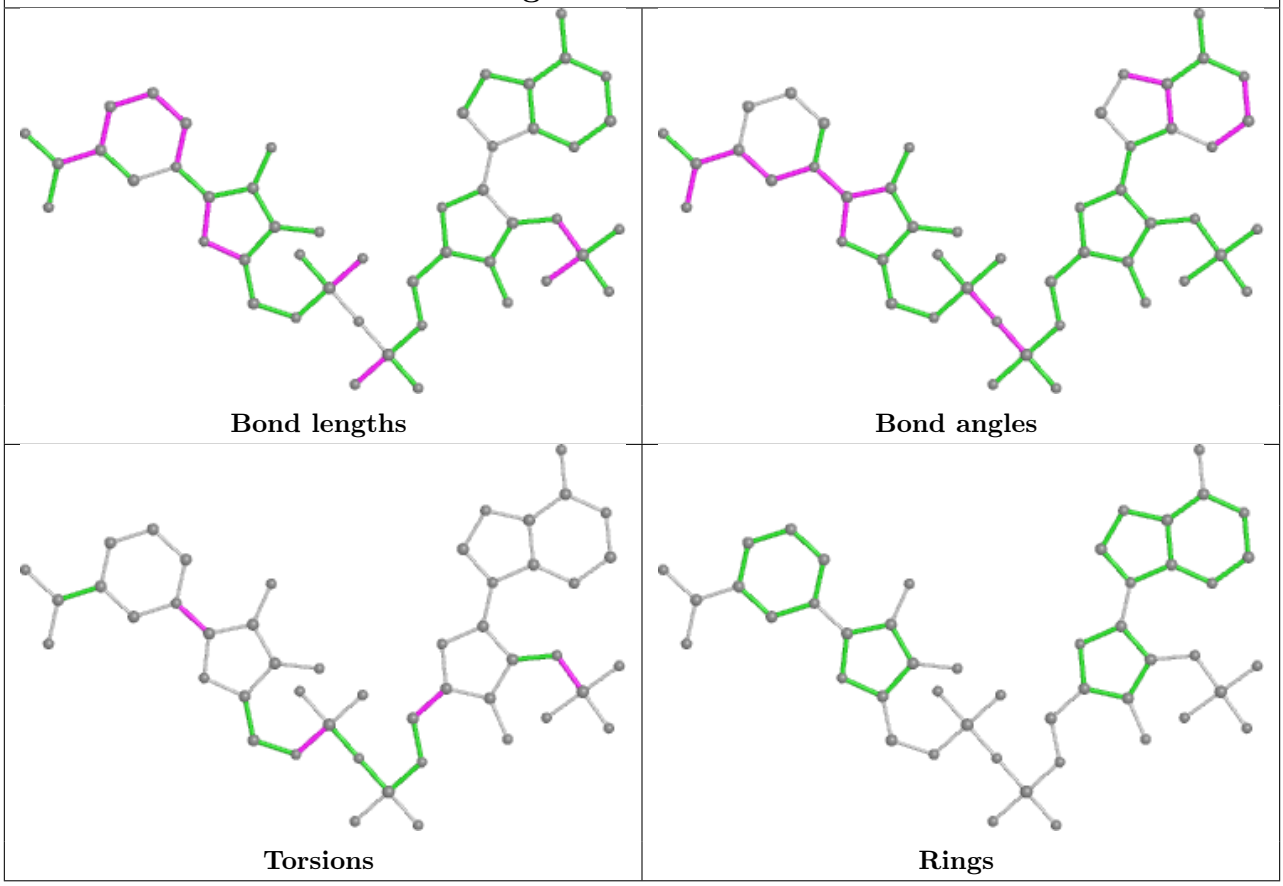


Torsions



Rings

Ligand NDP B 800



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	490/495 (98%)	-0.45	4 (0%)	86	87	13, 24, 41, 55	2 (0%)
1	B	486/495 (98%)	-0.33	5 (1%)	82	84	16, 29, 51, 66	0
1	C	490/495 (98%)	-0.49	1 (0%)	95	95	14, 24, 38, 50	0
1	D	487/495 (98%)	-0.38	5 (1%)	82	84	15, 26, 47, 59	1 (0%)
All	All	1953/1980 (98%)	-0.41	15 (0%)	86	87	13, 25, 47, 66	3 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	SER	5.2
1	B	352	ASN	3.8
1	B	354	PRO	3.3
1	B	320	PRO	3.2
1	A	352	ASN	3.1
1	D	352	ASN	3.1
1	B	144	LYS	2.8
1	A	353	LYS	2.7
1	A	306	LYS	2.7
1	D	305	PRO	2.3
1	B	305	PRO	2.2
1	C	305	PRO	2.1
1	D	420	SER	2.0
1	D	150	ARG	2.0
1	A	396	PHE	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)

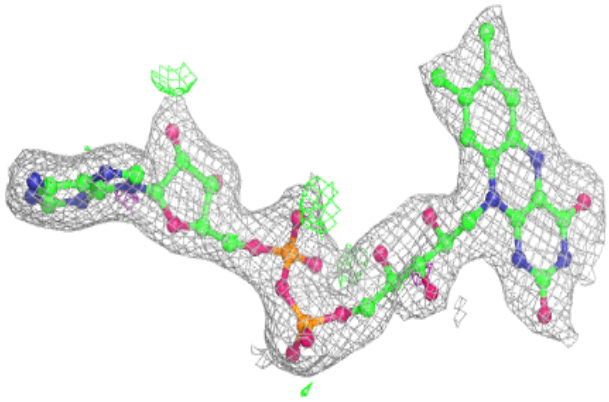
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

