



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:53 PM UTC

PDB ID : 3MJ4 / pdb_00003mj4
Title : Crystal structure of UDP-galactopyranose mutase in complex with phosphate analog of UDP-galactopyranose
Authors : Karunan Partha, S.; Sadeghi-Khomami, A.; Slowski, K.; Kotake, T.; Thomas, N.R.; Jakeman, D.L.; Sanders, D.A.R.
Deposited on : 2010-04-12
Resolution : 2.65 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

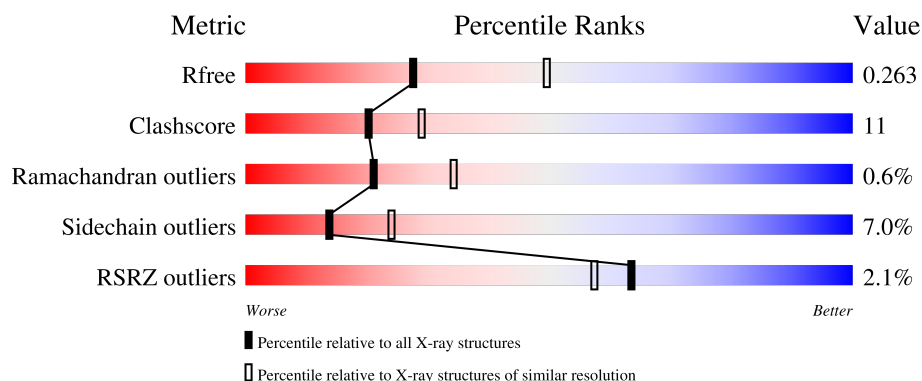
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	397	% 67% 21% • 8%
1	B	397	5% 62% 25% • 9%
1	C	397	2% 68% 21% • 9%
1	D	397	% 66% 22% • 10%

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Mol	Chain	Length	Quality of chain
1	E	397	
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
6	XYL	I	401	-	X	-	-

2 Entry composition

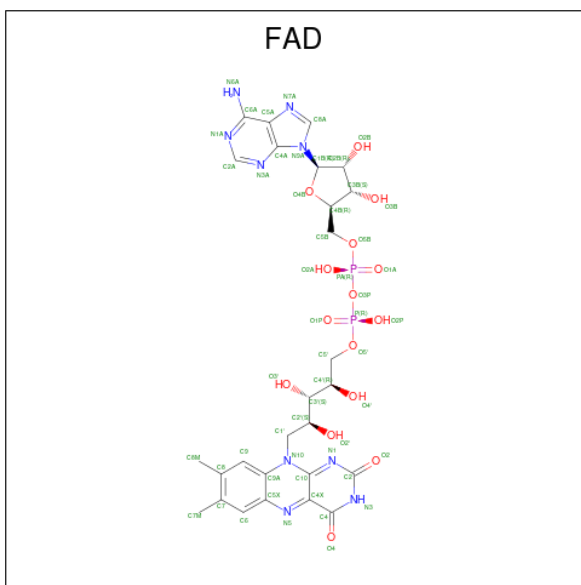
There are 7 unique types of molecules in this entry. The entry contains 31256 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

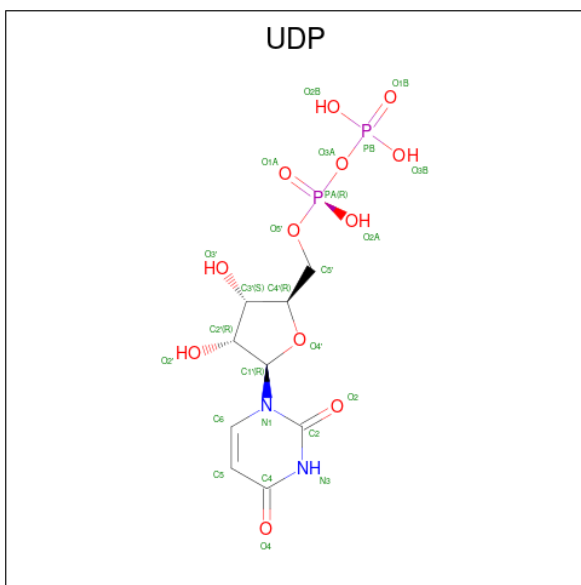
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	1	1	0
			2992	1909	521	554	8			
1	B	363	Total	C	N	O	S	1	0	0
			2969	1896	516	549	8			
1	C	363	Total	C	N	O	S	1	0	0
			2969	1896	516	549	8			
1	D	359	Total	C	N	O	S	0	0	0
			2943	1881	510	544	8			
1	E	361	Total	C	N	O	S	2	0	0
			2951	1885	512	546	8			
1	F	364	Total	C	N	O	S	1	1	0
			2984	1906	520	550	8			
1	G	363	Total	C	N	O	S	1	0	0
			2966	1894	515	549	8			
1	H	364	Total	C	N	O	S	0	0	0
			2975	1899	517	551	8			
1	I	364	Total	C	N	O	S	1	0	0
			2975	1899	516	552	8			
1	J	363	Total	C	N	O	S	2	0	0
			2966	1894	515	549	8			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



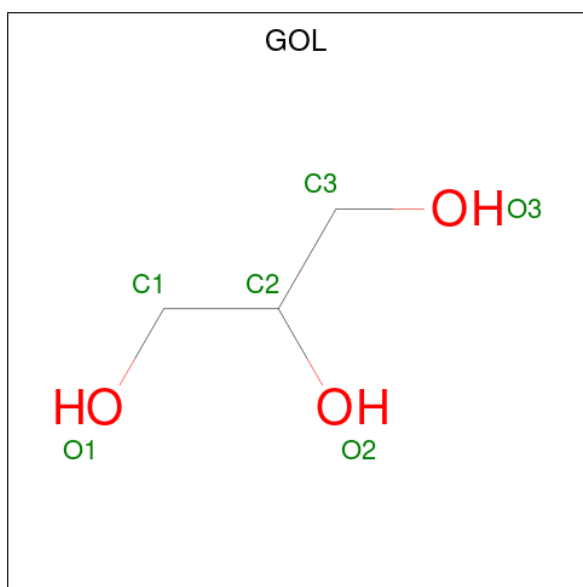
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	D	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	E	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	F	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	G	1	Total 53	C 27	N 9	O 15	P 2	0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

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $\text{C}_9\text{H}_{14}\text{N}_2\text{O}_{12}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 25	C 9	N 2	O 12	P 2	0	0
3	B	1	Total 25	C 9	N 2	O 12	P 2	0	0
3	C	1	Total 25	C 9	N 2	O 12	P 2	0	0
3	E	1	Total 21	C 9	N 2	O 9	P 1	0	0
3	F	1	Total 25	C 9	N 2	O 12	P 2	0	0
3	G	1	Total 25	C 9	N 2	O 12	P 2	0	0
3	H	1	Total 25	C 9	N 2	O 12	P 2	0	0
3	I	1	Total 21	C 9	N 2	O 9	P 1	0	0
3	J	1	Total 25	C 9	N 2	O 12	P 2	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



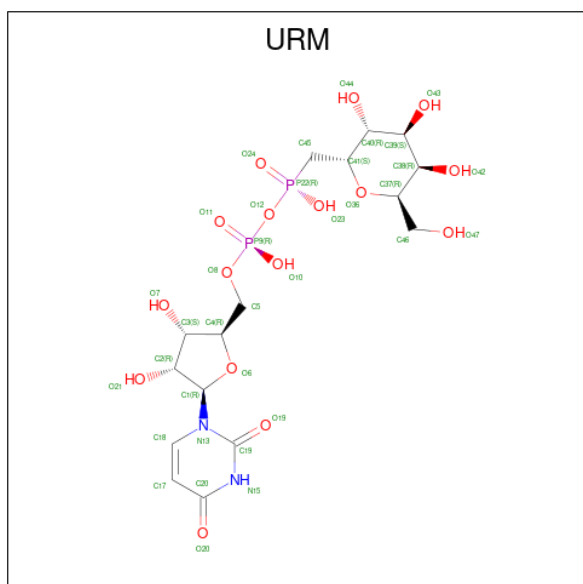
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total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

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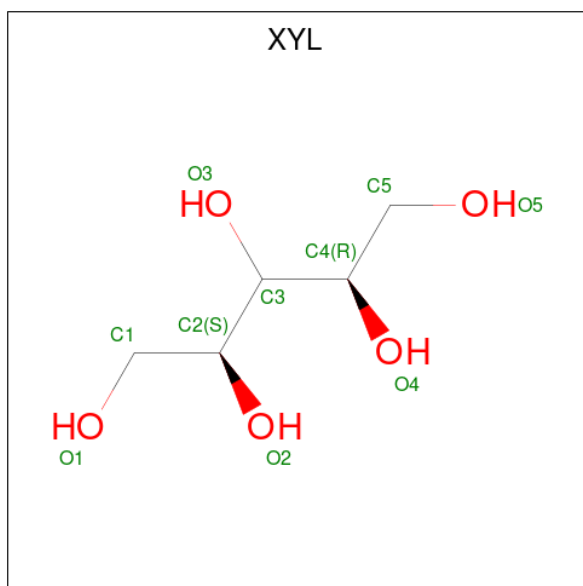
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		
4	J	1	Total	C	O	0	0
			6	3	3		
4	J	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is (((2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)methyl)phosphonic (((2R,3S,4R,5R)-5-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-3,4-dihydroxytetrahydrofuran-2-yl)methyl phosphoric) anhydride (CCD ID: URM) (formula: C₁₆H₂₆N₂O₁₆P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	P	0	0
			36	16	2	16	2		

- Molecule 6 is Xylitol (CCD ID: XYL) (formula: $C_5H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	C	O	0	0
			10	5	5		
6	I	1	Total	C	O	0	0
			10	5	5		

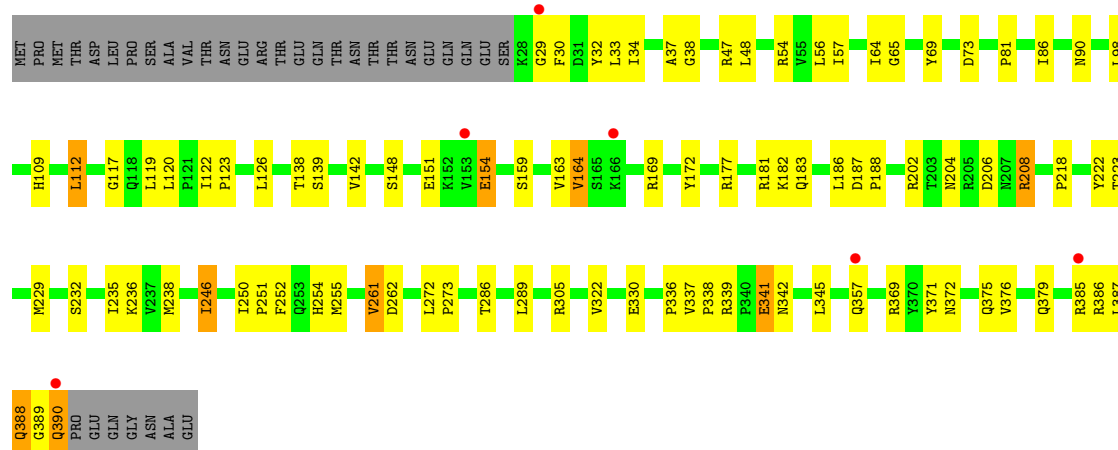
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	89	Total	O	0	0
			89	89		
7	B	68	Total	O	0	0
			68	68		
7	C	60	Total	O	0	0
			60	60		
7	D	46	Total	O	0	0
			46	46		
7	E	51	Total	O	0	0
			51	51		
7	F	60	Total	O	0	0
			60	60		
7	G	53	Total	O	0	0
			53	53		

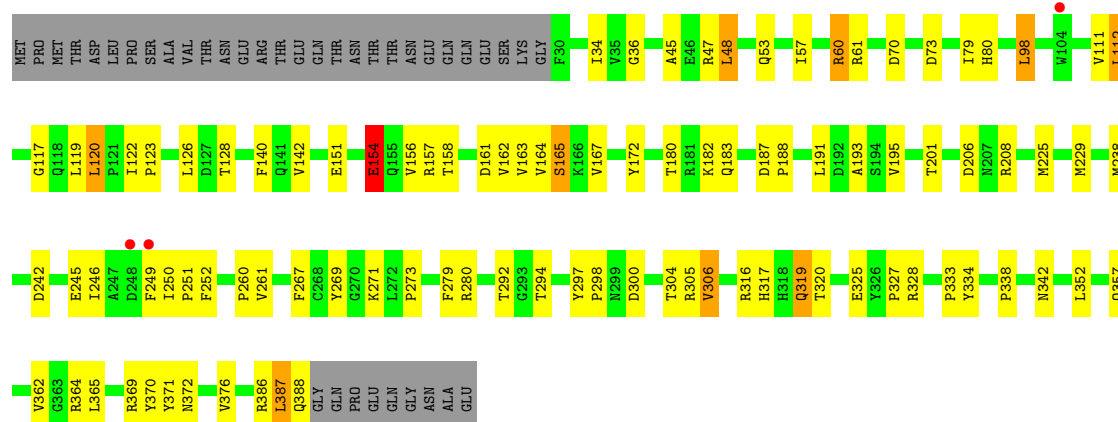
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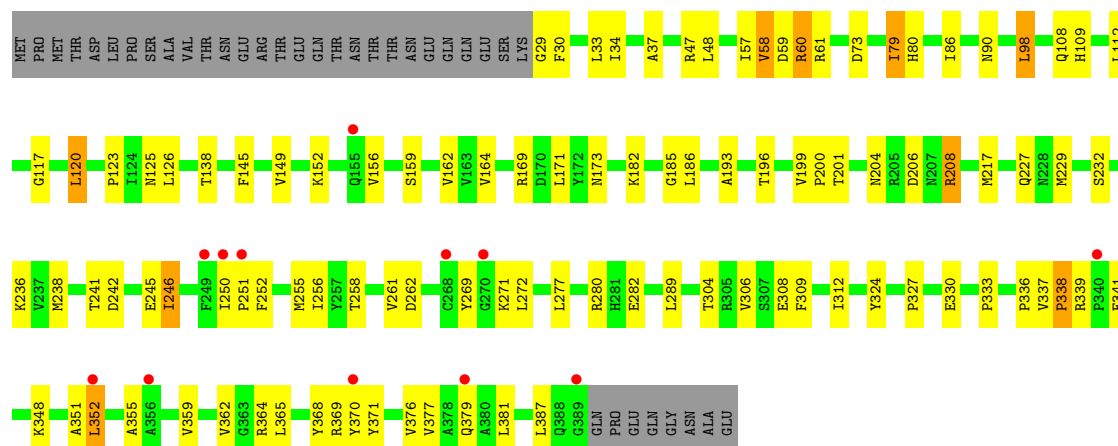
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	75	Total 75	O 75	0	0
7	I	65	Total 65	O 65	0	0
7	J	46	Total 46	O 46	0	0



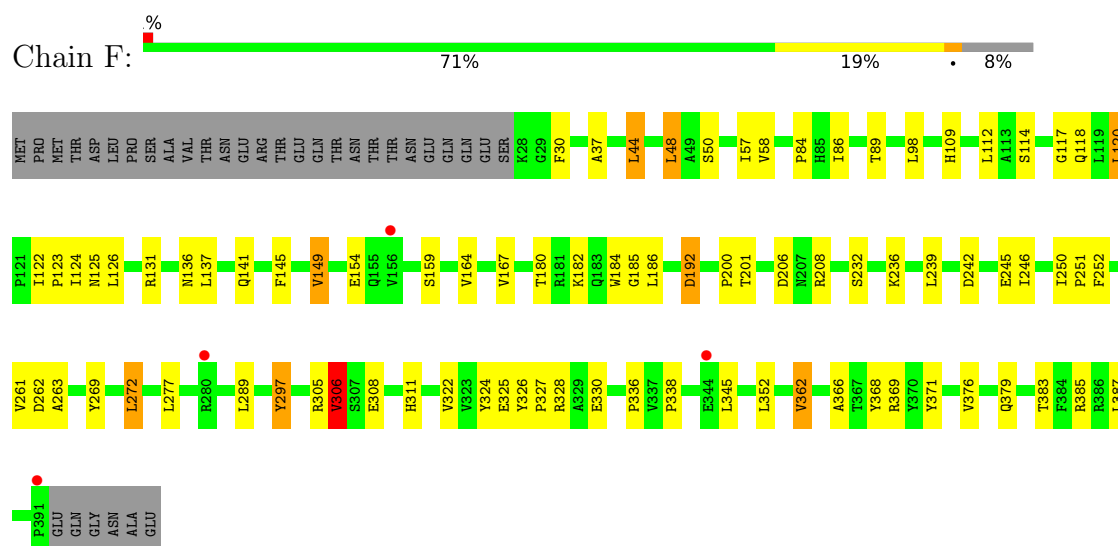
• Molecule 1: UDP-galactopyranose mutase



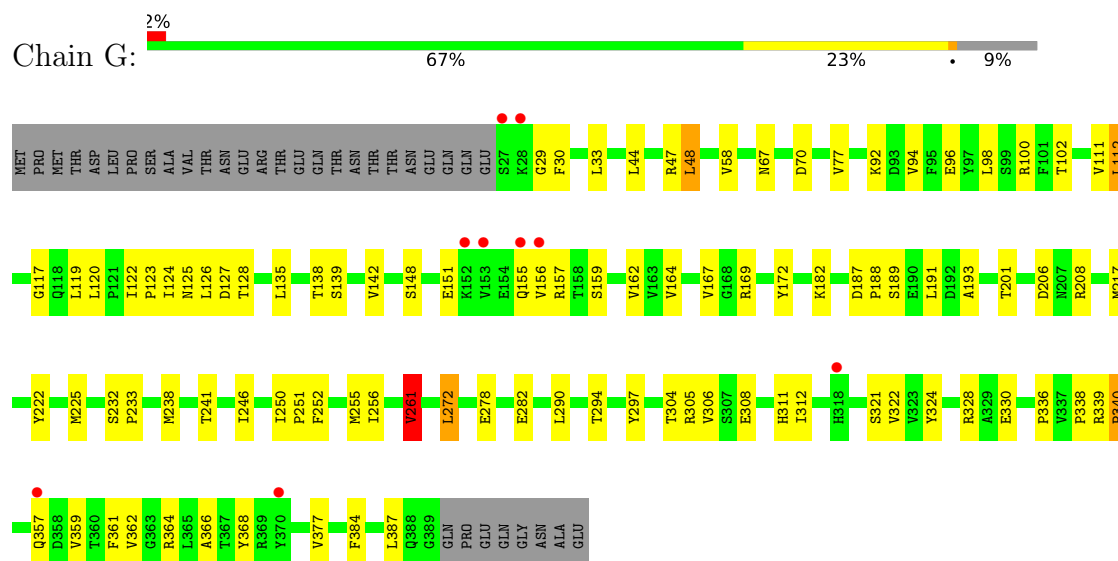
• Molecule 1: UDP-galactopyranose mutase



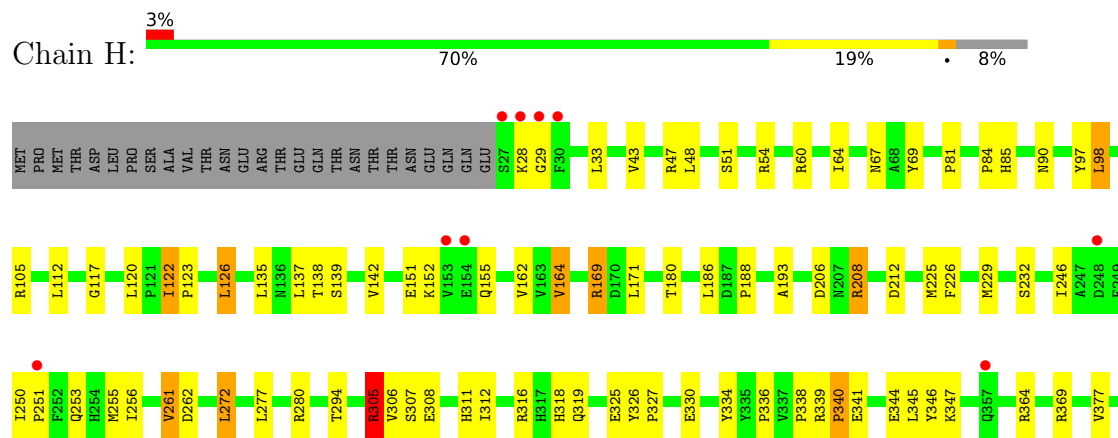
• Molecule 1: UDP-galactopyranose mutase

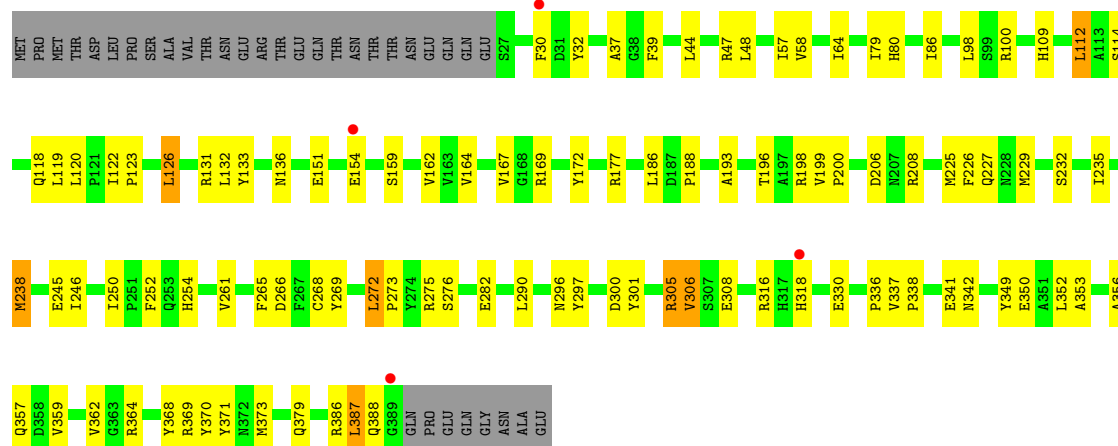


- Molecule 1: UDP-galactopyranose mutase



- 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	134.15Å 175.72Å 223.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.54 – 2.65 44.54 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.54-2.65) 99.5 (44.54-2.65)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.65Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.207 , 0.262 (Not available) , 0.263	Depositor DCC
R_{free} test set	7713 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	31256	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XYL, GOL, FAD, URM, UDP

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	0.60	0/3079	0.90	4/4185 (0.1%)
1	B	0.56	0/3053	0.90	5/4151 (0.1%)
1	C	0.55	0/3053	0.90	2/4151 (0.0%)
1	D	0.50	0/3027	0.83	0/4118
1	E	0.49	0/3035	0.86	4/4128 (0.1%)
1	F	0.53	0/3072	0.90	8/4177 (0.2%)
1	G	0.53	0/3050	0.90	1/4147 (0.0%)
1	H	0.56	0/3059	0.86	2/4159 (0.0%)
1	I	0.57	0/3059	0.90	7/4159 (0.2%)
1	J	0.53	0/3050	0.87	5/4147 (0.1%)
All	All	0.54	0/30537	0.88	38/41522 (0.1%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	297	TYR	CA-C-N	7.60	127.15	119.24
1	F	297	TYR	C-N-CA	7.60	127.15	119.24
1	C	261	VAL	CB-CA-C	-7.55	101.95	112.14
1	B	261	VAL	CB-CA-C	-7.13	102.52	112.14
1	A	249	PHE	CA-C-N	-7.06	117.51	122.59
1	A	249	PHE	C-N-CA	-7.06	117.51	122.59
1	E	232	SER	CA-C-N	6.70	126.39	119.56
1	E	232	SER	C-N-CA	6.70	126.39	119.56
1	J	199	VAL	CA-C-N	6.47	127.00	120.14
1	J	199	VAL	C-N-CA	6.47	127.00	120.14
1	B	162	VAL	N-CA-C	-6.25	105.17	112.98
1	I	80	HIS	CA-C-N	5.99	125.67	119.56
1	I	80	HIS	C-N-CA	5.99	125.67	119.56
1	A	246	ILE	CB-CA-C	-5.77	104.39	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	167	VAL	N-CA-C	5.75	118.42	112.90
1	B	309	PHE	N-CA-C	5.72	117.52	111.28
1	E	199	VAL	CA-C-N	5.69	125.59	119.85
1	E	199	VAL	C-N-CA	5.69	125.59	119.85
1	I	261	VAL	CB-CA-C	-5.56	104.86	111.97
1	I	306	VAL	CB-CA-C	-5.54	102.39	110.81
1	F	305	ARG	N-CA-C	5.38	116.71	108.42
1	I	60	ARG	N-CA-C	-5.36	105.52	111.36
1	H	261	VAL	CB-CA-C	-5.36	104.96	111.87
1	C	305	ARG	N-CA-C	5.33	116.64	108.42
1	F	326	TYR	CA-C-N	-5.31	114.49	119.85
1	F	326	TYR	C-N-CA	-5.31	114.49	119.85
1	B	187	ASP	CA-C-N	5.25	126.40	119.84
1	B	187	ASP	C-N-CA	5.25	126.40	119.84
1	F	232	SER	N-CA-C	5.20	115.58	109.60
1	G	261	VAL	CB-CA-C	-5.20	105.22	112.02
1	F	306	VAL	CB-CA-C	-5.18	102.94	110.81
1	J	80	HIS	CA-C-N	5.15	125.19	119.32
1	J	80	HIS	C-N-CA	5.15	125.19	119.32
1	H	305	ARG	N-CA-C	5.13	116.64	108.79
1	I	290	LEU	CA-C-N	5.05	124.66	119.56
1	I	290	LEU	C-N-CA	5.05	124.66	119.56
1	F	50	SER	N-CA-C	-5.03	106.65	112.89
1	A	65	GLY	N-CA-C	5.02	120.66	114.69

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2992	0	2867	79	0
1	B	2969	0	2843	119	0
1	C	2969	0	2843	62	0
1	D	2943	0	2816	70	0
1	E	2951	0	2822	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2984	0	2863	54	0
1	G	2966	0	2840	66	0
1	H	2975	0	2848	49	0
1	I	2975	0	2846	72	0
1	J	2966	0	2840	67	0
2	A	53	0	31	3	0
2	B	53	0	31	1	0
2	C	53	0	31	1	0
2	D	53	0	31	4	0
2	E	53	0	31	3	0
2	F	53	0	31	0	0
2	G	53	0	31	3	0
2	H	53	0	31	0	0
2	I	53	0	31	4	0
2	J	53	0	31	1	0
3	A	25	0	11	1	0
3	B	25	0	11	4	0
3	C	25	0	11	0	0
3	E	21	0	11	0	0
3	F	25	0	11	0	0
3	G	25	0	11	1	0
3	H	25	0	11	0	0
3	I	21	0	11	0	0
3	J	25	0	11	1	0
4	A	18	0	24	1	0
4	B	6	0	8	2	0
4	C	12	0	16	2	0
4	D	12	0	16	1	0
4	E	24	0	32	2	0
4	F	12	0	16	2	0
4	G	18	0	24	0	0
4	H	12	0	16	2	0
4	I	24	0	32	5	0
4	J	12	0	16	0	0
5	D	36	0	24	1	0
6	F	10	0	11	0	0
6	I	10	0	12	1	0
7	A	89	0	0	3	0
7	B	68	0	0	2	0
7	C	60	0	0	2	0
7	D	46	0	0	2	0
7	E	51	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	F	60	0	0	1	0
7	G	53	0	0	1	0
7	H	75	0	0	0	0
7	I	65	0	0	2	0
7	J	46	0	0	3	0
All	All	31256	0	29084	675	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 11.

