



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:22 PM UTC

PDB ID : 3HDY / pdb_00003hdy
Title : Crystal Structure of UDP-galactopyranose mutase (reduced form) in complex with substrate
Authors : Partha, S.K.; van Straaten, K.E.; Sanders, D.A.R.
Deposited on : 2009-05-07
Resolution : 2.40 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:

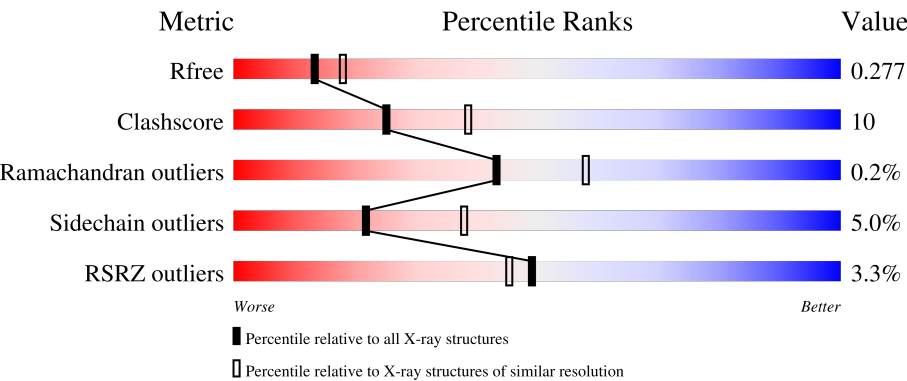
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

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

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	397	2% 70% 21% • 8%
1	B	397	% 73% 16% • 9%
1	C	397	14% 58% 26% • • 12%
1	D	397	4% 66% 23% • 9%
1	E	397	2% 69% 20% • 9%

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Mol	Chain	Length	Quality of chain
1	F	397	
1	G	397	
1	H	397	
1	I	397	
1	J	397	

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
4	FDA	B	1385	X	-	-	-
4	FDA	D	1385	X	-	-	-
4	FDA	G	1385	X	-	-	-

2 Entry composition

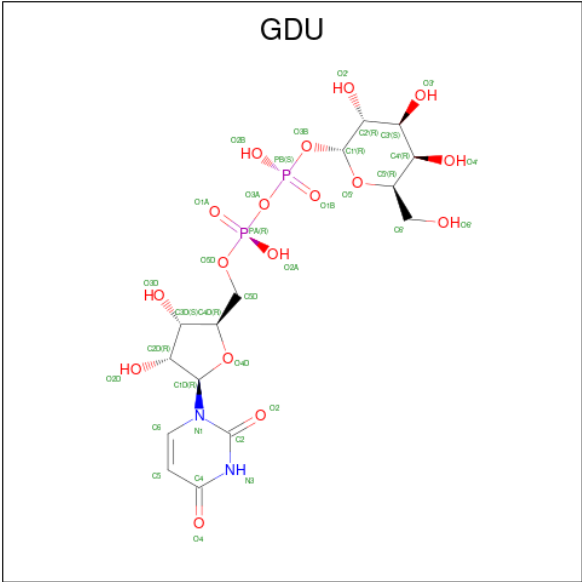
There are 5 unique types of molecules in this entry. The entry contains 30890 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 UDP-galactopyranose mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2984	1904	518	554	8			
1	B	361	Total	C	N	O	S	0	0	0
			2951	1885	512	546	8			
1	C	349	Total	C	N	O	S	12	0	0
			2850	1820	493	529	8			
1	D	361	Total	C	N	O	S	9	0	0
			2951	1885	512	546	8			
1	E	361	Total	C	N	O	S	12	0	0
			2951	1885	512	546	8			
1	F	362	Total	C	N	O	S	19	0	0
			2960	1891	514	547	8			
1	G	360	Total	C	N	O	S	0	0	0
			2947	1883	511	545	8			
1	H	361	Total	C	N	O	S	0	0	0
			2956	1889	513	546	8			
1	I	361	Total	C	N	O	S	1	0	0
			2951	1885	512	546	8			
1	J	359	Total	C	N	O	S	1	0	0
			2943	1881	510	544	8			

- Molecule 2 is GALACTOSE-URIDINE-5'-DIPHOSPHATE (CCD ID: GDU) (formula: $C_{15}H_{24}N_2O_{17}P_2$).



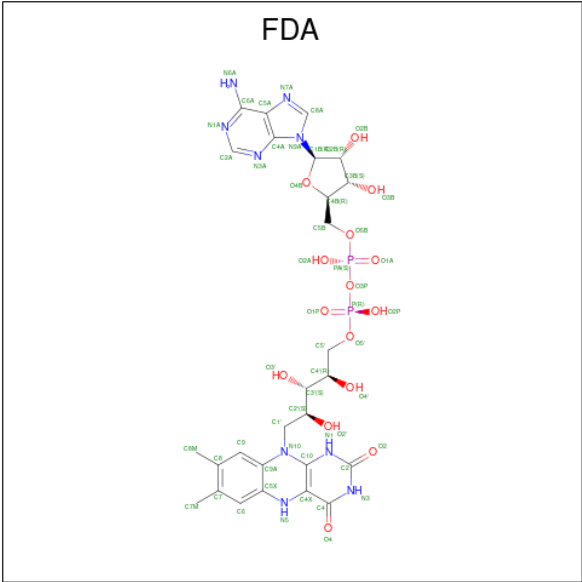
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
2	B	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
2	C	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
2	D	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
2	E	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
2	F	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
2	G	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
2	H	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
2	I	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
2	J	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	I	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	J	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (CCD ID: FDA) (formula: C₂₇H₃₅N₉O₁₅P₂).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	70	Total	O	0	0
			70	70		
5	B	51	Total	O	0	0
			51	51		
5	C	41	Total	O	0	0
			41	41		
5	D	48	Total	O	0	0
			48	48		
5	E	44	Total	O	0	0
			44	44		
5	F	60	Total	O	0	0
			60	60		
5	G	47	Total	O	0	0
			47	47		
5	H	75	Total	O	0	0
			75	75		
5	I	53	Total	O	0	0
			53	53		

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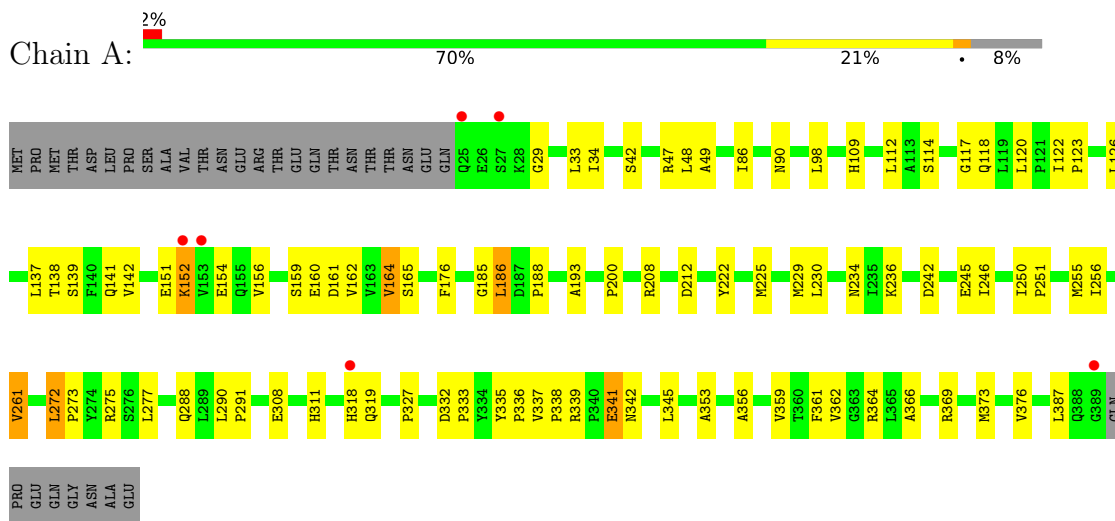
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	67	Total	O	0	0
			67	67		

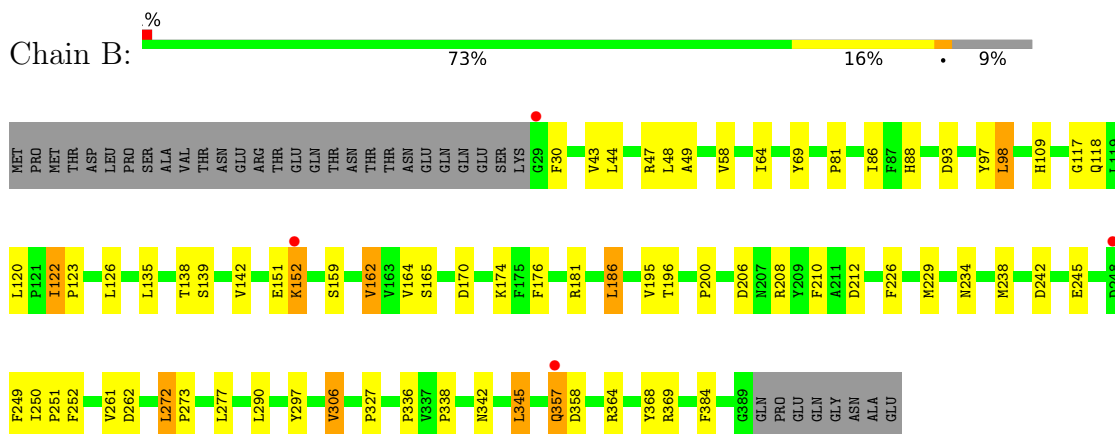
3 Residue-property plots

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.

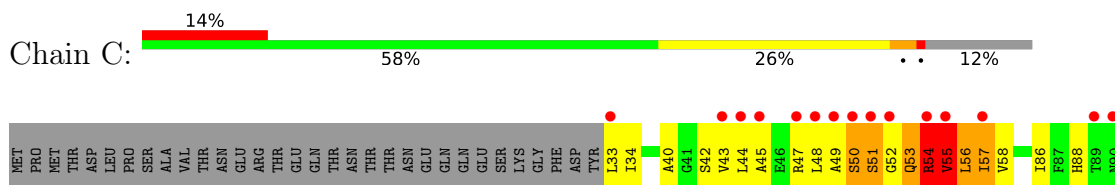
- Molecule 1: UDP-galactopyranose mutase

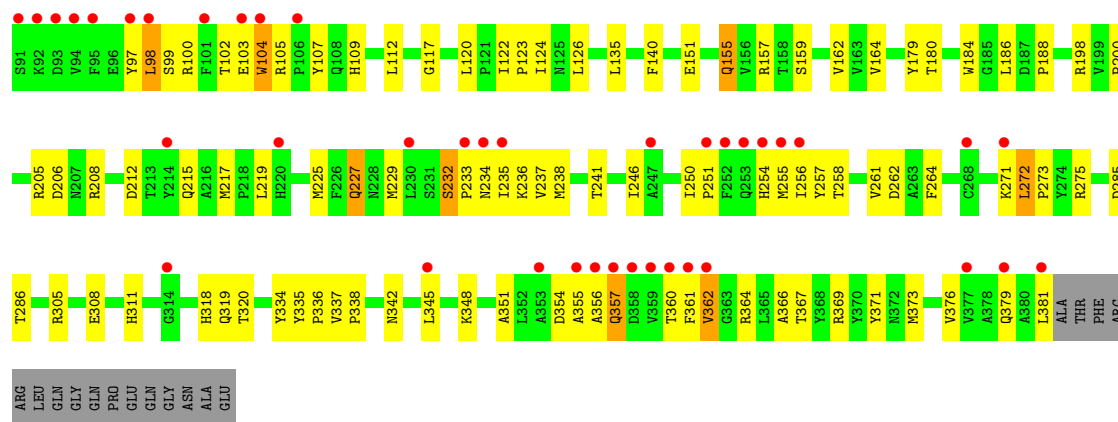


- Molecule 1: UDP-galactopyranose mutase

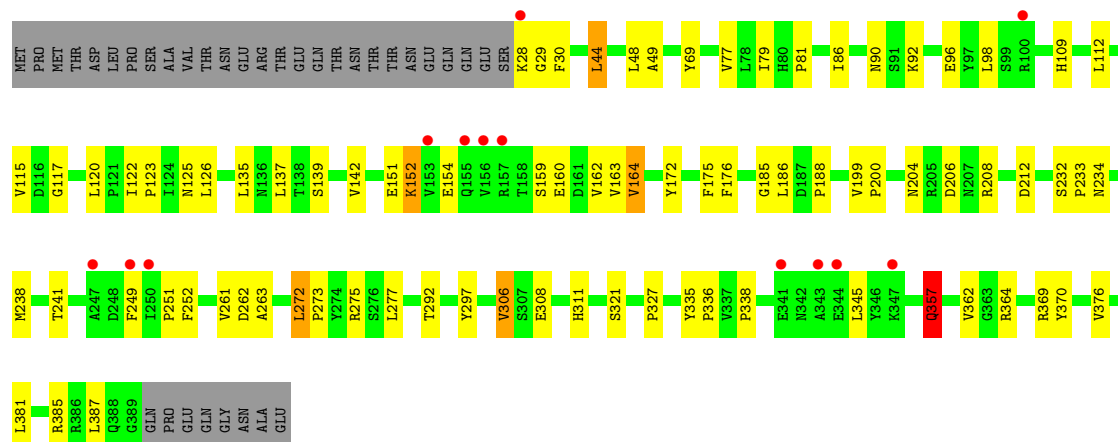


- Molecule 1: UDP-galactopyranose mutase



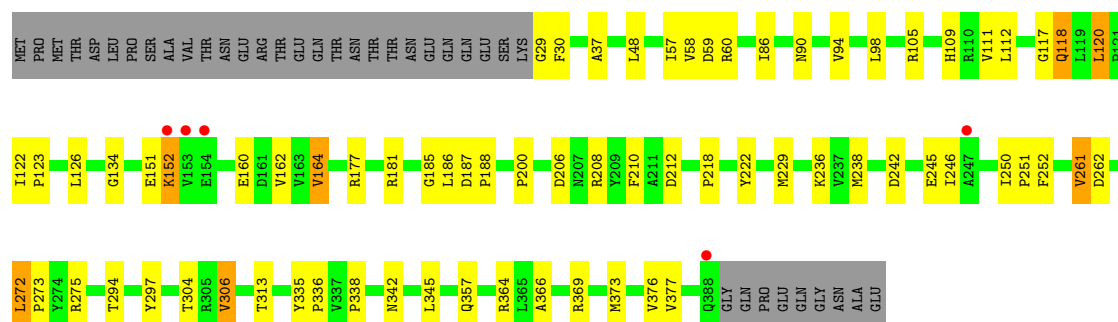


Chain F: 3% 70% 19% 9%



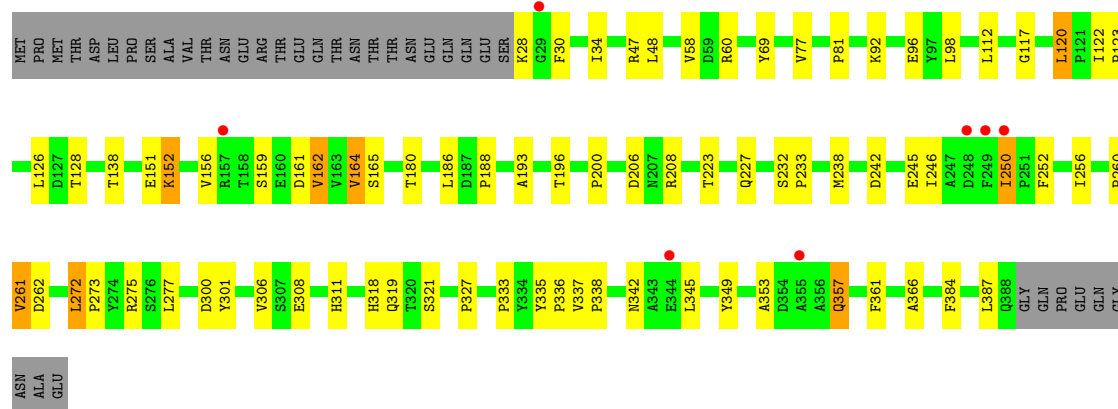
• Molecule 1: UDP-galactopyranose mutase

Chain G: % 73% 16% 9%



• Molecule 1: UDP-galactopyranose mutase

Chain H: 2% 71% 18% 9%

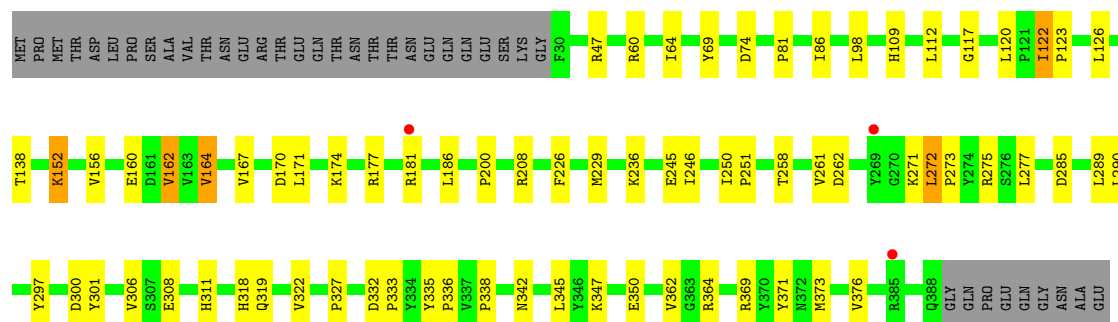
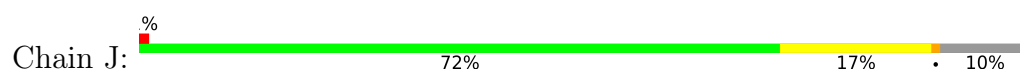


• Molecule 1: UDP-galactopyranose mutase

Chain I: 2% 69% 20% 9%



- Molecule 1: UDP-galactopyranose mutase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.82Å 174.63Å 218.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.94 – 2.40 39.94 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.8 (39.94-2.40) 95.7 (39.94-2.40)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	0.19	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.235 , 0.280 0.236 , 0.277	Depositor DCC
R_{free} test set	9506 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	30890	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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: FDA, GDU, FAD

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	0.33	0/3068	0.71	0/4171
1	B	0.37	0/3035	0.73	2/4128 (0.0%)
1	C	0.55	2/2931 (0.1%)	0.84	8/3989 (0.2%)
1	D	0.35	1/3035 (0.0%)	0.72	0/4128
1	E	0.35	1/3035 (0.0%)	0.71	0/4128
1	F	0.33	0/3044	0.73	0/4139
1	G	0.35	0/3031	0.72	0/4123
1	H	0.33	0/3040	0.73	2/4134 (0.0%)
1	I	0.31	0/3035	0.73	0/4128
1	J	0.35	2/3027 (0.1%)	0.73	2/4118 (0.0%)
All	All	0.37	6/30281 (0.0%)	0.74	14/41186 (0.0%)

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

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	301	TYR	C-N	-7.89	1.21	1.33
1	J	300	ASP	C-N	-6.94	1.24	1.33
1	C	57	ILE	CA-CB	-6.67	1.46	1.54
1	D	263	ALA	C-N	-6.64	1.24	1.33
1	E	302	ALA	CA-CB	-5.30	1.44	1.53
1	C	124	ILE	C-O	-5.06	1.18	1.24

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	104	TRP	N-CA-C	9.56	122.66	110.33
1	C	105	ARG	CA-C-N	8.66	129.20	119.93
1	C	105	ARG	C-N-CA	8.66	129.20	119.93
1	C	55	VAL	N-CA-C	7.27	119.30	108.46
1	C	357	GLN	N-CA-C	6.88	121.95	112.04
1	C	54	ARG	CA-C-N	-6.37	114.09	122.94
1	C	54	ARG	C-N-CA	-6.37	114.09	122.94
1	C	53	GLN	N-CA-C	-5.82	101.58	110.14
1	H	250	ILE	CA-C-N	5.77	126.67	119.98
1	H	250	ILE	C-N-CA	5.77	126.67	119.98
1	B	290	LEU	CA-C-N	5.55	125.17	119.56
1	B	290	LEU	C-N-CA	5.55	125.17	119.56
1	J	300	ASP	CA-C-N	5.45	131.95	121.54
1	J	300	ASP	C-N-CA	5.45	131.95	121.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	50	SER	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2984	0	2854	57	0
1	B	2951	0	2822	54	0
1	C	2850	0	2728	104	0
1	D	2951	0	2822	69	0
1	E	2951	0	2822	48	0
1	F	2960	0	2835	58	0
1	G	2947	0	2819	48	0
1	H	2956	0	2832	51	0
1	I	2951	0	2822	51	0
1	J	2943	0	2816	46	0
2	A	36	0	22	4	0
2	B	36	0	22	4	0
2	C	36	0	22	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	36	0	22	6	0
2	E	36	0	22	2	0
2	F	36	0	22	3	0
2	G	36	0	22	2	0
2	H	36	0	22	1	0
2	I	36	0	22	1	0
2	J	36	0	22	0	0
3	A	53	0	31	3	0
3	C	53	0	31	6	0
3	E	53	0	31	2	0
3	F	53	0	31	4	0
3	H	53	0	31	2	0
3	I	53	0	31	3	0
3	J	53	0	31	3	0
4	B	53	0	28	2	0
4	D	53	0	29	5	0
4	G	53	0	28	6	0
5	A	70	0	0	1	0
5	B	51	0	0	0	0
5	C	41	0	0	3	0
5	D	48	0	0	2	0
5	E	44	0	0	0	0
5	F	60	0	0	0	0
5	G	47	0	0	1	0
5	H	75	0	0	0	0
5	I	53	0	0	1	0
5	J	67	0	0	0	0
All	All	30890	0	28694	572	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 10.