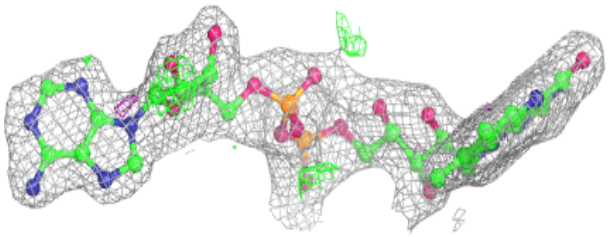
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NA	D	1490	1/1	0.78	0.18	58,58,58,58	0
4	NA	C	1489	1/1	0.88	0.10	34,34,34,34	0
4	NA	A	1489	1/1	0.89	0.13	40,40,40,40	0
4	NA	C	1490	1/1	0.92	0.06	23,23,23,23	0
4	NA	B	1489	1/1	0.92	0.10	41,41,41,41	0
4	NA	D	1489	1/1	0.94	0.22	35,35,35,35	0
4	NA	B	1488	1/1	0.94	0.12	32,32,32,32	0
3	FAD	B	998	53/53	0.97	0.11	10,22,30,31	0
2	NDP	B	800	48/48	0.97	0.10	16,26,29,30	0
2	NDP	C	800	48/48	0.97	0.10	15,23,28,29	0
2	NDP	D	800	48/48	0.97	0.10	20,26,28,29	0
3	FAD	D	998	53/53	0.98	0.09	5,20,25,26	0
3	FAD	A	998	53/53	0.98	0.09	6,13,19,22	0
2	NDP	A	800	48/48	0.98	0.09	15,24,30,33	0
3	FAD	C	998	53/53	0.98	0.10	9,16,20,23	0

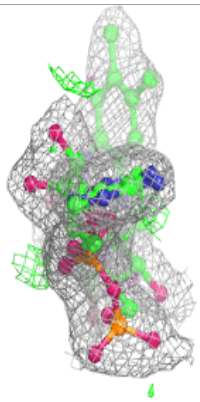
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 998:

