



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:27 AM UTC

PDB ID : 8OWM / pdb_00008owm
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

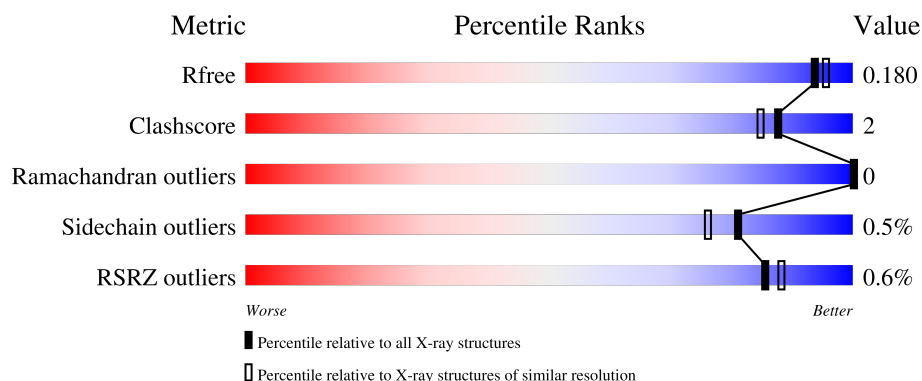
1 Overall quality at a glance

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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 $\leq 5\%$. 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	94% 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:

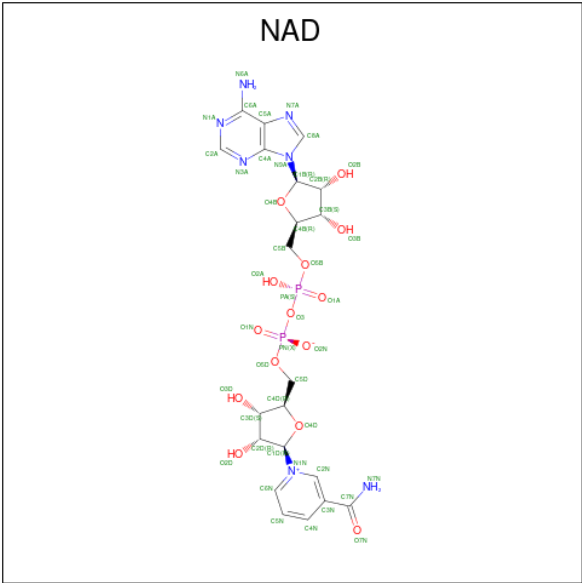
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q38946
A	-1	ASN	-	expression tag	UNP Q38946
A	0	ALA	-	expression tag	UNP Q38946
B	-2	SER	-	expression tag	UNP Q38946
B	-1	ASN	-	expression tag	UNP Q38946
B	0	ALA	-	expression tag	UNP Q38946
C	-2	SER	-	expression tag	UNP Q38946
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 (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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 (CCD ID: GOL) (formula: C₃H₈O₃).



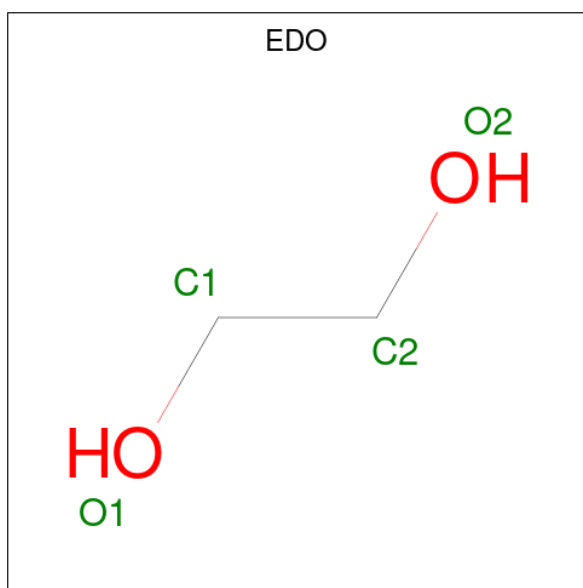
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total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

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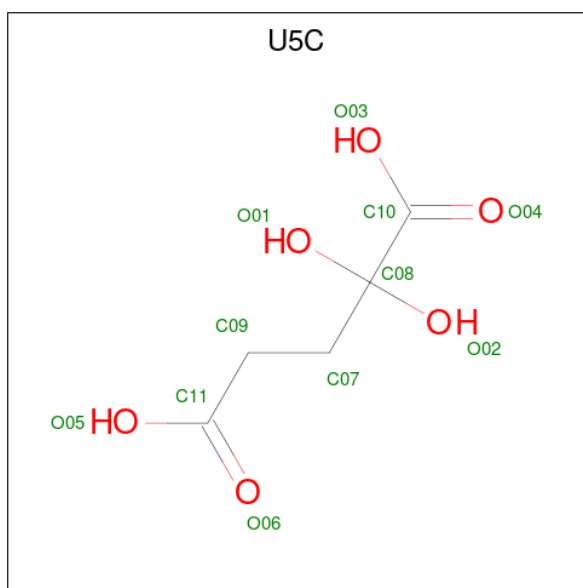
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: 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 (CCD ID: U5C) (formula: C₅H₈O₆) (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 (CCD ID: 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 (CCD ID: 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 (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 9 is water.

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

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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



- Molecule 1: Glutamate dehydrogenase 2



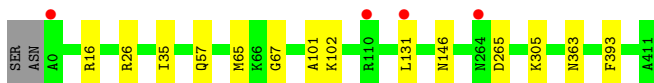
- Molecule 1: Glutamate dehydrogenase 2



- Molecule 1: Glutamate dehydrogenase 2



- Molecule 1: Glutamate dehydrogenase 2



- Molecule 1: Glutamate dehydrogenase 2



4 Data and refinement statistics

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 65.70 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.0 (65.70-1.70) 97.0 (65.70-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, R_{free}	0.144 , 0.172 0.154 , 0.180	Depositor DCC
R_{free} test set	3189 reflections (0.97%)	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)	0.38 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: NA, PEG, U5C, EDO, GOL, CA, NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.45	0/3288	0.61	0/4448
1	B	0.41	0/3238	0.58	0/4382
1	C	0.43	0/3293	0.60	0/4453
1	D	0.42	0/3264	0.56	0/4416
1	E	0.43	0/3289	0.59	0/4449
1	F	0.41	0/3224	0.57	0/4364
All	All	0.42	0/19596	0.59	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 [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	3225	0	3204	14	0
1	B	3175	0	3158	11	0
1	C	3230	0	3212	17	0
1	D	3201	0	3186	9	0
1	E	3226	0	3213	12	0
1	F	3161	0	3142	11	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	2	0
5	E	11	0	0	1	0
5	F	11	0	0	2	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	5	0
9	B	358	0	0	1	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	78	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 (78) 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:A:255:LYS:NZ	9:A:604:HOH:O	2.41	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:36:LYS:CE	9:F:759:HOH:O	2.63	0.46
1:B:67:GLY:HA3	1:B:101:ALA:O	2.15	0.46
1:F:316:ASP:OD1	1:F:316:ASP:C	2.60	0.45
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:D:277:LEU:C	1:D:277:LEU:HD13	2.42	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: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:F:66:LYS:NZ	5:F:506:U5C:O05	2.52	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:C:277:LEU:HD13	1:C:277:LEU:C	2.45	0.41
1:D:153:ILE:HG21	1:D:168[B]:VAL:HG21	2.03	0.41
1:C:275:ASP:C	1:C:275:ASP:OD1	2.63	0.41
1:B:316:ASP:OD1	1:B:316:ASP:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:208:THR:HA	1:F:231:LYS:O	2.21	0.41
1:B:50:SER:O	1:E:26[B]:ARG:NH1	2.51	0.40
1:D:66:LYS:NZ	5:D:506:U5C:O05	2.52	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%)	78	72
1	B	333/332 (100%)	332 (100%)	1 (0%)	86	83
1	C	339/332 (102%)	338 (100%)	1 (0%)	86	83
1	D	336/332 (101%)	333 (99%)	3 (1%)	70	62
1	E	338/332 (102%)	337 (100%)	1 (0%)	86	83
1	F	332/332 (100%)	331 (100%)	1 (0%)	86	83
All	All	2017/1992 (101%)	2008 (100%)	9 (0%)	81	80

All (9) 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	211	ILE
1	D	393	PHE
1	E	393	PHE
1	F	393	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	205	GLN
1	A	212	GLN
1	B	81	ASN
1	B	212	GLN
1	B	384	HIS
1	C	81	ASN
1	C	226	HIS
1	C	264	ASN
1	C	375	HIS
1	D	212	GLN
1	D	376	ASN
1	E	81	ASN
1	E	212	GLN
1	F	81	ASN
1	F	212	GLN