All (572) 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:F:152:LYS:HE2	1:F:152:LYS:HA	1.48	0.96
1:J:152:LYS:HE2	1:J:152:LYS:HA	1.50	0.91
1:I:152:LYS:HE2	1:I:152:LYS:HA	1.52	0.91
1:D:152:LYS:HE2	1:D:152:LYS:HA	1.51	0.89
1:B:152:LYS:HA	1:B:152:LYS:HE2	1.55	0.88
1:F:117:GLY:HA2	1:H:208:ARG:HD2	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:152:LYS:HE2	1:H:152:LYS:HA	1.55	0.88
1:G:152:LYS:HA	1:G:152:LYS:HE2	1.57	0.87
1:E:152:LYS:HA	1:E:152:LYS:HE2	1.57	0.84
1:D:208:ARG:HD2	1:I:117:GLY:HA2	1.61	0.83
1:I:44:LEU:HD13	1:I:256:ILE:HD13	1.61	0.83
1:B:208:ARG:HD2	1:G:117:GLY:CA	2.08	0.82
1:E:58:VAL:HG23	1:E:238:MET:HB3	1.61	0.82
1:A:152:LYS:HE2	1:A:152:LYS:HA	1.63	0.81
1:B:208:ARG:HD2	1:G:117:GLY:HA3	1.61	0.80
2:C:500:GDU:H6'1	5:C:405:HOH:O	1.81	0.79
1:A:117:GLY:HA2	1:G:208:ARG:HD2	1.65	0.79
1:C:57:ILE:CG2	1:C:57:ILE:O	2.30	0.78
1:F:117:GLY:CA	1:H:208:ARG:HD2	2.15	0.77
1:C:99:SER:HB2	1:C:104:TRP:HE1	1.50	0.76
1:C:57:ILE:O	1:C:57:ILE:HG23	1.85	0.76
1:I:376:VAL:HG21	3:I:450:FAD:H5'2	1.67	0.74
1:H:246:ILE:HB	1:H:250:ILE:HD12	1.68	0.74
1:C:246:ILE:HD12	1:C:250:ILE:HD12	1.71	0.73
1:D:265:PHE:O	1:D:266:ASP:HB2	1.87	0.72
1:F:376:VAL:HG21	3:F:450:FAD:H5'2	1.71	0.72
1:F:308:GLU:HB3	1:F:311:HIS:HD2	1.55	0.72
1:C:53:GLN:O	1:C:234:ASN:ND2	2.23	0.71
1:F:275:ARG:HB3	1:F:335:TYR:HB2	1.72	0.71
1:E:117:GLY:HA2	1:I:208:ARG:HD2	1.72	0.71
1:B:357:GLN:HE21	1:B:357:GLN:HA	1.57	0.70
1:J:275:ARG:HB3	1:J:335:TYR:HB2	1.74	0.69
1:D:208:ARG:HD2	1:I:117:GLY:CA	2.22	0.68
1:D:336:PRO:O	1:D:338:PRO:HD3	1.94	0.68
1:A:122:ILE:HA	1:A:123:PRO:C	2.19	0.68
1:D:69:TYR:O	1:D:81:PRO:HD2	1.93	0.68
1:F:152:LYS:HA	1:F:152:LYS:CE	2.23	0.68
1:C:238:MET:HE2	1:C:241:THR:HG21	1.77	0.67
1:A:29:GLY:HA3	1:A:251:PRO:HB2	1.77	0.67
1:F:206:ASP:OD1	1:F:208:ARG:HD3	1.95	0.66
1:I:29:GLY:HA3	1:I:251:PRO:HB2	1.78	0.66
1:E:125:ASN:HB2	1:E:204:ASN:O	1.96	0.66
1:E:37:ALA:HA	1:E:57:ILE:HD11	1.78	0.66
1:E:336:PRO:O	1:E:338:PRO:HD3	1.95	0.66
1:F:122:ILE:HD12	1:F:123:PRO:HA	1.77	0.66
1:D:117:GLY:CA	1:F:208:ARG:HD2	2.26	0.65
1:E:376:VAL:HG21	3:E:450:FAD:H5'2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:SER:O	1:C:234:ASN:N	2.30	0.65
1:I:272:LEU:HD23	1:I:273:PRO:HD2	1.77	0.65
1:F:272:LEU:HD23	1:F:273:PRO:HD2	1.79	0.64
1:E:272:LEU:HD23	1:E:273:PRO:HD2	1.80	0.64
1:C:102:THR:HB	1:C:225:MET:HB2	1.80	0.64
1:C:232:SER:C	1:C:234:ASN:H	2.04	0.64
1:E:246:ILE:HB	1:E:250:ILE:HD12	1.77	0.64
1:I:242:ASP:HB3	1:I:245:GLU:HG3	1.78	0.64
1:D:373:MET:HE2	4:D:1385:FDA:C2	2.27	0.64
1:D:272:LEU:HD23	1:D:273:PRO:HD2	1.79	0.64
1:E:162:VAL:HG13	1:E:193:ALA:HB1	1.79	0.64
1:A:208:ARG:HD2	1:J:117:GLY:HA2	1.79	0.63
1:E:44:LEU:HD13	1:E:256:ILE:HD13	1.80	0.63
1:I:275:ARG:HB3	1:I:335:TYR:HB2	1.80	0.63
1:C:50:SER:C	1:C:52:GLY:N	2.55	0.62
1:I:58:VAL:HG23	1:I:238:MET:HB3	1.81	0.62
1:C:257:TYR:CD2	1:C:361:PHE:CE1	2.88	0.62
1:H:180:THR:HB	1:H:188:PRO:HG3	1.81	0.62
1:H:308:GLU:HB3	1:H:311:HIS:HD2	1.64	0.62
1:J:290:LEU:HD12	1:J:308:GLU:HB2	1.81	0.62
1:B:117:GLY:CA	1:C:208:ARG:HD2	2.29	0.62
1:B:122:ILE:HA	1:B:123:PRO:C	2.25	0.62
1:D:206:ASP:OD1	1:D:208:ARG:HD3	2.00	0.62
1:G:262:ASP:HB3	1:G:272:LEU:HB2	1.80	0.62
1:A:117:GLY:CA	1:G:208:ARG:HD2	2.31	0.61
1:B:249:PHE:HE1	1:H:28:LYS:O	1.83	0.61
1:A:151:GLU:HB2	1:A:164:VAL:CG1	2.31	0.61
1:B:336:PRO:O	1:B:338:PRO:HD3	2.01	0.61
1:C:49:ALA:HA	1:C:234:ASN:HD22	1.64	0.61
1:G:273:PRO:HG2	1:G:342:ASN:OD1	2.01	0.61
1:H:336:PRO:O	1:H:338:PRO:HD3	2.00	0.61
1:C:56:LEU:HD23	1:C:236:LYS:O	2.01	0.60
1:I:277:LEU:HD23	1:I:327:PRO:HA	1.83	0.60
1:F:122:ILE:HA	1:F:123:PRO:C	2.26	0.60
1:I:308:GLU:HB3	1:I:311:HIS:HD2	1.66	0.60
1:D:44:LEU:HD13	1:D:256:ILE:HD13	1.83	0.60
1:C:50:SER:C	1:C:52:GLY:H	2.08	0.60
1:D:122:ILE:HA	1:D:123:PRO:C	2.25	0.60
1:C:262:ASP:OD2	1:C:271:LYS:HD2	2.01	0.60
1:F:29:GLY:HA3	1:F:251:PRO:HB2	1.84	0.60
1:I:123:PRO:HB3	1:I:200:PRO:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ARG:HD2	1:G:117:GLY:HA2	1.82	0.60
2:A:500:GDU:O5D	2:A:500:GDU:H6	2.03	0.59
1:C:57:ILE:CG2	1:C:237:VAL:HG13	2.32	0.59
1:D:275:ARG:HB3	1:D:335:TYR:HB2	1.83	0.59
1:H:92:LYS:HE2	1:H:96:GLU:OE2	2.03	0.59
1:E:262:ASP:HB3	1:E:272:LEU:HB2	1.85	0.59
1:A:49:ALA:HB1	1:A:234:ASN:HB2	1.85	0.58
1:H:357:GLN:HE21	1:H:357:GLN:HA	1.66	0.58
1:B:273:PRO:HG2	1:B:342:ASN:OD1	2.03	0.58
1:C:49:ALA:HA	1:C:234:ASN:ND2	2.18	0.58
1:J:318:HIS:CD2	1:J:319:GLN:HG3	2.38	0.58
1:F:238:MET:HE2	1:F:241:THR:HG21	1.85	0.58
1:G:123:PRO:HB3	1:G:200:PRO:O	2.04	0.58
1:C:232:SER:C	1:C:234:ASN:N	2.62	0.58
1:B:206:ASP:OD1	1:B:208:ARG:HD3	2.03	0.57
1:C:97:TYR:HD2	1:C:98:LEU:HD13	1.69	0.57
1:C:155:GLN:HB3	1:C:157:ARG:HG3	1.85	0.57
1:G:151:GLU:HB2	1:G:164:VAL:HG13	1.87	0.57
1:H:77:VAL:HG11	1:H:321:SER:HB2	1.87	0.57
1:A:318:HIS:CD2	1:A:319:GLN:HG3	2.39	0.57
1:C:257:TYR:HD2	1:C:361:PHE:CE1	2.23	0.57
1:G:376:VAL:HG21	4:G:1385:FDA:H5'2	1.86	0.57
1:C:250:ILE:HG23	1:C:251:PRO:HD2	1.87	0.57
1:E:122:ILE:HA	1:E:123:PRO:C	2.29	0.57
1:B:117:GLY:HA2	1:C:208:ARG:HD2	1.86	0.57
1:C:86:ILE:HG21	1:C:109:HIS:HB2	1.86	0.56
1:G:364:ARG:HG3	1:G:369:ARG:O	2.05	0.56
1:H:277:LEU:HD23	1:H:327:PRO:HA	1.87	0.56
1:D:364:ARG:HG3	1:D:369:ARG:O	2.04	0.56
1:A:356:ALA:HB1	1:A:359:VAL:HB	1.87	0.56
1:D:117:GLY:HA2	1:F:208:ARG:HD2	1.87	0.56
1:C:57:ILE:HG23	1:C:237:VAL:HG13	1.87	0.56
1:G:261:VAL:HG13	1:G:366:ALA:O	2.06	0.56
1:I:261:VAL:HG13	1:I:366:ALA:O	2.06	0.56
1:G:246:ILE:HB	1:G:250:ILE:HD12	1.88	0.56
1:E:162:VAL:CG1	1:E:193:ALA:HB1	2.35	0.56
1:D:37:ALA:HA	1:D:57:ILE:HD11	1.88	0.56
1:H:275:ARG:HB3	1:H:335:TYR:HB2	1.88	0.55
1:C:47:ARG:NE	1:C:47:ARG:HA	2.21	0.55
1:G:86:ILE:HG21	1:G:109:HIS:HB2	1.88	0.55
1:J:123:PRO:HB3	1:J:200:PRO:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:ARG:HD3	2:C:500:GDU:H5'2	1.87	0.55
1:H:122:ILE:HA	1:H:123:PRO:C	2.30	0.55
1:I:37:ALA:HA	1:I:57:ILE:HD11	1.87	0.55
1:C:376:VAL:HG21	3:C:450:FAD:H5'2	1.88	0.55
2:G:500:GDU:H2'	4:G:1385:FDA:C4	2.36	0.55
1:H:123:PRO:HB3	1:H:200:PRO:O	2.07	0.55
1:B:242:ASP:HB3	1:B:245:GLU:HG3	1.88	0.55
1:E:123:PRO:HB3	1:E:200:PRO:O	2.07	0.55
1:J:336:PRO:O	1:J:338:PRO:HD3	2.07	0.54
1:B:30:PHE:O	1:B:252:PHE:HA	2.07	0.54
1:C:184:TRP:NE1	2:C:500:GDU:O3D	2.31	0.54
1:E:47:ARG:NE	1:E:47:ARG:HA	2.23	0.54
1:F:69:TYR:O	1:F:81:PRO:HD2	2.08	0.54
1:G:122:ILE:HA	1:G:123:PRO:C	2.32	0.54
1:J:272:LEU:HD23	1:J:273:PRO:HD2	1.89	0.54
1:C:236:LYS:HG3	1:F:238:MET:HE3	1.88	0.54
1:D:185:GLY:C	1:D:186:LEU:HD12	2.32	0.54
1:E:29:GLY:HA3	1:E:251:PRO:HB2	1.89	0.54
1:G:152:LYS:HA	1:G:152:LYS:CE	2.28	0.54
1:C:117:GLY:HA2	1:J:208:ARG:HD2	1.90	0.53
1:C:122:ILE:HA	1:C:123:PRO:C	2.33	0.53
1:B:69:TYR:O	1:B:81:PRO:HD2	2.08	0.53
1:B:123:PRO:HB3	1:B:200:PRO:O	2.08	0.53
1:D:170:ASP:O	1:D:174:LYS:HG3	2.09	0.53
1:B:138:THR:HG22	1:G:134:GLY:O	2.09	0.53
1:A:376:VAL:HG21	3:A:450:FAD:H5'2	1.88	0.53
1:D:265:PHE:CE1	1:D:352:LEU:HB2	2.44	0.53
1:H:30:PHE:O	1:H:252:PHE:HA	2.07	0.53
1:H:58:VAL:HG23	1:H:238:MET:HB3	1.90	0.53
1:C:48:LEU:C	1:C:50:SER:H	2.16	0.53
1:A:138:THR:OG1	1:A:141:GLN:HG3	2.09	0.53
1:C:285:ASP:HA	1:C:319:GLN:HG2	1.89	0.53
1:D:117:GLY:HA3	1:F:208:ARG:HD2	1.89	0.53
1:I:86:ILE:HG21	1:I:109:HIS:HB2	1.91	0.53
1:F:92:LYS:HE2	1:F:96:GLU:OE2	2.09	0.53
1:J:69:TYR:O	1:J:81:PRO:HD2	2.08	0.53
1:D:79:ILE:HB	1:D:309:PHE:CE1	2.44	0.53
1:G:185:GLY:O	1:G:186:LEU:HD12	2.09	0.53
1:F:77:VAL:HG11	1:F:321:SER:HB2	1.91	0.52
1:J:152:LYS:HA	1:J:152:LYS:CE	2.31	0.52
1:C:47:ARG:NH1	1:C:100:ARG:NH2	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:272:LEU:HD23	1:H:273:PRO:HD2	1.91	0.52
1:I:185:GLY:C	1:I:186:LEU:HD12	2.34	0.52
1:A:151:GLU:HB2	1:A:164:VAL:HG13	1.90	0.52
1:F:364:ARG:HG3	1:F:369:ARG:O	2.09	0.52
1:G:177:ARG:HD2	1:G:181:ARG:NH2	2.24	0.52
1:G:210:PHE:HZ	2:G:500:GDU:O4'	1.92	0.52
1:D:305:ARG:HH12	2:D:500:GDU:H5'	1.73	0.52
1:E:126:LEU:HD22	1:E:130:ASN:ND2	2.24	0.52
1:A:246:ILE:HB	1:A:250:ILE:HD12	1.91	0.52
1:I:139:SER:O	1:I:142:VAL:HG12	2.10	0.52
2:A:500:GDU:H2'	3:A:450:FAD:C4	2.40	0.52
1:G:111:VAL:HG22	1:G:294:THR:HB	1.90	0.52
1:B:210:PHE:HZ	2:B:500:GDU:O4'	1.94	0.51
1:C:135:LEU:HD23	1:J:138:THR:HG21	1.92	0.51
1:C:206:ASP:OD1	1:C:208:ARG:HD3	2.10	0.51
2:B:500:GDU:H2'	4:B:1385:FDA:C4	2.40	0.51
1:D:273:PRO:HG2	1:D:342:ASN:OD1	2.10	0.51
1:G:206:ASP:OD1	1:G:208:ARG:HD3	2.10	0.51
1:D:308:GLU:HB3	1:D:311:HIS:HD2	1.75	0.51
1:A:123:PRO:HB3	1:A:200:PRO:O	2.10	0.51
1:A:242:ASP:HB3	1:A:245:GLU:HG3	1.92	0.51
1:A:272:LEU:HD23	1:A:273:PRO:HD2	1.91	0.51
1:C:57:ILE:HG22	1:C:237:VAL:HA	1.93	0.51
1:D:246:ILE:HD12	1:D:250:ILE:HD12	1.92	0.51
1:I:151:GLU:O	1:I:165:SER:HA	2.11	0.51
1:C:42:SER:HB3	1:C:229:MET:HE2	1.93	0.51
1:C:355:ALA:O	1:C:356:ALA:C	2.53	0.51
1:J:167:VAL:HB	1:J:171:LEU:HD12	1.92	0.51
1:D:60:ARG:HD3	5:D:424:HOH:O	2.09	0.51
1:G:151:GLU:HB2	1:G:164:VAL:CG1	2.40	0.51
1:B:272:LEU:HD23	1:B:273:PRO:HD2	1.93	0.51
1:B:297:TYR:HE1	1:B:306:VAL:HG23	1.75	0.51
1:G:37:ALA:HA	1:G:57:ILE:HD11	1.93	0.51
1:G:59:ASP:OD1	4:G:1385:FDA:O2B	2.29	0.51
1:C:43:VAL:HA	1:C:229:MET:HE3	1.93	0.50
1:D:266:ASP:O	1:D:267:PHE:HB2	2.11	0.50
1:B:135:LEU:HD21	1:C:140:PHE:HE2	1.76	0.50
2:H:500:GDU:O1A	2:H:500:GDU:H3'	2.11	0.50
1:J:122:ILE:HA	1:J:123:PRO:C	2.36	0.50
1:G:60:ARG:HD3	5:G:422:HOH:O	2.12	0.50
1:H:262:ASP:HA	1:H:349:TYR:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:170:ASP:O	1:J:174:LYS:HG3	2.11	0.50
1:E:208:ARG:HD2	1:H:117:GLY:HA2	1.94	0.50
1:G:242:ASP:HB3	1:G:245:GLU:HG3	1.93	0.50
1:C:286:THR:O	1:C:320:THR:HG22	2.11	0.50
1:C:348:LYS:O	1:C:351:ALA:HB3	2.11	0.50
1:C:43:VAL:HG23	1:C:44:LEU:N	2.27	0.50
1:C:103:GLU:O	1:C:219:LEU:CB	2.60	0.50
3:C:450:FAD:O2'	3:C:450:FAD:O4'	2.30	0.50
1:F:125:ASN:HB2	1:F:204:ASN:O	2.12	0.50
1:H:180:THR:CB	1:H:188:PRO:HG3	2.42	0.50
1:D:205:ARG:HB2	1:I:118:GLN:OE1	2.12	0.50
1:F:151:GLU:HB2	1:F:164:VAL:HG13	1.94	0.50
1:I:30:PHE:CE2	1:I:56:LEU:HB2	2.47	0.50
1:B:249:PHE:CE1	1:H:28:LYS:O	2.63	0.49
1:J:273:PRO:HG2	1:J:342:ASN:OD1	2.12	0.49
1:F:262:ASP:HB3	1:F:272:LEU:HB2	1.94	0.49
1:D:123:PRO:HB3	1:D:200:PRO:O	2.12	0.49
1:I:122:ILE:HA	1:I:123:PRO:C	2.36	0.49
1:B:118:GLN:OE1	1:C:205:ARG:HB2	2.11	0.49
1:C:88:HIS:HD2	1:C:212:ASP:OD1	1.95	0.49
1:C:336:PRO:O	1:C:338:PRO:HD3	2.11	0.49
1:G:90:ASN:OD1	1:G:212:ASP:HA	2.13	0.49
1:G:272:LEU:HD23	1:G:273:PRO:HD2	1.94	0.49
1:A:152:LYS:HA	1:A:152:LYS:CE	2.32	0.49
1:D:162:VAL:HG13	1:D:193:ALA:HB1	1.94	0.49
1:E:176:PHE:HA	2:E:500:GDU:O2	2.13	0.49
1:J:289:LEU:HD23	1:J:322:VAL:HG11	1.94	0.49
1:A:86:ILE:HG21	1:A:109:HIS:HB2	1.95	0.49
1:I:246:ILE:HD12	1:I:250:ILE:HD12	1.95	0.49
1:J:64:ILE:HD12	1:J:226:PHE:HB3	1.94	0.49
1:B:170:ASP:O	1:B:174:LYS:HG3	2.13	0.48
1:C:57:ILE:HG21	1:C:237:VAL:HG22	1.95	0.48
1:F:49:ALA:HB1	1:F:234:ASN:HB2	1.94	0.48
1:J:376:VAL:HG21	3:J:450:FAD:H5'2	1.95	0.48
1:D:151:GLU:O	1:D:165:SER:HA	2.12	0.48
1:I:217:MET:HG3	1:I:312:ILE:O	2.14	0.48
1:A:33:LEU:HD23	1:A:255:MET:HE2	1.96	0.48
1:G:187:ASP:CG	1:G:188:PRO:HD2	2.39	0.48
1:A:308:GLU:HB3	1:A:311:HIS:HD2	1.79	0.48
1:B:151:GLU:HB2	1:B:164:VAL:HG12	1.96	0.48
1:D:58:VAL:HG23	1:D:238:MET:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:275:ARG:HB3	1:E:335:TYR:HB2	1.94	0.48
1:I:133:TYR:HB2	1:I:135:LEU:HG	1.95	0.48
1:A:208:ARG:CD	1:J:117:GLY:HA2	2.44	0.48
1:D:176:PHE:HA	2:D:500:GDU:O2	2.14	0.48
1:I:176:PHE:HA	2:I:500:GDU:O2	2.14	0.48
1:C:236:LYS:HB3	1:F:238:MET:HE3	1.96	0.48
1:H:34:ILE:HG12	1:H:256:ILE:HB	1.96	0.48
1:A:156:VAL:HG13	1:A:161:ASP:CB	2.44	0.48
1:A:336:PRO:O	1:A:338:PRO:HD3	2.13	0.48
1:D:269:TYR:HB2	1:D:349:TYR:CE1	2.48	0.48
1:B:159:SER:O	1:B:162:VAL:HG23	2.13	0.48
1:D:111:VAL:HG22	1:D:294:THR:HB	1.95	0.48
1:E:152:LYS:HA	1:E:152:LYS:CE	2.34	0.48
1:A:339:ARG:HG3	1:A:341:GLU:HG2	1.96	0.47
1:C:275:ARG:HB3	1:C:335:TYR:HB2	1.95	0.47
1:F:160:GLU:O	1:F:164:VAL:HB	2.14	0.47
1:C:238:MET:HE2	1:C:241:THR:CG2	2.42	0.47
1:F:277:LEU:HD11	1:F:335:TYR:HE1	1.79	0.47
1:H:151:GLU:HB2	1:H:164:VAL:CG1	2.43	0.47
1:I:69:TYR:O	1:I:81:PRO:HD2	2.14	0.47
1:I:151:GLU:HB2	1:I:164:VAL:CG1	2.44	0.47
1:J:277:LEU:HD23	1:J:327:PRO:HA	1.95	0.47
1:A:47:ARG:HA	1:A:47:ARG:NE	2.28	0.47
1:C:236:LYS:HG3	1:F:238:MET:CE	2.45	0.47
1:C:103:GLU:O	1:C:219:LEU:HB2	2.15	0.47
1:G:105:ARG:HD2	1:G:313:THR:O	2.14	0.47
1:C:97:TYR:CD2	1:C:98:LEU:HD13	2.50	0.47
1:D:382:ALA:HA	1:D:385:ARG:HH11	1.78	0.47
1:I:30:PHE:CD2	1:I:56:LEU:HB2	2.49	0.47
1:B:277:LEU:HD23	1:B:327:PRO:HA	1.96	0.47
1:C:57:ILE:CG2	1:C:237:VAL:HG22	2.45	0.47
1:F:86:ILE:HG21	1:F:109:HIS:HB2	1.97	0.47
1:F:381:LEU:O	1:F:385:ARG:HG3	2.15	0.47
1:G:58:VAL:HG23	1:G:238:MET:HB3	1.96	0.47
3:I:450:FAD:O2'	3:I:450:FAD:O4'	2.30	0.47
1:B:64:ILE:HD12	1:B:226:PHE:HB3	1.97	0.47
1:G:236:LYS:HA	1:G:236:LYS:HD3	1.82	0.47
1:H:47:ARG:HB3	1:H:384:PHE:CD1	2.50	0.47
1:J:262:ASP:OD2	1:J:271:LYS:HD2	2.15	0.47
1:D:250:ILE:O	1:D:252:PHE:HD2	1.97	0.47
1:H:159:SER:HB3	1:H:196:THR:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:386:ARG:C	1:I:388:GLN:H	2.23	0.47
1:A:156:VAL:HG13	1:A:161:ASP:HB2	1.97	0.47
1:A:261:VAL:HG13	1:A:366:ALA:O	2.15	0.47
1:B:117:GLY:HA3	1:C:208:ARG:HD2	1.96	0.47
1:C:43:VAL:HG23	1:C:44:LEU:H	1.79	0.47
1:C:45:ALA:O	1:C:49:ALA:HB2	2.15	0.47
1:C:250:ILE:CG2	1:C:251:PRO:HD2	2.45	0.47
1:F:139:SER:O	1:F:142:VAL:HG12	2.15	0.47
1:J:177:ARG:HD2	1:J:181:ARG:NH2	2.29	0.47
1:J:285:ASP:HA	1:J:319:GLN:HG2	1.95	0.47
1:A:229:MET:HB2	1:A:229:MET:HE3	1.80	0.46
1:A:277:LEU:HD23	1:A:327:PRO:HA	1.97	0.46
1:A:222:TYR:OH	1:A:373:MET:HE1	2.15	0.46
1:B:47:ARG:HA	1:B:47:ARG:NE	2.30	0.46
1:B:48:LEU:HD12	1:B:384:PHE:CD1	2.50	0.46
1:G:118:GLN:HB2	1:G:120:LEU:HD13	1.96	0.46
1:H:318:HIS:CD2	1:H:319:GLN:HG3	2.50	0.46
1:I:162:VAL:HG13	1:I:193:ALA:HB1	1.98	0.46
1:B:176:PHE:HA	2:B:500:GDU:O2	2.15	0.46
1:C:47:ARG:NH1	1:C:100:ARG:HH21	2.13	0.46
1:D:29:GLY:N	1:D:251:PRO:HB2	2.30	0.46
1:D:265:PHE:O	1:D:266:ASP:CB	2.56	0.46
1:I:111:VAL:HG22	1:I:294:THR:HB	1.96	0.46
1:I:182:LYS:HD2	1:I:302:ALA:O	2.14	0.46
1:J:86:ILE:HG21	1:J:109:HIS:HB2	1.96	0.46
1:D:160:GLU:O	1:D:164:VAL:HB	2.14	0.46
1:G:94:VAL:HG13	1:G:377:VAL:HG11	1.96	0.46
1:A:114:SER:HA	1:A:118:GLN:O	2.15	0.46
1:D:130:ASN:HA	1:D:135:LEU:HB2	1.98	0.46
1:F:176:PHE:HA	2:F:500:GDU:O2	2.15	0.46
1:B:272:LEU:HD22	1:B:368:TYR:CE1	2.50	0.46
1:C:49:ALA:CA	1:C:234:ASN:HD22	2.29	0.46
1:D:112:LEU:HD12	1:D:120:LEU:C	2.40	0.46
1:E:297:TYR:HE1	1:E:306:VAL:HG23	1.81	0.46
1:B:364:ARG:HG3	1:B:369:ARG:O	2.16	0.46
1:C:334:TYR:O	1:C:364:ARG:NH1	2.44	0.46
1:C:362:VAL:O	1:C:366:ALA:HB3	2.15	0.46
1:E:305:ARG:HE	1:E:325:GLU:CD	2.22	0.46
1:D:305:ARG:NH1	2:D:500:GDU:H5'	2.30	0.46
1:F:29:GLY:CA	1:F:251:PRO:HB2	2.44	0.46
1:C:155:GLN:HB2	1:C:157:ARG:NH1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:GLU:O	1:E:164:VAL:HB	2.15	0.46
1:G:336:PRO:O	1:G:338:PRO:HD3	2.16	0.46
1:B:135:LEU:HD21	1:C:140:PHE:CE2	2.51	0.46
1:B:159:SER:HB3	1:B:196:THR:HG23	1.98	0.46
1:D:47:ARG:HA	1:D:47:ARG:NE	2.31	0.46
1:C:246:ILE:HB	1:C:250:ILE:CD1	2.46	0.45
1:E:69:TYR:O	1:E:81:PRO:HD2	2.16	0.45
1:E:250:ILE:O	1:E:252:PHE:HD2	1.99	0.45
1:J:246:ILE:HD12	1:J:250:ILE:HD12	1.98	0.45
1:C:318:HIS:HB3	5:C:399:HOH:O	2.16	0.45
2:D:500:GDU:H1'	4:D:1385:FDA:C5X	2.47	0.45
1:H:260:PRO:HG3	1:H:333:PRO:HG2	1.98	0.45
1:A:275:ARG:HB3	1:A:335:TYR:HB2	1.97	0.45
1:C:235:ILE:C	1:C:236:LYS:HD3	2.41	0.45
1:D:242:ASP:HB3	1:D:245:GLU:HG3	1.97	0.45
3:H:450:FAD:O2'	3:H:450:FAD:O4'	2.30	0.45
1:J:60:ARG:H	3:J:450:FAD:C2A	2.30	0.45
1:J:160:GLU:O	1:J:164:VAL:HB	2.15	0.45
1:H:242:ASP:HB3	1:H:245:GLU:HG3	1.98	0.45
1:J:258:THR:HG22	1:J:362:VAL:HG13	1.98	0.45
1:B:159:SER:OG	1:B:195:VAL:HB	2.17	0.45
1:E:187:ASP:CG	1:E:188:PRO:HD2	2.41	0.45
1:H:47:ARG:HA	1:H:47:ARG:NE	2.32	0.45
1:J:86:ILE:HD12	1:J:86:ILE:N	2.31	0.45
1:B:151:GLU:HB2	1:B:164:VAL:CG1	2.47	0.45
1:C:34:ILE:HG12	1:C:256:ILE:HD12	1.99	0.45
1:J:47:ARG:NE	1:J:47:ARG:HA	2.32	0.45
1:C:262:ASP:HB3	1:C:272:LEU:HB2	1.99	0.45
1:C:264:PHE:CG	1:C:361:PHE:HZ	2.34	0.45
1:I:86:ILE:N	1:I:86:ILE:HD12	2.31	0.45
1:B:97:TYR:HD2	1:B:98:LEU:HD13	1.81	0.45
1:E:225:MET:HE3	1:E:229:MET:HE1	1.99	0.45
1:F:163:VAL:HG12	1:F:172:TYR:HB2	1.98	0.45
1:H:156:VAL:HG13	1:H:161:ASP:HB2	1.98	0.45
1:H:261:VAL:HG13	1:H:366:ALA:O	2.16	0.45
1:B:97:TYR:CD2	1:B:98:LEU:HD13	2.51	0.45
1:D:36:GLY:O	1:D:41:GLY:HA3	2.17	0.45
1:D:220:HIS:CE1	1:J:74:ASP:HB3	2.52	0.45
1:G:30:PHE:O	1:G:252:PHE:HA	2.17	0.45
1:H:206:ASP:OD1	1:H:208:ARG:HD3	2.17	0.45
1:F:135:LEU:HD23	1:H:138:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:297:TYR:HE1	1:I:306:VAL:HG23	1.82	0.44
1:C:54:ARG:NH2	1:F:249:PHE:CE1	2.86	0.44
2:D:500:GDU:C1'	4:D:1385:FDA:N5	2.80	0.44
1:F:123:PRO:HB3	1:F:200:PRO:O	2.17	0.44
1:C:381:LEU:HD23	1:C:381:LEU:N	2.32	0.44
1:E:169:ARG:O	1:E:172:TYR:HB3	2.17	0.44
1:F:151:GLU:HB2	1:F:164:VAL:CG1	2.48	0.44
1:D:367:THR:O	1:D:369:ARG:HG3	2.17	0.44
1:H:159:SER:HB3	1:H:196:THR:HG23	1.98	0.44
1:I:36:GLY:O	1:I:41:GLY:HA3	2.17	0.44
1:A:160:GLU:O	1:A:164:VAL:HB	2.18	0.44
1:C:57:ILE:O	1:C:57:ILE:HG22	2.16	0.44
1:C:360:THR:HG22	1:C:362:VAL:CG1	2.47	0.44
1:F:272:LEU:HD23	1:F:273:PRO:CD	2.48	0.44
1:B:262:ASP:HB3	1:B:272:LEU:HB2	1.98	0.44
2:B:500:GDU:H2'	4:B:1385:FDA:C4X	2.47	0.44
1:C:367:THR:HG21	1:C:379:GLN:NE2	2.33	0.44
1:D:151:GLU:HB2	1:D:164:VAL:CG1	2.48	0.44
1:A:137:LEU:HA	1:A:141:GLN:OE1	2.18	0.44
1:C:40:ALA:HB1	1:C:362:VAL:HG23	2.00	0.44
1:C:180:THR:HB	1:C:188:PRO:HG3	1.99	0.44
1:C:308:GLU:HB3	1:C:311:HIS:HD2	1.83	0.44
1:D:64:ILE:HD12	1:D:226:PHE:HB3	1.99	0.44
1:G:373:MET:HE2	4:G:1385:FDA:C2	2.47	0.44
1:G:376:VAL:HG21	4:G:1385:FDA:C5'	2.47	0.44
1:H:223:THR:HG22	1:H:227:GLN:HE21	1.82	0.44
1:D:86:ILE:N	1:D:86:ILE:HD12	2.32	0.44
1:E:236:LYS:HA	1:E:236:LYS:HD3	1.84	0.44
1:B:229:MET:HE3	1:B:229:MET:HB2	1.81	0.44
1:C:369:ARG:HD3	1:C:371:TYR:OH	2.18	0.44
1:E:86:ILE:HG21	1:E:109:HIS:HB2	1.99	0.44
1:F:30:PHE:O	1:F:252:PHE:HA	2.18	0.44
1:H:151:GLU:O	1:H:165:SER:HA	2.17	0.44
1:A:369:ARG:HD3	5:A:581:HOH:O	2.18	0.43
1:C:305:ARG:HG3	5:C:411:HOH:O	2.17	0.43
1:H:156:VAL:HG13	1:H:161:ASP:CB	2.48	0.43
1:I:162:VAL:CG1	1:I:193:ALA:HB1	2.48	0.43
1:H:120:LEU:HB3	1:H:128:THR:HG23	2.00	0.43
1:I:229:MET:HE3	1:I:229:MET:HB2	1.87	0.43
1:B:86:ILE:HG21	1:B:109:HIS:HB2	2.01	0.43
1:H:159:SER:HB2	1:H:188:PRO:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:92:LYS:HE2	1:H:96:GLU:CD	2.43	0.43
1:H:262:ASP:HB3	1:H:272:LEU:HB2	2.01	0.43
1:A:162:VAL:HG13	1:A:193:ALA:HB1	2.01	0.43
1:A:236:LYS:HA	1:A:236:LYS:HD3	1.89	0.43
1:B:88:HIS:HD1	1:B:212:ASP:CG	2.27	0.43
1:D:262:ASP:HB3	1:D:272:LEU:HB2	2.00	0.43
1:D:332:ASP:HA	1:D:333:PRO:HD3	1.89	0.43
1:I:284:HIS:HE1	5:I:404:HOH:O	2.00	0.43
1:C:123:PRO:HB3	1:C:200:PRO:O	2.18	0.43
1:C:351:ALA:O	1:C:354:ASP:HB2	2.19	0.43
1:G:275:ARG:HB3	1:G:335:TYR:HB2	1.99	0.43
1:C:55:VAL:HG23	1:C:235:ILE:HG12	1.99	0.43
1:D:92:LYS:O	1:D:96:GLU:HG3	2.19	0.43
1:E:67:ASN:HB3	1:E:85:HIS:NE2	2.34	0.43
1:J:371:TYR:HB3	1:J:376:VAL:HG23	2.00	0.43
1:A:42:SER:HA	1:A:230:LEU:HD21	2.01	0.43
1:C:107:TYR:O	1:C:215:GLN:HB3	2.19	0.43
1:E:242:ASP:HB3	1:E:245:GLU:HG3	2.00	0.43
1:G:29:GLY:HA3	1:G:251:PRO:HB2	2.01	0.43
1:I:34:ILE:HG12	1:I:256:ILE:HB	2.01	0.43
1:J:364:ARG:HG3	1:J:369:ARG:O	2.19	0.43
1:C:151:GLU:HB2	1:C:164:VAL:CG1	2.48	0.43
1:F:122:ILE:HD11	1:F:199:VAL:HG11	2.01	0.43
1:F:172:TYR:OH	1:F:188:PRO:HG2	2.18	0.43
1:B:86:ILE:N	1:B:86:ILE:HD12	2.34	0.43
1:C:373:MET:HE2	3:C:450:FAD:C2	2.48	0.43
1:C:373:MET:HG3	3:C:450:FAD:H2'	1.99	0.43
1:D:261:VAL:HG13	1:D:366:ALA:O	2.19	0.43
1:I:285:ASP:OD2	1:J:318:HIS:NE2	2.52	0.43
1:A:139:SER:O	1:A:142:VAL:HG12	2.18	0.42
1:A:159:SER:HB2	1:A:188:PRO:O	2.19	0.42
1:C:254:HIS:HD2	1:C:254:HIS:O	2.02	0.42
1:D:32:TYR:CD2	1:D:48:LEU:HD23	2.53	0.42
1:D:269:TYR:CE2	1:D:348:LYS:HB3	2.54	0.42
1:E:277:LEU:HD23	1:E:327:PRO:HA	2.01	0.42
1:G:160:GLU:O	1:G:164:VAL:HB	2.19	0.42
1:C:86:ILE:HA	1:C:217:MET:SD	2.59	0.42
2:E:500:GDU:O5D	2:E:500:GDU:H6	2.19	0.42
1:F:86:ILE:N	1:F:86:ILE:HD12	2.34	0.42
1:H:300:ASP:O	1:H:301:TYR:HB2	2.19	0.42
1:F:90:ASN:OD1	1:F:212:ASP:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:236:LYS:HA	1:J:236:LYS:HD3	1.81	0.42
1:A:337:VAL:HB	1:A:342:ASN:HD22	1.84	0.42
1:B:250:ILE:HA	1:B:251:PRO:HD3	1.86	0.42
1:C:97:TYR:O	1:C:100:ARG:HB2	2.19	0.42
1:F:199:VAL:HA	1:F:200:PRO:HD2	1.89	0.42
4:G:1385:FDA:HM83	4:G:1385:FDA:HM71	1.79	0.42
1:B:272:LEU:HG	1:B:345:LEU:HD13	2.02	0.42
1:C:34:ILE:O	1:C:57:ILE:HA	2.20	0.42
1:D:151:GLU:HB2	1:D:164:VAL:HG13	2.00	0.42
1:E:265:PHE:CE2	1:E:352:LEU:HB3	2.55	0.42
1:E:300:ASP:O	1:E:301:TYR:HB2	2.19	0.42
1:F:357:GLN:HA	1:F:357:GLN:HE21	1.85	0.42
1:H:308:GLU:HB3	1:H:311:HIS:CD2	2.50	0.42
1:F:277:LEU:HD23	1:F:327:PRO:HA	2.02	0.42
1:H:69:TYR:O	1:H:81:PRO:HD2	2.20	0.42
1:H:162:VAL:CG1	1:H:193:ALA:HB1	2.49	0.42
1:I:232:SER:HA	1:I:233:PRO:HD3	1.93	0.42
1:C:33:LEU:HA	1:C:56:LEU:O	2.19	0.42
1:D:250:ILE:O	1:D:252:PHE:CD2	2.73	0.42
1:F:308:GLU:HB3	1:F:311:HIS:CD2	2.45	0.42
1:J:156:VAL:HG11	1:J:162:VAL:HG13	2.02	0.42
1:J:273:PRO:HG2	1:J:342:ASN:CG	2.45	0.42
1:A:34:ILE:HG12	1:A:256:ILE:HB	2.02	0.42
1:B:49:ALA:HB1	1:B:234:ASN:HB2	2.02	0.42
1:D:243:TYR:CE2	1:D:244:ARG:HG3	2.55	0.42
1:E:353:ALA:HB1	1:E:361:PHE:CD1	2.55	0.42
1:F:115:VAL:HG21	1:F:175:PHE:CE2	2.54	0.42
1:G:250:ILE:HA	1:G:251:PRO:HD3	1.78	0.42
1:J:308:GLU:HB3	1:J:311:HIS:HD2	1.84	0.42
1:A:176:PHE:HA	2:A:500:GDU:O2	2.20	0.42
1:E:156:VAL:HG13	1:E:161:ASP:CB	2.50	0.42
1:A:151:GLU:O	1:A:165:SER:HA	2.19	0.41
1:B:44:LEU:O	1:B:48:LEU:HD13	2.20	0.41
1:B:58:VAL:HA	1:B:238:MET:O	2.20	0.41
1:B:181:ARG:HA	1:B:186:LEU:O	2.20	0.41
1:D:162:VAL:CG1	1:D:193:ALA:HB1	2.49	0.41
1:E:30:PHE:O	1:E:252:PHE:HA	2.20	0.41
1:E:232:SER:HA	1:E:233:PRO:HD3	1.96	0.41
1:E:262:ASP:OD1	1:E:263:ALA:N	2.52	0.41
1:J:373:MET:HG3	3:J:450:FAD:H2'	2.02	0.41
1:A:250:ILE:HA	1:A:251:PRO:HD3	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:500:GDU:H2'	3:A:450:FAD:C4X	2.49	0.41
1:D:373:MET:HE2	4:D:1385:FDA:N3	2.35	0.41
3:F:450:FAD:C4	2:F:500:GDU:H2'	2.50	0.41
1:B:139:SER:O	1:B:142:VAL:HG12	2.20	0.41
1:C:272:LEU:HD23	1:C:273:PRO:HD2	2.02	0.41
1:E:332:ASP:HA	1:E:333:PRO:HD3	1.88	0.41
1:G:218:PRO:HG2	1:G:222:TYR:CD2	2.55	0.41
1:I:336:PRO:O	1:I:338:PRO:HD3	2.20	0.41
1:J:297:TYR:HE1	1:J:306:VAL:HG23	1.86	0.41
1:C:179:TYR:CD2	2:C:500:GDU:H2D	2.55	0.41
1:G:229:MET:HE3	1:G:229:MET:HB2	1.89	0.41
1:C:254:HIS:CD2	1:C:254:HIS:C	2.98	0.41
1:G:86:ILE:N	1:G:86:ILE:HD12	2.35	0.41
1:I:30:PHE:O	1:I:252:PHE:HA	2.20	0.41
1:I:250:ILE:HA	1:I:251:PRO:HD3	1.81	0.41
1:A:353:ALA:HB1	1:A:361:PHE:CD1	2.56	0.41
1:C:48:LEU:C	1:C:50:SER:N	2.75	0.41
3:F:450:FAD:C4X	2:F:500:GDU:H2'	2.50	0.41
1:I:332:ASP:HA	1:I:333:PRO:HD3	1.87	0.41
1:J:229:MET:HE3	1:J:229:MET:HB2	1.92	0.41
1:A:288:GLN:HA	1:A:308:GLU:OE1	2.21	0.41
1:A:337:VAL:HB	1:A:342:ASN:ND2	2.36	0.41
1:A:364:ARG:HG3	1:A:369:ARG:O	2.21	0.41
1:D:32:TYR:CG	1:D:48:LEU:HD23	2.56	0.41
1:H:337:VAL:HB	1:H:342:ASN:HD22	1.86	0.41
1:J:332:ASP:HA	1:J:333:PRO:HD3	1.91	0.41
3:C:450:FAD:N5	2:C:500:GDU:H2'	2.35	0.41
1:D:277:LEU:HD23	1:D:327:PRO:HA	2.02	0.41
1:F:185:GLY:O	1:F:186:LEU:HD12	2.20	0.41
1:I:47:ARG:HA	1:I:47:ARG:NE	2.36	0.41
1:J:250:ILE:HA	1:J:251:PRO:HD3	1.70	0.41
1:C:337:VAL:HB	1:C:342:ASN:HD22	1.86	0.41
3:C:450:FAD:C4X	2:C:500:GDU:H2'	2.51	0.41
2:D:500:GDU:H1'	4:D:1385:FDA:N5	2.35	0.41
1:E:337:VAL:HB	1:E:342:ASN:HD22	1.86	0.41
1:F:297:TYR:HE1	1:F:306:VAL:HG23	1.86	0.41
1:H:353:ALA:HB1	1:H:361:PHE:CD1	2.55	0.41
1:A:90:ASN:OD1	1:A:212:ASP:HA	2.21	0.41
1:B:151:GLU:O	1:B:165:SER:HA	2.21	0.41
1:G:297:TYR:HE1	1:G:306:VAL:HG23	1.86	0.41
1:A:185:GLY:O	1:A:186:LEU:HD12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:LEU:HA	1:A:291:PRO:HD3	1.93	0.40
1:E:308:GLU:HB3	1:E:311:HIS:HD2	1.86	0.40
3:E:450:FAD:O2'	3:E:450:FAD:O4'	2.30	0.40
1:F:44:LEU:CD1	1:F:362:VAL:HG11	2.51	0.40
1:F:79:ILE:O	1:F:81:PRO:HD3	2.21	0.40
1:H:60:ARG:H	3:H:450:FAD:C2A	2.34	0.40
1:A:272:LEU:CD2	1:A:273:PRO:HD2	2.51	0.40
1:A:332:ASP:HA	1:A:333:PRO:HD3	1.88	0.40
1:C:33:LEU:O	1:C:255:MET:HA	2.21	0.40
1:D:73:ASP:HB2	5:D:637:HOH:O	2.20	0.40
1:D:268:CYS:SG	1:D:352:LEU:HD11	2.62	0.40
1:F:137:LEU:HD12	1:F:142:VAL:HG23	2.04	0.40
1:H:122:ILE:HD12	1:H:123:PRO:HA	2.03	0.40
1:J:347:LYS:HG2	1:J:350:GLU:OE2	2.20	0.40
1:A:162:VAL:CG1	1:A:193:ALA:HB1	2.52	0.40
1:B:43:VAL:HG22	1:B:97:TYR:HE2	1.87	0.40
1:D:236:LYS:HE3	1:J:245:GLU:OE2	2.22	0.40
1:E:86:ILE:HD12	1:E:86:ILE:N	2.36	0.40
1:F:262:ASP:OD1	1:F:263:ALA:N	2.53	0.40
1:F:336:PRO:O	1:F:338:PRO:HD3	2.22	0.40
3:F:450:FAD:O2'	3:F:450:FAD:O4'	2.30	0.40
1:I:255:MET:HG2	1:I:359:VAL:HG13	2.04	0.40
1:A:225:MET:HE2	1:A:225:MET:HB3	2.01	0.40
1:C:238:MET:HE1	1:C:246:ILE:HG21	2.02	0.40
1:C:246:ILE:HB	1:C:250:ILE:HG13	2.03	0.40
1:E:261:VAL:HG13	1:E:366:ALA:O	2.22	0.40
1:E:290:LEU:HD12	1:E:308:GLU:HB2	2.03	0.40
1:H:232:SER:HA	1:H:233:PRO:HD3	1.86	0.40
1:I:337:VAL:HB	1:I:342:ASN:HD22	1.85	0.40
1:D:77:VAL:O	1:D:79:ILE:HG23	2.21	0.40
1:D:158:THR:O	1:D:161:ASP:HB2	2.21	0.40
1:F:232:SER:HA	1:F:233:PRO:HD3	1.90	0.40
1:I:60:ARG:HD2	3:I:450:FAD:C5A	2.52	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	363/397 (91%)	347 (96%)	16 (4%)	0	100	100
1	B	359/397 (90%)	347 (97%)	12 (3%)	0	100	100
1	C	347/397 (87%)	314 (90%)	30 (9%)	3 (1%)	14	22
1	D	359/397 (90%)	342 (95%)	17 (5%)	0	100	100
1	E	359/397 (90%)	347 (97%)	12 (3%)	0	100	100
1	F	360/397 (91%)	343 (95%)	15 (4%)	2 (1%)	21	32
1	G	358/397 (90%)	342 (96%)	16 (4%)	0	100	100
1	H	359/397 (90%)	347 (97%)	12 (3%)	0	100	100
1	I	359/397 (90%)	343 (96%)	15 (4%)	1 (0%)	36	50
1	J	357/397 (90%)	341 (96%)	16 (4%)	0	100	100
All	All	3580/3970 (90%)	3413 (95%)	161 (4%)	6 (0%)	43	58