All (675) 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:C:388:GLN:HA	1:C:388:GLN:NE2	1.45	1.12
1:A:153:VAL:HA	1:A:154:GLU:HB3	1.31	1.11
1:C:388:GLN:HE21	1:C:388:GLN:CA	1.66	1.08
1:C:389:GLY:C	1:C:390:GLN:HG2	1.74	1.02
1:G:58:VAL:HG23	1:G:238:MET:HB3	1.41	0.99
1:A:153:VAL:HA	1:A:154:GLU:CB	1.94	0.98
1:C:388:GLN:HA	1:C:388:GLN:HE21	0.78	0.94
1:C:389:GLY:O	1:C:390:GLN:HG2	1.68	0.93
1:A:154:GLU:HG2	1:A:155:GLN:H	1.36	0.91
1:I:371:TYR:HE2	1:I:379:GLN:HE21	1.19	0.90
1:C:388:GLN:NE2	1:C:388:GLN:CA	2.30	0.89
1:B:194:SER:O	1:B:198:ARG:HG3	1.78	0.84
1:B:189:SER:HA	1:B:190:GLU:HB2	1.56	0.84
1:B:187:ASP:CG	1:B:188:PRO:HD2	2.02	0.84
1:B:169:ARG:HH11	1:B:169:ARG:HB3	1.42	0.83
1:D:151:GLU:HB2	1:D:164:VAL:HG12	1.60	0.83
1:A:225:MET:HE3	1:A:229:MET:HE1	1.61	0.82
1:B:198:ARG:HG2	1:B:198:ARG:HH11	1.44	0.82
1:G:151:GLU:HB2	1:G:164:VAL:HG12	1.62	0.81
1:B:169:ARG:HB3	1:B:169:ARG:NH1	1.94	0.81
1:I:67:ASN:HD21	2:I:450:FAD:HM82	1.45	0.81
1:A:153:VAL:CA	1:A:154:GLU:HB3	2.08	0.81
1:C:90:ASN:HD22	4:C:398:GOL:H2	1.44	0.80
1:F:167:VAL:CG1	1:F:201:THR:HG21	2.12	0.80
1:D:267:PHE:CD1	1:D:271:LYS:HG2	2.17	0.80
1:B:376:VAL:HG21	2:B:450:FAD:H5'2	1.63	0.79
1:B:192:ASP:OD1	1:B:194:SER:HB3	1.81	0.79
1:G:304:THR:HG23	1:G:305:ARG:HG2	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:GLY:O	1:C:390:GLN:CG	2.30	0.79
1:F:167:VAL:HG11	1:F:201:THR:HG21	1.66	0.78
1:J:246:ILE:HD12	1:J:250:ILE:HD12	1.66	0.78
1:D:162:VAL:HG23	1:D:193:ALA:HB1	1.63	0.78
1:C:117:GLY:HA2	1:J:208:ARG:HD2	1.66	0.77
1:A:92:LYS:HE2	1:A:96:GLU:OE2	1.85	0.77
1:C:262:ASP:HB3	1:C:272:LEU:HD12	1.65	0.76
1:I:371:TYR:HE2	1:I:379:GLN:NE2	1.81	0.76
1:B:238:MET:HE1	1:B:246:ILE:HG21	1.67	0.76
1:E:162:VAL:CG2	1:E:193:ALA:HB1	2.15	0.76
1:J:151:GLU:HB2	1:J:164:VAL:HG12	1.67	0.76
1:D:162:VAL:CG2	1:D:193:ALA:HB1	2.16	0.75
1:A:239:LEU:HD23	7:A:523:HOH:O	1.85	0.75
1:B:159:SER:OG	1:B:195:VAL:HB	1.87	0.74
1:E:162:VAL:HG23	1:E:193:ALA:HB1	1.69	0.74
1:G:336:PRO:O	1:G:338:PRO:HD3	1.87	0.74
1:D:280:ARG:HB3	7:D:584:HOH:O	1.86	0.74
1:B:318:HIS:CE1	1:H:316:ARG:HD3	2.22	0.74
1:B:238:MET:HE2	1:B:241:THR:HG21	1.69	0.73
1:A:173:ASN:OD1	1:A:177:ARG:NE	2.21	0.73
1:B:161:ASP:H	1:B:164:VAL:HG23	1.53	0.73
1:C:177:ARG:NH1	1:C:181:ARG:HH12	1.87	0.73
1:B:318:HIS:CD2	1:B:318:HIS:H	2.05	0.72
1:E:37:ALA:HA	1:E:57:ILE:HD11	1.70	0.72
1:I:152:LYS:HA	7:I:629:HOH:O	1.90	0.71
1:B:187:ASP:CB	1:B:188:PRO:HD2	2.20	0.70
1:I:371:TYR:CE2	1:I:379:GLN:NE2	2.59	0.70
1:J:162:VAL:CG2	1:J:193:ALA:HB1	2.21	0.70
1:B:388:GLN:HB2	7:B:656:HOH:O	1.92	0.70
1:F:117:GLY:HA2	1:H:208:ARG:HD2	1.75	0.69
1:G:162:VAL:CG2	1:G:193:ALA:HB1	2.23	0.69
1:B:206:ASP:OD1	1:B:208:ARG:HD3	1.94	0.68
1:G:272:LEU:HD22	1:G:368:TYR:CE1	2.29	0.68
1:I:269:TYR:CE2	1:I:348:LYS:HB3	2.29	0.68
1:I:122:ILE:HA	1:I:123:PRO:C	2.19	0.68
1:J:86:ILE:HG21	1:J:109:HIS:HB2	1.75	0.68
1:A:376:VAL:HG21	2:A:450:FAD:H5'2	1.76	0.67
1:D:48:LEU:HD12	1:D:53:GLN:HG3	1.77	0.67
1:E:29:GLY:HA2	1:E:251:PRO:HG2	1.76	0.67
1:E:255:MET:HB3	1:E:359:VAL:HG22	1.77	0.67
1:E:280:ARG:NH1	1:E:282:GLU:OE2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:29:GLY:HA3	1:H:251:PRO:HB2	1.77	0.66
1:F:89:THR:HA	4:F:398:GOL:H11	1.78	0.66
1:F:206:ASP:OD1	1:F:208:ARG:HD3	1.95	0.66
1:J:64:ILE:HD12	1:J:226:PHE:HB3	1.76	0.66
1:B:30:PHE:O	1:B:252:PHE:HA	1.96	0.66
1:I:371:TYR:HB3	1:I:376:VAL:HG23	1.78	0.66
1:D:208:ARG:HD2	1:I:117:GLY:HA2	1.78	0.66
1:H:246:ILE:HB	1:H:250:ILE:HD12	1.77	0.66
1:E:90:ASN:HD22	4:E:398:GOL:H2	1.61	0.65
1:I:207:ASN:HD21	4:I:402:GOL:H2	1.59	0.65
1:C:90:ASN:ND2	4:C:398:GOL:H2	2.10	0.65
1:C:336:PRO:O	1:C:338:PRO:HD3	1.96	0.65
1:G:162:VAL:HG23	1:G:193:ALA:HB1	1.79	0.65
1:I:336:PRO:O	1:I:338:PRO:HD3	1.97	0.65
1:J:206:ASP:OD1	1:J:208:ARG:HD3	1.97	0.65
1:B:150:ALA:O	1:B:151:GLU:HG3	1.96	0.65
1:B:160:GLU:HG2	1:B:164:VAL:CG2	2.26	0.65
1:H:253:GLN:HE21	1:H:253:GLN:HA	1.62	0.65
1:B:138:THR:HG23	1:B:140:PHE:H	1.62	0.64
1:B:158:THR:HA	1:B:191:LEU:O	1.97	0.64
1:E:262:ASP:OD2	1:E:271:LYS:HD2	1.96	0.64
1:A:250:ILE:HG12	1:I:250:ILE:HD13	1.80	0.63
1:D:167:VAL:CG1	1:D:201:THR:HG21	2.29	0.63
1:A:92:LYS:HE2	1:A:96:GLU:CD	2.24	0.62
1:B:138:THR:HG22	1:B:141:GLN:H	1.64	0.62
1:D:34:ILE:HD12	1:D:45:ALA:HB2	1.81	0.62
1:E:246:ILE:HD13	1:E:250:ILE:HD12	1.80	0.62
1:A:246:ILE:HB	1:A:250:ILE:HD12	1.82	0.62
1:J:112:LEU:HG	1:J:119:LEU:HB3	1.82	0.62
1:J:296:ASN:HA	1:J:305:ARG:HB3	1.82	0.61
1:G:206:ASP:OD1	1:G:208:ARG:HD3	2.00	0.61
1:B:117:GLY:CA	1:C:208:ARG:HD2	2.30	0.61
1:B:280:ARG:NH1	1:B:282:GLU:OE2	2.33	0.61
1:F:131:ARG:HD2	7:F:603:HOH:O	2.00	0.61
1:D:297:TYR:HE1	1:D:306:VAL:HG23	1.64	0.61
1:A:155:GLN:HB2	1:A:157[B]:ARG:HG3	1.82	0.61
1:B:185:GLY:O	1:B:186:LEU:HB3	2.01	0.61
1:B:187:ASP:OD1	1:B:188:PRO:HD2	2.01	0.61
1:E:306:VAL:HG22	1:E:324:TYR:CD1	2.36	0.60
1:A:212:ASP:OD2	1:A:212:ASP:N	2.31	0.60
1:B:160:GLU:HG2	1:B:164:VAL:HG21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:37:ALA:HA	1:I:57:ILE:HD11	1.82	0.60
1:G:304:THR:HG23	1:G:305:ARG:CG	2.31	0.60
1:I:39:PHE:O	1:I:43:VAL:HG23	2.02	0.60
1:B:163:VAL:HG23	1:B:164:VAL:N	2.16	0.60
1:D:249:PHE:HE2	1:J:250:ILE:HG23	1.67	0.60
1:C:30:PHE:O	1:C:252:PHE:HA	2.02	0.60
1:E:206:ASP:OD1	1:E:208:ARG:HD3	2.02	0.60
1:B:126:LEU:HD23	1:B:142:VAL:CG2	2.32	0.59
1:D:269:TYR:HE2	1:D:352:LEU:HD11	1.67	0.59
1:D:183:GLN:HE22	1:D:305:ARG:HH12	1.51	0.59
1:G:122:ILE:HD12	1:G:123:PRO:HA	1.84	0.59
1:H:225:MET:HE3	1:H:229:MET:HE1	1.83	0.59
1:G:58:VAL:HG23	1:G:238:MET:CB	2.25	0.59
1:B:164:VAL:HG22	1:B:172:TYR:CD1	2.37	0.59
1:D:122:ILE:HA	1:D:123:PRO:C	2.28	0.59
1:D:376:VAL:HG21	2:D:450:FAD:H5'2	1.83	0.59
1:H:64:ILE:HD12	1:H:226:PHE:HB3	1.84	0.59
1:E:336:PRO:O	1:E:338:PRO:HD3	2.03	0.59
1:H:162:VAL:CG2	1:H:193:ALA:HB1	2.32	0.59
1:E:123:PRO:HB3	1:E:200:PRO:O	2.03	0.58
1:C:372:ASN:HB2	1:C:375:GLN:HG3	1.84	0.58
1:J:272:LEU:HD22	1:J:368:TYR:CE1	2.39	0.58
1:B:255:MET:HB3	1:B:359:VAL:HG22	1.86	0.58
1:B:195:VAL:CG2	1:B:338:PRO:HG2	2.34	0.58
1:I:151:GLU:HB2	1:I:164:VAL:HG13	1.85	0.58
1:B:138:THR:O	1:B:142:VAL:HG23	2.04	0.57
1:B:198:ARG:HG2	1:B:198:ARG:NH1	2.15	0.57
1:D:208:ARG:HD2	1:I:117:GLY:CA	2.33	0.57
1:G:29:GLY:HA3	1:G:251:PRO:HB2	1.85	0.57
1:G:272:LEU:HD22	1:G:368:TYR:CZ	2.39	0.57
1:A:154:GLU:HG2	1:A:155:GLN:N	2.13	0.57
1:B:138:THR:OG1	1:G:135:LEU:HD23	2.04	0.57
1:J:297:TYR:HE1	1:J:306:VAL:HG23	1.69	0.57
1:D:163:VAL:HG12	1:D:172:TYR:HB2	1.86	0.57
1:F:262:ASP:HB3	1:F:272:LEU:HB2	1.87	0.57
1:J:369:ARG:HD3	1:J:371:TYR:CZ	2.39	0.57
1:B:117:GLY:HA3	1:C:208:ARG:HD2	1.85	0.57
1:B:339:ARG:HB3	1:B:341:GLU:OE2	2.05	0.57
1:C:37:ALA:HA	1:C:57:ILE:HD11	1.86	0.57
1:C:177:ARG:HH11	1:C:181:ARG:HH12	1.52	0.57
1:I:125:ASN:HB2	1:I:204:ASN:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:306:VAL:HG13	1:I:324:TYR:CD1	2.39	0.57
1:A:334:TYR:O	1:A:364:ARG:NH1	2.37	0.57
1:D:47:ARG:HA	1:D:47:ARG:NE	2.19	0.57
1:G:112:LEU:HG	1:G:119:LEU:HB3	1.87	0.57
1:I:67:ASN:HD21	2:I:450:FAD:C8M	2.17	0.57
1:A:284:HIS:CD2	1:A:289:LEU:HD22	2.40	0.56
1:D:151:GLU:HB2	1:D:164:VAL:CG1	2.34	0.56
1:F:192:ASP:HB2	1:F:338:PRO:O	2.05	0.56
1:F:327:PRO:O	1:F:328:ARG:HD3	2.04	0.56
1:I:269:TYR:CD2	1:I:348:LYS:HB3	2.40	0.56
1:B:47:ARG:HA	1:B:47:ARG:NE	2.19	0.56
1:D:370:TYR:HE1	2:D:450:FAD:H1'1	1.71	0.56
1:H:336:PRO:O	1:H:338:PRO:HD3	2.05	0.56
1:D:225:MET:HE3	1:D:229:MET:HE1	1.87	0.56
1:B:169:ARG:HH11	1:B:169:ARG:CB	2.14	0.56
1:D:269:TYR:CE2	1:D:352:LEU:HD11	2.41	0.56
1:D:195:VAL:CG2	1:D:338:PRO:HG2	2.36	0.56
1:J:131:ARG:HD2	7:J:432:HOH:O	2.06	0.56
1:J:272:LEU:HD22	1:J:368:TYR:CZ	2.40	0.56
1:C:289:LEU:HD23	1:C:322:VAL:HG11	1.87	0.56
1:D:297:TYR:HE1	1:D:306:VAL:CG2	2.19	0.56
1:A:122:ILE:HD12	1:A:123:PRO:HA	1.87	0.56
1:A:153:VAL:CA	1:A:154:GLU:CB	2.72	0.56
1:E:29:GLY:CA	1:E:251:PRO:HG2	2.36	0.56
1:A:39:PHE:CE2	1:A:225:MET:HE1	2.41	0.55
1:C:117:GLY:CA	1:J:208:ARG:HD2	2.33	0.55
1:J:371:TYR:HE2	1:J:379:GLN:NE2	2.02	0.55
1:A:123:PRO:HB3	1:A:200:PRO:O	2.05	0.55
1:F:84:PRO:HD2	1:F:325:GLU:OE1	2.05	0.55
1:B:246:ILE:HB	1:B:250:ILE:HD12	1.89	0.55
1:I:280:ARG:NH1	1:I:282:GLU:OE2	2.39	0.55
1:I:308:GLU:HB3	1:I:311:HIS:HD2	1.70	0.55
1:J:126:LEU:O	1:J:126:LEU:HD22	2.05	0.55
1:B:196:THR:HG22	3:B:500:UDP:H1'	1.89	0.55
1:E:86:ILE:HD12	1:E:86:ILE:N	2.22	0.55
1:H:122:ILE:HA	1:H:123:PRO:C	2.31	0.55
1:F:30:PHE:O	1:F:252:PHE:HA	2.07	0.55
1:F:336:PRO:O	1:F:338:PRO:HD3	2.05	0.55
1:J:151:GLU:OE2	1:J:164:VAL:HG11	2.07	0.55
1:H:151:GLU:HB2	1:H:164:VAL:CG1	2.36	0.55
1:A:117:GLY:CA	1:G:208:ARG:HD2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:ARG:HG3	1:D:365:LEU:HG	1.89	0.55
1:E:206:ASP:OD2	1:E:208:ARG:NH1	2.39	0.55
1:C:151:GLU:HB2	1:C:164:VAL:HG13	1.88	0.54
1:A:316:ARG:HD3	1:I:318:HIS:CD2	2.42	0.54
1:B:362:VAL:HG23	1:B:379:GLN:HG2	1.88	0.54
1:D:117:GLY:HA2	1:F:208:ARG:HD2	1.89	0.54
1:A:153:VAL:HG13	1:A:154:GLU:HB3	1.90	0.54
1:B:158:THR:HG22	1:B:191:LEU:O	2.08	0.54
1:G:111:VAL:HG22	1:G:294:THR:HB	1.87	0.54
1:J:58:VAL:HG23	1:J:238:MET:HG2	1.90	0.54
1:C:232:SER:HB3	1:C:235:ILE:HG13	1.90	0.54
1:B:327:PRO:O	1:B:328:ARG:HD3	2.08	0.54
1:J:269:TYR:CZ	1:J:352:LEU:HD11	2.43	0.54
1:D:273:PRO:HG2	1:D:342:ASN:OD1	2.08	0.54
1:D:316:ARG:HD3	1:J:318:HIS:CD2	2.42	0.54
1:E:371:TYR:HE2	1:E:379:GLN:NE2	2.06	0.54
1:A:117:GLY:HA3	1:G:208:ARG:HD2	1.89	0.54
1:E:272:LEU:HD22	1:E:368:TYR:CZ	2.43	0.54
1:J:172:TYR:OH	1:J:188:PRO:HG2	2.07	0.54
1:D:195:VAL:HG23	1:D:338:PRO:HG2	1.89	0.53
1:B:159:SER:O	1:B:196:THR:OG1	2.19	0.53
1:B:186:LEU:O	1:B:187:ASP:CB	2.57	0.53
1:I:310:LYS:HG3	7:I:406:HOH:O	2.08	0.53
1:B:86:ILE:HG21	1:B:109:HIS:HB2	1.88	0.53
1:B:160:GLU:C	1:B:162:VAL:H	2.17	0.53
1:F:289:LEU:HD23	1:F:322:VAL:HG11	1.89	0.53
1:D:140:PHE:CD2	4:D:399:GOL:H2	2.43	0.53
1:B:208:ARG:HD2	1:G:117:GLY:CA	2.38	0.53
1:D:70:ASP:HB3	1:D:80:HIS:HD2	1.72	0.53
1:E:60:ARG:HA	1:E:241:THR:H	1.73	0.53
1:J:387:LEU:O	1:J:388:GLN:HG2	2.09	0.53
1:C:371:TYR:CE1	1:C:379:GLN:NE2	2.77	0.53
1:G:261:VAL:HG22	1:G:366:ALA:O	2.09	0.52
1:E:182:LYS:HG2	1:E:304:THR:HG22	1.91	0.52
1:J:159:SER:HB3	1:J:196:THR:HG23	1.91	0.52
1:A:153:VAL:CG1	1:A:154:GLU:HB3	2.39	0.52
1:B:172:TYR:OH	1:B:177:ARG:HG3	2.09	0.52
1:H:162:VAL:HG23	1:H:193:ALA:HB1	1.91	0.52
1:I:376:VAL:HG21	2:I:450:FAD:H5'2	1.91	0.52
1:J:122:ILE:HA	1:J:123:PRO:C	2.35	0.52
1:A:139:SER:O	1:A:142:VAL:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:MET:HE1	1:D:246:ILE:HG21	1.92	0.52
3:G:500:UDP:O2B	3:G:500:UDP:H5'1	2.09	0.52
1:I:151:GLU:HB2	1:I:164:VAL:CG1	2.39	0.52
1:C:151:GLU:HB2	1:C:164:VAL:CG1	2.40	0.52
1:J:47:ARG:NE	1:J:47:ARG:HA	2.25	0.52
1:A:272:LEU:HD22	1:A:368:TYR:CZ	2.45	0.52
1:D:316:ARG:HD3	1:J:318:HIS:NE2	2.25	0.52
1:E:159:SER:HA	1:E:193:ALA:HA	1.91	0.51
1:A:250:ILE:HG12	1:I:250:ILE:CD1	2.40	0.51
1:G:357:GLN:OE1	1:G:357:GLN:HA	2.08	0.51
1:A:47:ARG:HA	1:A:47:ARG:NE	2.26	0.51
1:A:167:VAL:CG1	1:A:201:THR:HG21	2.40	0.51
1:E:79:ILE:HG12	1:E:80:HIS:N	2.21	0.51
1:E:60:ARG:HD2	2:E:450:FAD:C4A	2.41	0.51
1:B:33:LEU:HD23	1:B:255:MET:HE2	1.91	0.51
1:H:69:TYR:O	1:H:81:PRO:HD2	2.09	0.51
1:A:297:TYR:HE1	1:A:306:VAL:HG23	1.75	0.51
1:J:337:VAL:HB	1:J:342:ASN:HD22	1.75	0.51
1:A:172:TYR:OH	1:A:188:PRO:HG2	2.11	0.51
1:J:86:ILE:HD12	1:J:86:ILE:N	2.26	0.51
1:A:336:PRO:O	1:A:338:PRO:HD3	2.10	0.51
1:A:277:LEU:HD23	1:A:327:PRO:HA	1.92	0.50
1:B:186:LEU:O	1:B:187:ASP:HB2	2.09	0.50
1:C:246:ILE:HB	1:C:250:ILE:HD12	1.92	0.50
1:B:172:TYR:CE2	1:B:177:ARG:HD3	2.45	0.50
1:D:36:GLY:O	1:D:57:ILE:HD11	2.12	0.50
1:C:139:SER:O	1:C:142:VAL:HG12	2.11	0.50
1:D:120:LEU:HB3	1:D:128:THR:HG23	1.93	0.50
1:A:56:LEU:HD13	1:I:238:MET:HE3	1.92	0.50
1:B:39:PHE:O	1:B:43:VAL:HG23	2.12	0.50
1:E:162:VAL:HG21	1:E:193:ALA:HB1	1.90	0.50
1:F:117:GLY:CA	1:H:208:ARG:HD2	2.40	0.50
1:I:102:THR:HB	1:I:225:MET:HG3	1.93	0.50
1:C:389:GLY:O	1:C:390:GLN:CD	2.55	0.50
1:H:33:LEU:HD23	1:H:255:MET:HE2	1.93	0.50
1:H:180:THR:HB	1:H:188:PRO:HG3	1.94	0.50
1:B:199:VAL:HG22	3:B:500:UDP:O2A	2.11	0.50
1:C:376:VAL:HG21	2:C:450:FAD:H5'2	1.92	0.50
1:E:117:GLY:CA	1:I:208:ARG:HD2	2.42	0.50
1:F:262:ASP:OD1	1:F:263:ALA:N	2.44	0.50
1:J:275:ARG:HG3	1:J:276:SER:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:80:HIS:HB2	1:I:309:PHE:CE2	2.46	0.50
1:B:162:VAL:HG21	1:B:197:ALA:HB2	1.92	0.50
1:C:47:ARG:NE	1:C:47:ARG:HA	2.26	0.50
1:F:269:TYR:CE2	1:F:352:LEU:HD11	2.46	0.50
1:G:217:MET:HE2	1:G:312:ILE:HG22	1.93	0.50
1:D:279:PHE:CD2	1:D:325:GLU:HG2	2.47	0.50
1:E:159:SER:HB3	1:E:196:THR:HG23	1.93	0.50
1:F:369:ARG:HD2	1:F:371:TYR:CZ	2.46	0.50
1:I:30:PHE:O	1:I:252:PHE:HA	2.11	0.50
1:F:272:LEU:HD22	1:F:368:TYR:CZ	2.47	0.49
1:I:294:THR:HG21	1:I:305:ARG:CZ	2.43	0.49
1:I:253:GLN:NE2	1:I:253:GLN:HA	2.27	0.49
1:J:30:PHE:O	1:J:252:PHE:HA	2.12	0.49
1:B:273:PRO:HG2	1:B:342:ASN:OD1	2.12	0.49
1:H:206:ASP:OD1	1:H:208:ARG:HD3	2.12	0.49
1:A:376:VAL:HG21	2:A:450:FAD:C5'	2.41	0.49
1:J:169:ARG:HD2	7:J:641:HOH:O	2.13	0.49
1:A:151:GLU:HB2	1:A:164:VAL:HG13	1.95	0.49
1:G:308:GLU:HG3	1:G:322:VAL:HG12	1.95	0.49
1:J:269:TYR:OH	1:J:352:LEU:HD21	2.12	0.49
1:J:337:VAL:HB	1:J:342:ASN:ND2	2.28	0.49
1:B:135:LEU:HD23	1:C:138:THR:HG21	1.93	0.49
1:B:336:PRO:O	1:B:338:PRO:HD3	2.12	0.49
1:C:151:GLU:OE2	1:C:169:ARG:NH2	2.45	0.49
1:E:145:PHE:O	1:E:149:VAL:HG22	2.12	0.49
1:G:111:VAL:HG12	1:G:122:ILE:CG2	2.42	0.49
1:J:58:VAL:HG23	1:J:238:MET:HB3	1.95	0.49
1:H:90:ASN:ND2	4:H:398:GOL:H2	2.28	0.49
1:H:97:TYR:HD2	1:H:98:LEU:HD13	1.77	0.49
1:J:275:ARG:HG3	1:J:276:SER:H	1.78	0.49
1:A:29:GLY:HA3	1:A:251:PRO:HB2	1.93	0.49
1:B:163:VAL:CG2	1:B:164:VAL:N	2.75	0.49
1:G:297:TYR:HE1	1:G:306:VAL:HG23	1.76	0.49
1:I:90:ASN:HD22	4:I:398:GOL:H32	1.78	0.49
1:A:90:ASN:HD22	4:A:398:GOL:H12	1.76	0.49
1:C:273:PRO:HG2	1:C:342:ASN:OD1	2.13	0.49
1:D:117:GLY:CA	1:F:208:ARG:HD2	2.42	0.49
1:D:249:PHE:CE2	1:J:250:ILE:HG23	2.46	0.49
1:E:125:ASN:HB2	1:E:204:ASN:O	2.12	0.49
1:G:162:VAL:HG21	1:G:193:ALA:HB1	1.94	0.49
1:G:167:VAL:HG12	1:G:201:THR:HG21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ASP:HB3	1:A:79:ILE:HD13	1.95	0.49
1:B:32:TYR:CD1	1:B:254:HIS:HB3	2.47	0.48
1:D:122:ILE:HG13	1:D:123:PRO:HA	1.95	0.48
1:E:371:TYR:CE2	1:E:379:GLN:NE2	2.80	0.48
1:I:90:ASN:HD22	4:I:398:GOL:C3	2.26	0.48
1:B:90:ASN:ND2	4:B:398:GOL:H2	2.28	0.48
1:B:199:VAL:HG21	3:B:500:UDP:C6	2.48	0.48
1:H:280:ARG:NH2	1:H:326:TYR:OH	2.46	0.48
1:I:212:ASP:OD1	4:I:398:GOL:H2	2.13	0.48
1:I:364:ARG:NH2	1:I:370:TYR:CD2	2.82	0.48
1:B:386:ARG:HD2	7:B:505:HOH:O	2.13	0.48
1:A:280:ARG:NH1	1:A:282:GLU:OE1	2.46	0.48
1:D:60:ARG:HD3	2:D:450:FAD:C5A	2.43	0.48
1:H:294:THR:HG21	1:H:305:ARG:HH11	1.79	0.48
1:B:47:ARG:HA	1:B:47:ARG:HE	1.77	0.48
1:G:58:VAL:HG22	1:G:241:THR:HB	1.95	0.48
1:I:373:MET:HE2	2:I:450:FAD:C2	2.44	0.48
1:J:132:LEU:HD23	1:J:133:TYR:CZ	2.48	0.48
1:A:327:PRO:O	1:A:328:ARG:HD3	2.13	0.48
1:E:86:ILE:HG21	1:E:109:HIS:HB2	1.94	0.48
1:E:369:ARG:HD2	1:E:371:TYR:CE2	2.48	0.48
1:H:67:ASN:HB3	1:H:85:HIS:NE2	2.29	0.48
1:B:199:VAL:HG21	3:B:500:UDP:H6	1.79	0.48
1:E:61:ARG:HG3	2:E:450:FAD:O2B	2.14	0.48
1:G:125:ASN:C	1:G:125:ASN:OD1	2.56	0.48
1:D:250:ILE:O	1:D:252:PHE:HD2	1.97	0.48
1:G:187:ASP:CG	1:G:188:PRO:HD2	2.38	0.48
1:B:163:VAL:O	1:B:166:LYS:N	2.47	0.48
1:E:336:PRO:C	1:E:338:PRO:HD3	2.38	0.48
1:G:306:VAL:HG22	1:G:324:TYR:CD1	2.49	0.48
1:C:69:TYR:O	1:C:81:PRO:HD2	2.14	0.47
1:F:86:ILE:HG21	1:F:109:HIS:HB2	1.96	0.47
1:I:77:VAL:HG11	1:I:321:SER:HB2	1.95	0.47
1:I:112:LEU:HG	1:I:119:LEU:HB3	1.95	0.47
1:I:142:VAL:HG13	1:I:203:THR:HG22	1.95	0.47
1:B:138:THR:HG23	1:B:140:PHE:N	2.28	0.47
1:B:160:GLU:O	1:B:161:ASP:HB2	2.14	0.47
1:F:44:LEU:HD13	1:F:362:VAL:HG11	1.96	0.47
1:F:123:PRO:HB3	1:F:200:PRO:O	2.14	0.47
1:A:44:LEU:O	1:A:48:LEU:HB2	2.14	0.47
1:B:150:ALA:HB1	1:B:165:SER:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:ARG:C	1:C:388:GLN:H	2.23	0.47
1:D:112:LEU:HG	1:D:119:LEU:HB3	1.96	0.47
1:G:208:ARG:HB3	7:G:401:HOH:O	2.13	0.47
1:H:364:ARG:HG3	1:H:369:ARG:O	2.14	0.47
1:J:39:PHE:CZ	1:J:225:MET:HE1	2.49	0.47
1:F:180:THR:HG23	1:F:184:TRP:CD1	2.50	0.47
1:G:70:ASP:OD1	1:G:222:TYR:N	2.48	0.47
1:B:187:ASP:CG	1:B:188:PRO:CD	2.83	0.47
1:B:246:ILE:HD12	1:B:246:ILE:C	2.39	0.47
1:B:386:ARG:C	1:B:388:GLN:H	2.23	0.47
1:D:182:LYS:HG2	1:D:304:THR:HG22	1.97	0.47
1:E:364:ARG:NH2	1:E:370:TYR:CD1	2.82	0.47
1:F:369:ARG:NH1	1:F:379:GLN:HE21	2.12	0.47
1:H:28:LYS:HE2	1:H:28:LYS:HA	1.96	0.47
1:I:253:GLN:HA	1:I:253:GLN:HE21	1.78	0.47
1:B:306:VAL:HG13	1:B:324:TYR:CD1	2.50	0.47
1:G:151:GLU:OE2	1:G:164:VAL:HG11	2.14	0.47
1:F:272:LEU:HD22	1:F:368:TYR:CE1	2.49	0.47
1:B:246:ILE:HD12	1:B:247:ALA:N	2.30	0.47
1:G:189:SER:C	1:G:191:LEU:H	2.23	0.47
1:I:123:PRO:HB3	1:I:200:PRO:O	2.15	0.47
1:I:279:PHE:CE2	1:I:325:GLU:HG2	2.50	0.47
1:F:137:LEU:HA	1:F:141:GLN:OE1	2.15	0.46
1:G:44:LEU:HD13	1:G:256:ILE:HG21	1.96	0.46
1:G:67:ASN:ND2	2:G:450:FAD:HM83	2.30	0.46
1:H:90:ASN:HD22	4:H:398:GOL:H2	1.81	0.46
1:I:180:THR:HG21	1:I:188:PRO:HG3	1.98	0.46
1:A:225:MET:HE3	1:A:229:MET:CE	2.38	0.46
1:B:195:VAL:HG23	1:B:338:PRO:HG2	1.96	0.46
1:B:318:HIS:CD2	1:B:318:HIS:N	2.80	0.46
1:D:161:ASP:O	1:D:165:SER:HB3	2.16	0.46
1:H:305:ARG:HD2	1:H:325:GLU:OE1	2.15	0.46
1:J:177:ARG:HD2	7:J:642:HOH:O	2.15	0.46
1:B:34:ILE:HD12	1:B:55:VAL:HG11	1.96	0.46
1:I:262:ASP:HB3	1:I:272:LEU:HB2	1.97	0.46
1:B:120:LEU:HB3	1:B:128:THR:HG23	1.96	0.46
1:B:385:ARG:HG2	1:B:390:GLN:OE1	2.16	0.46
1:C:86:ILE:HG21	1:C:109:HIS:HB2	1.98	0.46
1:D:327:PRO:O	1:D:328:ARG:HD3	2.16	0.46
1:E:217:MET:HE2	1:E:312:ILE:HG22	1.96	0.46
1:J:364:ARG:NH2	1:J:370:TYR:HD1	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:208:ARG:HD2	1:H:117:GLY:CA	2.45	0.46
1:H:29:GLY:O	1:H:54:ARG:CZ	2.63	0.46
1:A:278:GLU:HG3	1:A:328:ARG:CG	2.46	0.46
1:F:277:LEU:HD23	1:F:327:PRO:HA	1.98	0.46
1:A:289:LEU:HD23	1:A:322:VAL:HG11	1.98	0.46
1:B:185:GLY:O	1:B:186:LEU:CB	2.63	0.46
1:D:229:MET:HB2	1:D:229:MET:HE3	1.76	0.46
1:E:30:PHE:O	1:E:252:PHE:HA	2.16	0.46
1:F:118:GLN:HB3	1:F:120:LEU:HD13	1.96	0.46
1:I:153:VAL:HG23	1:I:165:SER:HB3	1.97	0.46
1:D:111:VAL:HG22	1:D:294:THR:HB	1.96	0.46
1:I:47:ARG:NH1	1:I:100:ARG:HH12	2.14	0.46
1:B:58:VAL:HG12	1:B:238:MET:HB3	1.97	0.46
1:C:163:VAL:HG12	1:C:172:TYR:HB2	1.97	0.46
1:D:206:ASP:OD1	1:D:208:ARG:HD3	2.16	0.46
1:E:236:LYS:HA	1:E:236:LYS:HD3	1.70	0.46
1:G:47:ARG:HA	1:G:47:ARG:NE	2.30	0.46
1:B:389:GLY:O	1:B:390:GLN:C	2.58	0.46
1:C:29:GLY:O	1:C:54:ARG:NH1	2.49	0.46
1:G:246:ILE:HB	1:G:250:ILE:HD12	1.96	0.46
1:I:185:GLY:O	1:I:186:LEU:HD13	2.16	0.46
1:A:272:LEU:HD13	1:A:368:TYR:CD1	2.52	0.45
1:I:207:ASN:ND2	4:I:402:GOL:H2	2.30	0.45
1:J:225:MET:HG2	1:J:229:MET:CE	2.46	0.45
1:D:122:ILE:HD13	5:D:600:URM:O20	2.15	0.45
1:E:204:ASN:C	1:E:204:ASN:OD1	2.59	0.45
1:H:308:GLU:HB3	1:H:311:HIS:HD2	1.81	0.45
1:I:80:HIS:HB2	1:I:309:PHE:HE2	1.82	0.45
1:D:246:ILE:HB	1:D:250:ILE:HD12	1.99	0.45
1:B:90:ASN:HD22	4:B:398:GOL:H2	1.81	0.45
1:B:182:LYS:HG2	1:B:327:PRO:HG2	1.99	0.45
1:B:229:MET:HE2	1:B:229:MET:HB2	1.84	0.45
1:D:372:ASN:HB3	2:D:450:FAD:O2	2.17	0.45
1:F:44:LEU:O	1:F:48:LEU:HB2	2.17	0.45
1:I:86:ILE:HG21	1:I:109:HIS:HB2	1.98	0.45
1:A:59:ASP:N	7:A:523:HOH:O	2.48	0.45
1:F:236:LYS:HA	1:F:236:LYS:HD3	1.81	0.45
1:H:84:PRO:HG3	1:H:307:SER:OG	2.16	0.45
1:H:318:HIS:CD2	1:H:319:GLN:HG3	2.52	0.45
1:B:172:TYR:HE2	1:B:177:ARG:HD3	1.81	0.45
1:H:47:ARG:HA	1:H:47:ARG:NE	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:232:SER:HB3	1:J:235:ILE:HG13	1.97	0.45
1:C:206:ASP:OD1	1:C:208:ARG:HD3	2.16	0.45
1:H:43:VAL:HG21	1:H:377:VAL:HG13	1.99	0.45
1:C:208:ARG:HB3	7:C:401:HOH:O	2.17	0.45
1:E:376:VAL:HG21	2:E:450:FAD:H5'2	1.99	0.45
1:G:30:PHE:O	1:G:252:PHE:HA	2.17	0.45
1:H:339:ARG:O	1:H:340:PRO:C	2.60	0.45
1:B:138:THR:HG22	1:B:141:GLN:N	2.31	0.44
1:E:269:TYR:OH	1:E:352:LEU:HD21	2.17	0.44
1:J:305:ARG:NH2	3:J:500:UDP:O3B	2.50	0.44
1:J:336:PRO:O	1:J:338:PRO:HD3	2.17	0.44
1:D:158:THR:HA	1:D:191:LEU:O	2.17	0.44
1:I:162:VAL:CG2	1:I:193:ALA:HB1	2.48	0.44
1:A:155:GLN:HB2	1:A:157[A]:ARG:HG3	1.98	0.44
1:B:138:THR:HG23	1:B:139:SER:N	2.30	0.44
1:E:79:ILE:HB	1:E:309:PHE:CD1	2.51	0.44
1:F:242:ASP:HB3	1:F:245:GLU:HG3	1.99	0.44
1:I:206:ASP:OD1	1:I:208:ARG:HD3	2.17	0.44
1:D:298:PRO:HD2	7:D:410:HOH:O	2.16	0.44
1:J:37:ALA:HA	1:J:57:ILE:HD11	1.99	0.44
1:B:144:GLU:O	1:B:145:PHE:C	2.60	0.44
1:D:369:ARG:HB3	1:D:371:TYR:CE2	2.53	0.44
1:F:289:LEU:CD2	1:F:322:VAL:HG11	2.47	0.44
1:F:297:TYR:HE1	1:F:306:VAL:CG2	2.30	0.44
1:G:48:LEU:HD13	1:G:384:PHE:HD1	1.83	0.44
1:I:364:ARG:NH2	1:I:370:TYR:HD2	2.14	0.44
1:E:138:THR:HG21	1:H:135:LEU:HD23	1.99	0.44
1:E:337:VAL:O	1:E:339:ARG:HG2	2.18	0.44
4:E:400:GOL:O3	4:E:400:GOL:O1	2.30	0.44
1:I:272:LEU:HD22	1:I:368:TYR:CZ	2.52	0.44
1:A:58:VAL:HG12	1:A:238:MET:HB3	1.99	0.44
1:B:122:ILE:HA	1:B:123:PRO:C	2.43	0.44
1:B:318:HIS:H	1:B:318:HIS:HD2	1.56	0.44
1:C:238:MET:HE3	1:F:236:LYS:HB3	2.00	0.44
1:D:250:ILE:HA	1:D:251:PRO:HD3	1.85	0.44
1:E:289:LEU:N	1:E:308:GLU:OE1	2.48	0.44
1:H:334:TYR:O	1:H:364:ARG:HD3	2.17	0.44
1:B:267:PHE:C	1:B:269:TYR:H	2.26	0.44
1:A:364:ARG:HG3	1:A:369:ARG:O	2.18	0.44
1:B:306:VAL:HG13	1:B:324:TYR:CE1	2.52	0.44
1:C:385:ARG:O	1:C:389:GLY:HA2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:HIS:CE1	1:D:319:GLN:HG3	2.53	0.44
1:H:169:ARG:HE	1:H:169:ARG:HB2	1.63	0.44
1:J:386:ARG:C	1:J:388:GLN:H	2.26	0.44
1:A:155:GLN:C	1:A:156:VAL:HG23	2.43	0.43
1:B:387:LEU:HD12	1:B:387:LEU:HA	1.83	0.43
1:C:112:LEU:HG	1:C:119:LEU:HB3	2.00	0.43
1:D:187:ASP:CG	1:D:188:PRO:HD2	2.44	0.43
1:E:246:ILE:CD1	1:E:250:ILE:HD12	2.47	0.43
1:E:333:PRO:HG2	1:E:365:LEU:HD13	2.00	0.43
1:G:139:SER:O	1:G:142:VAL:HG12	2.17	0.43
1:I:167:VAL:CG1	1:I:201:THR:HG21	2.47	0.43
1:J:162:VAL:HG21	1:J:193:ALA:HB1	1.97	0.43
1:B:160:GLU:HG2	1:B:164:VAL:HG23	2.00	0.43
1:C:229:MET:HE3	1:C:229:MET:HB2	1.76	0.43
1:F:269:TYR:CE2	1:F:352:LEU:CD1	3.01	0.43
1:G:47:ARG:NH1	1:G:100:ARG:HH12	2.16	0.43
1:B:172:TYR:CZ	1:B:177:ARG:HG3	2.53	0.43
1:B:189:SER:HA	1:B:190:GLU:CB	2.30	0.43
1:F:180:THR:HG23	1:F:184:TRP:HD1	1.82	0.43
1:H:105:ARG:NH1	1:H:312:ILE:O	2.51	0.43
1:B:269:TYR:HB2	1:B:349:TYR:CZ	2.54	0.43
1:F:145:PHE:O	1:F:149:VAL:HG22	2.18	0.43
1:F:385:ARG:HE	4:F:400:GOL:C1	2.31	0.43
1:G:124:ILE:HG23	1:G:128:THR:HB	2.00	0.43
1:I:70:ASP:HB2	1:I:79:ILE:O	2.18	0.43
1:B:208:ARG:HD2	1:G:117:GLY:HA2	2.01	0.43
1:C:337:VAL:HG12	1:C:339:ARG:HG3	2.01	0.43
1:C:388:GLN:N	1:C:389:GLY:HA2	2.32	0.43
1:J:100:ARG:HE	1:J:100:ARG:HB3	1.48	0.43
1:A:77:VAL:O	1:A:79:ILE:HG23	2.19	0.43
1:A:81:PRO:HD2	7:A:537:HOH:O	2.19	0.43
1:B:189:SER:CA	1:B:190:GLU:HB2	2.39	0.43
1:B:191:LEU:CD2	1:B:338:PRO:HD2	2.49	0.43
1:C:218:PRO:HG2	1:C:222:TYR:CD2	2.53	0.43
1:C:236:LYS:HE3	1:F:245:GLU:OE2	2.18	0.43
1:E:364:ARG:HG2	1:E:365:LEU:HD23	2.00	0.43
1:H:277:LEU:HD23	1:H:327:PRO:HA	2.01	0.43
1:I:31:ASP:O	1:I:253:GLN:HB2	2.19	0.43
1:B:289:LEU:HD12	1:B:289:LEU:HA	1.76	0.43
1:D:73:ASP:C	1:D:73:ASP:OD1	2.62	0.43
1:G:125:ASN:OD1	1:G:127:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:232:SER:HA	1:G:233:PRO:HD3	1.90	0.43
1:J:151:GLU:HB2	1:J:164:VAL:CG1	2.44	0.43
1:J:290:LEU:HD12	1:J:308:GLU:HB2	2.01	0.43
1:D:180:THR:HB	1:D:188:PRO:HG3	2.00	0.43
1:D:242:ASP:HB3	1:D:245:GLU:HG3	1.99	0.43
1:I:383:THR:HG22	1:I:387:LEU:HD22	2.00	0.43
1:A:373:MET:HE2	2:A:450:FAD:C2	2.49	0.43
1:B:223:THR:O	1:B:227:GLN:HG3	2.19	0.43
1:F:269:TYR:CZ	1:F:352:LEU:HD11	2.54	0.43
1:G:278:GLU:HB2	1:G:328:ARG:HG3	2.01	0.43
1:J:349:TYR:O	1:J:350:GLU:C	2.60	0.43
1:A:134:GLY:O	1:G:138:THR:HG22	2.19	0.42
1:D:260:PRO:HA	1:D:365:LEU:O	2.19	0.42
1:E:47:ARG:NE	1:E:47:ARG:HA	2.33	0.42
1:E:58:VAL:HB	1:E:238:MET:HB3	2.01	0.42
1:E:59:ASP:OD1	1:E:61:ARG:HG3	2.19	0.42
1:F:122:ILE:HA	1:F:123:PRO:C	2.44	0.42
1:F:261:VAL:HB	1:F:366:ALA:O	2.19	0.42
1:H:29:GLY:CA	1:H:251:PRO:HB2	2.48	0.42
1:J:44:LEU:CD1	1:J:362:VAL:HG11	2.49	0.42
1:J:356:ALA:HB1	1:J:359:VAL:HB	2.00	0.42
1:A:122:ILE:HA	1:A:123:PRO:C	2.44	0.42
1:B:116:ASP:OD2	1:B:174:LYS:HE2	2.18	0.42
1:B:159:SER:C	1:B:162:VAL:HG12	2.44	0.42
1:C:202:ARG:HB3	1:C:204:ASN:OD1	2.18	0.42
1:D:369:ARG:HE	1:D:369:ARG:HB2	1.66	0.42
1:G:94:VAL:HG13	1:G:377:VAL:HG11	2.01	0.42
1:H:126:LEU:HD23	1:H:142:VAL:HB	2.01	0.42
1:H:262:ASP:HB3	1:H:272:LEU:HB2	2.00	0.42
1:A:250:ILE:HA	1:A:251:PRO:HD3	1.91	0.42
1:B:208:ARG:HD2	1:G:117:GLY:HA3	2.00	0.42
1:C:386:ARG:O	1:C:388:GLN:N	2.53	0.42
1:D:386:ARG:C	1:D:388:GLN:N	2.75	0.42
1:E:277:LEU:HD23	1:E:327:PRO:HA	2.01	0.42
1:F:48:LEU:HD12	1:F:48:LEU:HA	1.95	0.42
1:B:160:GLU:C	1:B:162:VAL:N	2.77	0.42
1:D:334:TYR:HA	1:D:364:ARG:NH2	2.35	0.42
1:G:339:ARG:O	1:G:340:PRO:C	2.62	0.42
1:I:125:ASN:OD1	1:I:127:ASP:N	2.51	0.42
1:J:373:MET:HG3	2:J:450:FAD:H2'	2.02	0.42
1:C:238:MET:HE1	1:C:246:ILE:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:359:VAL:HG12	1:G:361:PHE:CE1	2.54	0.42
1:J:47:ARG:HA	1:J:47:ARG:HE	1.85	0.42
1:J:364:ARG:NH2	1:J:370:TYR:CD1	2.88	0.42
1:A:177:ARG:NH1	1:A:181:ARG:HH12	2.18	0.42
1:D:154:GLU:OE1	1:D:154:GLU:HA	2.20	0.42
1:I:44:LEU:CD1	1:I:362:VAL:HG11	2.49	0.42
1:B:158:THR:C	1:B:193:ALA:HA	2.45	0.42
1:B:277:LEU:HB2	1:B:334:TYR:CE1	2.54	0.42
1:E:73:ASP:OD1	1:E:73:ASP:C	2.62	0.42
1:G:206:ASP:OD2	1:G:208:ARG:NH1	2.52	0.42
1:I:279:PHE:HE2	1:I:325:GLU:HG2	1.84	0.42
1:I:306:VAL:HG13	1:I:324:TYR:CE1	2.54	0.42
1:D:98:LEU:HD12	1:D:98:LEU:HA	1.86	0.42
1:E:108:GLN:HB3	1:E:208:ARG:HG2	2.01	0.42
1:E:171:LEU:HD23	1:E:171:LEU:HA	1.85	0.42
1:E:208:ARG:HD2	1:H:117:GLY:HA3	2.02	0.42
1:G:169:ARG:HE	1:G:169:ARG:HB2	1.71	0.42
1:A:155:GLN:O	1:A:156:VAL:HG23	2.19	0.42
1:H:90:ASN:OD1	1:H:212:ASP:HA	2.20	0.42
1:H:341:GLU:O	1:H:344:GLU:HG2	2.20	0.42
1:J:198:ARG:O	1:J:200:PRO:HD3	2.20	0.41
1:A:179:TYR:CD2	3:A:500:UDP:H2'	2.55	0.41
1:C:386:ARG:C	1:C:388:GLN:N	2.78	0.41
1:E:58:VAL:HA	1:E:238:MET:O	2.20	0.41
1:G:250:ILE:HA	1:G:251:PRO:HD3	1.82	0.41
1:G:290:LEU:HD12	1:G:308:GLU:HB2	2.01	0.41
1:I:79:ILE:O	1:I:80:HIS:HD2	2.02	0.41
1:I:362:VAL:HG23	1:I:379:GLN:OE1	2.21	0.41
1:A:169:ARG:HG2	1:A:173:ASN:HD21	1.86	0.41
1:A:226:PHE:HA	1:A:229:MET:HE3	2.02	0.41
1:B:246:ILE:HD13	1:B:250:ILE:HD12	2.01	0.41
1:C:32:TYR:HA	1:C:254:HIS:O	2.21	0.41
1:C:33:LEU:HD23	1:C:255:MET:HE2	2.00	0.41
1:F:250:ILE:HA	1:F:251:PRO:HD3	1.84	0.41
1:F:306:VAL:HG13	1:F:324:TYR:CD1	2.55	0.41
1:G:102:THR:HB	1:G:225:MET:HB2	2.02	0.41
1:G:119:LEU:HD23	1:G:119:LEU:HA	1.84	0.41
1:H:138:THR:O	1:H:139:SER:C	2.63	0.41
1:C:222:TYR:O	1:C:223:THR:C	2.63	0.41
1:D:250:ILE:O	1:D:252:PHE:CD2	2.73	0.41
1:D:320:THR:O	1:D:320:THR:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:GLY:HA3	1:I:208:ARG:HD2	2.02	0.41
1:F:125:ASN:OD1	1:F:125:ASN:C	2.63	0.41
1:F:185:GLY:O	1:F:186:LEU:HD12	2.20	0.41
1:A:155:GLN:HB2	1:A:157[A]:ARG:CG	2.51	0.41
1:B:126:LEU:HD23	1:B:142:VAL:HG21	2.00	0.41
1:B:338:PRO:O	1:B:339:ARG:HG3	2.20	0.41
1:E:242:ASP:HB3	1:E:245:GLU:HG3	2.02	0.41
1:F:114:SER:HA	1:F:118:GLN:O	2.20	0.41
1:J:32:TYR:HA	1:J:254:HIS:O	2.21	0.41
1:A:154:GLU:CG	1:A:155:GLN:H	2.16	0.41
1:C:122:ILE:HA	1:C:123:PRO:C	2.45	0.41
1:D:182:LYS:HG2	1:D:304:THR:CG2	2.50	0.41
1:E:364:ARG:NH2	1:E:370:TYR:HD1	2.18	0.41
1:E:377:VAL:O	1:E:381:LEU:HG	2.20	0.41
1:G:92:LYS:HZ3	1:G:96:GLU:CD	2.28	0.41
1:A:238:MET:HE3	1:I:56:LEU:HD13	2.01	0.41
1:C:187:ASP:CG	1:C:188:PRO:HD2	2.45	0.41
1:E:34:ILE:HG12	1:E:256:ILE:HB	2.01	0.41
1:E:98:LEU:HD12	1:E:98:LEU:HA	1.94	0.41
1:F:124:ILE:HB	1:F:201:THR:HG23	2.03	0.41
2:G:450:FAD:HM81	2:G:450:FAD:HM73	1.83	0.41
1:H:171:LEU:HD23	1:H:171:LEU:HA	1.90	0.41
1:H:346:TYR:O	1:H:347:LYS:C	2.63	0.41
1:A:85:HIS:O	1:A:217:MET:HE1	2.20	0.41
1:E:348:LYS:O	1:E:351:ALA:HB3	2.21	0.41
1:A:162:VAL:O	1:A:166:LYS:HE3	2.21	0.41
1:A:163:VAL:O	1:A:164:VAL:C	2.64	0.41
1:E:120:LEU:HD12	1:E:120:LEU:HA	1.97	0.41
1:E:185:GLY:C	1:E:186:LEU:HD12	2.46	0.41
1:E:371:TYR:HE2	1:E:379:GLN:HE22	1.68	0.41
1:F:37:ALA:HA	1:F:57:ILE:HD11	2.03	0.41
1:F:154:GLU:OE1	1:F:154:GLU:HA	2.21	0.41
1:G:122:ILE:HA	1:G:123:PRO:C	2.45	0.41
1:G:308:GLU:HB3	1:G:311:HIS:HD2	1.86	0.41
1:I:159:SER:HB3	1:I:196:THR:HG23	2.03	0.41
1:J:273:PRO:HG2	1:J:342:ASN:OD1	2.21	0.41
1:A:97:TYR:O	1:A:100:ARG:HG3	2.21	0.41
1:A:159:SER:HB2	1:A:188:PRO:O	2.21	0.41
1:B:163:VAL:C	1:B:165:SER:H	2.29	0.41
1:C:38:GLY:HA2	1:C:65:GLY:C	2.46	0.41
1:E:169:ARG:HG3	1:E:173:ASN:HD21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:33:LEU:HD23	1:G:255:MET:HE2	2.03	0.41
1:G:364:ARG:HD3	2:G:450:FAD:H3'	2.03	0.41
1:I:275:ARG:HB3	1:I:335:TYR:HB2	2.02	0.41
1:A:169:ARG:HG2	1:A:173:ASN:ND2	2.35	0.40
1:B:277:LEU:HB2	1:B:334:TYR:CD1	2.57	0.40
1:C:30:PHE:CE1	1:C:56:LEU:HD22	2.56	0.40
1:C:250:ILE:HA	1:C:251:PRO:HD3	1.82	0.40
1:E:289:LEU:HD11	6:I:401:XYL:H4	2.04	0.40
1:J:162:VAL:HG23	1:J:193:ALA:HB1	1.99	0.40
1:A:102:THR:HB	1:A:225:MET:HG3	2.03	0.40
1:A:318:HIS:CD2	1:A:318:HIS:H	2.39	0.40
1:A:345:LEU:HD23	1:A:345:LEU:HA	1.80	0.40
1:B:163:VAL:C	1:B:165:SER:N	2.79	0.40
1:C:341:GLU:H	1:C:341:GLU:HG3	1.41	0.40
1:F:308:GLU:HB3	1:F:311:HIS:HD2	1.86	0.40
1:I:373:MET:O	1:I:377:VAL:HG23	2.21	0.40
1:A:104:TRP:HB3	1:A:216:ALA:HB1	2.04	0.40
1:G:77:VAL:HG11	1:G:321:SER:HB2	2.03	0.40
1:G:172:TYR:OH	1:G:188:PRO:HG2	2.21	0.40
1:J:265:PHE:HZ	1:J:353:ALA:HA	1.86	0.40
1:A:210:PHE:HB3	1:A:212:ASP:OD2	2.21	0.40
1:B:217:MET:HE3	1:B:218:PRO:HD2	2.03	0.40
1:D:333:PRO:O	1:D:364:ARG:NH2	2.47	0.40
1:H:137:LEU:HD12	1:H:142:VAL:HG23	2.03	0.40
1:J:159:SER:HB3	1:J:196:THR:CG2	2.52	0.40
1:J:300:ASP:O	1:J:301:TYR:HB2	2.20	0.40
1:A:306:VAL:HG22	1:A:324:TYR:CD1	2.57	0.40
1:B:160:GLU:HB2	1:B:189:SER:OG	2.21	0.40
1:C:73:ASP:HB2	7:C:438:HOH:O	2.22	0.40
1:F:371:TYR:HB3	1:F:376:VAL:HG23	2.03	0.40
1:J:114:SER:HA	1:J:118:GLN:O	2.21	0.40
1:J:272:LEU:CD2	1:J:368:TYR:CZ	3.05	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	364/397 (92%)	349 (96%)	12 (3%)	3 (1%)	16	27
1	B	361/397 (91%)	331 (92%)	24 (7%)	6 (2%)	7	12
1	C	361/397 (91%)	341 (94%)	17 (5%)	3 (1%)	16	27
1	D	357/397 (90%)	333 (93%)	22 (6%)	2 (1%)	21	34
1	E	359/397 (90%)	329 (92%)	27 (8%)	3 (1%)	16	27
1	F	363/397 (91%)	351 (97%)	12 (3%)	0	100	100
1	G	361/397 (91%)	345 (96%)	15 (4%)	1 (0%)	36	52
1	H	362/397 (91%)	342 (94%)	20 (6%)	0	100	100
1	I	362/397 (91%)	342 (94%)	20 (6%)	0	100	100
1	J	361/397 (91%)	340 (94%)	17 (5%)	4 (1%)	11	19
All	All	3611/3970 (91%)	3403 (94%)	186 (5%)	22 (1%)	21	34