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Mol	Chain	Res	Type
1	F	273	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
4	EDO	C	509	-	3,3,3	0.42	0	2,2,2	0.64	0
4	EDO	B	504	-	3,3,3	0.60	0	2,2,2	0.24	0
4	EDO	A	505	-	3,3,3	0.35	0	2,2,2	0.76	0
2	NAD	D	501	-	46,48,48	0.81	2 (4%)	64,73,73	0.67	1 (1%)
3	GOL	B	512	7	5,5,5	0.71	0	5,5,5	0.94	0
8	PEG	B	511	-	6,6,6	0.25	0	5,5,5	0.11	0
3	GOL	D	502	-	5,5,5	1.27	0	5,5,5	1.06	0
3	GOL	C	503	-	5,5,5	1.29	0	5,5,5	1.10	0
4	EDO	F	505	-	3,3,3	0.50	0	2,2,2	0.31	0
2	NAD	F	501	-	46,48,48	0.74	2 (4%)	64,73,73	0.77	2 (3%)
3	GOL	C	511	7	5,5,5	0.94	0	5,5,5	1.11	1 (20%)
3	GOL	D	505	7	5,5,5	1.20	0	5,5,5	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PEG	E	4208	-	6,6,6	0.18	0	5,5,5	0.11	0
4	EDO	E	4204	-	3,3,3	0.46	0	2,2,2	0.24	0
3	GOL	E	4205	-	5,5,5	0.76	0	5,5,5	1.38	1 (20%)
4	EDO	E	4206	-	3,3,3	0.69	0	2,2,2	0.18	0
2	NAD	E	4202	-	46,48,48	0.54	0	64,73,73	0.73	1 (1%)
5	U5C	B	514	-	8,10,10	1.03	0	9,14,14	2.92	5 (55%)
3	GOL	B	510	-	5,5,5	0.91	0	5,5,5	1.15	0
3	GOL	A	509	-	5,5,5	1.45	1 (20%)	5,5,5	0.67	0
5	U5C	D	506	-	8,10,10	1.37	1 (12%)	9,14,14	1.98	2 (22%)
8	PEG	B	502	-	6,6,6	0.18	0	5,5,5	0.18	0
4	EDO	B	505	-	3,3,3	0.50	0	2,2,2	0.44	0
2	NAD	B	501	-	46,48,48	0.63	1 (2%)	64,73,73	0.71	1 (1%)
2	NAD	A	501	-	46,48,48	0.61	1 (2%)	64,73,73	0.75	0
3	GOL	B	513	7	5,5,5	1.03	0	5,5,5	1.19	1 (20%)
3	GOL	C	510	-	5,5,5	1.20	0	5,5,5	0.97	0
3	GOL	C	507	-	5,5,5	1.00	0	5,5,5	1.11	0
3	GOL	D	503	-	5,5,5	1.04	0	5,5,5	1.06	0
4	EDO	C	506	-	3,3,3	0.54	0	2,2,2	0.34	0
3	GOL	B	507	-	5,5,5	0.86	0	5,5,5	0.92	0
4	EDO	B	509	-	3,3,3	0.30	0	2,2,2	0.51	0
8	PEG	D	504	-	6,6,6	0.19	0	5,5,5	0.13	0
5	U5C	C	512	-	8,10,10	1.11	0	9,14,14	3.10	5 (55%)
8	PEG	F	504	-	6,6,6	0.16	0	5,5,5	0.13	0
3	GOL	A	502	-	5,5,5	1.10	0	5,5,5	1.26	0
8	PEG	C	504	-	6,6,6	0.21	0	5,5,5	0.14	0
3	GOL	A	506	-	5,5,5	1.00	0	5,5,5	0.86	0
3	GOL	B	503	-	5,5,5	1.07	0	5,5,5	1.31	0
4	EDO	F	503	-	3,3,3	0.51	0	2,2,2	0.42	0
5	U5C	A	508	-	8,10,10	1.16	0	9,14,14	2.40	3 (33%)
3	GOL	E	4201	7	5,5,5	1.00	0	5,5,5	1.07	0
8	PEG	C	502	-	6,6,6	0.13	0	5,5,5	0.09	0
5	U5C	E	4210	-	8,10,10	1.60	1 (12%)	9,14,14	1.43	1 (11%)
3	GOL	B	506	-	5,5,5	1.04	0	5,5,5	0.93	0
3	GOL	A	504	-	5,5,5	1.20	0	5,5,5	0.74	0
4	EDO	E	4209	-	3,3,3	0.46	0	2,2,2	0.31	0
4	EDO	C	505	-	3,3,3	0.51	0	2,2,2	0.39	0
2	NAD	C	501	-	46,48,48	0.70	1 (2%)	64,73,73	0.76	2 (3%)
3	GOL	F	502	-	5,5,5	1.14	0	5,5,5	0.96	0
3	GOL	E	4207	-	5,5,5	0.96	0	5,5,5	1.23	1 (20%)
3	GOL	A	507	7	5,5,5	0.94	0	5,5,5	1.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	B	508	-	5,5,5	1.06	0	5,5,5	1.51	1 (20%)
3	GOL	C	508	-	5,5,5	1.27	0	5,5,5	1.35	1 (20%)
3	GOL	E	4203	-	5,5,5	1.00	0	5,5,5	1.19	0
3	GOL	A	503	-	5,5,5	1.00	0	5,5,5	0.96	0
5	U5C	F	506	-	8,10,10	1.27	0	9,14,14	2.13	1 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	509	-	-	0/1/1/1	-
4	EDO	B	504	-	-	1/1/1/1	-
4	EDO	A	505	-	-	0/1/1/1	-
2	NAD	D	501	-	-	3/30/62/62	0/5/5/5
3	GOL	B	512	7	-	4/4/4/4	-
8	PEG	B	511	-	-	0/4/4/4	-
3	GOL	D	502	-	-	3/4/4/4	-
3	GOL	C	503	-	-	2/4/4/4	-
4	EDO	F	505	-	-	1/1/1/1	-
2	NAD	F	501	-	-	3/30/62/62	0/5/5/5
3	GOL	C	511	7	-	0/4/4/4	-
3	GOL	D	505	7	-	2/4/4/4	-
8	PEG	E	4208	-	-	1/4/4/4	-
4	EDO	E	4204	-	-	1/1/1/1	-
3	GOL	E	4205	-	-	0/4/4/4	-
4	EDO	E	4206	-	-	1/1/1/1	-
2	NAD	E	4202	-	-	4/30/62/62	0/5/5/5
5	U5C	B	514	-	-	9/12/12/12	-
3	GOL	B	510	-	-	1/4/4/4	-
3	GOL	A	509	-	-	2/4/4/4	-
5	U5C	D	506	-	-	6/12/12/12	-
8	PEG	B	502	-	-	1/4/4/4	-
4	EDO	B	505	-	-	1/1/1/1	-
2	NAD	B	501	-	-	3/30/62/62	0/5/5/5
2	NAD	A	501	-	-	3/30/62/62	0/5/5/5
3	GOL	B	513	7	-	0/4/4/4	-
3	GOL	C	510	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	507	-	-	2/4/4/4	-
3	GOL	D	503	-	-	4/4/4/4	-
4	EDO	C	506	-	-	1/1/1/1	-
3	GOL	B	507	-	-	2/4/4/4	-
4	EDO	B	509	-	-	0/1/1/1	-
8	PEG	D	504	-	-	2/4/4/4	-
5	U5C	C	512	-	-	9/12/12/12	-
8	PEG	F	504	-	-	0/4/4/4	-
3	GOL	A	502	-	-	2/4/4/4	-
8	PEG	C	504	-	-	0/4/4/4	-
3	GOL	A	506	-	-	2/4/4/4	-
3	GOL	B	503	-	-	3/4/4/4	-
4	EDO	F	503	-	-	1/1/1/1	-
5	U5C	A	508	-	-	11/12/12/12	-
3	GOL	E	4201	7	-	2/4/4/4	-
8	PEG	C	502	-	-	1/4/4/4	-
5	U5C	E	4210	-	-	7/12/12/12	-
3	GOL	B	506	-	-	1/4/4/4	-
3	GOL	A	504	-	-	2/4/4/4	-
4	EDO	E	4209	-	-	0/1/1/1	-
4	EDO	C	505	-	-	0/1/1/1	-
2	NAD	C	501	-	-	3/30/62/62	0/5/5/5
3	GOL	F	502	-	-	2/4/4/4	-
3	GOL	E	4207	-	-	2/4/4/4	-
3	GOL	A	507	7	-	0/4/4/4	-
3	GOL	B	508	-	-	3/4/4/4	-
3	GOL	C	508	-	-	2/4/4/4	-
3	GOL	E	4203	-	-	3/4/4/4	-
3	GOL	A	503	-	-	4/4/4/4	-
5	U5C	F	506	-	-	6/12/12/12	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	NAD	C2N-N1N	3.62	1.39	1.35
2	F	501	NAD	C2N-N1N	2.87	1.38	1.35
2	C	501	NAD	C2N-N1N	2.77	1.38	1.35
2	A	501	NAD	C2N-N1N	2.72	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	NAD	O4D-C1D	2.58	1.44	1.40
3	A	509	GOL	C3-C2	2.46	1.61	1.51
2	D	501	NAD	PN-O3	2.42	1.62	1.59
2	B	501	NAD	O4D-C1D	2.35	1.44	1.40
5	D	506	U5C	O05-C11	-2.19	1.23	1.30
5	E	4210	U5C	O01-C08	2.10	1.42	1.39

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	506	U5C	C09-C07-C08	-6.02	100.51	117.46
5	C	512	U5C	C09-C07-C08	-5.92	100.79	117.46
5	B	514	U5C	C09-C07-C08	-5.72	101.36	117.46
5	D	506	U5C	C09-C07-C08	-4.81	103.92	117.46
5	B	514	U5C	O04-C10-C08	-4.60	115.79	123.77
5	C	512	U5C	O04-C10-C08	-4.45	116.06	123.77
5	A	508	U5C	O04-C10-C08	-4.24	116.42	123.77
5	C	512	U5C	O03-C10-C08	4.14	122.10	113.70
5	A	508	U5C	C09-C07-C08	-3.88	106.55	117.46
5	B	514	U5C	O03-C10-C08	3.58	120.97	113.70
5	E	4210	U5C	C09-C07-C08	-3.41	107.87	117.46
5	A	508	U5C	O03-C10-C08	3.09	119.97	113.70
2	F	501	NAD	C6N-N1N-C2N	-2.73	119.55	121.88
3	E	4205	GOL	C3-C2-C1	-2.71	101.86	111.80
3	B	508	GOL	C3-C2-C1	-2.70	101.90	111.80
5	C	512	U5C	O05-C11-C09	2.70	122.52	114.00
2	E	4202	NAD	C6N-N1N-C2N	-2.64	119.63	121.88
2	C	501	NAD	C6N-N1N-C2N	-2.32	119.90	121.88
3	C	508	GOL	C3-C2-C1	-2.31	103.33	111.80
5	B	514	U5C	O05-C11-C09	2.27	121.17	114.00
5	C	512	U5C	O06-C11-C09	-2.26	115.92	123.09
2	B	501	NAD	C6N-N1N-C2N	-2.26	119.96	121.88
2	F	501	NAD	C3B-C2B-C1B	-2.17	97.35	101.46
5	D	506	U5C	O03-C10-C08	2.16	118.09	113.70
3	B	513	GOL	C3-C2-C1	-2.12	104.02	111.80
2	D	501	NAD	C6N-N1N-C2N	-2.10	120.09	121.88
3	E	4207	GOL	C3-C2-C1	-2.07	104.22	111.80
2	C	501	NAD	O3D-C3D-C2D	-2.06	105.22	111.82
3	C	511	GOL	C3-C2-C1	-2.02	104.39	111.80
5	B	514	U5C	O06-C11-C09	-2.02	116.70	123.09

There are no chirality outliers.

All (131) 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
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	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

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Mol	Chain	Res	Type	Atoms
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
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	502	GOL	C1-C2-C3-O3
3	D	503	GOL	O1-C1-C2-C3
3	D	503	GOL	C1-C2-C3-O3
3	D	505	GOL	C1-C2-C3-O3
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

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Mol	Chain	Res	Type	Atoms
3	B	512	GOL	O1-C1-C2-O2
3	C	503	GOL	O2-C2-C3-O3
3	D	502	GOL	O2-C2-C3-O3
3	E	4207	GOL	O1-C1-C2-O2
3	F	502	GOL	O1-C1-C2-O2
8	D	504	PEG	O2-C3-C4-O4
4	B	504	EDO	O1-C1-C2-O2
4	E	4204	EDO	O1-C1-C2-O2
4	F	505	EDO	O1-C1-C2-O2
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	C	506	EDO	O1-C1-C2-O2
4	E	4206	EDO	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
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
3	E	4203	GOL	O1-C1-C2-C3
3	E	4203	GOL	C1-C2-C3-O3
4	B	505	EDO	O1-C1-C2-O2
4	F	503	EDO	O1-C1-C2-O2
5	F	506	U5C	O01-C08-C10-O03
8	E	4208	PEG	O2-C3-C4-O4
3	A	503	GOL	O1-C1-C2-O2
3	B	508	GOL	O1-C1-C2-O2
3	B	512	GOL	O2-C2-C3-O3
8	D	504	PEG	C4-C3-O2-C2
8	C	502	PEG	C4-C3-O2-C2
2	E	4202	NAD	C2D-C1D-N1N-C2N
5	D	506	U5C	O01-C08-C10-O03
3	D	505	GOL	O2-C2-C3-O3
5	A	508	U5C	C07-C09-C11-O06
5	A	508	U5C	C07-C09-C11-O05

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Mol	Chain	Res	Type	Atoms
5	E	4210	U5C	C07-C09-C11-O05
3	B	503	GOL	O1-C1-C2-O2
3	B	508	GOL	O2-C2-C3-O3
5	E	4210	U5C	C07-C09-C11-O06
8	B	502	PEG	O2-C3-C4-O4

