Full wwPDB X-ray Structure Validation Report ⓘ

Aug 2, 2023 – 04:35 pm BST

PDB ID	:	8OWM
Title	:	Crystal structure of glutamate dehydrogenase 2 from Arabidopsis thaliana binding Ca, NAD and 2,2-dihydroxyglutarate
Authors	:	Grzechowiak, M.; Ruszkowski, M.
Deposited on	:	2023-04-28
Resolution	:	1.70 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 ⓘ 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 ⓘ) were used in the production of this report:

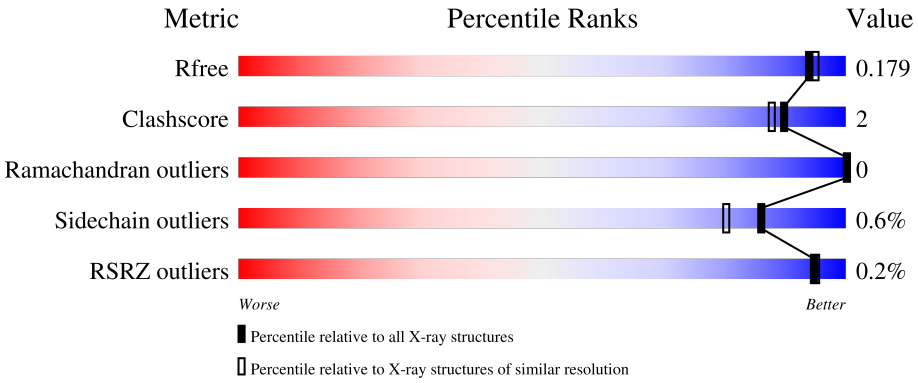
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	414	95% 5%
1	B	414	97% .
1	C	414	95% 5%
1	D	414	96% .
1	E	414	96% .

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Mol	Chain	Length	Quality of chain
1	F	414	96%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 21903 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 Glutamate dehydrogenase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	9	0
			3225	2026	577	604	18			
1	B	412	Total	C	N	O	S	0	3	0
			3175	1997	566	595	17			
1	C	413	Total	C	N	O	S	0	8	0
			3230	2027	582	603	18			
1	D	412	Total	C	N	O	S	0	6	0
			3201	2013	572	598	18			
1	E	412	Total	C	N	O	S	0	8	0
			3226	2027	581	601	17			
1	F	412	Total	C	N	O	S	0	2	0
			3161	1990	559	594	18			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q38946
A	-1	ASN	-	expression tag	UNP Q38946
A	0	ALA	-	expression tag	UNP Q38946
B	-2	SER	-	expression tag	UNP Q38946
B	-1	ASN	-	expression tag	UNP Q38946
B	0	ALA	-	expression tag	UNP Q38946
C	-2	SER	-	expression tag	UNP Q38946
C	-1	ASN	-	expression tag	UNP Q38946
C	0	ALA	-	expression tag	UNP Q38946
D	-2	SER	-	expression tag	UNP Q38946
D	-1	ASN	-	expression tag	UNP Q38946
D	0	ALA	-	expression tag	UNP Q38946
E	-2	SER	-	expression tag	UNP Q38946
E	-1	ASN	-	expression tag	UNP Q38946
E	0	ALA	-	expression tag	UNP Q38946
F	-2	SER	-	expression tag	UNP Q38946
F	-1	ASN	-	expression tag	UNP Q38946

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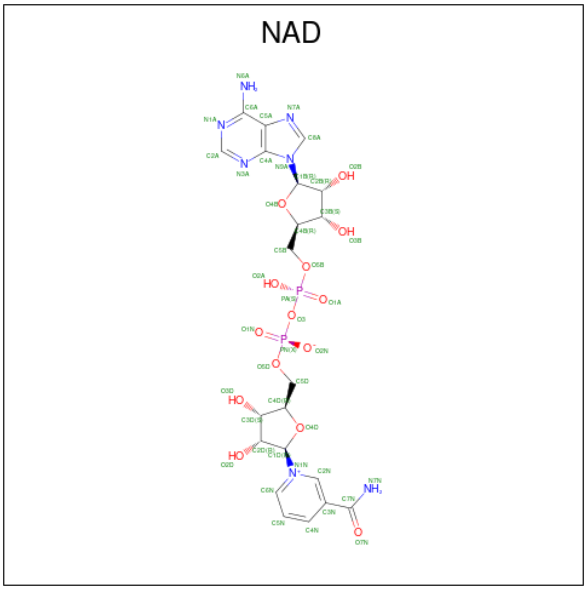
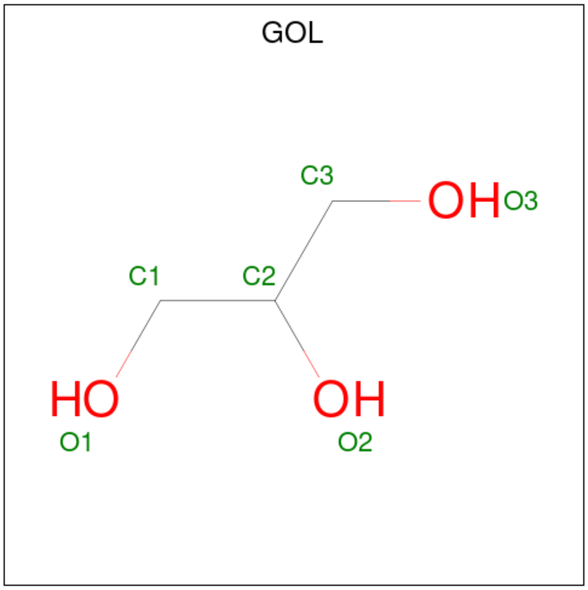
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	expression tag	UNP Q38946

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



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0

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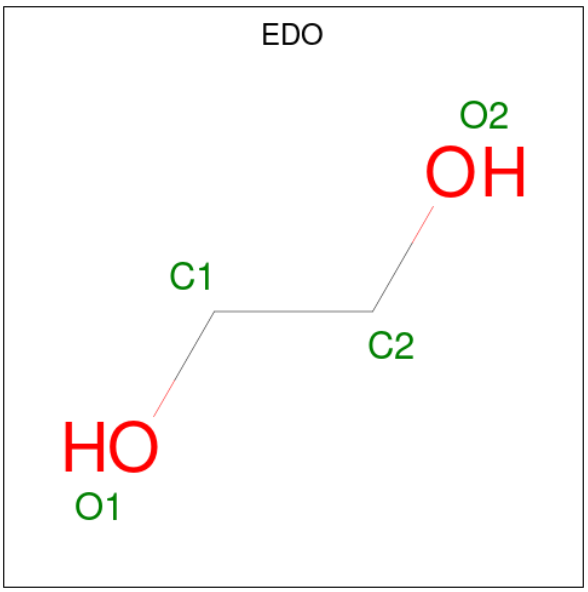
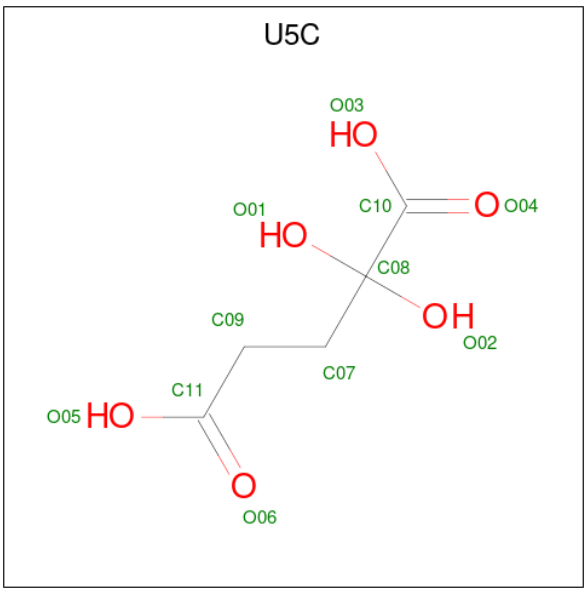
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0

- Molecule 5 is 2,2-bis(oxidanyl)pentanedioic acid (three-letter code: U5C) (formula: $C_5H_8O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 11 5 6	0	0
5	B	1	Total C O 11 5 6	0	0
5	C	1	Total C O 11 5 6	0	0
5	D	1	Total C O 11 5 6	0	0
5	E	1	Total C O 11 5 6	0	0
5	F	1	Total C O 11 5 6	0	0

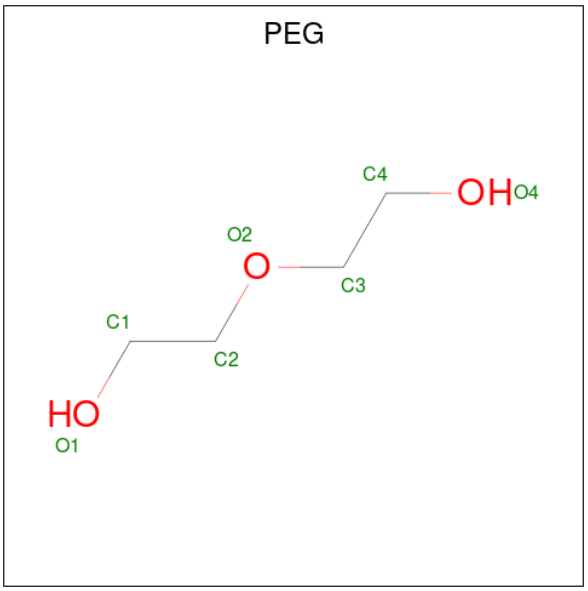
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Ca 1 1	0	0
6	B	1	Total Ca 1 1	0	0
6	C	1	Total Ca 1 1	0	0
6	D	1	Total Ca 1 1	0	0
6	E	1	Total Ca 1 1	0	0
6	F	1	Total Ca 1 1	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Na 1 1	0	0
7	B	1	Total Na 1 1	0	0
7	C	1	Total Na 1 1	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 7 4 3	0	0
8	B	1	Total C O 7 4 3	0	0
8	C	1	Total C O 7 4 3	0	0
8	C	1	Total C O 7 4 3	0	0
8	D	1	Total C O 7 4 3	0	0
8	E	1	Total C O 7 4 3	0	0
8	F	1	Total C O 7 4 3	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	391	Total O 392 392	0	1
9	B	358	Total O 358 358	0	0
9	C	393	Total O 394 394	0	1
9	D	291	Total O 291 291	0	0
9	E	361	Total O 362 362	0	1

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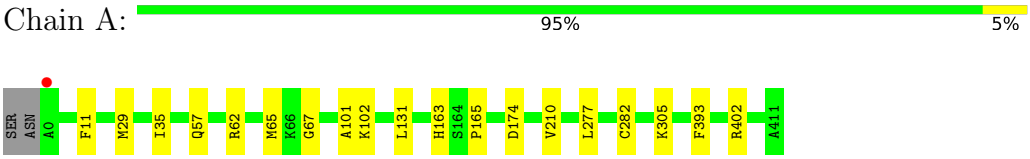
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	F	296	Total 296	O 296	0	0

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.

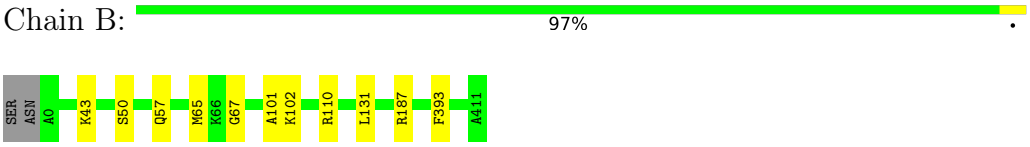
• Molecule 1: Glutamate dehydrogenase 2

Chain A:



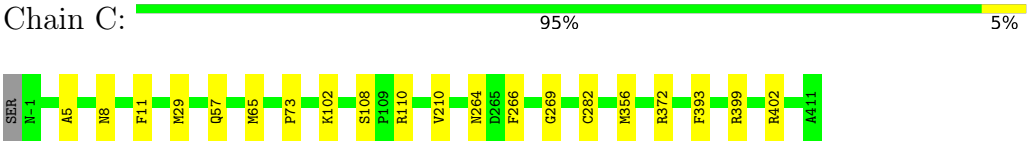
• Molecule 1: Glutamate dehydrogenase 2

Chain B:



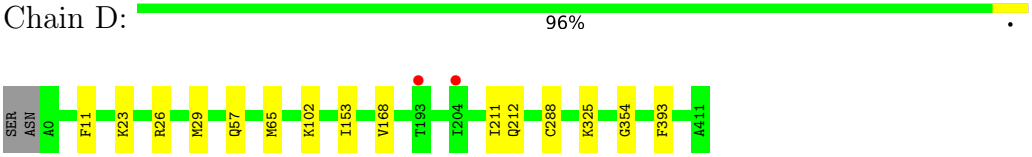
• Molecule 1: Glutamate dehydrogenase 2

Chain C:



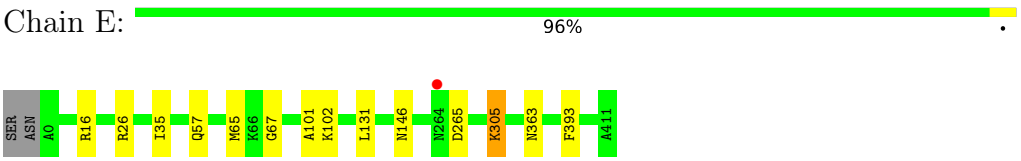
• Molecule 1: Glutamate dehydrogenase 2

Chain D:



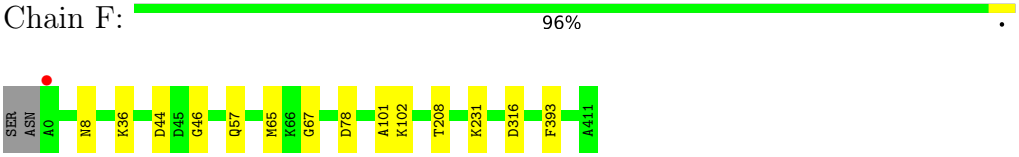
• Molecule 1: Glutamate dehydrogenase 2

Chain E:



• Molecule 1: Glutamate dehydrogenase 2

Chain F:


96%
SER
ASN
A0
N8
K36
D44
D45
G46
Q57
M65
K66
G67
D78
A101
K102
T208
K231
D316
F393
A411

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	95.54Å 95.63Å 95.84Å 90.42° 93.59° 117.78°	Depositor
Resolution (Å)	65.70 – 1.70 95.57 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.0 (65.70-1.70) 97.0 (95.57-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, R_{free}	0.144 , 0.172 0.154 , 0.179	Depositor DCC
R_{free} test set	3189 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	23.4	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 49.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.004 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	21903	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CA, U5C, NAD, EDO, PEG, 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	0.48	0/3288	0.61	0/4448
1	B	0.45	0/3238	0.59	0/4382
1	C	0.47	0/3293	0.61	0/4453
1	D	0.45	0/3264	0.58	0/4416
1	E	0.46	0/3289	0.60	0/4449
1	F	0.44	0/3224	0.58	0/4364
All	All	0.46	0/19596	0.60	0/26512

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3225	0	3204	13	0
1	B	3175	0	3158	11	0
1	C	3230	0	3212	15	0
1	D	3201	0	3186	7	0
1	E	3226	0	3213	12	0
1	F	3161	0	3142	10	0
2	A	44	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
2	E	44	0	26	0	0
2	F	44	0	26	0	0
3	A	36	0	47	4	0
3	B	42	0	53	4	0
3	C	30	0	38	2	0
3	D	18	0	23	2	0
3	E	24	0	32	1	0
3	F	6	0	8	0	0
4	A	4	0	6	0	0
4	B	12	0	18	0	0
4	C	12	0	18	1	0
4	E	12	0	18	0	0
4	F	8	0	12	0	0
5	A	11	0	0	1	0
5	B	11	0	0	1	0
5	C	11	0	0	1	0
5	D	11	0	0	1	0
5	E	11	0	0	1	0
5	F	11	0	0	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	14	0	20	3	0
8	C	14	0	20	4	0
8	D	7	0	10	0	0
8	E	7	0	10	2	0
8	F	7	0	10	2	0
9	A	392	0	0	4	0
9	B	358	0	0	2	0
9	C	394	0	0	4	0
9	D	291	0	0	2	0
9	E	362	0	0	2	0
9	F	296	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	21903	0	19614	72	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 2.