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	51	SER
1	C	233	PRO
1	F	357	GLN
1	F	370	TYR
1	I	370	TYR
1	C	227	GLN

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	317/346 (92%)	302 (95%)	15 (5%)	23	41
1	B	313/346 (90%)	299 (96%)	14 (4%)	24	42
1	C	304/346 (88%)	283 (93%)	21 (7%)	14	24
1	D	313/346 (90%)	299 (96%)	14 (4%)	24	42
1	E	313/346 (90%)	299 (96%)	14 (4%)	24	42
1	F	314/346 (91%)	295 (94%)	19 (6%)	17	30
1	G	313/346 (90%)	298 (95%)	15 (5%)	23	40
1	H	314/346 (91%)	299 (95%)	15 (5%)	23	40
1	I	313/346 (90%)	297 (95%)	16 (5%)	21	37
1	J	313/346 (90%)	301 (96%)	12 (4%)	29	49
All	All	3127/3460 (90%)	2972 (95%)	155 (5%)	22	38

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	98	LEU
1	A	112	LEU
1	A	120	LEU
1	A	126	LEU
1	A	152	LYS
1	A	154	GLU
1	A	164	VAL
1	A	186	LEU
1	A	261	VAL
1	A	272	LEU
1	A	341	GLU
1	A	345	LEU
1	A	362	VAL
1	A	387	LEU
1	B	93	ASP
1	B	98	LEU
1	B	120	LEU
1	B	122	ILE
1	B	126	LEU
1	B	152	LYS
1	B	162	VAL
1	B	186	LEU
1	B	261	VAL

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Mol	Chain	Res	Type
1	B	272	LEU
1	B	306	VAL
1	B	345	LEU
1	B	357	GLN
1	B	358	ASP
1	C	51	SER
1	C	54	ARG
1	C	55	VAL
1	C	56	LEU
1	C	58	VAL
1	C	98	LEU
1	C	112	LEU
1	C	120	LEU
1	C	126	LEU
1	C	155	GLN
1	C	159	SER
1	C	162	VAL
1	C	186	LEU
1	C	227	GLN
1	C	232	SER
1	C	258	THR
1	C	261	VAL
1	C	272	LEU
1	C	345	LEU
1	C	357	GLN
1	C	362	VAL
1	D	98	LEU
1	D	112	LEU
1	D	120	LEU
1	D	122	ILE
1	D	126	LEU
1	D	142	VAL
1	D	152	LYS
1	D	154	GLU
1	D	159	SER
1	D	162	VAL
1	D	164	VAL
1	D	261	VAL
1	D	272	LEU
1	D	345	LEU
1	E	48	LEU
1	E	98	LEU

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Mol	Chain	Res	Type
1	E	112	LEU
1	E	120	LEU
1	E	126	LEU
1	E	152	LYS
1	E	154	GLU
1	E	164	VAL
1	E	186	LEU
1	E	261	VAL
1	E	272	LEU
1	E	304	THR
1	E	306	VAL
1	E	345	LEU
1	F	28	LYS
1	F	44	LEU
1	F	48	LEU
1	F	98	LEU
1	F	112	LEU
1	F	120	LEU
1	F	126	LEU
1	F	152	LYS
1	F	154	GLU
1	F	159	SER
1	F	162	VAL
1	F	164	VAL
1	F	261	VAL
1	F	272	LEU
1	F	292	THR
1	F	306	VAL
1	F	345	LEU
1	F	357	GLN
1	F	387	LEU
1	G	48	LEU
1	G	98	LEU
1	G	112	LEU
1	G	118	GLN
1	G	120	LEU
1	G	126	LEU
1	G	152	LYS
1	G	162	VAL
1	G	164	VAL
1	G	261	VAL
1	G	272	LEU

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Mol	Chain	Res	Type
1	G	304	THR
1	G	306	VAL
1	G	345	LEU
1	G	357	GLN
1	H	48	LEU
1	H	98	LEU
1	H	112	LEU
1	H	120	LEU
1	H	126	LEU
1	H	152	LYS
1	H	162	VAL
1	H	164	VAL
1	H	186	LEU
1	H	261	VAL
1	H	272	LEU
1	H	306	VAL
1	H	345	LEU
1	H	357	GLN
1	H	387	LEU
1	I	48	LEU
1	I	98	LEU
1	I	112	LEU
1	I	118	GLN
1	I	120	LEU
1	I	122	ILE
1	I	126	LEU
1	I	152	LYS
1	I	164	VAL
1	I	261	VAL
1	I	272	LEU
1	I	306	VAL
1	I	345	LEU
1	I	357	GLN
1	I	371	TYR
1	I	387	LEU
1	J	98	LEU
1	J	112	LEU
1	J	120	LEU
1	J	122	ILE
1	J	126	LEU
1	J	152	LYS
1	J	162	VAL

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Mol	Chain	Res	Type
1	J	164	VAL
1	J	186	LEU
1	J	261	VAL
1	J	272	LEU
1	J	345	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	118	GLN
1	A	220	HIS
1	A	284	HIS
1	A	357	GLN
1	B	220	HIS
1	B	357	GLN
1	B	388	GLN
1	C	88	HIS
1	C	155	GLN
1	C	220	HIS
1	C	254	HIS
1	C	299	ASN
1	C	311	HIS
1	D	220	HIS
1	D	284	HIS
1	D	311	HIS
1	D	318	HIS
1	D	319	GLN
1	D	357	GLN
1	E	53	GLN
1	E	311	HIS
1	E	357	GLN
1	F	53	GLN
1	F	299	ASN
1	F	357	GLN
1	G	220	HIS
1	H	220	HIS
1	H	227	GLN
1	H	357	GLN
1	I	220	HIS
1	I	284	HIS
1	I	311	HIS

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Mol	Chain	Res	Type
1	I	319	GLN
1	I	357	GLN
1	J	53	GLN
1	J	118	GLN
1	J	284	HIS
1	J	311	HIS
1	J	357	GLN

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 ⓘ

20 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	E	450	-	58,58,58	1.23	5 (8%)	85,89,89	1.61	13 (15%)
2	GDU	J	500	-	37,38,38	2.67	4 (10%)	55,58,58	3.56	16 (29%)
3	FAD	H	450	-	58,58,58	1.23	5 (8%)	85,89,89	1.60	12 (14%)
2	GDU	B	500	-	37,38,38	2.64	4 (10%)	55,58,58	3.61	20 (36%)
3	FAD	F	450	-	58,58,58	1.23	5 (8%)	85,89,89	1.60	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GDU	H	500	-	37,38,38	2.67	4 (10%)	55,58,58	3.54	18 (32%)
2	GDU	C	500	-	37,38,38	2.66	4 (10%)	55,58,58	3.65	19 (34%)
3	FAD	C	450	-	58,58,58	1.23	5 (8%)	85,89,89	1.61	13 (15%)
4	FDA	B	1385	-	57,58,58	2.79	28 (49%)	78,89,89	2.60	30 (38%)
2	GDU	F	500	-	37,38,38	2.66	4 (10%)	55,58,58	3.58	17 (30%)
2	GDU	G	500	-	37,38,38	2.68	4 (10%)	55,58,58	3.58	18 (32%)
3	FAD	J	450	-	58,58,58	1.23	5 (8%)	85,89,89	1.60	12 (14%)
4	FDA	G	1385	-	57,58,58	2.80	27 (47%)	78,89,89	2.60	31 (39%)
2	GDU	E	500	-	37,38,38	2.66	4 (10%)	55,58,58	3.60	19 (34%)
3	FAD	A	450	-	58,58,58	1.23	5 (8%)	85,89,89	1.61	12 (14%)
2	GDU	D	500	-	37,38,38	2.66	4 (10%)	55,58,58	3.63	17 (30%)
2	GDU	I	500	-	37,38,38	2.67	4 (10%)	55,58,58	3.57	17 (30%)
4	FDA	D	1385	-	57,58,58	2.50	17 (29%)	78,89,89	2.47	28 (35%)
2	GDU	A	500	-	37,38,38	2.70	4 (10%)	55,58,58	3.60	21 (38%)
3	FAD	I	450	-	58,58,58	1.23	5 (8%)	85,89,89	1.61	12 (14%)

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
3	FAD	E	450	-	-	0/34/50/50	0/6/6/6
2	GDU	J	500	-	-	7/23/59/59	0/3/3/3
3	FAD	H	450	-	-	0/34/50/50	0/6/6/6
2	GDU	B	500	-	-	8/23/59/59	0/3/3/3
3	FAD	F	450	-	-	0/34/50/50	0/6/6/6
2	GDU	H	500	-	-	7/23/59/59	0/3/3/3
2	GDU	C	500	-	-	12/23/59/59	0/3/3/3
3	FAD	C	450	-	-	0/34/50/50	0/6/6/6
4	FDA	B	1385	-	2/2/9/9	2/34/50/50	0/6/6/6
2	GDU	F	500	-	-	8/23/59/59	0/3/3/3
2	GDU	G	500	-	-	9/23/59/59	0/3/3/3
3	FAD	J	450	-	-	0/34/50/50	0/6/6/6
4	FDA	G	1385	-	2/2/9/9	5/34/50/50	0/6/6/6
2	GDU	E	500	-	-	6/23/59/59	0/3/3/3
3	FAD	A	450	-	-	0/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GDU	D	500	-	-	10/23/59/59	0/3/3/3
2	GDU	I	500	-	-	8/23/59/59	0/3/3/3
4	FDA	D	1385	-	4/4/9/9	5/34/50/50	0/6/6/6
2	GDU	A	500	-	-	4/23/59/59	0/3/3/3
3	FAD	I	450	-	-	0/34/50/50	0/6/6/6

All (147) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	GDU	O2-C2	11.58	1.43	1.23
2	F	500	GDU	O2-C2	11.57	1.43	1.23
2	H	500	GDU	O2-C2	11.56	1.43	1.23
2	A	500	GDU	O2-C2	11.53	1.43	1.23
2	B	500	GDU	O2-C2	11.53	1.43	1.23
2	C	500	GDU	O2-C2	11.53	1.43	1.23
2	G	500	GDU	O2-C2	11.51	1.43	1.23
2	E	500	GDU	O2-C2	11.48	1.43	1.23
2	J	500	GDU	O2-C2	11.29	1.43	1.23
2	I	500	GDU	O2-C2	11.28	1.43	1.23
4	D	1385	FDA	O4-C4	8.90	1.40	1.23
4	D	1385	FDA	O2-C2	8.12	1.40	1.23
2	A	500	GDU	C2-N1	-8.07	1.25	1.38
2	I	500	GDU	C2-N1	-7.99	1.25	1.38
2	J	500	GDU	C2-N1	-7.93	1.26	1.38
2	E	500	GDU	C2-N1	-7.78	1.26	1.38
2	G	500	GDU	C2-N1	-7.74	1.26	1.38
2	B	500	GDU	C2-N1	-7.73	1.26	1.38
2	H	500	GDU	C2-N1	-7.72	1.26	1.38
2	D	500	GDU	C2-N1	-7.63	1.26	1.38
2	F	500	GDU	C2-N1	-7.54	1.26	1.38
2	C	500	GDU	C2-N1	-7.47	1.26	1.38
4	B	1385	FDA	O4-C4	6.73	1.36	1.23
4	G	1385	FDA	O4-C4	6.66	1.36	1.23
2	C	500	GDU	C2-N3	-6.60	1.26	1.38
4	G	1385	FDA	C3B-C4B	-6.59	1.36	1.53
2	J	500	GDU	C2-N3	-6.59	1.26	1.38
4	B	1385	FDA	O2-C2	6.59	1.37	1.23
2	G	500	GDU	C2-N3	-6.58	1.26	1.38
2	A	500	GDU	C2-N3	-6.57	1.26	1.38
2	H	500	GDU	C2-N3	-6.55	1.26	1.38
2	F	500	GDU	C2-N3	-6.52	1.26	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	500	GDU	C2-N3	-6.49	1.26	1.38
2	D	500	GDU	C2-N3	-6.42	1.26	1.38
2	E	500	GDU	C2-N3	-6.40	1.26	1.38
2	B	500	GDU	C2-N3	-6.35	1.26	1.38
4	G	1385	FDA	O2-C2	6.22	1.36	1.23
4	B	1385	FDA	C3B-C4B	-5.66	1.38	1.53
4	G	1385	FDA	C9A-N10	-5.38	1.31	1.41
4	B	1385	FDA	C2B-C3B	-5.06	1.39	1.53
4	G	1385	FDA	C2B-C3B	-4.89	1.40	1.53
4	B	1385	FDA	C9A-N10	-4.88	1.32	1.41
4	D	1385	FDA	C3B-C4B	-4.71	1.41	1.53
4	G	1385	FDA	C8A-N9A	-4.68	1.29	1.37
4	G	1385	FDA	C5A-C4A	-4.66	1.30	1.39
4	B	1385	FDA	C2-N1	-4.53	1.30	1.37
4	D	1385	FDA	C6A-N6A	4.45	1.45	1.34
4	D	1385	FDA	C9A-N10	-4.39	1.33	1.41
4	G	1385	FDA	C2B-C1B	-4.24	1.40	1.53
4	B	1385	FDA	C8A-N9A	-4.23	1.30	1.37
4	B	1385	FDA	C4X-N5	-4.12	1.27	1.35
4	B	1385	FDA	C5A-C4A	-4.07	1.31	1.39
4	B	1385	FDA	PA-O3P	-4.05	1.55	1.59
4	B	1385	FDA	C2B-C1B	-4.04	1.40	1.53
4	D	1385	FDA	C2B-C3B	-3.92	1.42	1.53
4	G	1385	FDA	C5X-C9A	-3.89	1.36	1.40
4	B	1385	FDA	PA-O2A	-3.89	1.37	1.55
4	G	1385	FDA	C6A-N6A	3.85	1.44	1.34
4	G	1385	FDA	C4X-N5	-3.81	1.28	1.35
4	B	1385	FDA	C5X-C9A	-3.80	1.36	1.40
4	D	1385	FDA	C2B-C1B	-3.67	1.42	1.53
4	B	1385	FDA	C6A-N6A	3.63	1.43	1.34
4	D	1385	FDA	C8A-N7A	3.59	1.38	1.31
4	G	1385	FDA	C2-N1	-3.48	1.31	1.37
4	D	1385	FDA	C10-N10	3.47	1.44	1.38
4	G	1385	FDA	PA-O2A	-3.31	1.40	1.55
4	G	1385	FDA	P-O2P	-3.17	1.40	1.55
4	G	1385	FDA	C4-N3	-3.11	1.33	1.38
4	B	1385	FDA	O2'-C2'	-3.11	1.36	1.43
4	B	1385	FDA	P-O2P	-3.07	1.41	1.55
4	G	1385	FDA	O4'-C4'	-3.01	1.37	1.43
4	D	1385	FDA	C4X-N5	-2.97	1.30	1.35
4	D	1385	FDA	C5X-N5	2.92	1.44	1.39
3	I	450	FAD	C4X-N5	2.84	1.36	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1385	FDA	P-O3P	-2.84	1.56	1.59
3	E	450	FAD	C4X-N5	2.83	1.36	1.30
3	F	450	FAD	C4X-N5	2.83	1.36	1.30
3	J	450	FAD	C4X-N5	2.83	1.36	1.30
3	A	450	FAD	C4X-N5	2.81	1.36	1.30
4	D	1385	FDA	PA-O1A	2.80	1.60	1.50
4	D	1385	FDA	P-O1P	2.80	1.60	1.50
4	B	1385	FDA	C4-N3	-2.80	1.33	1.38
3	C	450	FAD	C4X-N5	2.77	1.36	1.30
4	G	1385	FDA	O3B-C3B	-2.77	1.36	1.43
3	H	450	FAD	C4X-N5	2.76	1.36	1.30
4	D	1385	FDA	C5X-C9A	-2.71	1.37	1.40
4	G	1385	FDA	C5A-N7A	-2.69	1.34	1.39
4	B	1385	FDA	C4X-C4	-2.69	1.34	1.41
4	G	1385	FDA	O2'-C2'	-2.65	1.37	1.43
3	F	450	FAD	C5A-N7A	-2.58	1.34	1.39
3	E	450	FAD	C5A-N7A	-2.57	1.34	1.39
3	J	450	FAD	C5A-N7A	-2.56	1.34	1.39
4	D	1385	FDA	C5A-C4A	-2.55	1.34	1.39
3	A	450	FAD	C5A-N7A	-2.55	1.34	1.39
3	H	450	FAD	C5A-N7A	-2.54	1.34	1.39
3	C	450	FAD	C5A-N7A	-2.51	1.34	1.39
3	I	450	FAD	C5A-N7A	-2.49	1.34	1.39
3	C	450	FAD	O4B-C4B	-2.46	1.39	1.45
3	F	450	FAD	O4B-C4B	-2.46	1.39	1.45
3	H	450	FAD	O4B-C4B	-2.44	1.39	1.45
3	A	450	FAD	O4B-C4B	-2.44	1.39	1.45
4	B	1385	FDA	C9-C8	-2.43	1.36	1.39
4	B	1385	FDA	C8A-N7A	2.43	1.36	1.31
3	I	450	FAD	O4B-C4B	-2.42	1.39	1.45
3	J	450	FAD	O4B-C4B	-2.41	1.39	1.45
3	E	450	FAD	O4B-C4B	-2.41	1.39	1.45
4	G	1385	FDA	P-O3P	-2.40	1.56	1.59
4	D	1385	FDA	C8A-N9A	-2.39	1.33	1.37
4	G	1385	FDA	O4B-C1B	-2.38	1.36	1.42
4	G	1385	FDA	C4X-C4	-2.37	1.34	1.41
2	F	500	GDU	C4-N3	-2.34	1.34	1.38
2	A	500	GDU	C4-N3	-2.34	1.34	1.38
4	D	1385	FDA	C10-N1	2.33	1.41	1.37
2	G	500	GDU	C4-N3	-2.31	1.34	1.38
4	G	1385	FDA	O4B-C4B	-2.31	1.39	1.45
4	G	1385	FDA	PA-O3P	-2.28	1.57	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	GDU	C4-N3	-2.27	1.34	1.38
4	B	1385	FDA	O5B-C5B	-2.25	1.36	1.44
4	B	1385	FDA	O3'-C3'	-2.24	1.37	1.43
4	G	1385	FDA	C9-C8	-2.24	1.36	1.39
2	D	500	GDU	C4-N3	-2.22	1.34	1.38
2	J	500	GDU	C4-N3	-2.22	1.34	1.38
2	H	500	GDU	C4-N3	-2.21	1.34	1.38
3	C	450	FAD	C4X-C10	-2.21	1.37	1.44
3	E	450	FAD	C4X-C10	-2.21	1.37	1.44
3	A	450	FAD	C4X-C10	-2.20	1.37	1.44
3	I	450	FAD	C4X-C10	-2.20	1.37	1.44
3	F	450	FAD	C4X-C10	-2.20	1.37	1.44
3	J	450	FAD	C4X-C10	-2.18	1.37	1.44
3	H	450	FAD	C4X-C10	-2.18	1.37	1.44
4	B	1385	FDA	O4B-C1B	-2.17	1.37	1.42
4	B	1385	FDA	C5A-N7A	-2.16	1.35	1.39
4	B	1385	FDA	O4'-C4'	-2.15	1.38	1.43
2	I	500	GDU	C4-N3	-2.13	1.35	1.38
4	B	1385	FDA	C6-C7	-2.12	1.36	1.39
4	B	1385	FDA	O3B-C3B	-2.11	1.37	1.43
2	E	500	GDU	C4-N3	-2.10	1.35	1.38
3	H	450	FAD	C4X-C4	-2.08	1.36	1.44
3	E	450	FAD	C4X-C4	-2.07	1.36	1.44
3	J	450	FAD	C4X-C4	-2.06	1.37	1.44
3	A	450	FAD	C4X-C4	-2.06	1.37	1.44
3	F	450	FAD	C4X-C4	-2.06	1.37	1.44
3	C	450	FAD	C4X-C4	-2.06	1.37	1.44
3	I	450	FAD	C4X-C4	-2.05	1.37	1.44
4	G	1385	FDA	C5A-C6A	-2.04	1.35	1.41
4	G	1385	FDA	C2-N3	-2.02	1.34	1.37
2	B	500	GDU	C4-N3	-2.01	1.35	1.38