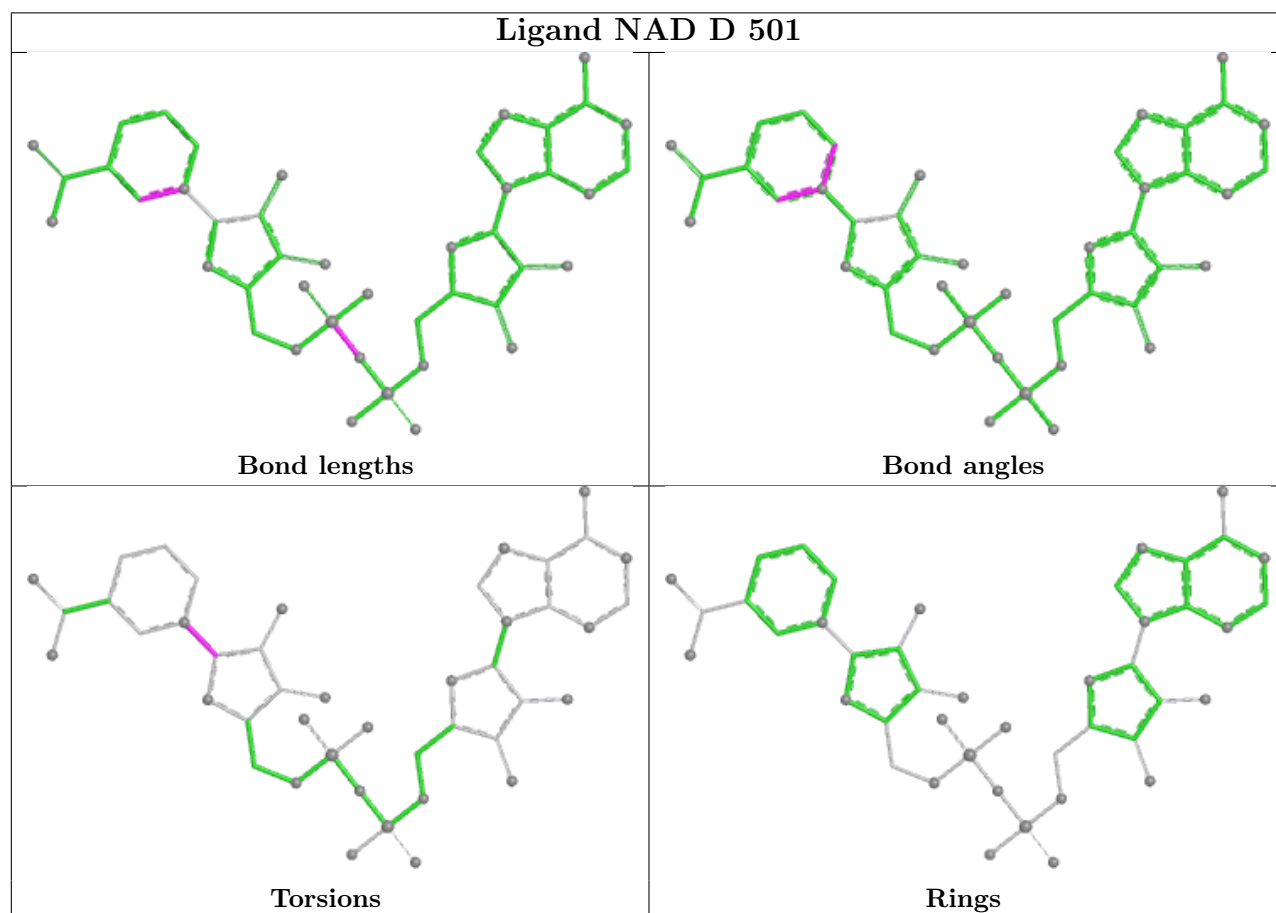
There are no ring outliers.

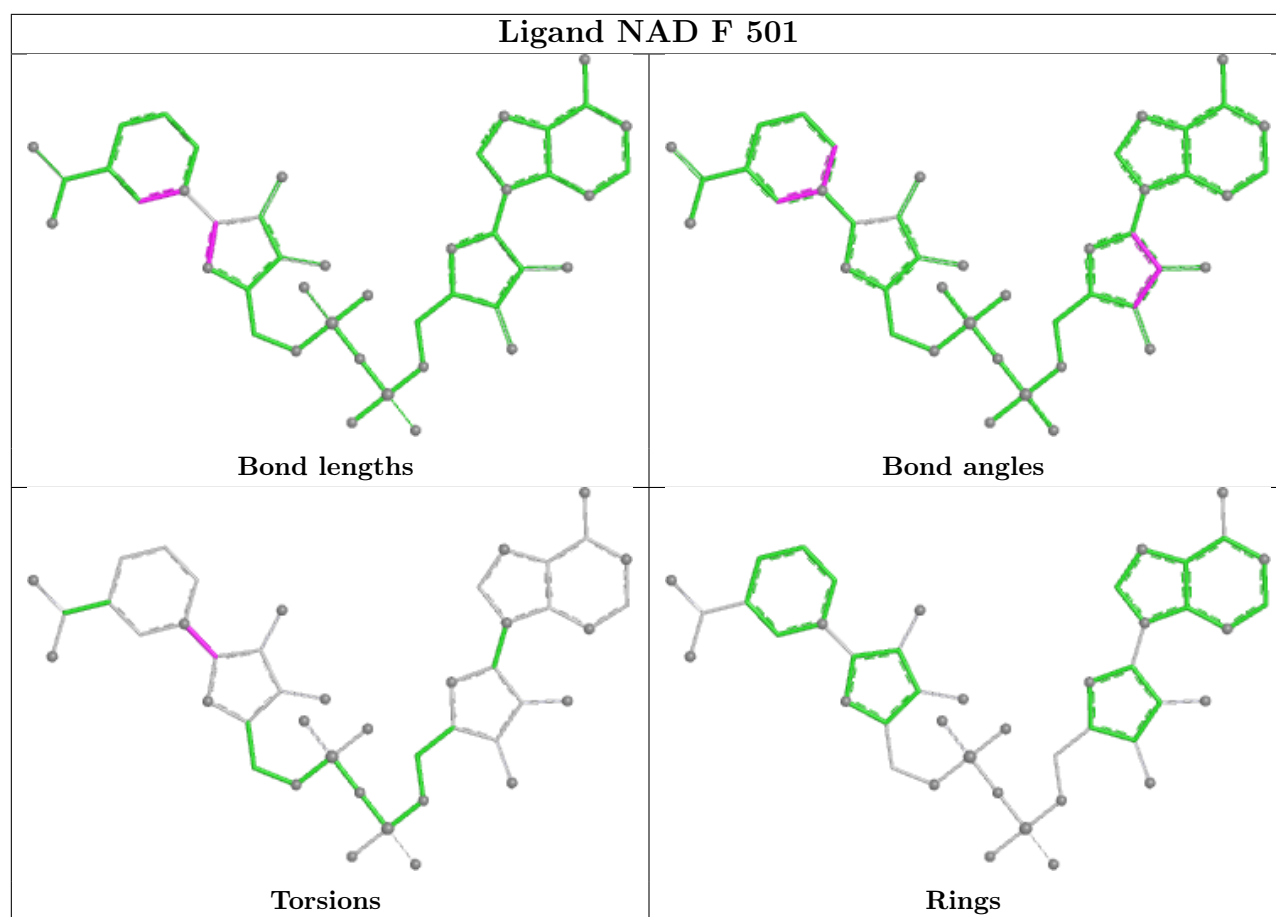
21 monomers are involved in 33 short contacts:

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

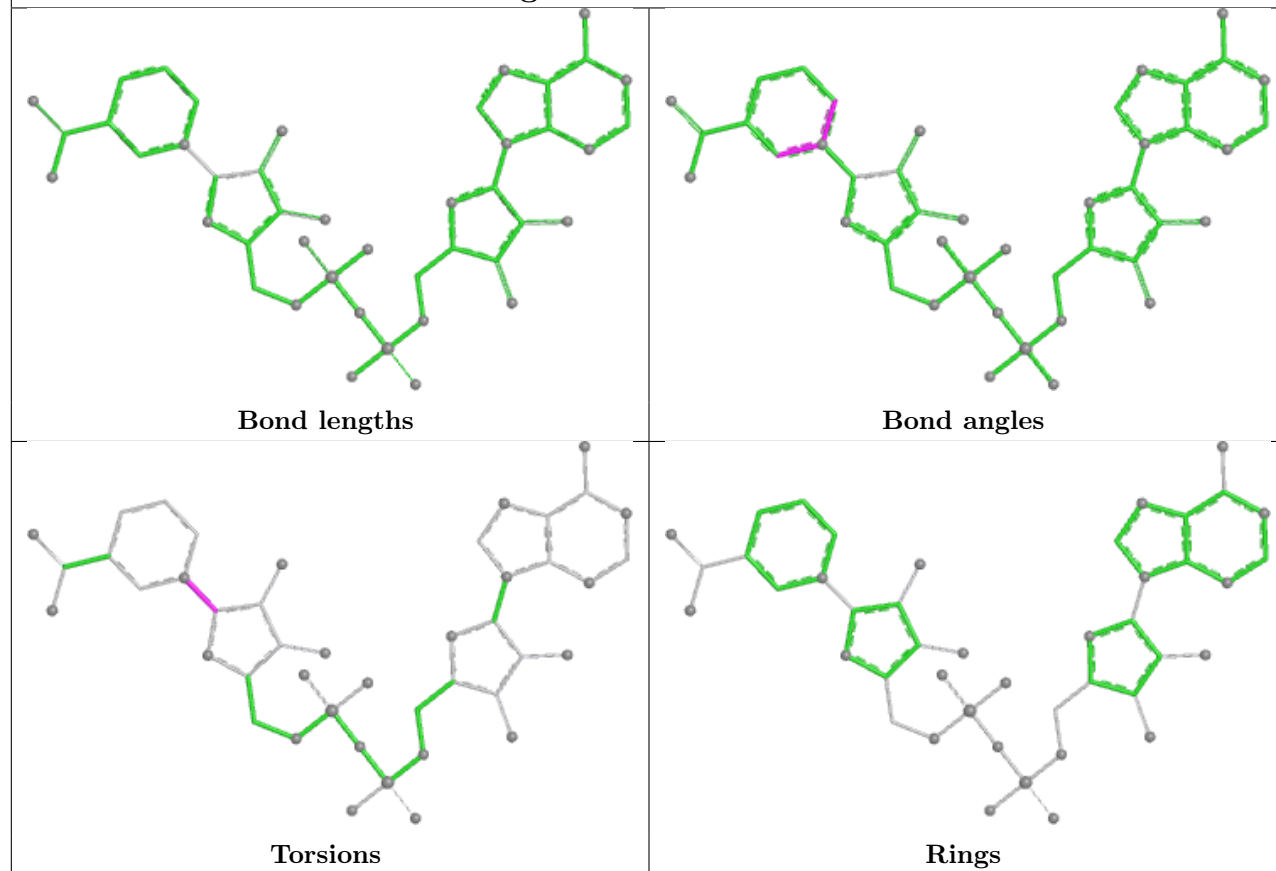
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