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	GLU
1	B	150	ALA
1	B	188	PRO
1	C	357	GLN
1	B	186	LEU
1	B	200	PRO
1	B	167	VAL
1	C	154	GLU
1	E	355	ALA
1	J	357	GLN
1	E	156	VAL
1	J	154	GLU
1	J	268	CYS
1	C	387	LEU
1	D	154	GLU
1	D	387	LEU
1	G	340	PRO
1	J	266	ASP
1	A	195	VAL
1	A	164	VAL

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Mol	Chain	Res	Type
1	B	187	ASP
1	E	338	PRO

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	318/346 (92%)	293 (92%)	25 (8%)	11	19
1	B	315/346 (91%)	292 (93%)	23 (7%)	13	22
1	C	315/346 (91%)	291 (92%)	24 (8%)	12	21
1	D	313/346 (90%)	292 (93%)	21 (7%)	15	25
1	E	313/346 (90%)	290 (93%)	23 (7%)	13	22
1	F	317/346 (92%)	295 (93%)	22 (7%)	14	24
1	G	315/346 (91%)	298 (95%)	17 (5%)	20	35
1	H	316/346 (91%)	292 (92%)	24 (8%)	12	21
1	I	316/346 (91%)	295 (93%)	21 (7%)	15	26
1	J	315/346 (91%)	295 (94%)	20 (6%)	16	29
All	All	3153/3460 (91%)	2933 (93%)	220 (7%)	14	24

All (220) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	44	LEU
1	A	48	LEU
1	A	98	LEU
1	A	112	LEU
1	A	120	LEU
1	A	156	VAL
1	A	157[A]	ARG
1	A	157[B]	ARG
1	A	159	SER
1	A	164	VAL

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Mol	Chain	Res	Type
1	A	166	LYS
1	A	186	LEU
1	A	208	ARG
1	A	212	ASP
1	A	261	VAL
1	A	272	LEU
1	A	282	GLU
1	A	306	VAL
1	A	330	GLU
1	A	341	GLU
1	A	344	GLU
1	A	345	LEU
1	A	362	VAL
1	A	387	LEU
1	B	28	LYS
1	B	44	LEU
1	B	98	LEU
1	B	112	LEU
1	B	120	LEU
1	B	126	LEU
1	B	138	THR
1	B	154	GLU
1	B	164	VAL
1	B	169	ARG
1	B	187	ASP
1	B	199	VAL
1	B	208	ARG
1	B	256	ILE
1	B	261	VAL
1	B	292	THR
1	B	306	VAL
1	B	318	HIS
1	B	319	GLN
1	B	330	GLU
1	B	341	GLU
1	B	345	LEU
1	B	387	LEU
1	C	34	ILE
1	C	48	LEU
1	C	64	ILE
1	C	98	LEU
1	C	112	LEU

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Mol	Chain	Res	Type
1	C	120	LEU
1	C	126	LEU
1	C	148	SER
1	C	154	GLU
1	C	159	SER
1	C	164	VAL
1	C	182	LYS
1	C	183	GLN
1	C	186	LEU
1	C	208	ARG
1	C	246	ILE
1	C	261	VAL
1	C	286	THR
1	C	330	GLU
1	C	341	GLU
1	C	345	LEU
1	C	369	ARG
1	C	388	GLN
1	C	390	GLN
1	D	48	LEU
1	D	60	ARG
1	D	61	ARG
1	D	79	ILE
1	D	98	LEU
1	D	112	LEU
1	D	120	LEU
1	D	126	LEU
1	D	142	VAL
1	D	154	GLU
1	D	156	VAL
1	D	157	ARG
1	D	165	SER
1	D	261	VAL
1	D	292	THR
1	D	300	ASP
1	D	306	VAL
1	D	319	GLN
1	D	357	GLN
1	D	362	VAL
1	D	387	LEU
1	E	33	LEU
1	E	48	LEU

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Mol	Chain	Res	Type
1	E	58	VAL
1	E	60	ARG
1	E	79	ILE
1	E	98	LEU
1	E	112	LEU
1	E	120	LEU
1	E	126	LEU
1	E	152	LYS
1	E	164	VAL
1	E	201	THR
1	E	208	ARG
1	E	227	GLN
1	E	229	MET
1	E	246	ILE
1	E	258	THR
1	E	261	VAL
1	E	330	GLU
1	E	341	GLU
1	E	352	LEU
1	E	362	VAL
1	E	387	LEU
1	F	44	LEU
1	F	48	LEU
1	F	58	VAL
1	F	98	LEU
1	F	112	LEU
1	F	120	LEU
1	F	126	LEU
1	F	136	ASN
1	F	149	VAL
1	F	159	SER
1	F	164	VAL
1	F	182	LYS
1	F	192	ASP
1	F	239	LEU
1	F	246	ILE
1	F	272	LEU
1	F	306	VAL
1	F	330	GLU
1	F	345	LEU
1	F	362	VAL
1	F	383	THR

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Mol	Chain	Res	Type
1	F	387	LEU
1	G	48	LEU
1	G	98	LEU
1	G	112	LEU
1	G	120	LEU
1	G	126	LEU
1	G	148	SER
1	G	155	GLN
1	G	156	VAL
1	G	157	ARG
1	G	159	SER
1	G	182	LYS
1	G	261	VAL
1	G	272	LEU
1	G	282	GLU
1	G	330	GLU
1	G	362	VAL
1	G	387	LEU
1	H	48	LEU
1	H	51	SER
1	H	60	ARG
1	H	98	LEU
1	H	112	LEU
1	H	120	LEU
1	H	122	ILE
1	H	126	LEU
1	H	152	LYS
1	H	155	GLN
1	H	164	VAL
1	H	169	ARG
1	H	186	LEU
1	H	208	ARG
1	H	232	SER
1	H	256	ILE
1	H	261	VAL
1	H	272	LEU
1	H	305	ARG
1	H	306	VAL
1	H	330	GLU
1	H	340	PRO
1	H	345	LEU
1	H	387	LEU