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

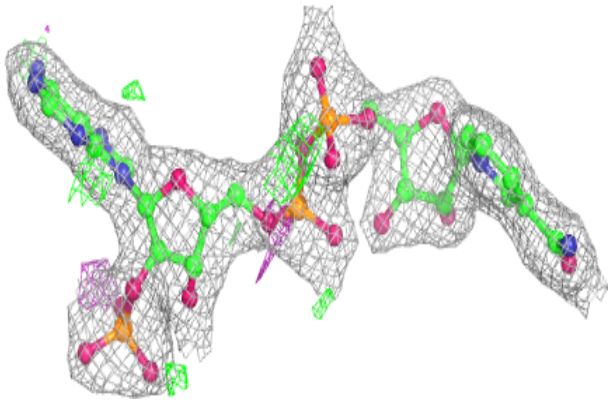


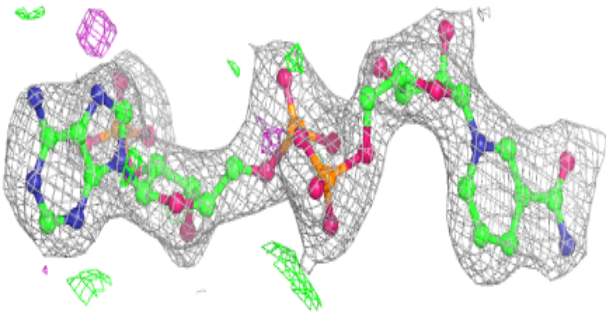


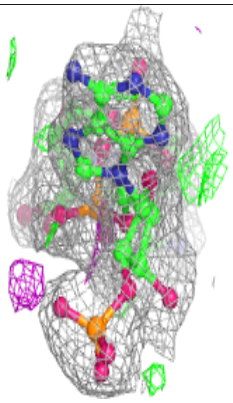


Electron density around NDP B 800:

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







Electron density around NDP C 800:

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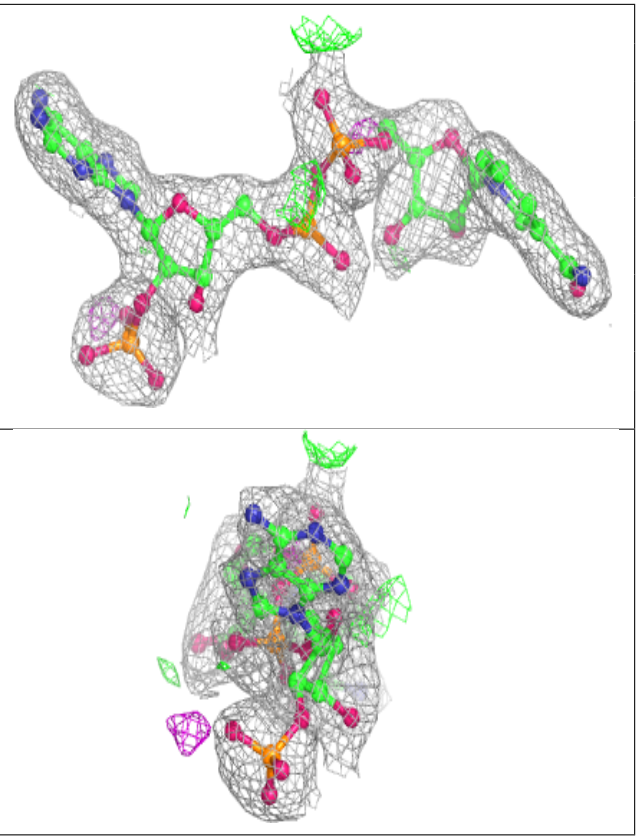
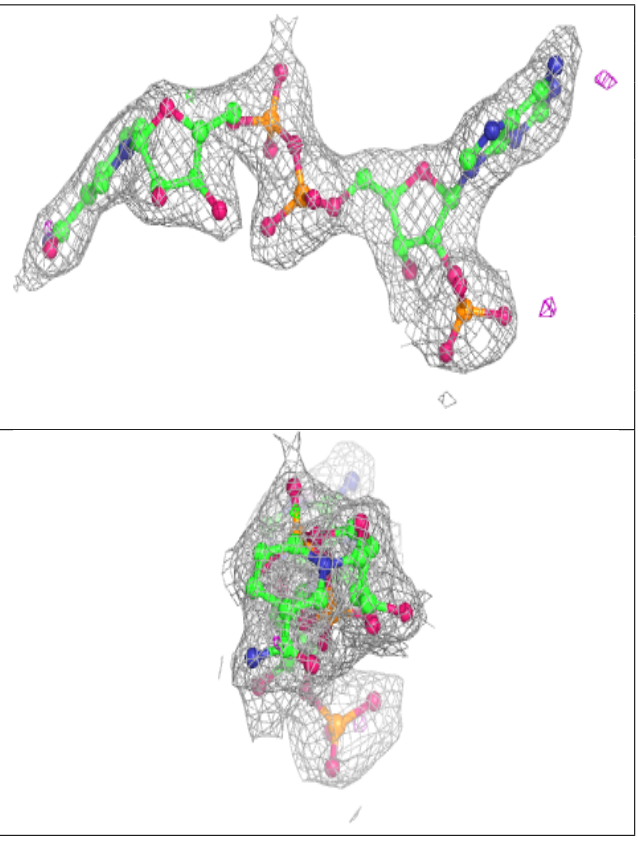
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