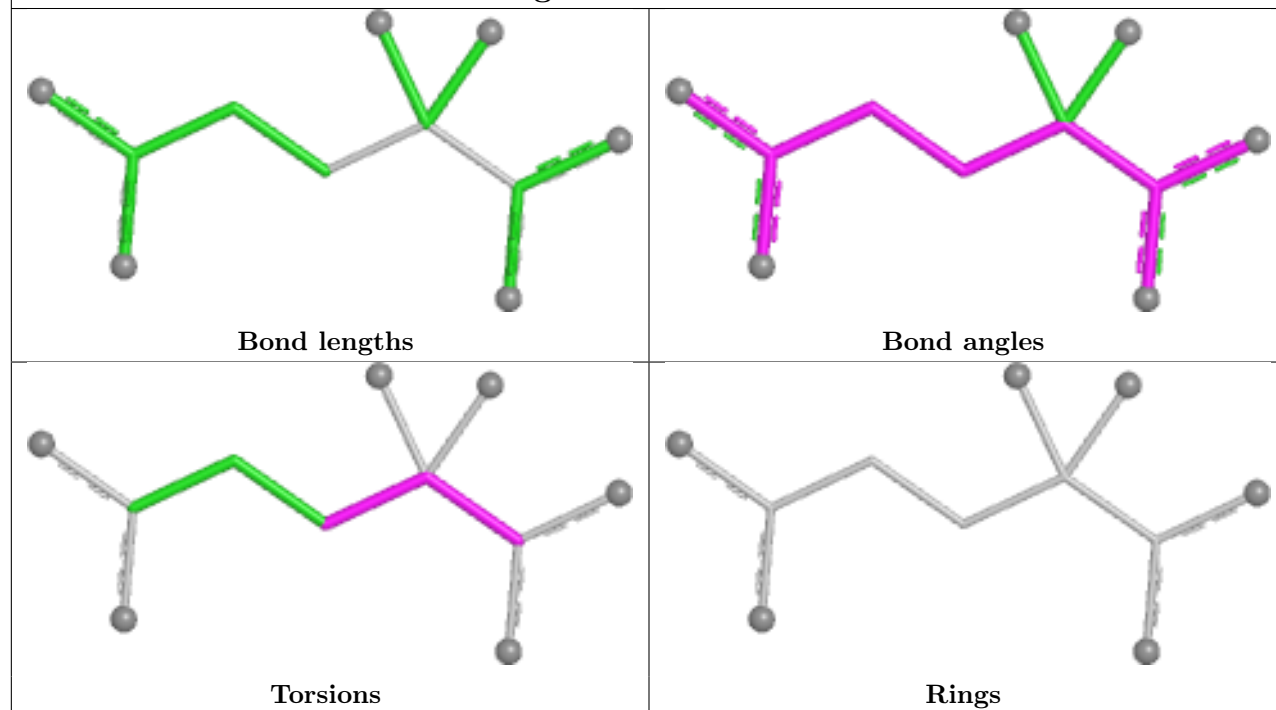


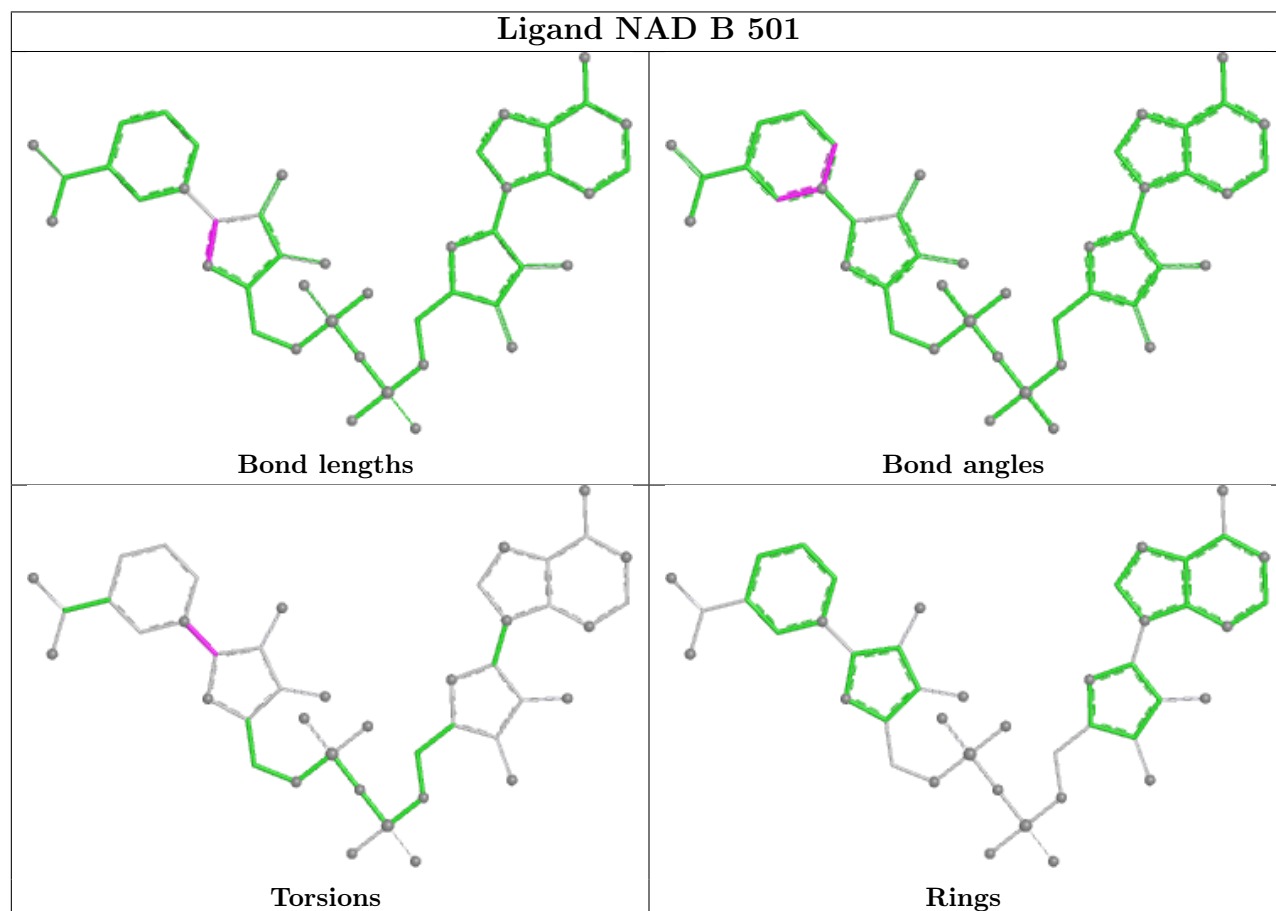
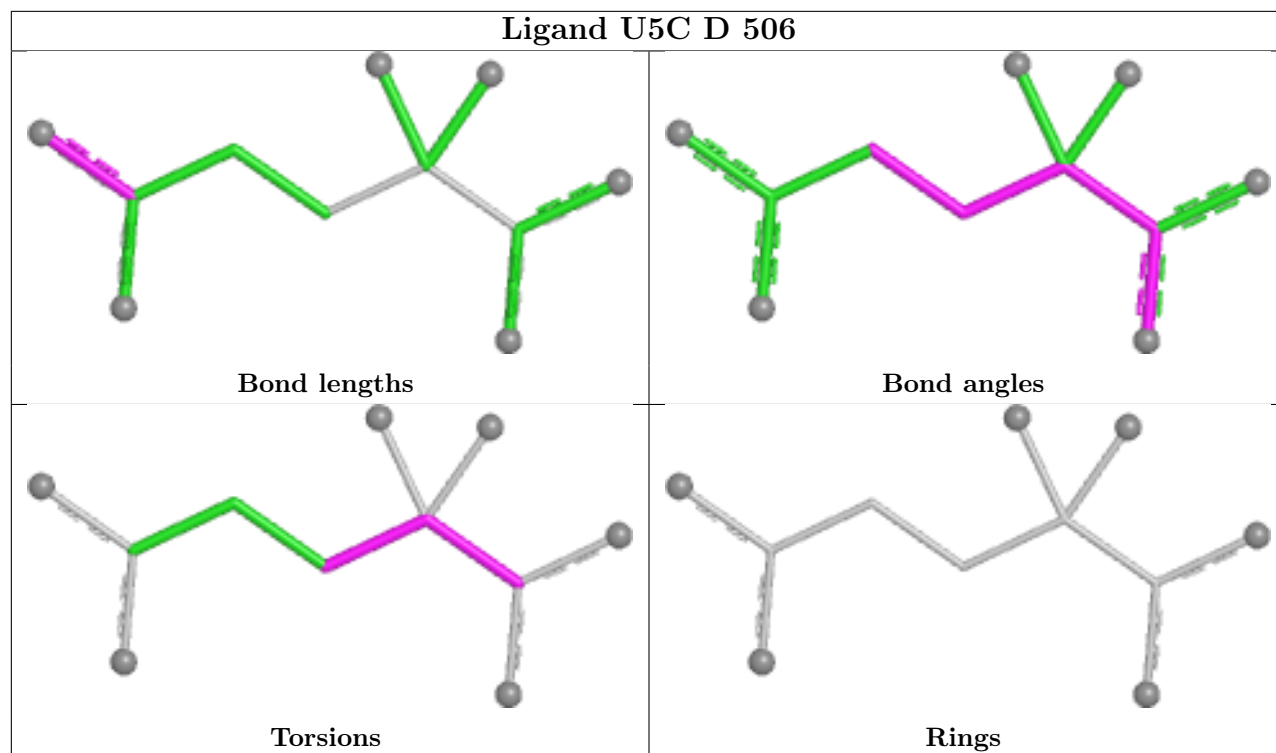