All (357) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	GDU	N3-C2-N1	16.64	136.55	114.89
2	J	500	GDU	N3-C2-N1	16.35	136.18	114.89
2	I	500	GDU	N3-C2-N1	16.27	136.07	114.89
2	B	500	GDU	N3-C2-N1	16.26	136.05	114.89
2	C	500	GDU	N3-C2-N1	16.25	136.03	114.89
2	F	500	GDU	N3-C2-N1	16.24	136.03	114.89
2	E	500	GDU	N3-C2-N1	16.21	135.99	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	GDU	N3-C2-N1	16.16	135.92	114.89
2	H	500	GDU	N3-C2-N1	16.05	135.78	114.89
2	G	500	GDU	N3-C2-N1	15.99	135.70	114.89
2	E	500	GDU	C4-N3-C2	-10.97	112.98	126.61
2	I	500	GDU	C4-N3-C2	-10.97	112.99	126.61
2	J	500	GDU	C4-N3-C2	-10.97	112.99	126.61
2	A	500	GDU	C4-N3-C2	-10.86	113.13	126.61
2	D	500	GDU	C4-N3-C2	-10.82	113.17	126.61
2	B	500	GDU	C4-N3-C2	-10.72	113.30	126.61
2	C	500	GDU	C4-N3-C2	-10.72	113.30	126.61
2	F	500	GDU	C4-N3-C2	-10.72	113.30	126.61
2	G	500	GDU	C4-N3-C2	-10.68	113.35	126.61
2	H	500	GDU	C4-N3-C2	-10.66	113.38	126.61
4	B	1385	FDA	O4B-C1B-N9A	9.31	125.97	108.09
4	D	1385	FDA	O4B-C1B-N9A	9.24	125.83	108.09
4	G	1385	FDA	O4B-C1B-N9A	9.22	125.80	108.09
2	A	500	GDU	O2-C2-N1	-8.06	112.31	122.80
2	B	500	GDU	O2-C2-N1	-7.64	112.85	122.80
2	J	500	GDU	O2-C2-N1	-7.57	112.94	122.80
2	E	500	GDU	O2-C2-N1	-7.56	112.95	122.80
2	I	500	GDU	O2-C2-N1	-7.55	112.97	122.80
2	D	500	GDU	O2-C2-N1	-7.33	113.25	122.80
2	H	500	GDU	O2-C2-N1	-7.17	113.47	122.80
2	F	500	GDU	O2-C2-N1	-6.96	113.73	122.80
2	C	500	GDU	O2-C2-N1	-6.78	113.97	122.80
2	G	500	GDU	O2-C2-N1	-6.63	114.17	122.80
2	C	500	GDU	O2-C2-N3	-6.23	109.99	121.49
2	G	500	GDU	O2-C2-N3	-6.16	110.12	121.49
2	F	500	GDU	O2-C2-N3	-6.10	110.24	121.49
2	F	500	GDU	O5'-C5'-C4'	6.09	120.68	109.70
2	G	500	GDU	O5'-C5'-C4'	6.09	120.67	109.70
2	C	500	GDU	O5'-C5'-C4'	6.09	120.67	109.70
2	C	500	GDU	C6-N1-C2	-6.05	113.63	121.00
2	I	500	GDU	O5'-C5'-C4'	6.02	120.55	109.70
2	C	500	GDU	O5'-C1'-O3B	-6.02	103.50	111.36
2	A	500	GDU	C6-N1-C2	-6.00	113.69	121.00
2	F	500	GDU	C6-N1-C2	-6.00	113.69	121.00
4	B	1385	FDA	N3A-C2A-N1A	-5.95	119.57	128.58
2	B	500	GDU	C6-N1-C2	-5.95	113.76	121.00
2	D	500	GDU	C6-N1-C2	-5.93	113.78	121.00
2	G	500	GDU	C1D-N1-C2	5.92	128.23	117.59
4	G	1385	FDA	C4-N3-C2	-5.90	118.24	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	450	FAD	N3A-C2A-N1A	-5.89	119.67	128.58
3	C	450	FAD	N3A-C2A-N1A	-5.89	119.67	128.58
2	C	500	GDU	C1D-N1-C2	5.88	128.16	117.59
2	A	500	GDU	O5'-C5'-C4'	5.88	120.29	109.70
3	E	450	FAD	N3A-C2A-N1A	-5.87	119.69	128.58
3	A	450	FAD	N3A-C2A-N1A	-5.87	119.70	128.58
2	G	500	GDU	C6-N1-C2	-5.87	113.86	121.00
3	J	450	FAD	N3A-C2A-N1A	-5.87	119.70	128.58
3	H	450	FAD	N3A-C2A-N1A	-5.86	119.71	128.58
2	D	500	GDU	C1D-N1-C2	5.86	128.12	117.59
2	H	500	GDU	O5'-C5'-C4'	5.86	120.25	109.70
3	F	450	FAD	N3A-C2A-N1A	-5.85	119.73	128.58
2	H	500	GDU	O2-C2-N3	-5.83	110.75	121.49
2	H	500	GDU	C6-N1-C2	-5.81	113.92	121.00
2	D	500	GDU	O2-C2-N3	-5.78	110.83	121.49
2	E	500	GDU	C6-N1-C2	-5.77	113.97	121.00
2	J	500	GDU	O2-C2-N3	-5.75	110.88	121.49
2	E	500	GDU	O5'-C5'-C4'	5.73	120.02	109.70
4	G	1385	FDA	C5A-C4A-N3A	-5.73	118.83	126.72
2	J	500	GDU	C6-N1-C2	-5.73	114.03	121.00
2	I	500	GDU	O2-C2-N3	-5.71	110.96	121.49
2	F	500	GDU	C1D-N1-C2	5.69	127.81	117.59
2	B	500	GDU	C1D-N1-C2	5.69	127.81	117.59
4	D	1385	FDA	N3A-C2A-N1A	-5.67	120.00	128.58
2	E	500	GDU	O2-C2-N3	-5.66	111.05	121.49
2	I	500	GDU	C6-N1-C2	-5.65	114.12	121.00
2	B	500	GDU	O2-C2-N3	-5.64	111.10	121.49
2	A	500	GDU	O2-C2-N3	-5.61	111.14	121.49
2	J	500	GDU	O5'-C5'-C4'	5.57	119.74	109.70
2	D	500	GDU	O5'-C5'-C4'	5.53	119.66	109.70
2	B	500	GDU	O5'-C5'-C4'	5.52	119.65	109.70
4	B	1385	FDA	C5A-C4A-N3A	-5.50	119.14	126.72
2	H	500	GDU	C1D-N1-C2	5.50	127.47	117.59
4	G	1385	FDA	C2B-C1B-N9A	5.47	126.89	113.30
4	B	1385	FDA	C2B-C1B-N9A	5.45	126.85	113.30
2	D	500	GDU	O5'-C1'-O3B	-5.25	104.50	111.36
2	J	500	GDU	C1D-N1-C2	5.23	126.99	117.59
2	E	500	GDU	C1D-N1-C2	5.23	126.99	117.59
4	D	1385	FDA	O3B-C3B-C4B	5.23	126.10	111.08
2	I	500	GDU	C1D-N1-C2	5.22	126.97	117.59
4	D	1385	FDA	O4B-C4B-C5B	5.19	125.95	109.33
4	B	1385	FDA	O2B-C2B-C1B	5.16	127.89	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1385	FDA	O3B-C3B-C4B	5.13	125.82	111.08
4	G	1385	FDA	N3A-C2A-N1A	-5.11	120.84	128.58
4	G	1385	FDA	O4B-C4B-C5B	5.05	125.51	109.33
4	D	1385	FDA	C2B-C1B-N9A	5.00	125.73	113.30
4	D	1385	FDA	C5A-C4A-N3A	-4.88	119.99	126.72
4	B	1385	FDA	C4-N3-C2	-4.81	119.74	126.37
4	B	1385	FDA	O4B-C4B-C5B	4.77	124.60	109.33
2	D	500	GDU	O2B-PB-O3A	4.75	120.10	107.27
2	E	500	GDU	O5'-C1'-O3B	-4.68	105.25	111.36
2	G	500	GDU	O5'-C1'-O3B	-4.68	105.25	111.36
4	D	1385	FDA	O2B-C2B-C1B	4.60	125.96	110.10
2	H	500	GDU	O5'-C1'-O3B	-4.60	105.35	111.36
3	C	450	FAD	C5A-C4A-N3A	-4.60	120.39	126.72
3	E	450	FAD	C5A-C4A-N3A	-4.60	120.39	126.72
2	B	500	GDU	O5'-C1'-O3B	-4.59	105.37	111.36
3	H	450	FAD	C5A-C4A-N3A	-4.59	120.40	126.72
3	I	450	FAD	C5A-C4A-N3A	-4.58	120.41	126.72
3	A	450	FAD	C5A-C4A-N3A	-4.58	120.41	126.72
4	D	1385	FDA	C4-N3-C2	-4.57	120.08	126.37
3	J	450	FAD	C5A-C4A-N3A	-4.56	120.44	126.72
2	C	500	GDU	O2B-PB-O3A	4.55	119.57	107.27
3	F	450	FAD	C5A-C4A-N3A	-4.55	120.45	126.72
4	G	1385	FDA	O2B-C2B-C1B	4.47	125.48	110.10
4	B	1385	FDA	N9A-C8A-N7A	-4.44	107.64	113.94
4	D	1385	FDA	O3B-C3B-C2B	4.44	126.04	111.82
2	A	500	GDU	O5'-C1'-O3B	-4.41	105.60	111.36
4	D	1385	FDA	O2B-C2B-C3B	4.41	125.94	111.82
2	J	500	GDU	O5'-C1'-O3B	-4.40	105.61	111.36
2	F	500	GDU	O5'-C1'-O3B	-4.39	105.62	111.36
4	G	1385	FDA	N9A-C8A-N7A	-4.37	107.74	113.94
2	A	500	GDU	C1D-N1-C2	4.35	125.41	117.59
2	G	500	GDU	O2B-PB-O3A	4.29	118.86	107.27
2	F	500	GDU	O2B-PB-O3A	4.25	118.77	107.27
2	J	500	GDU	O2B-PB-O3A	4.21	118.66	107.27
4	D	1385	FDA	N9A-C8A-N7A	-4.20	107.97	113.94
2	B	500	GDU	O2B-PB-O3A	4.15	118.49	107.27
4	G	1385	FDA	O3B-C3B-C2B	4.10	124.95	111.82
2	I	500	GDU	O2B-PB-O3A	4.04	118.18	107.27
4	G	1385	FDA	O2B-C2B-C3B	4.02	124.70	111.82
3	A	450	FAD	N9A-C8A-N7A	-4.02	108.24	113.94
2	E	500	GDU	O2B-PB-O3A	4.01	118.12	107.27
3	J	450	FAD	N9A-C8A-N7A	-4.01	108.24	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	500	GDU	O5'-C1'-O3B	-4.01	106.12	111.36
3	C	450	FAD	N9A-C8A-N7A	-4.00	108.25	113.94
3	I	450	FAD	N9A-C8A-N7A	-4.00	108.26	113.94
3	F	450	FAD	N9A-C8A-N7A	-4.00	108.26	113.94
3	E	450	FAD	N9A-C8A-N7A	-4.00	108.27	113.94
2	H	500	GDU	O2B-PB-O3A	3.99	118.07	107.27
3	H	450	FAD	N9A-C8A-N7A	-3.98	108.28	113.94
4	G	1385	FDA	N3A-C4A-N9A	3.93	133.86	127.17
4	G	1385	FDA	N3-C2-N1	3.92	121.91	115.74
3	F	450	FAD	C4-N3-C2	-3.84	118.82	125.64
3	I	450	FAD	C4-N3-C2	-3.84	118.83	125.64
3	J	450	FAD	C4-N3-C2	-3.83	118.84	125.64
3	A	450	FAD	C4-N3-C2	-3.83	118.84	125.64
3	H	450	FAD	C4-N3-C2	-3.82	118.85	125.64
3	E	450	FAD	C4-N3-C2	-3.82	118.85	125.64
3	C	450	FAD	C4-N3-C2	-3.82	118.86	125.64
4	G	1385	FDA	O3B-C3B-C4B	3.80	121.99	111.08
4	B	1385	FDA	O4-C4-C4X	-3.77	118.17	127.26
2	A	500	GDU	O2B-PB-O3A	3.76	117.44	107.27
4	B	1385	FDA	C3B-C2B-C1B	3.76	108.57	101.46
4	B	1385	FDA	C2A-N3A-C4A	3.75	121.00	111.83
3	E	450	FAD	C2A-N3A-C4A	3.67	120.81	111.83
3	C	450	FAD	C2A-N3A-C4A	3.67	120.79	111.83
3	I	450	FAD	C2A-N3A-C4A	3.67	120.78	111.83
3	A	450	FAD	C2A-N3A-C4A	3.66	120.78	111.83
3	H	450	FAD	C2A-N3A-C4A	3.66	120.76	111.83
3	J	450	FAD	C2A-N3A-C4A	3.65	120.75	111.83
3	F	450	FAD	C2A-N3A-C4A	3.64	120.72	111.83
4	G	1385	FDA	C4X-C4-N3	3.60	122.01	112.13
4	B	1385	FDA	C4X-C4-N3	3.59	121.99	112.13
2	D	500	GDU	O4-C4-C5	-3.57	119.00	125.16
4	B	1385	FDA	O2B-C2B-C3B	3.57	123.26	111.82
2	E	500	GDU	O4-C4-C5	-3.56	119.02	125.16
2	G	500	GDU	O4D-C4D-C5D	3.56	120.74	109.33
3	H	450	FAD	C5A-N7A-C8A	3.53	109.00	103.45
3	F	450	FAD	C5A-N7A-C8A	3.52	108.99	103.45
3	J	450	FAD	C5A-N7A-C8A	3.52	108.97	103.45
3	A	450	FAD	C5A-N7A-C8A	3.51	108.97	103.45
3	E	450	FAD	C5A-N7A-C8A	3.51	108.96	103.45
3	C	450	FAD	C5A-N7A-C8A	3.50	108.95	103.45
2	G	500	GDU	O4-C4-C5	-3.50	119.12	125.16
2	E	500	GDU	O3B-C1'-C2'	3.49	114.78	108.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1385	FDA	C2A-N3A-C4A	3.49	120.34	111.83
3	I	450	FAD	C5A-N7A-C8A	3.48	108.92	103.45
2	B	500	GDU	O4-C4-C5	-3.48	119.15	125.16
4	G	1385	FDA	O4-C4-C4X	-3.48	118.88	127.26
2	I	500	GDU	O3B-C1'-C2'	3.44	114.69	108.38
2	I	500	GDU	O4-C4-C5	-3.43	119.24	125.16
2	D	500	GDU	PB-O3B-C1'	3.43	135.18	121.21
2	H	500	GDU	O4-C4-C5	-3.42	119.27	125.16
2	C	500	GDU	O4-C4-C5	-3.38	119.33	125.16
4	D	1385	FDA	C2A-N3A-C4A	3.35	120.02	111.83
2	J	500	GDU	O4-C4-C5	-3.35	119.38	125.16
4	B	1385	FDA	C5A-N7A-C8A	3.31	108.65	103.45
2	F	500	GDU	C2D-C1D-N1	3.30	122.44	113.25
2	C	500	GDU	O4D-C4D-C5D	3.29	119.86	109.33
2	B	500	GDU	O3A-PB-O1B	-3.28	100.82	110.70
4	D	1385	FDA	C3B-C2B-C1B	3.28	107.67	101.46
2	F	500	GDU	O4-C4-C5	-3.26	119.54	125.16
4	B	1385	FDA	O3B-C3B-C2B	3.23	122.16	111.82
2	D	500	GDU	O4D-C4D-C5D	3.17	119.50	109.33
4	B	1385	FDA	C4A-C5A-N7A	-3.17	106.96	110.58
4	D	1385	FDA	O4-C4-C4X	-3.16	119.65	127.26
3	C	450	FAD	O4-C4-C4X	-3.15	118.22	126.53
3	J	450	FAD	O4-C4-C4X	-3.14	118.24	126.53
3	I	450	FAD	O4-C4-C4X	-3.14	118.25	126.53
3	A	450	FAD	O4-C4-C4X	-3.13	118.26	126.53
3	F	450	FAD	O4-C4-C4X	-3.13	118.27	126.53
3	E	450	FAD	O4-C4-C4X	-3.12	118.28	126.53
3	H	450	FAD	O4-C4-C4X	-3.12	118.29	126.53
2	F	500	GDU	O3B-C1'-C2'	3.12	114.09	108.38
2	E	500	GDU	PB-O3B-C1'	3.12	133.91	121.21
4	D	1385	FDA	C4X-C4-N3	3.11	120.68	112.13
2	E	500	GDU	O3A-PB-O1B	-3.10	101.37	110.70
2	F	500	GDU	O3A-PB-O1B	-3.10	101.37	110.70
2	D	500	GDU	O2A-PA-O3A	3.10	115.65	107.27
2	A	500	GDU	O4-C4-C5	-3.09	119.83	125.16
4	D	1385	FDA	O5'-C5'-C4'	3.08	117.60	109.36
4	G	1385	FDA	O3'-C3'-C2'	3.08	115.94	108.93
2	E	500	GDU	O4D-C4D-C5D	3.08	119.20	109.33
2	D	500	GDU	O3B-C1'-C2'	3.08	114.02	108.38
2	G	500	GDU	O3B-C1'-C2'	3.08	114.02	108.38
2	B	500	GDU	O4D-C4D-C5D	3.08	119.19	109.33
4	G	1385	FDA	C5A-N7A-C8A	3.07	108.27	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	GDU	O3A-PB-O1B	-3.04	101.57	110.70
2	C	500	GDU	O2A-PA-O3A	3.02	115.43	107.27
2	I	500	GDU	O3A-PB-O1B	-3.01	101.64	110.70
2	I	500	GDU	O4D-C4D-C5D	3.01	118.98	109.33
2	J	500	GDU	O4D-C4D-C5D	2.99	118.93	109.33
2	G	500	GDU	O2A-PA-O3A	2.99	115.34	107.27
4	B	1385	FDA	N3A-C4A-N9A	2.98	132.24	127.17
2	F	500	GDU	O4D-C4D-C5D	2.97	118.84	109.33
2	H	500	GDU	O2A-PA-O3A	2.97	115.29	107.27
2	A	500	GDU	PB-O3B-C1'	2.96	133.26	121.21
4	D	1385	FDA	C5B-C4B-C3B	2.95	125.83	115.21
2	J	500	GDU	O3A-PB-O1B	-2.95	101.84	110.70
4	D	1385	FDA	C5A-N7A-C8A	2.94	108.07	103.45
3	H	450	FAD	C4X-C4-N3	2.93	120.71	113.25
4	B	1385	FDA	C5B-C4B-C3B	2.93	125.76	115.21
4	G	1385	FDA	C6A-C5A-C4A	2.93	121.17	117.18
3	C	450	FAD	C4X-C4-N3	2.93	120.70	113.25
2	H	500	GDU	O4D-C4D-C5D	2.92	118.70	109.33
3	F	450	FAD	C4X-C4-N3	2.92	120.69	113.25
3	E	450	FAD	C4X-C4-N3	2.92	120.69	113.25
3	I	450	FAD	C4X-C4-N3	2.92	120.69	113.25
3	J	450	FAD	C4X-C4-N3	2.91	120.67	113.25
3	A	450	FAD	C4X-C4-N3	2.91	120.67	113.25
2	C	500	GDU	PB-O3B-C1'	2.91	133.06	121.21
3	E	450	FAD	N3A-C4A-N9A	2.90	132.10	127.17
3	I	450	FAD	N3A-C4A-N9A	2.89	132.08	127.17
3	C	450	FAD	N3A-C4A-N9A	2.88	132.07	127.17
3	J	450	FAD	N3A-C4A-N9A	2.88	132.06	127.17
3	A	450	FAD	N3A-C4A-N9A	2.88	132.06	127.17
2	E	500	GDU	C2D-C1D-N1	2.88	121.25	113.25
4	D	1385	FDA	N3A-C4A-N9A	2.87	132.06	127.17
4	B	1385	FDA	O5B-C5B-C4B	2.87	118.77	108.99
2	I	500	GDU	PB-O3B-C1'	2.86	132.87	121.21
3	H	450	FAD	N3A-C4A-N9A	2.86	132.03	127.17
3	F	450	FAD	N3A-C4A-N9A	2.85	132.02	127.17
2	I	500	GDU	O2A-PA-O3A	2.84	114.94	107.27
2	B	500	GDU	O2A-PA-O3A	2.82	114.88	107.27
2	A	500	GDU	C2D-C1D-N1	2.80	121.03	113.25
3	H	450	FAD	C4A-C5A-N7A	-2.79	107.39	110.58
2	C	500	GDU	O3A-PB-O1B	-2.78	102.33	110.70
2	E	500	GDU	O2A-PA-O3A	2.77	114.77	107.27
4	G	1385	FDA	C5B-C4B-C3B	2.77	125.19	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	500	GDU	O2A-PA-O3A	2.75	114.69	107.27
3	C	450	FAD	C4A-C5A-N7A	-2.74	107.45	110.58
3	F	450	FAD	C4A-C5A-N7A	-2.73	107.45	110.58
3	E	450	FAD	C4A-C5A-N7A	-2.73	107.46	110.58
3	A	450	FAD	C4A-C5A-N7A	-2.73	107.46	110.58
3	I	450	FAD	C4A-C5A-N7A	-2.73	107.47	110.58
2	C	500	GDU	C2D-C1D-N1	2.72	120.83	113.25
4	B	1385	FDA	N3-C2-N1	2.71	120.00	115.74
2	G	500	GDU	PB-O3B-C1'	2.71	132.26	121.21
3	J	450	FAD	C4A-C5A-N7A	-2.71	107.48	110.58
4	G	1385	FDA	C5X-C9A-N10	2.70	121.07	118.01
2	I	500	GDU	C5-C4-N3	2.69	118.57	114.80
2	J	500	GDU	C5-C4-N3	2.69	118.57	114.80
4	G	1385	FDA	O3'-C3'-C4'	2.69	115.04	108.93
4	G	1385	FDA	C3B-C2B-C1B	2.69	106.55	101.46
2	B	500	GDU	C4'-C3'-C2'	-2.68	106.12	110.83
2	A	500	GDU	O2A-PA-O3A	2.67	114.50	107.27
4	B	1385	FDA	O4'-C4'-C3'	2.67	115.50	109.25
2	B	500	GDU	C2D-C1D-N1	2.67	120.67	113.25
2	E	500	GDU	C5-C4-N3	2.66	118.52	114.80
2	J	500	GDU	C2D-C1D-N1	2.65	120.63	113.25
2	G	500	GDU	O3A-PB-O1B	-2.65	102.73	110.70
2	A	500	GDU	O3A-PB-O1B	-2.64	102.75	110.70
2	D	500	GDU	C5-C4-N3	2.64	118.49	114.80
2	G	500	GDU	C5-C4-N3	2.64	118.49	114.80
4	G	1385	FDA	C4A-N9A-C8A	2.62	108.49	105.74
2	F	500	GDU	C5-C4-N3	2.62	118.46	114.80
2	H	500	GDU	PB-O3B-C1'	2.61	131.86	121.21
2	F	500	GDU	O2A-PA-O3A	2.59	114.28	107.27
4	G	1385	FDA	C2B-C3B-C4B	2.59	107.61	102.61
4	D	1385	FDA	C2B-C3B-C4B	2.58	107.60	102.61
2	H	500	GDU	C5-C4-N3	2.58	118.41	114.80
4	B	1385	FDA	C5A-C4A-N9A	2.57	108.61	105.81
2	A	500	GDU	O4D-C1D-C2D	-2.57	101.12	106.62
2	B	500	GDU	PB-O3B-C1'	2.57	131.66	121.21
2	H	500	GDU	O3A-PB-O1B	-2.56	103.01	110.70
2	F	500	GDU	PB-O3B-C1'	2.55	131.59	121.21
2	H	500	GDU	O3B-C1'-C2'	2.54	113.04	108.38
4	D	1385	FDA	O5B-C5B-C4B	2.54	117.65	108.99
4	D	1385	FDA	N3-C2-N1	2.54	119.73	115.74
3	E	450	FAD	C4X-C10-N10	2.53	120.11	116.48
2	H	500	GDU	C2D-C1D-N1	2.52	120.27	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	450	FAD	C4X-C10-N10	2.51	120.08	116.48
3	C	450	FAD	C4X-C10-N10	2.51	120.08	116.48
4	G	1385	FDA	C9-C9A-N10	-2.50	118.49	121.85
3	A	450	FAD	C4X-C10-N10	2.50	120.06	116.48
2	A	500	GDU	C4'-C3'-C2'	-2.48	106.47	110.83
3	J	450	FAD	C4X-C10-N10	2.48	120.03	116.48
2	A	500	GDU	O4D-C4D-C5D	2.48	117.28	109.33
2	B	500	GDU	O4-C4-N3	2.48	122.87	119.27
3	F	450	FAD	C4X-C10-N10	2.48	120.03	116.48
2	J	500	GDU	PB-O3B-C1'	2.48	131.30	121.21
3	H	450	FAD	C4X-C10-N10	2.46	120.00	116.48
2	B	500	GDU	O3B-C1'-C2'	2.45	112.87	108.38
2	C	500	GDU	C5-C4-N3	2.44	118.22	114.80
4	G	1385	FDA	O5B-C5B-C4B	2.44	117.29	108.99
2	C	500	GDU	O3B-C1'-C2'	2.36	112.71	108.38
4	G	1385	FDA	O5'-C5'-C4'	2.33	115.59	109.36
3	I	450	FAD	C4X-C10-N1	-2.30	118.94	124.59
2	B	500	GDU	C1'-C2'-C3'	-2.30	105.17	110.01
4	D	1385	FDA	C4A-C5A-N7A	-2.29	107.96	110.58
3	E	450	FAD	C4X-C10-N1	-2.29	118.99	124.59
3	A	450	FAD	C4X-C10-N1	-2.28	119.00	124.59
3	C	450	FAD	C4X-C10-N1	-2.28	119.00	124.59
3	J	450	FAD	C4X-C10-N1	-2.28	119.00	124.59
2	A	500	GDU	C5-C4-N3	2.28	117.99	114.80
4	B	1385	FDA	O3'-C3'-C2'	2.28	114.10	108.93
3	F	450	FAD	C4X-C10-N1	-2.27	119.02	124.59
2	B	500	GDU	C5-C4-N3	2.26	117.97	114.80
3	H	450	FAD	C4X-C10-N1	-2.26	119.05	124.59
4	B	1385	FDA	C4A-N9A-C8A	2.26	108.11	105.74
2	G	500	GDU	C2D-C1D-N1	2.23	119.45	113.25
2	D	500	GDU	O4-C4-N3	2.23	122.50	119.27
2	E	500	GDU	O4-C4-N3	2.20	122.47	119.27
4	D	1385	FDA	C4A-N9A-C8A	2.19	108.04	105.74
2	C	500	GDU	O4-C4-N3	2.19	122.45	119.27
2	E	500	GDU	O4D-C1D-C2D	-2.18	101.96	106.62
2	G	500	GDU	O4-C4-N3	2.14	122.38	119.27
2	A	500	GDU	O3B-C1'-C2'	2.13	112.28	108.38
4	D	1385	FDA	O3'-C3'-C4'	2.12	113.74	108.93
4	B	1385	FDA	C5X-N5-C4X	-2.11	116.21	121.08
4	D	1385	FDA	O3'-C3'-C2'	2.10	113.71	108.93
4	G	1385	FDA	O2-C2-N3	-2.10	118.13	121.86
2	A	500	GDU	O4D-C1D-N1	2.10	113.11	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	500	GDU	O4-C4-N3	2.10	122.32	119.27
4	G	1385	FDA	C4A-C5A-N7A	-2.09	108.19	110.58
4	G	1385	FDA	C5'-C4'-C3'	2.09	116.16	112.22
2	C	500	GDU	C3D-C2D-C1D	2.04	105.33	101.46
4	D	1385	FDA	C6A-C5A-C4A	2.04	119.97	117.18
4	B	1385	FDA	C9A-C5X-N5	2.03	121.85	119.37
4	B	1385	FDA	C5X-C9A-N10	2.03	120.31	118.01
4	D	1385	FDA	O2'-C2'-C3'	2.03	114.00	109.25
3	E	450	FAD	C10-C4X-N5	-2.01	120.69	124.81
4	B	1385	FDA	O3P-PA-O1A	-2.01	104.64	110.70
2	I	500	GDU	O4-C4-N3	2.01	122.19	119.27
4	B	1385	FDA	C6A-C5A-C4A	2.01	119.92	117.18
3	C	450	FAD	C10-C4X-N5	-2.01	120.71	124.81
2	A	500	GDU	O4-C4-N3	2.01	122.18	119.27

