



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 08:03 PM UTC

PDB ID : 8S3D / pdb_00008s3d
Title : Crystal structure of Medicago truncatula glutamate dehydrogenase 2 in complex with 2-amino-2-hydroxyglutarate (reaction intermediate) and NAD
Authors : Grzechowiak, M.; Ruszkowski, M.
Deposited on : 2024-02-19
Resolution : 1.65 Å(reported)

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

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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:

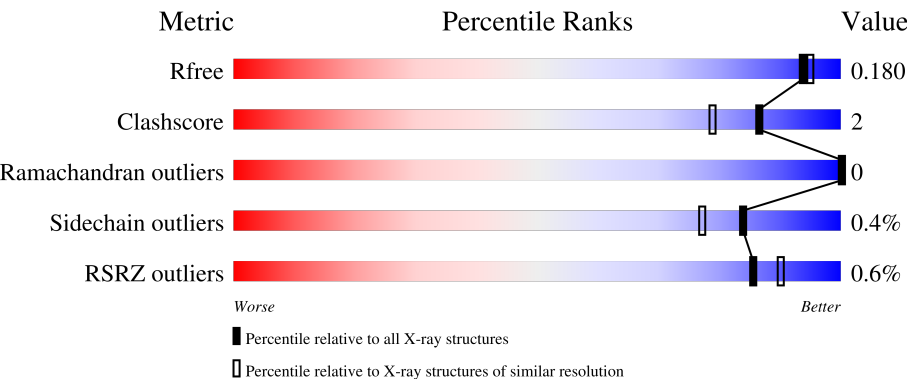
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

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

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	96%
1	B	414	96%
1	C	414	% 96%
1	D	414	% 94% 6%
1	E	414	96%

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Mol	Chain	Length	Quality of chain
1	F	414	% 97%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	GLY	A	514	-	X	-	-
9	GLY	B	503	-	X	-	-
9	GLY	D	511	-	X	-	-
9	GLY	E	504	-	X	-	-
9	GLY	F	2313	-	X	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 22384 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	4	0
			3168	1998	555	598	17			
1	B	412	Total	C	N	O	S	0	5	0
			3181	2004	561	599	17			
1	C	412	Total	C	N	O	S	0	8	0
			3206	2020	564	605	17			
1	D	412	Total	C	N	O	S	0	5	0
			3182	2005	560	600	17			
1	E	412	Total	C	N	O	S	0	8	0
			3202	2020	561	604	17			
1	F	412	Total	C	N	O	S	0	6	0
			3180	2006	556	601	17			

There are 18 discrepancies between the modelled and reference sequences:

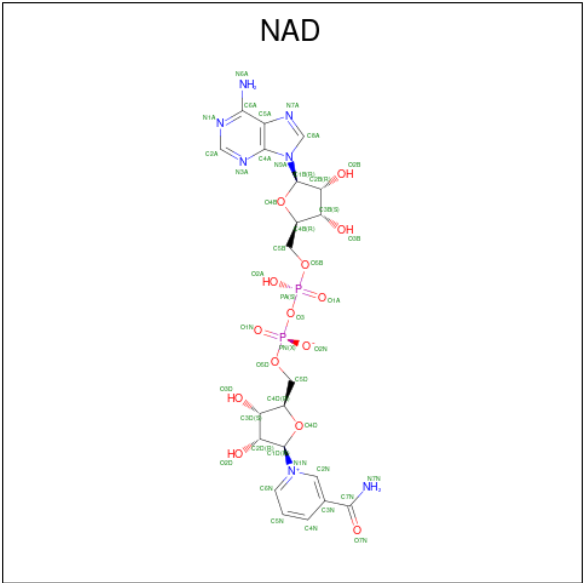
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP G7JYL4
A	-1	ASN	-	expression tag	UNP G7JYL4
A	0	ALA	-	expression tag	UNP G7JYL4
B	-2	SER	-	expression tag	UNP G7JYL4
B	-1	ASN	-	expression tag	UNP G7JYL4
B	0	ALA	-	expression tag	UNP G7JYL4
C	-2	SER	-	expression tag	UNP G7JYL4
C	-1	ASN	-	expression tag	UNP G7JYL4
C	0	ALA	-	expression tag	UNP G7JYL4
D	-2	SER	-	expression tag	UNP G7JYL4
D	-1	ASN	-	expression tag	UNP G7JYL4
D	0	ALA	-	expression tag	UNP G7JYL4
E	-2	SER	-	expression tag	UNP G7JYL4
E	-1	ASN	-	expression tag	UNP G7JYL4
E	0	ALA	-	expression tag	UNP G7JYL4
F	-2	SER	-	expression tag	UNP G7JYL4
F	-1	ASN	-	expression tag	UNP G7JYL4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	expression tag	UNP G7JYL4

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



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 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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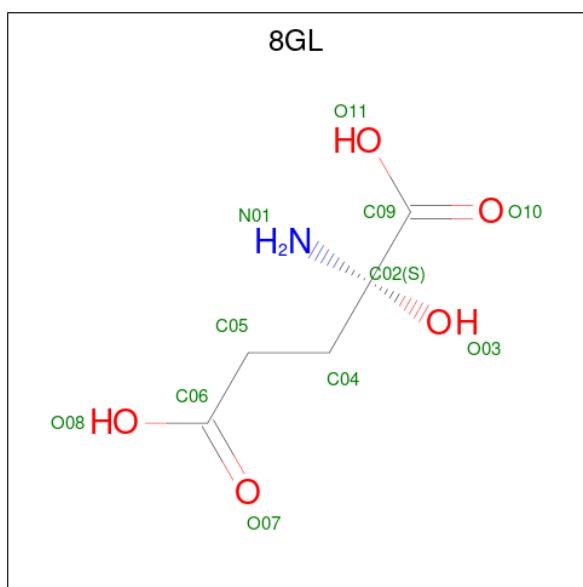
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



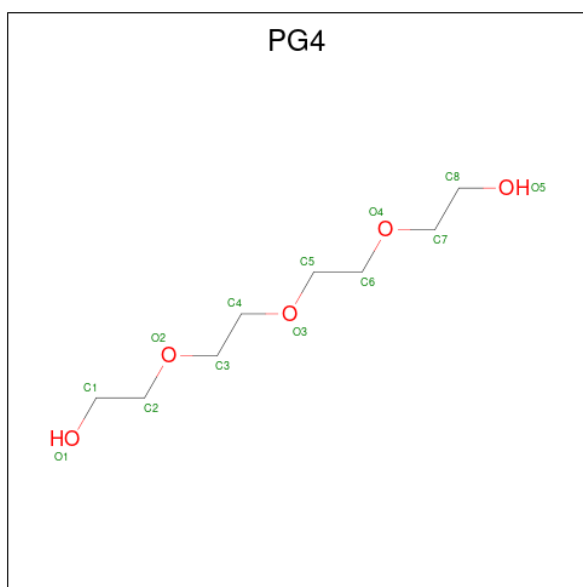
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	F	1	Total	C	O	0	0
			7	4	3		
4	F	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is (2S)-2-azanyl-2-oxidanyl-pentanedioic acid (CCD ID: 8GL) (formula: $C_5H_9NO_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	8	5		
6	B	1	Total	C	O	0	0
			13	8	5		
6	D	1	Total	C	O	0	0
			13	8	5		
6	E	1	Total	C	O	0	0
			13	8	5		
6	E	1	Total	C	O	0	0
			13	8	5		

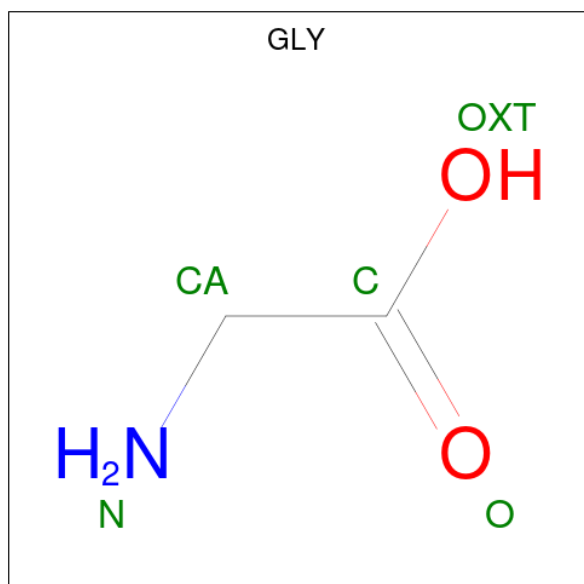
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

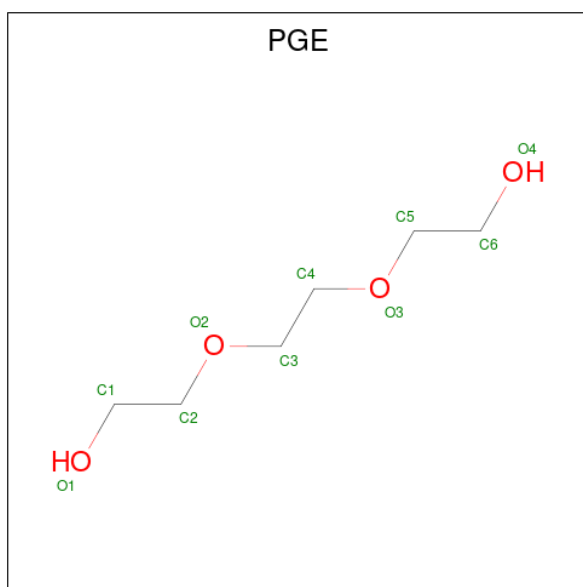
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Na	0	0
			1	1		
8	B	1	Total	Na	0	0
			1	1		
8	D	1	Total	Na	0	0
			1	1		

- Molecule 9 is GLYCINE (CCD ID: GLY) (formula: C₂H₅NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			5	2	1	2		
9	B	1	Total	C	N	O	0	0
			5	2	1	2		
9	C	1	Total	C	N	O	0	0
			5	2	1	2		
9	D	1	Total	C	N	O	0	0
			5	2	1	2		
9	E	1	Total	C	N	O	0	0
			5	2	1	2		
9	F	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 10 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			10	6	4		

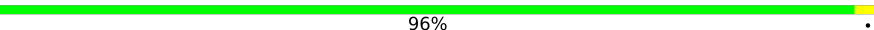
- Molecule 11 is water.

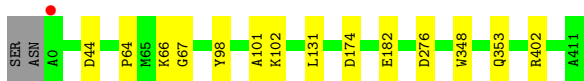
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	468	Total	O	0	2
			470	470		
11	B	430	Total	O	0	2
			432	432		
11	C	433	Total	O	0	2
			435	435		
11	D	380	Total	O	0	1
			381	381		
11	E	464	Total	O	0	4
			468	468		
11	F	461	Total	O	0	2
			463	463		

3 Residue-property plots [i](#)

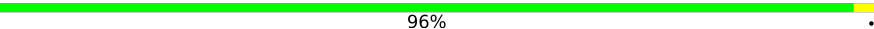
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

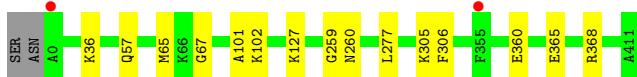
- Molecule 1: Glutamate dehydrogenase

Chain A:  96%

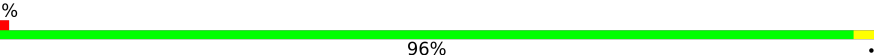


- Molecule 1: Glutamate dehydrogenase

Chain B:  96%

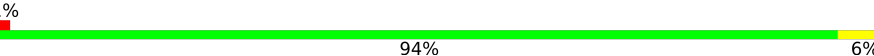


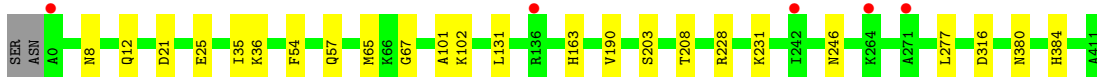
- Molecule 1: Glutamate dehydrogenase

Chain C:  96%

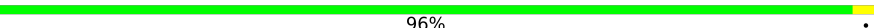


- Molecule 1: Glutamate dehydrogenase

Chain D:  94% 6%



- Molecule 1: Glutamate dehydrogenase

Chain E:  96%



- Molecule 1: Glutamate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.83Å 155.71Å 163.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.89 – 1.65 65.89 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.5 (65.89-1.65) 99.5 (65.89-1.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 1.65Å)	Xtriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, R_{free}	0.147 , 0.173 0.158 , 0.180	Depositor DCC
R_{free} test set	3377 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.2	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	22384	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.2690e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NAD, EDO, PGE, PEG, CA, 8GL, PG4, 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	0.55	0/3230	0.68	0/4370
1	B	0.53	0/3243	0.66	0/4387
1	C	0.55	0/3269	0.67	0/4423
1	D	0.51	0/3245	0.66	0/4391
1	E	0.54	0/3264	0.69	0/4417
1	F	0.53	0/3242	0.66	0/4388
All	All	0.54	0/19493	0.67	0/26376