All (72) 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)
8:E:4208:PEG:H42	9:E:4565:HOH:O	1.79	0.81
1:C:266:PHE:O	8:C:504:PEG:H32	1.89	0.72
1:D:102:LYS:NZ	5:D:506:U5C:O02	2.30	0.64
1:C:102:LYS:NZ	5:C:512:U5C:O02	2.31	0.62
1:B:131:LEU:HD21	1:E:131:LEU:HD21	1.83	0.59
1:C:5:ALA:HA	8:C:502:PEG:H32	1.84	0.59
9:A:619:HOH:O	3:B:512:GOL:H12	2.03	0.58
1:B:187[A]:ARG:HD3	8:B:511:PEG:H31	1.85	0.58
1:F:8:ASN:HD22	8:F:504:PEG:H11	1.68	0.58
1:A:35:ILE:HG13	1:A:131:LEU:HD13	1.86	0.57
1:A:131:LEU:HD11	9:A:684:HOH:O	2.06	0.56
1:A:402:ARG:HD2	9:A:669:HOH:O	2.06	0.55
3:A:509:GOL:H11	9:A:903:HOH:O	2.07	0.55
1:B:187[B]:ARG:HE	8:B:511:PEG:H31	1.73	0.53
1:C:269:GLY:O	8:C:504:PEG:H41	2.09	0.53
1:C:372[A]:ARG:HD2	9:C:862:HOH:O	2.11	0.50
3:A:503:GOL:H2	9:D:611:HOH:O	2.12	0.49
1:E:16[B]:ARG:NH1	9:E:4309:HOH:O	2.45	0.49
1:B:110:ARG:NH2	9:B:606:HOH:O	2.45	0.49
1:E:102:LYS:NZ	5:E:4210:U5C:O02	2.40	0.49
1:D:11:PHE:CE2	1:D:29[B]:MET:CG	2.96	0.49
3:B:513:GOL:H12	9:F:786:HOH:O	2.11	0.49
1:F:67:GLY:HA3	1:F:101:ALA:O	2.13	0.48
1:C:110:ARG:NH2	9:C:609:HOH:O	2.40	0.48
1:C:264:ASN:OD1	9:C:601:HOH:O	2.20	0.48
1:A:62:ARG:HE	3:A:506:GOL:H12	1.79	0.47
3:D:503:GOL:H12	9:F:791:HOH:O	2.14	0.47
1:A:11:PHE:CE2	1:A:29[B]:MET:CG	2.98	0.47
1:D:11:PHE:CE2	1:D:29[B]:MET:HG2	2.50	0.47
1:B:131:LEU:HD21	1:E:131:LEU:CD2	2.45	0.46
3:C:503:GOL:O2	9:C:602:HOH:O	2.21	0.46
1:A:11:PHE:CE2	1:A:29[B]:MET:HG3	2.51	0.46
1:F:36:LYS:CE	9:F:759:HOH:O	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:GLY:HA3	1:B:101:ALA:O	2.15	0.46
1:F:102:LYS:NZ	5:F:506:U5C:O02	2.48	0.45
1:A:163:HIS:NE2	1:A:165:PRO:HG3	2.31	0.45
1:C:8:ASN:HD22	8:C:502:PEG:H42	1.81	0.45
1:C:399:ARG:HB3	4:C:506:EDO:H12	1.98	0.45
1:F:78:ASP:OD2	8:F:504:PEG:H41	2.16	0.44
1:A:210:VAL:HG23	1:A:282:CYS:HB3	1.99	0.44
1:A:305:LYS:N	1:A:305:LYS:HD2	2.32	0.44
1:E:305:LYS:N	1:E:305:LYS:HD2	2.32	0.44
1:B:57:GLN:HB3	1:B:65:MET:SD	2.57	0.44
1:C:57:GLN:HB3	1:C:65:MET:SD	2.57	0.44
1:B:102:LYS:NZ	5:B:514:U5C:O02	2.48	0.43
1:C:11:PHE:CE2	1:C:29[A]:MET:CG	3.01	0.43
3:B:513:GOL:H2	1:F:44:ASP:HB3	2.00	0.43
1:D:354:GLY:HA2	3:D:503:GOL:H11	2.00	0.43
1:E:35:ILE:HG13	1:E:131:LEU:HD13	1.99	0.43
1:E:67:GLY:HA3	1:E:101:ALA:O	2.19	0.43
1:A:102:LYS:NZ	5:A:508:U5C:O02	2.41	0.43
1:B:43:LYS:NZ	9:B:617:HOH:O	2.52	0.42
1:C:73:PRO:HG3	1:C:108:SER:OG	2.18	0.42
1:E:57:GLN:HB3	1:E:65:MET:SD	2.58	0.42
1:A:174:ASP:OD2	1:C:402[A]:ARG:HD2	2.20	0.42
3:A:503:GOL:C2	9:D:611:HOH:O	2.68	0.42
1:E:265:ASP:OD1	1:E:265:ASP:N	2.45	0.42
1:F:57:GLN:HB3	1:F:65:MET:SD	2.59	0.42
1:B:187[A]:ARG:HH11	8:B:511:PEG:H31	1.84	0.42
1:D:57:GLN:HB3	1:D:65:MET:SD	2.59	0.41
3:B:512:GOL:H11	1:F:46:GLY:CA	2.50	0.41
1:C:210:VAL:HG23	1:C:282:CYS:HB3	2.02	0.41
1:A:57:GLN:HB3	1:A:65:MET:SD	2.60	0.41
1:E:363:ASN:HB3	8:E:4208:PEG:H41	2.03	0.41
1:D:153:ILE:HG21	1:D:168[B]:VAL:HG21	2.03	0.41
1:D:212:GLN:O	1:D:288:CYS:N	2.51	0.41
1:A:67:GLY:HA3	1:A:101:ALA:O	2.20	0.41
1:C:356:MET:SD	3:C:508:GOL:H12	2.61	0.41
1:F:208:THR:HA	1:F:231:LYS:O	2.21	0.41
1:F:316:ASP:OD1	1:F:316:ASP:C	2.60	0.41
1:B:50:SER:O	1:E:26[B]:ARG:NH1	2.51	0.40
1:E:146:ASN:HA	3:E:4203:GOL:H32	2.03	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	419/414 (101%)	408 (97%)	11 (3%)	0	100	100
1	B	413/414 (100%)	401 (97%)	12 (3%)	0	100	100
1	C	419/414 (101%)	405 (97%)	14 (3%)	0	100	100
1	D	416/414 (100%)	407 (98%)	9 (2%)	0	100	100
1	E	418/414 (101%)	407 (97%)	11 (3%)	0	100	100
1	F	412/414 (100%)	400 (97%)	12 (3%)	0	100	100
All	All	2497/2484 (100%)	2428 (97%)	69 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	339/332 (102%)	337 (99%)	2 (1%)	86	80
1	B	333/332 (100%)	332 (100%)	1 (0%)	92	89
1	C	339/332 (102%)	338 (100%)	1 (0%)	92	89
1	D	336/332 (101%)	330 (98%)	6 (2%)	59	43
1	E	338/332 (102%)	336 (99%)	2 (1%)	86	80
1	F	332/332 (100%)	331 (100%)	1 (0%)	92	89
All	All	2017/1992 (101%)	2004 (99%)	13 (1%)	86	80

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	LEU
1	A	393	PHE
1	B	393	PHE
1	C	393	PHE
1	D	23	LYS
1	D	26[A]	ARG
1	D	26[B]	ARG
1	D	211	ILE
1	D	325	LYS
1	D	393	PHE
1	E	305	LYS
1	E	393	PHE
1	F	393	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	264	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 66 ligands modelled in this entry, 9 are monoatomic - leaving 57 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	NAD	E	4202	-	42,48,48	0.64	0	50,73,73	0.91	2 (4%)
8	PEG	C	504	-	6,6,6	0.20	0	5,5,5	0.15	0
4	EDO	E	4204	-	3,3,3	0.49	0	2,2,2	0.19	0
5	U5C	A	508	-	8,10,10	1.11	0	8,14,14	2.55	3 (37%)
3	GOL	A	509	-	5,5,5	1.37	1 (20%)	5,5,5	0.61	0
4	EDO	C	509	-	3,3,3	0.46	0	2,2,2	0.61	0
3	GOL	B	513	7	5,5,5	1.00	0	5,5,5	1.11	0
4	EDO	C	506	-	3,3,3	0.56	0	2,2,2	0.38	0
2	NAD	F	501	-	42,48,48	0.77	2 (4%)	50,73,73	1.00	4 (8%)
3	GOL	E	4207	-	5,5,5	0.91	0	5,5,5	1.15	0
4	EDO	A	505	-	3,3,3	0.37	0	2,2,2	0.75	0
3	GOL	A	502	-	5,5,5	1.03	0	5,5,5	1.18	0
5	U5C	C	512	-	8,10,10	1.06	0	8,14,14	3.26	5 (62%)
5	U5C	D	506	-	8,10,10	1.31	1 (12%)	8,14,14	1.97	2 (25%)
4	EDO	B	505	-	3,3,3	0.53	0	2,2,2	0.40	0
4	EDO	E	4209	-	3,3,3	0.49	0	2,2,2	0.26	0
3	GOL	A	506	-	5,5,5	0.95	0	5,5,5	0.79	0
8	PEG	C	502	-	6,6,6	0.14	0	5,5,5	0.09	0
3	GOL	C	508	-	5,5,5	1.24	0	5,5,5	1.26	1 (20%)
5	U5C	E	4210	-	8,10,10	1.53	0	8,14,14	1.52	1 (12%)
3	GOL	C	507	-	5,5,5	0.95	0	5,5,5	1.03	0
4	EDO	F	505	-	3,3,3	0.54	0	2,2,2	0.28	0
8	PEG	E	4208	-	6,6,6	0.18	0	5,5,5	0.12	0
5	U5C	F	506	-	8,10,10	1.21	0	8,14,14	2.22	1 (12%)
3	GOL	A	504	-	5,5,5	1.14	0	5,5,5	0.68	0
8	PEG	B	502	-	6,6,6	0.18	0	5,5,5	0.18	0
3	GOL	D	505	7	5,5,5	1.13	0	5,5,5	0.88	0
3	GOL	B	508	-	5,5,5	1.04	0	5,5,5	1.41	1 (20%)
3	GOL	D	502	-	5,5,5	1.20	0	5,5,5	0.98	0
3	GOL	E	4201	7	5,5,5	0.94	0	5,5,5	1.00	0
2	NAD	C	501	-	42,48,48	0.73	1 (2%)	50,73,73	0.97	4 (8%)
8	PEG	D	504	-	6,6,6	0.19	0	5,5,5	0.14	0
3	GOL	C	503	-	5,5,5	1.23	0	5,5,5	1.02	0
2	NAD	D	501	-	42,48,48	0.77	1 (2%)	50,73,73	0.92	3 (6%)
3	GOL	A	507	7	5,5,5	0.89	0	5,5,5	1.04	0
3	GOL	F	502	-	5,5,5	1.08	0	5,5,5	0.89	0
8	PEG	B	511	-	6,6,6	0.25	0	5,5,5	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	A	503	-	5,5,5	0.96	0	5,5,5	0.90	0
4	EDO	E	4206	-	3,3,3	0.71	0	2,2,2	0.26	0
8	PEG	F	504	-	6,6,6	0.16	0	5,5,5	0.14	0
2	NAD	B	501	-	42,48,48	0.69	1 (2%)	50,73,73	0.91	2 (4%)
4	EDO	B	509	-	3,3,3	0.32	0	2,2,2	0.47	0
3	GOL	B	506	-	5,5,5	1.00	0	5,5,5	0.86	0
4	EDO	C	505	-	3,3,3	0.54	0	2,2,2	0.35	0
3	GOL	E	4205	-	5,5,5	0.74	0	5,5,5	1.29	1 (20%)
3	GOL	B	512	7	5,5,5	0.69	0	5,5,5	0.87	0
4	EDO	B	504	-	3,3,3	0.63	0	2,2,2	0.23	0
3	GOL	B	503	-	5,5,5	1.00	0	5,5,5	1.22	0
5	U5C	B	514	-	8,10,10	0.98	0	8,14,14	3.09	4 (50%)
3	GOL	B	510	-	5,5,5	0.86	0	5,5,5	1.07	0
3	GOL	B	507	-	5,5,5	0.84	0	5,5,5	0.85	0
3	GOL	C	510	-	5,5,5	1.13	0	5,5,5	0.90	0
3	GOL	D	503	-	5,5,5	1.01	0	5,5,5	0.98	0
3	GOL	E	4203	-	5,5,5	0.94	0	5,5,5	1.10	0
4	EDO	F	503	-	3,3,3	0.53	0	2,2,2	0.40	0
3	GOL	C	511	7	5,5,5	0.90	0	5,5,5	1.03	0
2	NAD	A	501	-	42,48,48	0.70	1 (2%)	50,73,73	0.94	2 (4%)