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Mol	Chain	Res	Type
1	I	44	LEU
1	I	48	LEU
1	I	54	ARG
1	I	58	VAL
1	I	64	ILE
1	I	98	LEU
1	I	112	LEU
1	I	120	LEU
1	I	122	ILE
1	I	126	LEU
1	I	153	VAL
1	I	164	VAL
1	I	186	LEU
1	I	261	VAL
1	I	272	LEU
1	I	306	VAL
1	I	330	GLU
1	I	344	GLU
1	I	345	LEU
1	I	364	ARG
1	I	387	LEU
1	J	48	LEU
1	J	79	ILE
1	J	98	LEU
1	J	112	LEU
1	J	120	LEU
1	J	126	LEU
1	J	136	ASN
1	J	186	LEU
1	J	227	GLN
1	J	238	MET
1	J	245	GLU
1	J	261	VAL
1	J	272	LEU
1	J	282	GLU
1	J	305	ARG
1	J	306	VAL
1	J	316	ARG
1	J	330	GLU
1	J	341	GLU
1	J	387	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	284	HIS
1	A	318	HIS
1	B	318	HIS
1	B	379	GLN
1	C	53	GLN
1	C	118	GLN
1	C	173	ASN
1	C	284	HIS
1	C	299	ASN
1	C	319	GLN
1	C	388	GLN
1	D	67	ASN
1	D	118	GLN
1	D	183	GLN
1	D	220	HIS
1	D	311	HIS
1	D	319	GLN
1	D	379	GLN
1	D	388	GLN
1	E	53	GLN
1	E	67	ASN
1	E	90	ASN
1	E	173	ASN
1	E	227	GLN
1	E	288	GLN
1	E	311	HIS
1	F	53	GLN
1	F	118	GLN
1	F	299	ASN
1	F	318	HIS
1	F	319	GLN
1	F	390	GLN
1	G	173	ASN
1	G	281	HIS
1	G	311	HIS
1	G	319	GLN
1	H	173	ASN
1	H	253	GLN
1	H	311	HIS
1	H	388	GLN
1	I	53	GLN
1	I	67	ASN

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Mol	Chain	Res	Type
1	I	90	ASN
1	I	253	GLN
1	I	311	HIS
1	J	53	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

47 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	$\# Z > 2$
4	GOL	I	398	-	5,5,5	0.40	0	5,5,5	0.79	0
4	GOL	I	399	-	5,5,5	0.43	0	5,5,5	0.51	0
2	FAD	F	450	-	58,58,58	1.08	6 (10%)	85,89,89	1.54	13 (15%)
4	GOL	A	398	-	5,5,5	0.34	0	5,5,5	0.53	0
6	XYL	I	401	-	9,9,9	1.28	2 (22%)	11,11,11	2.62	5 (45%)
3	UDP	J	500	-	25,26,26	0.97	0	38,40,40	1.76	7 (18%)
4	GOL	E	398	-	5,5,5	0.38	0	5,5,5	0.55	0
4	GOL	J	400	-	5,5,5	0.45	0	5,5,5	0.45	0
4	GOL	G	399	-	5,5,5	0.35	0	5,5,5	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	XYL	F	399	-	9,9,9	1.73	2 (22%)	11,11,11	1.75	3 (27%)
4	GOL	F	398	-	5,5,5	0.31	0	5,5,5	0.74	0
4	GOL	I	400	-	5,5,5	0.38	0	5,5,5	0.31	0
2	FAD	J	450	-	58,58,58	1.17	6 (10%)	85,89,89	1.63	16 (18%)
3	UDP	G	500	-	25,26,26	0.88	0	38,40,40	1.63	7 (18%)
4	GOL	A	400	-	5,5,5	0.38	0	5,5,5	0.14	0
2	FAD	I	450	-	58,58,58	1.06	5 (8%)	85,89,89	1.54	16 (18%)
4	GOL	G	400	-	5,5,5	0.40	0	5,5,5	0.41	0
4	GOL	F	400	-	5,5,5	0.44	0	5,5,5	0.36	0
4	GOL	E	399	-	5,5,5	0.40	0	5,5,5	0.16	0
4	GOL	E	401	-	5,5,5	0.39	0	5,5,5	0.36	0
2	FAD	G	450	-	58,58,58	1.14	6 (10%)	85,89,89	1.53	15 (17%)
4	GOL	B	398	-	5,5,5	0.45	0	5,5,5	0.34	0
4	GOL	D	398	-	5,5,5	0.35	0	5,5,5	0.65	0
4	GOL	E	400	-	5,5,5	0.31	0	5,5,5	0.50	0
3	UDP	B	500	-	25,26,26	0.95	1 (4%)	38,40,40	1.54	6 (15%)
4	GOL	H	398	-	5,5,5	0.37	0	5,5,5	0.40	0
4	GOL	H	399	-	5,5,5	0.46	0	5,5,5	0.32	0
4	GOL	C	398	-	5,5,5	0.35	0	5,5,5	0.31	0
4	GOL	C	399	-	5,5,5	0.39	0	5,5,5	0.37	0
2	FAD	E	450	-	58,58,58	1.21	7 (12%)	85,89,89	1.50	14 (16%)
4	GOL	G	398	-	5,5,5	0.42	0	5,5,5	0.36	0
4	GOL	D	399	-	5,5,5	0.47	0	5,5,5	0.52	0
2	FAD	B	450	-	58,58,58	1.11	5 (8%)	85,89,89	1.61	14 (16%)
3	UDP	C	500	-	25,26,26	0.92	1 (4%)	38,40,40	1.67	5 (13%)
5	URM	D	600	-	38,38,38	3.34	7 (18%)	51,58,58	3.42	12 (23%)
3	UDP	A	500	-	25,26,26	1.07	2 (8%)	38,40,40	1.78	8 (21%)
3	UDP	E	500	-	22,22,26	0.94	0	32,33,40	1.67	5 (15%)
4	GOL	I	402	-	5,5,5	0.42	0	5,5,5	0.45	0
3	UDP	H	500	-	25,26,26	0.97	0	38,40,40	1.76	7 (18%)
2	FAD	C	450	-	58,58,58	1.09	4 (6%)	85,89,89	1.67	19 (22%)
4	GOL	J	399	-	5,5,5	0.53	0	5,5,5	0.36	0
3	UDP	F	500	-	25,26,26	0.99	2 (8%)	38,40,40	1.60	5 (13%)
2	FAD	D	450	-	58,58,58	1.11	4 (6%)	85,89,89	1.66	15 (17%)
4	GOL	A	399	-	5,5,5	0.50	0	5,5,5	0.30	0
2	FAD	A	450	-	58,58,58	1.09	5 (8%)	85,89,89	1.62	18 (21%)
2	FAD	H	450	-	58,58,58	1.14	8 (13%)	85,89,89	1.48	16 (18%)
3	UDP	I	500	-	22,22,26	0.93	0	32,33,40	1.76	5 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	I	398	-	-	2/4/4/4	-
4	GOL	I	399	-	-	3/4/4/4	-
2	FAD	F	450	-	-	2/34/50/50	0/6/6/6
4	GOL	A	398	-	-	2/4/4/4	-
6	XYL	I	401	-	-	7/12/12/12	-
3	UDP	J	500	-	-	0/16/32/32	0/2/2/2
4	GOL	E	398	-	-	2/4/4/4	-
4	GOL	J	400	-	-	4/4/4/4	-
4	GOL	G	399	-	-	2/4/4/4	-
6	XYL	F	399	-	-	7/12/12/12	-
4	GOL	F	398	-	-	4/4/4/4	-
4	GOL	I	400	-	-	0/4/4/4	-
2	FAD	J	450	-	-	8/34/50/50	0/6/6/6
3	UDP	G	500	-	-	7/16/32/32	0/2/2/2
4	GOL	A	400	-	-	2/4/4/4	-
2	FAD	I	450	-	-	2/34/50/50	0/6/6/6
4	GOL	G	400	-	-	2/4/4/4	-
4	GOL	F	400	-	-	0/4/4/4	-
4	GOL	E	399	-	-	0/4/4/4	-
4	GOL	E	401	-	-	2/4/4/4	-
2	FAD	G	450	-	-	2/34/50/50	0/6/6/6
4	GOL	B	398	-	-	0/4/4/4	-
4	GOL	D	398	-	-	0/4/4/4	-
4	GOL	E	400	-	-	2/4/4/4	-
3	UDP	B	500	-	-	3/16/32/32	0/2/2/2
4	GOL	H	398	-	-	4/4/4/4	-
4	GOL	H	399	-	-	0/4/4/4	-
4	GOL	C	398	-	-	3/4/4/4	-
4	GOL	C	399	-	-	4/4/4/4	-
2	FAD	E	450	-	-	4/34/50/50	0/6/6/6
4	GOL	G	398	-	-	2/4/4/4	-
4	GOL	D	399	-	-	2/4/4/4	-
2	FAD	B	450	-	-	0/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UDP	C	500	-	-	2/16/32/32	0/2/2/2
5	URM	D	600	-	-	7/20/59/59	0/3/3/3
3	UDP	A	500	-	-	1/16/32/32	0/2/2/2
3	UDP	E	500	-	-	0/10/26/32	0/2/2/2
4	GOL	I	402	-	-	2/4/4/4	-
3	UDP	H	500	-	-	6/16/32/32	0/2/2/2
2	FAD	C	450	-	-	3/34/50/50	0/6/6/6
4	GOL	J	399	-	-	0/4/4/4	-
3	UDP	F	500	-	-	0/16/32/32	0/2/2/2
2	FAD	D	450	-	-	2/34/50/50	0/6/6/6
4	GOL	A	399	-	-	2/4/4/4	-
2	FAD	A	450	-	-	1/34/50/50	0/6/6/6
2	FAD	H	450	-	-	4/34/50/50	0/6/6/6
3	UDP	I	500	-	-	4/10/26/32	0/2/2/2

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	600	URM	P22-C45	-11.97	1.61	1.80
5	D	600	URM	O19-C19	11.87	1.44	1.23
5	D	600	URM	C19-N13	-7.06	1.27	1.38
5	D	600	URM	C19-N15	-6.20	1.27	1.38
2	F	450	FAD	C4X-N5	3.84	1.39	1.30
2	C	450	FAD	C4X-N5	3.77	1.38	1.30
6	F	399	XYL	O2-C2	-3.71	1.35	1.43
2	G	450	FAD	C4X-N5	3.54	1.38	1.30
2	E	450	FAD	P-O3P	3.53	1.63	1.59
2	E	450	FAD	C4X-N5	3.53	1.38	1.30
2	E	450	FAD	PA-O3P	3.44	1.63	1.59
2	A	450	FAD	C4X-N5	3.44	1.38	1.30
2	B	450	FAD	C4X-N5	3.42	1.38	1.30
2	H	450	FAD	C4X-N5	3.35	1.38	1.30
2	J	450	FAD	P-O3P	3.28	1.63	1.59
2	D	450	FAD	C4X-N5	3.21	1.37	1.30
2	I	450	FAD	C4X-N5	3.12	1.37	1.30
2	J	450	FAD	C4X-N5	3.12	1.37	1.30
2	C	450	FAD	C2A-N3A	2.98	1.39	1.33
2	I	450	FAD	C2A-N3A	2.94	1.39	1.33
2	G	450	FAD	C2A-N1A	2.91	1.39	1.33
2	J	450	FAD	PA-O3P	2.87	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	450	FAD	C2A-N3A	2.86	1.39	1.33
5	D	600	URM	C45-C41	-2.86	1.45	1.53
2	E	450	FAD	C2A-N1A	2.86	1.39	1.33
2	A	450	FAD	C2A-N3A	2.85	1.39	1.33
2	A	450	FAD	C2A-N1A	2.85	1.39	1.33
2	H	450	FAD	C2A-N1A	2.76	1.38	1.33
2	J	450	FAD	C2A-N3A	2.73	1.38	1.33
2	F	450	FAD	C2A-N1A	2.71	1.38	1.33
3	A	500	UDP	PA-O3A	2.71	1.62	1.59
2	C	450	FAD	C2A-N1A	2.70	1.38	1.33
2	G	450	FAD	P-O3P	2.69	1.62	1.59
6	F	399	XYL	O4-C4	-2.68	1.37	1.43
2	E	450	FAD	C2A-N3A	2.68	1.38	1.33
2	I	450	FAD	C2A-N1A	2.64	1.38	1.33
2	F	450	FAD	C10-N1	2.64	1.38	1.33
2	B	450	FAD	C2A-N1A	2.64	1.38	1.33
2	H	450	FAD	C2A-N3A	2.59	1.38	1.33
5	D	600	URM	P22-O23	-2.57	1.50	1.56
2	J	450	FAD	C10-N1	2.56	1.38	1.33
2	A	450	FAD	C10-N1	2.56	1.38	1.33
2	D	450	FAD	C2A-N3A	2.54	1.38	1.33
2	D	450	FAD	C2A-N1A	2.54	1.38	1.33
2	D	450	FAD	P-O3P	2.52	1.62	1.59
6	I	401	XYL	O2-C2	-2.51	1.38	1.43
2	C	450	FAD	C10-N1	2.48	1.38	1.33
2	I	450	FAD	C10-N1	2.48	1.38	1.33
2	H	450	FAD	C10-N1	2.47	1.38	1.33
2	J	450	FAD	C2A-N1A	2.46	1.38	1.33
2	B	450	FAD	C2A-N3A	2.43	1.38	1.33
2	F	450	FAD	C2A-N3A	2.40	1.38	1.33
2	G	450	FAD	C8A-N7A	2.38	1.36	1.31
2	H	450	FAD	PA-O3P	2.35	1.62	1.59
2	G	450	FAD	C10-N1	2.25	1.37	1.33
3	F	500	UDP	PA-O3A	2.24	1.61	1.59
2	E	450	FAD	C8A-N7A	2.21	1.35	1.31
2	E	450	FAD	C10-N1	2.20	1.37	1.33
2	H	450	FAD	C8A-N7A	2.20	1.35	1.31
2	A	450	FAD	PA-O3P	2.18	1.61	1.59
2	H	450	FAD	C5A-N7A	-2.17	1.35	1.39
2	B	450	FAD	C10-N1	2.15	1.37	1.33
2	H	450	FAD	P-O3P	2.12	1.61	1.59
2	I	450	FAD	C8A-N7A	2.12	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	401	XYL	O4-C4	-2.10	1.38	1.43
3	C	500	UDP	C6-C5	2.08	1.39	1.35
2	F	450	FAD	P-O3P	2.04	1.61	1.59
5	D	600	URM	P22-O12	2.04	1.60	1.58
3	F	500	UDP	C6-C5	2.04	1.39	1.35
3	B	500	UDP	PA-O3A	2.02	1.61	1.59
2	B	450	FAD	C5A-N7A	-2.01	1.35	1.39
2	F	450	FAD	C8A-N7A	2.01	1.35	1.31
3	A	500	UDP	C5-C4	-2.00	1.39	1.43

All (231) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	600	URM	N15-C19-N13	16.01	135.73	114.89
5	D	600	URM	C20-N15-C19	-11.10	112.83	126.61
5	D	600	URM	O19-C19-N13	-7.31	113.28	122.80
3	J	500	UDP	C4-N3-C2	-6.28	118.82	126.61
2	B	450	FAD	N3A-C2A-N1A	-6.26	119.10	128.58
3	H	500	UDP	C4-N3-C2	-6.24	118.86	126.61
3	A	500	UDP	C4-N3-C2	-6.01	119.16	126.61
2	F	450	FAD	N3A-C2A-N1A	-5.94	119.59	128.58
2	D	450	FAD	N3A-C2A-N1A	-5.79	119.81	128.58
2	G	450	FAD	N3A-C2A-N1A	-5.78	119.83	128.58
3	G	500	UDP	C4-N3-C2	-5.75	119.47	126.61
2	J	450	FAD	N3A-C2A-N1A	-5.71	119.94	128.58
3	I	500	UDP	C4-N3-C2	-5.71	119.52	126.61
5	D	600	URM	O19-C19-N15	-5.70	110.98	121.49
3	C	500	UDP	C4-N3-C2	-5.64	119.62	126.61
2	A	450	FAD	N3A-C2A-N1A	-5.46	120.32	128.58
3	F	500	UDP	C4-N3-C2	-5.41	119.90	126.61
6	I	401	XYL	O1-C1-C2	5.38	122.46	111.16
2	I	450	FAD	N3A-C2A-N1A	-5.36	120.47	128.58
3	E	500	UDP	C4-N3-C2	-5.26	120.08	126.61
5	D	600	URM	C18-N13-C19	-5.18	114.69	121.00
2	E	450	FAD	N3A-C2A-N1A	-5.16	120.78	128.58
2	H	450	FAD	N3A-C2A-N1A	-5.06	120.92	128.58
2	C	450	FAD	N3A-C2A-N1A	-5.00	121.01	128.58
3	B	500	UDP	C4-N3-C2	-4.94	120.48	126.61
3	C	500	UDP	N3-C2-N1	4.77	121.10	114.89
2	C	450	FAD	C5A-C4A-N3A	-4.67	120.29	126.72
2	J	450	FAD	C5A-C4A-N3A	-4.65	120.31	126.72
3	I	500	UDP	N3-C2-N1	4.63	120.92	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	600	URM	C1-N13-C19	4.61	125.87	117.59
2	D	450	FAD	C5A-C4A-N3A	-4.58	120.42	126.72
3	G	500	UDP	N3-C2-N1	4.57	120.84	114.89
2	B	450	FAD	C5A-C4A-N3A	-4.52	120.50	126.72
2	A	450	FAD	C5A-C4A-N3A	-4.51	120.50	126.72
2	D	450	FAD	N9A-C8A-N7A	-4.45	107.63	113.94
3	J	500	UDP	C5-C4-N3	4.43	121.00	114.80
2	I	450	FAD	C5A-C4A-N3A	-4.40	120.66	126.72
3	H	500	UDP	N3-C2-N1	4.35	120.55	114.89
2	B	450	FAD	N9A-C8A-N7A	-4.28	107.86	113.94
2	H	450	FAD	C5A-C4A-N3A	-4.26	120.85	126.72
3	E	500	UDP	N3-C2-N1	4.23	120.39	114.89
2	I	450	FAD	N9A-C8A-N7A	-4.16	108.04	113.94
2	G	450	FAD	N9A-C8A-N7A	-4.15	108.04	113.94
2	E	450	FAD	C5A-C4A-N3A	-4.14	121.02	126.72
2	C	450	FAD	N9A-C8A-N7A	-4.13	108.07	113.94
3	F	500	UDP	N3-C2-N1	4.12	120.26	114.89
2	F	450	FAD	N9A-C8A-N7A	-4.10	108.12	113.94
2	E	450	FAD	N9A-C8A-N7A	-4.06	108.18	113.94
2	A	450	FAD	N9A-C8A-N7A	-4.05	108.19	113.94
3	A	500	UDP	N3-C2-N1	3.99	120.09	114.89
2	G	450	FAD	C5A-C4A-N3A	-3.97	121.24	126.72
2	D	450	FAD	C5A-N7A-C8A	3.86	109.52	103.45
2	B	450	FAD	C5A-N7A-C8A	3.86	109.51	103.45
2	J	450	FAD	N9A-C8A-N7A	-3.86	108.47	113.94
3	B	500	UDP	N3-C2-N1	3.84	119.89	114.89
2	F	450	FAD	C5A-C4A-N3A	-3.83	121.45	126.72
2	B	450	FAD	C2A-N3A-C4A	3.77	121.03	111.83
2	A	450	FAD	C5A-N7A-C8A	3.74	109.33	103.45
6	I	401	XYL	O5-C5-C4	3.73	118.99	111.16
3	J	500	UDP	N3-C2-N1	3.72	119.73	114.89
3	A	500	UDP	O2-C2-N1	-3.66	118.03	122.80
2	J	450	FAD	C2A-N3A-C4A	3.66	120.76	111.83
6	F	399	XYL	O1-C1-C2	3.66	118.83	111.16
2	C	450	FAD	C5A-N7A-C8A	3.62	109.15	103.45
2	H	450	FAD	N9A-C8A-N7A	-3.62	108.79	113.94
3	H	500	UDP	C5-C4-N3	3.62	119.86	114.80
2	G	450	FAD	C5A-N7A-C8A	3.60	109.11	103.45
2	J	450	FAD	C4-N3-C2	-3.59	119.27	125.64
2	D	450	FAD	C2A-N3A-C4A	3.58	120.57	111.83
2	I	450	FAD	C5A-N7A-C8A	3.55	109.02	103.45
2	D	450	FAD	C4X-C10-N10	3.50	121.49	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	450	FAD	N3A-C4A-N9A	3.46	133.06	127.17
3	F	500	UDP	C5-C4-N3	3.46	119.64	114.80
2	A	450	FAD	O2A-PA-O3P	3.44	116.58	107.27
3	I	500	UDP	C5-C4-N3	3.44	119.62	114.80
3	J	500	UDP	O4-C4-C5	-3.41	119.29	125.16
2	J	450	FAD	C5A-N7A-C8A	3.39	108.78	103.45
2	E	450	FAD	C5A-N7A-C8A	3.38	108.76	103.45
5	D	600	URM	O20-C20-C17	-3.36	119.36	125.16
2	G	450	FAD	C2A-N3A-C4A	3.31	119.92	111.83
3	H	500	UDP	O4-C4-C5	-3.31	119.45	125.16
2	I	450	FAD	C4-N3-C2	-3.31	119.77	125.64
2	I	450	FAD	C2A-N3A-C4A	3.29	119.86	111.83
3	C	500	UDP	C5-C4-N3	3.29	119.40	114.80
2	D	450	FAD	N3A-C4A-N9A	3.29	132.76	127.17
2	A	450	FAD	C2A-N3A-C4A	3.27	119.81	111.83
2	B	450	FAD	C4-N3-C2	-3.26	119.85	125.64
2	C	450	FAD	C2A-N3A-C4A	3.22	119.69	111.83
2	F	450	FAD	C5A-N7A-C8A	3.21	108.50	103.45
2	A	450	FAD	N3A-C4A-N9A	3.20	132.61	127.17
2	H	450	FAD	C5A-N7A-C8A	3.20	108.48	103.45
3	E	500	UDP	C5-C4-N3	3.20	119.28	114.80
2	F	450	FAD	C2A-N3A-C4A	3.19	119.63	111.83
3	A	500	UDP	C5-C4-N3	3.18	119.26	114.80
2	E	450	FAD	C2A-N3A-C4A	3.18	119.59	111.83
5	D	600	URM	O6-C4-C5	3.17	119.48	109.33
2	C	450	FAD	C5X-C9A-N10	3.16	120.83	117.97
2	D	450	FAD	O4B-C1B-N9A	3.16	114.15	108.09
6	I	401	XYL	O3-C3-C2	3.16	116.10	108.93
2	B	450	FAD	C4X-C10-N10	3.15	120.99	116.48
2	J	450	FAD	N3A-C4A-N9A	3.10	132.44	127.17
2	E	450	FAD	C4X-C10-N10	3.09	120.91	116.48
2	H	450	FAD	C4-N3-C2	-3.09	120.16	125.64
2	B	450	FAD	C10-C4X-N5	-3.09	118.50	124.81
2	G	450	FAD	C4-N3-C2	-3.06	120.20	125.64
3	A	500	UDP	C5-C6-N1	-3.04	116.89	121.84
3	G	500	UDP	C5-C4-N3	3.04	119.06	114.80
3	B	500	UDP	C5-C4-N3	3.01	119.02	114.80
3	H	500	UDP	O2-C2-N1	-3.01	118.88	122.80
2	D	450	FAD	C4-N3-C2	-3.00	120.32	125.64
2	H	450	FAD	C2A-N3A-C4A	2.99	119.12	111.83
2	F	450	FAD	N3A-C4A-N9A	2.97	132.21	127.17
6	I	401	XYL	O3-C3-C4	2.95	115.64	108.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	450	FAD	N3A-C4A-N9A	2.95	132.18	127.17
2	J	450	FAD	C4X-C10-N10	2.93	120.67	116.48
3	A	500	UDP	C2'-C1'-N1	-2.91	105.16	113.25
2	E	450	FAD	C10-C4X-N5	-2.88	118.92	124.81
2	A	450	FAD	C4-N3-C2	-2.86	120.56	125.64
2	C	450	FAD	C4-N3-C2	-2.86	120.57	125.64
2	A	450	FAD	C4X-C10-N10	2.85	120.56	116.48
2	G	450	FAD	C4X-C10-N10	2.84	120.54	116.48
2	C	450	FAD	O4-C4-C4X	-2.84	119.05	126.53
2	I	450	FAD	N3A-C4A-N9A	2.81	131.94	127.17
2	F	450	FAD	C5A-C6A-N6A	-2.79	116.37	123.29
2	E	450	FAD	N3A-C4A-N9A	2.78	131.90	127.17
2	H	450	FAD	O4-C4-C4X	-2.78	119.20	126.53
2	B	450	FAD	O4B-C1B-N9A	2.75	113.37	108.09
2	H	450	FAD	N3A-C4A-N9A	2.75	131.84	127.17
2	F	450	FAD	O4B-C1B-N9A	2.74	113.35	108.09
2	B	450	FAD	C4A-C5A-N7A	-2.74	107.45	110.58
3	B	500	UDP	O2-C2-N1	-2.73	119.25	122.80
2	I	450	FAD	C4A-C5A-N7A	-2.71	107.49	110.58
3	I	500	UDP	O4-C4-C5	-2.70	120.51	125.16
2	G	450	FAD	C4A-C5A-N7A	-2.69	107.51	110.58
3	G	500	UDP	O2-C2-N1	-2.67	119.32	122.80
3	B	500	UDP	C2'-C1'-N1	-2.67	105.81	113.25
2	F	450	FAD	C4X-C10-N10	2.66	120.29	116.48
2	I	450	FAD	C4X-C10-N10	2.66	120.28	116.48
2	F	450	FAD	C4A-N9A-C8A	2.65	108.52	105.74
5	D	600	URM	O6-C1-N13	2.64	114.35	108.36
2	I	450	FAD	O4B-C1B-N9A	2.64	113.17	108.09
2	A	450	FAD	C4A-C5A-N7A	-2.63	107.57	110.58
2	C	450	FAD	C9A-C5X-N5	-2.62	119.67	122.45
2	C	450	FAD	C5'-C4'-C3'	-2.62	107.28	112.22
2	H	450	FAD	O4B-C1B-N9A	2.62	113.11	108.09
3	C	500	UDP	O4-C4-C5	-2.61	120.66	125.16
2	C	450	FAD	C4X-C4-N3	2.57	119.80	113.25
6	F	399	XYL	O5-C5-C4	2.57	116.56	111.16
2	F	450	FAD	C4-N3-C2	-2.57	121.08	125.64
2	C	450	FAD	C5A-C6A-N6A	-2.57	116.93	123.29
2	E	450	FAD	C4-N3-C2	-2.57	121.09	125.64
2	D	450	FAD	O4-C4-C4X	-2.56	119.78	126.53
2	A	450	FAD	C5A-C6A-N6A	-2.56	116.95	123.29
2	A	450	FAD	C10-C4X-N5	-2.55	119.60	124.81
2	C	450	FAD	O2A-PA-O3P	2.55	114.16	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	450	FAD	C9-C9A-N10	-2.54	118.43	121.85
3	A	500	UDP	O4-C4-C5	-2.53	120.79	125.16
5	D	600	URM	C17-C20-N15	2.53	118.34	114.80
3	G	500	UDP	C2'-C1'-N1	-2.53	106.22	113.25
2	D	450	FAD	O2-C2-N1	-2.51	117.63	121.80
2	G	450	FAD	N3A-C4A-N9A	2.50	131.42	127.17
2	F	450	FAD	C10-C4X-N5	-2.50	119.71	124.81
2	D	450	FAD	C10-C4X-N5	-2.49	119.72	124.81
2	C	450	FAD	C4A-N9A-C8A	2.49	108.36	105.74
3	E	500	UDP	O2-C2-N1	-2.47	119.58	122.80
2	C	450	FAD	C6A-C5A-C4A	2.47	120.54	117.18
2	C	450	FAD	C4A-C5A-N7A	-2.46	107.77	110.58
2	J	450	FAD	C10-C4X-N5	-2.45	119.81	124.81
2	J	450	FAD	C4X-C4-N3	2.45	119.48	113.25
3	J	500	UDP	O2-C2-N1	-2.44	119.62	122.80
2	J	450	FAD	O4-C4-C4X	-2.44	120.10	126.53
2	J	450	FAD	C4A-C5A-N7A	-2.43	107.80	110.58
2	H	450	FAD	C4X-C4-N3	2.41	119.40	113.25
2	J	450	FAD	O2A-PA-O3P	2.41	113.79	107.27
3	G	500	UDP	O4-C4-C5	-2.40	121.02	125.16
3	C	500	UDP	O2-C2-N1	-2.39	119.68	122.80
2	G	450	FAD	O4B-C1B-N9A	2.39	112.68	108.09
2	E	450	FAD	O2P-P-O3P	2.38	113.70	107.27
2	E	450	FAD	O2A-PA-O3P	2.37	113.69	107.27
2	F	450	FAD	C4X-C4-N3	2.36	119.26	113.25
2	A	450	FAD	C4X-C4-N3	2.35	119.22	113.25
2	H	450	FAD	C4X-C10-N10	2.35	119.84	116.48
2	J	450	FAD	C4-C4X-C10	2.34	120.95	116.93
2	E	450	FAD	C4A-C5A-N7A	-2.34	107.91	110.58
2	H	450	FAD	C6A-C5A-C4A	2.34	120.37	117.18
3	E	500	UDP	O4-C4-C5	-2.34	121.13	125.16
2	G	450	FAD	C10-C4X-N5	-2.32	120.07	124.81
2	D	450	FAD	C4A-C5A-N7A	-2.32	107.93	110.58
2	A	450	FAD	C6A-C5A-C4A	2.31	120.33	117.18
3	F	500	UDP	O4-C4-C5	-2.30	121.20	125.16
2	B	450	FAD	C4-C4X-N5	2.29	121.38	118.21
2	I	450	FAD	C4X-C4-N3	2.29	119.09	113.25
3	B	500	UDP	O4-C4-C5	-2.29	121.21	125.16
6	I	401	XYL	C4-C3-C2	2.29	117.38	113.57
2	B	450	FAD	C4X-C4-N3	2.28	119.06	113.25
3	I	500	UDP	C2'-C1'-N1	-2.27	106.93	113.25
2	G	450	FAD	C9A-C5X-N5	-2.26	120.05	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	450	FAD	C10-C4X-N5	-2.26	120.19	124.81
2	J	450	FAD	O4B-C1B-N9A	2.24	112.39	108.09
2	D	450	FAD	C4X-C4-N3	2.24	118.96	113.25
2	D	450	FAD	C4A-N9A-C8A	2.24	108.09	105.74
6	F	399	XYL	O2-C2-C3	-2.23	104.03	109.25
2	E	450	FAD	C4A-N9A-C8A	2.22	108.07	105.74
2	G	450	FAD	C4X-C4-N3	2.22	118.90	113.25
3	A	500	UDP	O2B-PB-O3A	2.21	112.05	104.64
2	I	450	FAD	C4A-N9A-C8A	2.21	108.06	105.74
3	H	500	UDP	O3A-PA-O1A	-2.20	104.10	110.70
2	A	450	FAD	C4X-C10-N1	-2.18	119.25	124.59
2	A	450	FAD	C4A-N9A-C8A	2.18	108.03	105.74
2	G	450	FAD	C5X-C9A-N10	2.17	119.93	117.97
3	J	500	UDP	C2'-C1'-N1	-2.17	107.21	113.25
2	H	450	FAD	C4A-C5A-N7A	-2.16	108.11	110.58
2	G	450	FAD	C4A-N9A-C8A	2.16	108.01	105.74
2	C	450	FAD	C4X-C10-N10	2.13	119.54	116.48
2	E	450	FAD	C9A-C5X-N5	-2.13	120.20	122.45
2	J	450	FAD	C4X-C10-N1	-2.12	119.39	124.59
3	H	500	UDP	O3B-PB-O3A	2.12	111.74	104.64
2	A	450	FAD	O4'-C4'-C5'	-2.09	105.37	109.99
2	I	450	FAD	C4-C4X-C10	2.09	120.52	116.93
2	I	450	FAD	O4-C4-C4X	-2.09	121.02	126.53
2	A	450	FAD	C4-C4X-C10	2.09	120.51	116.93
5	D	600	URM	O20-C20-N15	2.07	122.28	119.27
3	J	500	UDP	O2A-PA-O3A	2.07	112.86	107.27
3	F	500	UDP	O3B-PB-O3A	2.06	111.56	104.64
2	H	450	FAD	C9A-C5X-N5	-2.04	120.28	122.45
2	H	450	FAD	O2A-PA-O3P	2.04	112.80	107.27
2	I	450	FAD	C6A-C5A-C4A	2.03	119.96	117.18
3	G	500	UDP	C5-C6-N1	-2.03	118.54	121.84
5	D	600	URM	P22-O12-P9	-2.03	125.75	132.37
2	B	450	FAD	C4A-N9A-C8A	2.01	107.85	105.74
2	H	450	FAD	C10-C4X-N5	-2.01	120.71	124.81

There are no chirality outliers.