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	3168	0	3155	12	0
1	B	3181	0	3168	15	0
1	C	3206	0	3183	15	0
1	D	3182	0	3160	18	0
1	E	3202	0	3188	15	0
1	F	3180	0	3165	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	24	0	36	0	0
3	B	20	0	30	0	0
3	C	20	0	30	1	0
3	D	12	0	18	0	0
3	E	12	0	18	0	0
3	F	28	0	41	0	0
4	A	14	0	20	0	0
4	C	14	0	20	1	0
4	D	14	0	20	0	0
4	F	14	0	20	1	0
5	A	11	0	0	2	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	13	0	18	2	0
6	B	13	0	18	3	0
6	D	13	0	18	1	0
6	E	26	0	36	5	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
9	A	5	0	2	1	0
9	B	5	0	2	1	0
9	C	5	0	2	1	0
9	D	5	0	2	0	0
9	E	5	0	2	1	0
9	F	5	0	2	0	0
10	B	10	0	14	0	0
11	A	470	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	B	432	0	0	7	0
11	C	435	0	0	5	0
11	D	381	0	0	4	0
11	E	468	0	0	2	0
11	F	463	0	0	2	0
All	All	22384	0	19544	84	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 (84) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:LYS:HE2	6:B:506:PG4:H32	1.65	0.78
1:C:182[B]:GLU:OE2	9:C:503:GLY:N	2.20	0.74
4:C:506:PEG:H32	11:C:690:HOH:O	1.86	0.74
1:D:8:ASN:O	1:D:12:GLN:HG2	1.93	0.66
1:D:102:LYS:NZ	5:D:502:8GL:O03	2.29	0.66
1:B:102:LYS:NZ	5:B:502:8GL:O03	2.30	0.63
6:A:511:PG4:H41	11:A:809:HOH:O	1.99	0.63
1:F:102:LYS:NZ	5:F:2304:8GL:O03	2.32	0.62
1:E:402[B]:ARG:HD2	11:E:623:HOH:O	1.99	0.61
1:C:102:LYS:NZ	5:C:502:8GL:O03	2.31	0.61
1:A:402:ARG:HD2	11:A:639:HOH:O	2.02	0.60
1:E:182[B]:GLU:OE2	9:E:504:GLY:N	2.35	0.58
1:B:306:PHE:CE2	6:B:506:PG4:H21	2.39	0.57
1:B:36:LYS:NZ	11:B:608:HOH:O	2.38	0.56
1:A:276:ASP:HB3	11:A:765:HOH:O	2.05	0.56
1:D:163[A]:HIS:NE2	11:D:602:HOH:O	2.32	0.56
1:F:402:ARG:NH1	11:F:2404:HOH:O	2.36	0.54
1:D:163[B]:HIS:CE1	11:D:723:HOH:O	2.60	0.54
1:E:44:ASP:HB3	6:E:507:PG4:H71	1.90	0.53
9:B:503:GLY:N	11:B:610:HOH:O	2.41	0.53
1:D:384:HIS:HD2	11:D:929:HOH:O	1.92	0.52
1:C:402[A]:ARG:HD2	11:C:612:HOH:O	2.08	0.52
1:D:12:GLN:OE1	1:D:25:GLU:OE2	2.28	0.51
1:D:246:ASN:HA	6:D:503:PG4:H61	1.92	0.51
1:E:33:ARG:CZ	1:E:131:LEU:HD13	2.39	0.51
1:E:102:LYS:NZ	5:E:502:8GL:O03	2.40	0.51
1:C:163[B]:HIS:CE1	11:C:693:HOH:O	2.63	0.51
1:C:163[A]:HIS:CD2	1:E:64:PRO:HD3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:ILE:HG21	1:D:131:LEU:HD11	1.93	0.50
1:C:35:ILE:HG13	1:C:131:LEU:HD13	1.92	0.50
1:F:368:ARG:NH1	4:F:2305:PEG:O4	2.45	0.49
1:E:206:ASP:HB3	6:E:505:PG4:H62	1.92	0.49
1:C:35:ILE:HD13	1:F:35:ILE:HD13	1.95	0.49
1:A:44:ASP:HB3	6:A:511:PG4:H31	1.94	0.49
1:B:360:GLU:CG	11:B:753:HOH:O	2.61	0.48
1:E:57:GLN:HB3	1:E:65:MET:SD	2.54	0.48
1:E:367:LYS:HE3	11:E:603:HOH:O	2.14	0.48
1:C:35:ILE:CD1	1:F:35:ILE:CD1	2.91	0.47
1:E:202:LYS:HE2	6:E:505:PG4:H72	1.96	0.47
1:C:131:LEU:CD1	11:C:749:HOH:O	2.61	0.47
1:C:12[B]:GLN:OE1	1:C:25:GLU:OE2	2.33	0.47
1:F:57:GLN:HB3	1:F:65:MET:SD	2.55	0.47
1:E:202:LYS:HD3	6:E:505:PG4:H61	1.97	0.46
1:B:360:GLU:HG3	11:B:840:HOH:O	2.16	0.46
1:E:44:ASP:HB3	6:E:507:PG4:H62	1.98	0.46
11:A:953:HOH:O	1:D:163[A]:HIS:HD2	1.99	0.46
1:D:57:GLN:HB3	1:D:65:MET:SD	2.56	0.46
1:A:102:LYS:NZ	5:A:505:8GL:O03	2.45	0.45
1:B:277:LEU:C	1:B:277:LEU:HD13	2.40	0.45
1:C:131:LEU:HD21	1:F:131:LEU:HD21	1.97	0.45
1:F:277:LEU:C	1:F:277:LEU:HD13	2.41	0.45
1:C:67:GLY:HA3	1:C:101:ALA:O	2.17	0.45
1:A:98:TYR:HH	1:A:348:TRP:CG	2.34	0.45
1:B:127:LYS:NZ	11:B:603:HOH:O	2.34	0.45
1:A:131:LEU:HD21	1:E:131:LEU:HD21	1.97	0.45
1:A:182:GLU:HG3	11:A:614:HOH:O	2.17	0.44
1:B:36:LYS:CE	11:B:608:HOH:O	2.66	0.44
1:C:190:VAL:HG21	1:C:224:ALA:HB3	1.99	0.44
1:A:64:PRO:HD3	1:D:163[A]:HIS:CD2	2.52	0.44
1:D:67:GLY:HA3	1:D:101:ALA:O	2.18	0.43
3:C:509:EDO:O1	11:C:601:HOH:O	2.21	0.43
1:E:33:ARG:NH2	1:E:131:LEU:HD13	2.33	0.43
1:D:36:LYS:HG2	1:D:54:PHE:CD2	2.53	0.43
1:D:384:HIS:HE1	11:D:904:HOH:O	2.00	0.43
1:B:306:PHE:HE2	6:B:506:PG4:H21	1.82	0.42
1:C:12[B]:GLN:CD	1:C:25:GLU:OE2	2.62	0.42
1:B:365:GLU:OE1	1:B:368:ARG:NH2	2.50	0.42
1:D:208:THR:HA	1:D:231:LYS:O	2.20	0.42
1:F:76:ASP:HB2	1:F:77:PRO:CD	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:LYS:HD2	11:B:603:HOH:O	2.20	0.42
1:A:174:ASP:OD2	1:F:402:ARG:HD2	2.20	0.42
1:C:157:TYR:CZ	1:C:161:HIS:CD2	3.08	0.42
1:F:127:LYS:HD2	11:F:2401:HOH:O	2.19	0.41
1:B:57:GLN:HB3	1:B:65:MET:SD	2.60	0.41
1:A:353:GLN:OE1	11:A:601:HOH:O	2.22	0.41
1:D:316:ASP:OD1	1:D:316:ASP:C	2.62	0.41
1:D:277:LEU:C	1:D:277:LEU:HD13	2.46	0.41
1:E:277:LEU:HD13	1:E:277:LEU:C	2.45	0.41
9:A:514:GLY:N	11:A:614:HOH:O	2.53	0.41
1:B:67:GLY:HA3	1:B:101:ALA:O	2.21	0.41
1:D:190:VAL:HG11	1:D:228:ARG:HD2	2.03	0.41
1:A:66:LYS:NZ	5:A:505:8GL:O07	2.55	0.40
1:A:67:GLY:HA3	1:A:101:ALA:O	2.20	0.40
1:B:259:GLY:O	1:B:260:ASN:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	414/414 (100%)	403 (97%)	11 (3%)	0	100	100
1	B	415/414 (100%)	405 (98%)	10 (2%)	0	100	100
1	C	418/414 (101%)	408 (98%)	10 (2%)	0	100	100
1	D	415/414 (100%)	407 (98%)	8 (2%)	0	100	100
1	E	418/414 (101%)	407 (97%)	11 (3%)	0	100	100
1	F	416/414 (100%)	405 (97%)	11 (3%)	0	100	100
All	All	2496/2484 (100%)	2435 (98%)	61 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	334/332 (101%)	334 (100%)	0	100	100
1	B	335/332 (101%)	335 (100%)	0	100	100
1	C	338/332 (102%)	337 (100%)	1 (0%)	86	80
1	D	335/332 (101%)	332 (99%)	3 (1%)	70	56
1	E	338/332 (102%)	336 (99%)	2 (1%)	78	68
1	F	336/332 (101%)	335 (100%)	1 (0%)	86	80
All	All	2016/1992 (101%)	2009 (100%)	7 (0%)	84	80

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	380	ASN
1	D	21	ASP
1	D	203	SER
1	D	380	ASN
1	E	131	LEU
1	E	380	ASN
1	F	380	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	GLN
1	A	239	ASN
1	B	12	GLN
1	B	81	ASN
1	B	212	GLN
1	C	212	GLN
1	C	239	ASN
1	D	212	GLN
1	D	380	ASN
1	E	212	GLN

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Mol	Chain	Res	Type
1	E	216	ASN
1	E	246	ASN
1	F	216	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 70 ligands modelled in this entry, 9 are monoatomic - leaving 61 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	$\# Z > 2$
6	PG4	B	506	-	12,12,12	0.19	0	11,11,11	0.14	0
3	EDO	B	508	-	3,3,3	0.48	0	2,2,2	0.84	0
3	EDO	F	2310	-	3,3,3	0.34	0	2,2,2	1.17	0
3	EDO	C	504	-	3,3,3	0.59	0	2,2,2	0.49	0
5	8GL	C	502	-	9,10,10	1.37	1 (11%)	10,14,14	2.43	3 (30%)
3	EDO	D	505	-	3,3,3	0.48	0	2,2,2	0.88	0
3	EDO	E	506	-	3,3,3	0.55	0	2,2,2	0.24	0
9	GLY	F	2313	-	4,4,4	1.11	1 (25%)	3,4,4	2.08	2 (66%)
6	PG4	E	507	8	12,12,12	0.25	0	11,11,11	0.31	0
3	EDO	A	510	-	3,3,3	0.62	0	2,2,2	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GLY	C	503	-	4,4,4	1.09	1 (25%)	3,4,4	1.64	1 (33%)
3	EDO	B	510	8	3,3,3	0.48	0	2,2,2	0.44	0
3	EDO	B	509	-	3,3,3	0.52	0	2,2,2	0.72	0
3	EDO	A	506	-	3,3,3	0.41	0	2,2,2	0.97	0
2	NAD	A	501	-	46,48,48	0.54	0	64,73,73	0.83	1 (1%)
6	PG4	D	503	-	12,12,12	0.22	0	11,11,11	0.17	0
3	EDO	B	504	-	3,3,3	0.56	0	2,2,2	0.12	0
9	GLY	E	504	-	4,4,4	1.28	1 (25%)	3,4,4	2.21	1 (33%)
3	EDO	C	508	-	3,3,3	0.45	0	2,2,2	0.94	0
3	EDO	E	508	-	3,3,3	0.49	0	2,2,2	0.26	0
3	EDO	D	507	-	3,3,3	0.55	0	2,2,2	0.22	0
4	PEG	C	506	-	6,6,6	0.13	0	5,5,5	0.12	0
5	8GL	A	505	-	9,10,10	1.19	0	10,14,14	2.73	3 (30%)
9	GLY	D	511	-	4,4,4	1.13	1 (25%)	3,4,4	1.85	1 (33%)
5	8GL	B	502	-	9,10,10	1.27	1 (11%)	10,14,14	1.65	2 (20%)
4	PEG	A	504	-	6,6,6	0.19	0	5,5,5	0.22	0
4	PEG	D	508	-	6,6,6	0.22	0	5,5,5	0.29	0
3	EDO	A	502	-	3,3,3	0.54	0	2,2,2	0.10	0
4	PEG	F	2307	-	6,6,6	0.19	0	5,5,5	0.19	0
4	PEG	F	2305	-	6,6,6	0.20	0	5,5,5	0.18	0
2	NAD	F	2303	-	46,48,48	0.55	1 (2%)	64,73,73	0.81	2 (3%)
3	EDO	C	510	-	3,3,3	0.42	0	2,2,2	0.31	0
3	EDO	F	2301	8	3,3,3	0.35	0	2,2,2	0.48	0
2	NAD	D	501	-	46,48,48	0.57	1 (2%)	64,73,73	0.72	2 (3%)
3	EDO	A	507	-	3,3,3	0.41	0	2,2,2	0.74	0
3	EDO	F	2308	-	3,3,3	0.43	0	2,2,2	0.73	0
3	EDO	E	503	-	3,3,3	0.42	0	2,2,2	0.20	0
2	NAD	C	501	-	46,48,48	0.59	0	64,73,73	0.76	1 (1%)
2	NAD	E	501	-	46,48,48	0.59	1 (2%)	64,73,73	0.75	1 (1%)
6	PG4	A	511	8	12,12,12	0.20	0	11,11,11	0.26	0
2	NAD	B	501	-	46,48,48	0.56	1 (2%)	64,73,73	0.81	0
3	EDO	F	2309	-	3,3,3	0.52	0	2,2,2	0.28	0
3	EDO	D	506	-	3,3,3	0.50	0	2,2,2	0.55	0
4	PEG	A	509	-	6,6,6	0.30	0	5,5,5	0.14	0
4	PEG	C	505	-	6,6,6	0.14	0	5,5,5	0.15	0
5	8GL	D	502	-	9,10,10	1.18	0	10,14,14	2.23	3 (30%)
3	EDO	B	505	-	3,3,3	0.43	0	2,2,2	0.82	0
4	PEG	D	504	-	6,6,6	0.12	0	5,5,5	0.22	0
3	EDO	C	507	-	3,3,3	0.53	0	2,2,2	0.33	0
5	8GL	E	502	-	9,10,10	1.09	1 (11%)	10,14,14	2.91	4 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	F	2306	-	3,3,3	0.61	0	2,2,2	0.64	0
3	EDO	F	2302	-	3,3,3	0.39	0	2,2,2	1.57	0
3	EDO	F	2311	-	3,3,3	0.56	0	2,2,2	0.79	0
9	GLY	B	503	-	4,4,4	1.06	1 (25%)	3,4,4	2.42	2 (66%)
6	PG4	E	505	-	12,12,12	0.24	0	11,11,11	0.14	0
5	8GL	F	2304	-	9,10,10	0.95	0	10,14,14	2.93	3 (30%)
10	PGE	B	507	-	9,9,9	0.37	0	8,8,8	0.35	0
3	EDO	A	503	-	3,3,3	0.46	0	2,2,2	0.65	0
3	EDO	A	508	-	3,3,3	0.54	0	2,2,2	0.44	0
3	EDO	C	509	-	3,3,3	0.43	0	2,2,2	0.63	0
9	GLY	A	514	-	4,4,4	0.93	0	3,4,4	2.20	2 (66%)

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
6	PG4	B	506	-	-	1/10/10/10	-
3	EDO	B	508	-	-	1/1/1/1	-
3	EDO	F	2310	-	-	1/1/1/1	-
3	EDO	C	504	-	-	0/1/1/1	-
5	8GL	C	502	-	-	6/9/12/12	-
3	EDO	D	505	-	-	1/1/1/1	-
3	EDO	E	506	-	-	1/1/1/1	-
9	GLY	F	2313	-	-	2/2/2/2	-
6	PG4	E	507	8	-	4/10/10/10	-
3	EDO	A	510	-	-	1/1/1/1	-
9	GLY	C	503	-	-	0/2/2/2	-
3	EDO	B	510	8	-	1/1/1/1	-
3	EDO	B	509	-	-	0/1/1/1	-
3	EDO	A	506	-	-	1/1/1/1	-
2	NAD	A	501	-	-	3/30/62/62	0/5/5/5
6	PG4	D	503	-	-	1/10/10/10	-
3	EDO	B	504	-	-	0/1/1/1	-
9	GLY	E	504	-	-	2/2/2/2	-
3	EDO	C	508	-	-	1/1/1/1	-
3	EDO	E	508	-	-	1/1/1/1	-
3	EDO	D	507	-	-	0/1/1/1	-
4	PEG	C	506	-	-	0/4/4/4	-
5	8GL	A	505	-	-	6/9/12/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GLY	D	511	-	-	2/2/2/2	-
5	8GL	B	502	-	-	6/9/12/12	-
4	PEG	A	504	-	-	1/4/4/4	-
4	PEG	D	508	-	-	1/4/4/4	-
3	EDO	A	502	-	-	1/1/1/1	-
4	PEG	F	2307	-	-	0/4/4/4	-
4	PEG	F	2305	-	-	0/4/4/4	-
2	NAD	F	2303	-	-	3/30/62/62	0/5/5/5
3	EDO	C	510	-	-	0/1/1/1	-
3	EDO	F	2301	8	-	0/1/1/1	-
2	NAD	D	501	-	-	4/30/62/62	0/5/5/5
3	EDO	A	507	-	-	0/1/1/1	-
3	EDO	F	2308	-	-	0/1/1/1	-
3	EDO	E	503	-	-	1/1/1/1	-
2	NAD	C	501	-	-	4/30/62/62	0/5/5/5
2	NAD	E	501	-	-	3/30/62/62	0/5/5/5
6	PG4	A	511	8	-	2/10/10/10	-
2	NAD	B	501	-	-	3/30/62/62	0/5/5/5
3	EDO	F	2309	-	-	1/1/1/1	-
3	EDO	D	506	-	-	0/1/1/1	-
4	PEG	A	509	-	-	1/4/4/4	-
4	PEG	C	505	-	-	0/4/4/4	-
5	8GL	D	502	-	-	6/9/12/12	-
3	EDO	B	505	-	-	0/1/1/1	-
4	PEG	D	504	-	-	0/4/4/4	-
3	EDO	C	507	-	-	0/1/1/1	-
5	8GL	E	502	-	-	6/9/12/12	-
3	EDO	F	2306	-	-	1/1/1/1	-
3	EDO	F	2302	-	-	1/1/1/1	-
3	EDO	F	2311	-	-	1/1/1/1	-
9	GLY	B	503	-	-	2/2/2/2	-
6	PG4	E	505	-	-	2/10/10/10	-
5	8GL	F	2304	-	-	7/9/12/12	-
10	PGE	B	507	-	-	3/7/7/7	-
3	EDO	A	503	-	-	0/1/1/1	-
3	EDO	A	508	-	-	0/1/1/1	-
3	EDO	C	509	-	-	1/1/1/1	-
9	GLY	A	514	-	-	2/2/2/2	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	502	8GL	O08-C06	-2.56	1.22	1.30
5	B	502	8GL	O08-C06	-2.49	1.22	1.30
2	D	501	NAD	O4D-C1D	2.32	1.43	1.40
5	E	502	8GL	O08-C06	-2.32	1.23	1.30
9	E	504	GLY	OXT-C	-2.29	1.23	1.30
2	B	501	NAD	O4D-C1D	2.22	1.43	1.40
9	C	503	GLY	OXT-C	-2.09	1.23	1.30
9	F	2313	GLY	OXT-C	-2.08	1.23	1.30
2	F	2303	NAD	PN-O3	2.07	1.61	1.59
2	E	501	NAD	PN-O3	2.05	1.61	1.59
9	D	511	GLY	OXT-C	-2.04	1.24	1.30
9	B	503	GLY	OXT-C	-2.04	1.24	1.30

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	2304	8GL	O10-C09-C02	-7.13	115.83	123.22
5	E	502	8GL	O10-C09-C02	-7.13	115.84	123.22
5	A	505	8GL	O10-C09-C02	-6.70	116.28	123.22
5	D	502	8GL	O10-C09-C02	-5.29	117.74	123.22
5	C	502	8GL	O03-C02-C09	-4.78	102.23	108.97
5	C	502	8GL	O10-C09-C02	-4.18	118.90	123.22
5	A	505	8GL	O03-C02-C09	-3.48	104.05	108.97
5	F	2304	8GL	O03-C02-C09	-3.43	104.12	108.97
5	E	502	8GL	O11-C09-C02	3.42	119.66	113.09
9	E	504	GLY	OXT-C-O	-3.41	114.55	123.33
5	F	2304	8GL	O11-C09-C02	3.41	119.64	113.09
5	B	502	8GL	O03-C02-C09	-3.28	104.35	108.97
9	B	503	GLY	OXT-C-O	-3.19	115.12	123.33
5	E	502	8GL	O03-C02-C09	-3.16	104.51	108.97
5	C	502	8GL	O03-C02-C04	3.08	114.06	108.15
9	F	2313	GLY	OXT-C-O	-2.80	116.13	123.33
5	B	502	8GL	O10-C09-C02	-2.72	120.40	123.22
9	D	511	GLY	OXT-C-O	-2.71	116.37	123.33
9	B	503	GLY	OXT-C-CA	2.69	124.08	113.38
9	A	514	GLY	OXT-C-CA	2.67	124.00	113.38
9	A	514	GLY	OXT-C-O	-2.61	116.62	123.33
2	D	501	NAD	C6N-N1N-C2N	-2.55	119.71	121.88
5	E	502	8GL	C04-C05-C06	2.48	118.52	112.77
5	A	505	8GL	O11-C09-C02	2.46	117.81	113.09
9	F	2313	GLY	OXT-C-CA	2.26	122.38	113.38
5	D	502	8GL	O11-C09-C02	2.25	117.42	113.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	502	8GL	O03-C02-C09	-2.24	105.81	108.97
9	C	503	GLY	OXT-C-O	-2.22	117.63	123.33
2	F	2303	NAD	O2A-PA-O1A	2.11	122.25	112.44
2	D	501	NAD	O2A-PA-O3	2.09	112.93	107.27
2	E	501	NAD	C6N-N1N-C2N	-2.08	120.11	121.88
2	F	2303	NAD	C4D-O4D-C1D	-2.06	108.03	109.92
2	C	501	NAD	C6N-N1N-C2N	-2.05	120.13	121.88
2	A	501	NAD	C6N-N1N-C2N	-2.05	120.13	121.88

There are no chirality outliers.