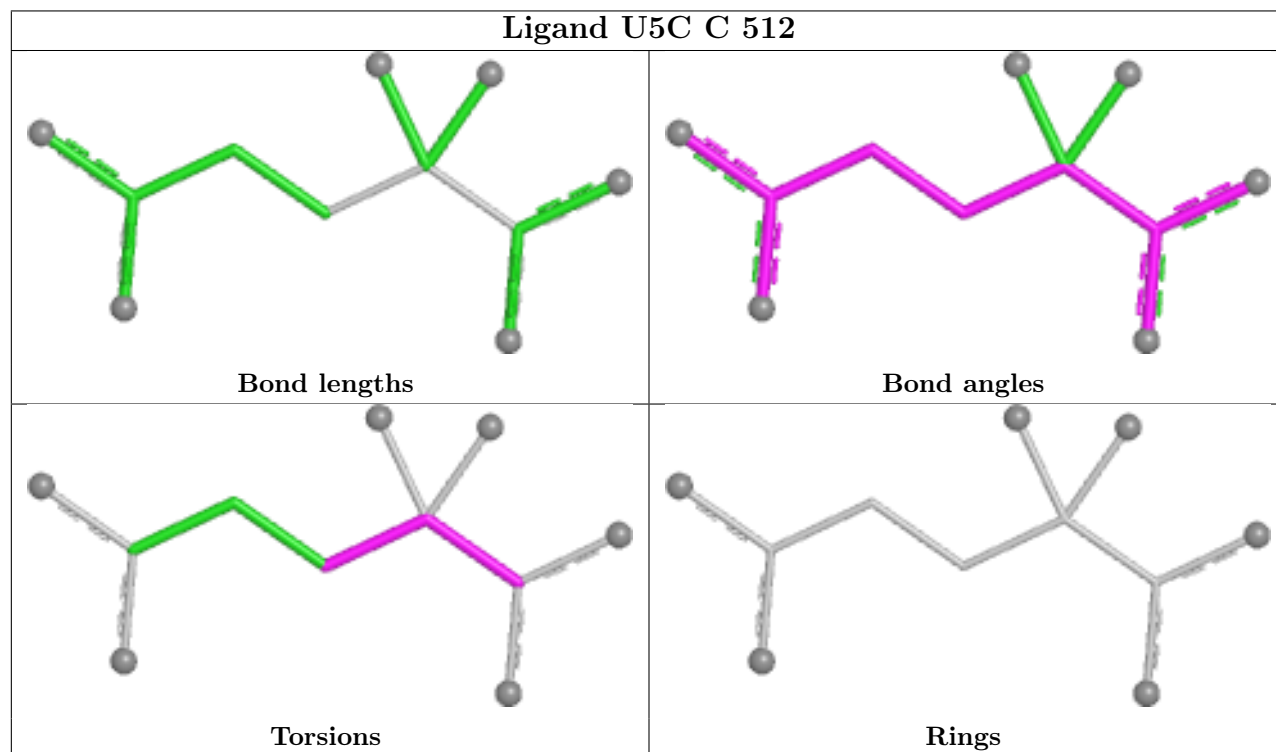
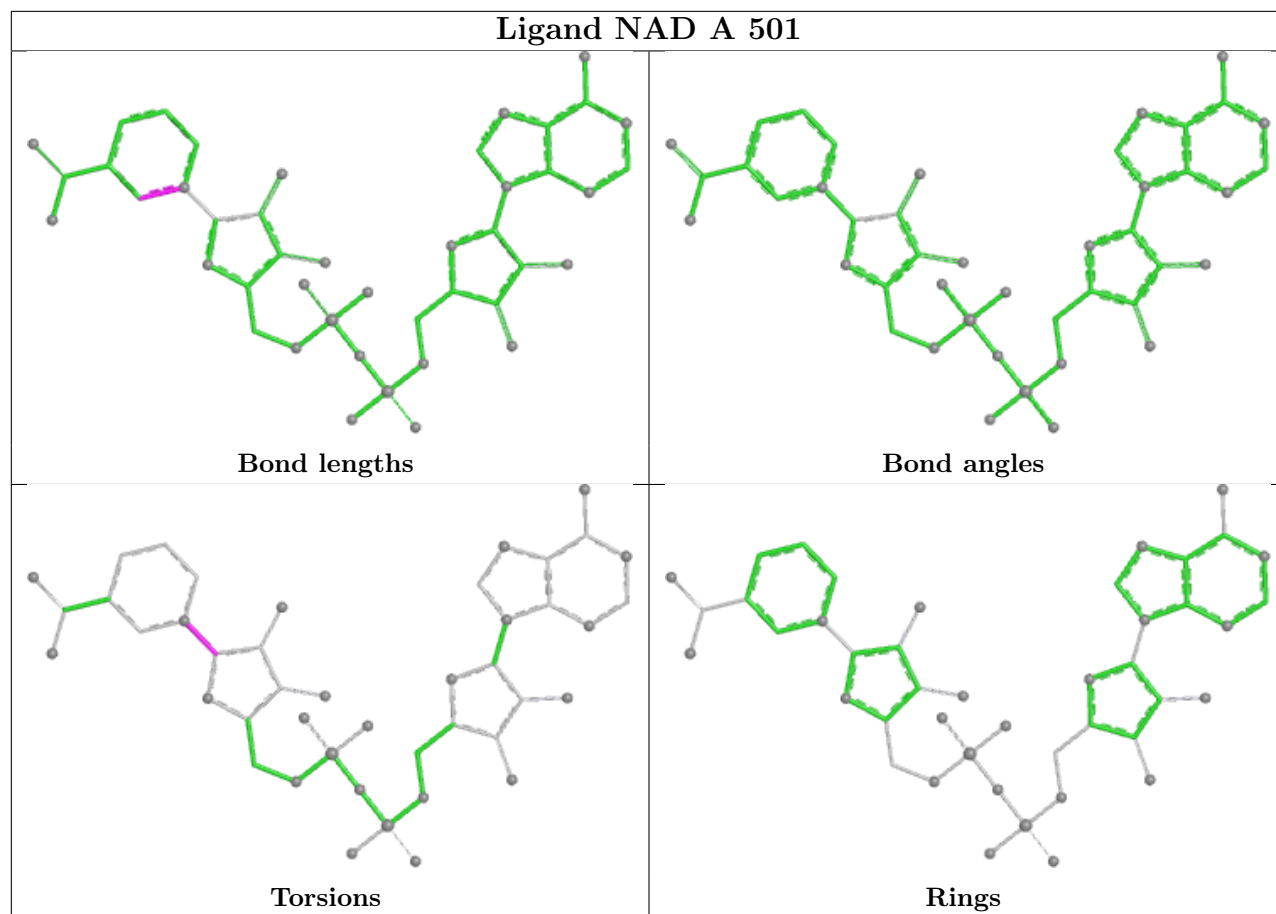
Ligand NAD E 4202



