



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:10 AM UTC

PDB ID : 4A99 / pdb_00004a99
Title : STRUCTURE OF THE TETRACYCLINE DEGRADING MONOOXYGENASE TETX IN COMPLEX WITH MINOCYCLINE
Authors : Volkers, G.; Palm, G.J.; Weiss, M.S.; Hinrichs, W.
Deposited on : 2011-11-25
Resolution : 2.18 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

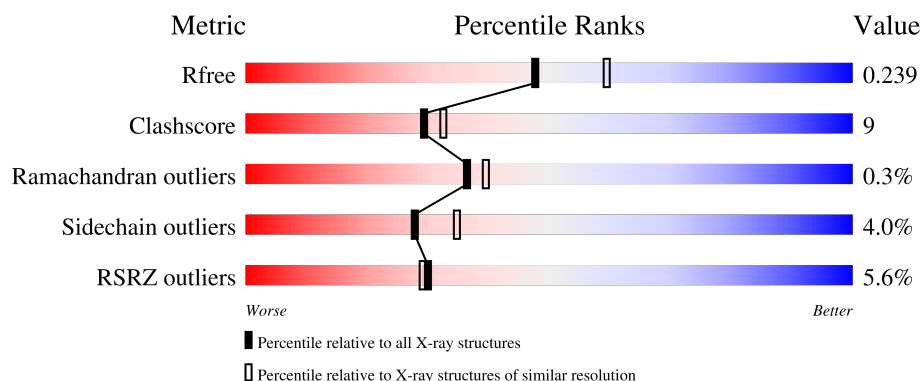
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	398	5% 76% 14% • 8%
1	B	398	5% 74% 15% • 8%
1	C	398	5% 77% 13% • 8%
1	D	398	6% 77% 12% • 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12662 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 TETX2 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2886	1826	489	559	12			
1	B	368	Total	C	N	O	S	0	0	0
			2883	1826	489	556	12			
1	C	367	Total	C	N	O	S	0	0	0
			2868	1817	485	554	12			
1	D	367	Total	C	N	O	S	0	0	0
			2859	1812	485	550	12			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	expression tag	UNP Q93L51
A	-8	GLY	-	expression tag	UNP Q93L51
A	-7	SER	-	expression tag	UNP Q93L51
A	-6	SER	-	expression tag	UNP Q93L51
A	-5	HIS	-	expression tag	UNP Q93L51
A	-4	HIS	-	expression tag	UNP Q93L51
A	-3	HIS	-	expression tag	UNP Q93L51
A	-2	HIS	-	expression tag	UNP Q93L51
A	-1	HIS	-	expression tag	UNP Q93L51
A	0	HIS	-	expression tag	UNP Q93L51
A	1	SER	-	expression tag	UNP Q93L51
A	2	SER	-	expression tag	UNP Q93L51
A	3	GLY	-	expression tag	UNP Q93L51
A	4	LEU	-	expression tag	UNP Q93L51
A	5	VAL	-	expression tag	UNP Q93L51
A	6	PRO	-	expression tag	UNP Q93L51
A	7	ARG	-	expression tag	UNP Q93L51
A	8	GLY	-	expression tag	UNP Q93L51
A	9	SER	-	expression tag	UNP Q93L51
A	10	HIS	-	expression tag	UNP Q93L51
B	-9	MET	-	expression tag	UNP Q93L51