All (99) 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	C5D-O5D-PN-O2N
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	501	NAD	O4D-C1D-N1N-C2N
2	E	501	NAD	O4D-C1D-N1N-C6N
2	E	501	NAD	C2D-C1D-N1N-C6N
2	F	2303	NAD	O4D-C1D-N1N-C2N
2	F	2303	NAD	O4D-C1D-N1N-C6N
2	F	2303	NAD	C2D-C1D-N1N-C6N
5	A	505	8GL	O03-C02-C04-C05
5	A	505	8GL	C09-C02-C04-C05
5	A	505	8GL	O03-C02-C09-O10
5	A	505	8GL	O03-C02-C09-O11
5	A	505	8GL	C04-C02-C09-O10
5	A	505	8GL	C04-C02-C09-O11
5	B	502	8GL	O03-C02-C04-C05
5	B	502	8GL	C09-C02-C04-C05
5	B	502	8GL	O03-C02-C09-O10
5	B	502	8GL	O03-C02-C09-O11

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Mol	Chain	Res	Type	Atoms
5	B	502	8GL	C04-C02-C09-O10
5	B	502	8GL	C04-C02-C09-O11
5	C	502	8GL	O03-C02-C04-C05
5	C	502	8GL	C09-C02-C04-C05
5	C	502	8GL	O03-C02-C09-O10
5	C	502	8GL	O03-C02-C09-O11
5	C	502	8GL	C04-C02-C09-O10
5	C	502	8GL	C04-C02-C09-O11
5	D	502	8GL	O03-C02-C04-C05
5	D	502	8GL	C09-C02-C04-C05
5	D	502	8GL	O03-C02-C09-O10
5	D	502	8GL	O03-C02-C09-O11
5	D	502	8GL	C04-C02-C09-O10
5	D	502	8GL	C04-C02-C09-O11
5	E	502	8GL	O03-C02-C04-C05
5	E	502	8GL	C09-C02-C04-C05
5	E	502	8GL	O03-C02-C09-O10
5	E	502	8GL	O03-C02-C09-O11
5	E	502	8GL	C04-C02-C09-O10
5	E	502	8GL	C04-C02-C09-O11
5	F	2304	8GL	O03-C02-C04-C05
5	F	2304	8GL	C09-C02-C04-C05
5	F	2304	8GL	O03-C02-C09-O10
5	F	2304	8GL	O03-C02-C09-O11
5	F	2304	8GL	C04-C02-C09-O10
5	F	2304	8GL	C04-C02-C09-O11
9	A	514	GLY	O-C-CA-N
9	A	514	GLY	OXT-C-CA-N
9	B	503	GLY	O-C-CA-N
9	B	503	GLY	OXT-C-CA-N
9	D	511	GLY	O-C-CA-N
9	D	511	GLY	OXT-C-CA-N
3	C	508	EDO	O1-C1-C2-O2
4	A	509	PEG	O1-C1-C2-O2
3	A	506	EDO	O1-C1-C2-O2
3	B	508	EDO	O1-C1-C2-O2
3	E	503	EDO	O1-C1-C2-O2
6	E	507	PG4	O1-C1-C2-O2
10	B	507	PGE	O3-C5-C6-O4
3	E	508	EDO	O1-C1-C2-O2
3	F	2302	EDO	O1-C1-C2-O2
3	F	2309	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	D	505	EDO	O1-C1-C2-O2
10	B	507	PGE	C6-C5-O3-C4
6	D	503	PG4	C6-C5-O3-C4
4	D	508	PEG	C1-C2-O2-C3
10	B	507	PGE	C4-C3-O2-C2
6	E	507	PG4	O4-C7-C8-O5
9	F	2313	GLY	O-C-CA-N
6	A	511	PG4	O1-C1-C2-O2
6	B	506	PG4	C8-C7-O4-C6
6	E	505	PG4	C5-C6-O4-C7
9	E	504	GLY	OXT-C-CA-N
9	F	2313	GLY	OXT-C-CA-N
2	D	501	NAD	C2D-C1D-N1N-C2N
6	E	505	PG4	O3-C5-C6-O4
3	A	510	EDO	O1-C1-C2-O2
3	C	509	EDO	O1-C1-C2-O2
6	E	507	PG4	C1-C2-O2-C3
3	B	510	EDO	O1-C1-C2-O2
3	E	506	EDO	O1-C1-C2-O2
3	F	2310	EDO	O1-C1-C2-O2
3	F	2311	EDO	O1-C1-C2-O2
5	F	2304	8GL	C04-C05-C06-O08
4	A	504	PEG	C1-C2-O2-C3
3	A	502	EDO	O1-C1-C2-O2
3	F	2306	EDO	O1-C1-C2-O2
6	E	507	PG4	C8-C7-O4-C6
9	E	504	GLY	O-C-CA-N
6	A	511	PG4	C5-C6-O4-C7

There are no ring outliers.

18 monomers are involved in 25 short contacts:

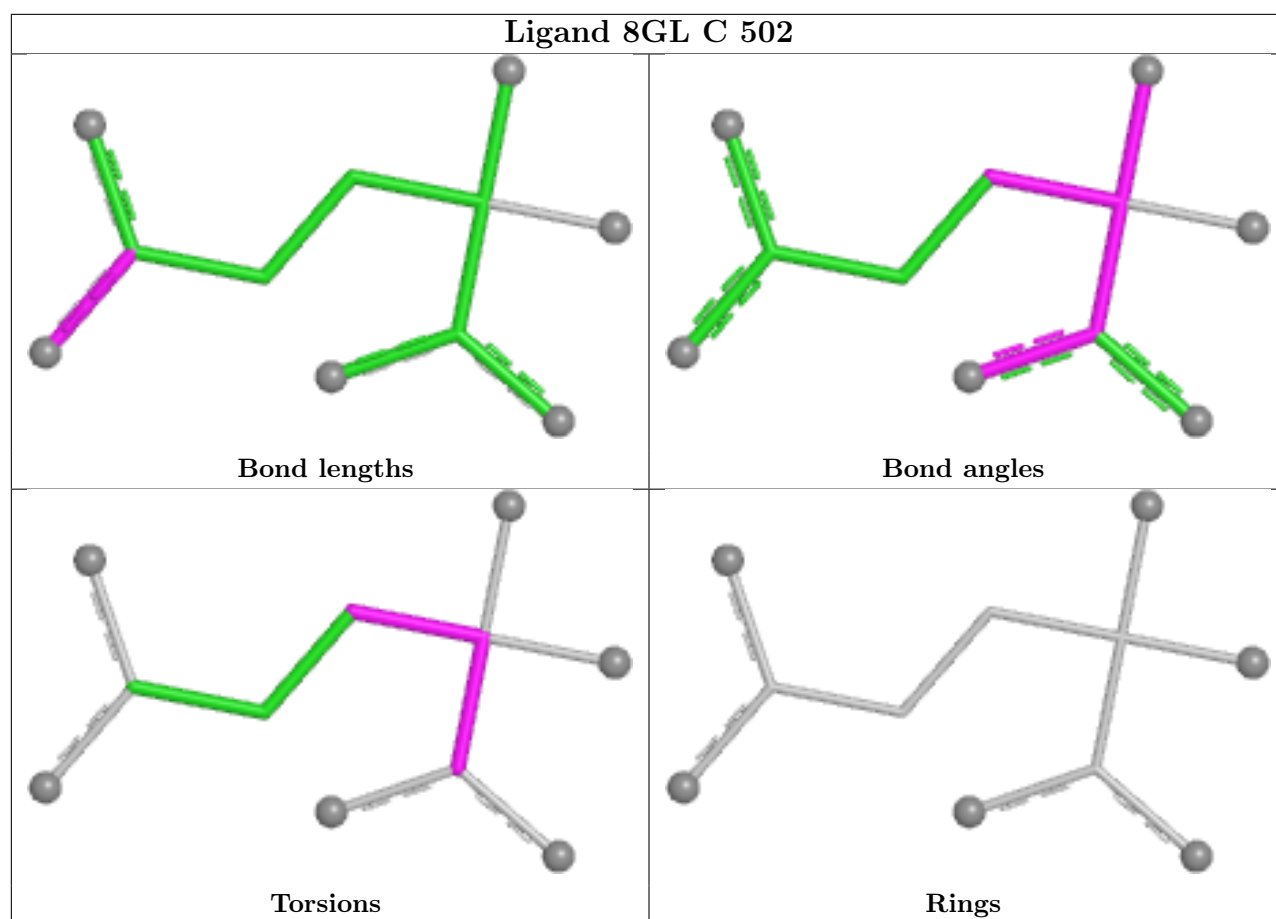
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	506	PG4	3	0
5	C	502	8GL	1	0
6	E	507	PG4	2	0
9	C	503	GLY	1	0
6	D	503	PG4	1	0
9	E	504	GLY	1	0
4	C	506	PEG	1	0
5	A	505	8GL	2	0
5	B	502	8GL	1	0

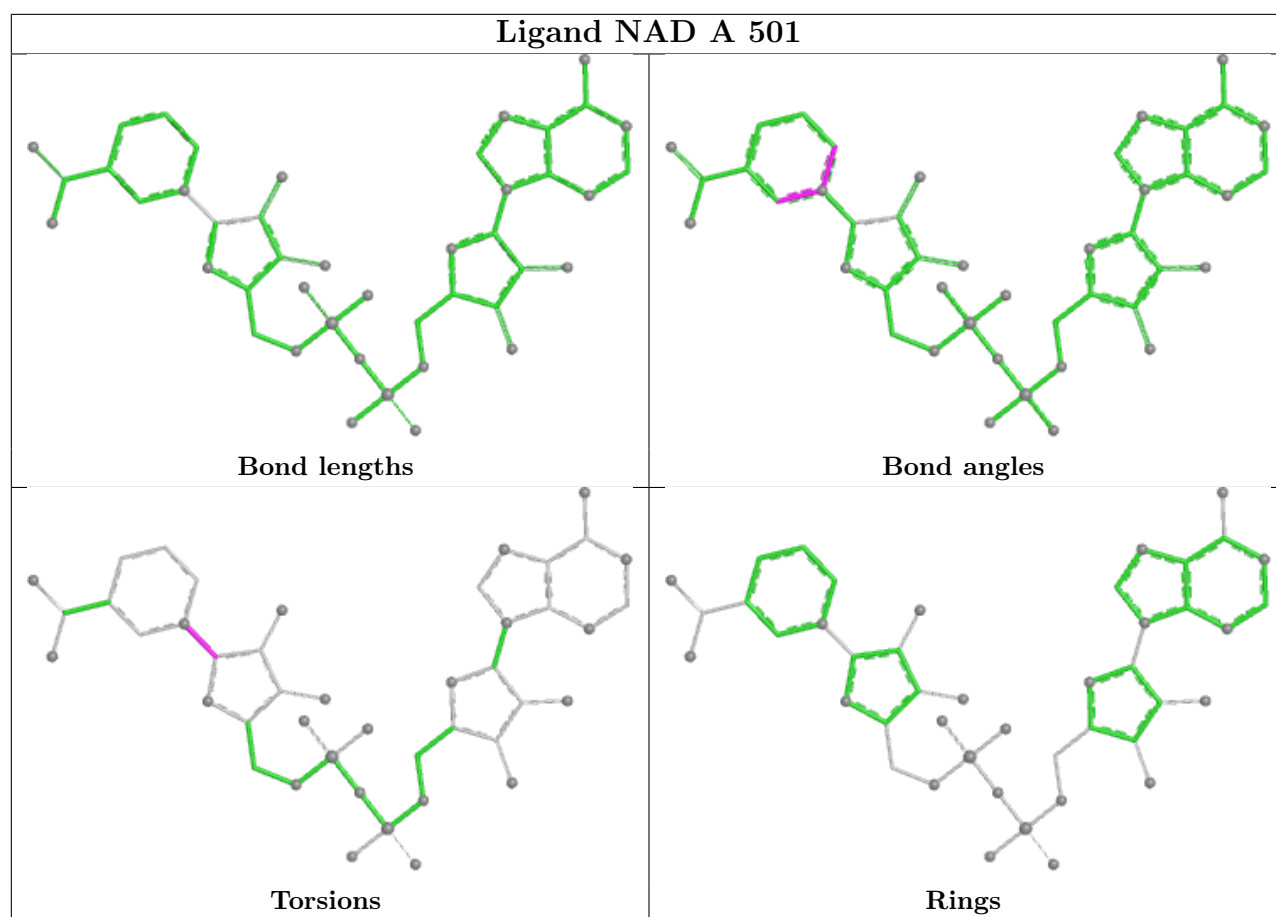
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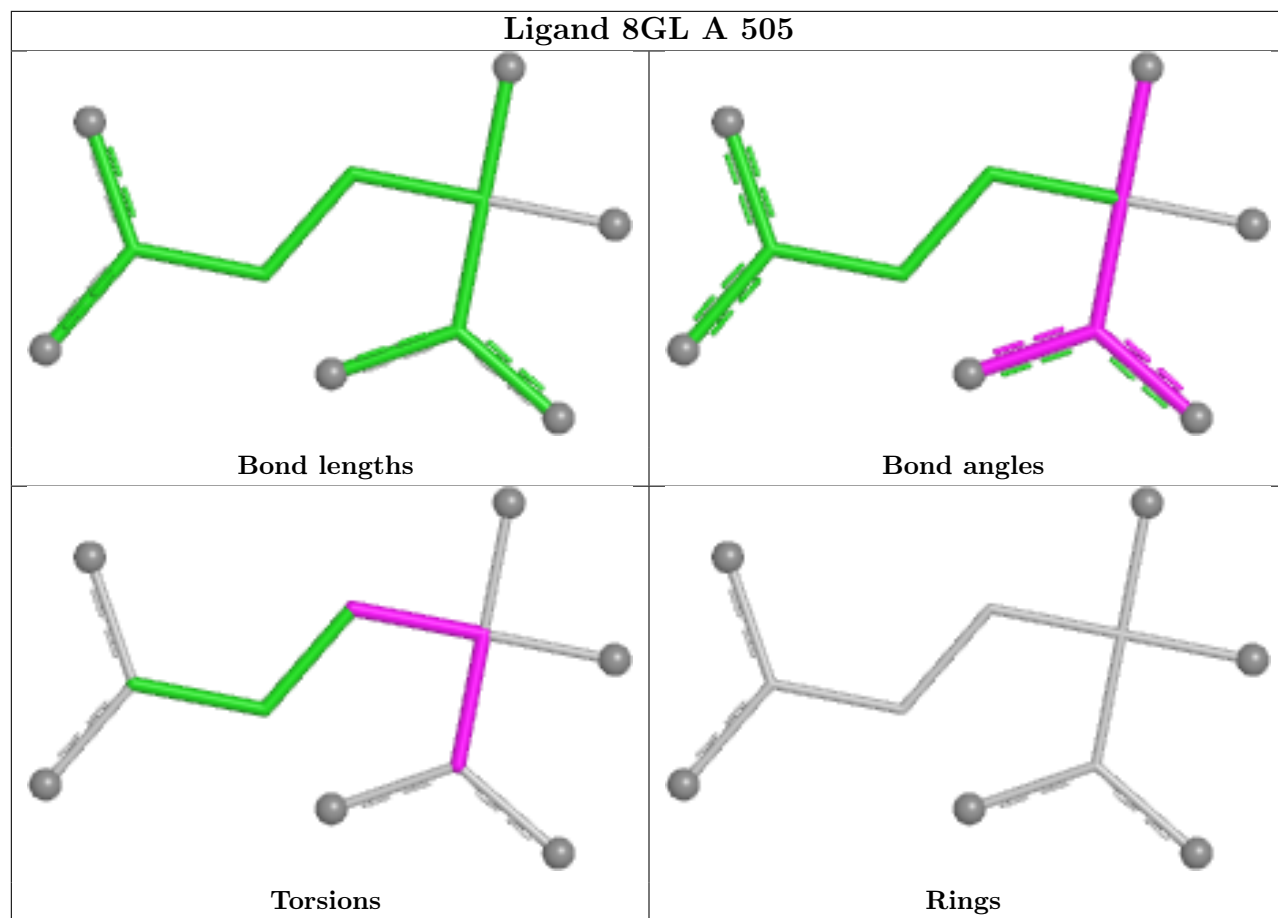
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	2305	PEG	1	0
6	A	511	PG4	2	0
5	D	502	8GL	1	0
5	E	502	8GL	1	0
9	B	503	GLY	1	0
6	E	505	PG4	3	0
5	F	2304	8GL	1	0
3	C	509	EDO	1	0
9	A	514	GLY	1	0