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1385	FDA	C1B
4	B	1385	FDA	C2B
4	D	1385	FDA	C3B
4	D	1385	FDA	C2B
4	D	1385	FDA	C4B
4	D	1385	FDA	C1B
4	G	1385	FDA	C3B
4	G	1385	FDA	C1B

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	GDU	O5'-C1'-O3B-PB
2	B	500	GDU	C1'-O3B-PB-O3A
2	B	500	GDU	C1'-O3B-PB-O2B
2	B	500	GDU	O5'-C1'-O3B-PB
2	C	500	GDU	O4D-C4D-C5D-O5D
2	C	500	GDU	C5D-O5D-PA-O1A
2	C	500	GDU	C5D-O5D-PA-O2A
2	C	500	GDU	O5'-C1'-O3B-PB
2	D	500	GDU	C1'-O3B-PB-O3A
2	D	500	GDU	C1'-O3B-PB-O2B
2	D	500	GDU	C2'-C1'-O3B-PB
2	D	500	GDU	O5'-C1'-O3B-PB

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Mol	Chain	Res	Type	Atoms
2	E	500	GDU	PA-O3A-PB-O3B
2	E	500	GDU	C1'-O3B-PB-O3A
2	E	500	GDU	C1'-O3B-PB-O2B
2	E	500	GDU	O5'-C1'-O3B-PB
2	F	500	GDU	PA-O3A-PB-O3B
2	F	500	GDU	C1'-O3B-PB-O3A
2	F	500	GDU	C1'-O3B-PB-O2B
2	F	500	GDU	O5'-C1'-O3B-PB
2	G	500	GDU	C5D-O5D-PA-O2A
2	G	500	GDU	C1'-O3B-PB-O3A
2	G	500	GDU	C1'-O3B-PB-O2B
2	G	500	GDU	O5'-C1'-O3B-PB
2	H	500	GDU	C1'-O3B-PB-O3A
2	H	500	GDU	C1'-O3B-PB-O2B
2	H	500	GDU	O5'-C1'-O3B-PB
2	I	500	GDU	C1'-O3B-PB-O3A
2	I	500	GDU	C1'-O3B-PB-O2B
2	I	500	GDU	O5'-C1'-O3B-PB
2	J	500	GDU	PA-O3A-PB-O3B
2	J	500	GDU	C1'-O3B-PB-O3A
2	J	500	GDU	C1'-O3B-PB-O2B
2	J	500	GDU	O5'-C1'-O3B-PB
4	G	1385	FDA	C5B-O5B-PA-O1A
4	G	1385	FDA	C5B-O5B-PA-O2A
4	G	1385	FDA	C5B-O5B-PA-O3P
4	G	1385	FDA	O4B-C4B-C5B-O5B
2	B	500	GDU	O5'-C5'-C6'-O6'
2	A	500	GDU	O5'-C5'-C6'-O6'
2	F	500	GDU	O5'-C5'-C6'-O6'
2	I	500	GDU	O5'-C5'-C6'-O6'
2	H	500	GDU	O5'-C5'-C6'-O6'
2	I	500	GDU	C4'-C5'-C6'-O6'
2	C	500	GDU	C3D-C4D-C5D-O5D
4	D	1385	FDA	O4B-C4B-C5B-O5B
4	D	1385	FDA	O3'-C3'-C4'-C5'
2	D	500	GDU	O5'-C5'-C6'-O6'
2	G	500	GDU	O5'-C5'-C6'-O6'
2	J	500	GDU	O5'-C5'-C6'-O6'
2	C	500	GDU	C4'-C5'-C6'-O6'
2	C	500	GDU	O5'-C5'-C6'-O6'
2	E	500	GDU	O5'-C5'-C6'-O6'
4	B	1385	FDA	O4B-C4B-C5B-O5B

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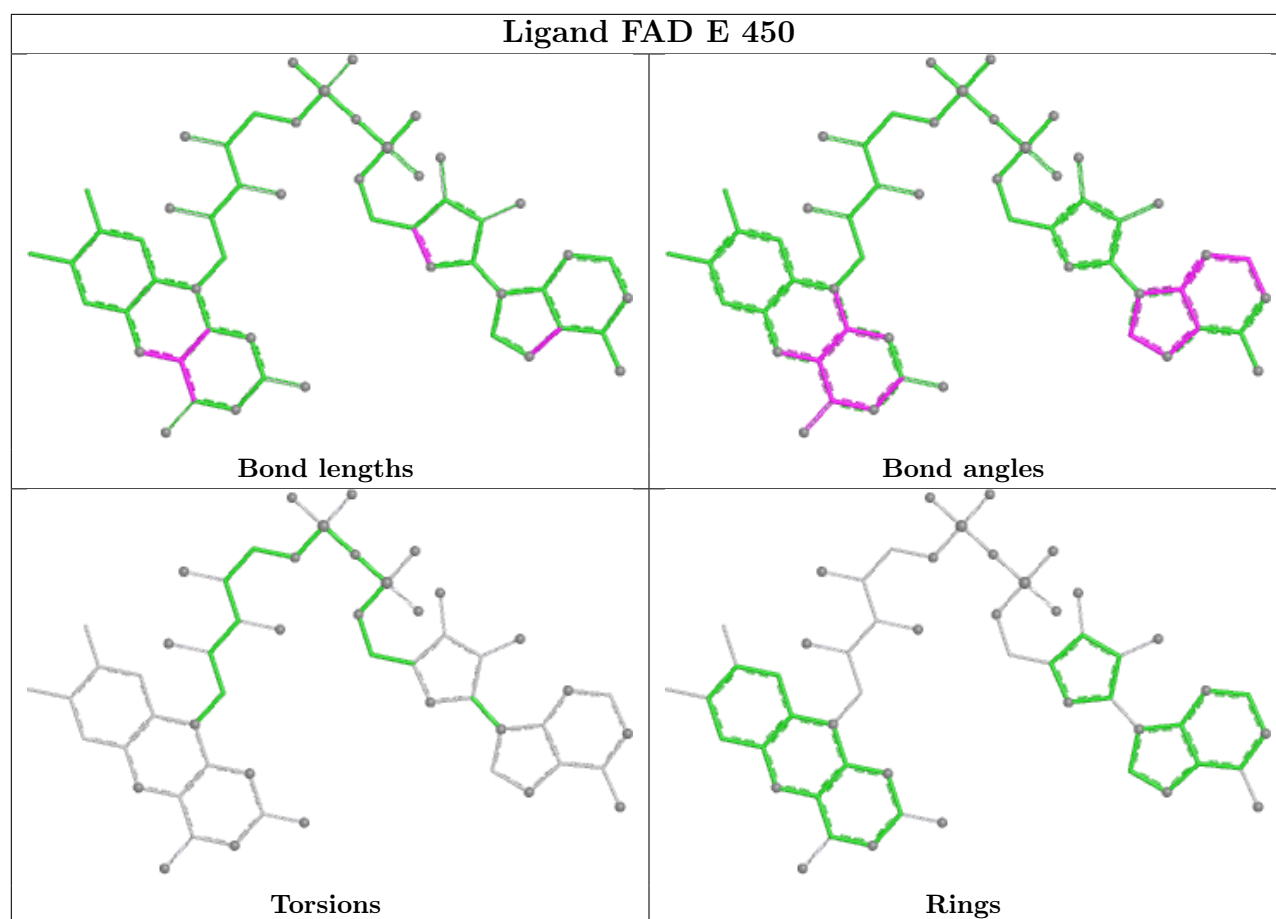
Mol	Chain	Res	Type	Atoms
2	F	500	GDU	C4'-C5'-C6'-O6'
2	B	500	GDU	PA-O3A-PB-O1B
4	G	1385	FDA	C3B-C4B-C5B-O5B
2	A	500	GDU	PA-O3A-PB-O3B
2	C	500	GDU	PA-O3A-PB-O3B
2	G	500	GDU	PA-O3A-PB-O3B
2	H	500	GDU	PA-O3A-PB-O3B
2	I	500	GDU	PA-O3A-PB-O3B
4	D	1385	FDA	O2'-C2'-C3'-C4'
2	B	500	GDU	C4'-C5'-C6'-O6'
2	A	500	GDU	PA-O3A-PB-O1B
2	C	500	GDU	C5D-O5D-PA-O3A
2	D	500	GDU	C5D-O5D-PA-O1A
2	D	500	GDU	C5D-O5D-PA-O3A
2	G	500	GDU	C5D-O5D-PA-O1A
2	G	500	GDU	C5D-O5D-PA-O3A
2	C	500	GDU	PA-O3A-PB-O1B
2	D	500	GDU	PA-O3A-PB-O1B
4	D	1385	FDA	C4'-C5'-O5'-P
2	D	500	GDU	PB-O3A-PA-O2A
2	H	500	GDU	PA-O3A-PB-O1B
2	B	500	GDU	PA-O3A-PB-O3B
2	C	500	GDU	C4D-C5D-O5D-PA
4	D	1385	FDA	O4'-C4'-C5'-O5'
2	C	500	GDU	C1'-O3B-PB-O1B
2	H	500	GDU	C2'-C1'-O3B-PB
2	F	500	GDU	PA-O3A-PB-O1B
2	F	500	GDU	PA-O3A-PB-O2B
2	I	500	GDU	PA-O3A-PB-O1B
2	J	500	GDU	PA-O3A-PB-O2B
4	B	1385	FDA	O4B-C1B-N9A-C8A
2	B	500	GDU	C2'-C1'-O3B-PB
2	D	500	GDU	PB-O3A-PA-O1A
2	E	500	GDU	PA-O3A-PB-O2B
2	I	500	GDU	PA-O3A-PB-O2B
2	J	500	GDU	PA-O3A-PB-O1B
2	G	500	GDU	C3D-C4D-C5D-O5D

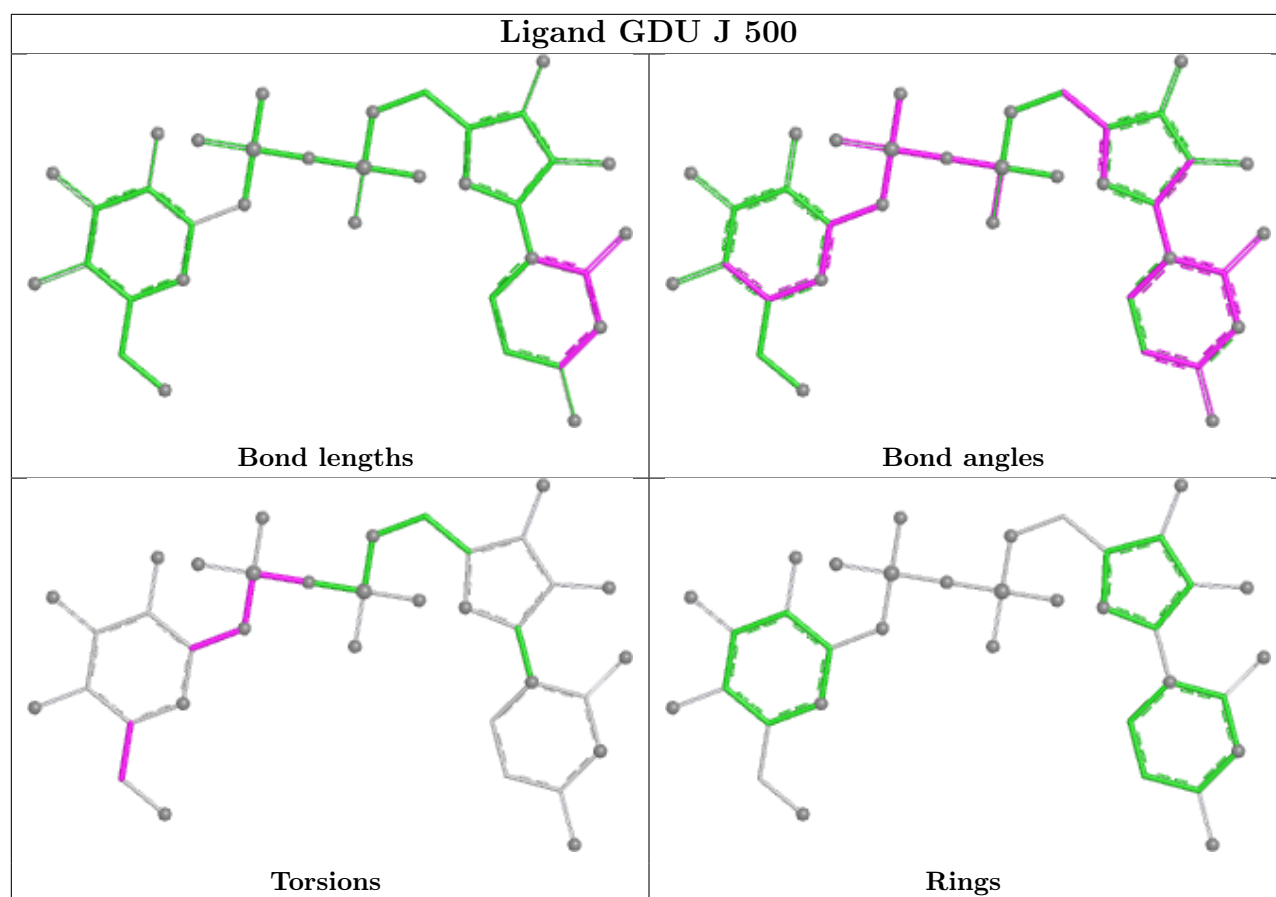
There are no ring outliers.

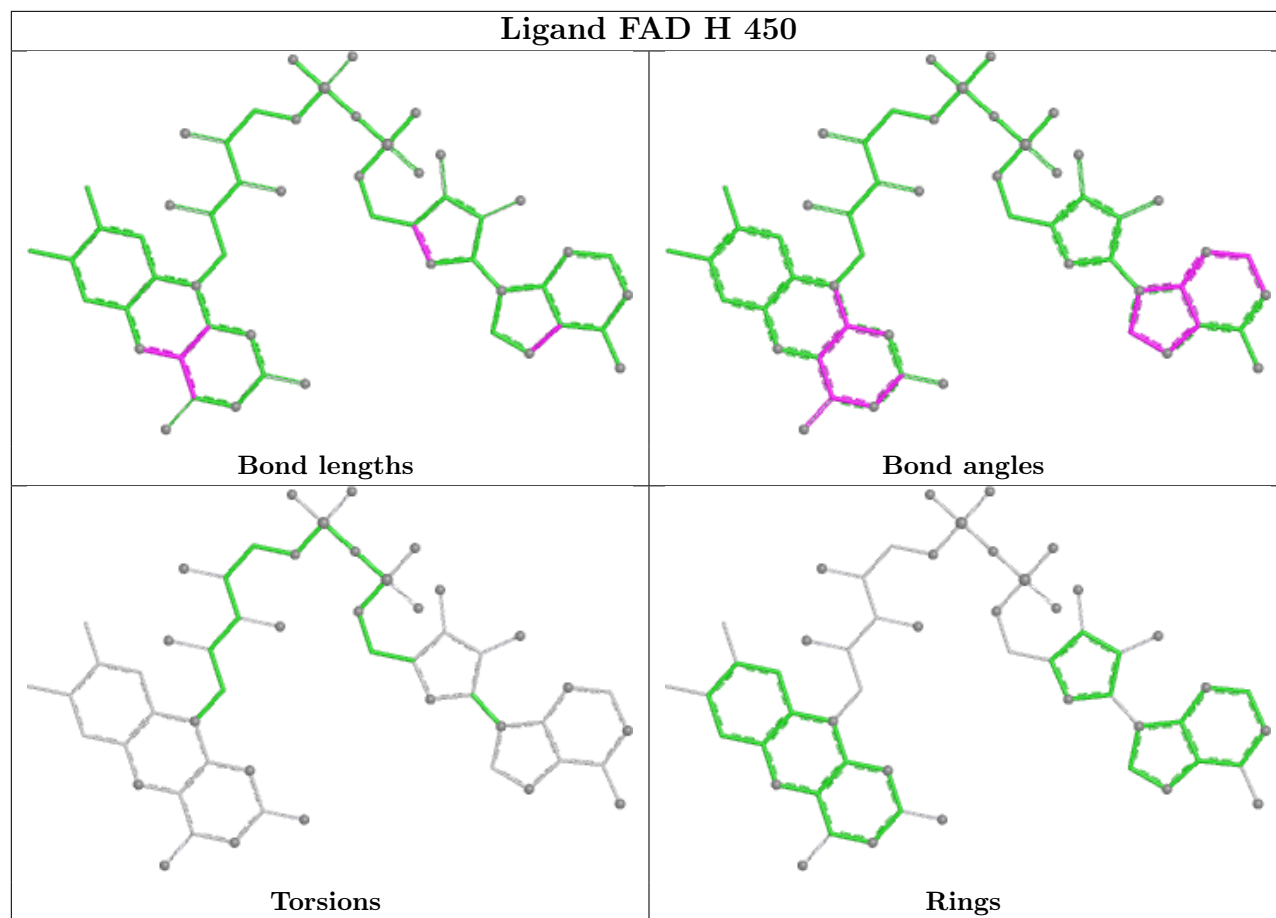
19 monomers are involved in 53 short contacts:

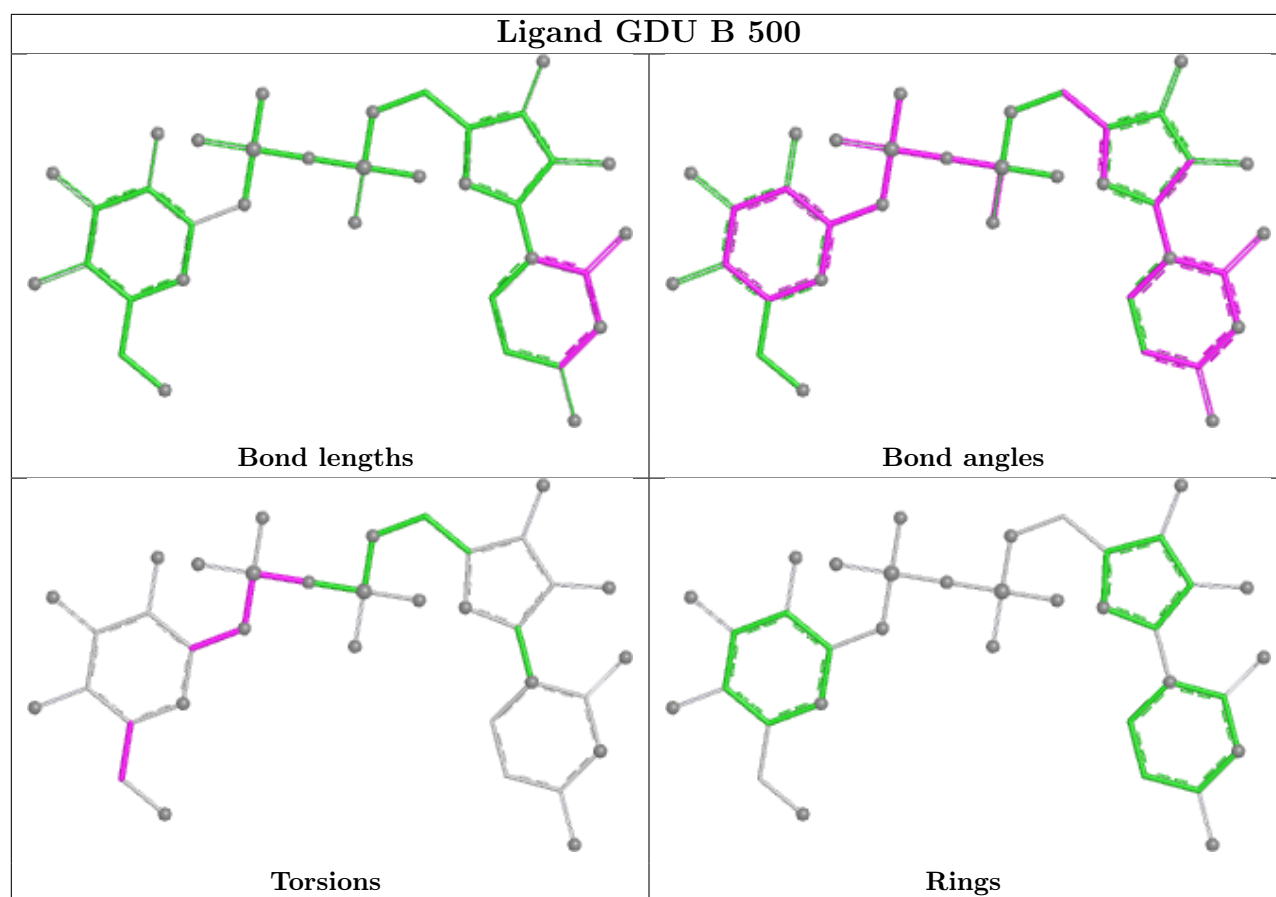
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	450	FAD	2	0
3	H	450	FAD	2	0
2	B	500	GDU	4	0
3	F	450	FAD	4	0
2	H	500	GDU	1	0
2	C	500	GDU	6	0
3	C	450	FAD	6	0
4	B	1385	FDA	2	0
2	F	500	GDU	3	0
2	G	500	GDU	2	0
3	J	450	FAD	3	0
4	G	1385	FDA	6	0
2	E	500	GDU	2	0
3	A	450	FAD	3	0
2	D	500	GDU	6	0
2	I	500	GDU	1	0
4	D	1385	FDA	5	0
2	A	500	GDU	4	0
3	I	450	FAD	3	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.

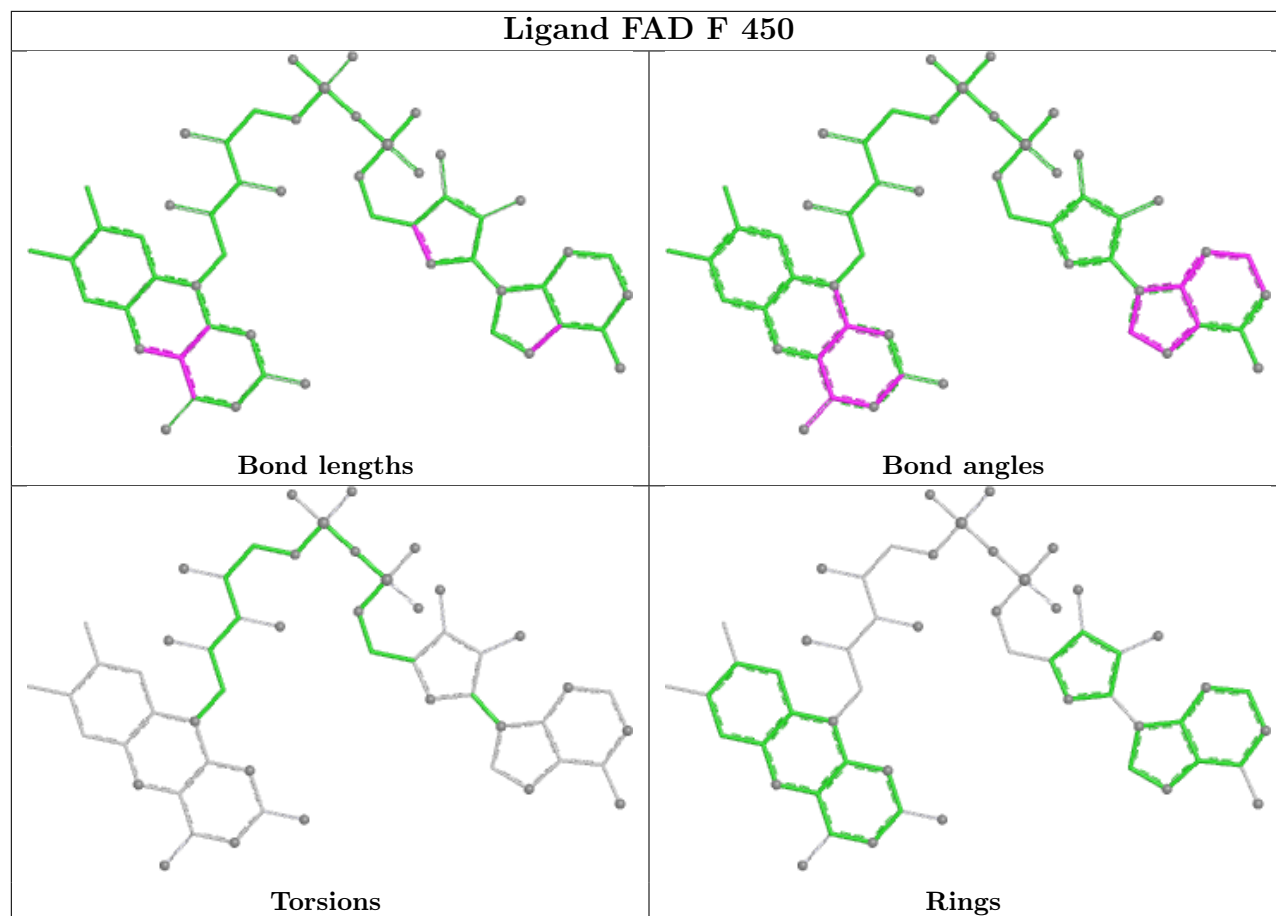


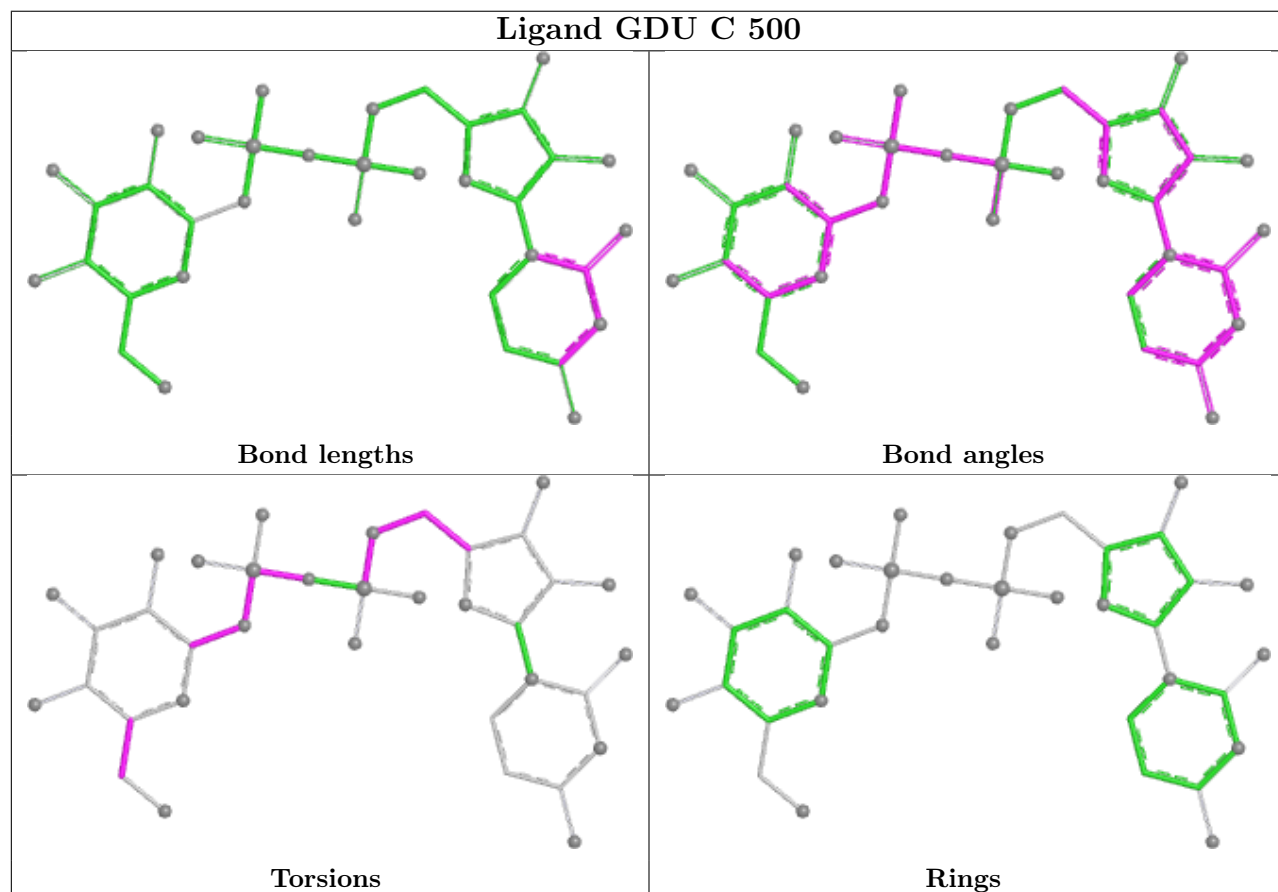
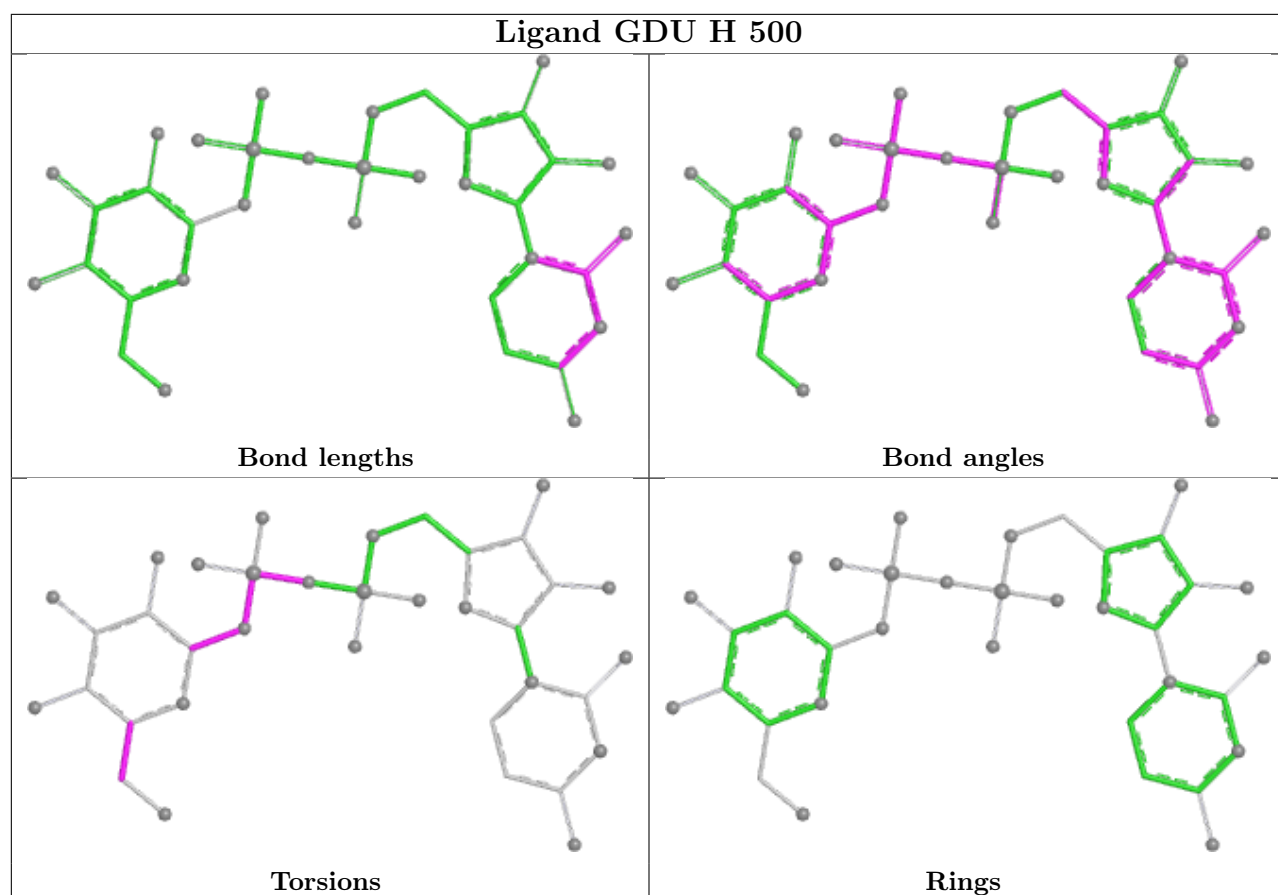