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	E	4202	-	-	5/26/62/62	0/5/5/5
8	PEG	C	504	-	-	0/4/4/4	-
4	EDO	E	4204	-	-	1/1/1/1	-
5	U5C	A	508	-	-	11/12/12/12	-
3	GOL	A	509	-	-	2/4/4/4	-
4	EDO	C	509	-	-	0/1/1/1	-
3	GOL	B	513	7	-	0/4/4/4	-
4	EDO	C	506	-	-	1/1/1/1	-
2	NAD	F	501	-	-	4/26/62/62	0/5/5/5
3	GOL	E	4207	-	-	2/4/4/4	-
4	EDO	A	505	-	-	0/1/1/1	-
3	GOL	A	502	-	-	2/4/4/4	-
5	U5C	C	512	-	-	9/12/12/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	U5C	D	506	-	-	7/12/12/12	-
4	EDO	B	505	-	-	1/1/1/1	-
4	EDO	E	4209	-	-	0/1/1/1	-
3	GOL	A	506	-	-	2/4/4/4	-
8	PEG	C	502	-	-	1/4/4/4	-
3	GOL	C	508	-	-	2/4/4/4	-
5	U5C	E	4210	-	-	7/12/12/12	-
3	GOL	C	507	-	-	2/4/4/4	-
4	EDO	F	505	-	-	1/1/1/1	-
8	PEG	E	4208	-	-	1/4/4/4	-
5	U5C	F	506	-	-	7/12/12/12	-
3	GOL	A	504	-	-	2/4/4/4	-
8	PEG	B	502	-	-	0/4/4/4	-
3	GOL	D	505	7	-	2/4/4/4	-
3	GOL	B	508	-	-	3/4/4/4	-
3	GOL	D	502	-	-	3/4/4/4	-
3	GOL	E	4201	7	-	2/4/4/4	-
2	NAD	C	501	-	-	4/26/62/62	0/5/5/5
8	PEG	D	504	-	-	2/4/4/4	-
3	GOL	C	503	-	-	2/4/4/4	-
2	NAD	D	501	-	-	4/26/62/62	0/5/5/5
3	GOL	A	507	7	-	0/4/4/4	-
3	GOL	F	502	-	-	2/4/4/4	-
8	PEG	B	511	-	-	0/4/4/4	-
3	GOL	A	503	-	-	4/4/4/4	-
4	EDO	E	4206	-	-	1/1/1/1	-
8	PEG	F	504	-	-	0/4/4/4	-
2	NAD	B	501	-	-	4/26/62/62	0/5/5/5
4	EDO	B	509	-	-	0/1/1/1	-
3	GOL	B	506	-	-	2/4/4/4	-
4	EDO	C	505	-	-	0/1/1/1	-
3	GOL	E	4205	-	-	0/4/4/4	-
3	GOL	B	512	7	-	4/4/4/4	-
4	EDO	B	504	-	-	1/1/1/1	-
3	GOL	B	503	-	-	3/4/4/4	-
5	U5C	B	514	-	-	9/12/12/12	-
3	GOL	B	510	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	507	-	-	2/4/4/4	-
3	GOL	C	510	-	-	2/4/4/4	-
3	GOL	D	503	-	-	4/4/4/4	-
3	GOL	E	4203	-	-	3/4/4/4	-
4	EDO	F	503	-	-	1/1/1/1	-
3	GOL	C	511	7	-	0/4/4/4	-
2	NAD	A	501	-	-	4/26/62/62	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	NAD	C2N-N1N	3.28	1.39	1.35
2	F	501	NAD	C2N-N1N	2.61	1.38	1.35
2	C	501	NAD	C2N-N1N	2.51	1.38	1.35
2	A	501	NAD	C2N-N1N	2.47	1.38	1.35
3	A	509	GOL	C3-C2	2.29	1.61	1.51
2	F	501	NAD	O4D-C1D	2.29	1.44	1.41
5	D	506	U5C	O05-C11	-2.13	1.23	1.30
2	B	501	NAD	O4D-C1D	2.08	1.44	1.41

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	506	U5C	C09-C07-C08	-6.00	100.51	117.87
5	C	512	U5C	C09-C07-C08	-5.90	100.79	117.87
5	B	514	U5C	C09-C07-C08	-5.70	101.36	117.87
5	B	514	U5C	O04-C10-C08	-4.84	115.79	123.49
5	D	506	U5C	C09-C07-C08	-4.82	103.92	117.87
5	C	512	U5C	O04-C10-C08	-4.67	116.06	123.49
5	A	508	U5C	O04-C10-C08	-4.44	116.42	123.49
5	C	512	U5C	O03-C10-C08	3.93	122.10	113.79
5	A	508	U5C	C09-C07-C08	-3.91	106.55	117.87
5	E	4210	U5C	C09-C07-C08	-3.45	107.87	117.87
5	B	514	U5C	O03-C10-C08	3.39	120.97	113.79
5	A	508	U5C	O03-C10-C08	2.92	119.97	113.79
2	C	501	NAD	O4D-C1D-C2D	-2.75	102.91	106.93
2	B	501	NAD	O4D-C1D-C2D	-2.69	102.99	106.93
2	F	501	NAD	C6N-N1N-C2N	-2.66	119.55	121.97
5	C	512	U5C	O05-C11-C09	2.64	122.52	114.03
2	E	4202	NAD	C6N-N1N-C2N	-2.57	119.63	121.97
2	D	501	NAD	C5A-C6A-N6A	2.56	124.24	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	4205	GOL	C3-C2-C1	-2.53	101.86	111.70
3	B	508	GOL	C3-C2-C1	-2.52	101.90	111.70
2	A	501	NAD	C5A-C6A-N6A	2.46	124.10	120.35
2	F	501	NAD	O4D-C1D-C2D	-2.44	103.36	106.93
2	F	501	NAD	C3B-C2B-C1B	-2.41	97.35	100.98
2	D	501	NAD	O4D-C1D-C2D	-2.31	103.55	106.93
2	C	501	NAD	C6N-N1N-C2N	-2.27	119.90	121.97
2	E	4202	NAD	C5A-C6A-N6A	2.26	123.79	120.35
5	C	512	U5C	O06-C11-C09	-2.23	115.92	123.08
5	B	514	U5C	O05-C11-C09	2.22	121.17	114.03
2	F	501	NAD	C5A-C6A-N6A	2.21	123.72	120.35
2	B	501	NAD	C6N-N1N-C2N	-2.21	119.96	121.97
3	C	508	GOL	C3-C2-C1	-2.15	103.33	111.70
2	A	501	NAD	O4D-C1D-C2D	-2.14	103.80	106.93
2	D	501	NAD	C6N-N1N-C2N	-2.07	120.09	121.97
2	C	501	NAD	C5A-C6A-N6A	2.06	123.48	120.35
2	C	501	NAD	O3D-C3D-C2D	-2.04	105.22	111.82
5	D	506	U5C	O03-C10-C08	2.03	118.09	113.79

There are no chirality outliers.

All (140) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAD	O4D-C1D-N1N-C2N
2	A	501	NAD	O4D-C1D-N1N-C6N
2	A	501	NAD	C2D-C1D-N1N-C6N
2	B	501	NAD	O4D-C1D-N1N-C2N
2	B	501	NAD	O4D-C1D-N1N-C6N
2	B	501	NAD	C2D-C1D-N1N-C6N
2	C	501	NAD	O4D-C1D-N1N-C2N
2	C	501	NAD	O4D-C1D-N1N-C6N
2	C	501	NAD	C2D-C1D-N1N-C6N
2	D	501	NAD	O4D-C1D-N1N-C2N
2	D	501	NAD	O4D-C1D-N1N-C6N
2	D	501	NAD	C2D-C1D-N1N-C6N
2	E	4202	NAD	O4D-C1D-N1N-C2N
2	E	4202	NAD	O4D-C1D-N1N-C6N
2	E	4202	NAD	C2D-C1D-N1N-C6N
2	F	501	NAD	O4D-C1D-N1N-C2N
2	F	501	NAD	O4D-C1D-N1N-C6N
2	F	501	NAD	C2D-C1D-N1N-C6N
3	A	503	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	504	GOL	C1-C2-C3-O3
3	A	504	GOL	O2-C2-C3-O3
3	C	503	GOL	C1-C2-C3-O3
3	D	502	GOL	C1-C2-C3-O3
3	D	503	GOL	O1-C1-C2-C3
3	E	4201	GOL	O1-C1-C2-O2
3	E	4201	GOL	O1-C1-C2-C3
3	E	4207	GOL	O1-C1-C2-C3
5	A	508	U5C	C09-C07-C08-C10
5	A	508	U5C	C09-C07-C08-O01
5	A	508	U5C	C09-C07-C08-O02
5	A	508	U5C	C07-C08-C10-O03
5	A	508	U5C	C07-C08-C10-O04
5	A	508	U5C	O01-C08-C10-O03
5	A	508	U5C	O01-C08-C10-O04
5	A	508	U5C	O02-C08-C10-O03
5	A	508	U5C	O02-C08-C10-O04
5	B	514	U5C	C09-C07-C08-C10
5	B	514	U5C	C09-C07-C08-O01
5	B	514	U5C	C07-C08-C10-O03
5	B	514	U5C	C07-C08-C10-O04
5	B	514	U5C	O01-C08-C10-O03
5	B	514	U5C	O01-C08-C10-O04
5	B	514	U5C	O02-C08-C10-O03
5	B	514	U5C	O02-C08-C10-O04
5	C	512	U5C	C09-C07-C08-C10
5	C	512	U5C	C09-C07-C08-O01
5	C	512	U5C	C07-C08-C10-O03
5	C	512	U5C	C07-C08-C10-O04
5	C	512	U5C	O01-C08-C10-O03
5	C	512	U5C	O01-C08-C10-O04
5	C	512	U5C	O02-C08-C10-O03
5	C	512	U5C	O02-C08-C10-O04
5	D	506	U5C	C09-C07-C08-C10
5	D	506	U5C	C09-C07-C08-O01
5	D	506	U5C	C07-C08-C10-O03
5	D	506	U5C	C07-C08-C10-O04
5	E	4210	U5C	C09-C07-C08-C10
5	E	4210	U5C	C09-C07-C08-O01
5	E	4210	U5C	C09-C07-C08-O02
5	E	4210	U5C	C07-C08-C10-O03
5	E	4210	U5C	C07-C08-C10-O04

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Mol	Chain	Res	Type	Atoms
5	F	506	U5C	C09-C07-C08-C10
5	F	506	U5C	C09-C07-C08-O01
5	F	506	U5C	C07-C08-C10-O03
5	F	506	U5C	C07-C08-C10-O04
3	A	502	GOL	C1-C2-C3-O3
3	A	503	GOL	O1-C1-C2-C3
3	A	506	GOL	C1-C2-C3-O3
3	A	509	GOL	O1-C1-C2-C3
3	B	503	GOL	O1-C1-C2-C3
3	B	507	GOL	C1-C2-C3-O3
3	B	508	GOL	C1-C2-C3-O3
3	B	512	GOL	O1-C1-C2-C3
3	B	512	GOL	C1-C2-C3-O3
3	C	507	GOL	O1-C1-C2-C3
3	C	508	GOL	O1-C1-C2-C3
3	C	510	GOL	C1-C2-C3-O3
3	D	502	GOL	O1-C1-C2-C3
3	D	503	GOL	C1-C2-C3-O3
3	D	505	GOL	C1-C2-C3-O3
3	E	4203	GOL	O1-C1-C2-C3
3	F	502	GOL	O1-C1-C2-C3
3	A	503	GOL	O2-C2-C3-O3
3	A	509	GOL	O1-C1-C2-O2
3	B	507	GOL	O2-C2-C3-O3
3	B	512	GOL	O1-C1-C2-O2
3	C	503	GOL	O2-C2-C3-O3
3	D	502	GOL	O2-C2-C3-O3
4	E	4204	EDO	O1-C1-C2-O2
4	F	505	EDO	O1-C1-C2-O2
8	D	504	PEG	O2-C3-C4-O4
3	E	4207	GOL	O1-C1-C2-O2
3	F	502	GOL	O1-C1-C2-O2
4	B	504	EDO	O1-C1-C2-O2
4	E	4206	EDO	O1-C1-C2-O2
3	E	4203	GOL	C1-C2-C3-O3
3	A	506	GOL	O2-C2-C3-O3
3	C	508	GOL	O1-C1-C2-O2
3	C	510	GOL	O2-C2-C3-O3
3	D	503	GOL	O2-C2-C3-O3
3	E	4203	GOL	O1-C1-C2-O2
4	B	505	EDO	O1-C1-C2-O2
4	C	506	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	F	503	EDO	O1-C1-C2-O2
3	A	502	GOL	O2-C2-C3-O3
3	B	503	GOL	O2-C2-C3-O3
3	B	506	GOL	O2-C2-C3-O3
3	B	510	GOL	O2-C2-C3-O3
3	C	507	GOL	O1-C1-C2-O2
3	D	503	GOL	O1-C1-C2-O2
5	B	514	U5C	C09-C07-C08-O02
5	C	512	U5C	C09-C07-C08-O02
5	D	506	U5C	C09-C07-C08-O02
5	F	506	U5C	C09-C07-C08-O02
8	E	4208	PEG	O2-C3-C4-O4
5	F	506	U5C	O01-C08-C10-O03
8	D	504	PEG	C4-C3-O2-C2
3	A	503	GOL	O1-C1-C2-O2
3	B	508	GOL	O1-C1-C2-O2
3	B	512	GOL	O2-C2-C3-O3
5	A	508	U5C	C07-C09-C11-O06
8	C	502	PEG	C4-C3-O2-C2
5	D	506	U5C	O01-C08-C10-O03
5	A	508	U5C	C07-C09-C11-O05
3	B	506	GOL	C1-C2-C3-O3
5	E	4210	U5C	C07-C09-C11-O05
3	D	505	GOL	O2-C2-C3-O3
5	E	4210	U5C	C07-C09-C11-O06
2	E	4202	NAD	C2D-C1D-N1N-C2N
3	B	503	GOL	O1-C1-C2-O2
3	B	508	GOL	O2-C2-C3-O3
2	A	501	NAD	O4B-C4B-C5B-O5B
2	B	501	NAD	O4B-C4B-C5B-O5B
2	C	501	NAD	O4B-C4B-C5B-O5B
2	D	501	NAD	O4B-C4B-C5B-O5B
2	F	501	NAD	O4B-C4B-C5B-O5B
3	B	510	GOL	C1-C2-C3-O3
2	E	4202	NAD	O4B-C4B-C5B-O5B
5	D	506	U5C	O01-C08-C10-O04
5	F	506	U5C	O01-C08-C10-O04

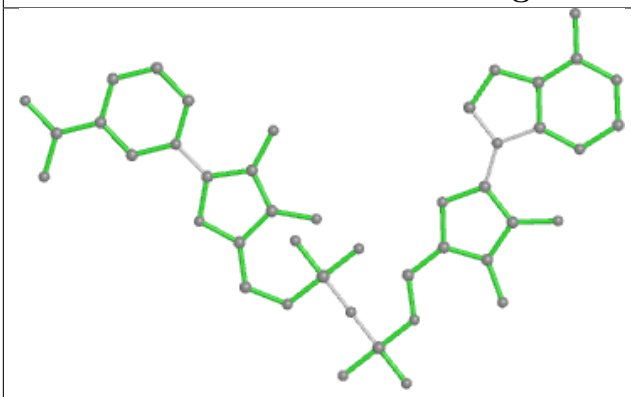
There are no ring outliers.