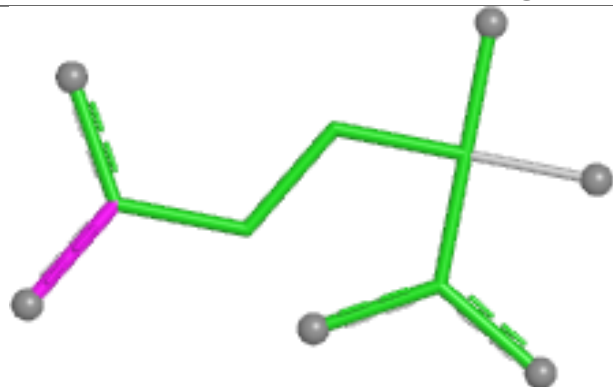
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



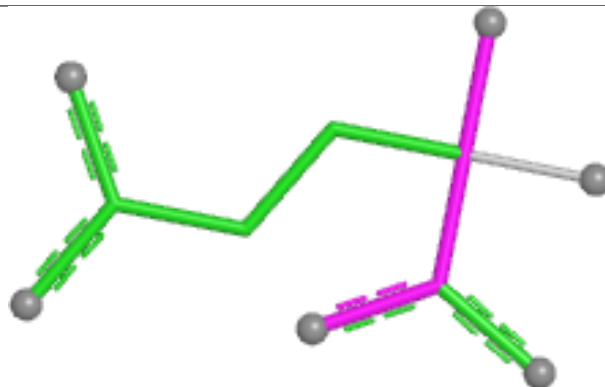




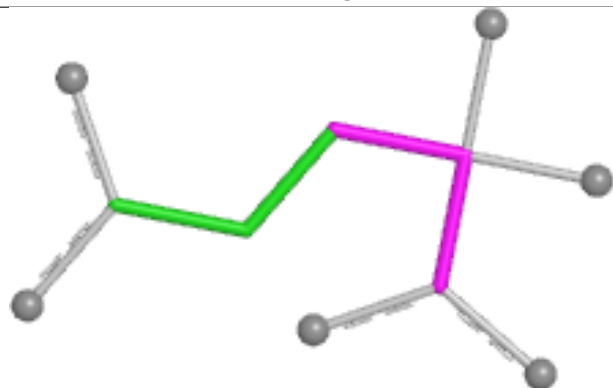
Ligand 8GL B 502



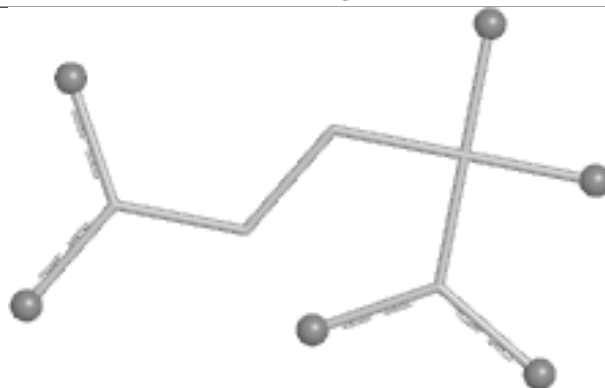
Bond lengths



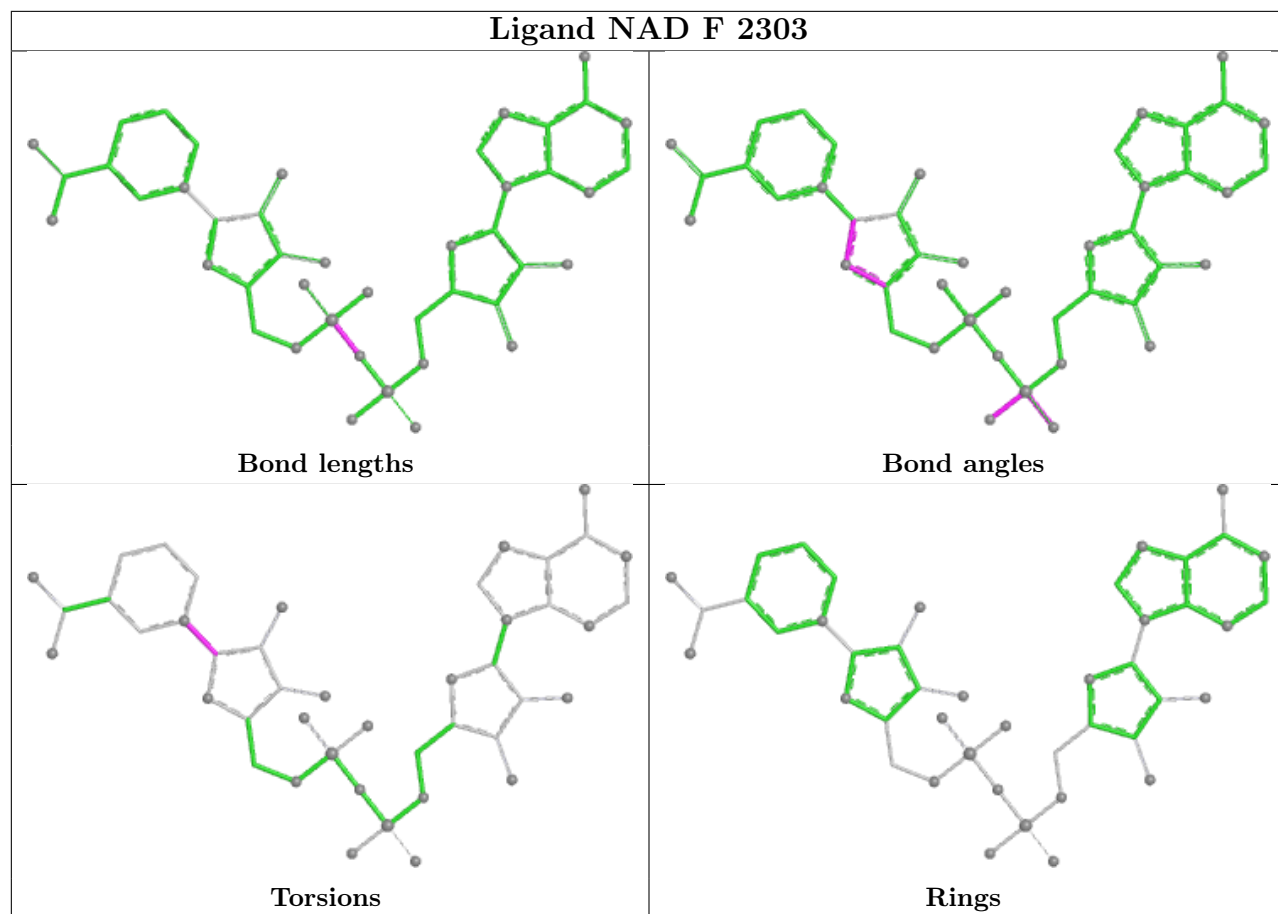
Bond angles

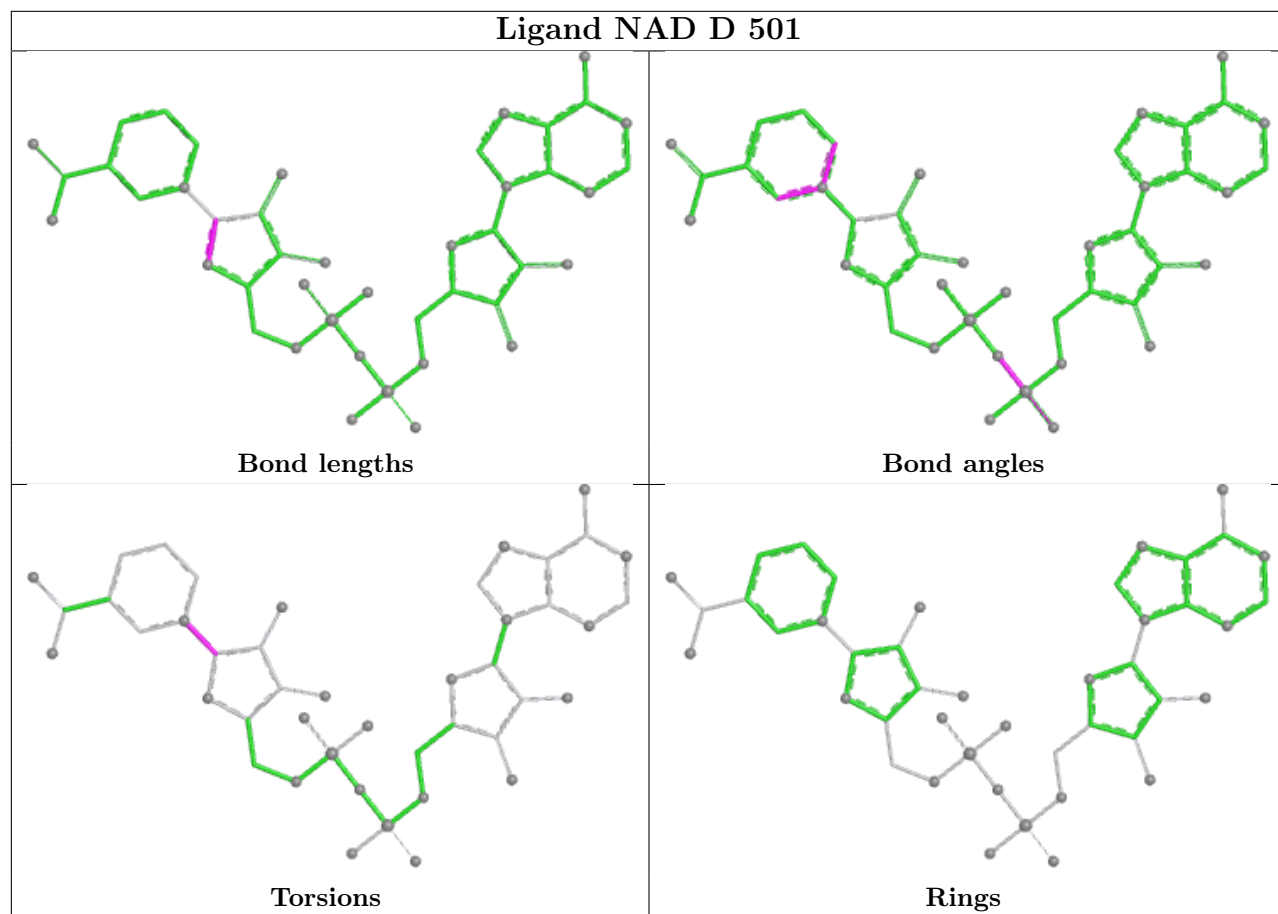


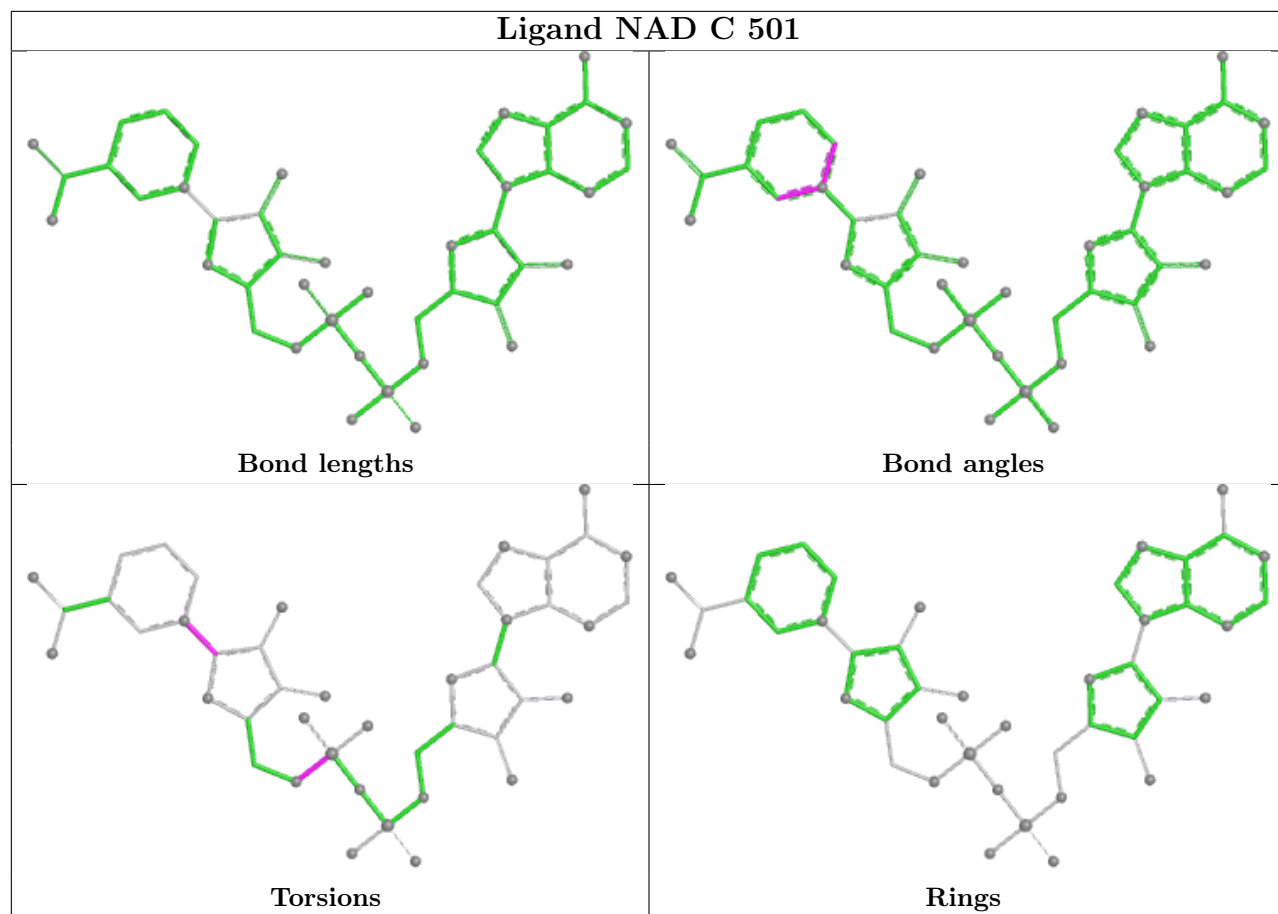
Torsions

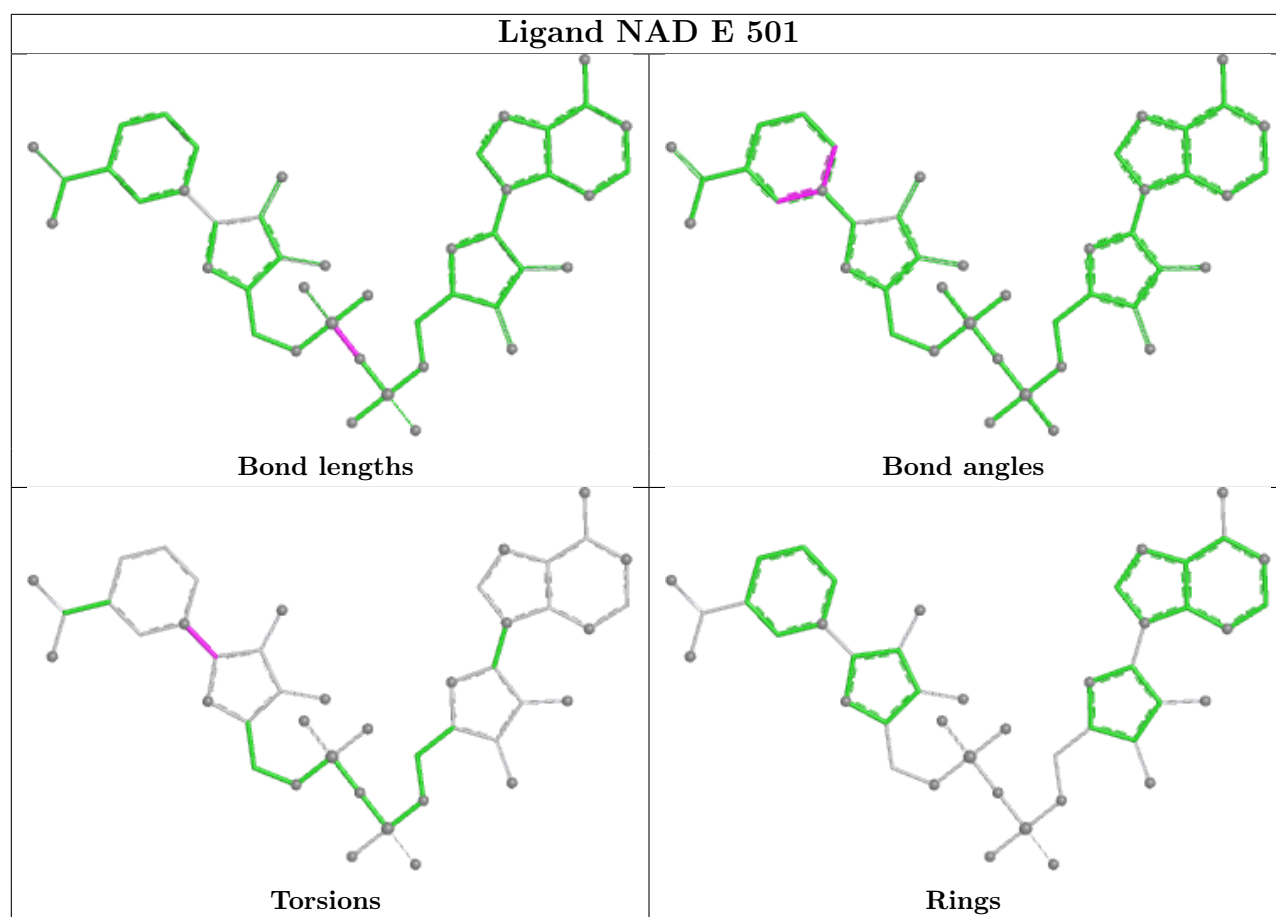


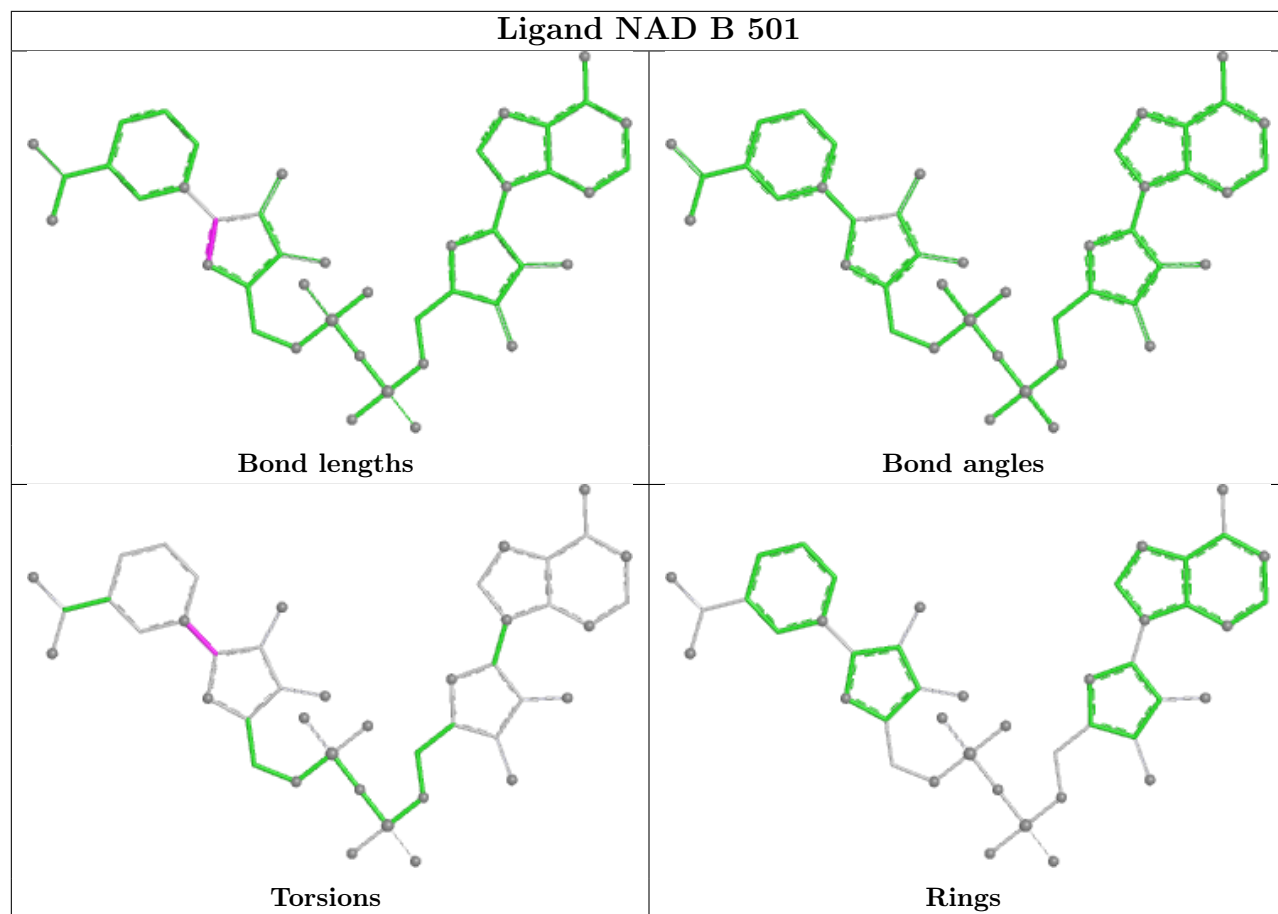
Rings

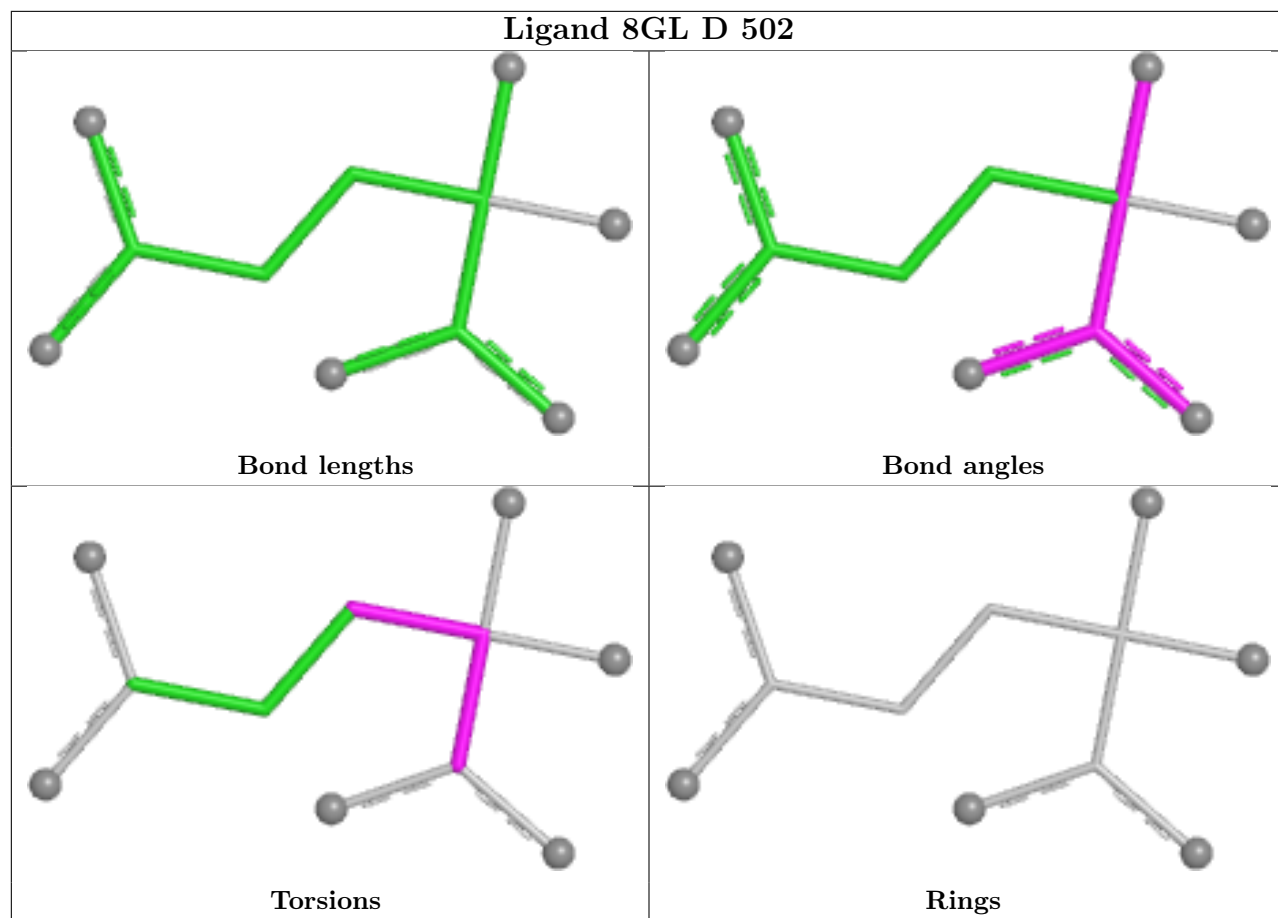


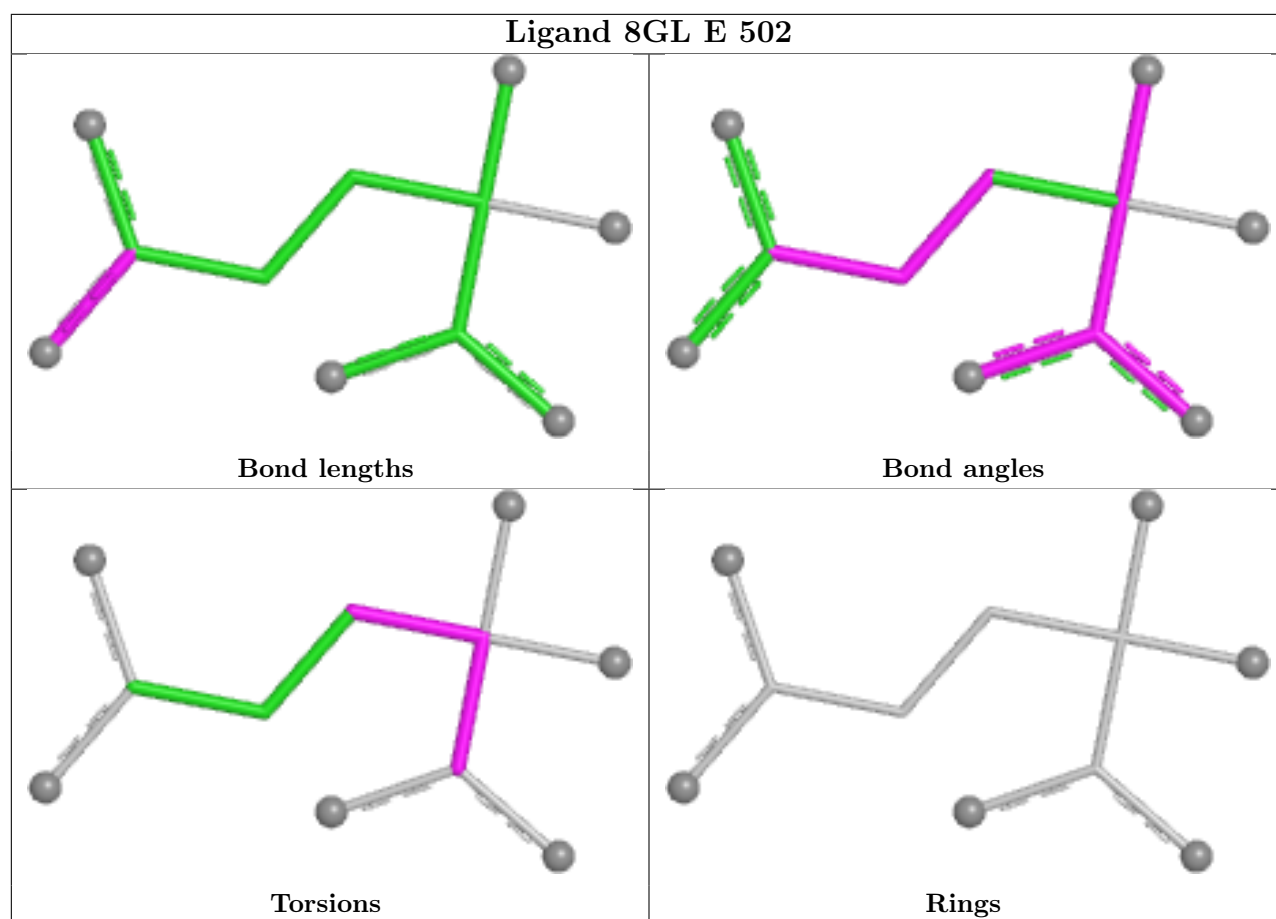


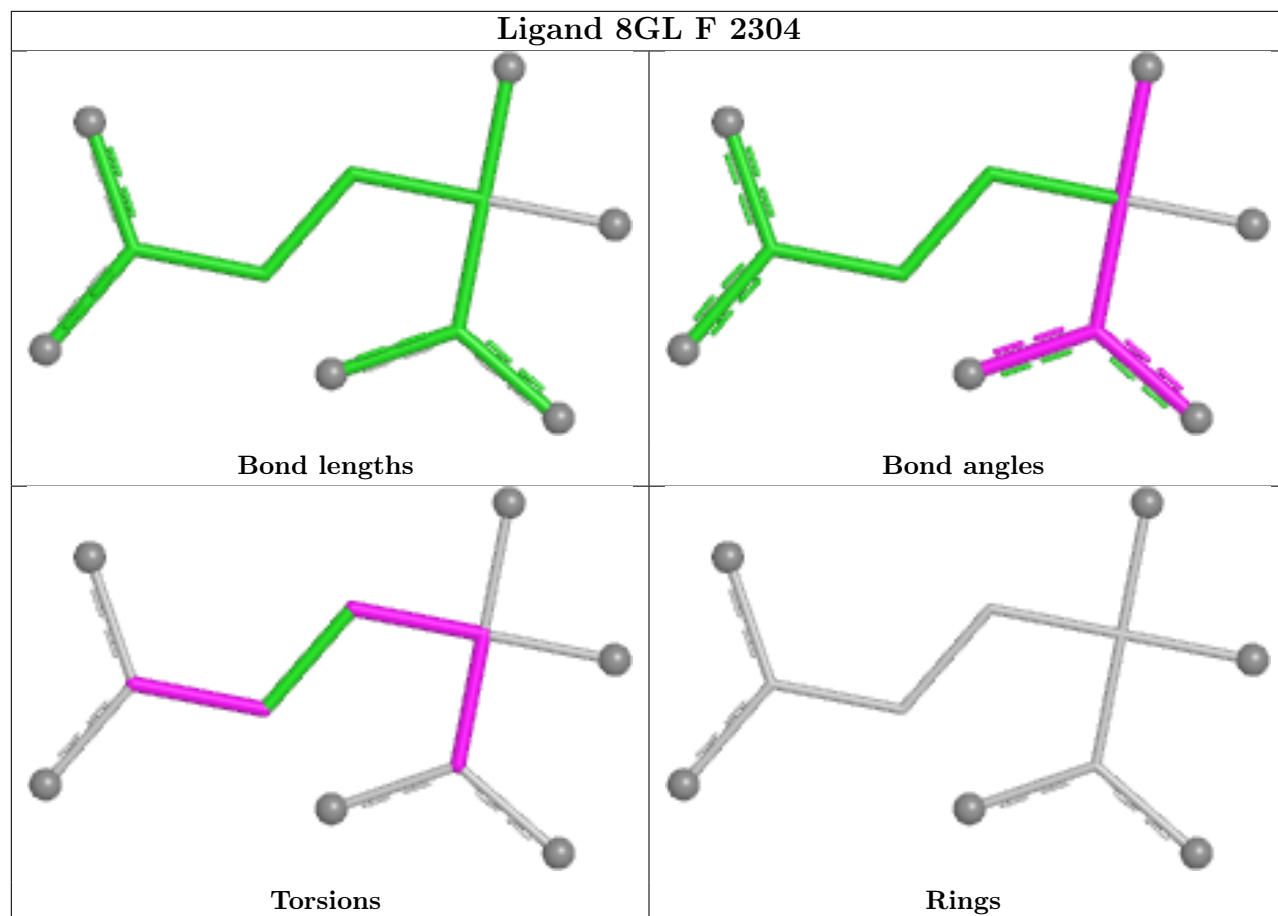












5.7 Other polymers [i](#)

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%)	-0.46	1 (0%) 91 93	9, 20, 33, 48	4 (0%)
1	B	412/414 (99%)	-0.38	2 (0%) 87 91	9, 22, 36, 70	5 (1%)
1	C	412/414 (99%)	-0.42	4 (0%) 79 84	9, 20, 36, 50	8 (1%)
1	D	412/414 (99%)	-0.03	5 (1%) 76 81	10, 25, 47, 65	5 (1%)
1	E	412/414 (99%)	-0.50	1 (0%) 91 93	8, 19, 31, 47	8 (1%)
1	F	412/414 (99%)	-0.47	3 (0%) 84 89	8, 20, 34, 53	6 (1%)
All	All	2472/2484 (99%)	-0.38	16 (0%) 85 90	8, 21, 37, 70	36 (1%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	0	ALA	5.1
1	B	355	PHE	4.0
1	B	0	ALA	3.6
1	F	355	PHE	3.2
1	A	0	ALA	3.1
1	F	0	ALA	3.0
1	E	0	ALA	2.8
1	C	352	ILE	2.8
1	C	355	PHE	2.7
1	F	131	LEU	2.5
1	C	131	LEU	2.5
1	D	242	ILE	2.4
1	D	136[A]	ARG	2.3
1	D	271	ALA	2.3
1	D	264	LYS	2.2
1	C	0	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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	EDO	D	506	4/4	0.76	0.17	39,43,45,54	0
4	PEG	C	506	7/7	0.76	0.15	44,51,60,63	0
6	PG4	E	507	13/13	0.76	0.17	34,45,54,58	0
4	PEG	A	509	7/7	0.77	0.16	42,47,60,60	0
6	PG4	E	505	13/13	0.78	0.16	42,50,63,66	0
6	PG4	A	511	13/13	0.78	0.17	34,50,56,56	0
3	EDO	F	2310	4/4	0.79	0.20	49,50,50,53	0