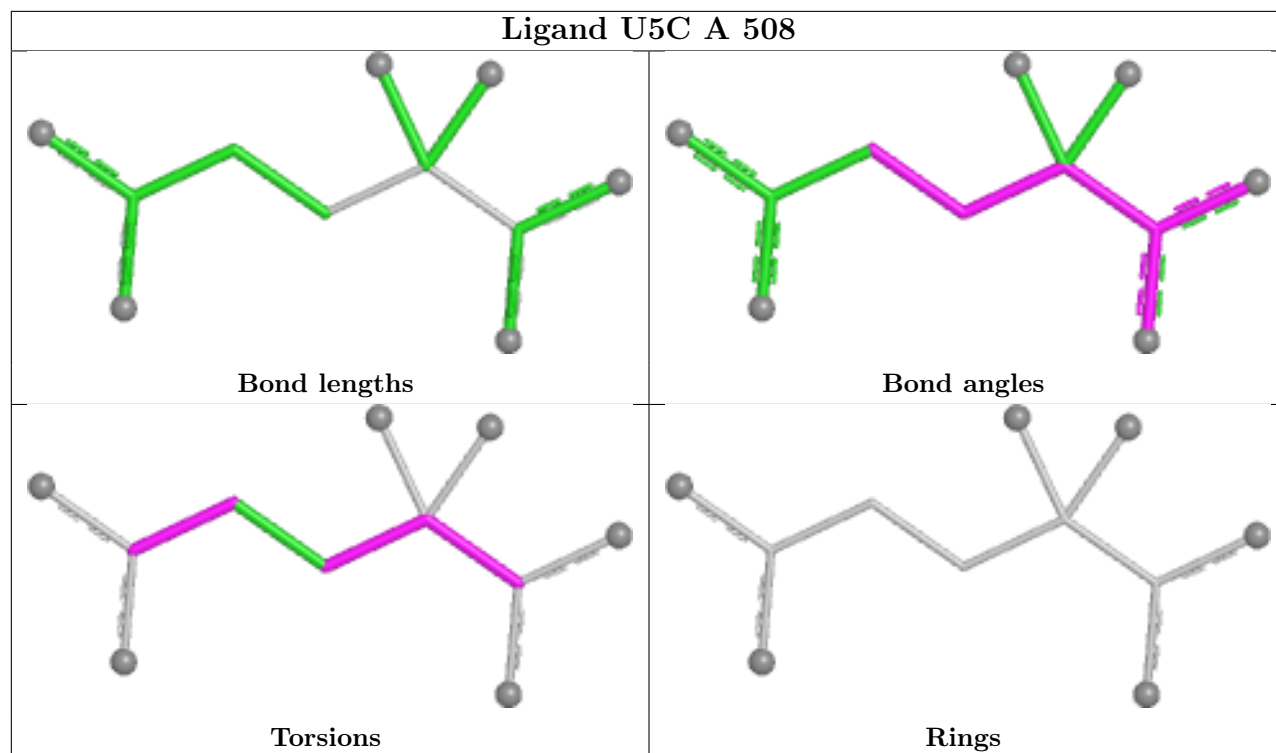
Ligand U5C B 514



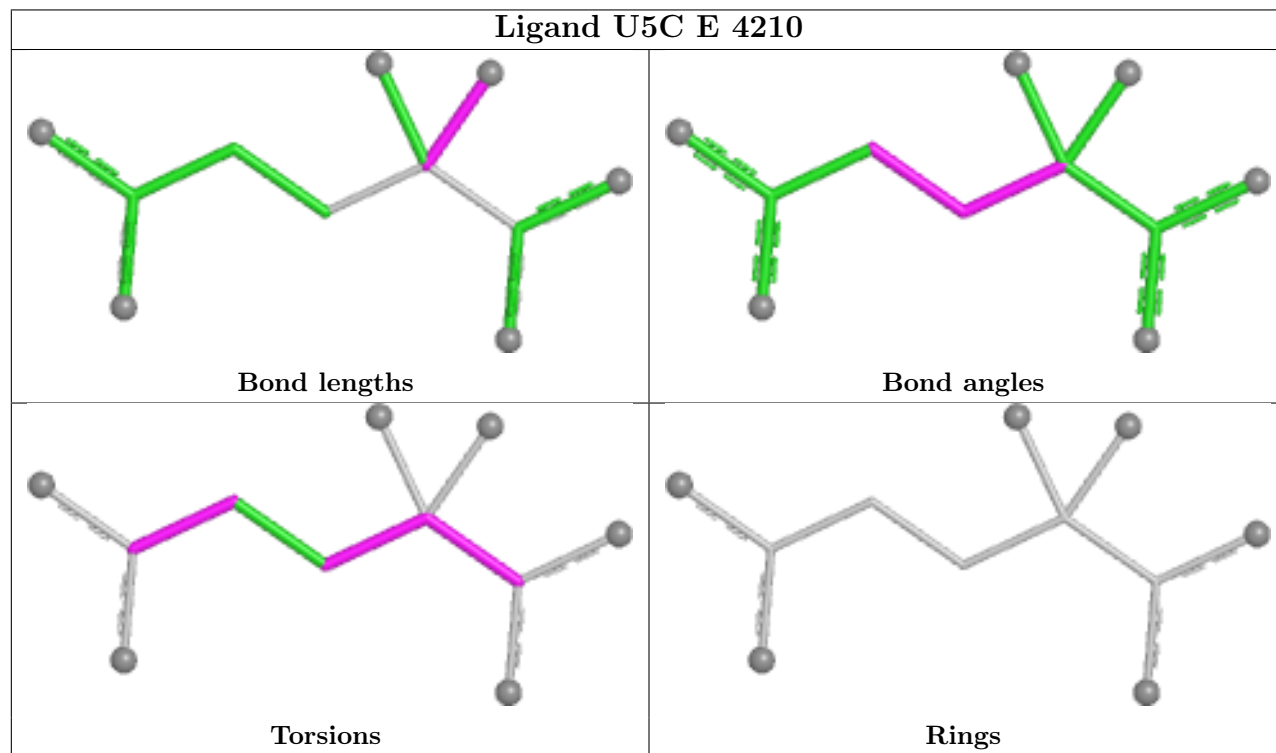


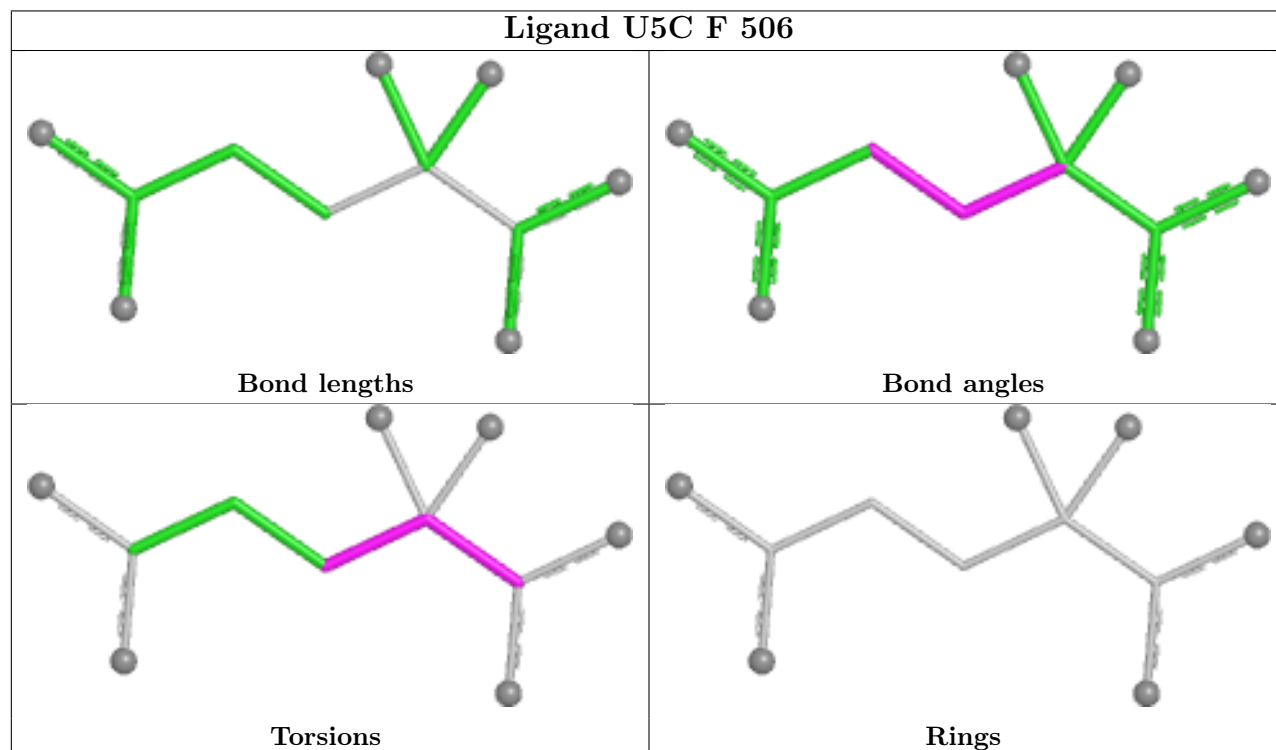
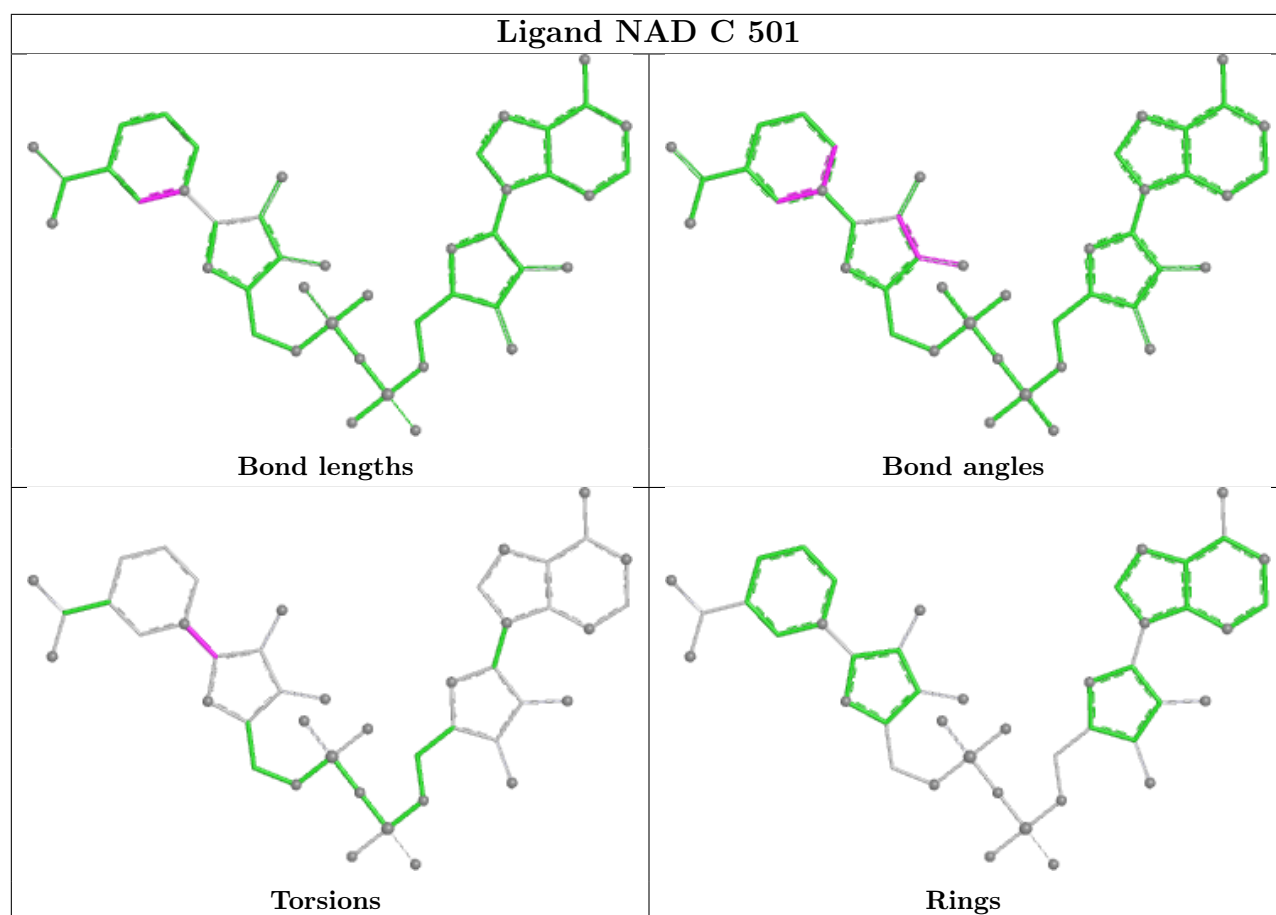


Ligand U5C A 508



Ligand U5C E 4210





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, 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	412/414 (99%)	-0.37	3 (0%) 84 86	11, 24, 42, 68	9 (2%)
1	B	412/414 (99%)	-0.30	2 (0%) 87 89	13, 28, 46, 66	3 (0%)
1	C	413/414 (99%)	-0.38	2 (0%) 87 89	12, 25, 42, 59	8 (1%)
1	D	412/414 (99%)	0.12	2 (0%) 87 89	12, 34, 58, 80	6 (1%)
1	E	412/414 (99%)	-0.33	4 (0%) 79 82	11, 26, 47, 66	8 (1%)
1	F	412/414 (99%)	-0.01	3 (0%) 84 86	13, 31, 59, 81	2 (0%)
All	All	2473/2484 (99%)	-0.21	16 (0%) 85 88	11, 27, 52, 81	36 (1%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	0	ALA	5.2
1	A	0	ALA	4.7
1	D	0	ALA	4.3
1	F	0	ALA	4.1
1	E	0	ALA	2.9
1	E	131	LEU	2.6
1	A	110	ARG	2.6
1	E	110	ARG	2.4
1	C	110	ARG	2.3
1	B	110	ARG	2.3
1	D	242	ILE	2.2
1	F	110	ARG	2.2
1	E	264	ASN	2.2
1	A	261	GLY	2.1
1	C	275	ASP	2.1
1	F	242	ILE	2.1

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	GOL	B	510	6/6	0.70	0.21	56,64,68,72	0
3	GOL	C	510	6/6	0.72	0.20	62,65,67,79	0
3	GOL	A	502	6/6	0.73	0.19	26,41,46,48	0
3	GOL	A	507	6/6	0.73	0.18	49,54,61,61	0
3	GOL	C	511	6/6	0.73	0.17	50,54,63,78	0
3	GOL	B	503	6/6	0.74	0.20	33,45,49,49	0
3	GOL	C	503	6/6	0.76	0.18	36,41,47,48	0
3	GOL	D	502	6/6	0.76	0.18	34,46,49,51	0
8	PEG	B	502	7/7	0.77	0.18	44,48,56,57	0
4	EDO	B	505	4/4	0.78	0.16	46,49,52,59	0
4	EDO	C	509	4/4	0.78	0.14	35,40,45,48	0
3	GOL	F	502	6/6	0.78	0.18	38,50,53,53	0
4	EDO	E	4209	4/4	0.79	0.16	61,63,64,68	0
8	PEG	B	511	7/7	0.79	0.15	32,40,51,66	0
3	GOL	E	4201	6/6	0.80	0.13	55,60,68,72	0
4	EDO	C	505	4/4	0.80	0.18	52,56,56,58	0
3	GOL	D	505	6/6	0.80	0.14	48,59,62,66	0
8	PEG	E	4208	7/7	0.81	0.16	32,43,47,56	0
3	GOL	B	512	6/6	0.82	0.16	45,49,56,62	6
3	GOL	B	513	6/6	0.82	0.16	46,49,54,58	6
3	GOL	C	508	6/6	0.83	0.18	33,34,37,42	6
8	PEG	C	504	7/7	0.83	0.15	38,45,51,55	0
8	PEG	D	504	7/7	0.83	0.15	36,55,59,66	0
3	GOL	E	4203	6/6	0.83	0.15	28,46,47,50	0
8	PEG	C	502	7/7	0.84	0.14	35,48,59,61	0
3	GOL	E	4205	6/6	0.84	0.15	26,36,40,42	6
3	GOL	E	4207	6/6	0.84	0.16	41,50,53,53	6

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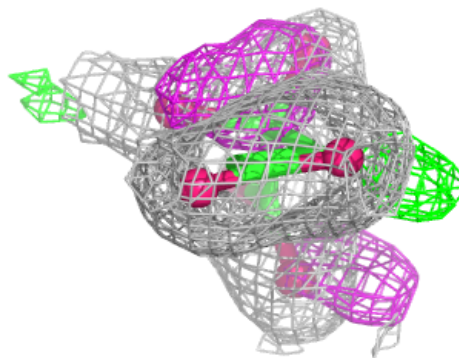
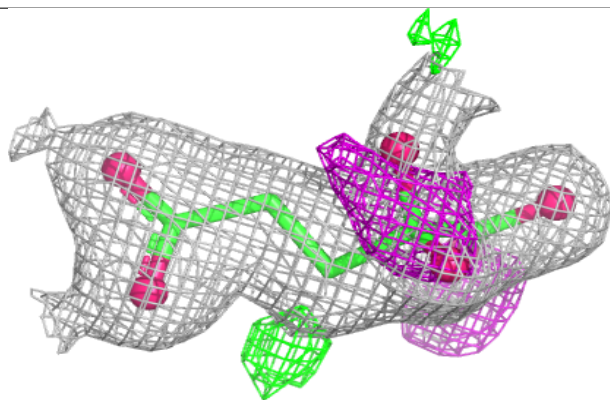
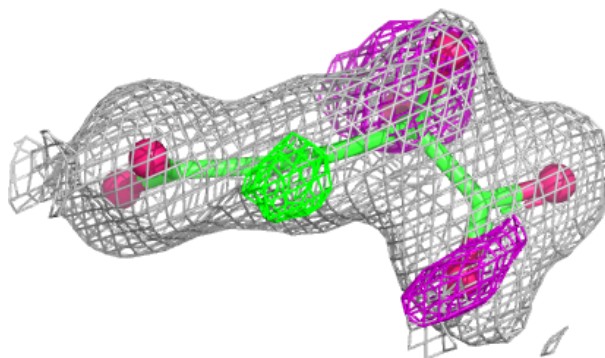
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	508	6/6	0.84	0.18	30,35,40,40	6
3	GOL	B	506	6/6	0.85	0.13	47,55,58,64	0
4	EDO	E	4206	4/4	0.85	0.17	44,46,50,53	0
3	GOL	C	507	6/6	0.85	0.13	41,51,60,66	0
8	PEG	F	504	7/7	0.85	0.14	45,49,66,70	0
4	EDO	A	505	4/4	0.86	0.13	31,40,50,52	0
4	EDO	B	504	4/4	0.86	0.14	36,42,47,51	0
3	GOL	A	509	6/6	0.87	0.14	26,45,51,51	0
3	GOL	B	507	6/6	0.87	0.16	35,40,54,54	6
4	EDO	F	503	4/4	0.88	0.15	41,45,46,51	0
4	EDO	C	506	4/4	0.88	0.15	40,41,42,55	0
3	GOL	D	503	6/6	0.89	0.15	39,42,46,48	6
3	GOL	A	503	6/6	0.89	0.13	35,36,39,40	6
4	EDO	B	509	4/4	0.89	0.12	36,46,50,51	0
3	GOL	A	504	6/6	0.89	0.12	39,47,51,54	6
4	EDO	F	505	4/4	0.89	0.12	36,42,54,60	0
3	GOL	A	506	6/6	0.89	0.13	44,48,53,57	0
4	EDO	E	4204	4/4	0.90	0.12	34,47,57,58	0
5	U5C	F	506	11/11	0.93	0.09	26,31,47,51	0
5	U5C	A	508	11/11	0.94	0.09	20,25,40,41	0
5	U5C	D	506	11/11	0.94	0.08	25,32,47,48	0
5	U5C	E	4210	11/11	0.95	0.08	21,28,39,41	0
5	U5C	C	512	11/11	0.95	0.08	20,28,42,43	0
5	U5C	B	514	11/11	0.95	0.08	22,28,46,48	0
2	NAD	F	501	44/44	0.97	0.06	23,28,34,39	0
7	NA	C	514	1/1	0.97	0.06	33,33,33,33	0
2	NAD	D	501	44/44	0.97	0.06	24,29,35,37	0
7	NA	A	511	1/1	0.98	0.07	34,34,34,34	0
7	NA	B	516	1/1	0.98	0.09	30,30,30,30	0
2	NAD	C	501	44/44	0.98	0.05	19,23,29,32	0
2	NAD	B	501	44/44	0.98	0.05	19,24,31,35	0
2	NAD	E	4202	44/44	0.98	0.05	18,23,29,34	0
6	CA	B	515	1/1	0.99	0.02	22,22,22,22	0
6	CA	D	507	1/1	0.99	0.04	21,21,21,21	0
2	NAD	A	501	44/44	0.99	0.04	18,22,27,30	0
6	CA	E	4211	1/1	1.00	0.03	19,19,19,19	0
6	CA	F	507	1/1	1.00	0.02	19,19,19,19	0
6	CA	C	513	1/1	1.00	0.04	20,20,20,20	0
6	CA	A	510	1/1	1.00	0.04	17,17,17,17	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.