All (118) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	450	FAD	C5'-O5'-P-O2P
2	H	450	FAD	PA-O3P-P-O5'
2	J	450	FAD	C1'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
3	B	500	UDP	C5'-O5'-PA-O2A
3	B	500	UDP	C5'-O5'-PA-O3A
3	C	500	UDP	C5'-O5'-PA-O2A
3	C	500	UDP	C5'-O5'-PA-O3A
3	G	500	UDP	C5'-O5'-PA-O1A
3	G	500	UDP	C5'-O5'-PA-O3A
3	G	500	UDP	PA-O3A-PB-O2B
3	H	500	UDP	C5'-O5'-PA-O1A
3	I	500	UDP	C5'-O5'-PA-O2A
4	A	398	GOL	C1-C2-C3-O3
4	A	398	GOL	O2-C2-C3-O3
4	A	400	GOL	O1-C1-C2-C3
4	C	398	GOL	O1-C1-C2-C3
4	D	399	GOL	O1-C1-C2-C3
4	E	398	GOL	O2-C2-C3-O3
4	E	401	GOL	C1-C2-C3-O3
4	E	400	GOL	O1-C1-C2-C3
4	F	398	GOL	O1-C1-C2-O2
4	F	398	GOL	O1-C1-C2-C3
4	G	398	GOL	C1-C2-C3-O3
4	G	399	GOL	C1-C2-C3-O3
4	G	400	GOL	O1-C1-C2-C3
4	H	398	GOL	O1-C1-C2-O2
4	H	398	GOL	O1-C1-C2-C3
4	I	398	GOL	O1-C1-C2-C3
4	I	399	GOL	O1-C1-C2-C3
4	I	402	GOL	O1-C1-C2-C3
5	D	600	URM	C5-O8-P9-O10
5	D	600	URM	C5-O8-P9-O11
5	D	600	URM	C5-O8-P9-O12
6	F	399	XYL	O1-C1-C2-O2
6	F	399	XYL	C1-C2-C3-O3
6	F	399	XYL	O2-C2-C3-C4
6	F	399	XYL	O2-C2-C3-O3
6	I	401	XYL	C1-C2-C3-O3
6	I	401	XYL	O2-C2-C3-C4
6	I	401	XYL	O4-C4-C5-O5
6	F	399	XYL	C1-C2-C3-C4
6	I	401	XYL	C1-C2-C3-C4
6	F	399	XYL	O1-C1-C2-C3
4	C	398	GOL	O1-C1-C2-O2
4	J	400	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	I	401	XYL	C3-C4-C5-O5
2	E	450	FAD	O4B-C4B-C5B-O5B
2	E	450	FAD	C3B-C4B-C5B-O5B
4	A	399	GOL	C1-C2-C3-O3
4	C	399	GOL	O1-C1-C2-C3
4	E	398	GOL	C1-C2-C3-O3
4	F	398	GOL	C1-C2-C3-O3
4	J	400	GOL	O1-C1-C2-C3
4	J	400	GOL	C1-C2-C3-O3
4	E	401	GOL	O2-C2-C3-O3
4	E	400	GOL	O1-C1-C2-O2
4	G	398	GOL	O2-C2-C3-O3
4	G	399	GOL	O2-C2-C3-O3
4	G	400	GOL	O1-C1-C2-O2
4	I	398	GOL	O1-C1-C2-O2
4	I	399	GOL	O1-C1-C2-O2
4	I	402	GOL	O1-C1-C2-O2
2	C	450	FAD	O4B-C4B-C5B-O5B
2	C	450	FAD	C3B-C4B-C5B-O5B
3	H	500	UDP	C3'-C4'-C5'-O5'
5	D	600	URM	C3-C4-C5-O8
6	I	401	XYL	O2-C2-C3-O3
2	G	450	FAD	O4B-C4B-C5B-O5B
2	G	450	FAD	C3B-C4B-C5B-O5B
2	I	450	FAD	O4B-C4B-C5B-O5B
2	I	450	FAD	C3B-C4B-C5B-O5B
3	H	500	UDP	O4'-C4'-C5'-O5'
2	J	450	FAD	O2'-C2'-C3'-C4'
5	D	600	URM	O36-C37-C46-O47
4	A	400	GOL	O1-C1-C2-O2
4	D	399	GOL	O1-C1-C2-O2
2	J	450	FAD	O4B-C4B-C5B-O5B
4	A	399	GOL	O2-C2-C3-O3
4	C	398	GOL	O2-C2-C3-O3
4	H	398	GOL	O2-C2-C3-O3
4	J	400	GOL	O2-C2-C3-O3
2	D	450	FAD	O4B-C4B-C5B-O5B
3	I	500	UDP	O4'-C4'-C5'-O5'
6	F	399	XYL	O4-C4-C5-O5
2	C	450	FAD	PA-O3P-P-O5'
3	B	500	UDP	PB-O3A-PA-O5'
4	C	399	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	I	399	GOL	O2-C2-C3-O3
2	J	450	FAD	C1'-C2'-C3'-O3'
3	G	500	UDP	O4'-C4'-C5'-O5'
3	I	500	UDP	C5'-O5'-PA-O3A
3	I	500	UDP	C3'-C4'-C5'-O5'
4	C	399	GOL	O1-C1-C2-O2
6	I	401	XYL	O3-C3-C4-O4
2	E	450	FAD	C5B-O5B-PA-O1A
2	E	450	FAD	C5B-O5B-PA-O2A
2	H	450	FAD	C5'-O5'-P-O1P
2	H	450	FAD	C5'-O5'-P-O3P
3	G	500	UDP	C5'-O5'-PA-O2A
3	H	500	UDP	C5'-O5'-PA-O2A
4	F	398	GOL	O2-C2-C3-O3
2	F	450	FAD	O4B-C4B-C5B-O5B
3	A	500	UDP	PB-O3A-PA-O1A
3	H	500	UDP	PB-O3A-PA-O1A
2	D	450	FAD	C3B-C4B-C5B-O5B
2	J	450	FAD	C3B-C4B-C5B-O5B
2	J	450	FAD	O3'-C3'-C4'-O4'
3	G	500	UDP	PA-O3A-PB-O1B
5	D	600	URM	P22-O12-P9-O10
2	A	450	FAD	O4B-C4B-C5B-O5B
2	J	450	FAD	O2'-C2'-C3'-O3'
2	J	450	FAD	O3'-C3'-C4'-C5'
4	C	399	GOL	C1-C2-C3-O3
4	H	398	GOL	C1-C2-C3-O3
2	F	450	FAD	C3B-C4B-C5B-O5B
3	G	500	UDP	C3'-C4'-C5'-O5'
3	H	500	UDP	PB-O3A-PA-O2A
5	D	600	URM	O6-C4-C5-O8

There are no ring outliers.

25 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	398	GOL	3	0
4	A	398	GOL	1	0
6	I	401	XYL	1	0
3	J	500	UDP	1	0
4	E	398	GOL	1	0
4	F	398	GOL	1	0

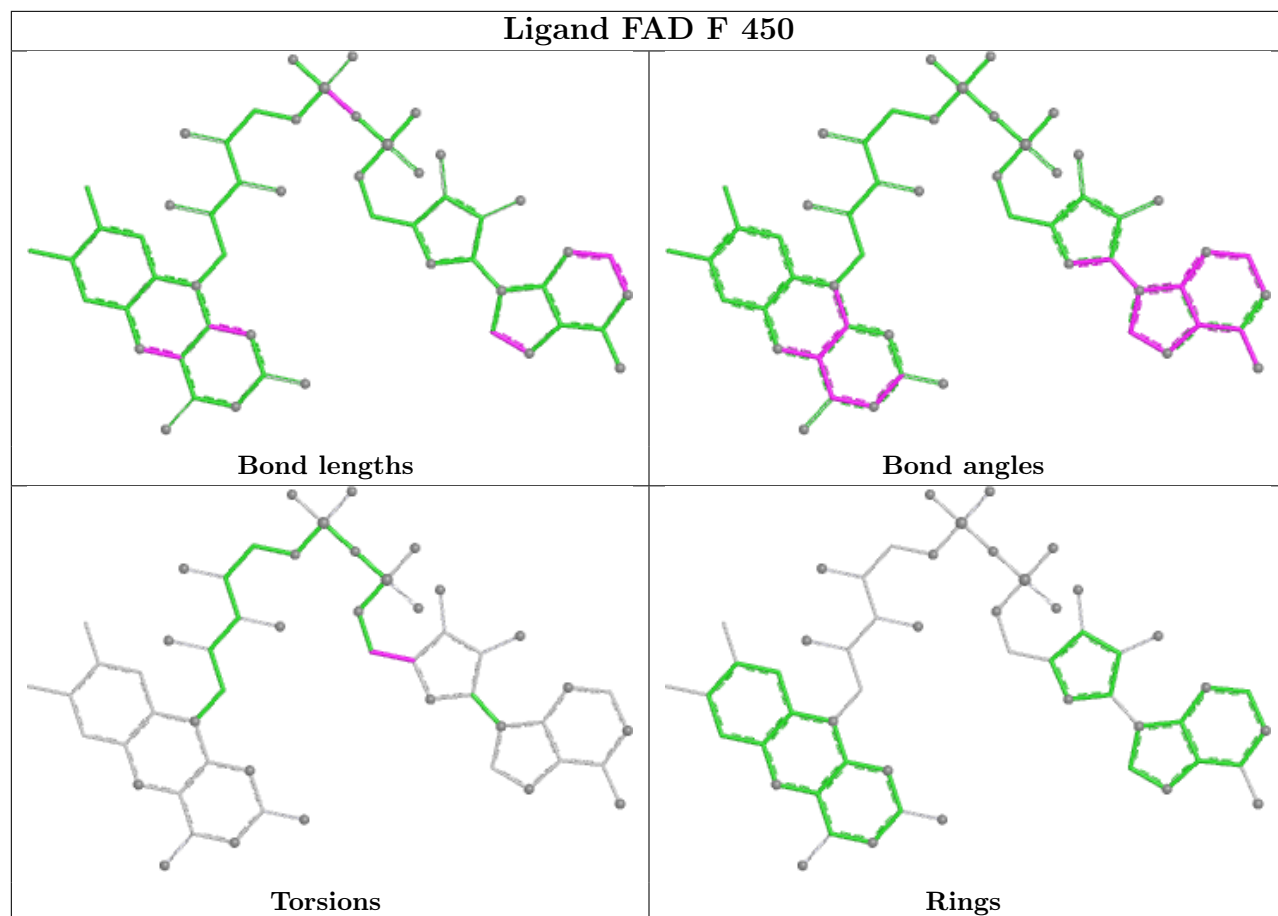
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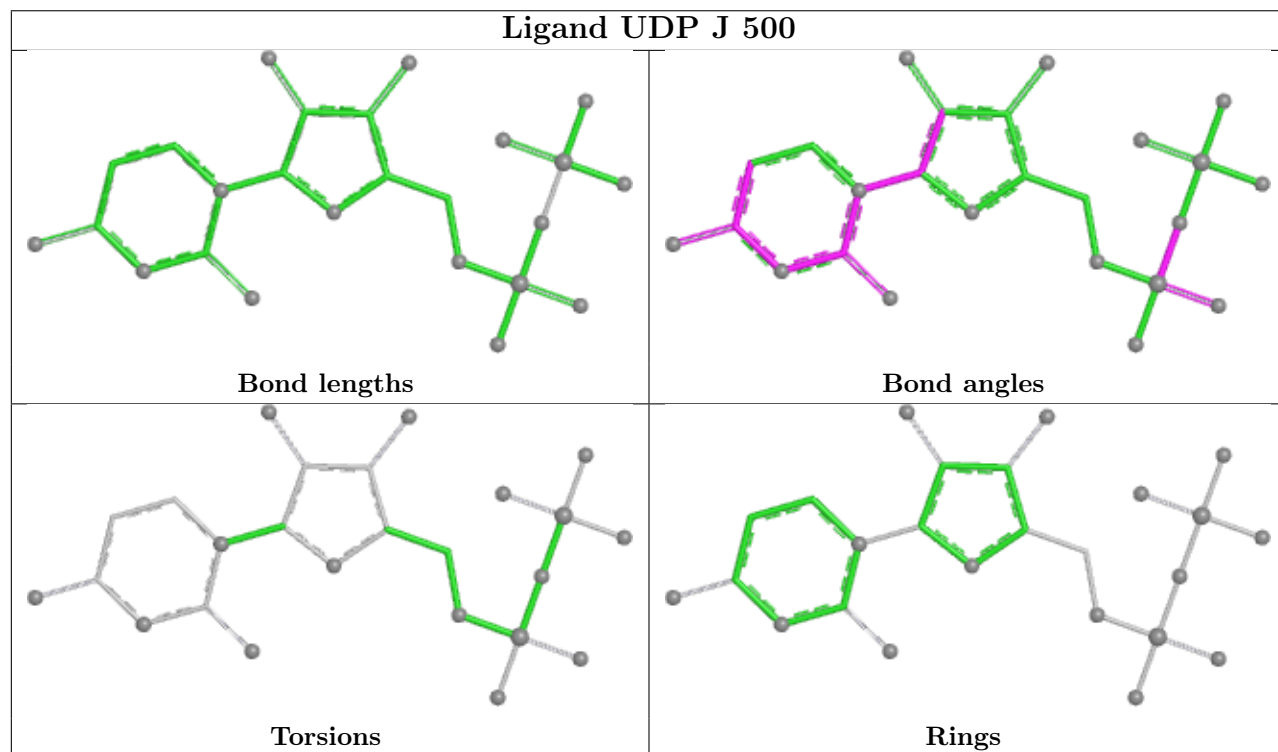
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	450	FAD	1	0
3	G	500	UDP	1	0
2	I	450	FAD	4	0
4	F	400	GOL	1	0
2	G	450	FAD	3	0
4	B	398	GOL	2	0
4	E	400	GOL	1	0
3	B	500	UDP	4	0
4	H	398	GOL	2	0
4	C	398	GOL	2	0
2	E	450	FAD	3	0
4	D	399	GOL	1	0
2	B	450	FAD	1	0
5	D	600	URM	1	0
3	A	500	UDP	1	0
4	I	402	GOL	2	0
2	C	450	FAD	1	0
2	D	450	FAD	4	0
2	A	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.