3	EDO	F	2301	4/4	0.79	0.17	38,43,45,60	0
3	EDO	F	2308	4/4	0.80	0.15	42,46,47,51	0
3	EDO	C	507	4/4	0.81	0.14	44,46,47,53	0
3	EDO	A	510	4/4	0.81	0.17	34,35,41,45	0
3	EDO	D	507	4/4	0.82	0.15	42,43,46,60	0
3	EDO	E	508	4/4	0.82	0.17	38,40,47,52	0
3	EDO	B	509	4/4	0.83	0.16	41,44,45,52	0
3	EDO	A	502	4/4	0.83	0.14	34,42,49,50	0
3	EDO	E	506	4/4	0.83	0.14	41,41,52,53	0
3	EDO	A	508	4/4	0.84	0.16	46,46,51,53	0
6	PG4	D	503	13/13	0.84	0.14	41,45,50,57	0
3	EDO	B	510	4/4	0.85	0.14	35,39,50,52	0
4	PEG	D	508	7/7	0.85	0.13	31,44,48,58	0
9	GLY	F	2313	5/5	0.85	0.18	63,64,65,66	0
3	EDO	F	2309	4/4	0.86	0.12	43,48,53,54	0
3	EDO	B	504	4/4	0.86	0.12	27,36,42,44	0
3	EDO	C	510	4/4	0.87	0.12	33,41,46,48	0
9	GLY	E	504	5/5	0.87	0.14	46,48,54,54	0
3	EDO	F	2311	4/4	0.87	0.13	28,34,37,50	0
10	PGE	B	507	10/10	0.87	0.14	34,42,47,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	B	508	4/4	0.88	0.12	20,35,45,48	0
9	GLY	A	514	5/5	0.88	0.15	48,53,61,61	0
3	EDO	A	507	4/4	0.88	0.12	35,37,38,57	0
4	PEG	C	505	7/7	0.88	0.12	38,43,48,54	0
3	EDO	F	2306	4/4	0.88	0.14	34,36,44,46	0
6	PG4	B	506	13/13	0.89	0.12	40,46,50,58	0
4	PEG	A	504	7/7	0.89	0.13	36,43,50,55	0
3	EDO	E	503	4/4	0.89	0.12	36,37,43,50	0
3	EDO	D	505	4/4	0.89	0.13	15,31,35,51	0
3	EDO	C	508	4/4	0.89	0.14	17,36,43,48	0
9	GLY	D	511	5/5	0.89	0.14	53,53,55,56	0
3	EDO	A	506	4/4	0.89	0.11	22,34,41,45	0
4	PEG	F	2307	7/7	0.89	0.13	42,44,50,52	0
3	EDO	F	2302	4/4	0.89	0.14	25,37,43,45	0
9	GLY	B	503	5/5	0.90	0.14	44,46,54,57	0
9	GLY	C	503	5/5	0.90	0.14	46,50,55,61	0
3	EDO	C	504	4/4	0.90	0.11	33,35,38,39	0
3	EDO	A	503	4/4	0.91	0.10	32,33,42,43	0
4	PEG	F	2305	7/7	0.91	0.10	34,36,48,48	0
3	EDO	B	505	4/4	0.91	0.10	38,38,39,45	0
3	EDO	C	509	4/4	0.91	0.10	34,35,41,46	0
4	PEG	D	504	7/7	0.91	0.10	38,39,45,47	0
5	8GL	D	502	11/11	0.94	0.08	17,22,29,31	0
8	NA	D	510	1/1	0.95	0.23	35,35,35,35	0