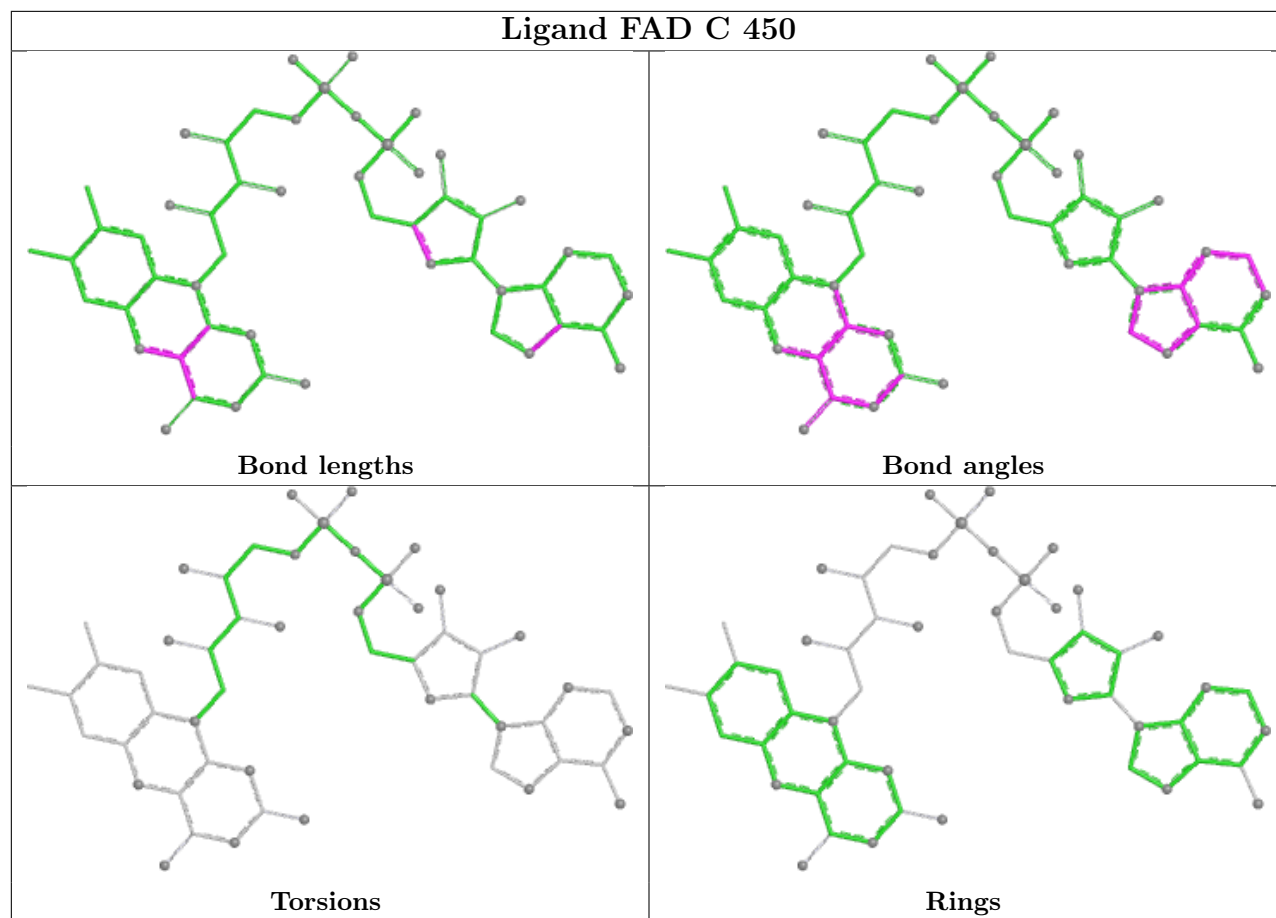


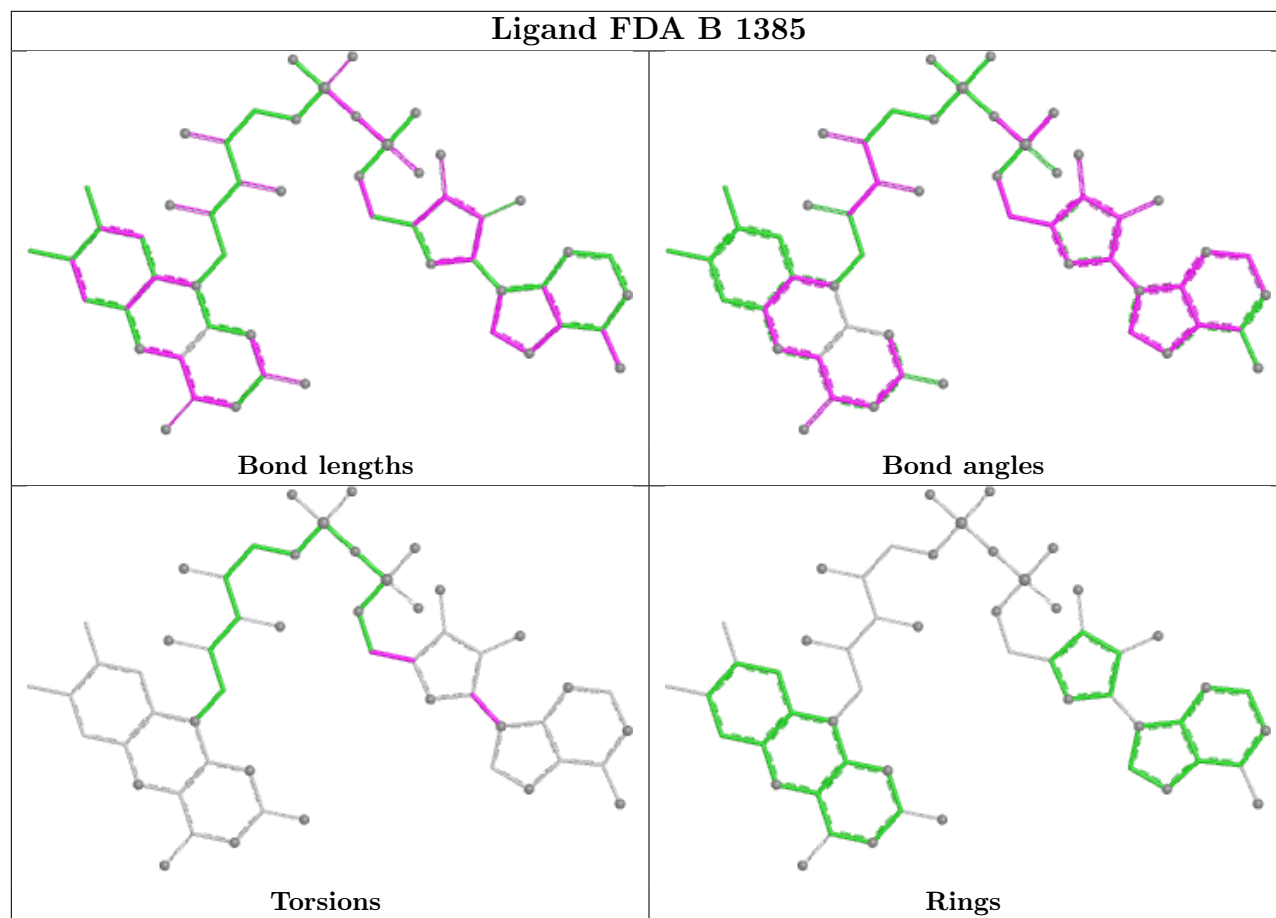


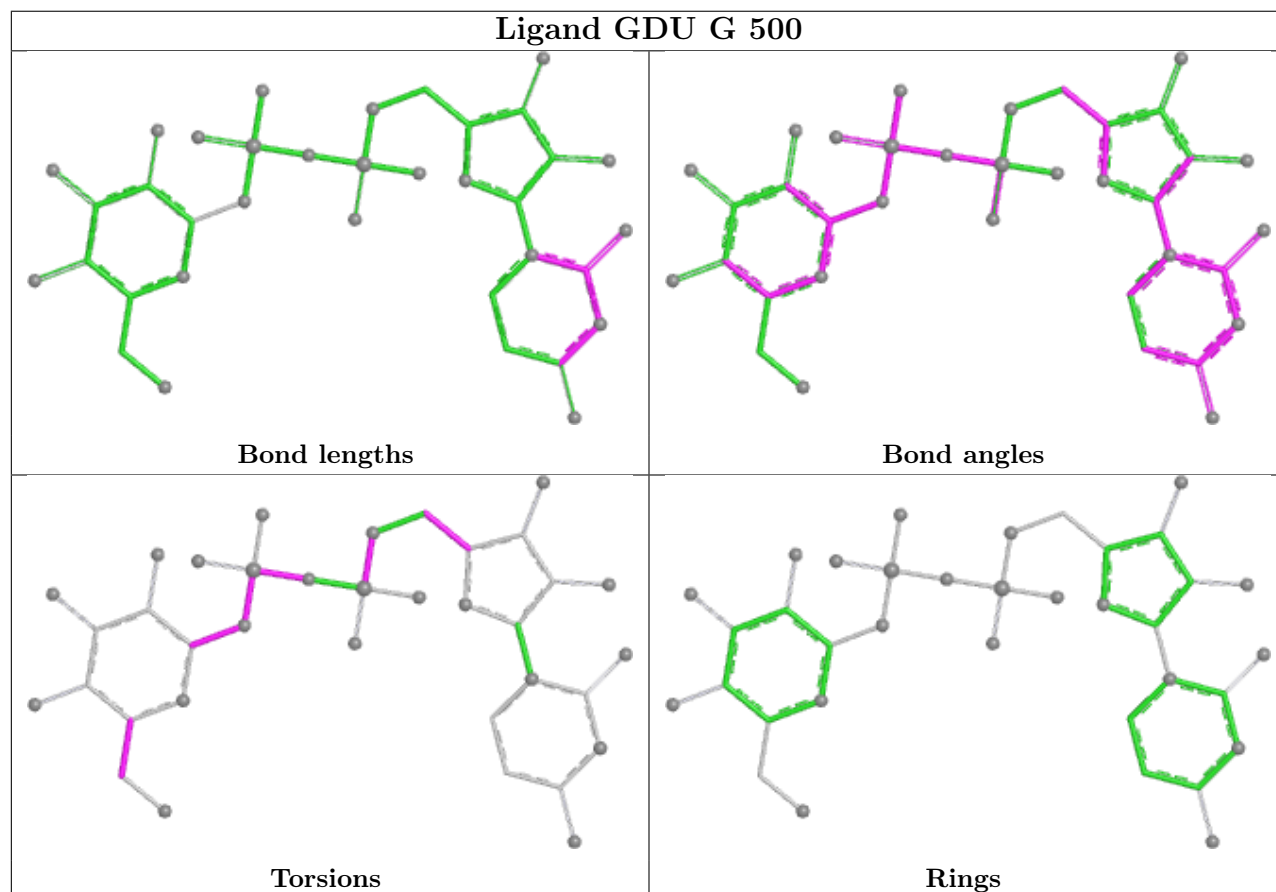
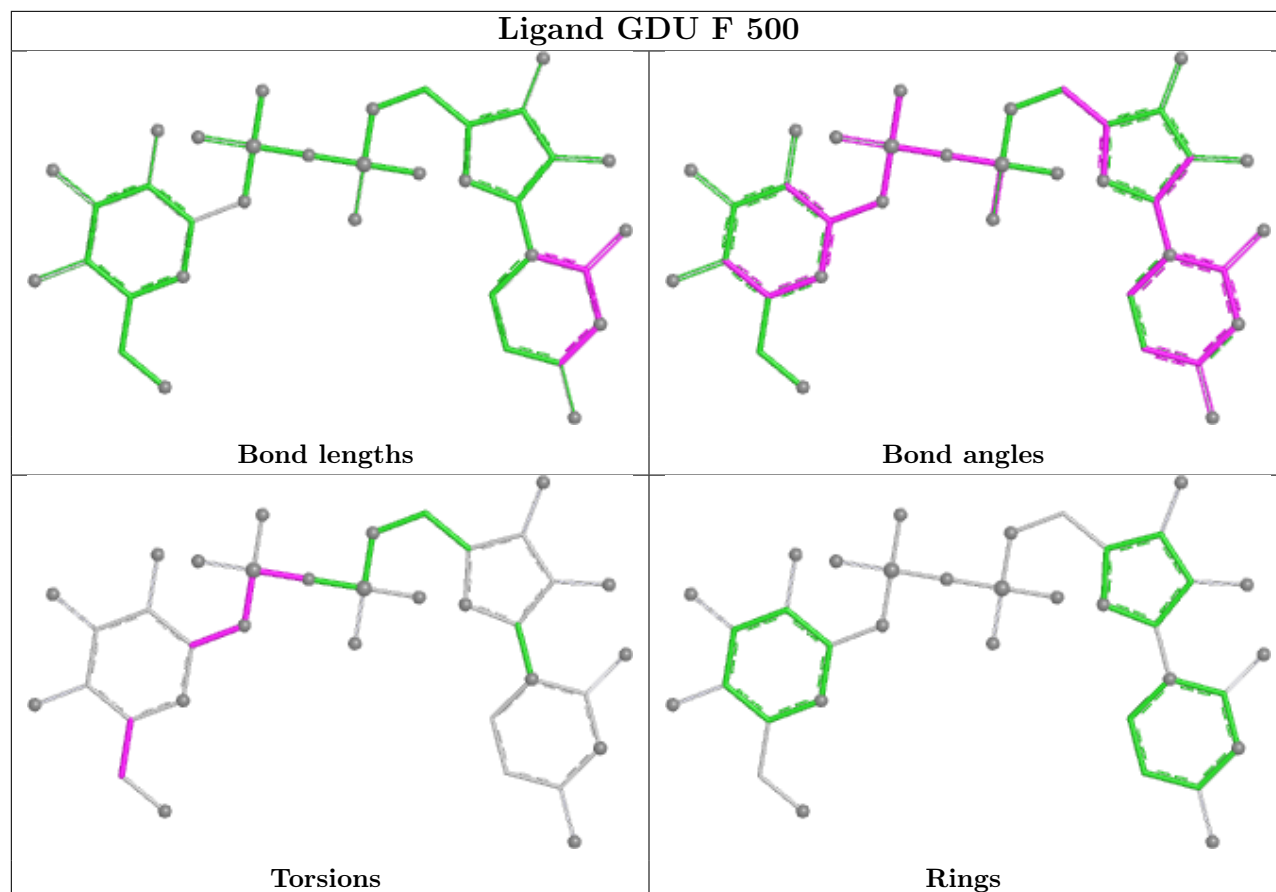
Ligand FAD F 450