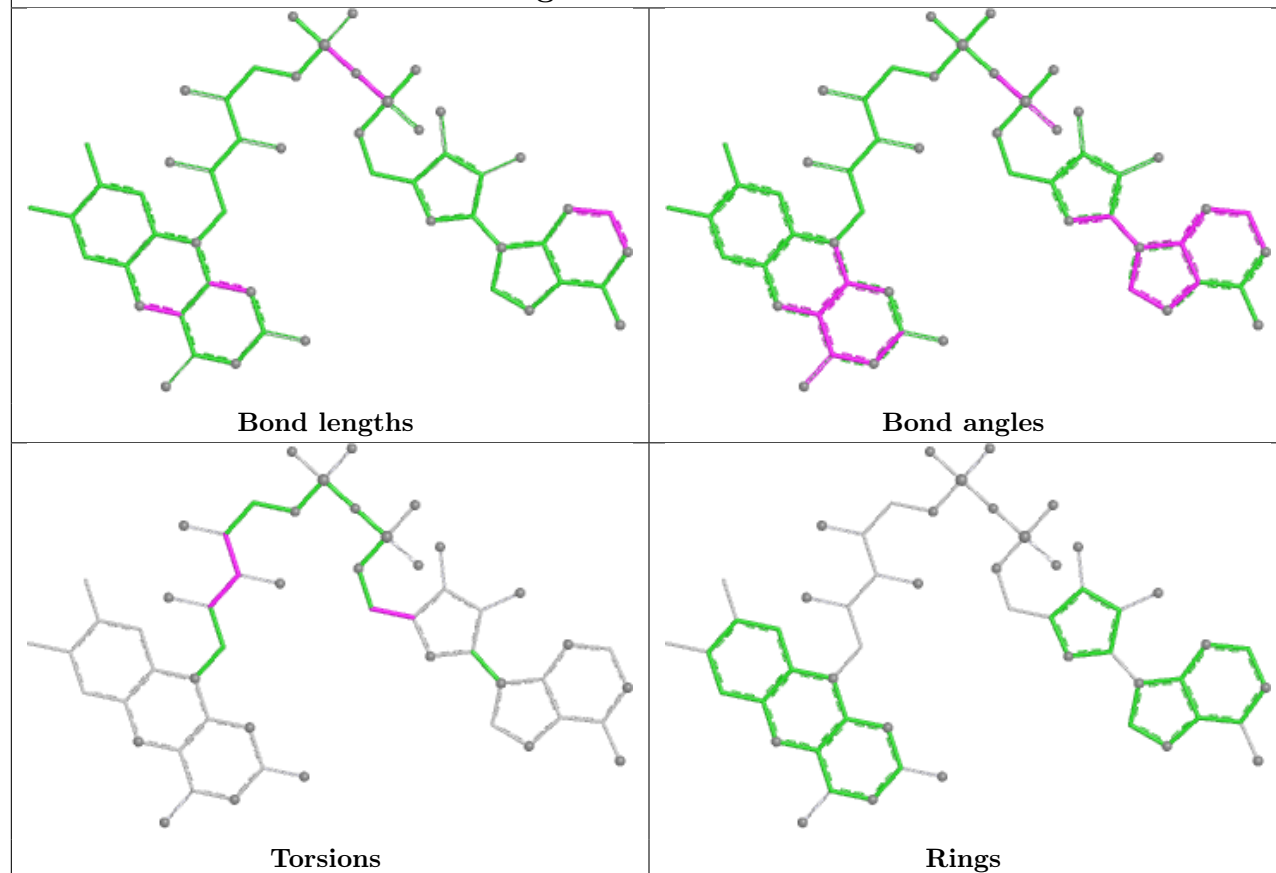
Ligand FAD F 450



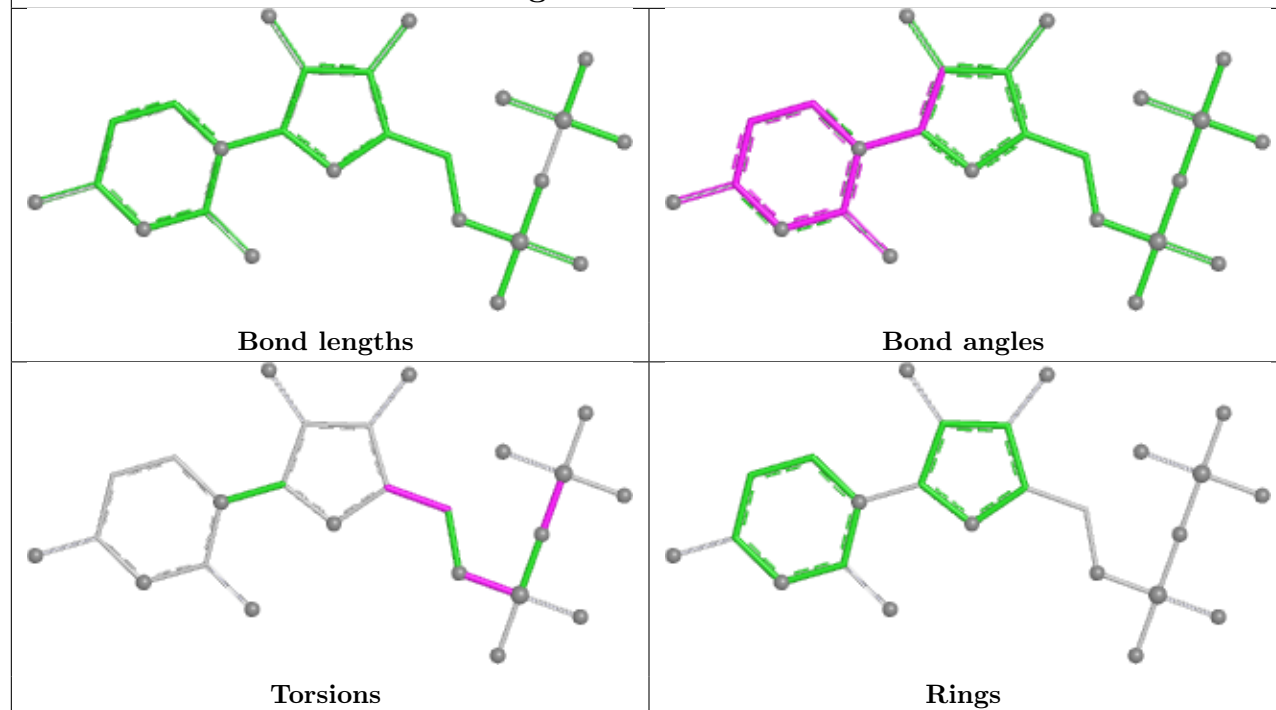
Ligand UDP J 500

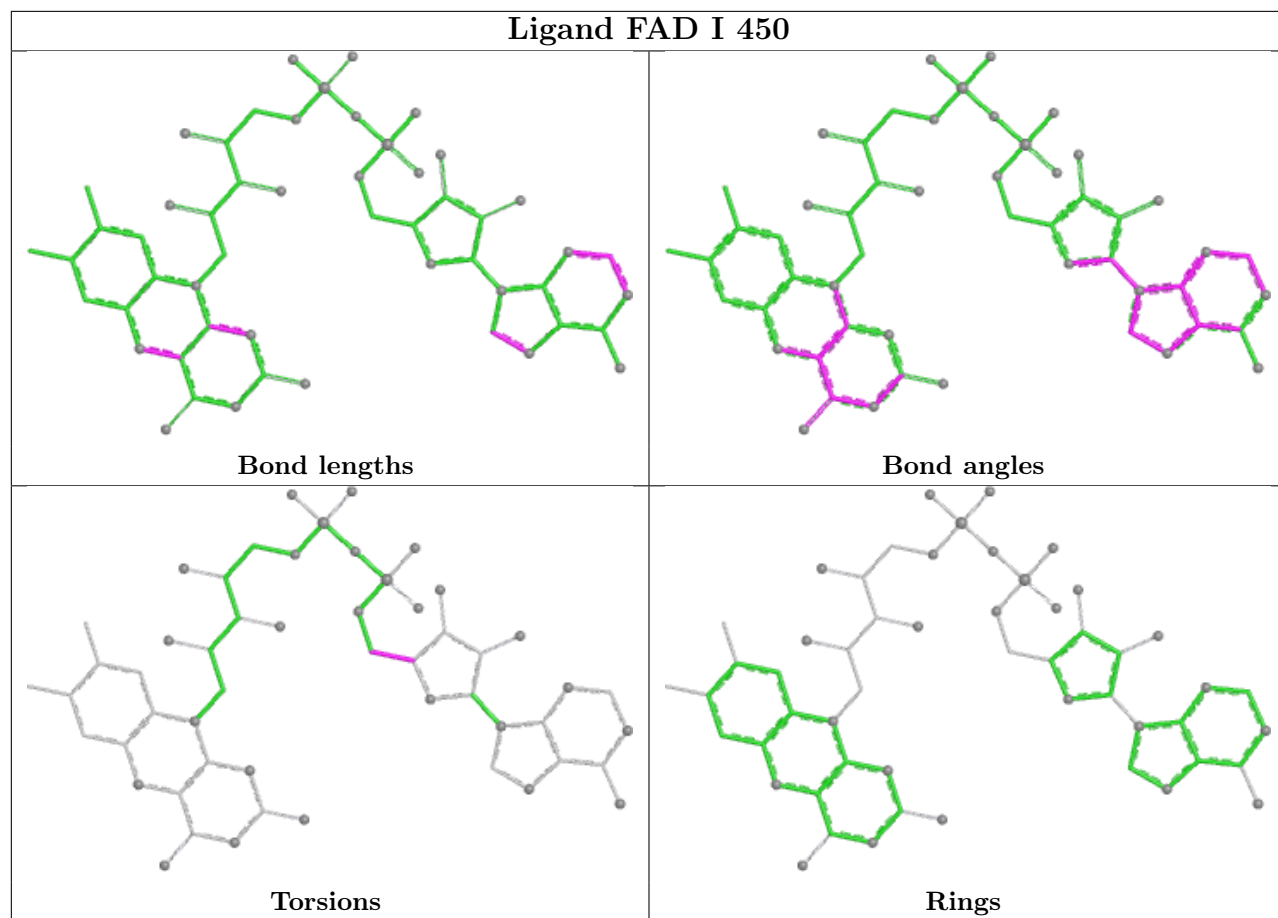


Ligand FAD J 450

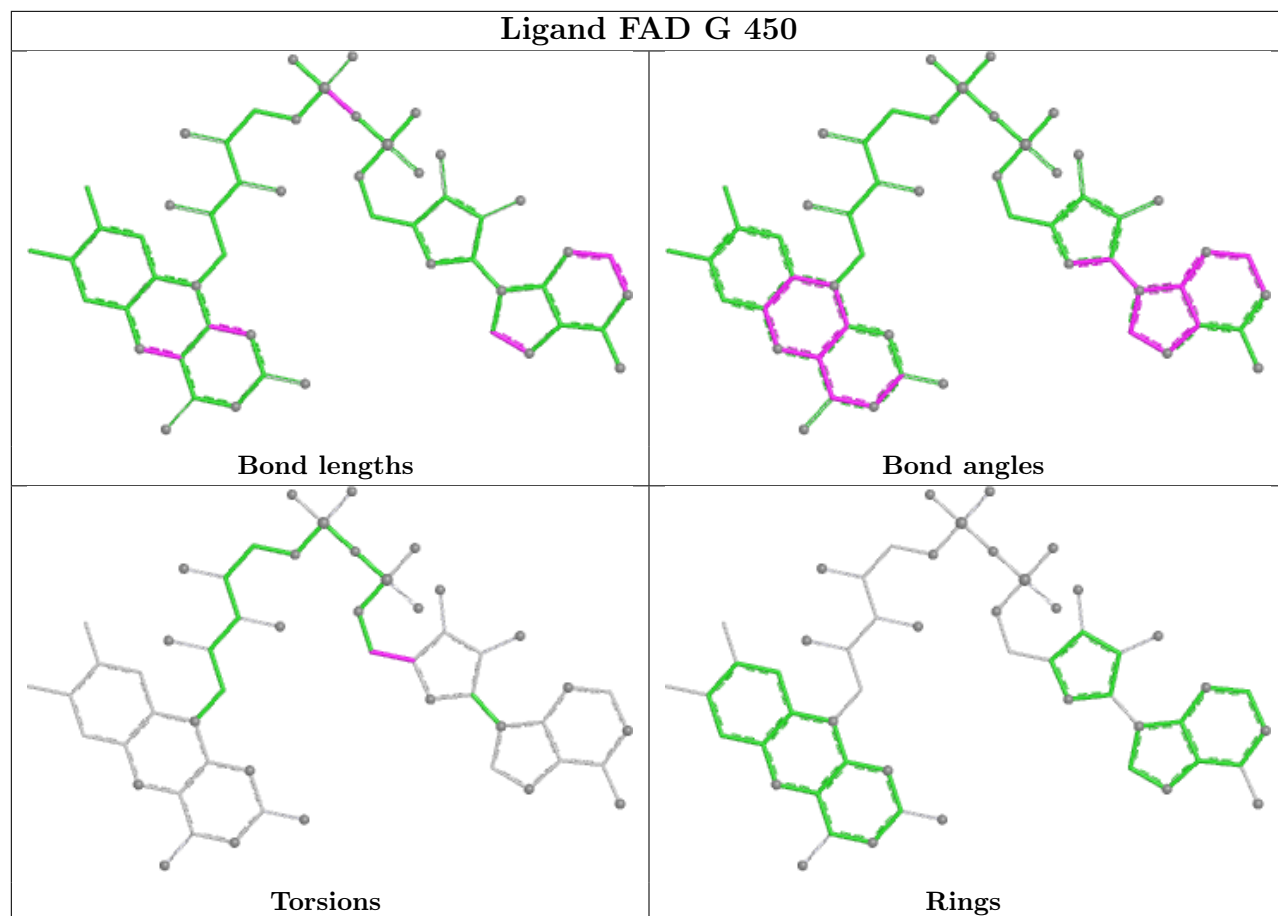


Ligand UDP G 500

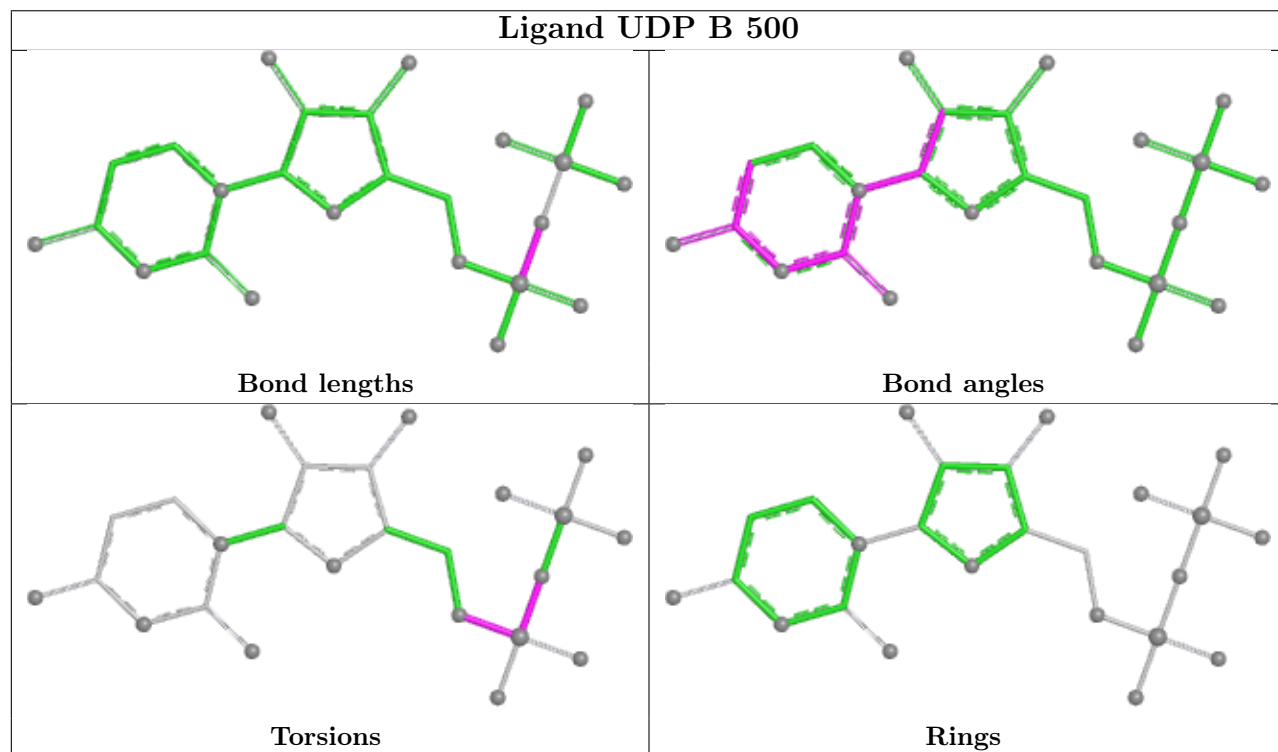




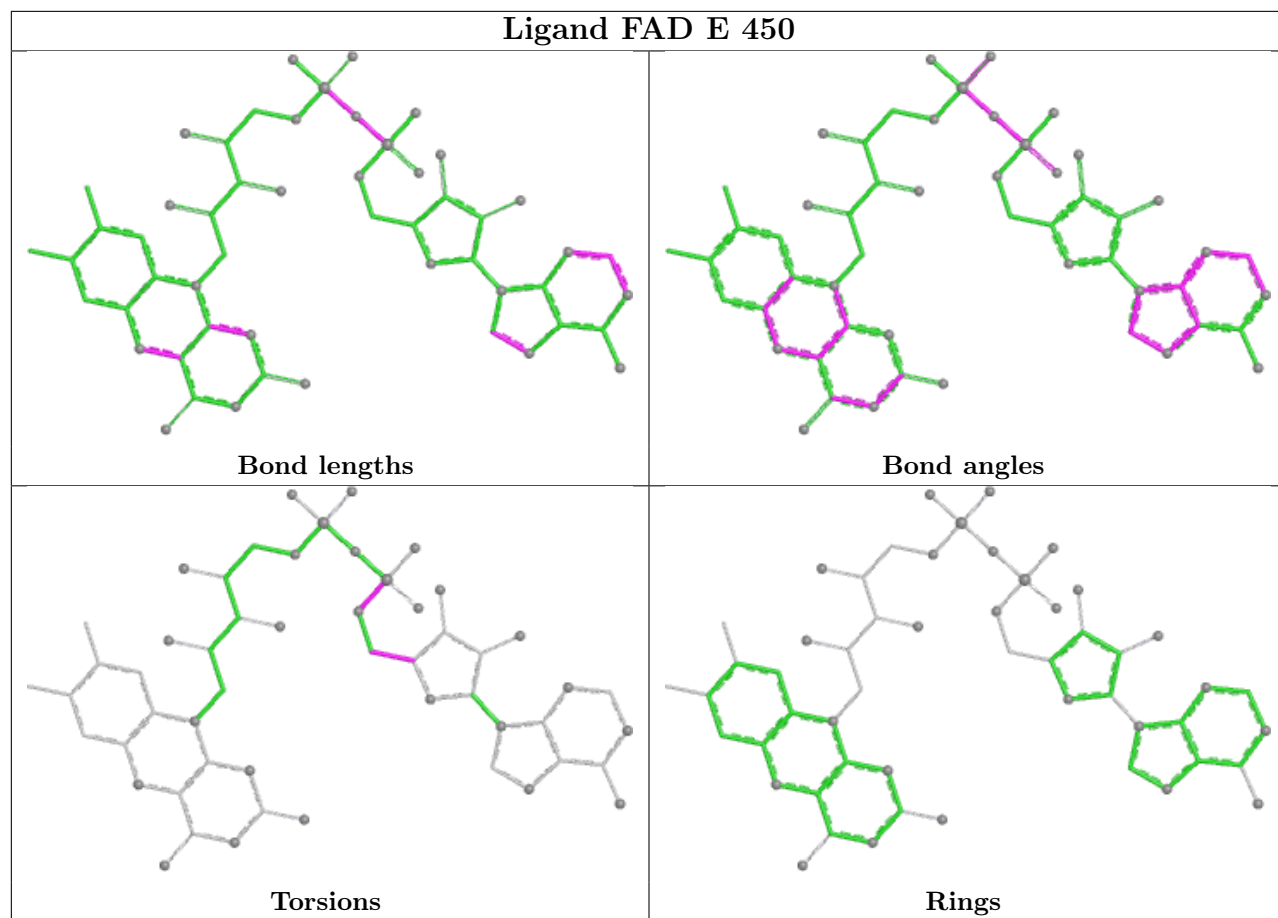
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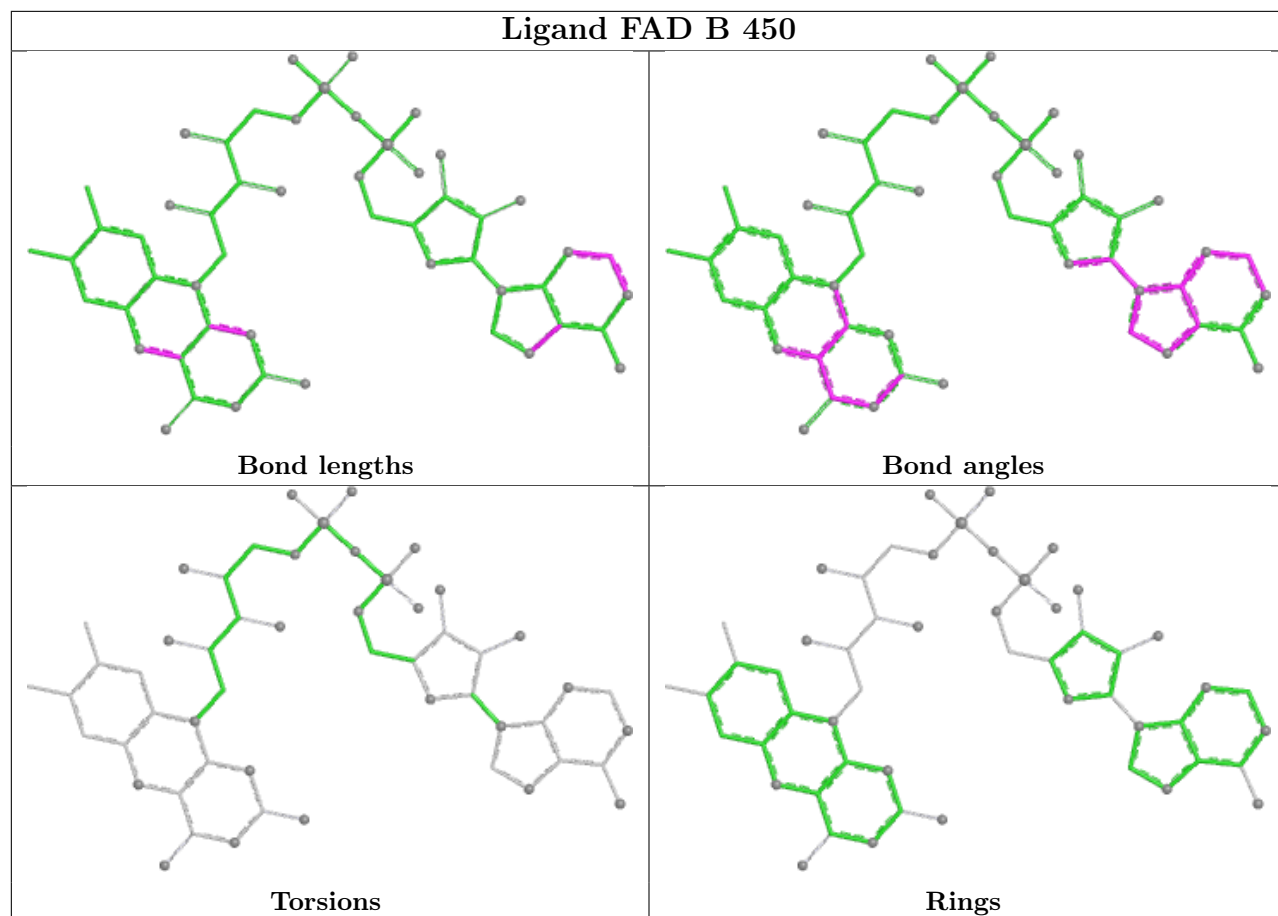
Ligand UDP B 500



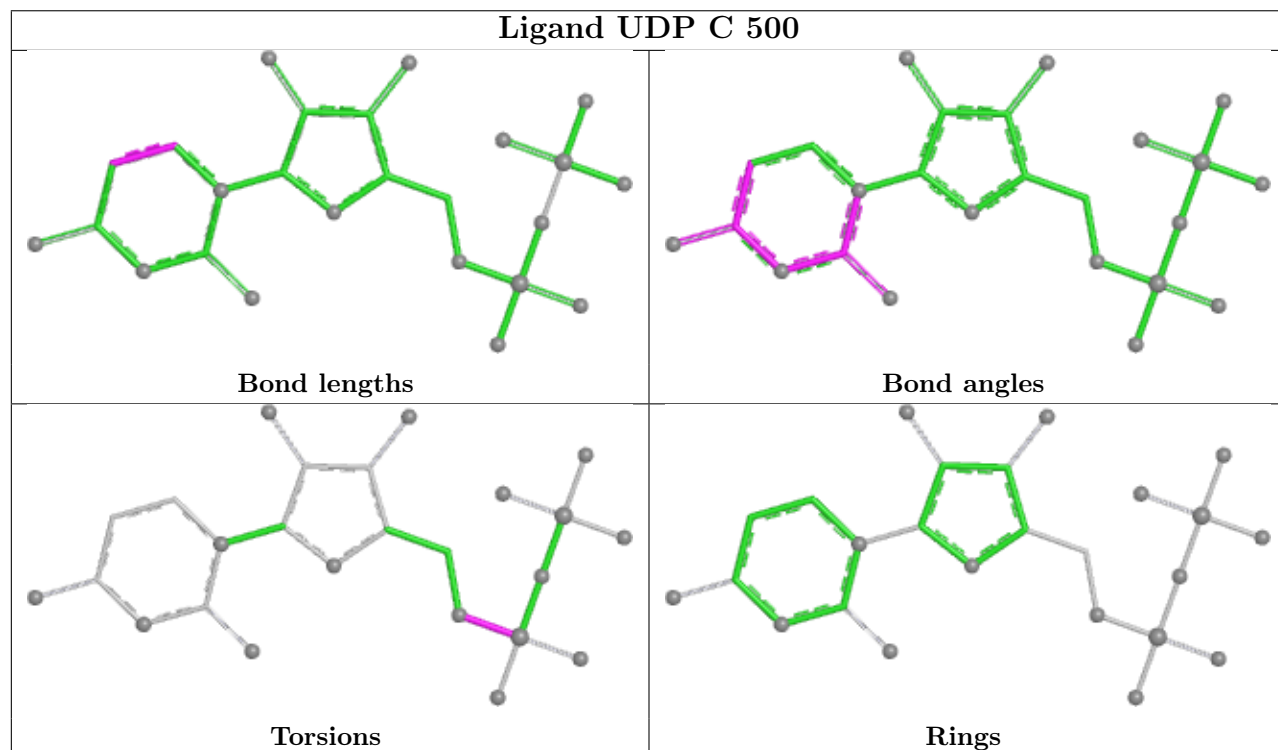
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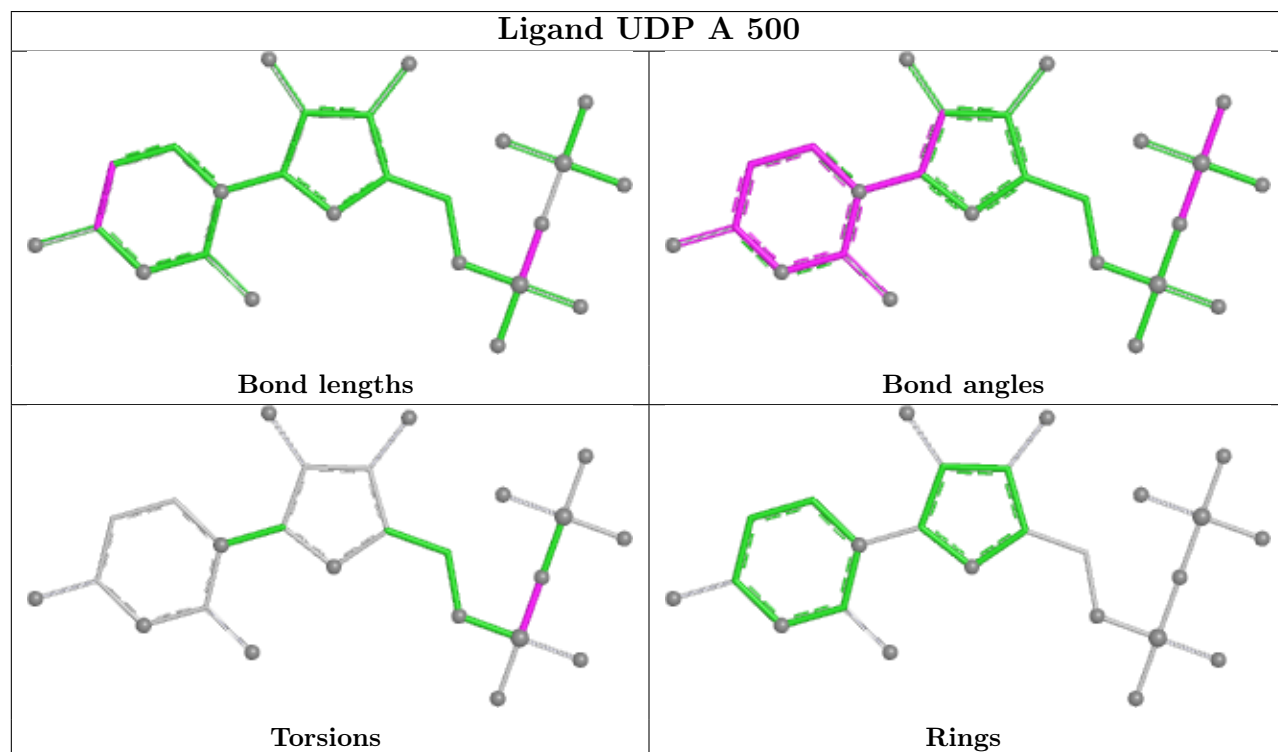
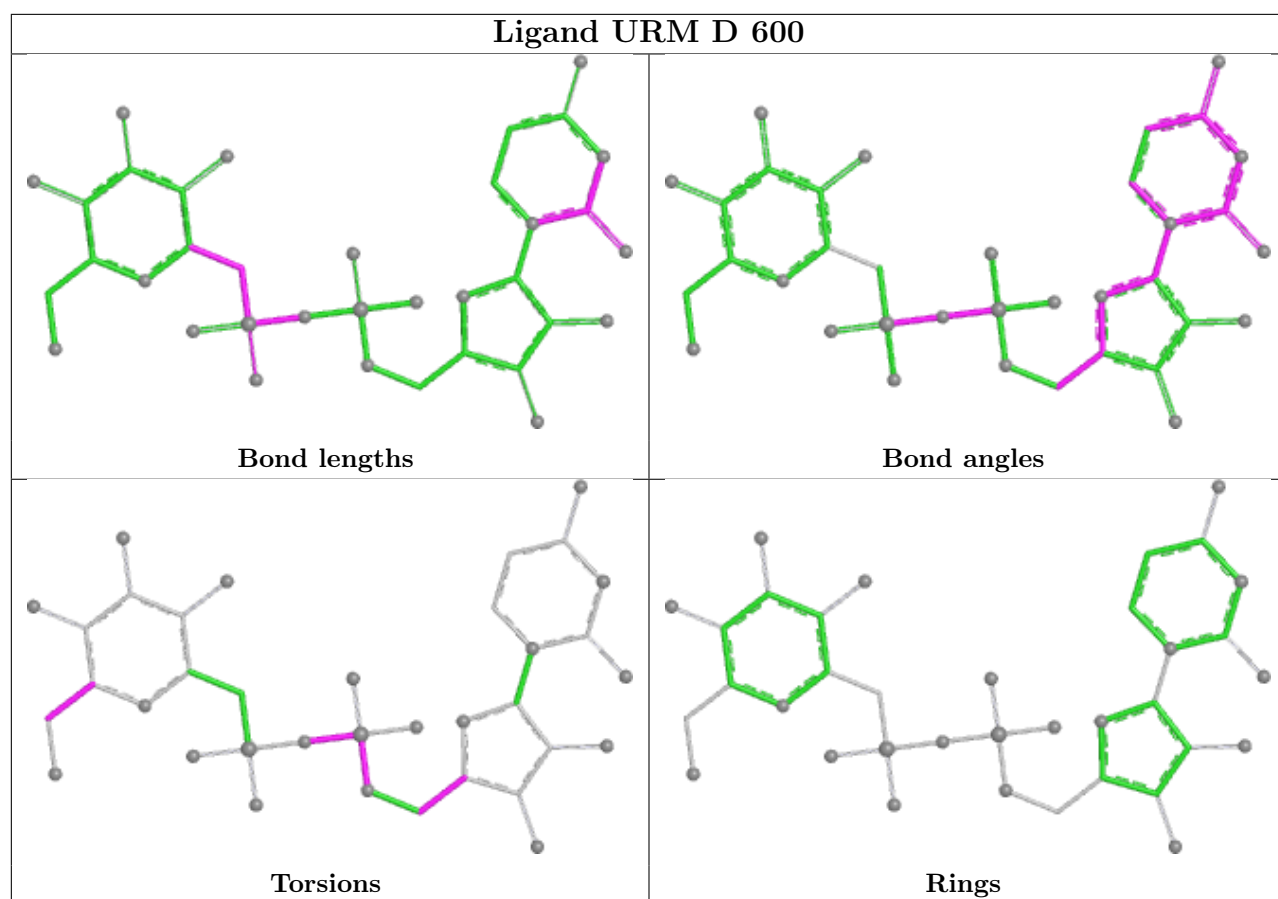


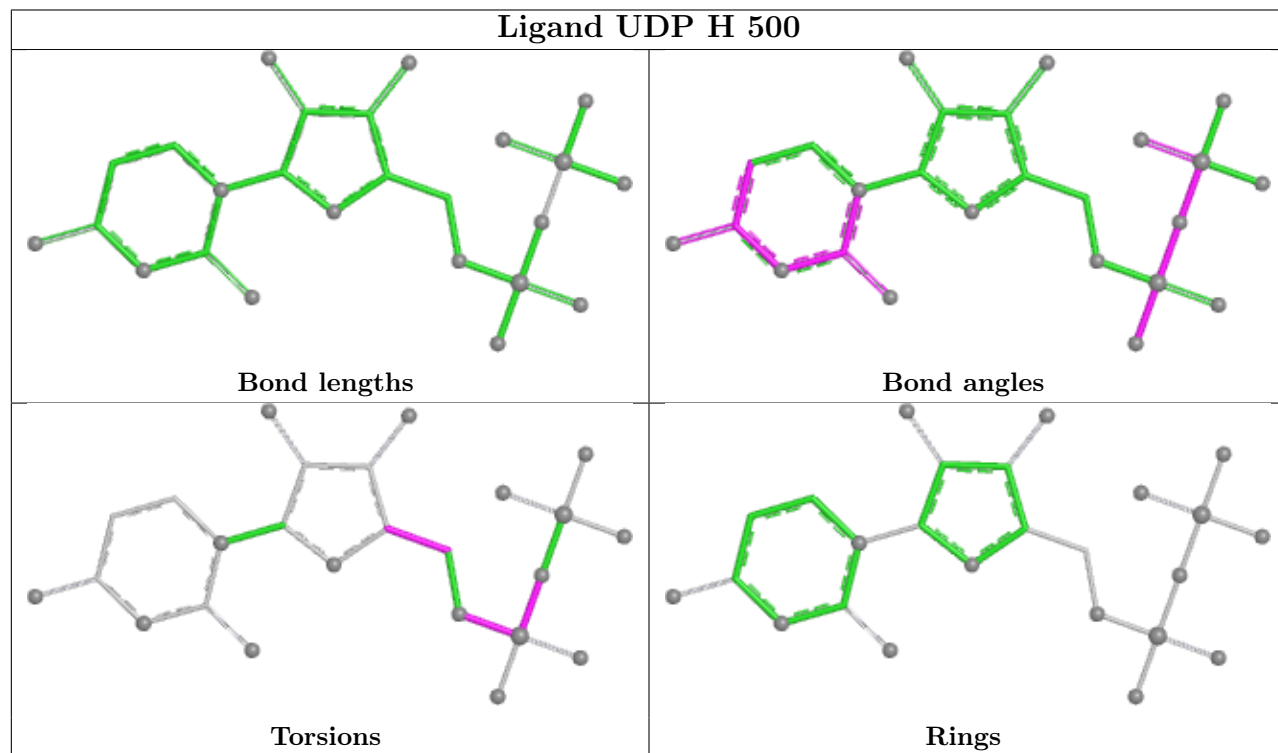
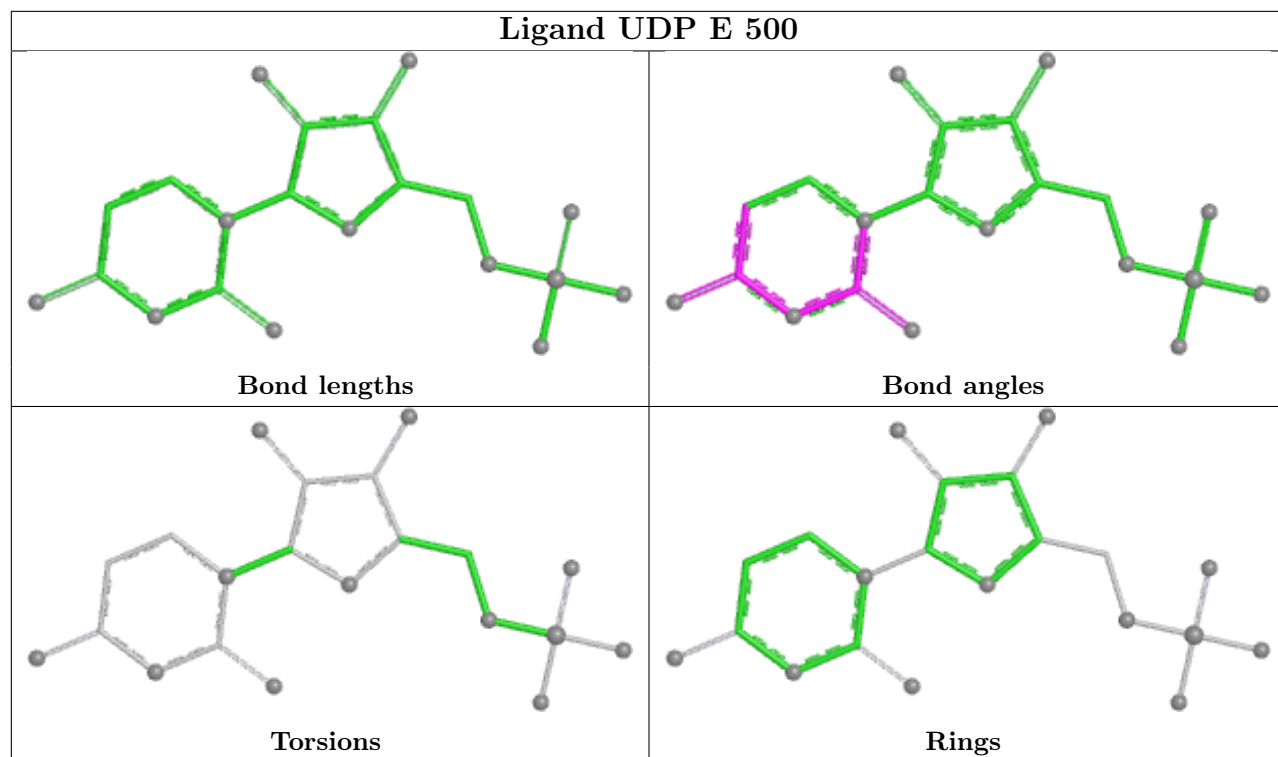
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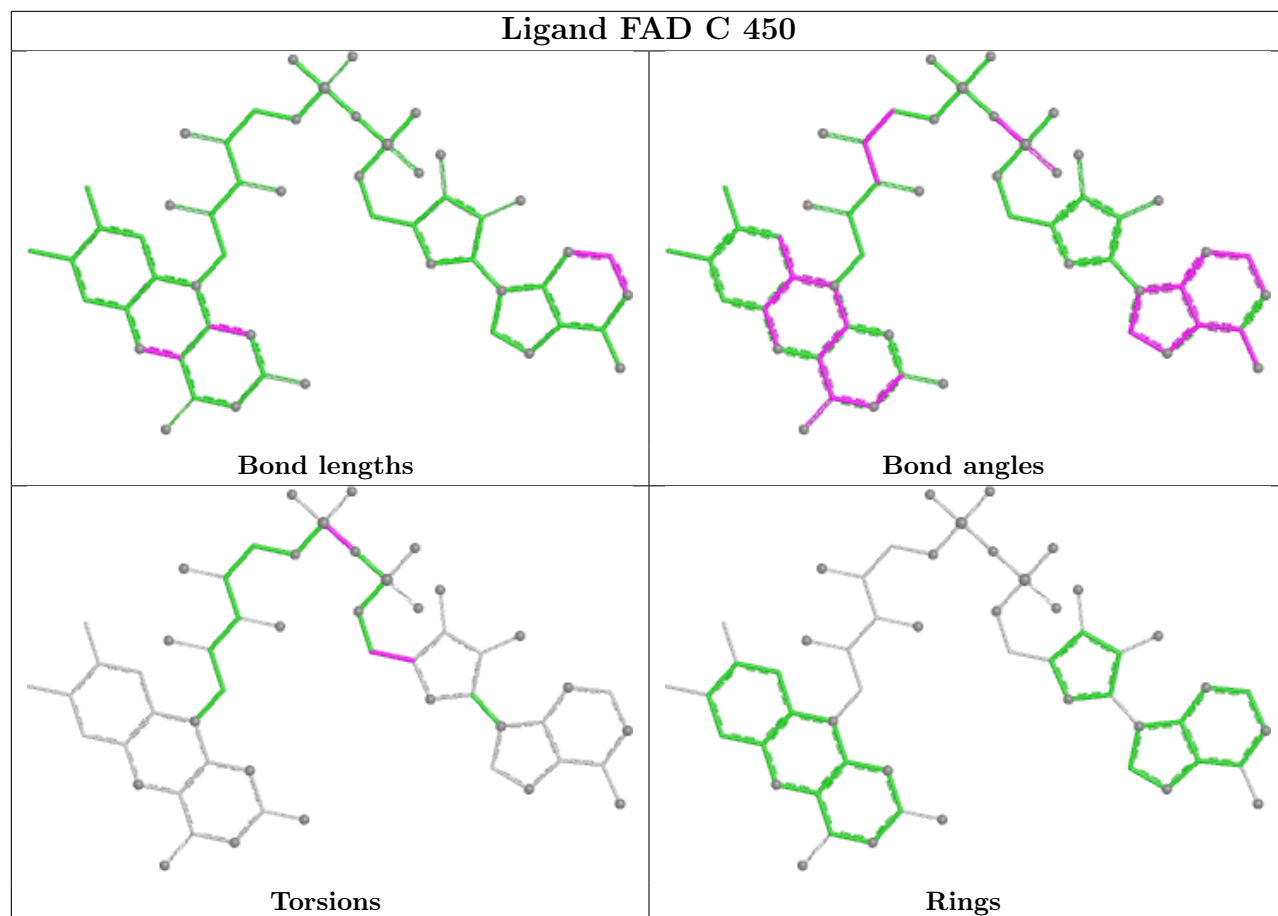
Ligand UDP C 500