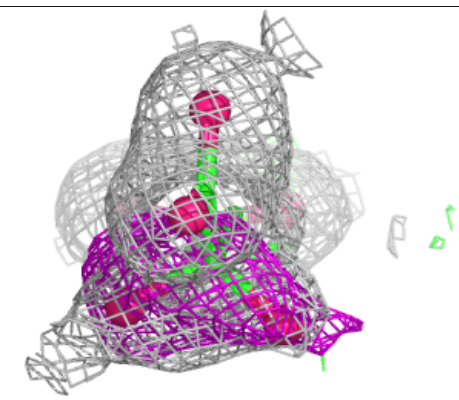
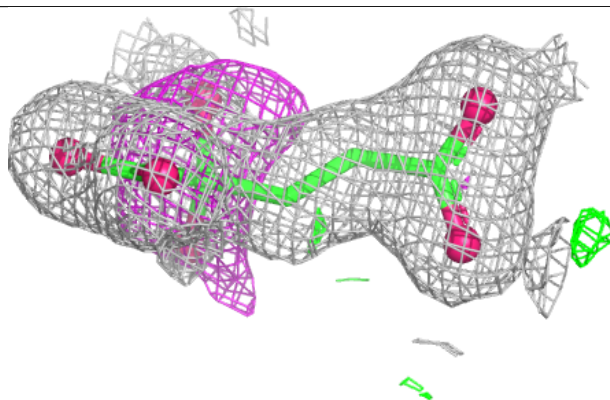
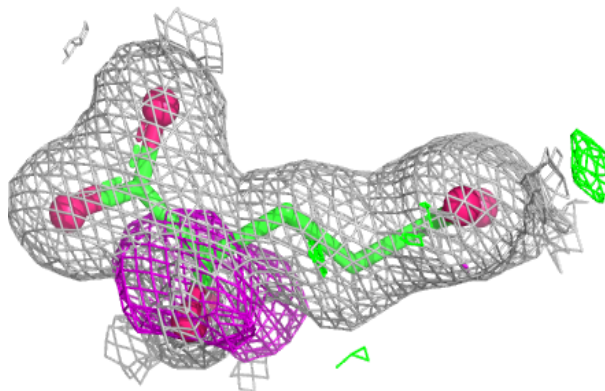
Electron density around U5C F 506:

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



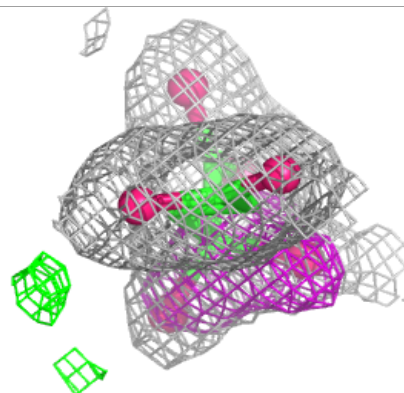
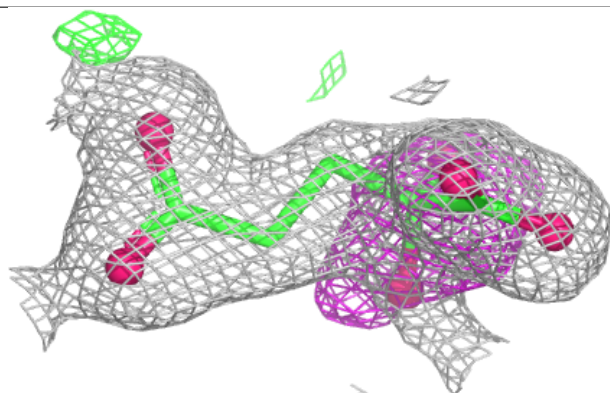
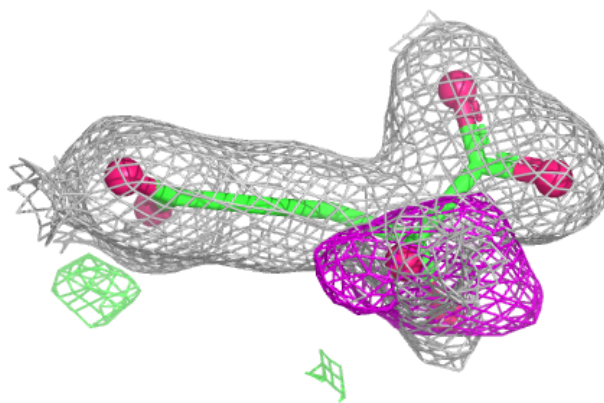
Electron density around U5C A 508:

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

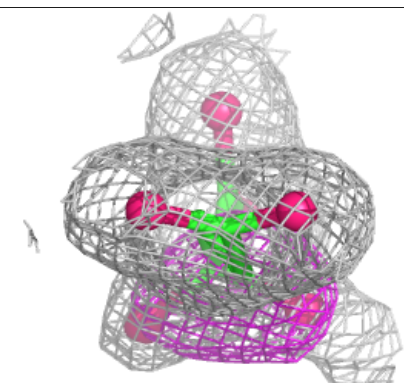
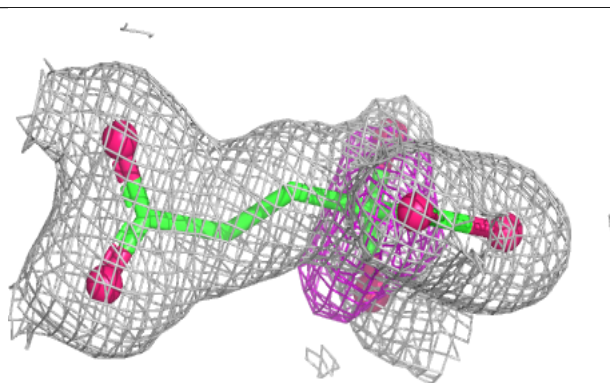
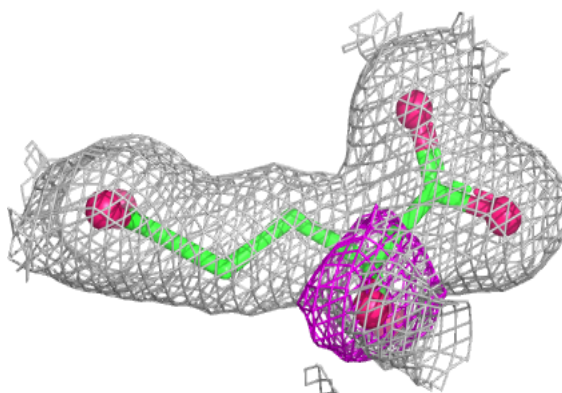


Electron density around U5C D 506:

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

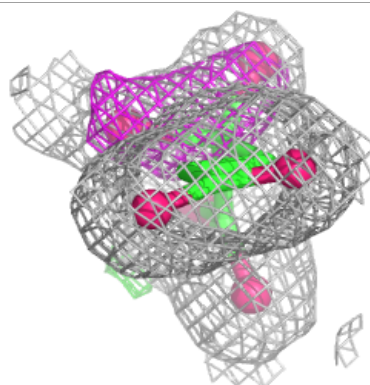
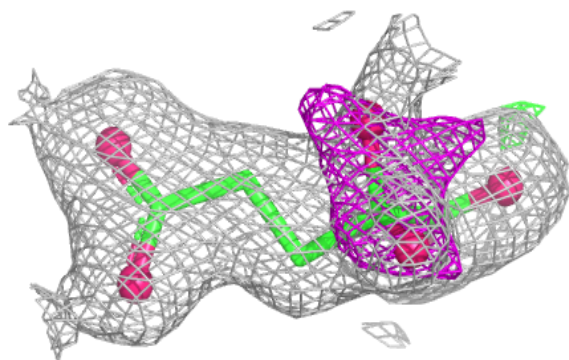
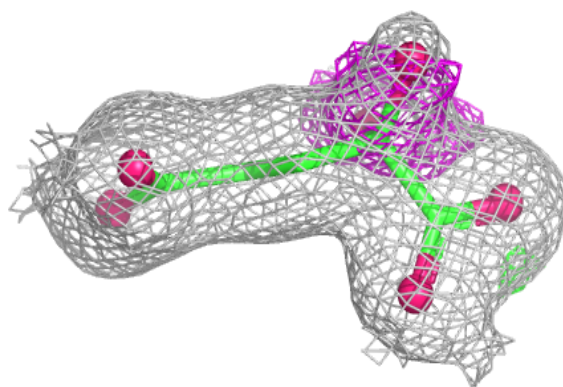
**Electron density around U5C E 4210:**