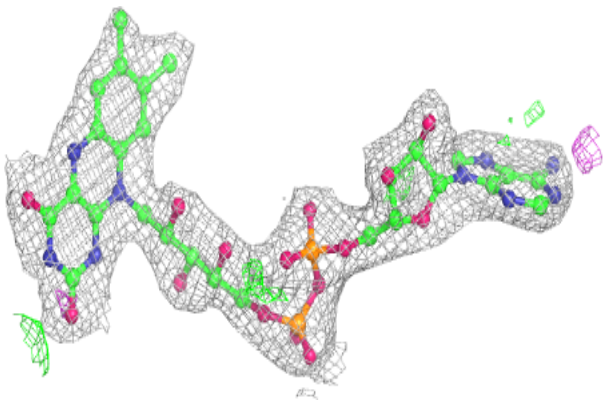
Electron density around NDP D 800:

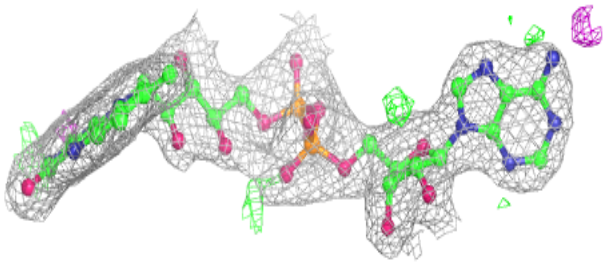
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

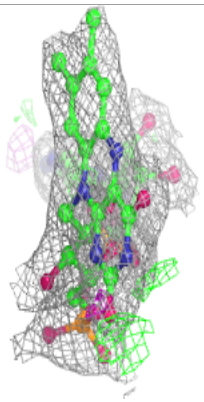


Electron density around FAD D 998:

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

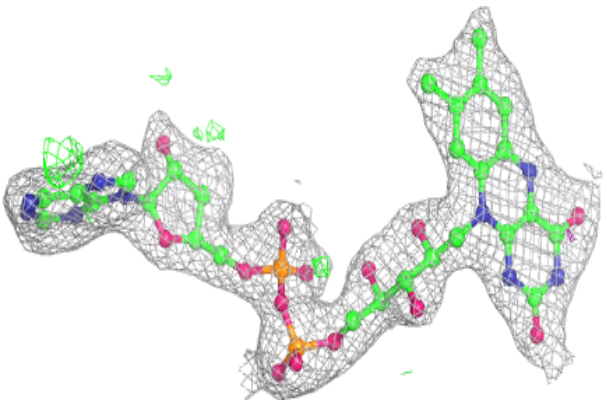


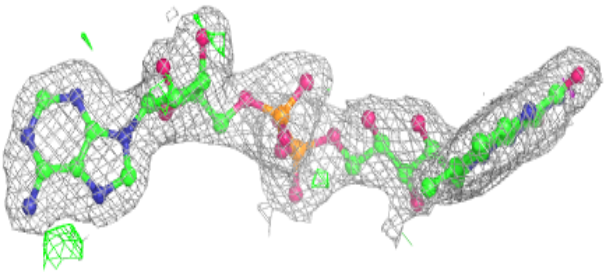


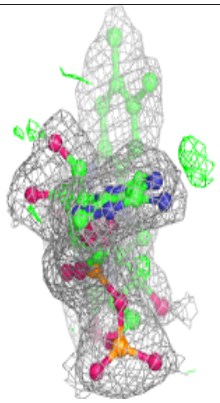


Electron density around FAD A 998:

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

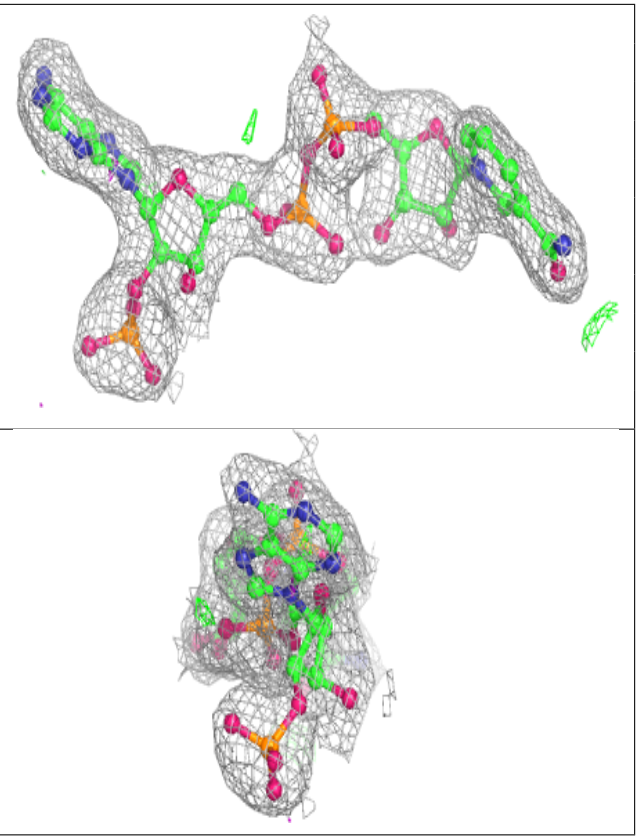






Electron density around NDP A 800:

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



Electron density around FAD C 998:

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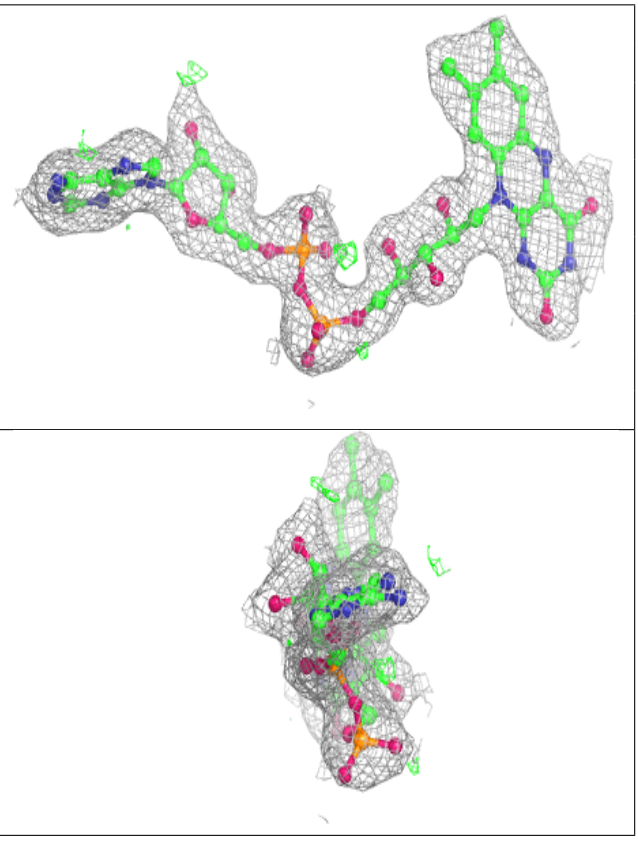
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.