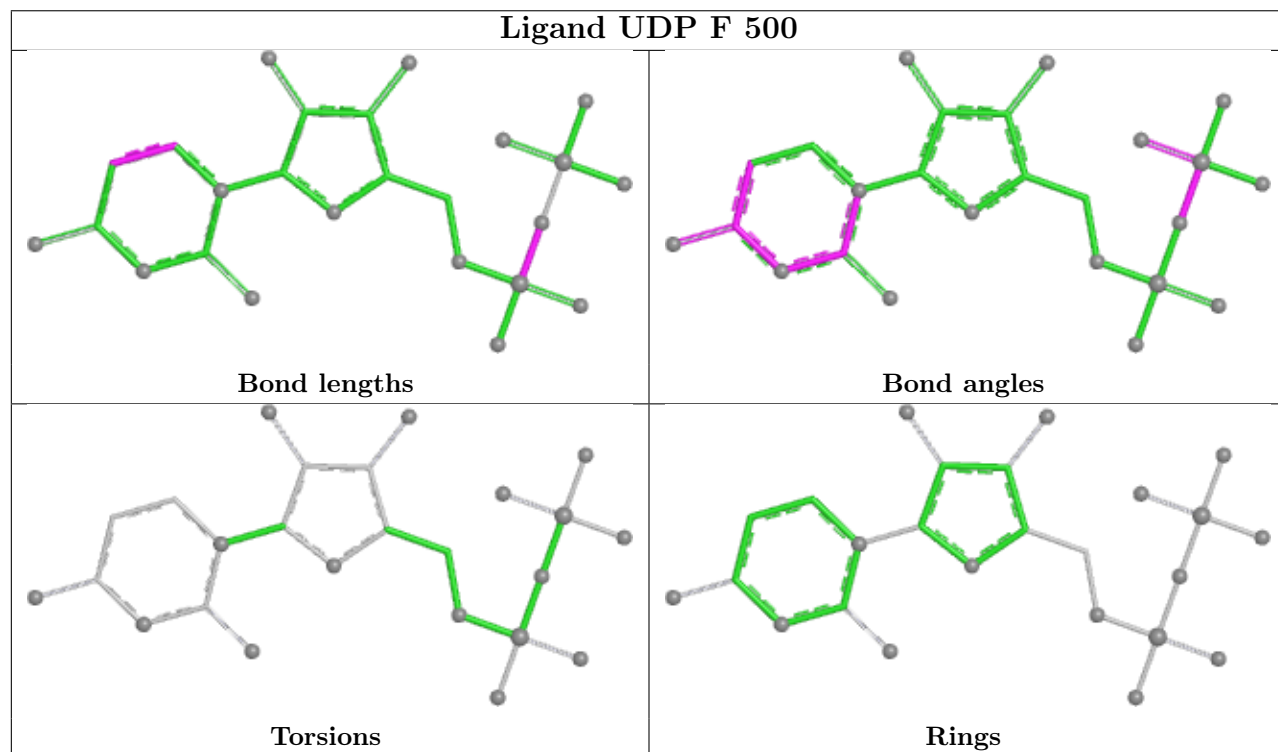


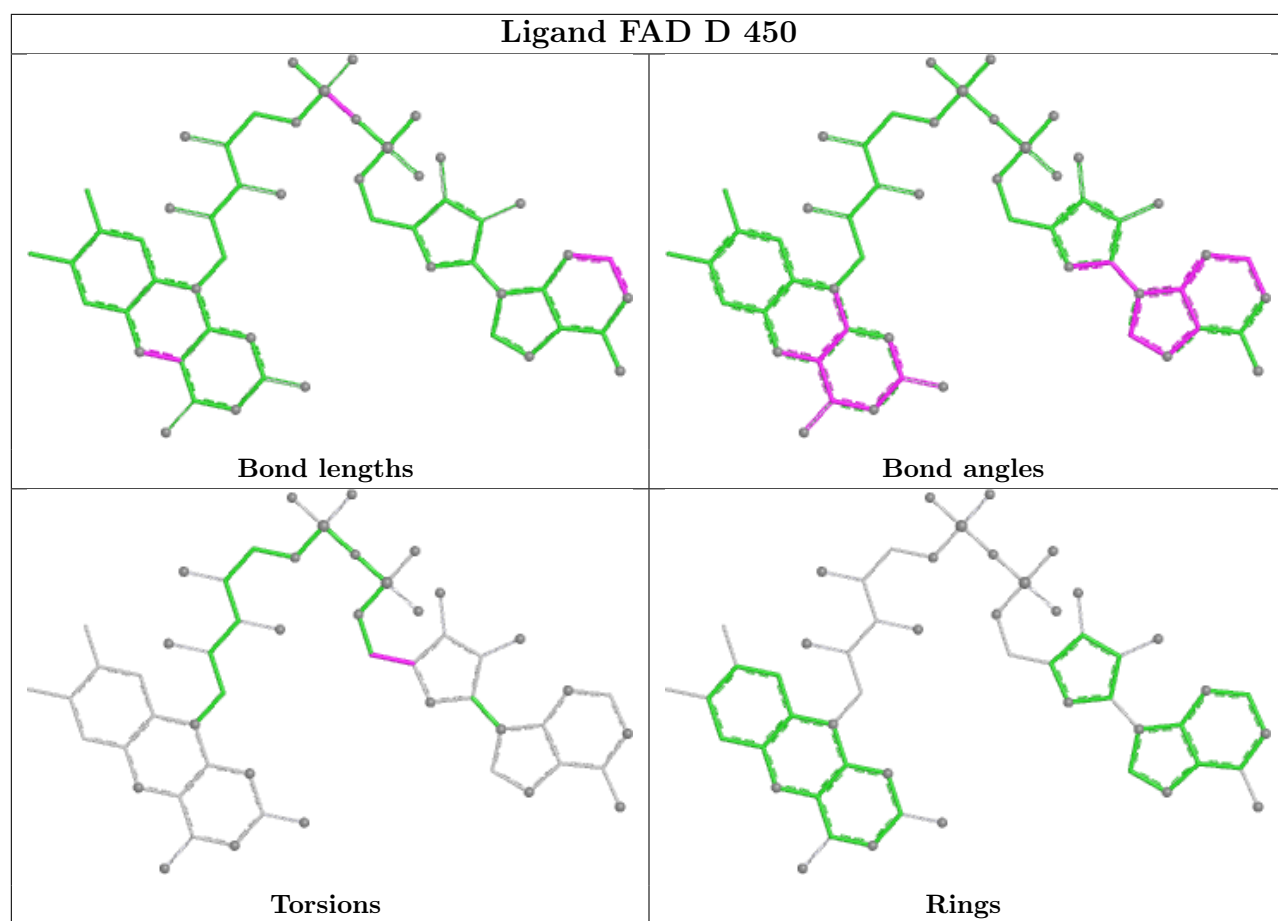


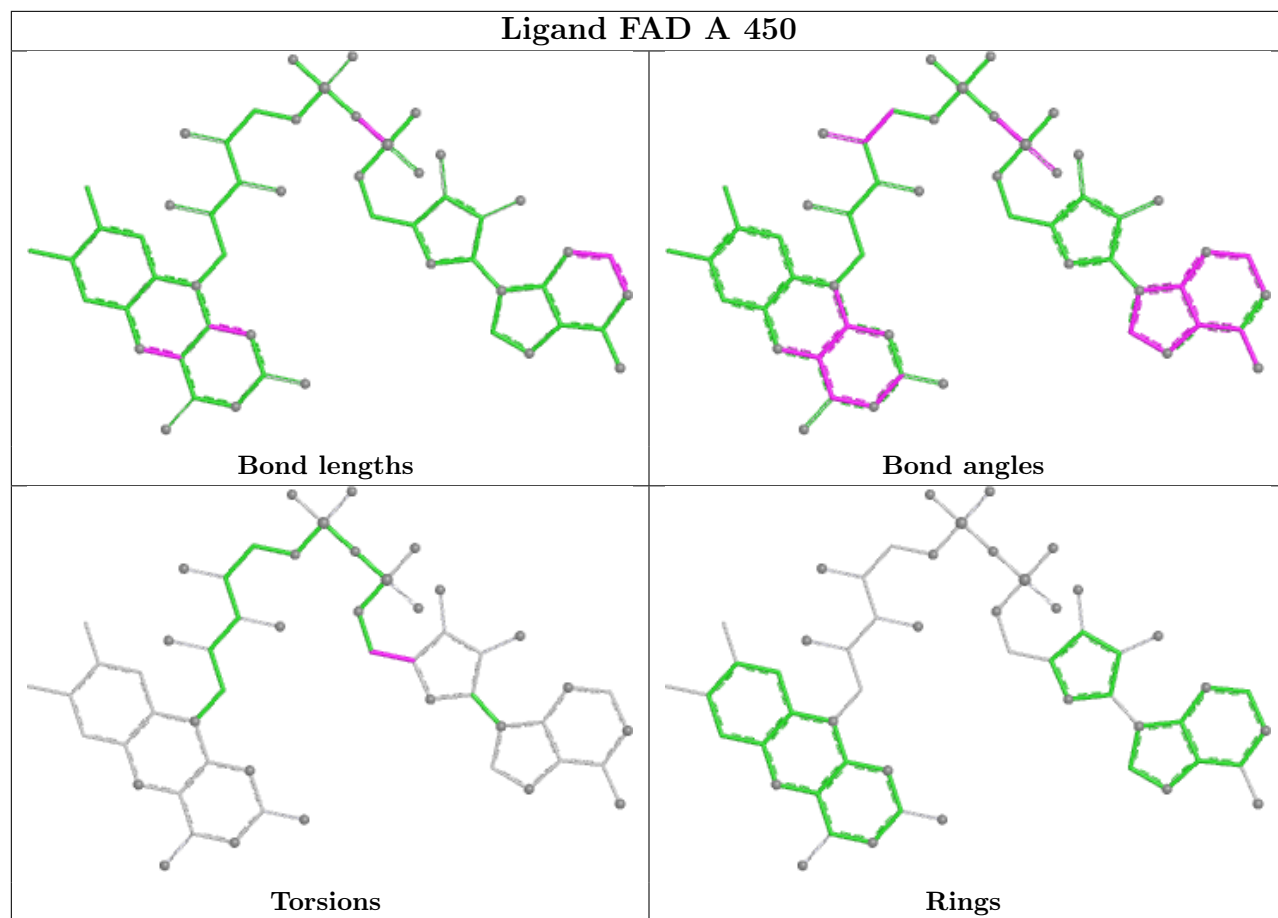
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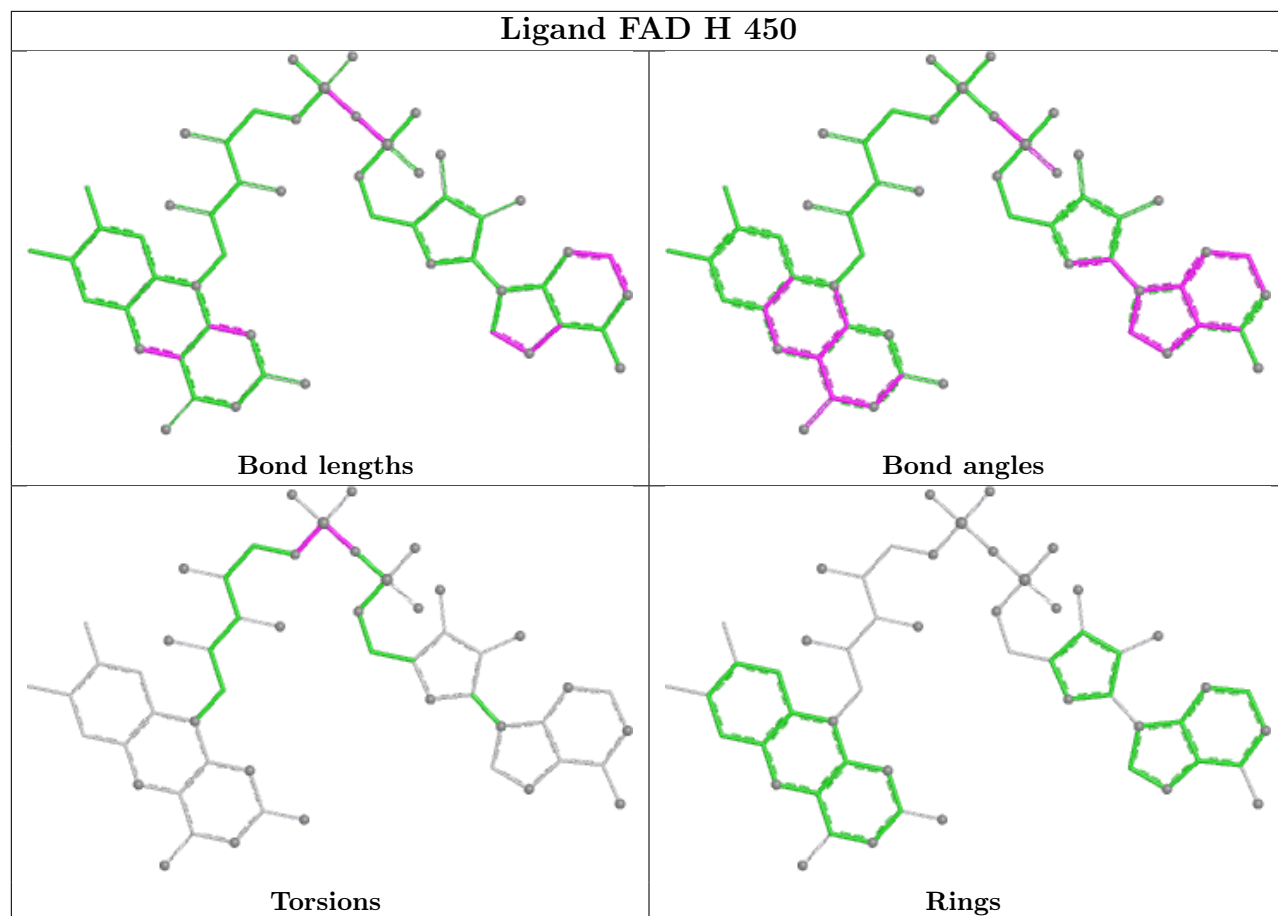
Ligand UDP F 500



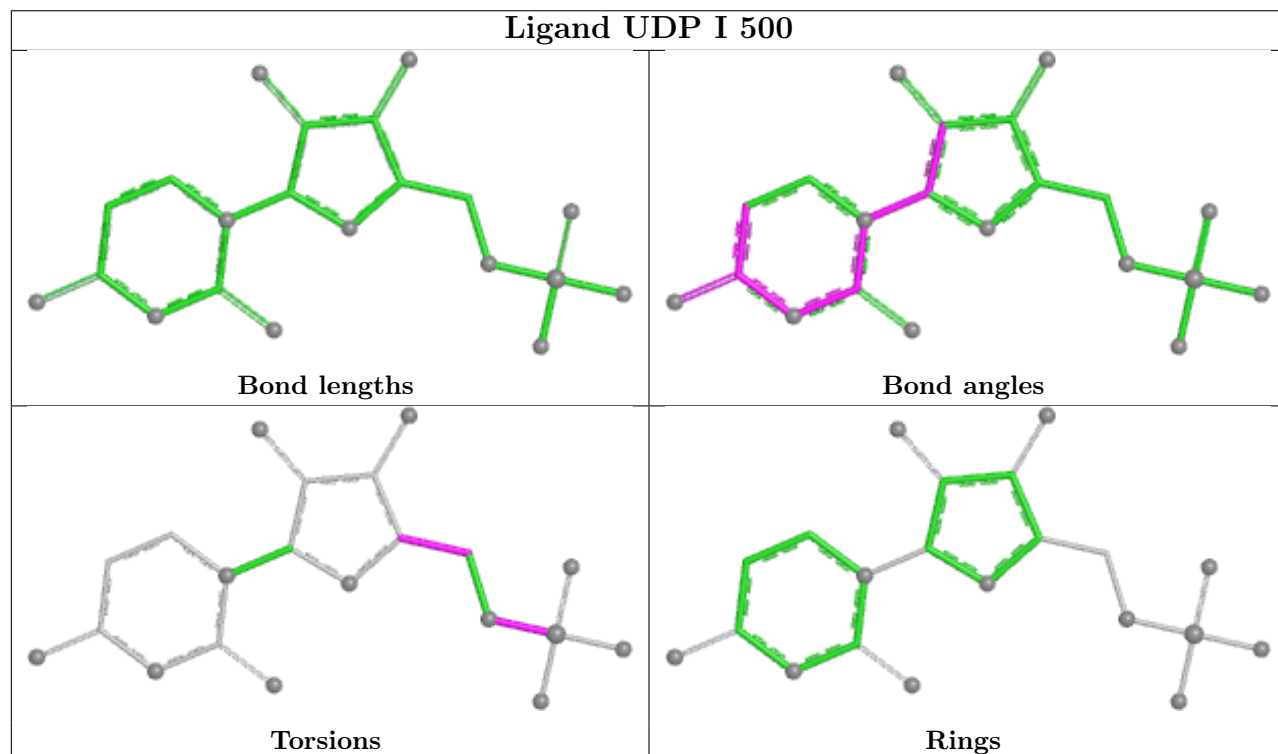




Ligand FAD H 450



Ligand UDP I 500



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.31	4 (1%) 78 75	32, 43, 59, 93	2 (0%)
1	B	363/397 (91%)	0.07	21 (5%) 29 22	33, 47, 94, 152	1 (0%)
1	C	363/397 (91%)	-0.10	6 (1%) 69 64	36, 49, 71, 104	1 (0%)
1	D	359/397 (90%)	-0.05	3 (0%) 82 79	38, 55, 80, 120	2 (0%)
1	E	361/397 (90%)	0.24	12 (3%) 49 40	38, 59, 91, 122	2 (0%)
1	F	364/397 (91%)	-0.17	4 (1%) 78 75	29, 48, 68, 95	3 (0%)
1	G	363/397 (91%)	0.02	9 (2%) 58 52	34, 53, 78, 126	2 (0%)
1	H	364/397 (91%)	-0.12	10 (2%) 56 49	35, 48, 69, 115	1 (0%)
1	I	364/397 (91%)	-0.25	5 (1%) 73 69	33, 46, 66, 106	1 (0%)
1	J	363/397 (91%)	0.00	4 (1%) 78 75	34, 53, 81, 109	3 (0%)
All	All	3629/3970 (91%)	-0.07	78 (2%) 63 57	29, 49, 81, 152	18 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	188	PRO	5.0
1	J	389	GLY	4.8
1	I	154	GLU	4.7
1	G	370	TYR	4.5
1	F	391	PRO	4.0
1	B	163	VAL	4.0
1	E	356	ALA	3.9
1	H	28	LYS	3.9
1	E	249	PHE	3.6
1	B	189	SER	3.6
1	B	162	VAL	3.5
1	H	29	GLY	3.3
1	F	280[A]	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	340	PRO	3.2
1	B	186	LEU	3.1
1	B	152	LYS	3.1
1	G	152	LYS	3.1
1	D	249	PHE	3.0
1	B	153	VAL	3.0
1	G	318	HIS	2.9
1	H	27	SER	2.9
1	C	29	GLY	2.8
1	B	197	ALA	2.8
1	H	154	GLU	2.8
1	B	156	VAL	2.8
1	B	28	LYS	2.7
1	H	357	GLN	2.7
1	B	157	ARG	2.5
1	B	164	VAL	2.5
1	G	28	LYS	2.5
1	B	200	PRO	2.5
1	H	30	PHE	2.5
1	E	250	ILE	2.5
1	I	389	GLY	2.5
1	E	155	GLN	2.5
1	G	27	SER	2.4
1	E	251	PRO	2.4
1	C	390	GLN	2.4
1	G	156	VAL	2.4
1	J	154	GLU	2.4
1	E	270	GLY	2.4
1	G	357	GLN	2.4
1	G	153	VAL	2.4
1	C	385	ARG	2.3
1	A	156	VAL	2.3
1	E	370	TYR	2.3
1	G	155	GLN	2.3
1	E	389	GLY	2.3
1	B	199	VAL	2.3
1	J	30	PHE	2.3
1	H	248	ASP	2.3
1	H	251	PRO	2.3
1	B	158	THR	2.2
1	A	157[A]	ARG	2.2
1	A	341	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	390	GLN	2.2
1	A	389	GLY	2.2
1	B	249	PHE	2.2
1	C	166	LYS	2.2
1	B	190	GLU	2.2
1	E	268	CYS	2.2
1	I	152	LYS	2.2
1	D	248	ASP	2.2
1	C	153	VAL	2.2
1	E	352	LEU	2.1
1	B	154	GLU	2.1
1	J	318	HIS	2.1
1	B	329	ALA	2.1
1	I	26	GLU	2.1
1	E	379	GLN	2.1
1	H	153	VAL	2.1
1	B	192	ASP	2.1
1	F	344	GLU	2.1
1	D	104	TRP	2.1
1	C	357	GLN	2.1
1	F	156	VAL	2.0
1	I	153	VAL	2.0
1	B	169	ARG	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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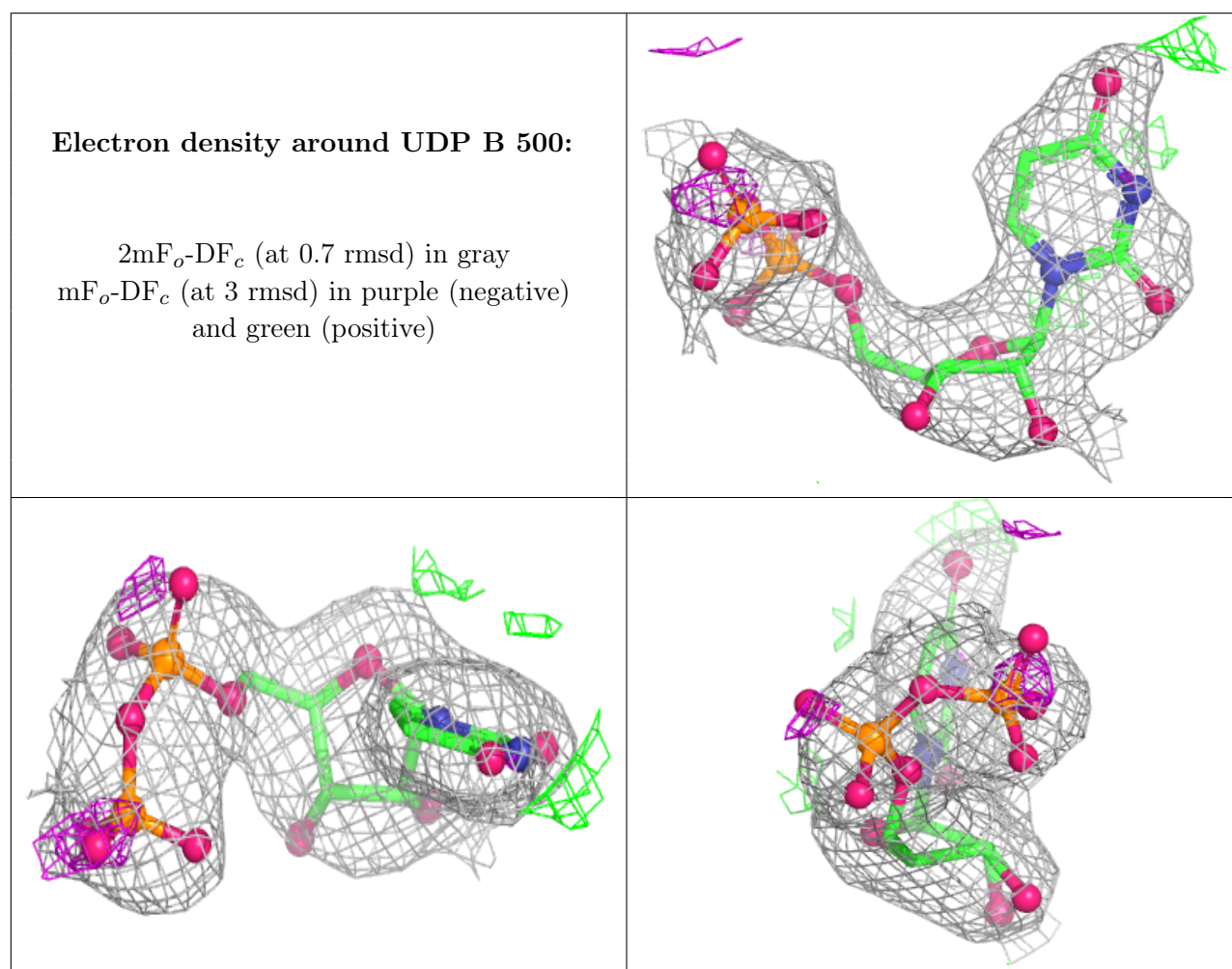
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	B	398	6/6	0.61	0.20	52,58,59,59	0
4	GOL	E	398	6/6	0.65	0.19	61,64,71,72	0
6	XYL	F	399	10/10	0.66	0.33	20,20,20,20	0
4	GOL	D	398	6/6	0.73	0.16	47,52,61,65	0
4	GOL	H	399	6/6	0.74	0.18	60,72,75,81	0
4	GOL	F	398	6/6	0.76	0.16	48,55,60,62	0
4	GOL	H	398	6/6	0.77	0.14	50,55,61,62	0
4	GOL	J	399	6/6	0.78	0.17	46,60,64,69	0
4	GOL	A	399	6/6	0.78	0.20	58,62,75,76	0
6	XYL	I	401	10/10	0.78	0.16	62,67,73,76	0
4	GOL	J	400	6/6	0.79	0.18	56,62,70,72	0
4	GOL	D	399	6/6	0.79	0.14	73,75,76,77	0
4	GOL	E	399	6/6	0.79	0.20	60,65,74,76	0
4	GOL	C	398	6/6	0.81	0.13	51,55,57,60	0
4	GOL	G	400	6/6	0.81	0.15	63,68,72,76	0
4	GOL	A	398	6/6	0.82	0.16	51,56,64,66	0
4	GOL	I	400	6/6	0.82	0.19	67,76,80,80	0
4	GOL	A	400	6/6	0.83	0.15	58,63,69,70	0
3	UDP	B	500	25/25	0.84	0.12	60,80,102,117	0
4	GOL	F	400	6/6	0.84	0.18	59,65,67,69	0
4	GOL	I	402	6/6	0.85	0.16	61,62,68,74	0
4	GOL	E	401	6/6	0.86	0.13	67,73,74,78	0
4	GOL	E	400	6/6	0.88	0.14	61,66,73,76	0
4	GOL	C	399	6/6	0.88	0.15	65,72,77,78	0
4	GOL	I	398	6/6	0.88	0.13	41,50,55,56	0
4	GOL	I	399	6/6	0.89	0.14	55,64,67,73	0
4	GOL	G	399	6/6	0.89	0.11	54,57,63,64	0
4	GOL	G	398	6/6	0.90	0.11	51,52,57,61	0
3	UDP	G	500	25/25	0.92	0.09	52,59,87,108	0
5	URM	D	600	36/36	0.92	0.10	54,63,76,85	0
3	UDP	F	500	25/25	0.93	0.08	47,52,90,107	0
3	UDP	C	500	25/25	0.93	0.09	50,58,85,108	0
3	UDP	H	500	25/25	0.94	0.08	41,48,73,90	0
3	UDP	J	500	25/25	0.94	0.09	38,47,85,108	0
3	UDP	E	500	21/25	0.94	0.08	57,63,72,76	0
2	FAD	D	450	53/53	0.94	0.08	50,57,65,66	0
3	UDP	A	500	25/25	0.94	0.09	39,46,72,90	0
2	FAD	E	450	53/53	0.95	0.08	45,60,70,74	0
2	FAD	G	450	53/53	0.95	0.09	46,54,65,67	0
2	FAD	J	450	53/53	0.95	0.08	44,57,64,65	0
2	FAD	A	450	53/53	0.96	0.07	38,46,51,55	0

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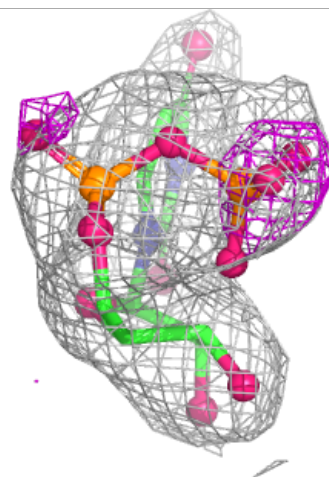
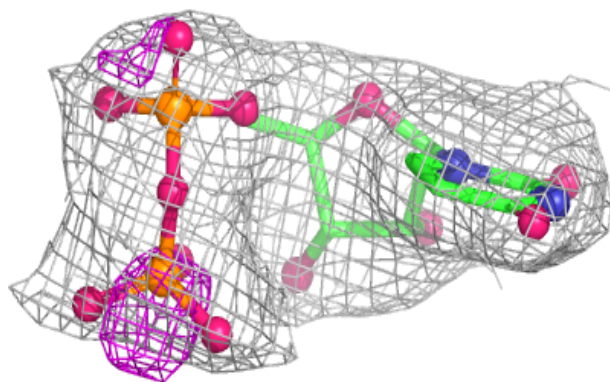
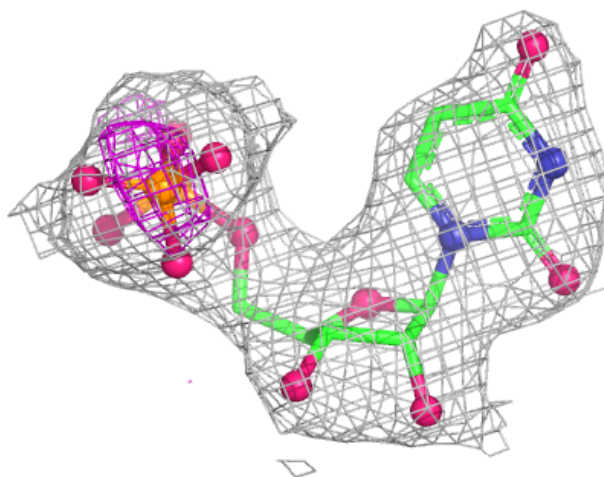
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	B	450	53/53	0.96	0.09	35,47,62,66	0
3	UDP	I	500	21/25	0.96	0.08	48,50,63,69	0
2	FAD	C	450	53/53	0.96	0.08	39,48,61,70	0
2	FAD	I	450	53/53	0.97	0.07	38,45,56,62	0
2	FAD	F	450	53/53	0.97	0.07	40,47,54,60	0
2	FAD	H	450	53/53	0.97	0.06	38,48,52,56	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.