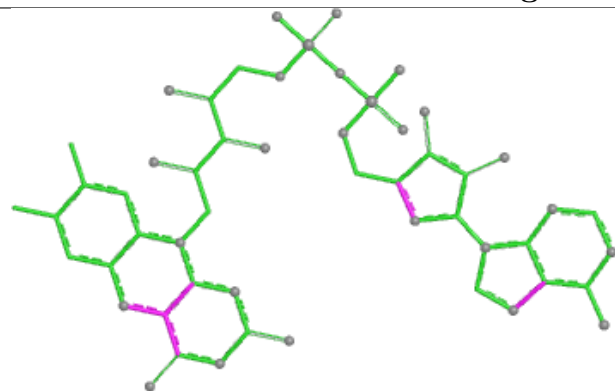




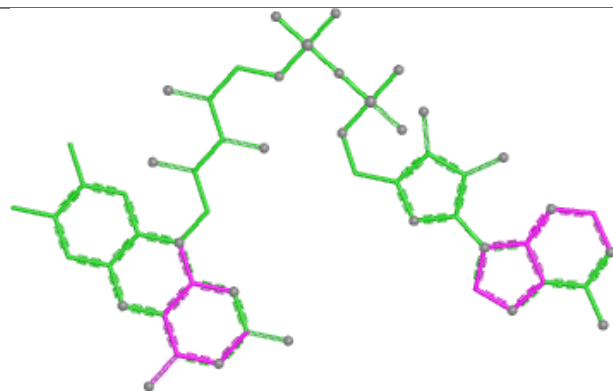




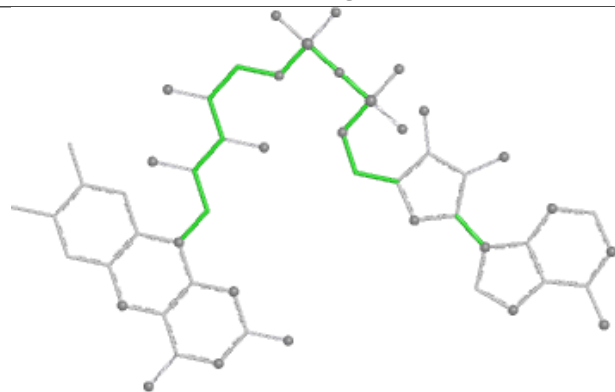
Ligand FAD J 450



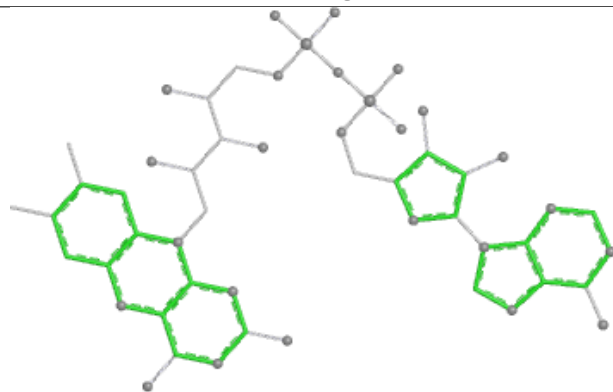
Bond lengths



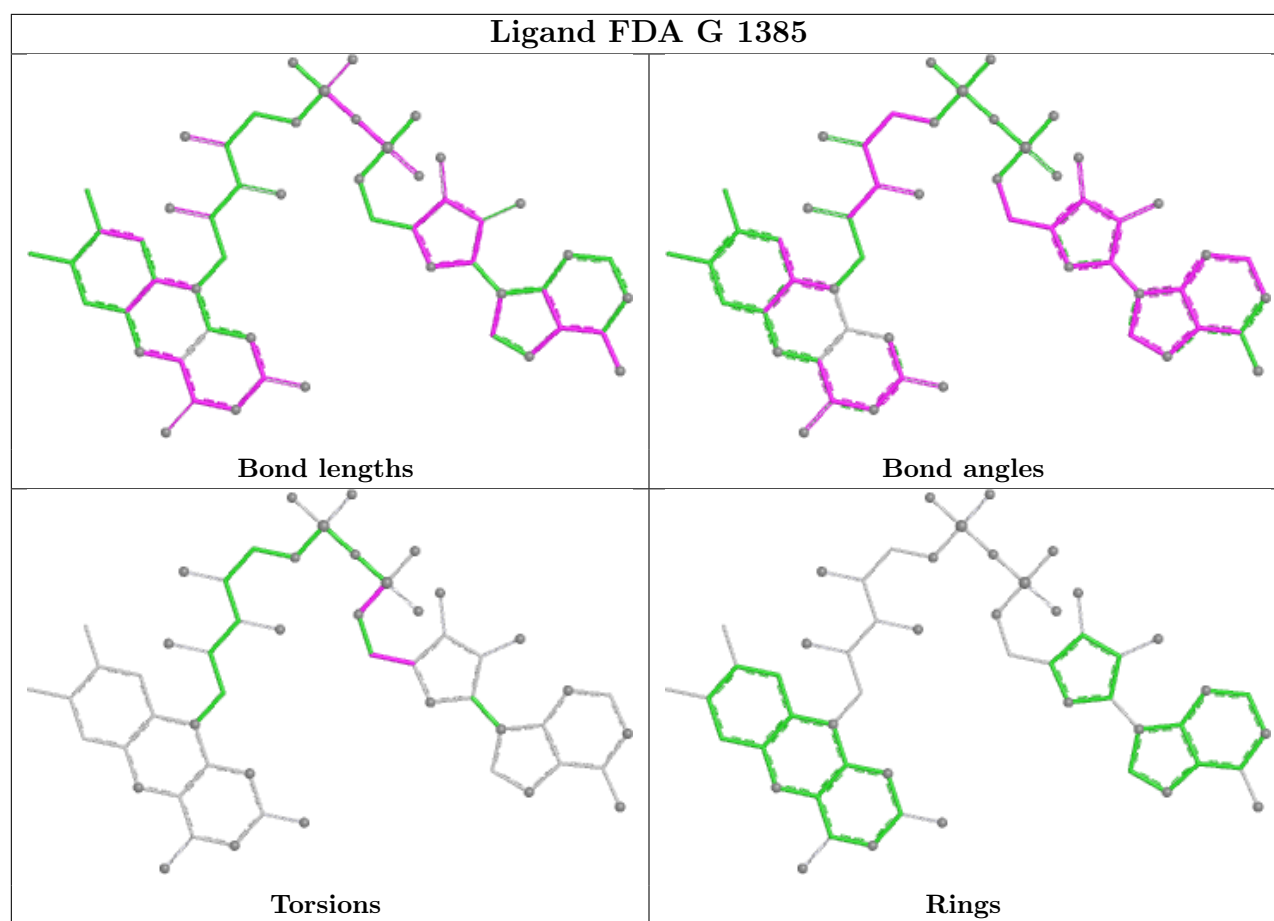
Bond angles

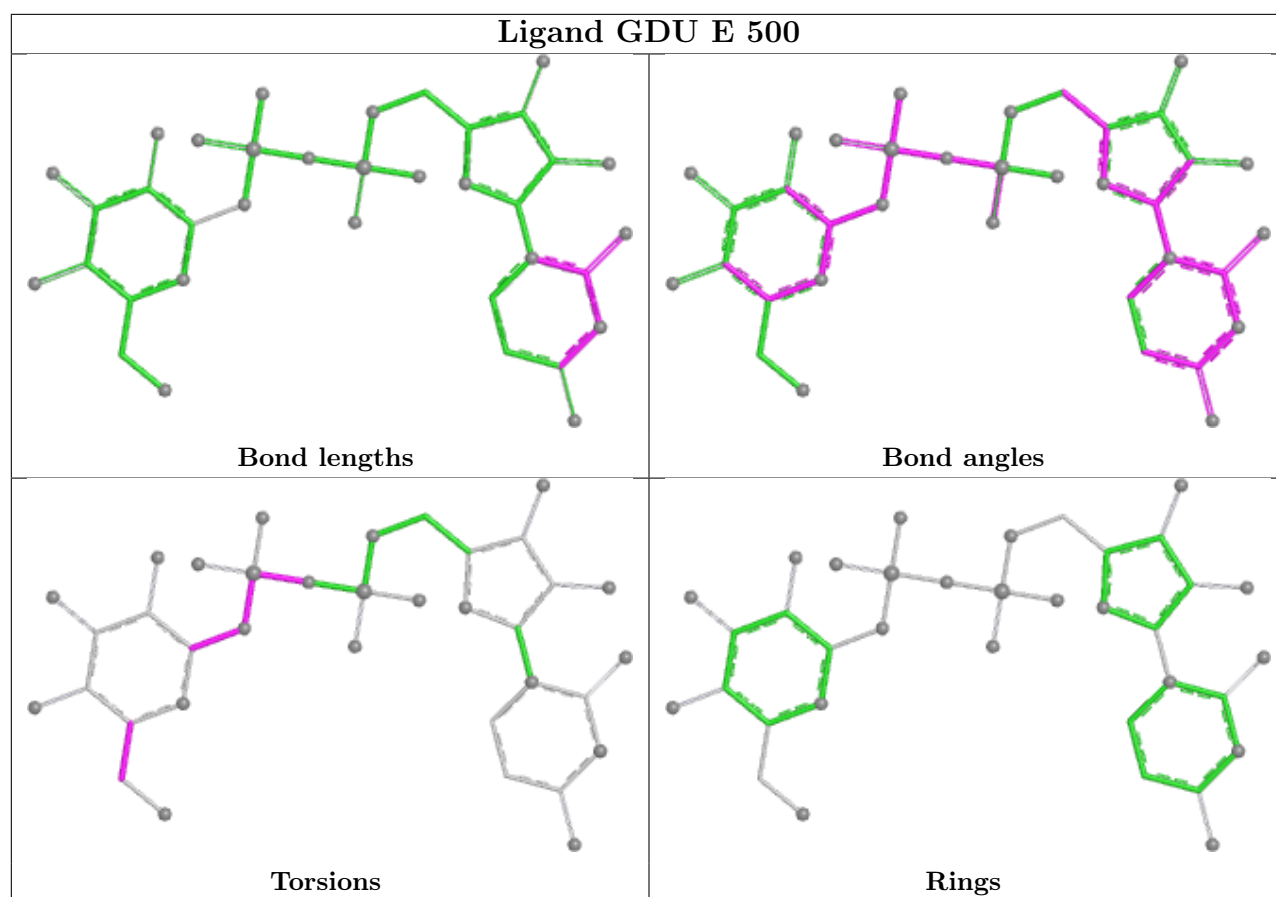


Torsions

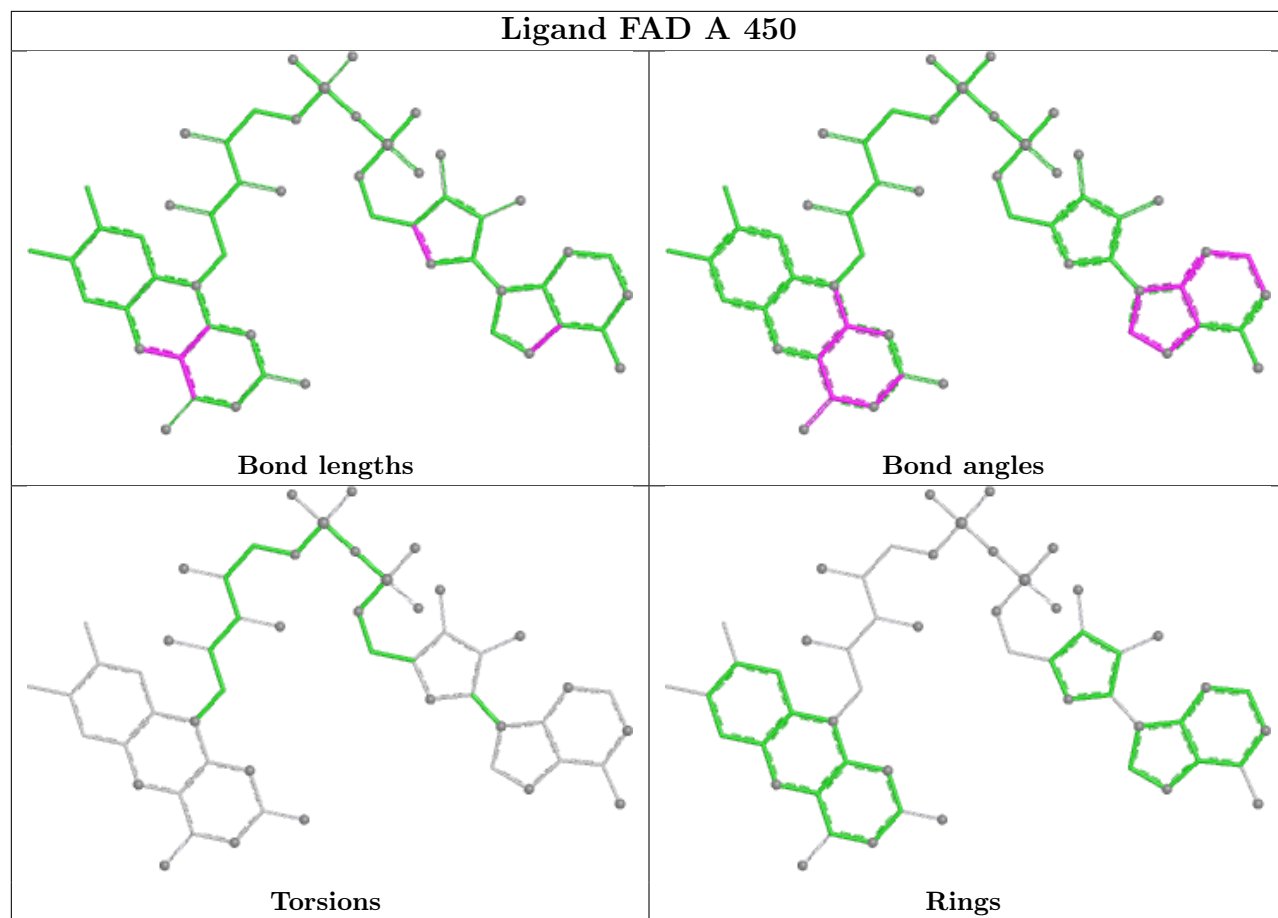


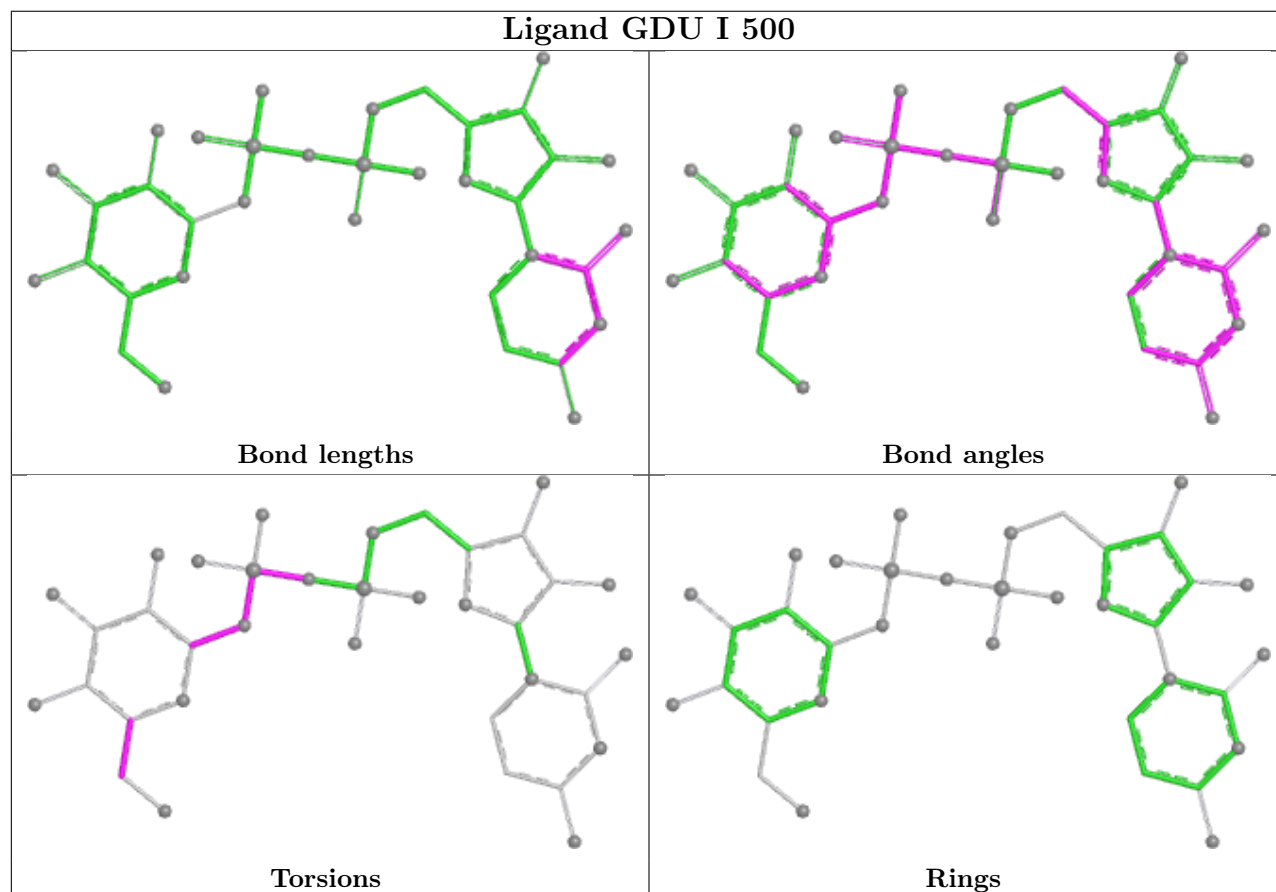
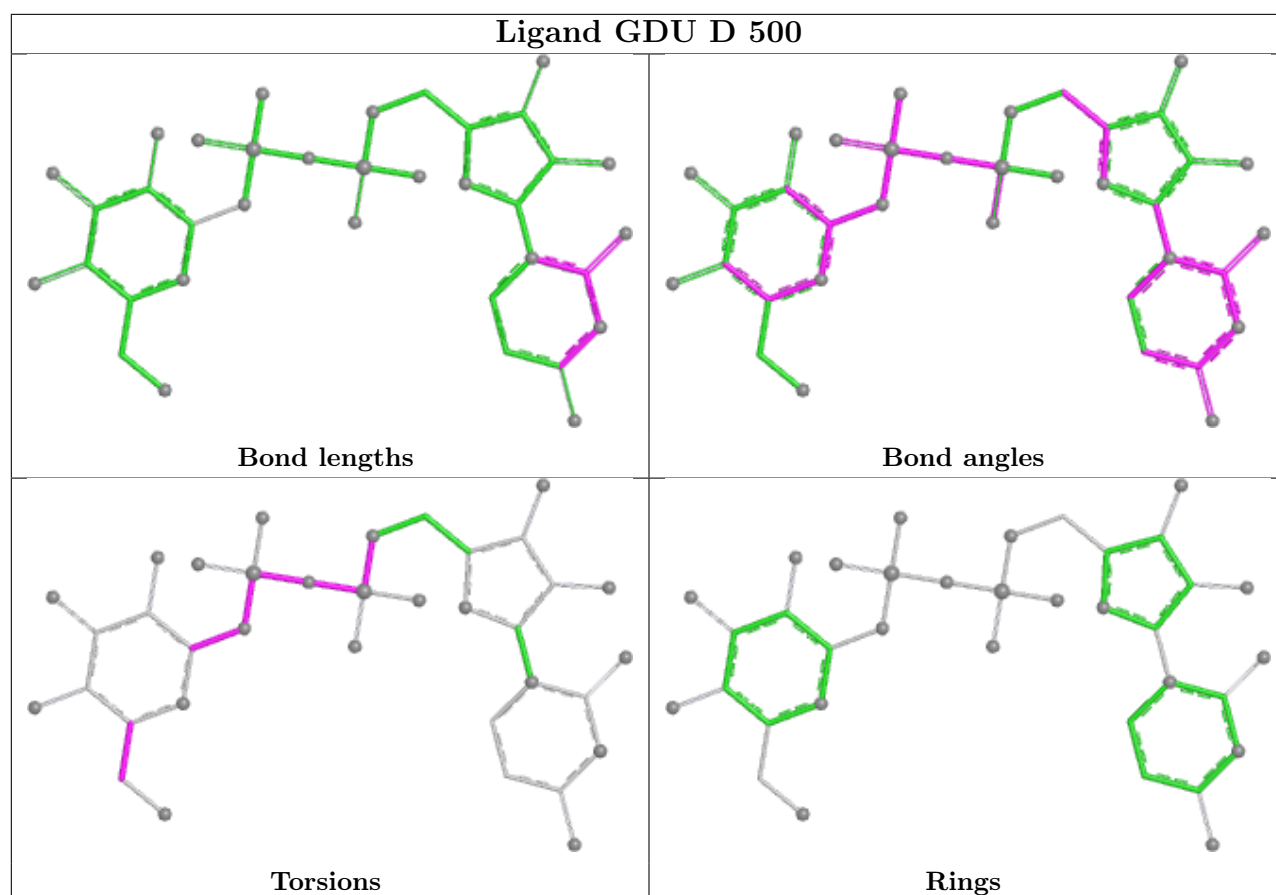
Rings

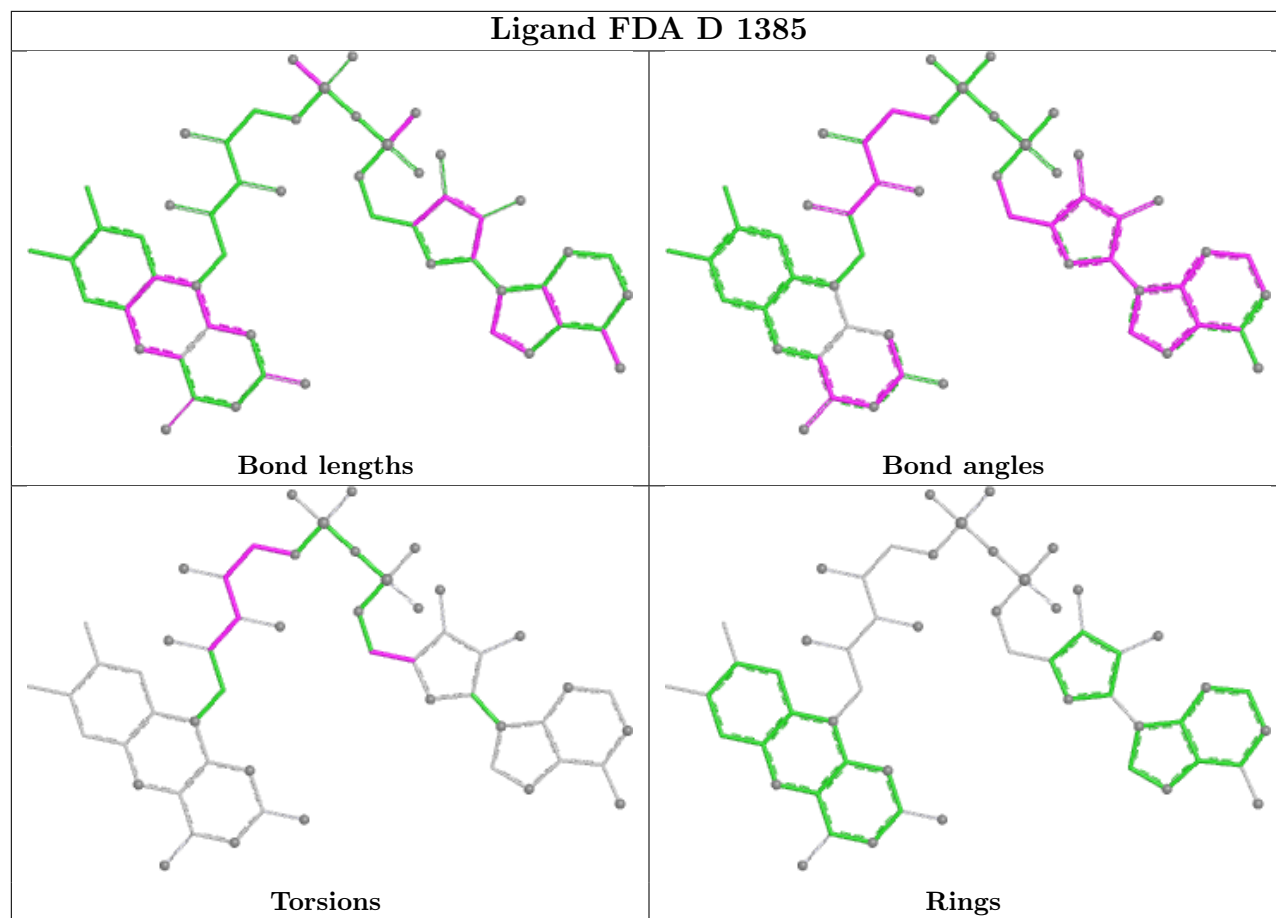


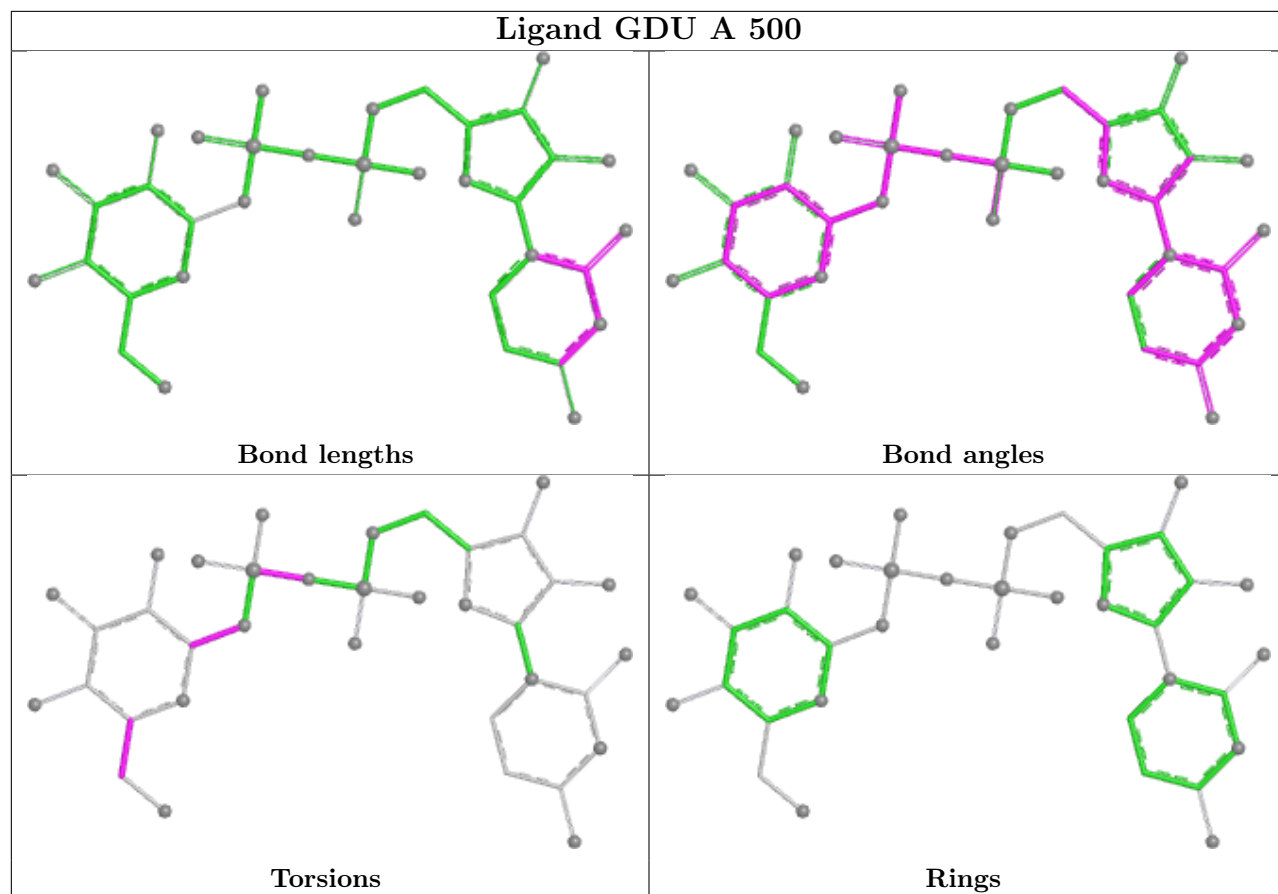


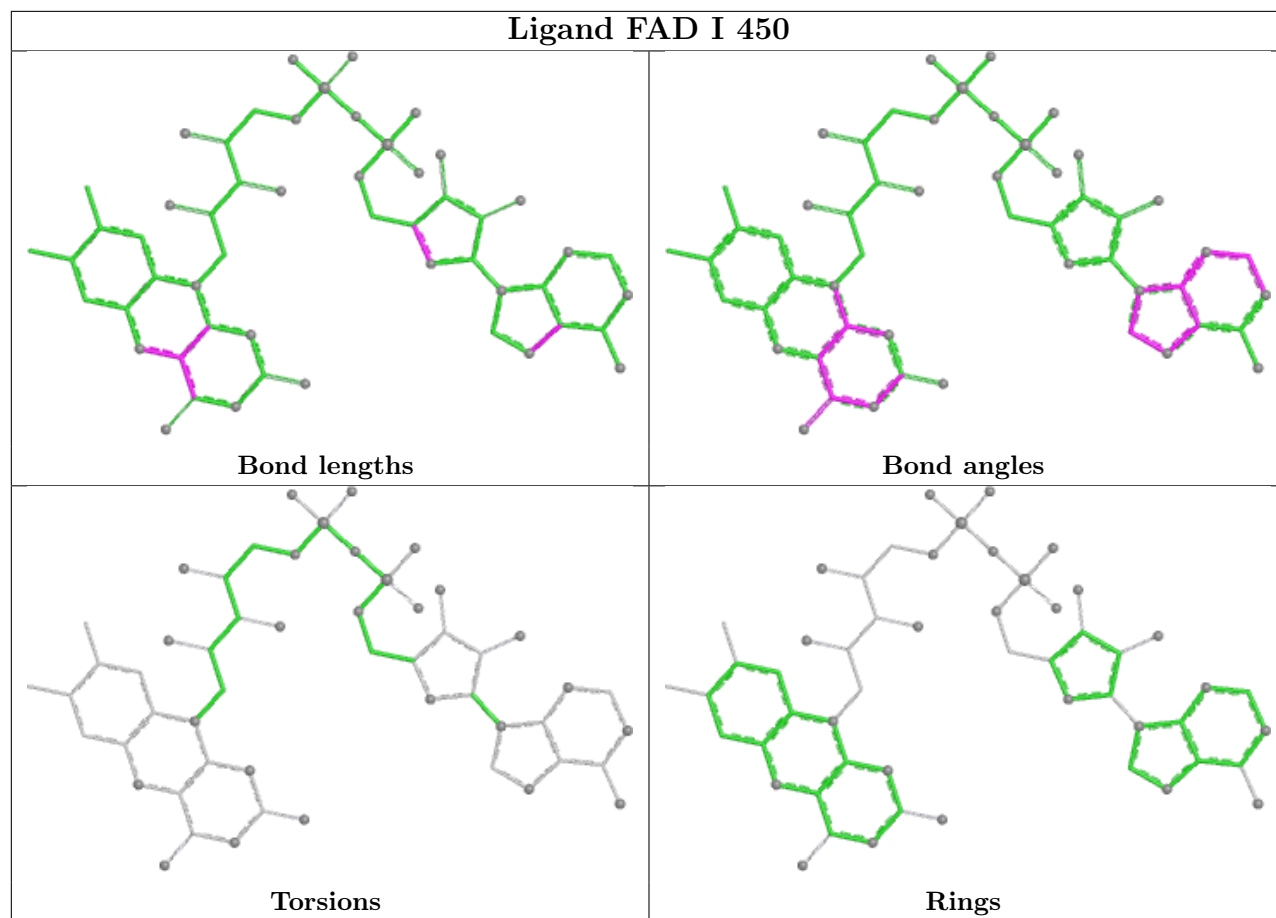
Ligand FAD A 450











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	365/397 (91%)	0.12	6 (1%)	70	66	35, 45, 65, 109	1 (0%)
1	B	361/397 (90%)	0.12	4 (1%)	78	74	36, 48, 66, 98	0
1	C	348/397 (87%)	0.91	55 (15%)	5	4	20, 55, 89, 122	1 (0%)
1	D	360/397 (90%)	0.36	15 (4%)	40	36	37, 53, 77, 102	1 (0%)
1	E	360/397 (90%)	0.36	6 (1%)	69	65	40, 55, 76, 101	1 (0%)
1	F	360/397 (90%)	0.20	13 (3%)	46	42	37, 48, 73, 97	1 (0%)
1	G	360/397 (90%)	0.27	5 (1%)	73	69	35, 50, 69, 102	0
1	H	361/397 (90%)	0.25	7 (1%)	66	62	37, 50, 70, 89	1 (0%)
1	I	361/397 (90%)	0.15	6 (1%)	69	65	38, 47, 65, 92	1 (0%)
1	J	359/397 (90%)	0.23	3 (0%)	82	80	36, 50, 74, 95	1 (0%)
All	All	3595/3970 (90%)	0.29	120 (3%)	49	45	20, 50, 75, 122	8 (0%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	55	VAL	7.0
1	C	360	THR	6.2
1	C	359	VAL	5.8
1	C	234	ASN	5.7
1	C	361	PHE	5.6
1	C	54	ARG	4.8
1	C	97	TYR	4.3
1	D	389	GLY	4.3
1	H	157	ARG	4.2
1	I	389	GLY	4.1
1	C	48	LEU	4.1
1	D	266	ASP	3.9
1	C	52	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	358	ASP	3.8
1	D	54	ARG	3.8
1	C	254	HIS	3.7
1	C	381	LEU	3.7
1	C	94	VAL	3.6
1	C	247	ALA	3.5
1	C	356	ALA	3.5
1	C	214	TYR	3.3
1	C	47	ARG	3.3
1	C	43	VAL	3.2
1	I	152	LYS	3.2
1	C	104	TRP	3.2
1	C	33	LEU	3.2
1	D	154	GLU	3.1
1	H	29	GLY	3.1
1	A	389	GLY	3.1
1	D	156	VAL	3.1
1	G	154	GLU	3.1
1	F	153	VAL	3.0
1	C	103	GLU	3.0
1	C	253	GLN	2.9
1	C	256	ILE	2.9
1	H	344	GLU	2.9
1	G	152	LYS	2.9
1	H	249	PHE	2.8
1	C	233	PRO	2.8
1	F	247	ALA	2.8
1	E	54	ARG	2.8
1	C	255	MET	2.8
1	B	152	LYS	2.8
1	A	152	LYS	2.7
1	D	152	LYS	2.7
1	D	268	CYS	2.7
1	I	29	GLY	2.7
1	D	265	PHE	2.7
1	F	156	VAL	2.7
1	C	235	ILE	2.6
1	C	362	VAL	2.6
1	J	269	TYR	2.6
1	H	250	ILE	2.6
1	C	95	PHE	2.6
1	C	252	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	344	GLU	2.6
1	J	181	ARG	2.5
1	D	29	GLY	2.5
1	E	178	GLY	2.5
1	E	154	GLU	2.5
1	I	330	GLU	2.5
1	C	98	LEU	2.5
1	J	385	ARG	2.5
1	C	89	THR	2.5
1	C	92	LYS	2.5
1	C	379	GLN	2.5
1	C	90	ASN	2.5
1	C	353	ALA	2.5
1	C	271	LYS	2.4
1	C	345	LEU	2.4
1	C	49	ALA	2.4
1	C	355	ALA	2.4
1	E	98	LEU	2.4
1	D	269	TYR	2.4
1	E	389	GLY	2.4
1	F	344	GLU	2.4
1	D	272	LEU	2.3
1	F	249	PHE	2.3
1	F	28	LYS	2.3
1	F	343	ALA	2.3
1	C	51	SER	2.3
1	A	318	HIS	2.3
1	C	44	LEU	2.3
1	C	45	ALA	2.3
1	H	355	ALA	2.3
1	A	25	GLN	2.3
1	A	27	SER	2.3
1	C	220	HIS	2.3
1	C	357	GLN	2.3
1	C	230	LEU	2.3
1	F	250	ILE	2.3
1	F	155	GLN	2.3
1	G	388	GLN	2.3
1	H	248	ASP	2.3
1	C	106	PRO	2.3
1	F	347	LYS	2.2
1	G	153	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	101	PHE	2.2
1	D	249	PHE	2.2
1	C	91	SER	2.2
1	F	341	GLU	2.2
1	D	385	ARG	2.2
1	B	29	GLY	2.2
1	C	57	ILE	2.2
1	I	153	VAL	2.1
1	B	357	GLN	2.1
1	D	330	GLU	2.1
1	F	100	ARG	2.1
1	C	377	VAL	2.1
1	C	314	GLY	2.1
1	D	345	LEU	2.1
1	E	29	GLY	2.1
1	B	248	ASP	2.1
1	C	50	SER	2.1
1	C	251	PRO	2.1
1	F	157	ARG	2.1
1	C	268	CYS	2.1
1	A	153	VAL	2.0
1	G	247	ALA	2.0
1	C	93	ASP	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.

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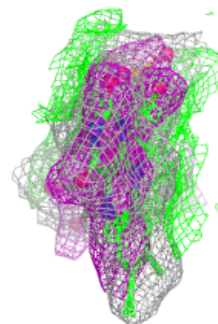
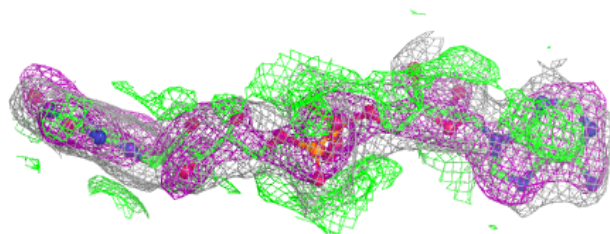
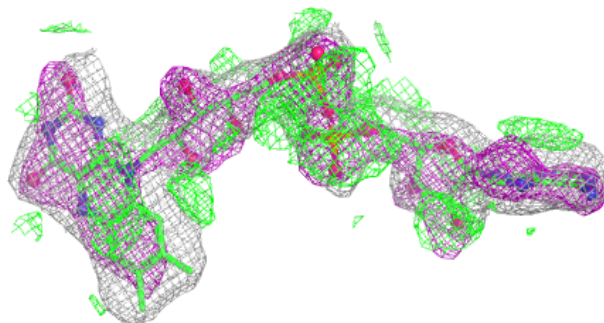
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FAD	C	450	53/53	0.84	0.12	20,20,20,20	0
3	FAD	E	450	53/53	0.88	0.11	20,20,20,20	0
3	FAD	H	450	53/53	0.88	0.11	20,20,20,20	0
3	FAD	I	450	53/53	0.88	0.11	20,20,20,20	0
3	FAD	J	450	53/53	0.88	0.11	20,20,20,20	0
3	FAD	F	450	53/53	0.89	0.10	20,20,20,20	0
2	GDU	C	500	36/36	0.90	0.12	36,48,61,68	0
4	FDA	D	1385	53/53	0.91	0.11	42,53,66,71	0
2	GDU	I	500	36/36	0.92	0.11	40,49,64,65	0
2	GDU	H	500	36/36	0.92	0.11	39,49,64,70	0
2	GDU	E	500	36/36	0.93	0.11	45,56,64,67	0
2	GDU	J	500	36/36	0.93	0.10	40,49,61,62	0
3	FAD	A	450	53/53	0.93	0.09	20,20,20,20	0
2	GDU	F	500	36/36	0.93	0.10	39,48,58,61	0
2	GDU	A	500	36/36	0.93	0.10	35,47,58,66	0
2	GDU	D	500	36/36	0.94	0.09	42,50,56,60	0
4	FDA	B	1385	53/53	0.94	0.08	42,49,55,57	0
2	GDU	B	500	36/36	0.94	0.08	43,50,59,64	0
4	FDA	G	1385	53/53	0.94	0.08	41,53,59,60	0
2	GDU	G	500	36/36	0.95	0.09	41,49,61,69	0

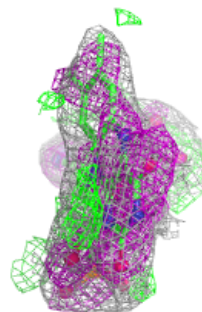
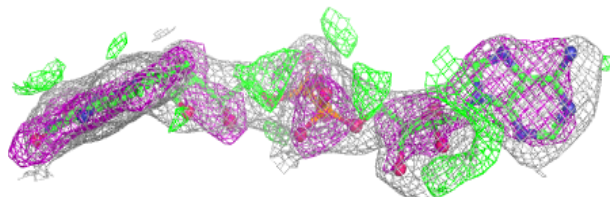
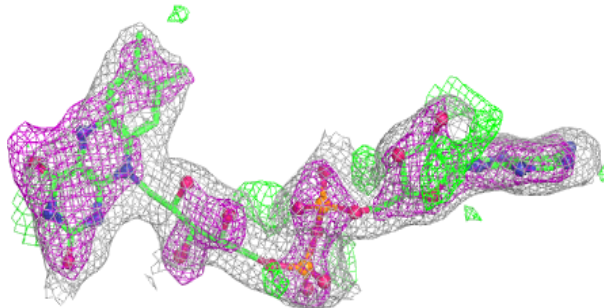
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD C 450:

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

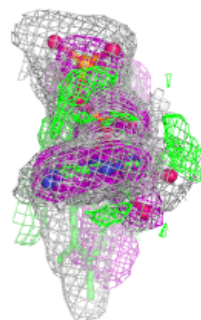
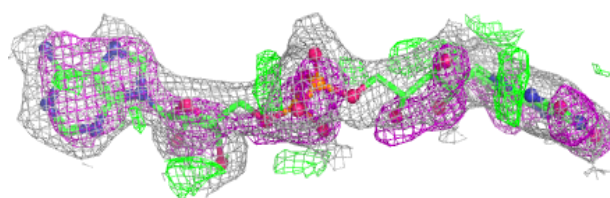
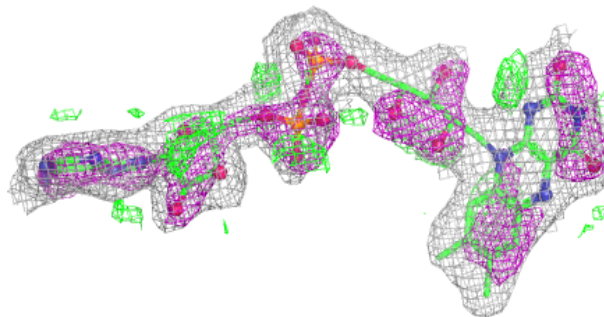
**Electron density around FAD E 450:**