21 monomers are involved in 31 short contacts:

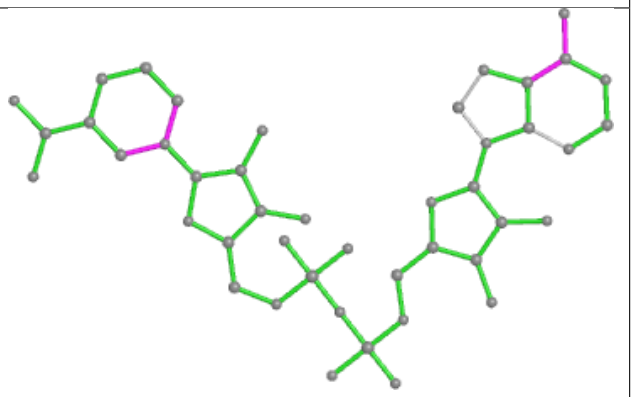
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	504	PEG	2	0
5	A	508	U5C	1	0
3	A	509	GOL	1	0
3	B	513	GOL	2	0
4	C	506	EDO	1	0
5	C	512	U5C	1	0
5	D	506	U5C	1	0
3	A	506	GOL	1	0
8	C	502	PEG	2	0
3	C	508	GOL	1	0
5	E	4210	U5C	1	0
8	E	4208	PEG	2	0
5	F	506	U5C	1	0
3	C	503	GOL	1	0
8	B	511	PEG	3	0
3	A	503	GOL	2	0
8	F	504	PEG	2	0
3	B	512	GOL	2	0
5	B	514	U5C	1	0
3	D	503	GOL	2	0
3	E	4203	GOL	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.

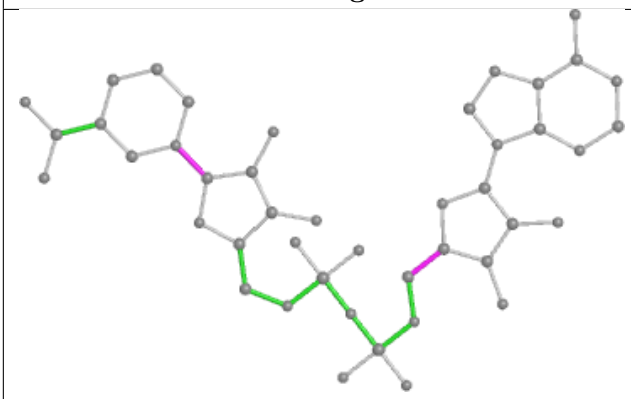
Ligand NAD E 4202



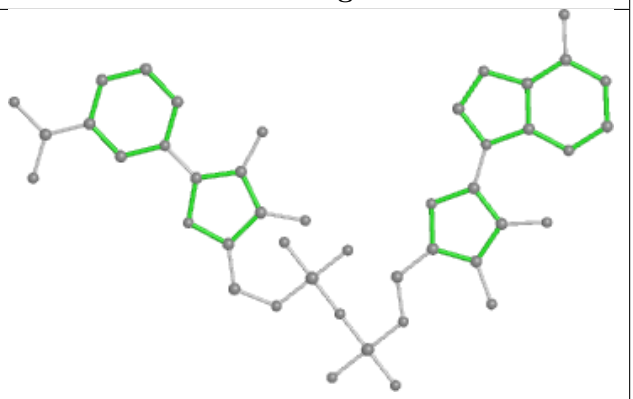
Bond lengths



Bond angles

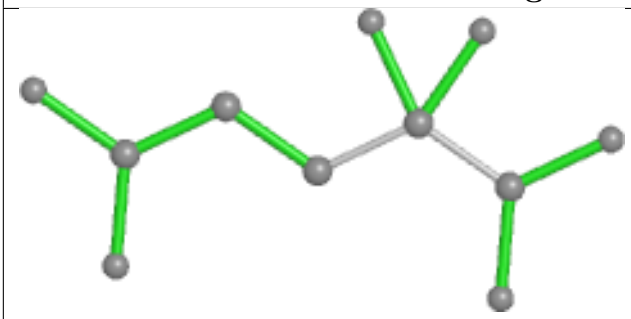


Torsions

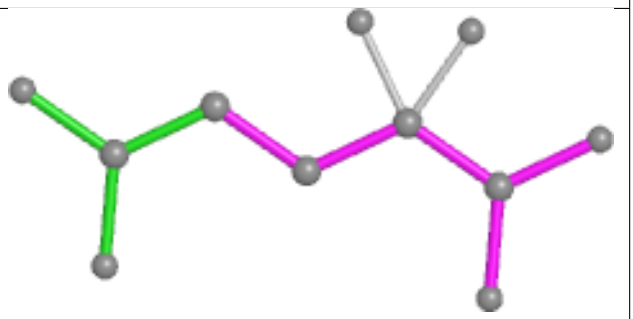


Rings

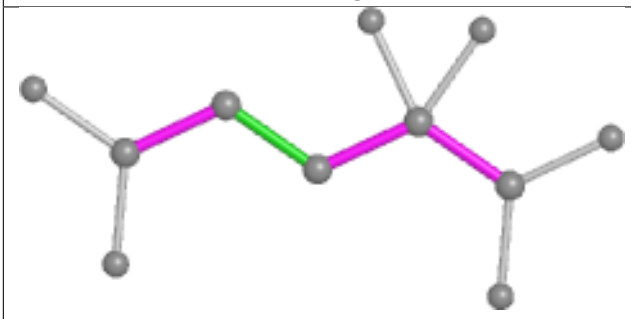
Ligand U5C A 508



Bond lengths



Bond angles



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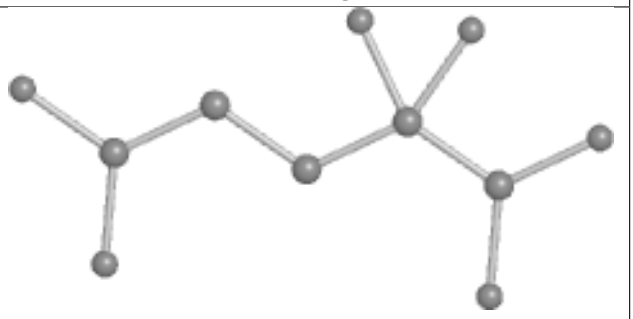
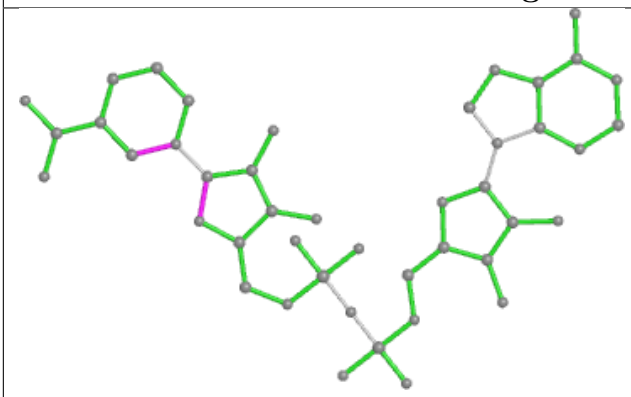
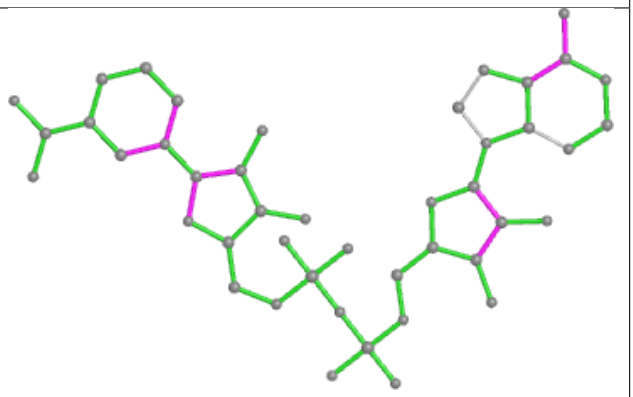