5	8GL	B	502	11/11	0.95	0.08	16,22,25,37	0
5	8GL	F	2304	11/11	0.96	0.07	16,20,26,36	0
5	8GL	C	502	11/11	0.96	0.07	15,21,28,37	0
5	8GL	A	505	11/11	0.96	0.07	16,20,28,41	0
8	NA	B	512	1/1	0.96	0.17	34,34,34,34	0
5	8GL	E	502	11/11	0.97	0.07	17,19,27,36	0
2	NAD	D	501	44/44	0.97	0.07	16,22,35,38	0
8	NA	A	513	1/1	0.98	0.14	28,28,28,28	0
2	NAD	A	501	44/44	0.99	0.04	13,16,21,23	0
7	CA	A	512	1/1	0.99	0.07	19,19,19,19	0
2	NAD	E	501	44/44	0.99	0.04	13,17,22,25	0
2	NAD	F	2303	44/44	0.99	0.04	15,18,22,27	0
2	NAD	B	501	44/44	0.99	0.04	14,18,24,29	0
2	NAD	C	501	44/44	0.99	0.04	13,16,22,24	0
7	CA	B	511	1/1	1.00	0.06	18,18,18,18	0
7	CA	C	511	1/1	1.00	0.03	19,19,19,19	0
7	CA	D	509	1/1	1.00	0.05	19,19,19,19	0
7	CA	E	509	1/1	1.00	0.05	18,18,18,18	0

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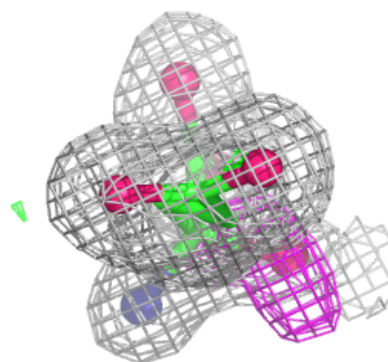
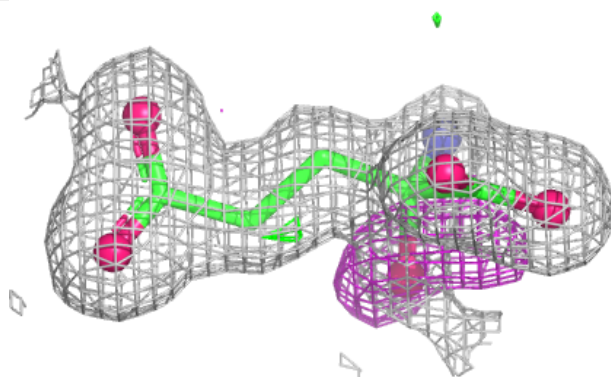
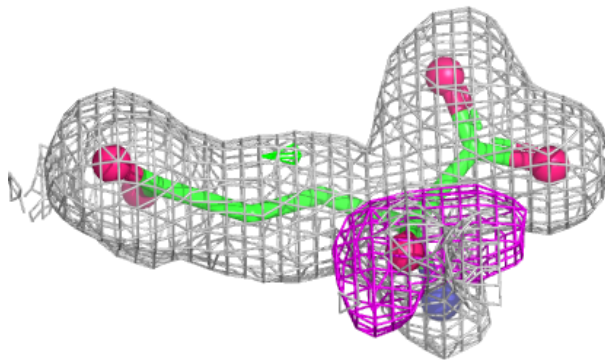
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	CA	F	2312	1/1	1.00	0.02	17,17,17,17	0

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.

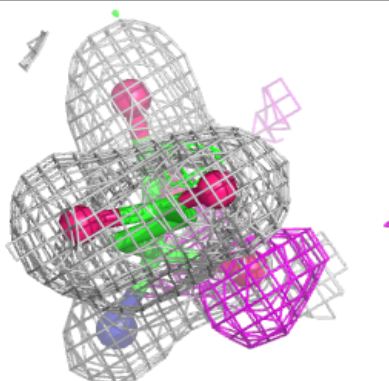
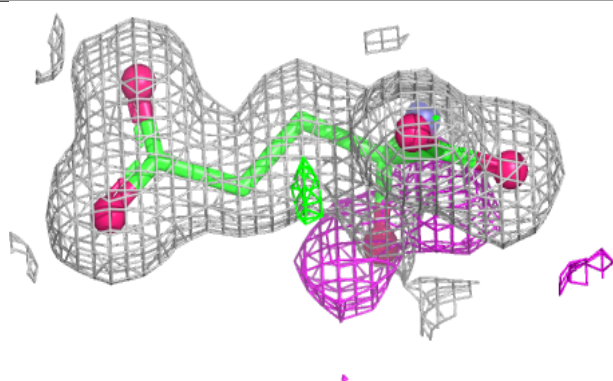
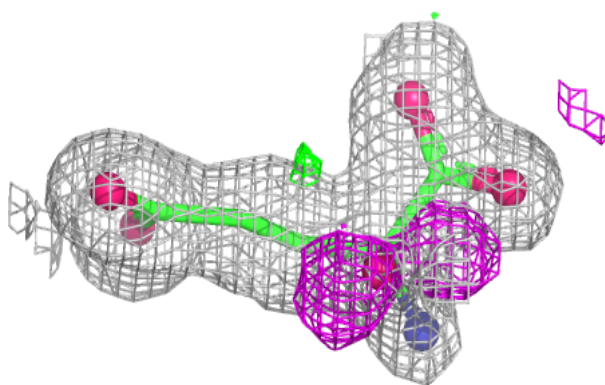
Electron density around 8GL D 502:

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

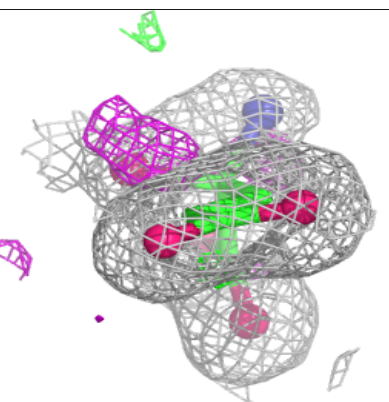
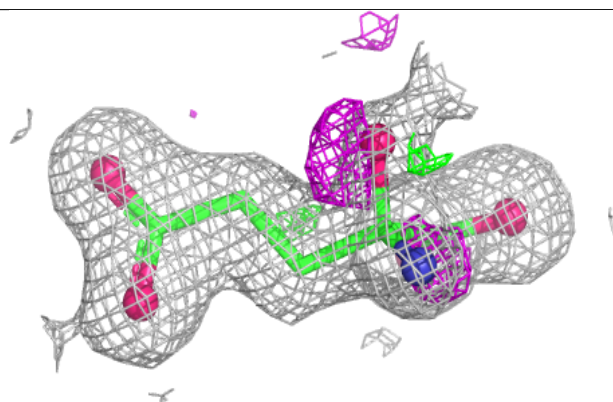
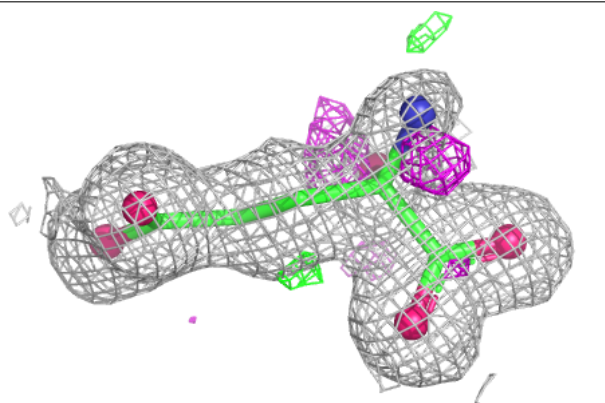


Electron density around 8GL B 502:

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

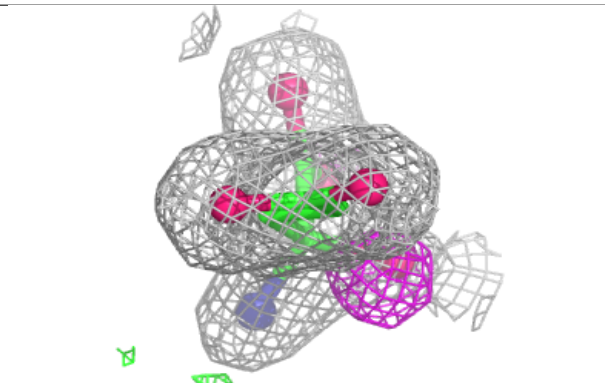
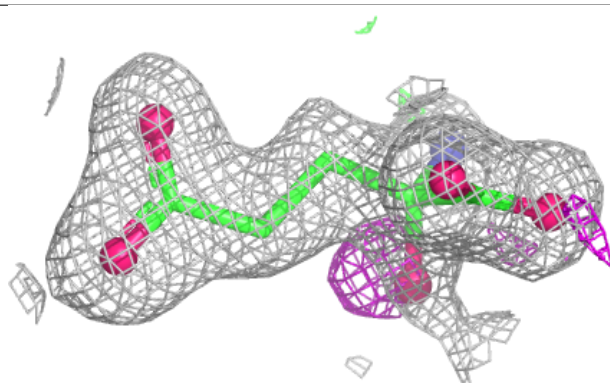
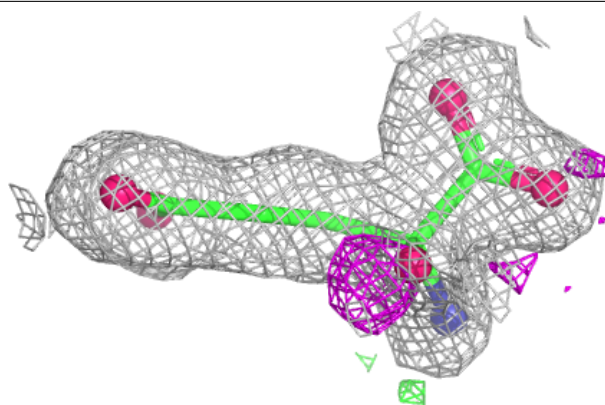
**Electron density around 8GL F 2304:**

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

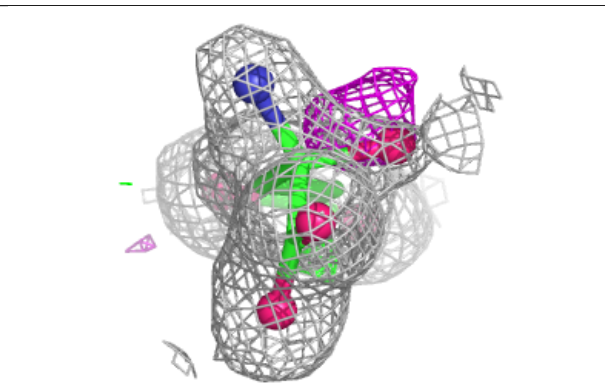
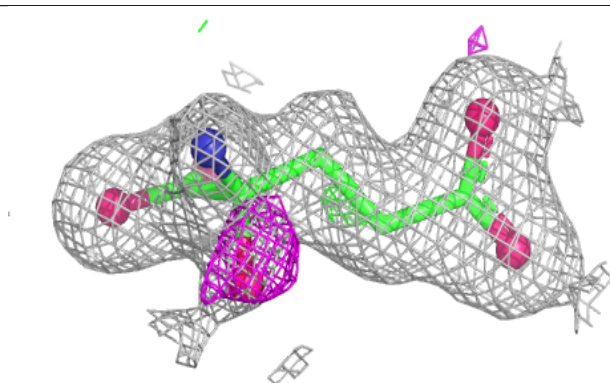
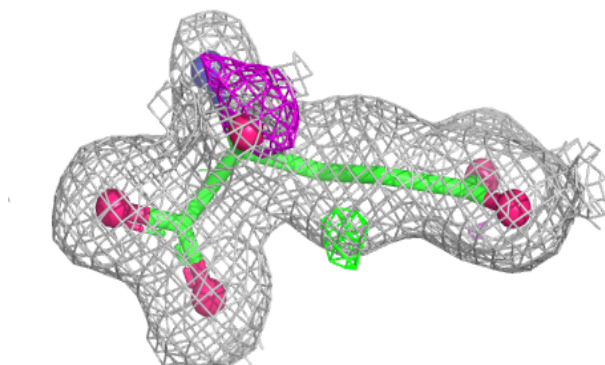