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

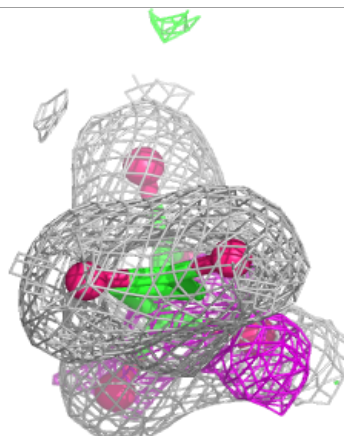
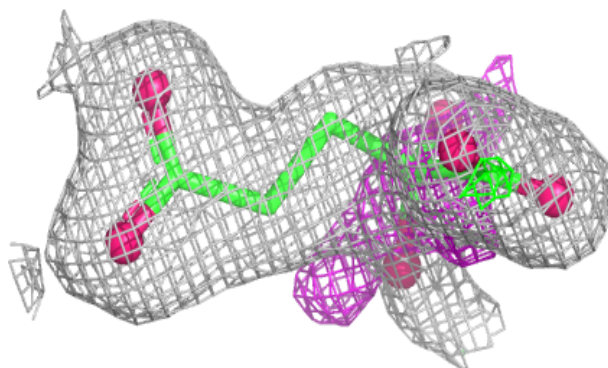
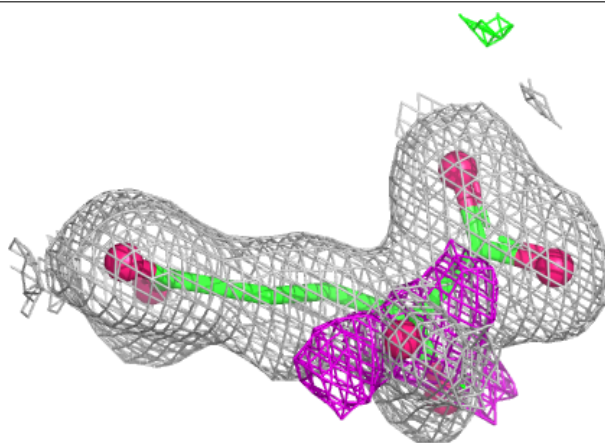


Electron density around U5C C 512:

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

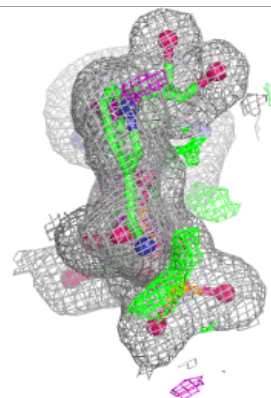
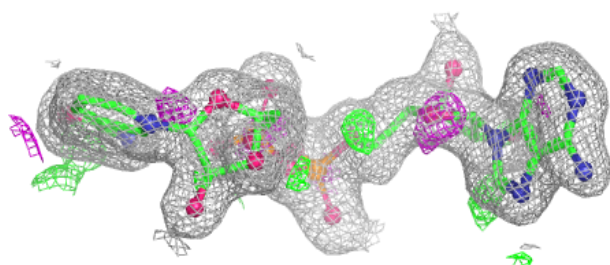
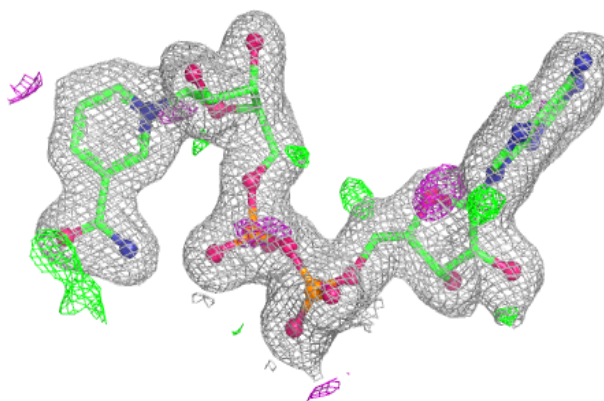
**Electron density around U5C B 514:**

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

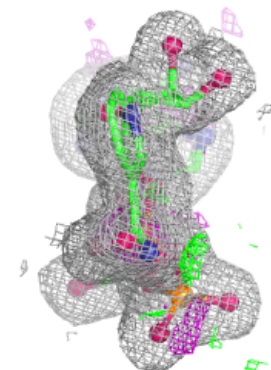
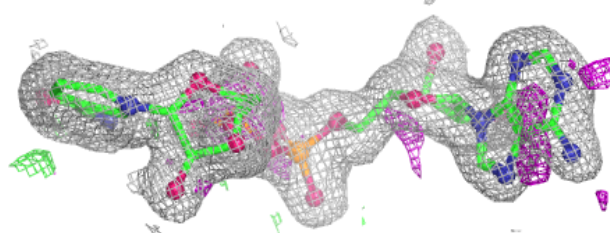
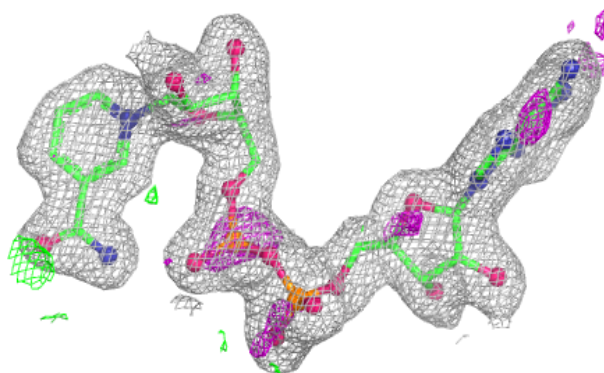


Electron density around NAD F 501:

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

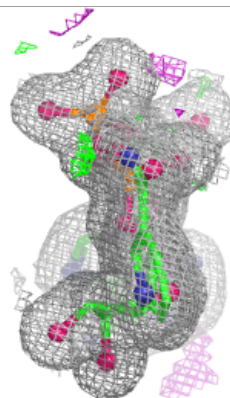
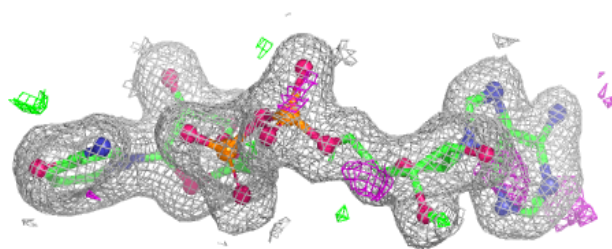
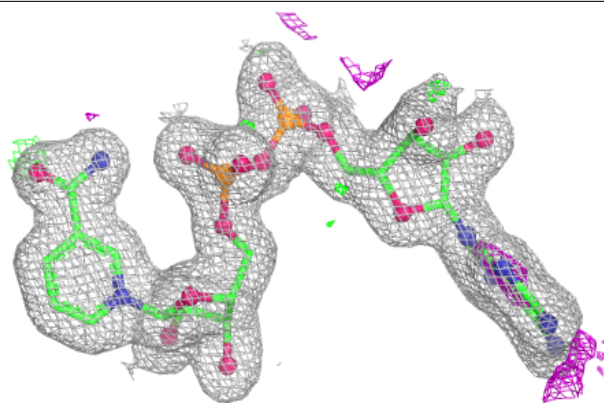
**Electron density around NAD D 501:**

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

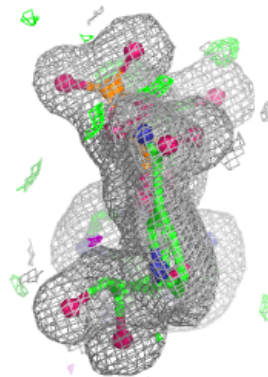
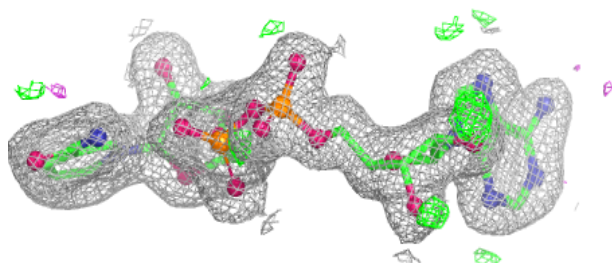
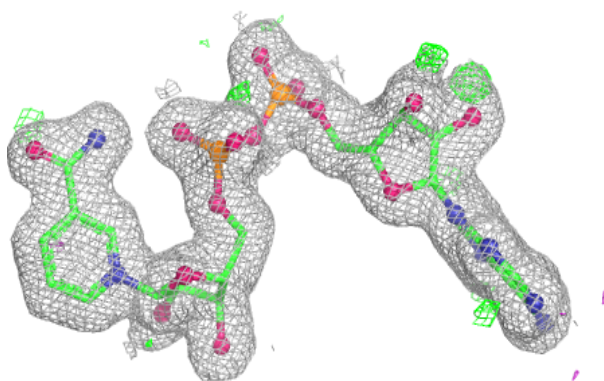


Electron density around NAD C 501:

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

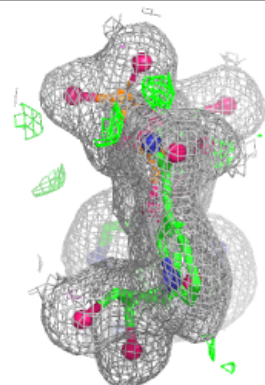
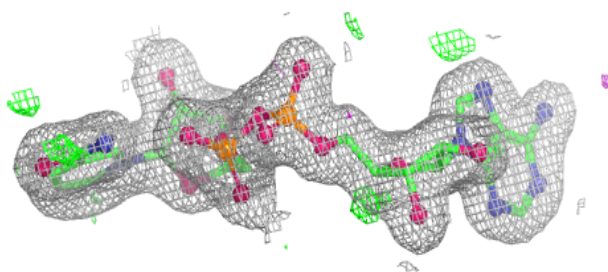
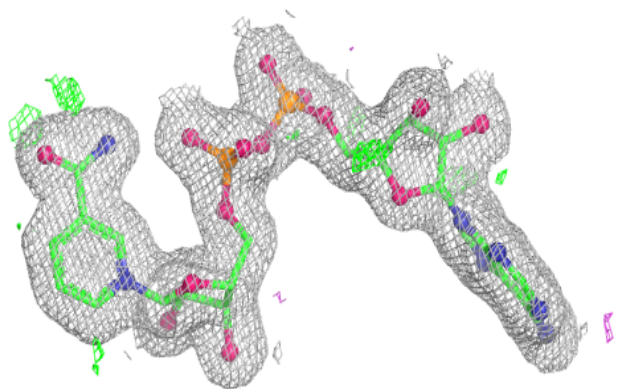
**Electron density around NAD B 501:**

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

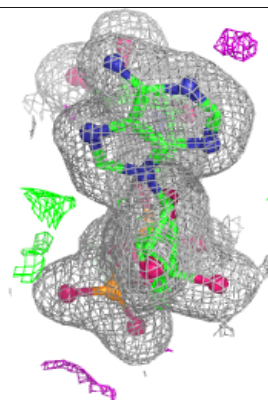
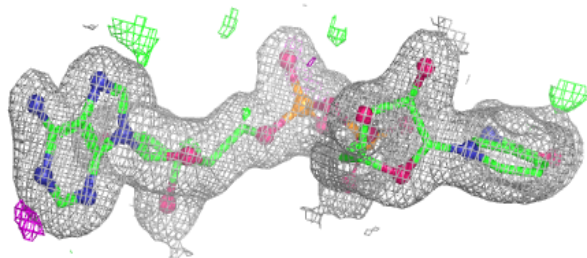
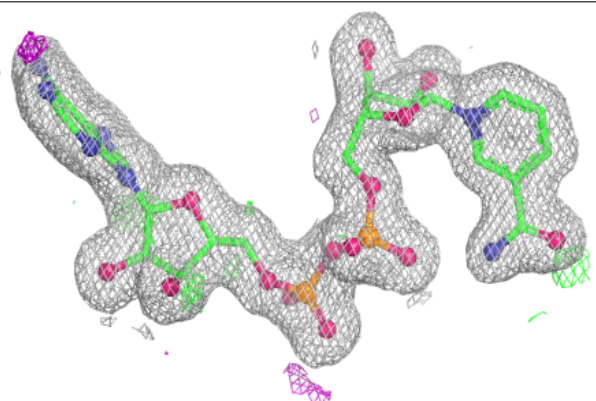


Electron density around NAD E 4202:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.