Rings

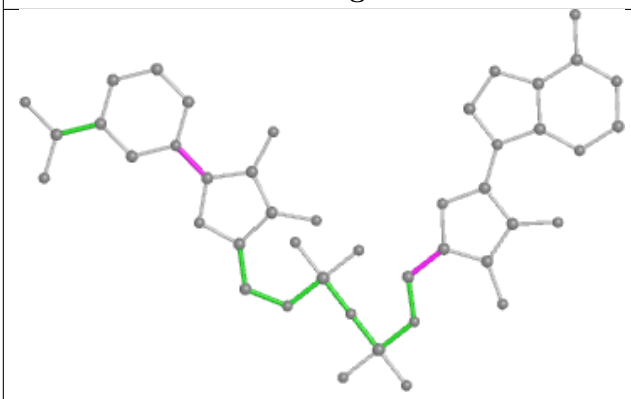
Ligand NAD F 501



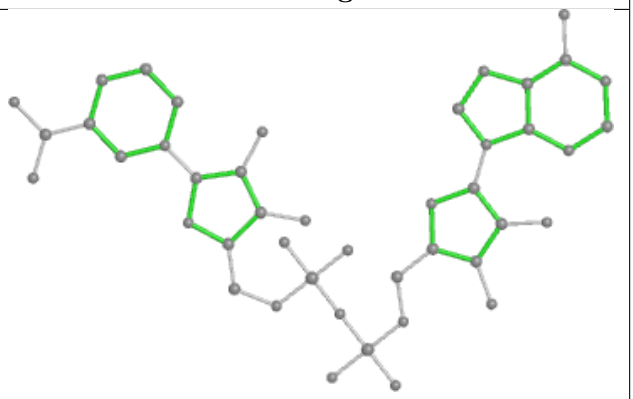
Bond lengths



Bond angles

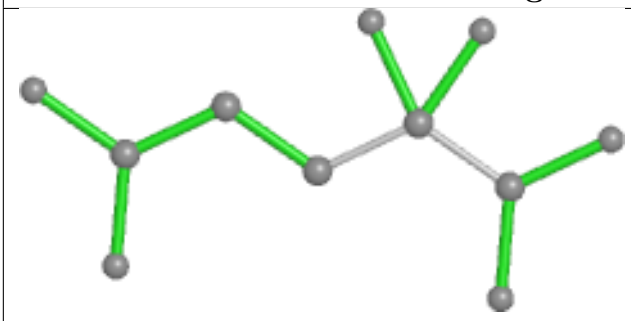


Torsions

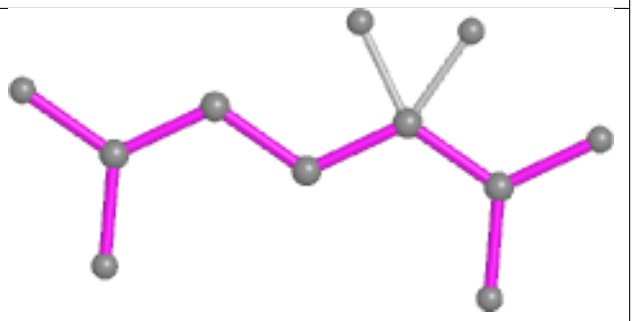


Rings

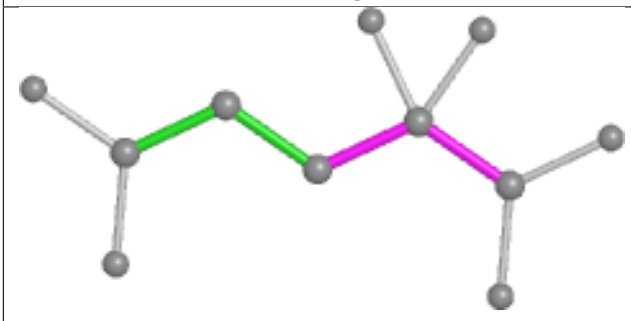
Ligand U5C C 512



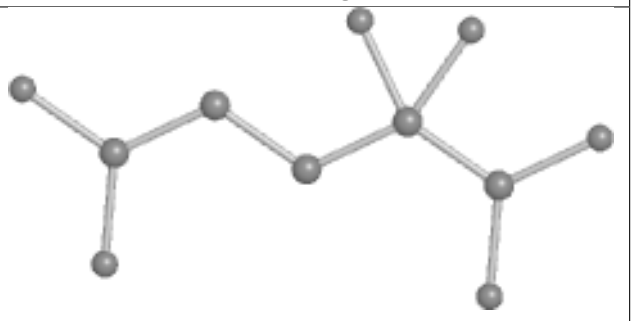
Bond lengths



Bond angles

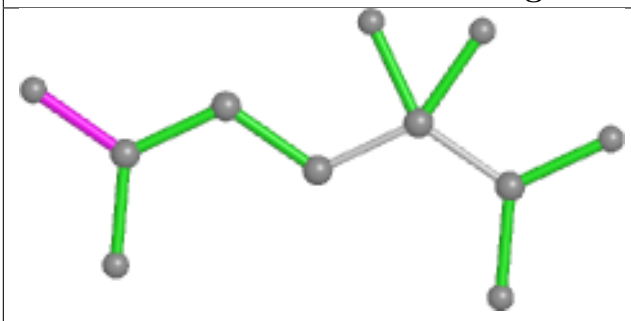


Torsions

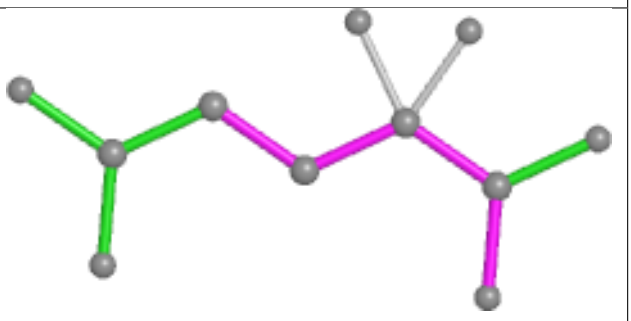


Rings

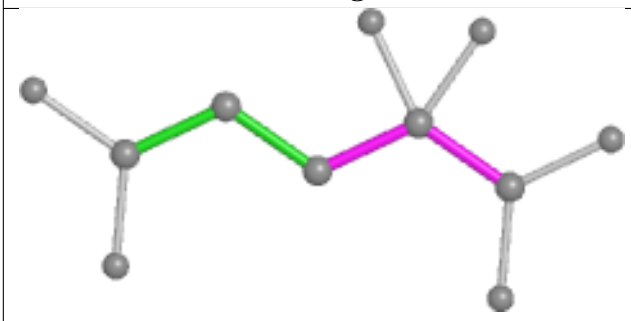
Ligand U5C D 506



Bond lengths



Bond angles



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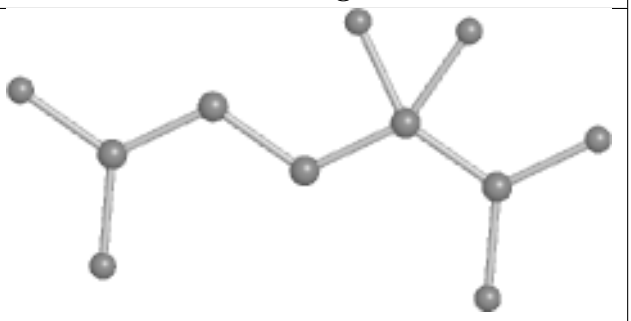
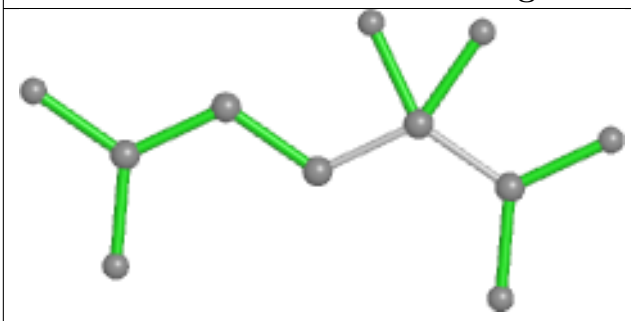
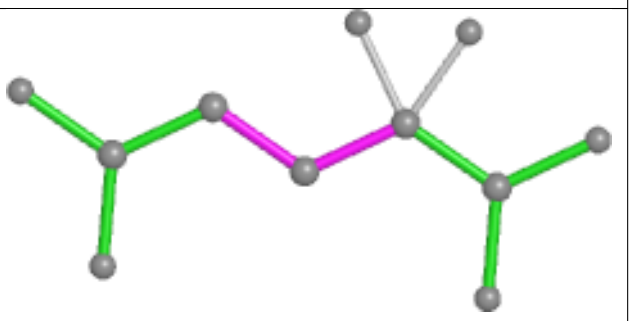