Electron density around 8GL C 502:

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

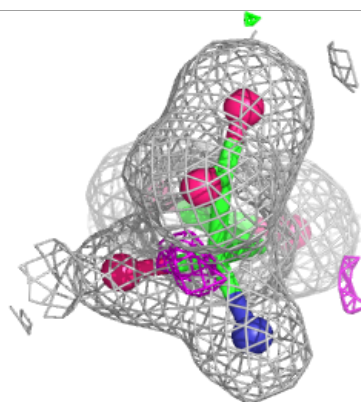
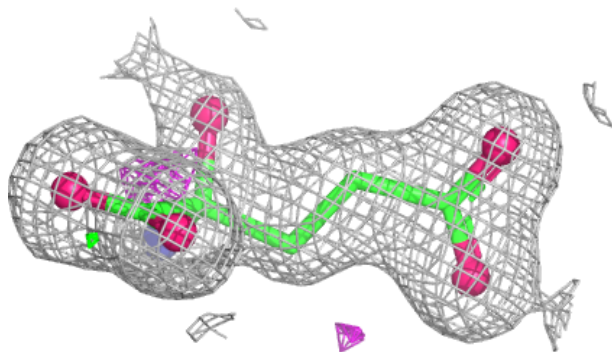
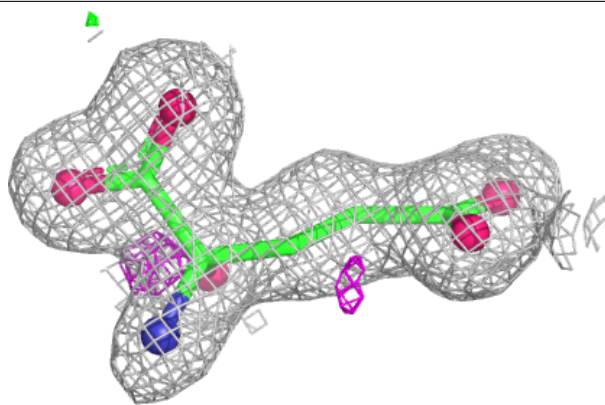
**Electron density around 8GL A 505:**

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

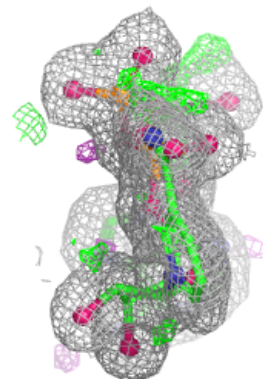
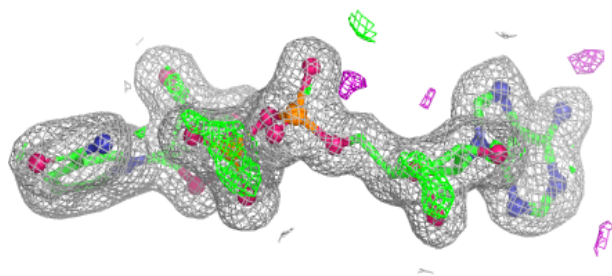
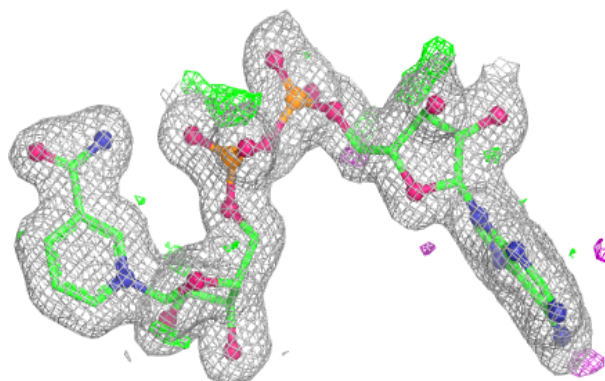


Electron density around 8GL E 502:

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

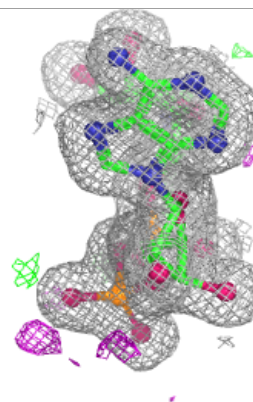
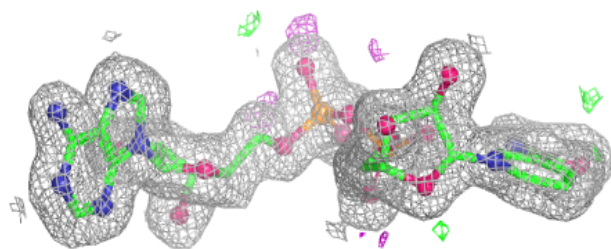
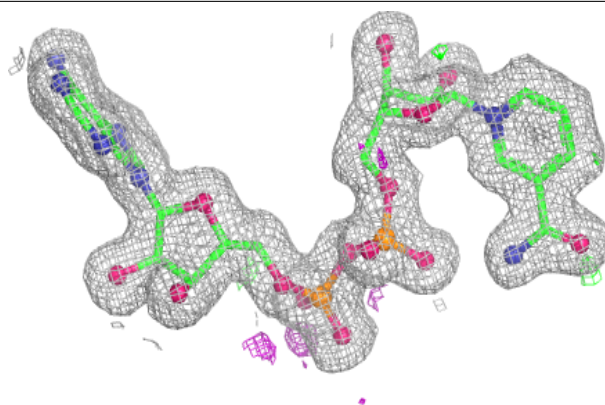
**Electron density around NAD D 501:**

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



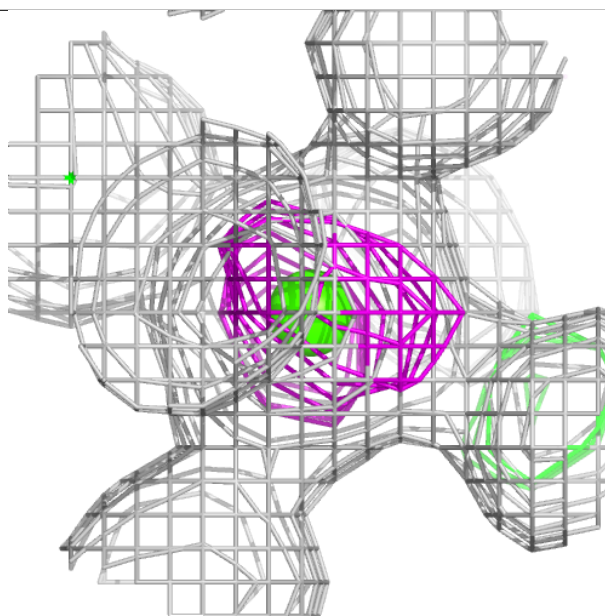
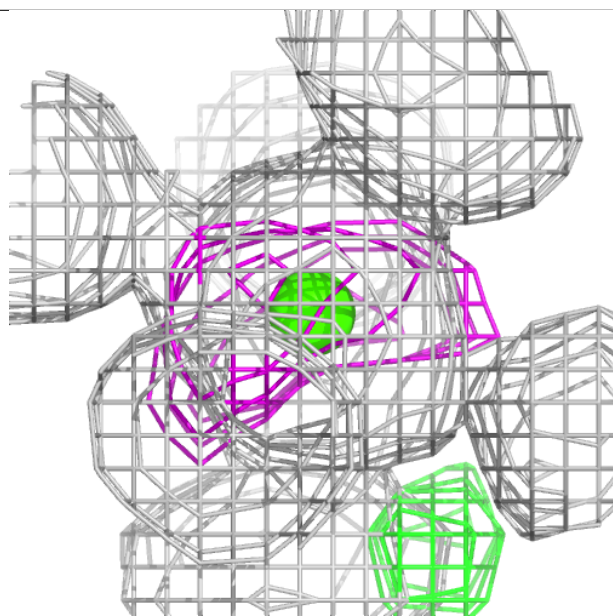
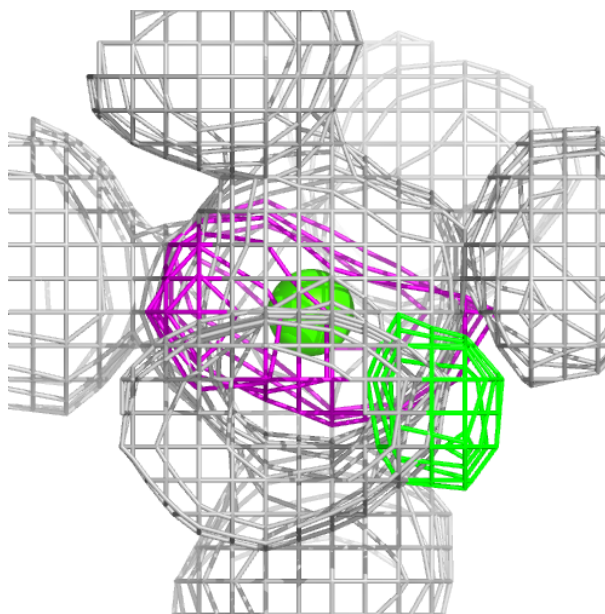
Electron density around NAD A 501:

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



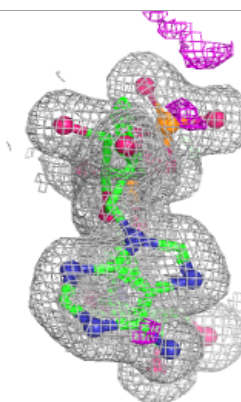
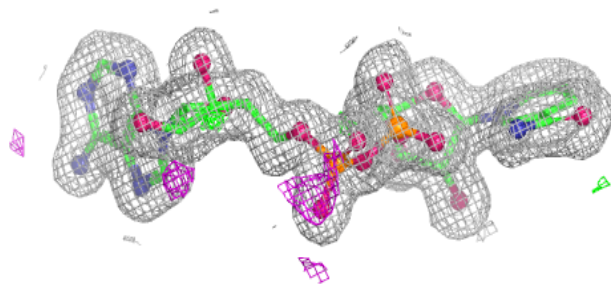
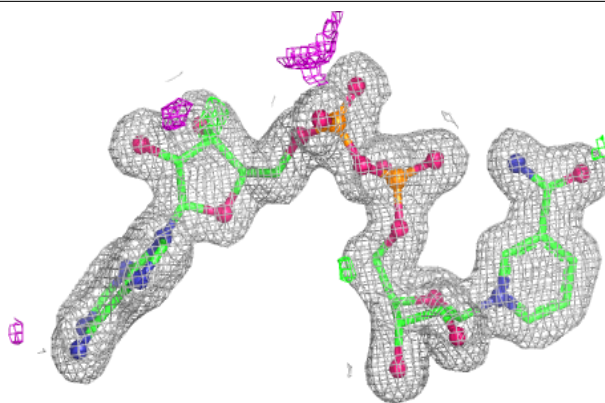
Electron density around CA A 512:

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

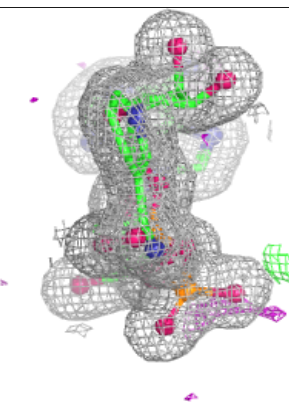
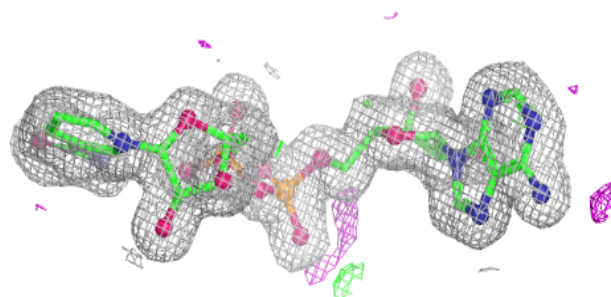
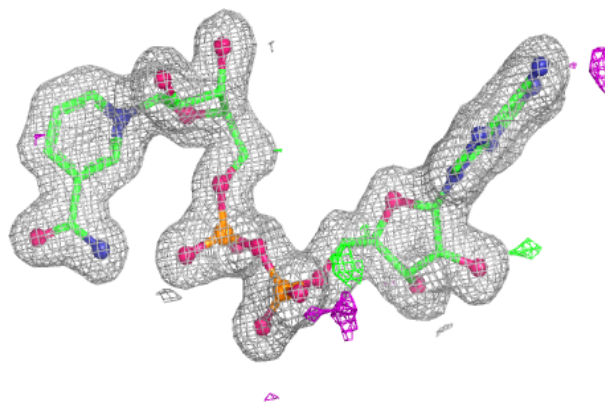


Electron density around NAD E 501:

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

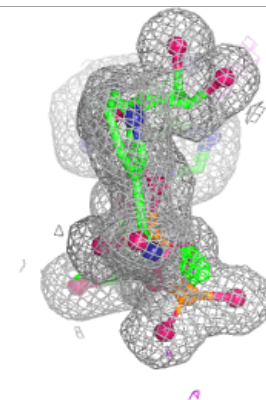
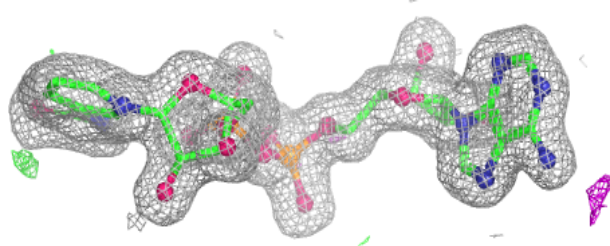
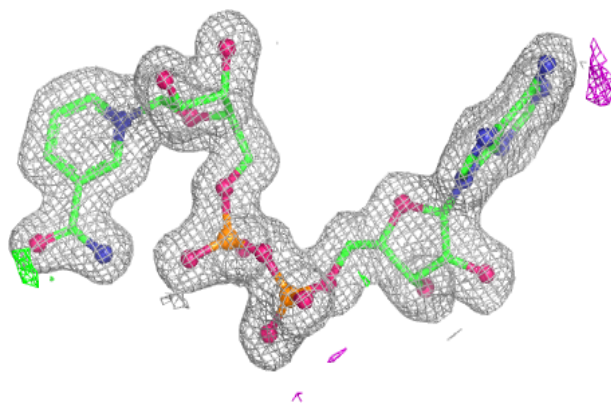
**Electron density around NAD F 2303:**

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

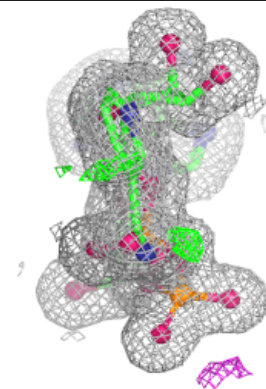
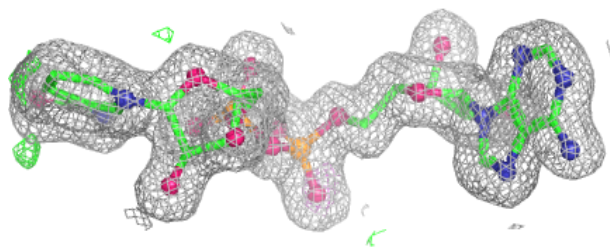
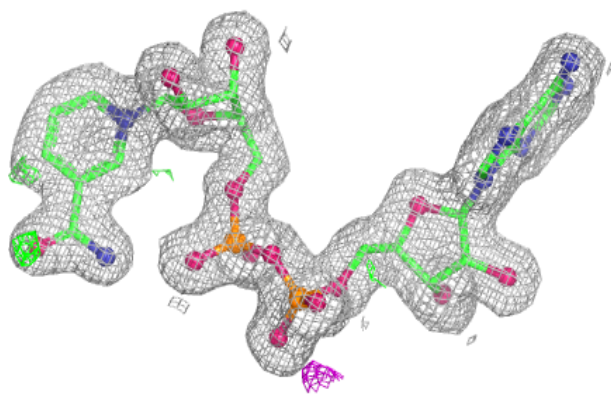


Electron density around NAD B 501:

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and green (positive)