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

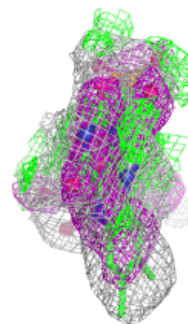
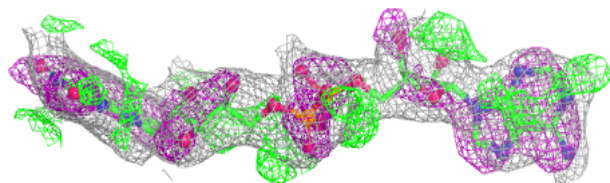
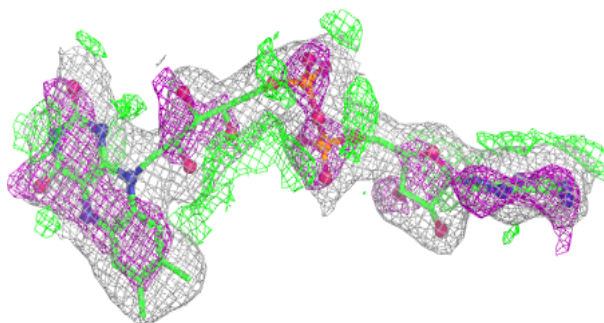


Electron density around FAD H 450:

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

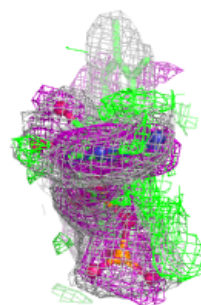
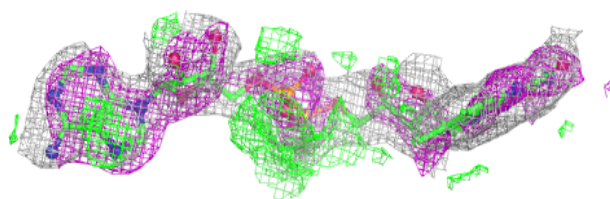
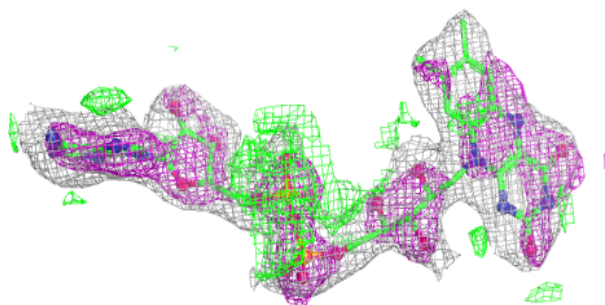
**Electron density around FAD I 450:**

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

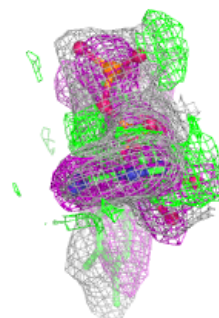
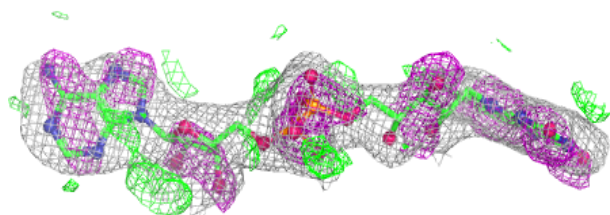
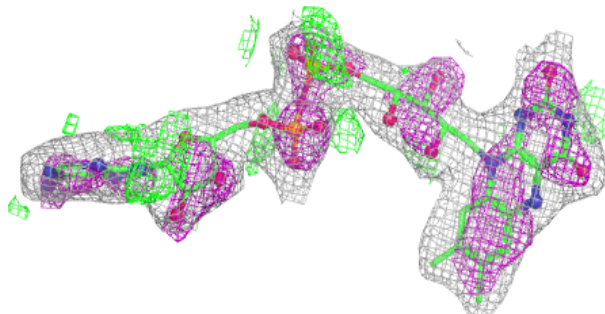


Electron density around FAD J 450:

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

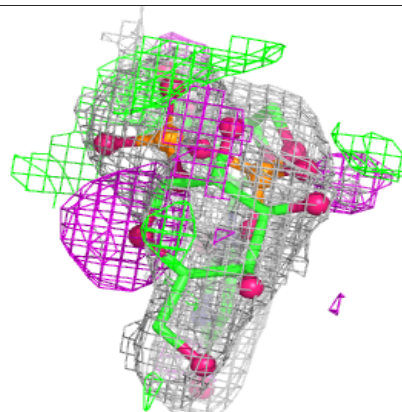
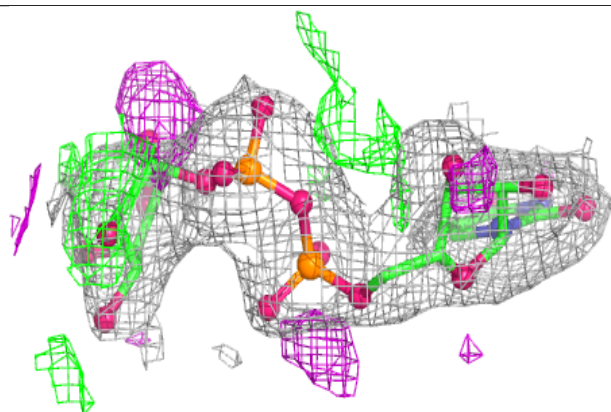
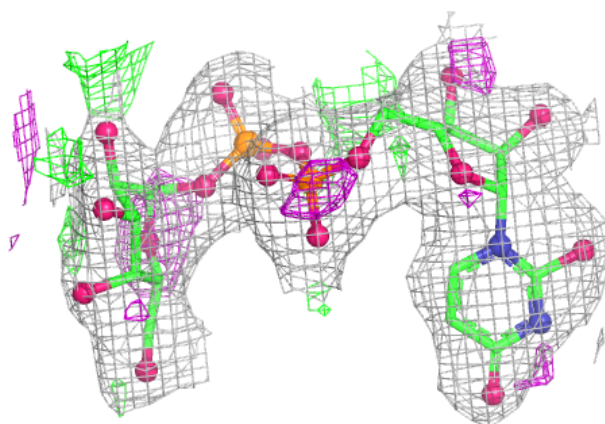
**Electron density around FAD F 450:**

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

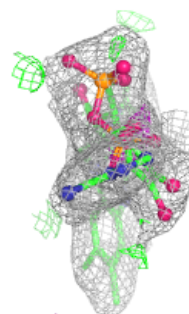
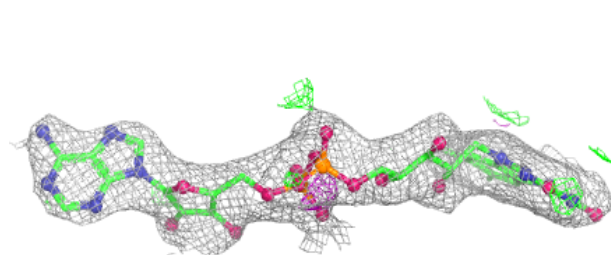
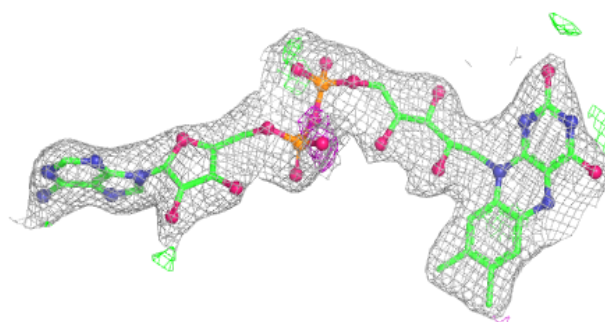


Electron density around GDU C 500:

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

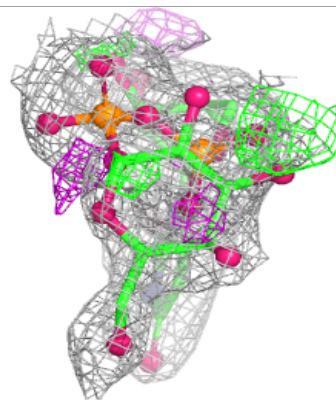
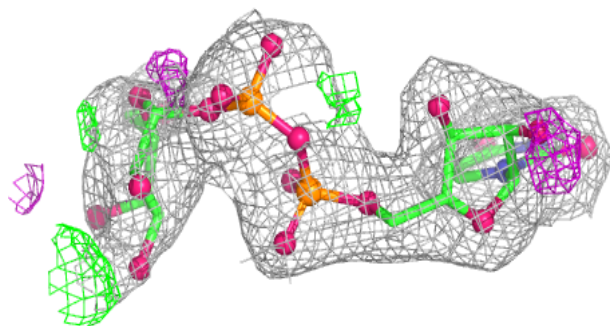
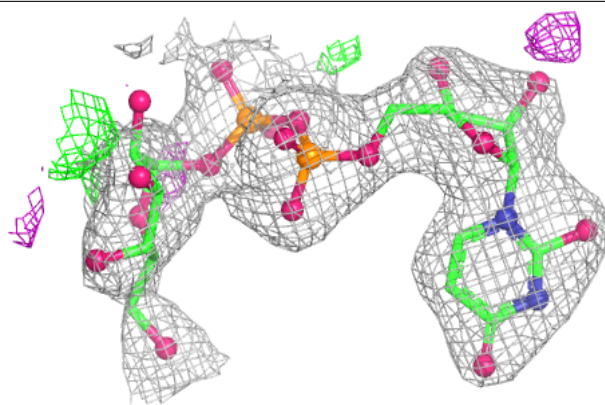
**Electron density around FDA D 1385:**

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

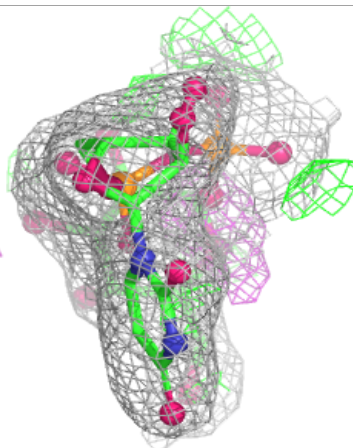
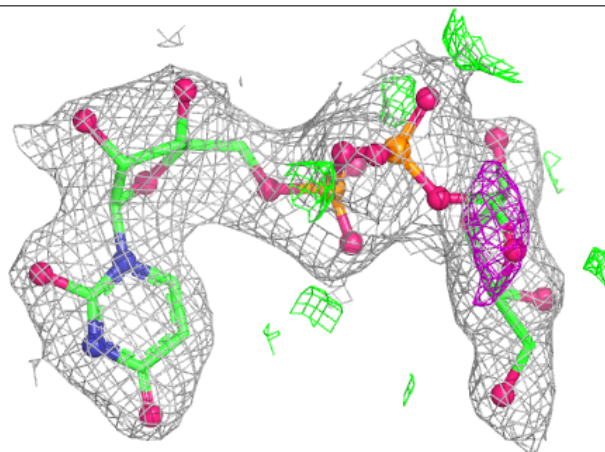


Electron density around GDU I 500:

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

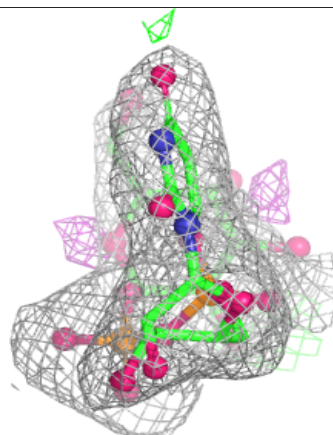
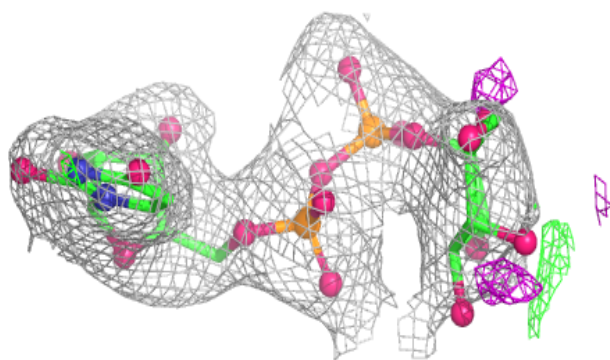
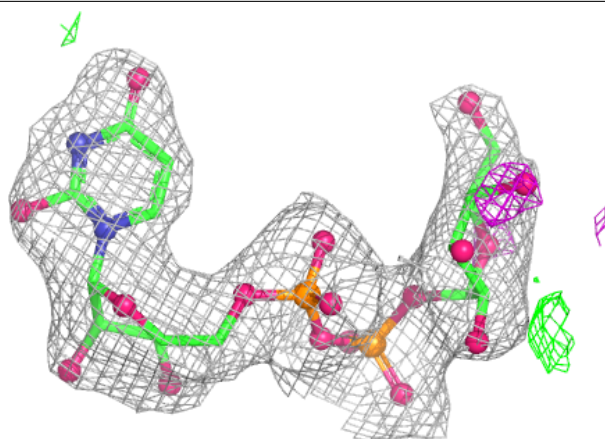
**Electron density around GDU H 500:**

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



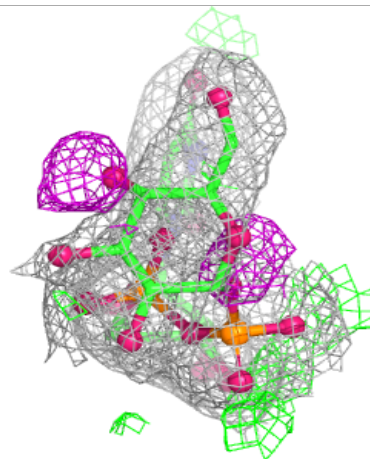
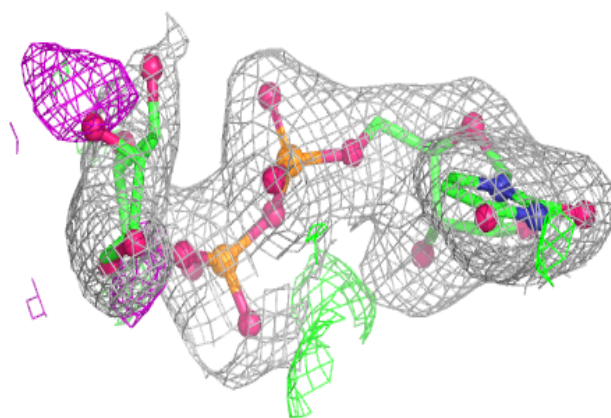
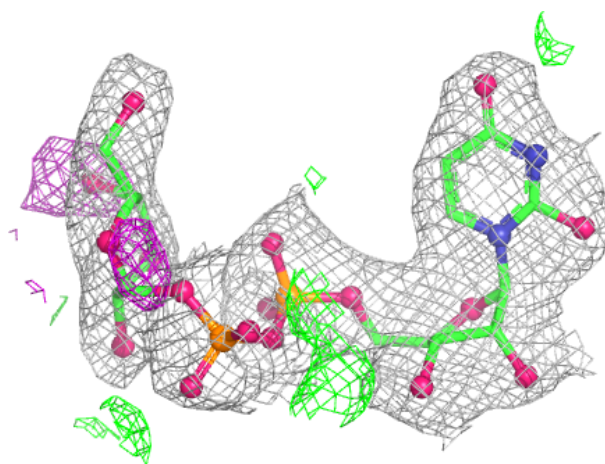
Electron density around GDU E 500:

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



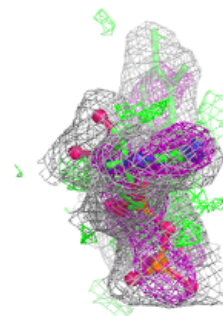
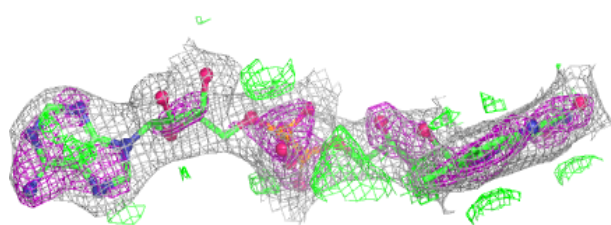
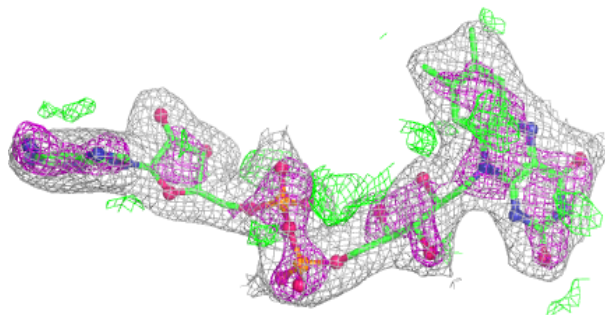
Electron density around GDU J 500:

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

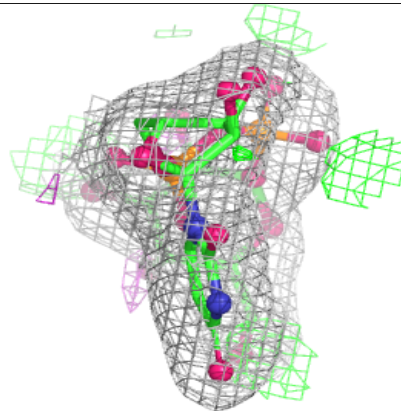
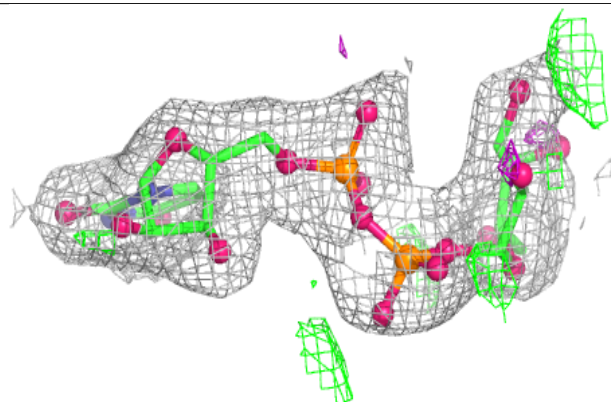
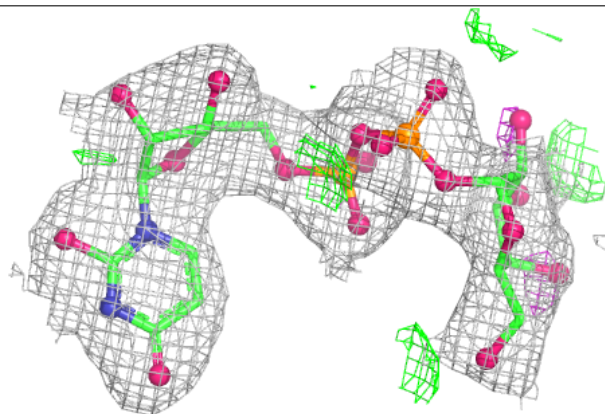


Electron density around FAD A 450:

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

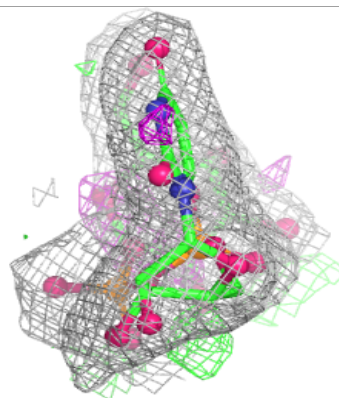
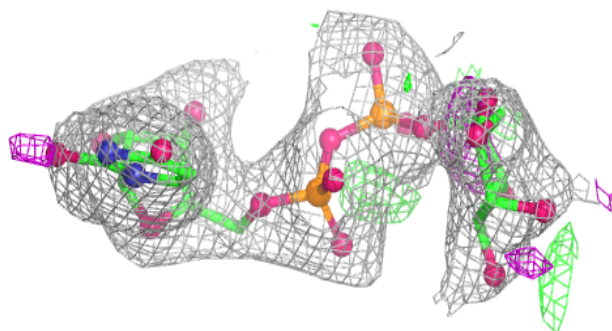
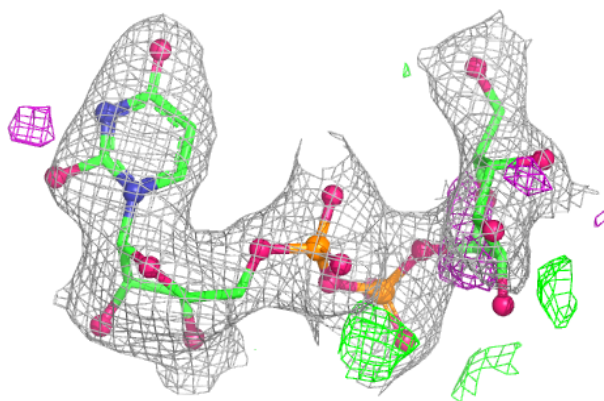
**Electron density around GDU F 500:**

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

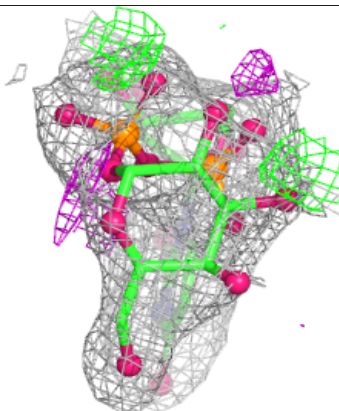
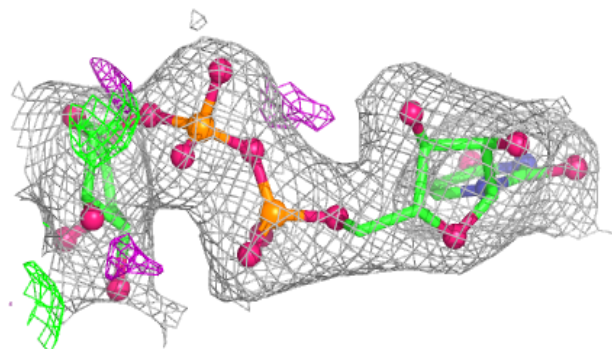
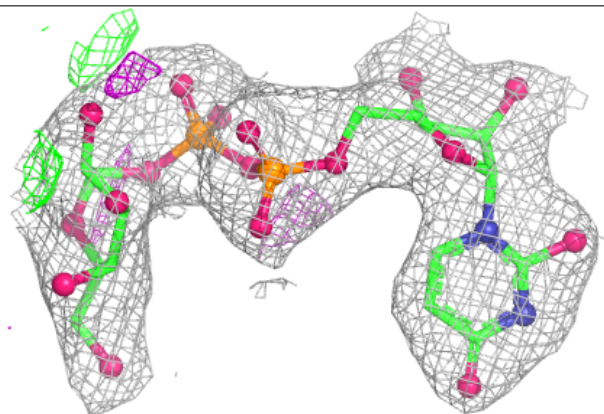


Electron density around GDU A 500:

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

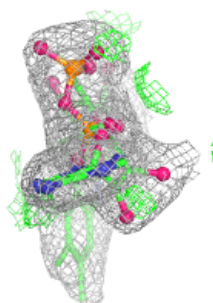
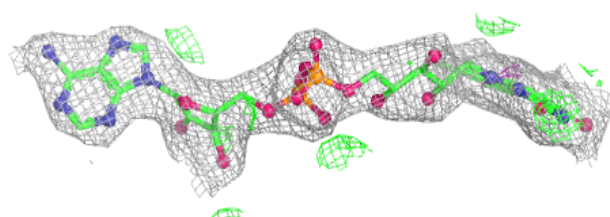
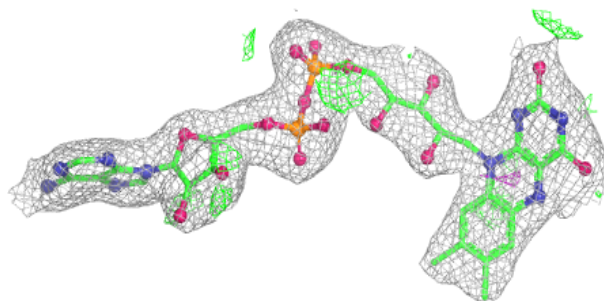
**Electron density around GDU D 500:**

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

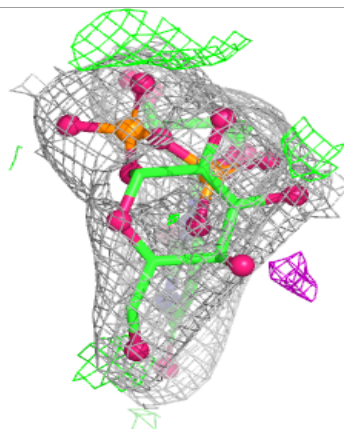
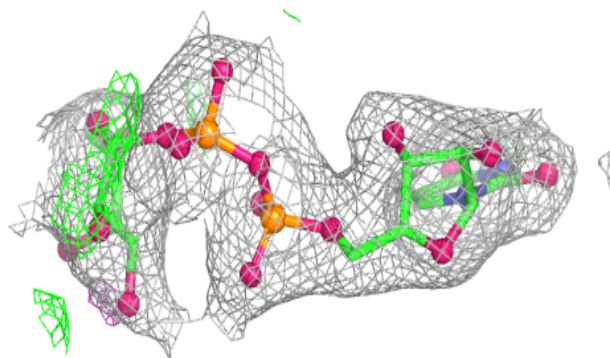
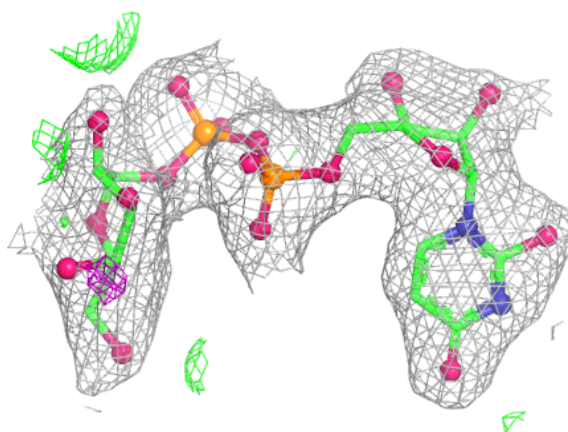


Electron density around FDA B 1385:

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

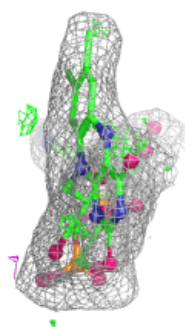
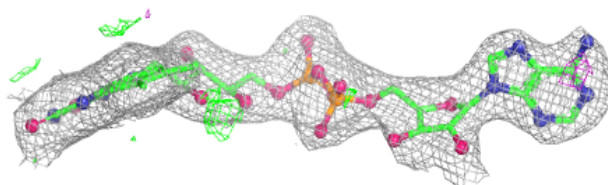
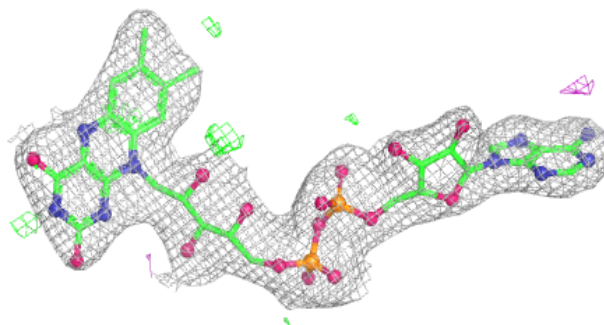
**Electron density around GDU B 500:**

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

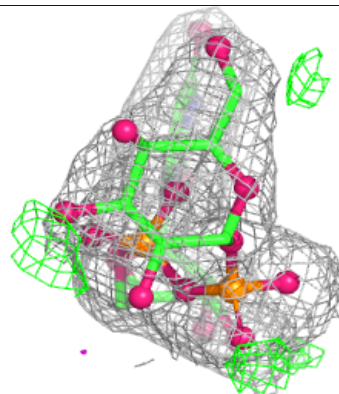
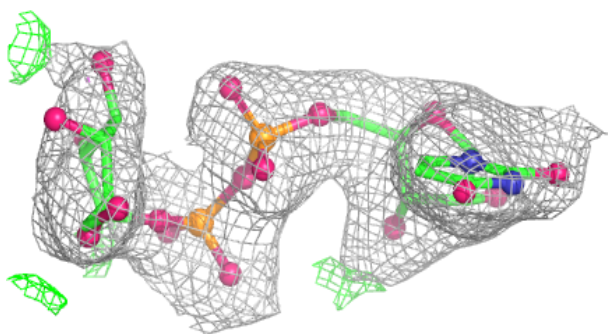
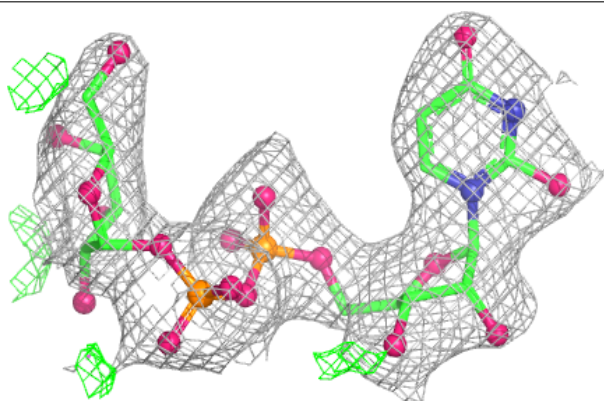


Electron density around FDA G 1385:

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

**Electron density around GDU G 500:**

$2mF_o-DF_c$ (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.