Rings

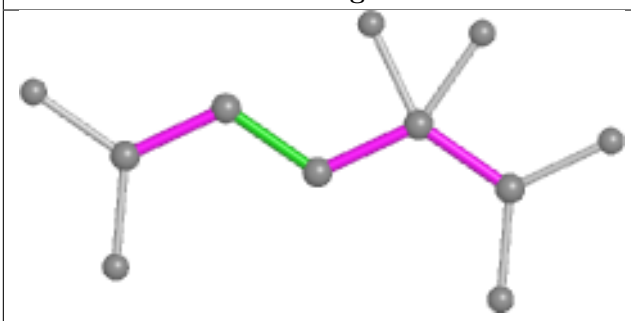
Ligand U5C E 4210



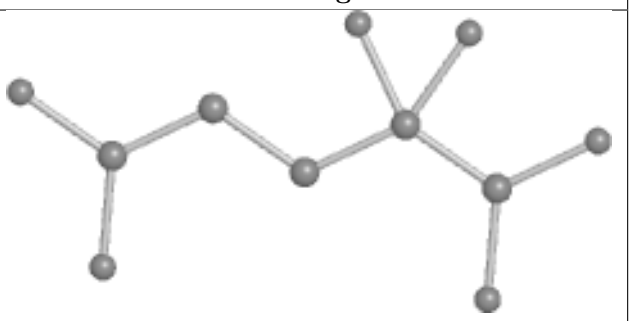
Bond lengths



Bond angles

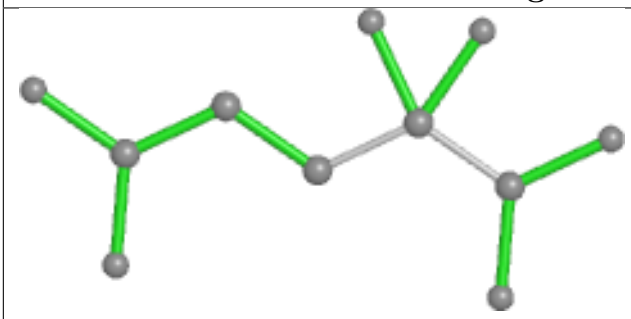


Torsions

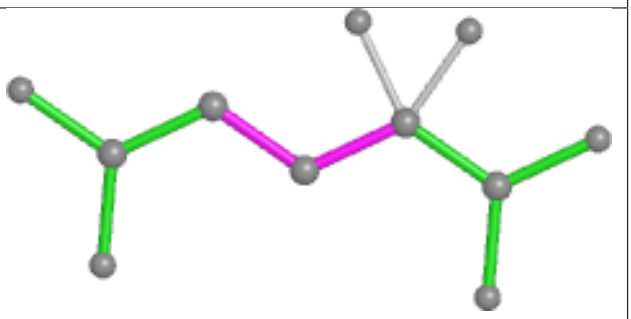


Rings

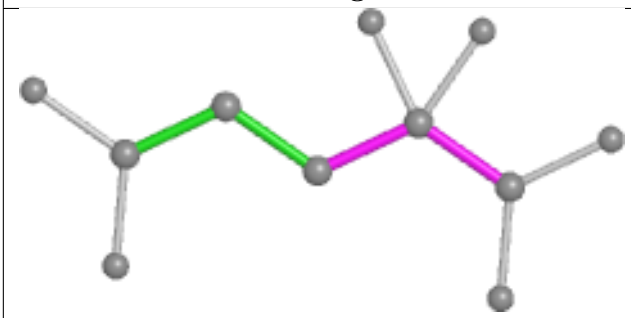
Ligand U5C F 506



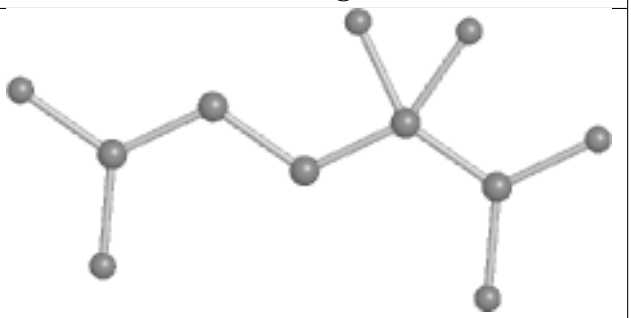
Bond lengths



Bond angles

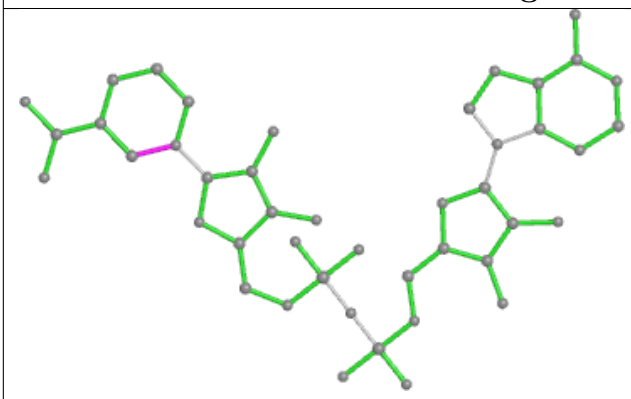


Torsions

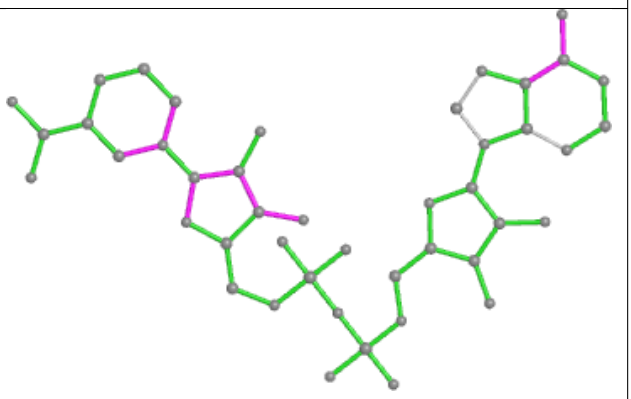


Rings

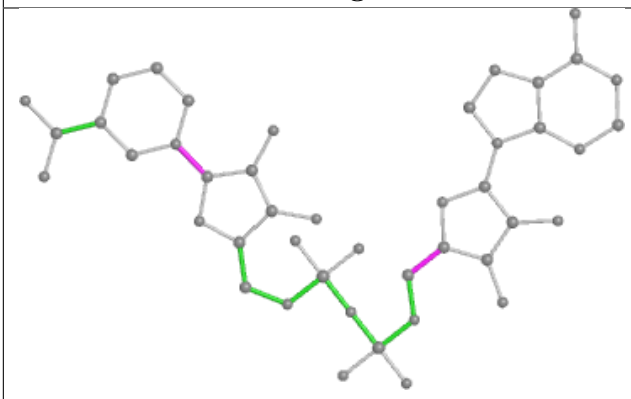
Ligand NAD C 501



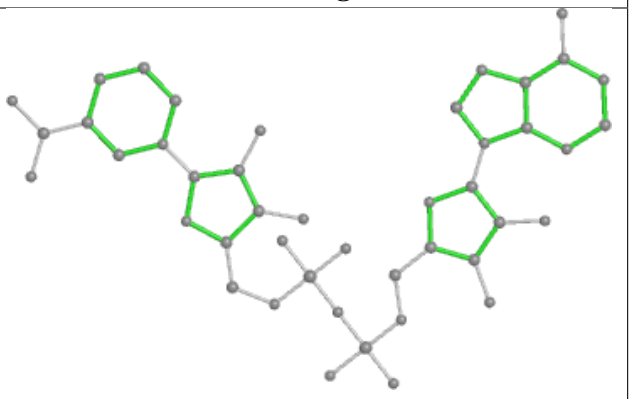
Bond lengths



Bond angles

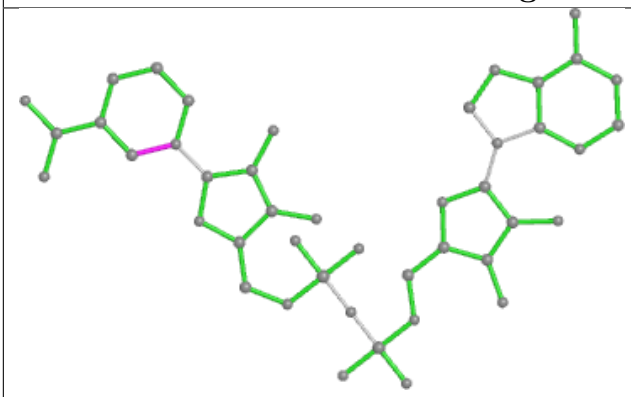


Torsions

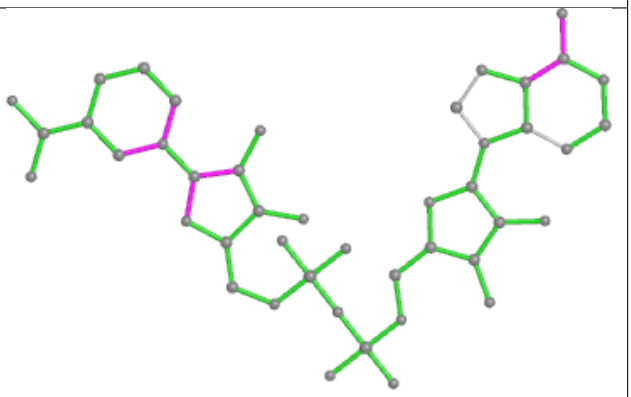


Rings

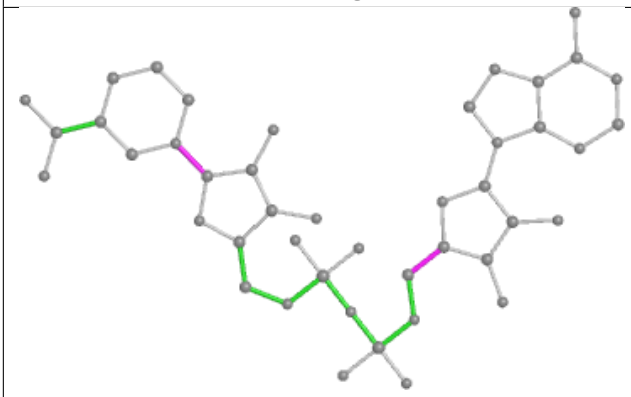
Ligand NAD D 501



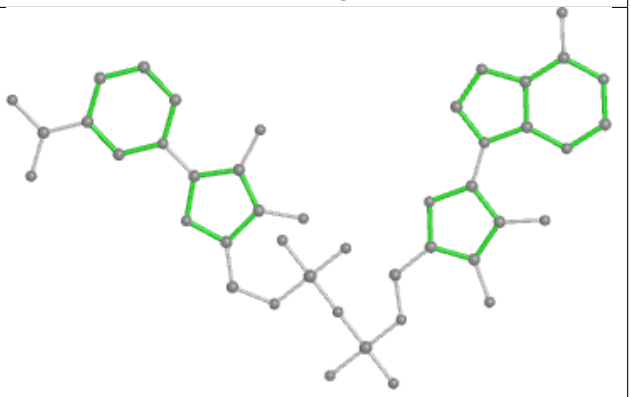
Bond lengths



Bond angles

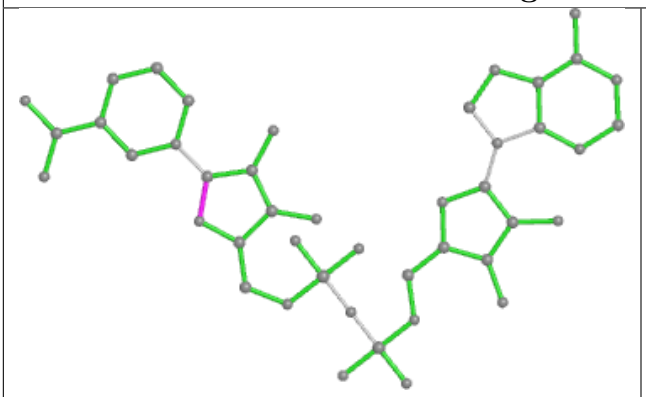


Torsions

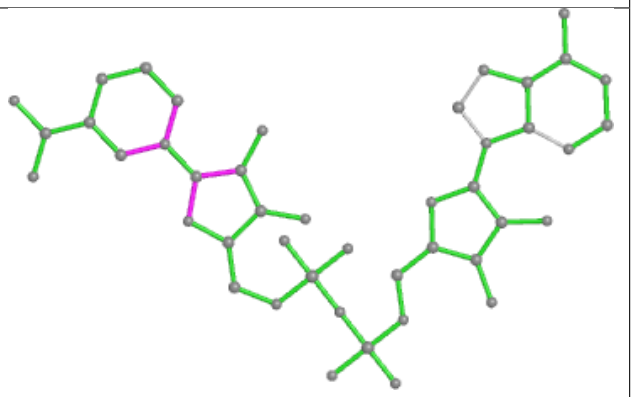


Rings

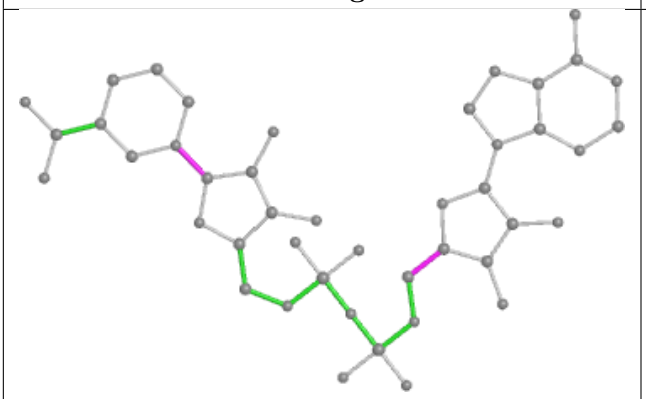
Ligand NAD B 501



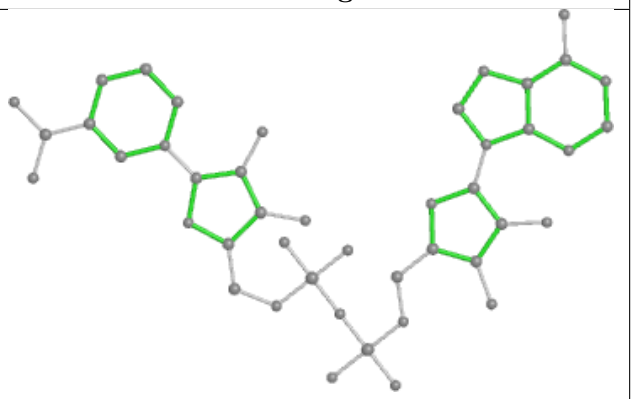
Bond lengths



Bond angles

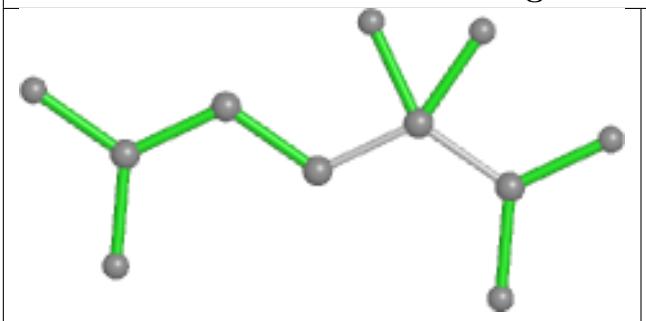


Torsions

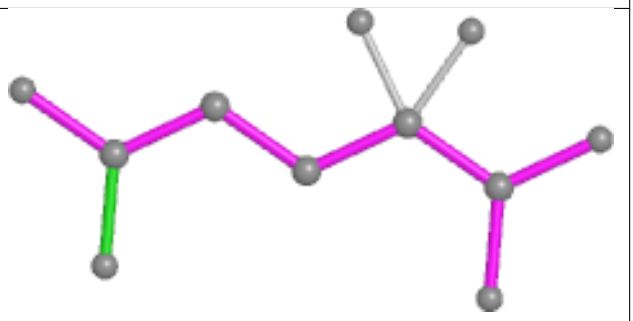


Rings

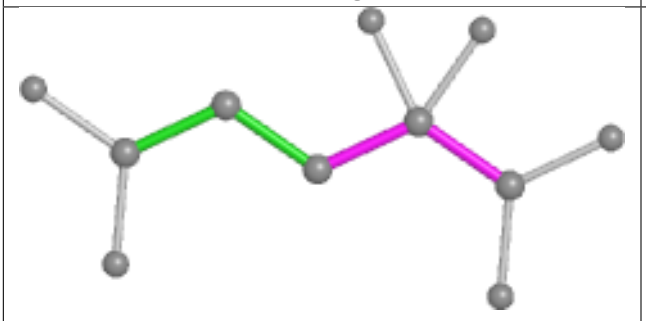
Ligand U5C B 514



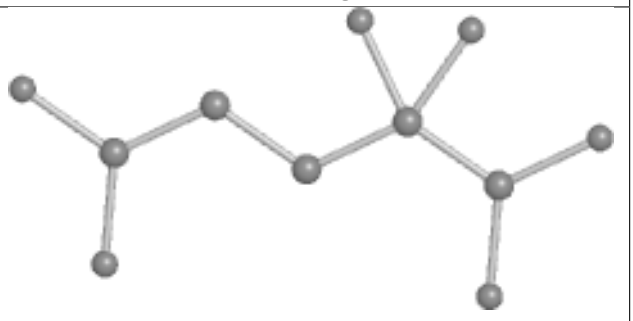
Bond lengths



Bond angles

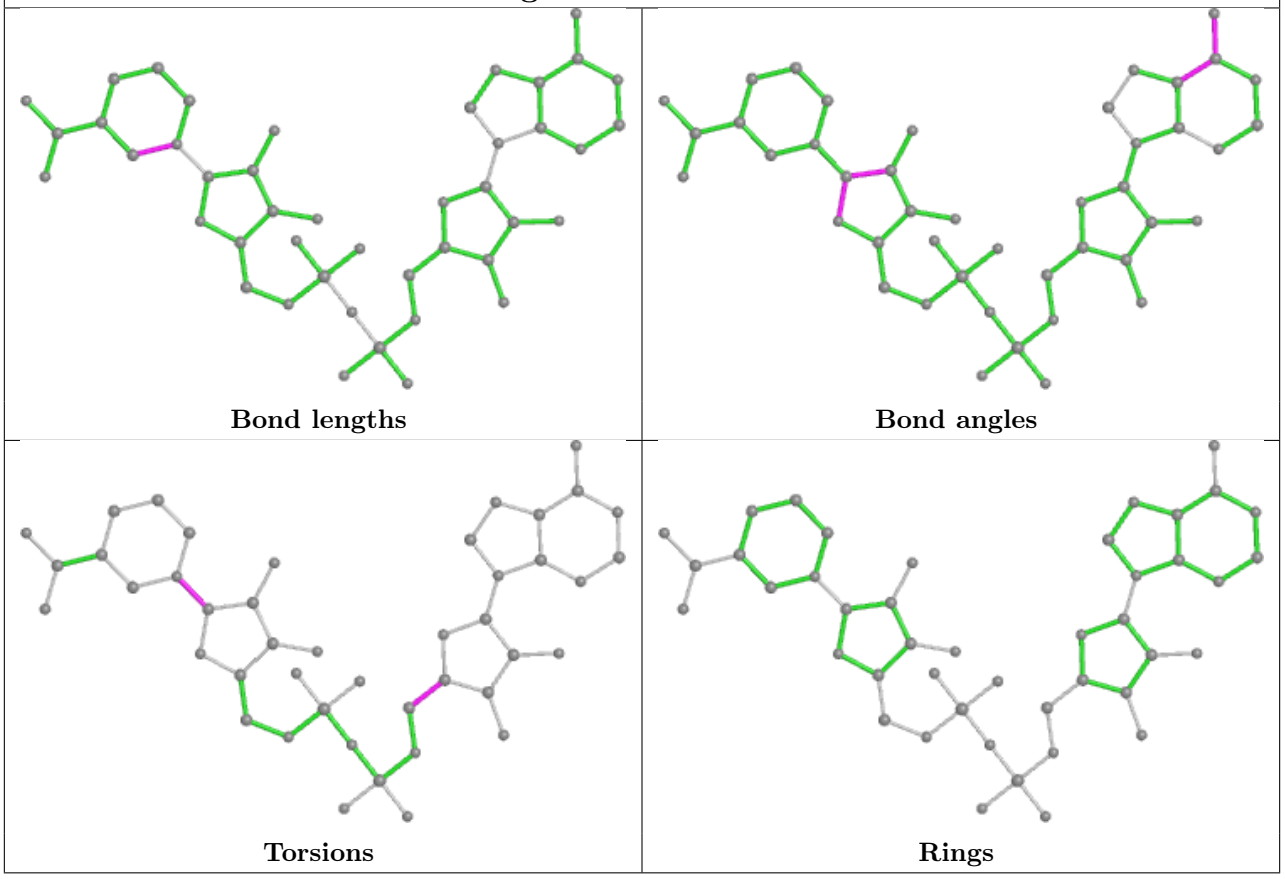


Torsions



Rings

Ligand NAD A 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	412/414 (99%)	-0.48	1 (0%)	95	95	17, 24, 43, 68	0
1	B	412/414 (99%)	-0.53	0	100	100	18, 28, 46, 66	0
1	C	413/414 (99%)	-0.52	0	100	100	19, 26, 42, 59	0
1	D	412/414 (99%)	-0.26	2 (0%)	91	92	20, 34, 58, 80	0
1	E	412/414 (99%)	-0.49	1 (0%)	95	95	19, 26, 47, 66	0
1	F	412/414 (99%)	-0.35	1 (0%)	95	95	20, 31, 59, 81	0
All	All	2473/2484 (99%)	-0.44	5 (0%)	95	95	17, 27, 52, 81	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	204	ILE	3.1
1	F	0	ALA	3.1
1	A	0	ALA	2.5
1	D	193	THR	2.3
1	E	264	ASN	2.2

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

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

6.3 Carbohydrates

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	C	510	6/6	0.60	0.15	62,65,67,79	0
3	GOL	B	510	6/6	0.67	0.21	56,64,68,72	0
3	GOL	E	4207	6/6	0.69	0.20	41,50,53,53	6
3	GOL	D	502	6/6	0.70	0.18	34,46,49,51	0
3	GOL	F	502	6/6	0.70	0.14	38,50,53,53	0
3	GOL	B	503	6/6	0.71	0.14	33,45,49,49	0
3	GOL	A	507	6/6	0.72	0.20	49,54,61,61	0
4	EDO	E	4206	4/4	0.72	0.13	44,46,50,53	0
3	GOL	C	503	6/6	0.73	0.17	36,41,47,48	0
4	EDO	B	504	4/4	0.74	0.11	36,42,47,51	0
8	PEG	B	502	7/7	0.74	0.18	44,48,56,57	0
8	PEG	F	504	7/7	0.74	0.22	45,49,66,70	0
8	PEG	E	4208	7/7	0.76	0.20	32,43,47,56	0
4	EDO	B	505	4/4	0.76	0.14	46,49,52,59	0
3	GOL	A	502	6/6	0.77	0.12	26,41,46,48	0
3	GOL	B	513	6/6	0.77	0.19	46,49,54,58	6
4	EDO	E	4209	4/4	0.77	0.11	61,63,64,68	0
4	EDO	C	506	4/4	0.78	0.12	40,41,42,55	0
8	PEG	B	511	7/7	0.78	0.15	32,40,51,66	0
3	GOL	E	4201	6/6	0.79	0.22	55,60,68,72	0
3	GOL	E	4205	6/6	0.80	0.19	26,36,40,42	6
3	GOL	C	508	6/6	0.80	0.13	33,34,37,42	6
3	GOL	B	512	6/6	0.81	0.17	45,49,56,62	6
8	PEG	D	504	7/7	0.81	0.14	36,55,59,66	0
4	EDO	F	505	4/4	0.82	0.12	36,42,54,60	0
3	GOL	E	4203	6/6	0.82	0.14	28,46,47,50	0
3	GOL	C	511	6/6	0.83	0.20	50,54,63,78	0
3	GOL	D	505	6/6	0.83	0.20	48,59,62,66	0
4	EDO	C	505	4/4	0.84	0.15	52,56,56,58	0
4	EDO	F	503	4/4	0.84	0.09	41,45,46,51	0
4	EDO	C	509	4/4	0.85	0.14	35,40,45,48	0
3	GOL	A	506	6/6	0.85	0.14	44,48,53,57	0
8	PEG	C	504	7/7	0.86	0.20	38,45,51,55	0
3	GOL	A	504	6/6	0.86	0.14	39,47,51,54	6
3	GOL	A	503	6/6	0.86	0.17	35,36,39,40	6
3	GOL	C	507	6/6	0.86	0.20	41,51,60,66	0
3	GOL	B	507	6/6	0.87	0.15	35,40,54,54	6

Continued on next page...