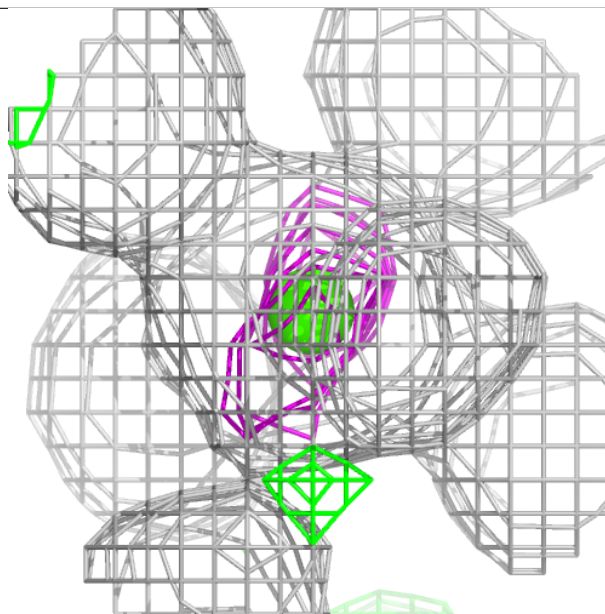
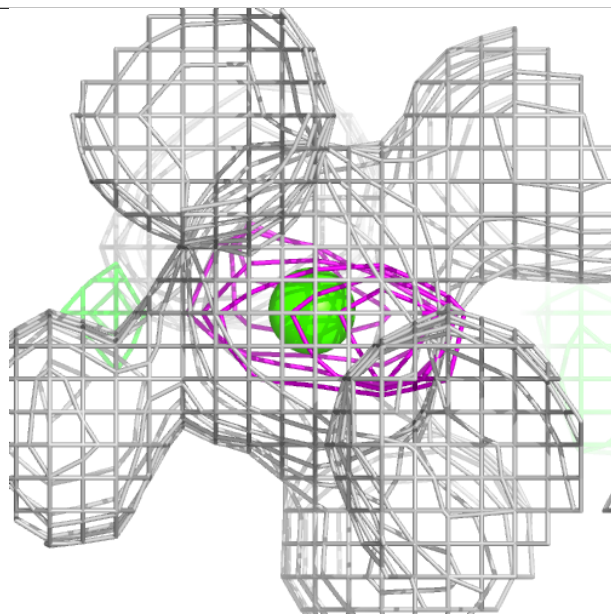
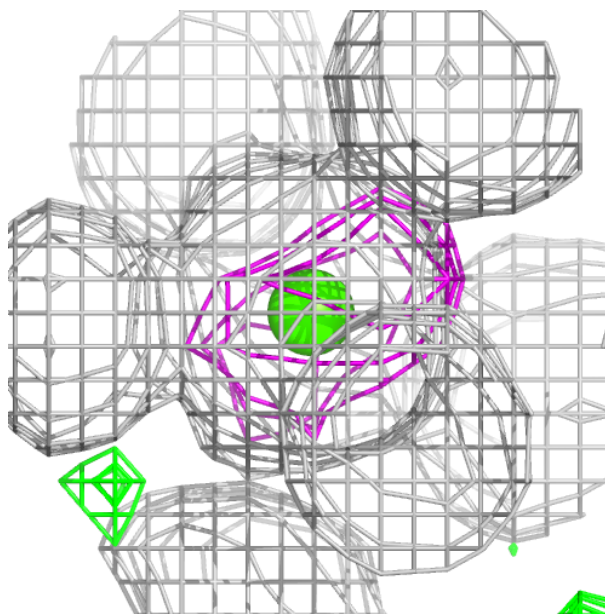
**Electron density around NAD C 501:**

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



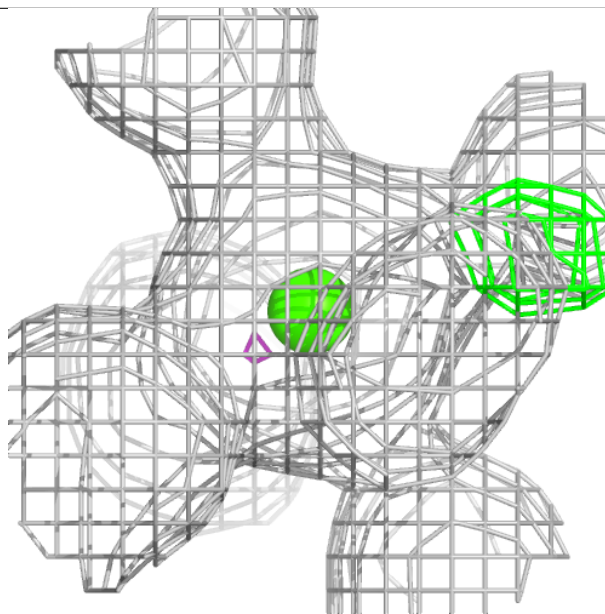
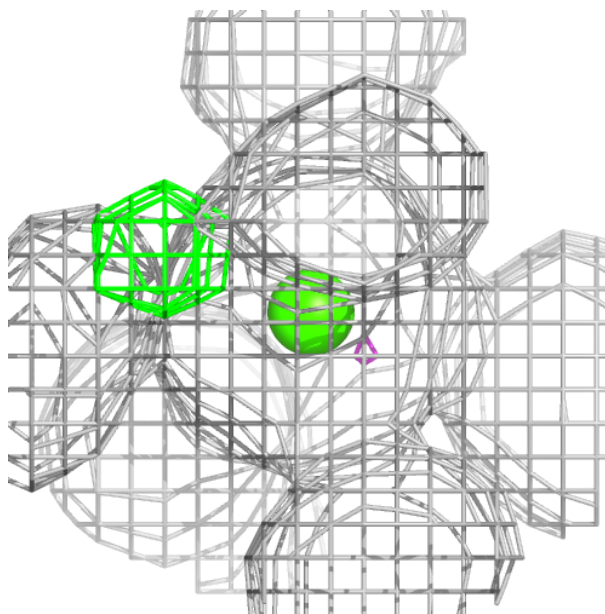
Electron density around CA B 511:

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and green (positive)



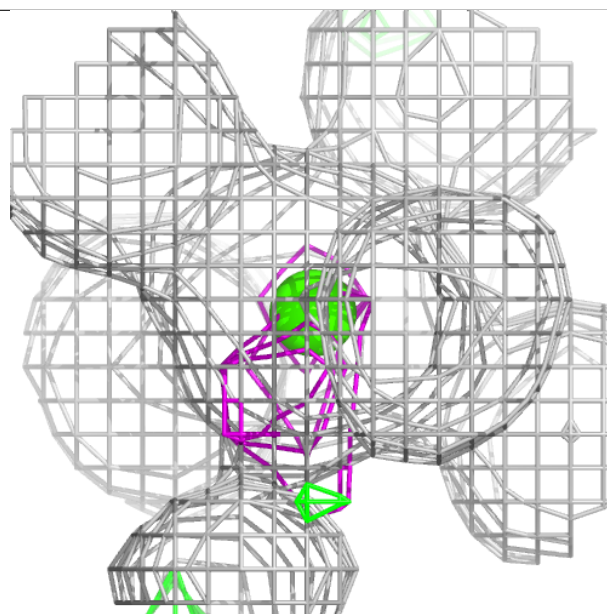
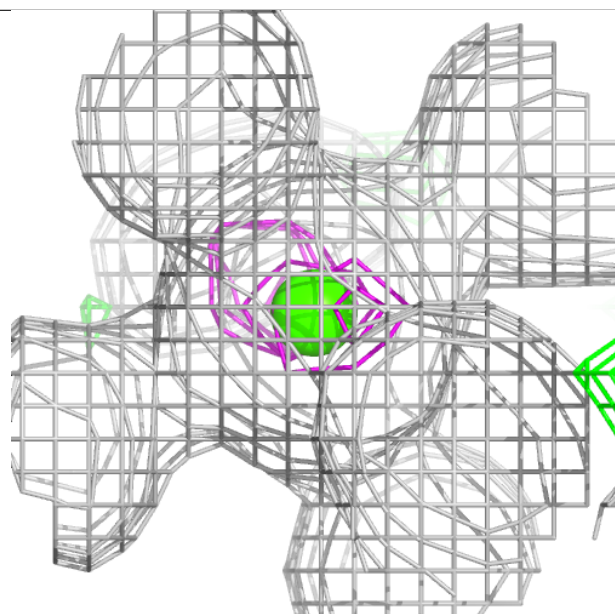
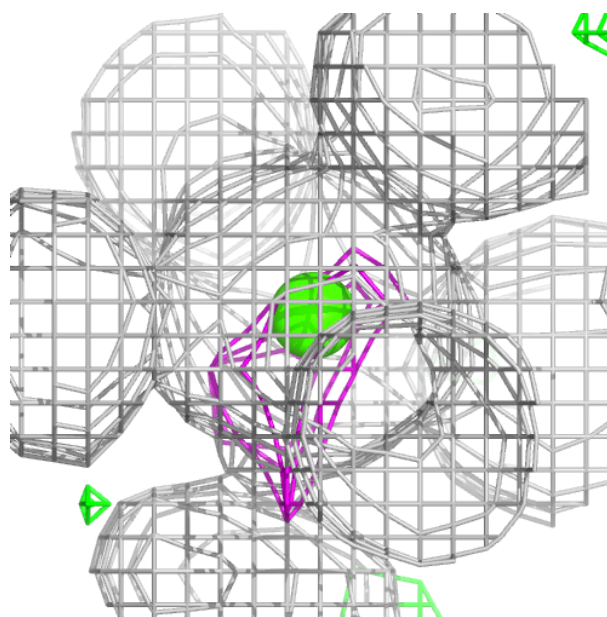
Electron density around CA C 511:

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and green (positive)



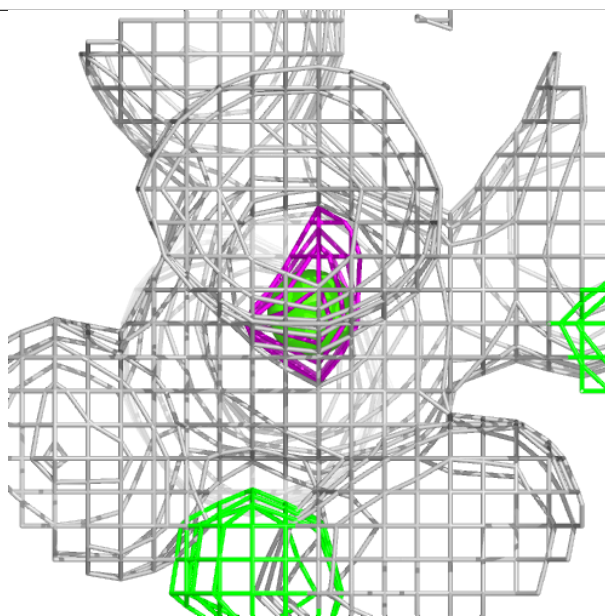
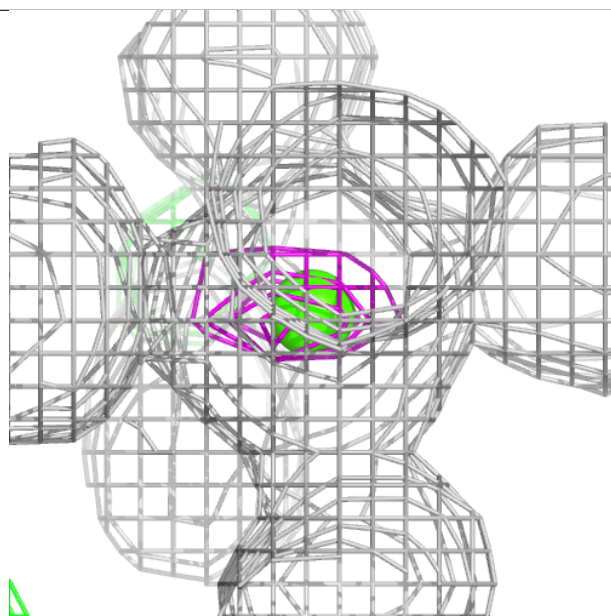
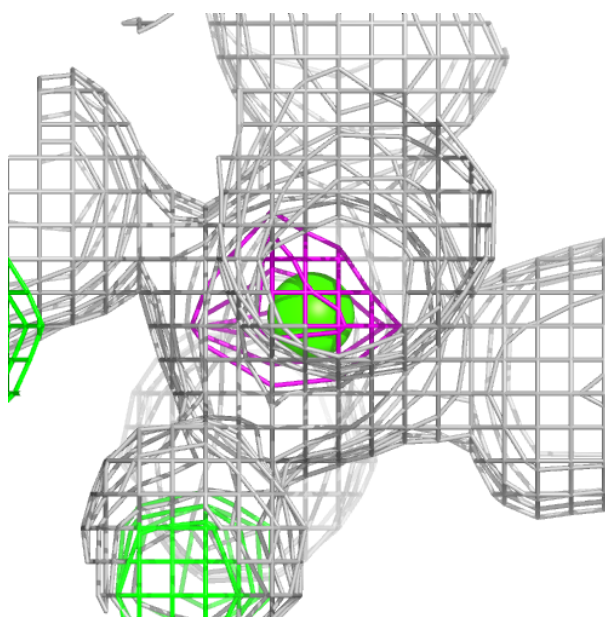
Electron density around CA D 509:

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and green (positive)



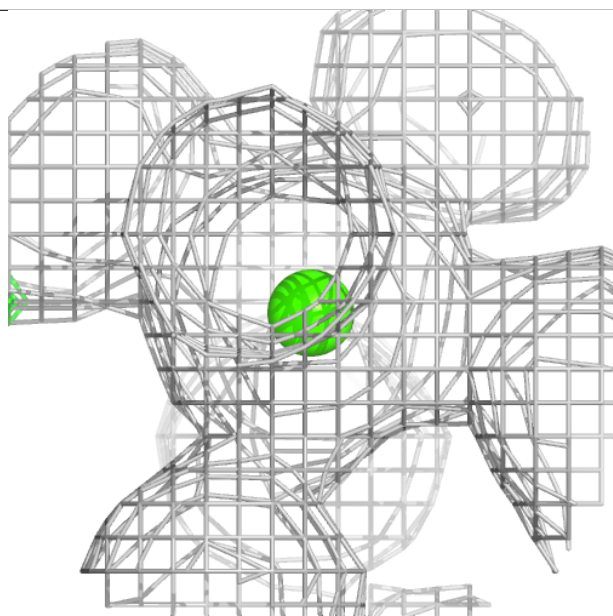
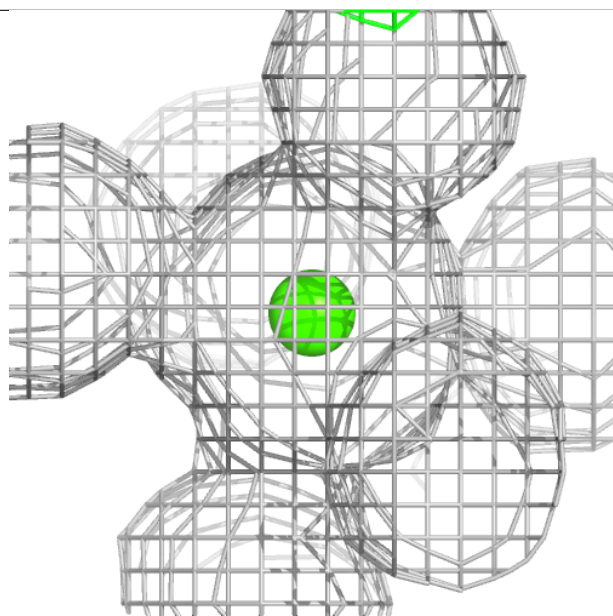
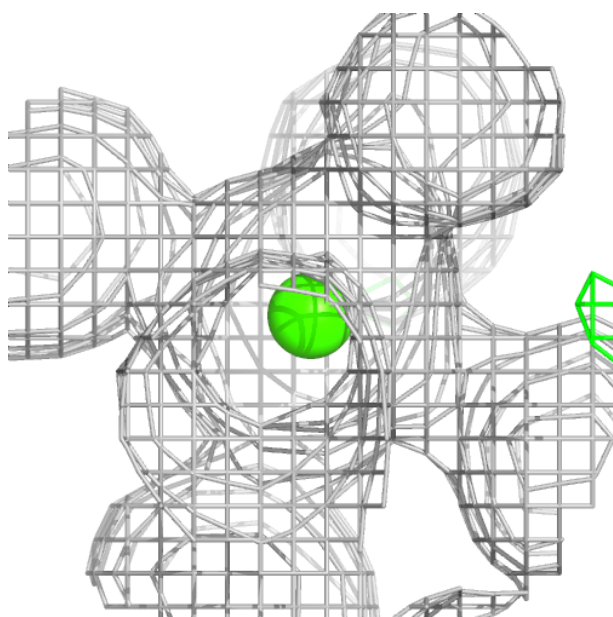
Electron density around CA E 509:

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and green (positive)



Electron density around CA F 2312:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.