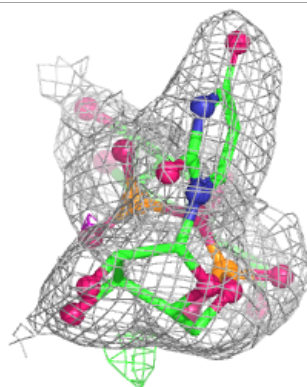
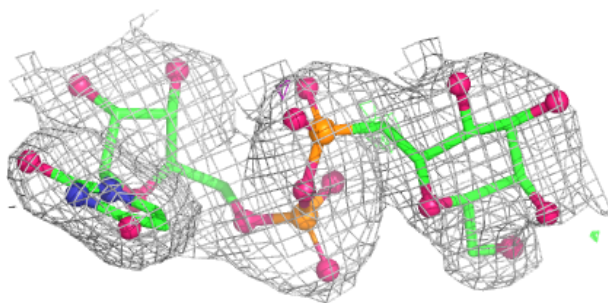
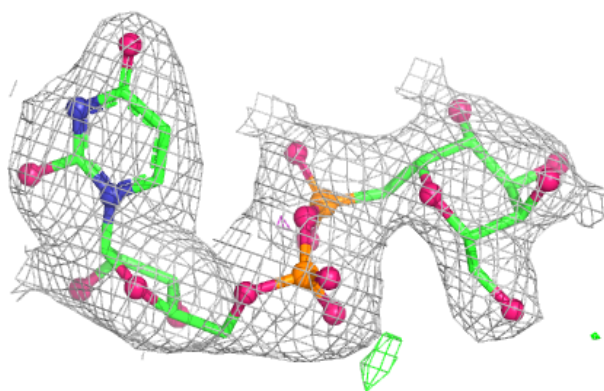
Electron density around UDP G 500:

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

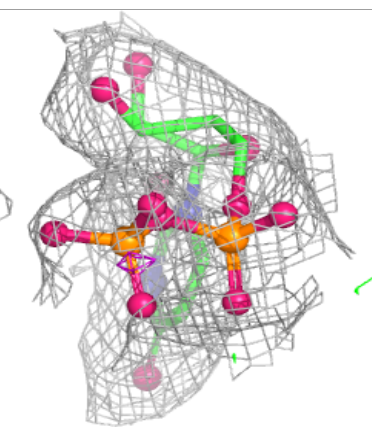
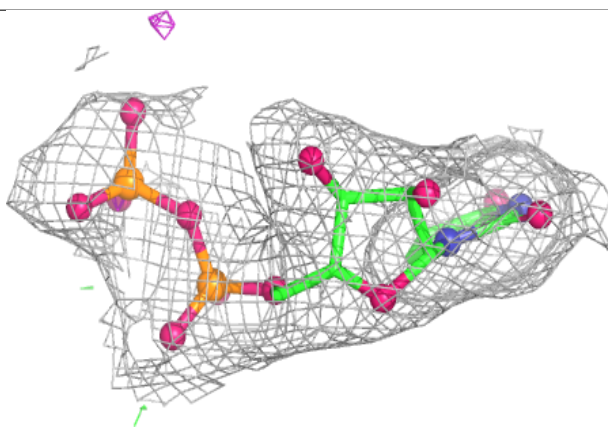
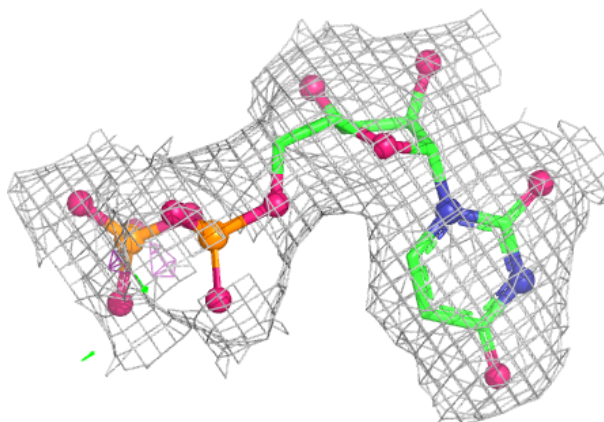


Electron density around URM D 600:

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

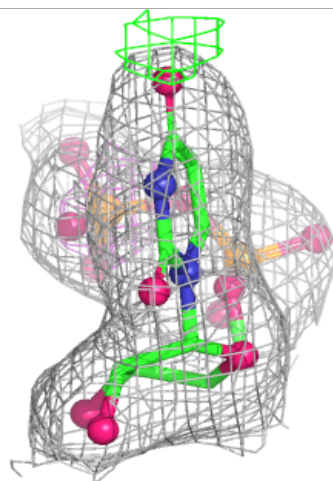
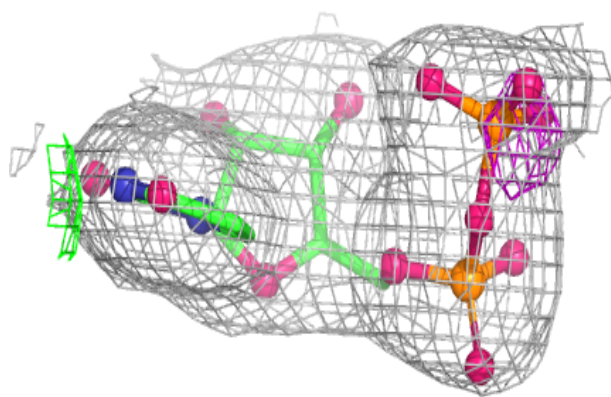
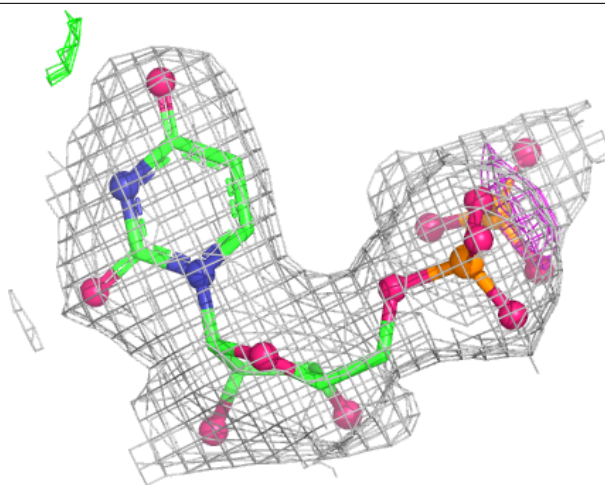
**Electron density around UDP F 500:**

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



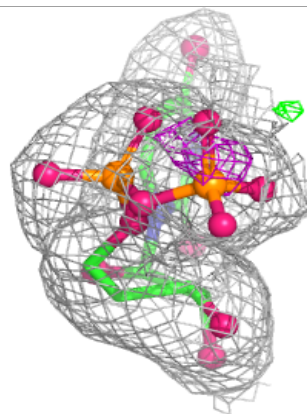
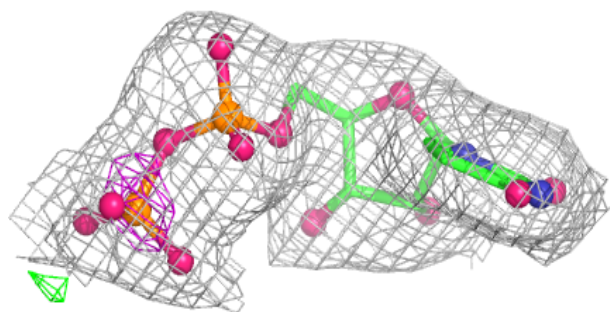
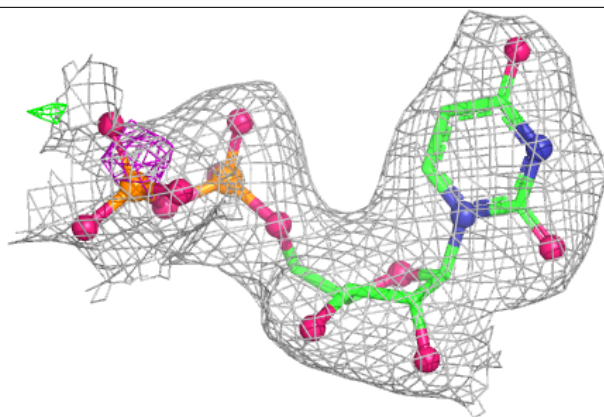
Electron density around UDP C 500:

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

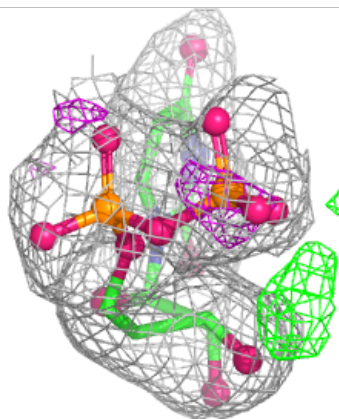
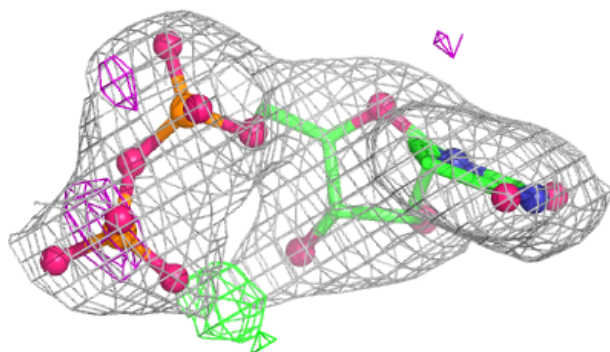
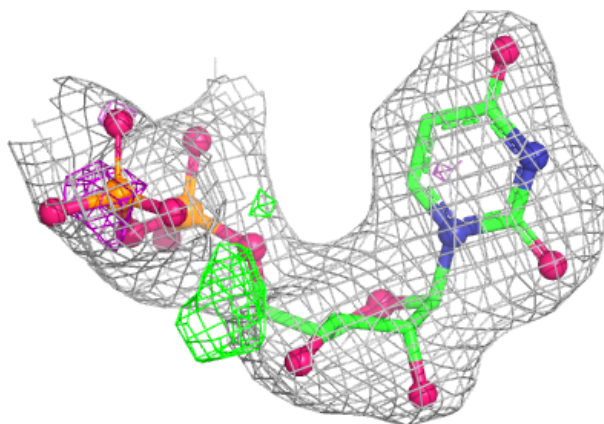


Electron density around UDP H 500:

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

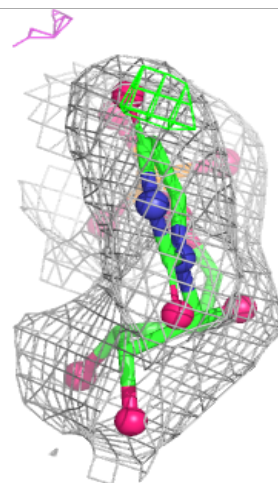
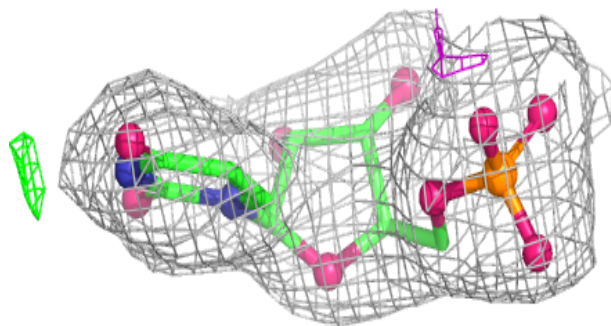
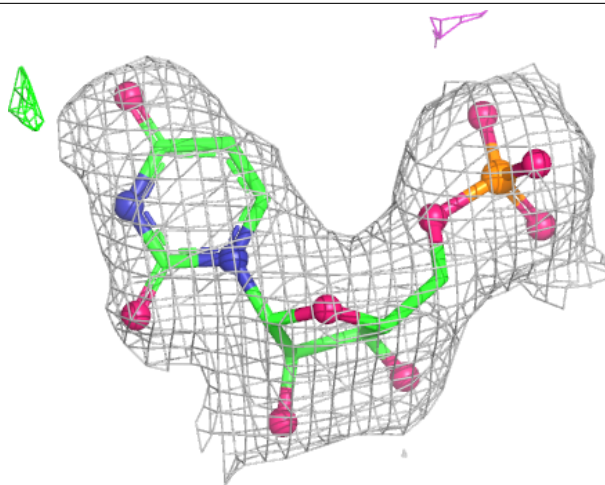
**Electron density around UDP J 500:**

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



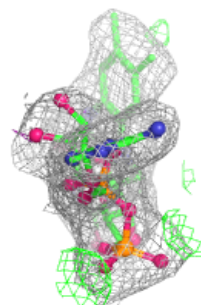
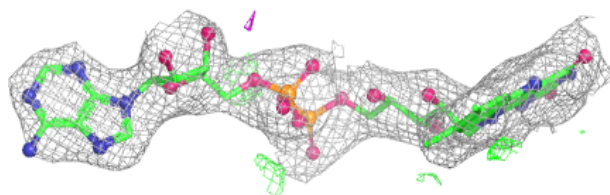
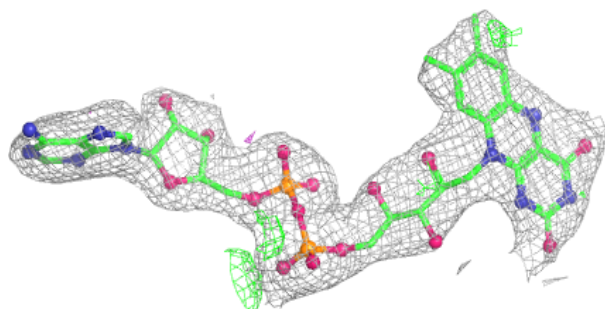
Electron density around UDP E 500:

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

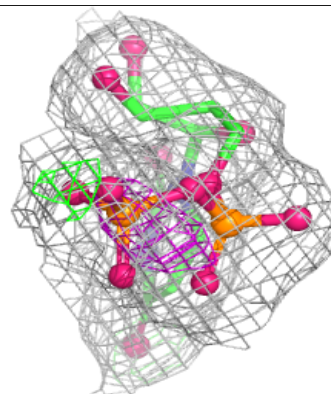
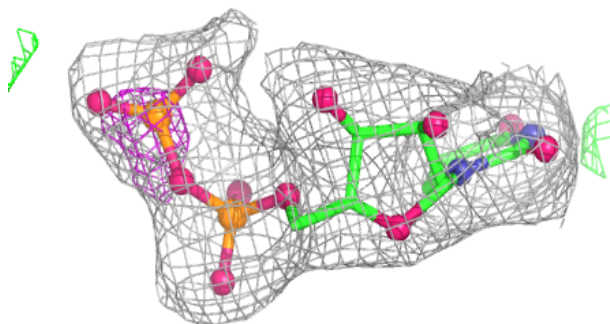
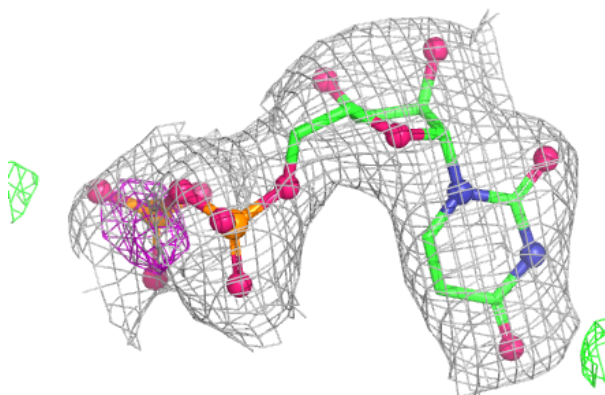


Electron density around FAD D 450:

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

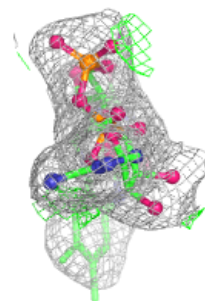
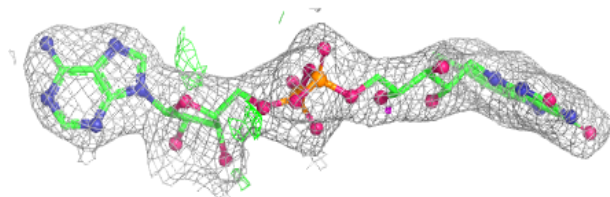
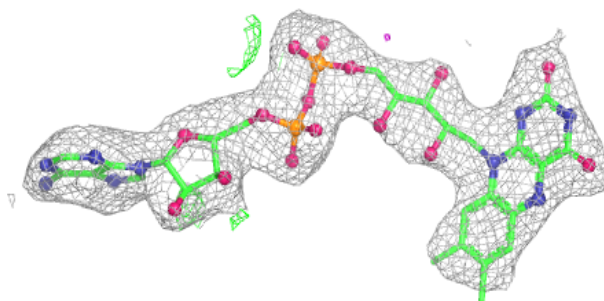
**Electron density around UDP A 500:**

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

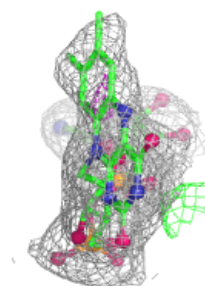
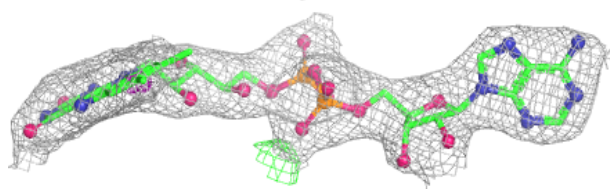
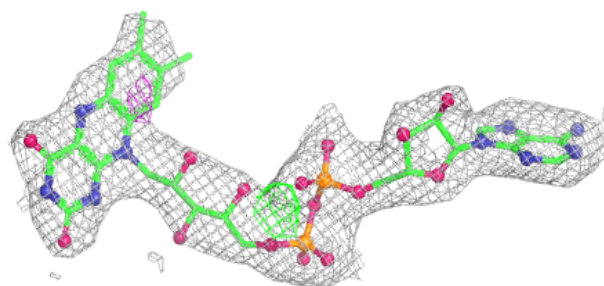


Electron density around FAD E 450:

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

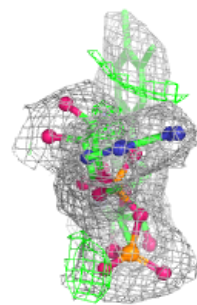
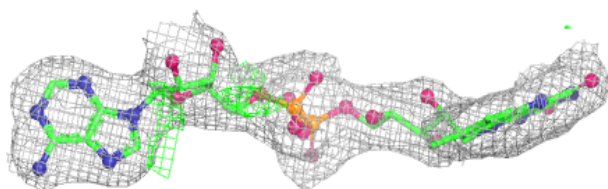
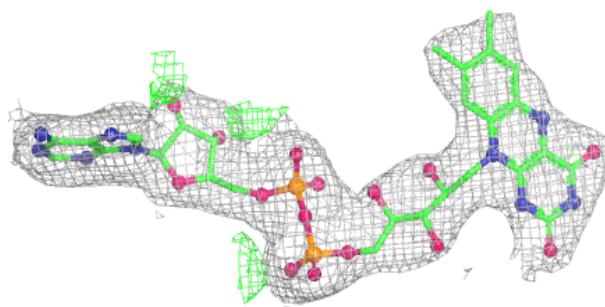
**Electron density around FAD G 450:**

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

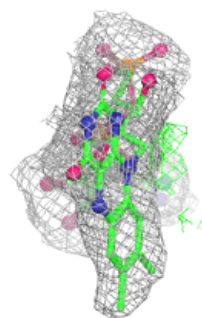
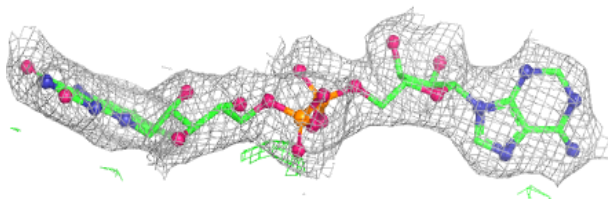
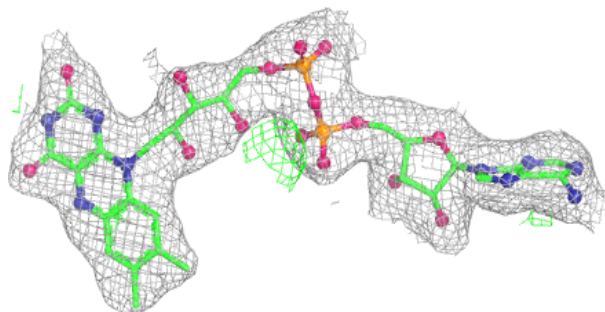


Electron density around FAD J 450:

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

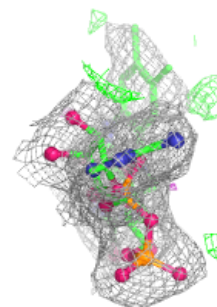
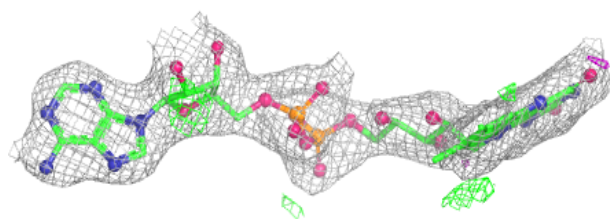
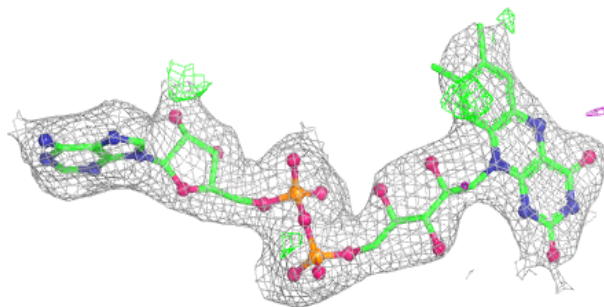
**Electron density around FAD A 450:**

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



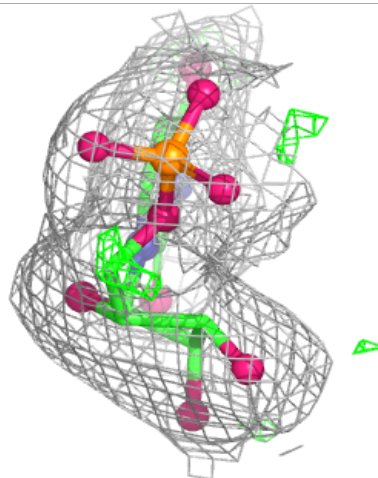
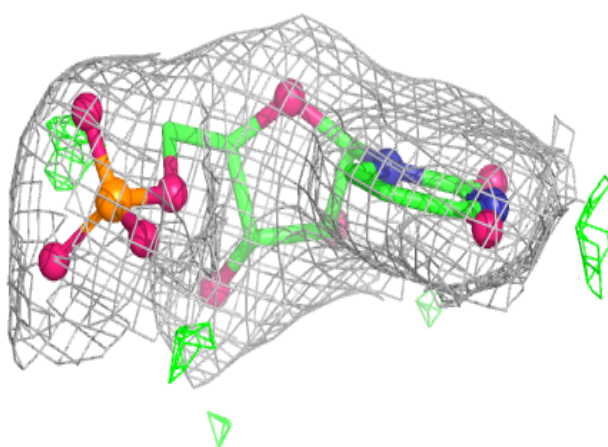
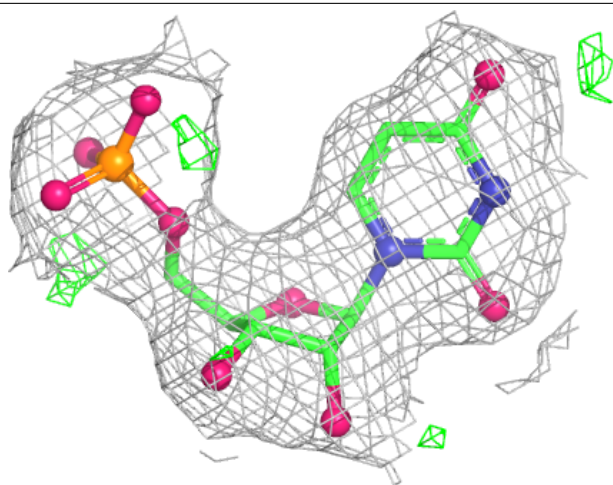
Electron density around FAD B 450:

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



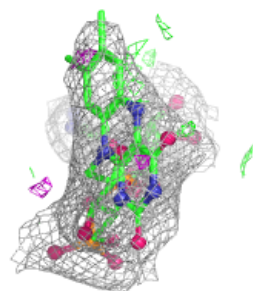
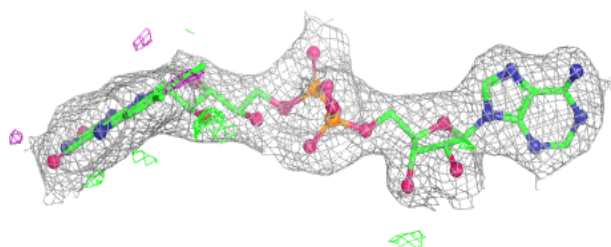
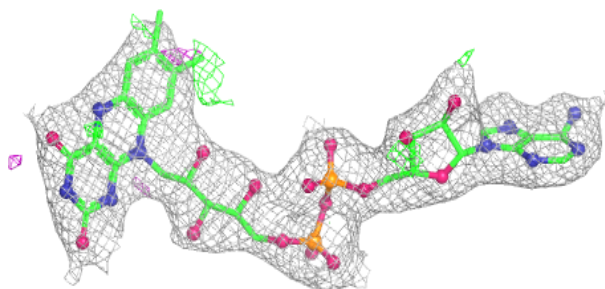
Electron density around UDP I 500:

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

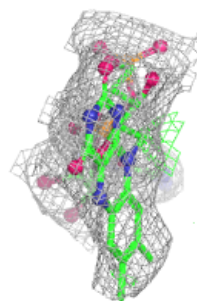
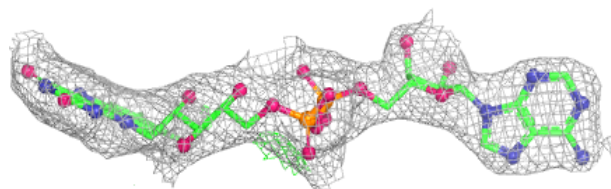
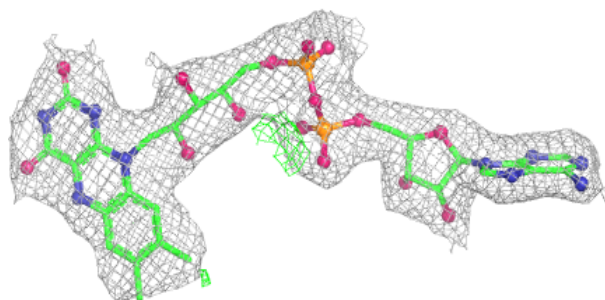


Electron density around FAD C 450:

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

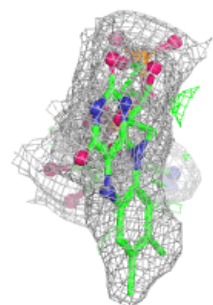
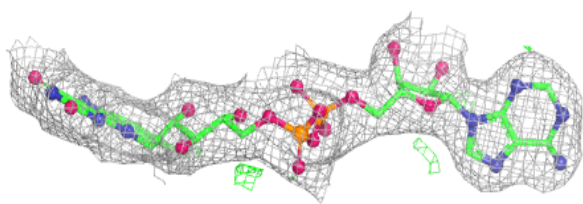
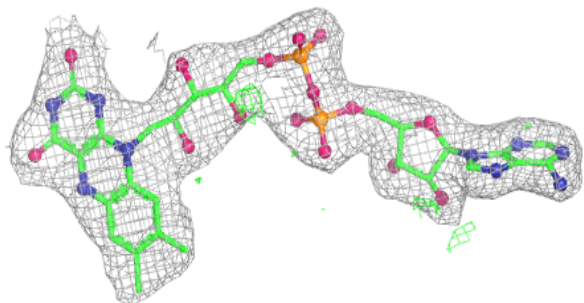
**Electron density around FAD I 450:**

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

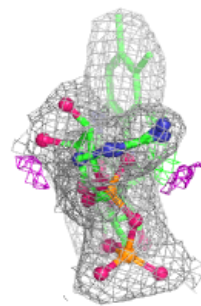
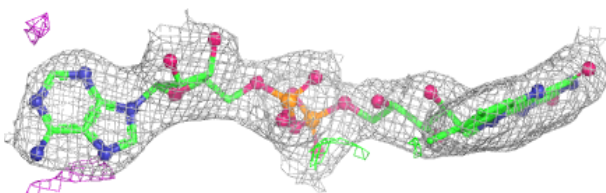
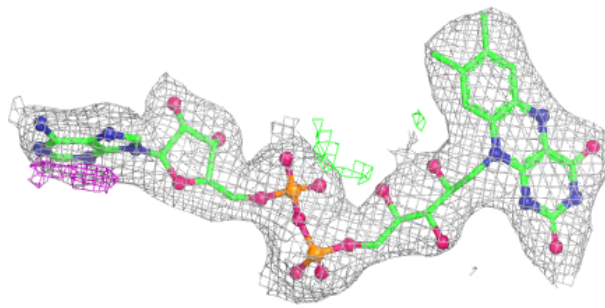


Electron density around FAD F 450:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.