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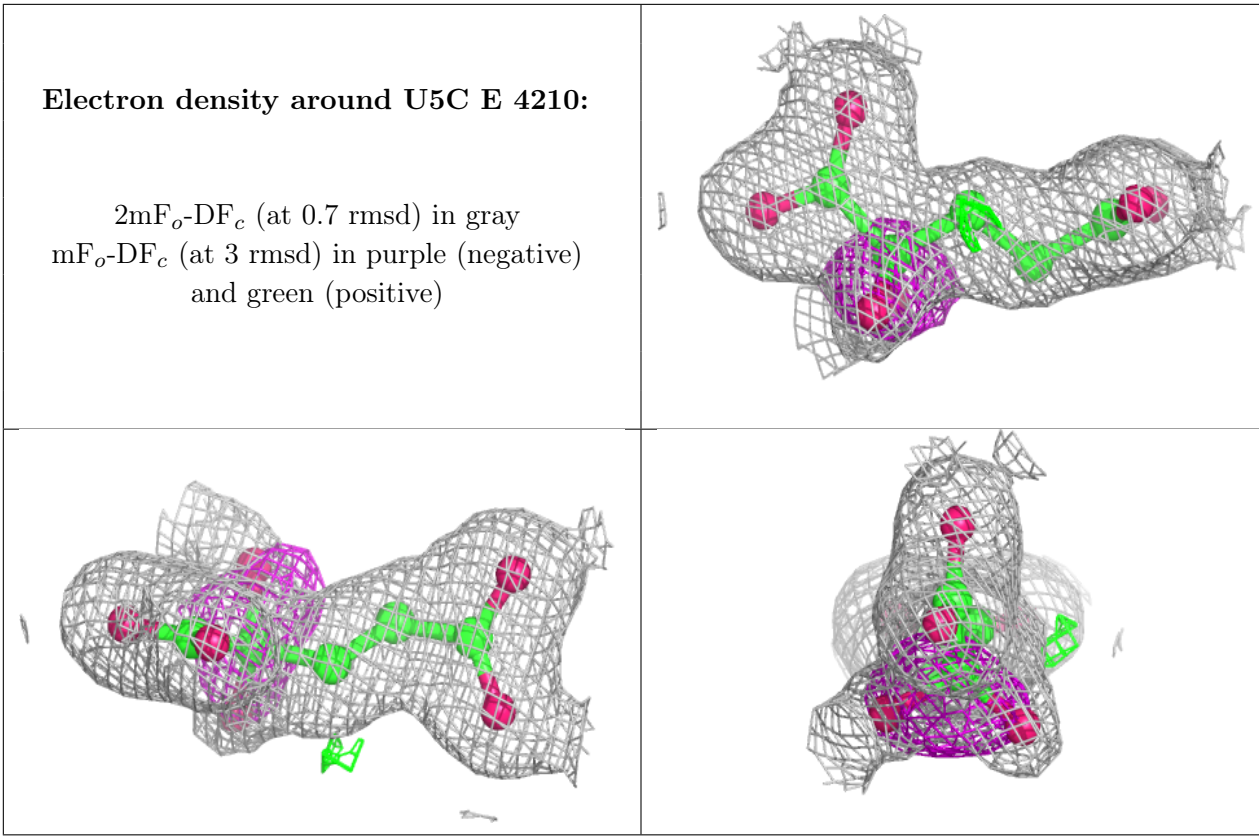
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	508	6/6	0.88	0.14	30,35,40,40	6
8	PEG	C	502	7/7	0.88	0.15	35,48,59,61	0
3	GOL	A	509	6/6	0.89	0.17	26,45,51,51	0
3	GOL	D	503	6/6	0.89	0.11	39,42,46,48	6
5	U5C	E	4210	11/11	0.91	0.11	21,28,39,41	0
5	U5C	F	506	11/11	0.91	0.14	26,31,47,51	0
5	U5C	D	506	11/11	0.91	0.15	25,32,47,48	0
3	GOL	B	506	6/6	0.92	0.21	47,55,58,64	0
5	U5C	A	508	11/11	0.92	0.13	20,25,40,41	0
4	EDO	A	505	4/4	0.92	0.21	31,40,50,52	0
4	EDO	B	509	4/4	0.93	0.23	36,46,50,51	0
5	U5C	C	512	11/11	0.93	0.12	20,28,42,43	0
4	EDO	E	4204	4/4	0.94	0.14	34,47,57,58	0
5	U5C	B	514	11/11	0.95	0.13	22,28,46,48	0
2	NAD	F	501	44/44	0.97	0.07	23,28,34,39	0
7	NA	B	516	1/1	0.97	0.08	30,30,30,30	0
2	NAD	D	501	44/44	0.97	0.08	24,29,35,37	0
2	NAD	B	501	44/44	0.98	0.07	19,24,31,35	0
2	NAD	C	501	44/44	0.98	0.07	19,23,29,32	0
7	NA	C	514	1/1	0.98	0.07	33,33,33,33	0
2	NAD	A	501	44/44	0.98	0.07	18,22,27,30	0
2	NAD	E	4202	44/44	0.98	0.07	18,23,29,34	0
7	NA	A	511	1/1	0.99	0.07	34,34,34,34	0
6	CA	B	515	1/1	0.99	0.10	22,22,22,22	0
6	CA	A	510	1/1	1.00	0.08	17,17,17,17	0
6	CA	C	513	1/1	1.00	0.07	20,20,20,20	0
6	CA	D	507	1/1	1.00	0.07	21,21,21,21	0
6	CA	E	4211	1/1	1.00	0.07	19,19,19,19	0
6	CA	F	507	1/1	1.00	0.10	19,19,19,19	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.

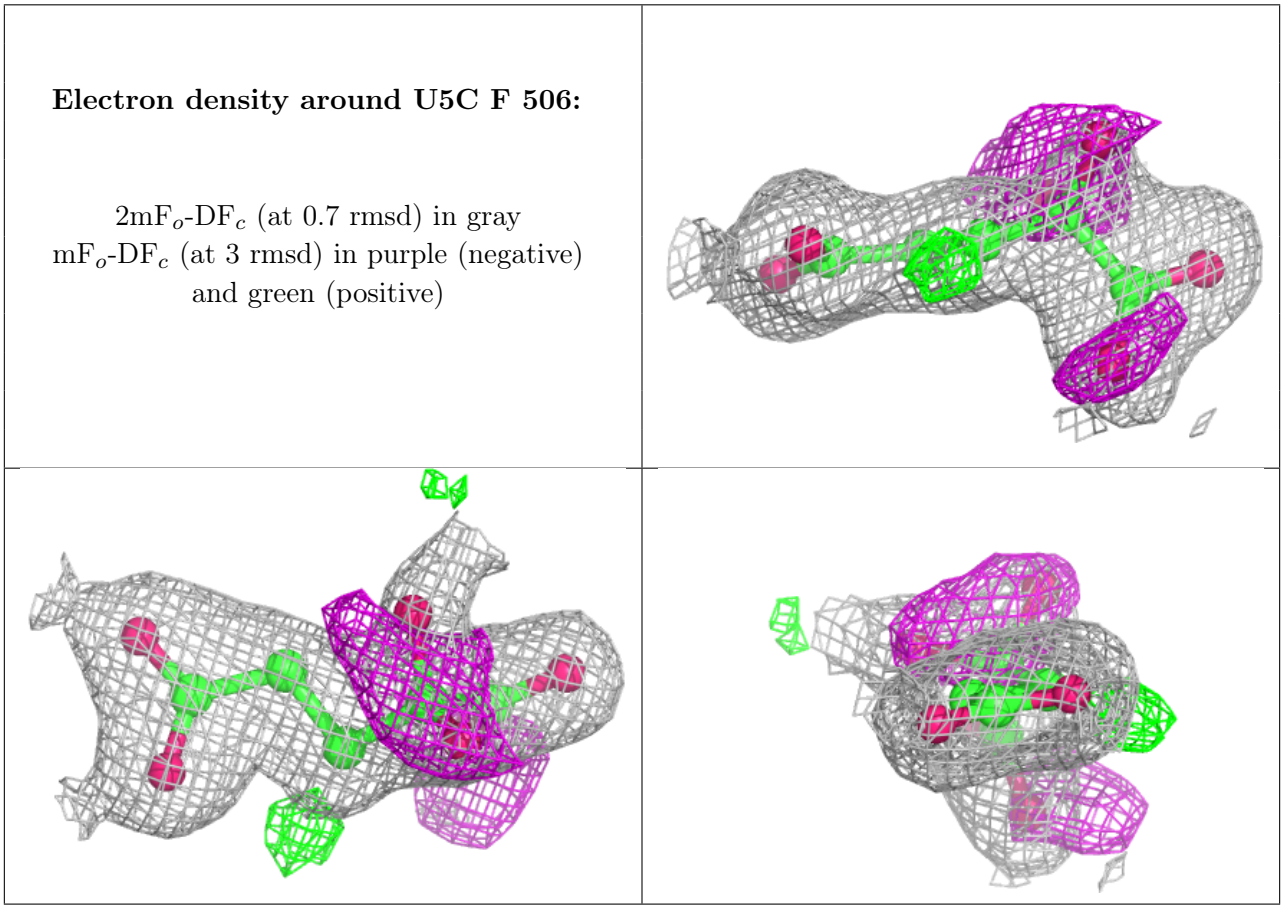
Electron density around U5C E 4210:

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



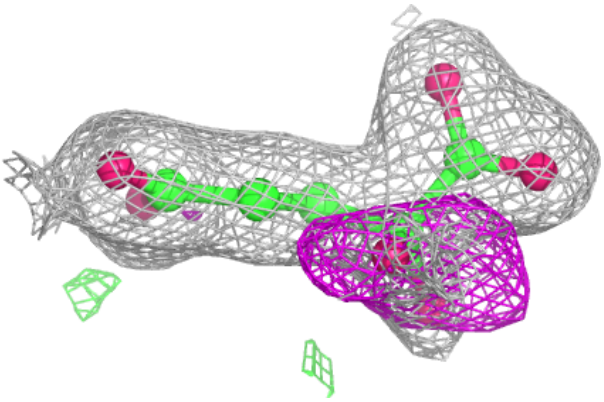
Electron density around U5C F 506:

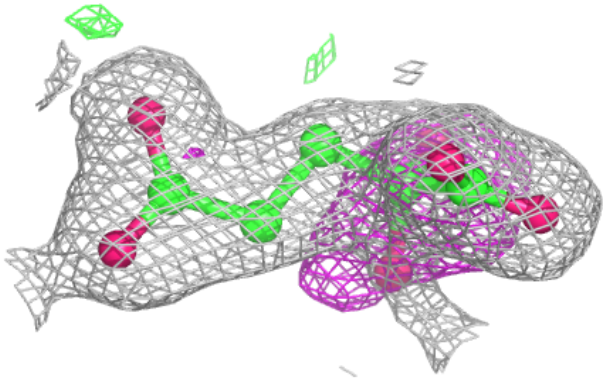
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

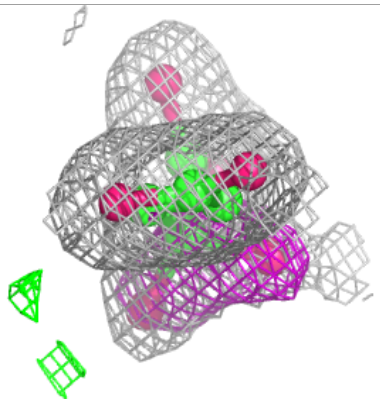


Electron density around U5C D 506:

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

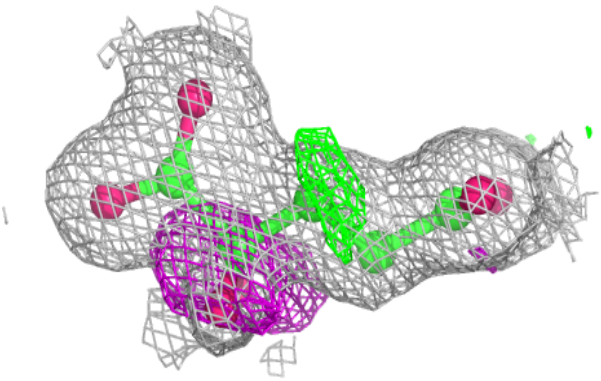


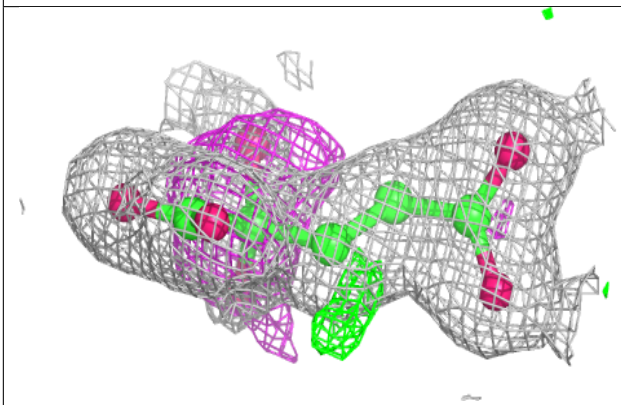


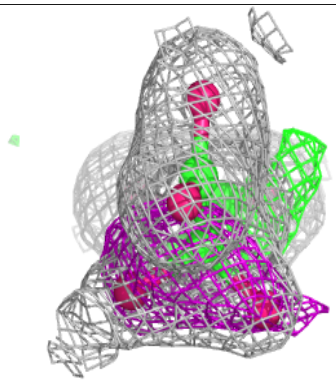


Electron density around U5C A 508:

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

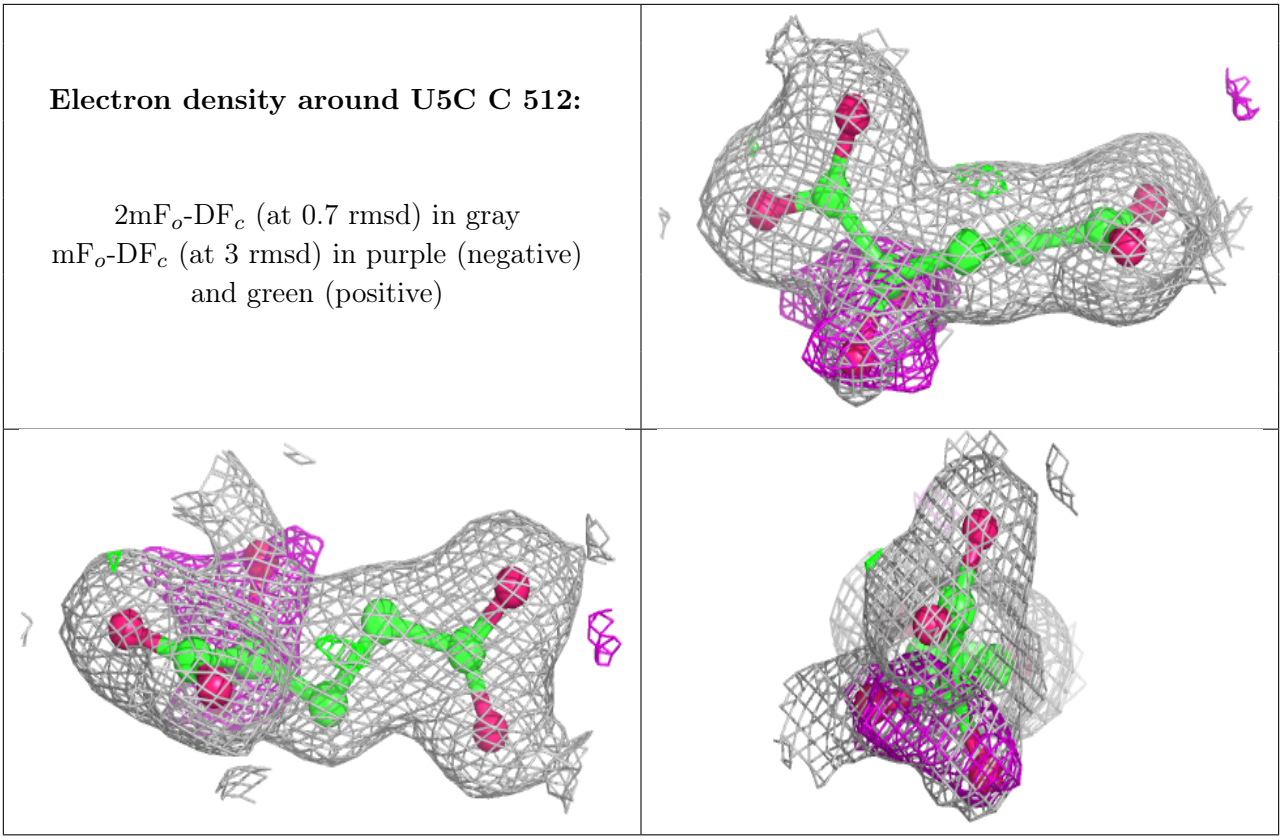






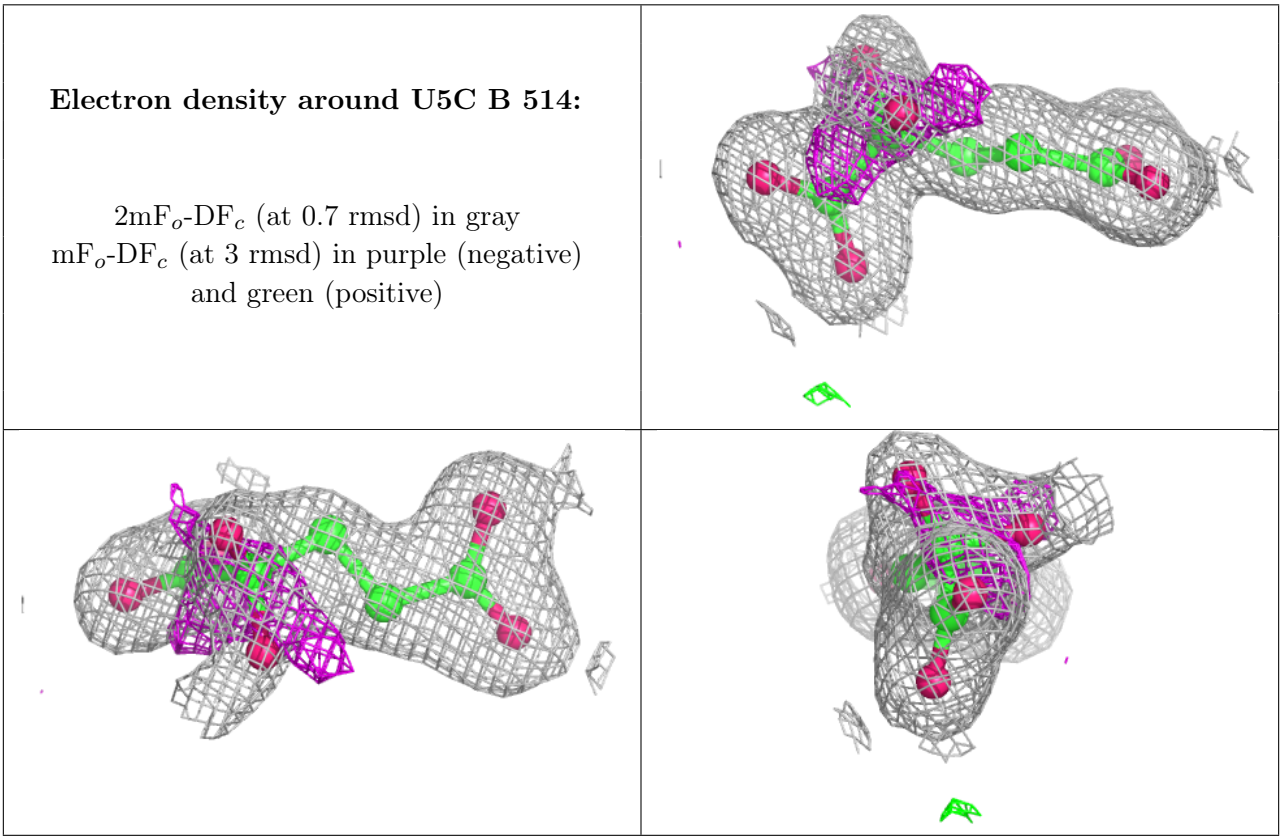
Electron density around U5C C 512:

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



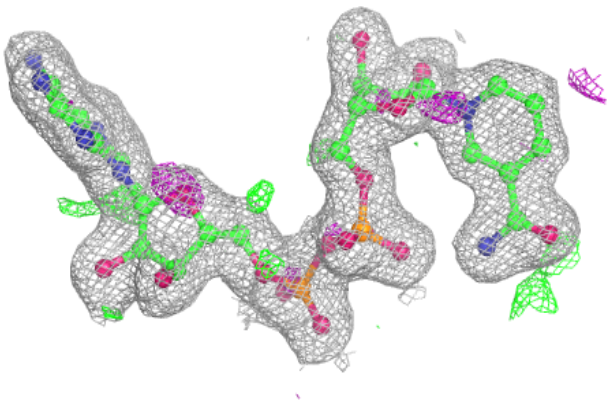
Electron density around U5C B 514:

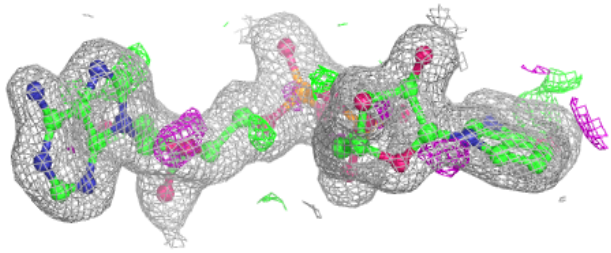
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

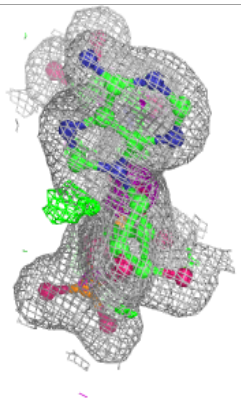


Electron density around NAD F 501:

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

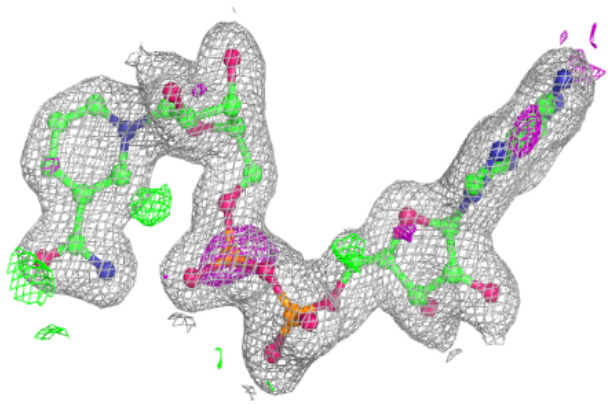


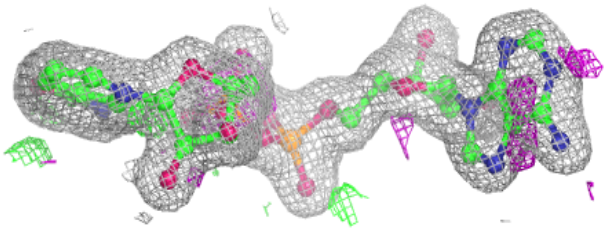


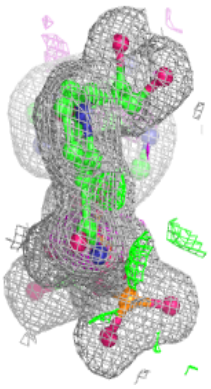


Electron density around NAD D 501:

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

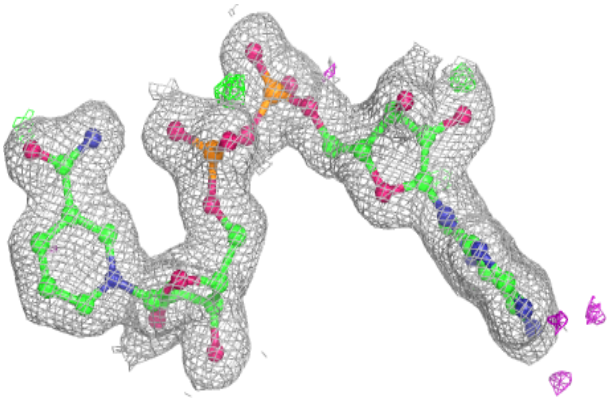


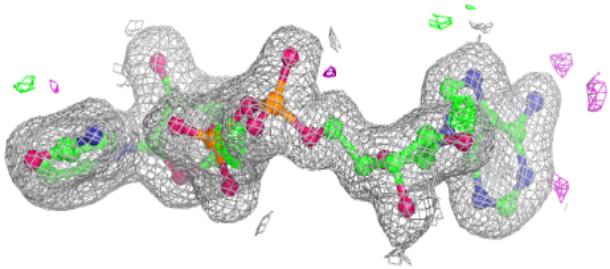


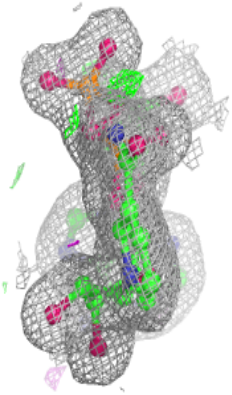


Electron density around NAD B 501:

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

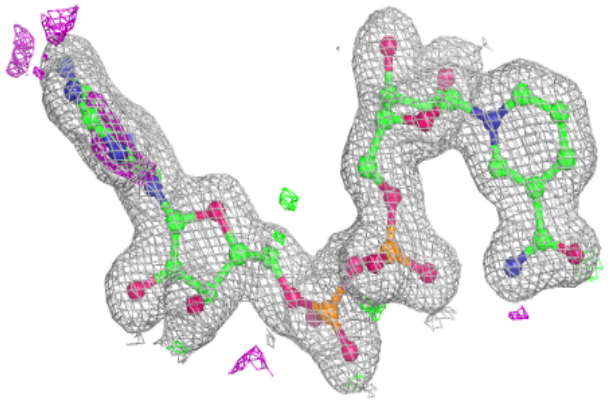


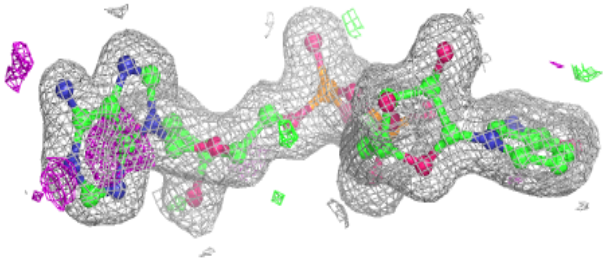


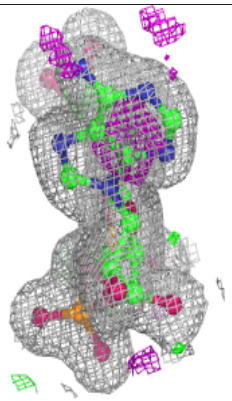


Electron density around NAD C 501:

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

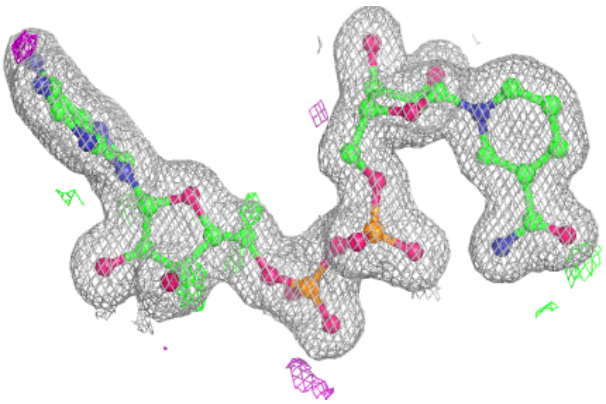


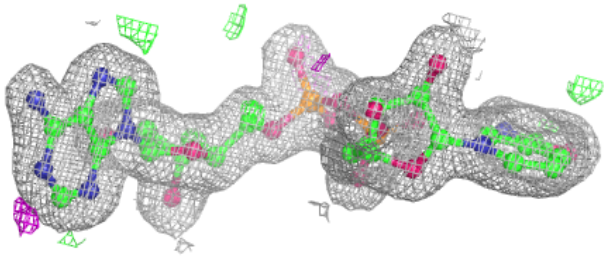


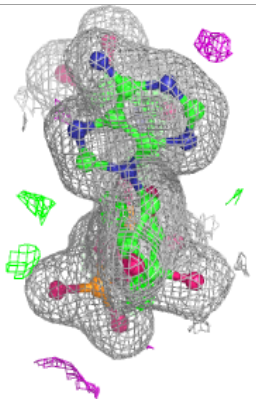


Electron density around NAD A 501:

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

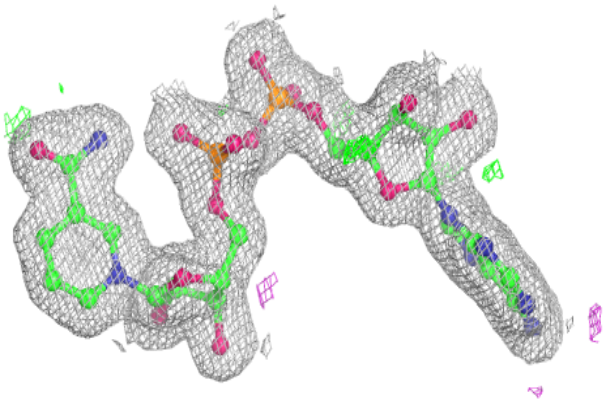


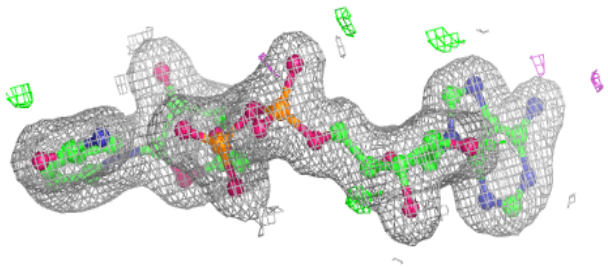


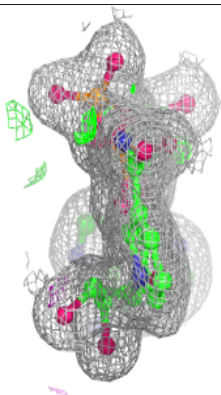


Electron density around NAD E 4202:

$2mF_o$-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.