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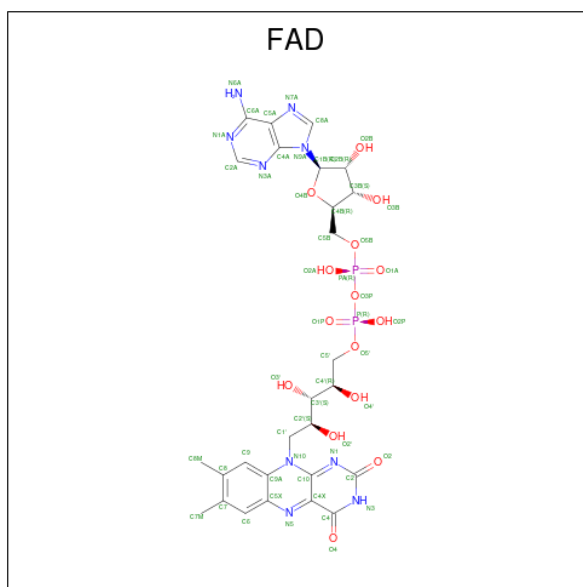
Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	expression tag	UNP Q93L51
B	-7	SER	-	expression tag	UNP Q93L51
B	-6	SER	-	expression tag	UNP Q93L51
B	-5	HIS	-	expression tag	UNP Q93L51
B	-4	HIS	-	expression tag	UNP Q93L51
B	-3	HIS	-	expression tag	UNP Q93L51
B	-2	HIS	-	expression tag	UNP Q93L51
B	-1	HIS	-	expression tag	UNP Q93L51
B	0	HIS	-	expression tag	UNP Q93L51
B	1	SER	-	expression tag	UNP Q93L51
B	2	SER	-	expression tag	UNP Q93L51
B	3	GLY	-	expression tag	UNP Q93L51
B	4	LEU	-	expression tag	UNP Q93L51
B	5	VAL	-	expression tag	UNP Q93L51
B	6	PRO	-	expression tag	UNP Q93L51
B	7	ARG	-	expression tag	UNP Q93L51
B	8	GLY	-	expression tag	UNP Q93L51
B	9	SER	-	expression tag	UNP Q93L51
B	10	HIS	-	expression tag	UNP Q93L51
C	-9	MET	-	expression tag	UNP Q93L51
C	-8	GLY	-	expression tag	UNP Q93L51
C	-7	SER	-	expression tag	UNP Q93L51
C	-6	SER	-	expression tag	UNP Q93L51
C	-5	HIS	-	expression tag	UNP Q93L51
C	-4	HIS	-	expression tag	UNP Q93L51
C	-3	HIS	-	expression tag	UNP Q93L51
C	-2	HIS	-	expression tag	UNP Q93L51
C	-1	HIS	-	expression tag	UNP Q93L51
C	0	HIS	-	expression tag	UNP Q93L51
C	1	SER	-	expression tag	UNP Q93L51
C	2	SER	-	expression tag	UNP Q93L51
C	3	GLY	-	expression tag	UNP Q93L51
C	4	LEU	-	expression tag	UNP Q93L51
C	5	VAL	-	expression tag	UNP Q93L51
C	6	PRO	-	expression tag	UNP Q93L51
C	7	ARG	-	expression tag	UNP Q93L51
C	8	GLY	-	expression tag	UNP Q93L51
C	9	SER	-	expression tag	UNP Q93L51
C	10	HIS	-	expression tag	UNP Q93L51
D	-9	MET	-	expression tag	UNP Q93L51
D	-8	GLY	-	expression tag	UNP Q93L51
D	-7	SER	-	expression tag	UNP Q93L51

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	SER	-	expression tag	UNP Q93L51
D	-5	HIS	-	expression tag	UNP Q93L51
D	-4	HIS	-	expression tag	UNP Q93L51
D	-3	HIS	-	expression tag	UNP Q93L51
D	-2	HIS	-	expression tag	UNP Q93L51
D	-1	HIS	-	expression tag	UNP Q93L51
D	0	HIS	-	expression tag	UNP Q93L51
D	1	SER	-	expression tag	UNP Q93L51
D	2	SER	-	expression tag	UNP Q93L51
D	3	GLY	-	expression tag	UNP Q93L51
D	4	LEU	-	expression tag	UNP Q93L51
D	5	VAL	-	expression tag	UNP Q93L51
D	6	PRO	-	expression tag	UNP Q93L51
D	7	ARG	-	expression tag	UNP Q93L51
D	8	GLY	-	expression tag	UNP Q93L51
D	9	SER	-	expression tag	UNP Q93L51
D	10	HIS	-	expression tag	UNP Q93L51

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



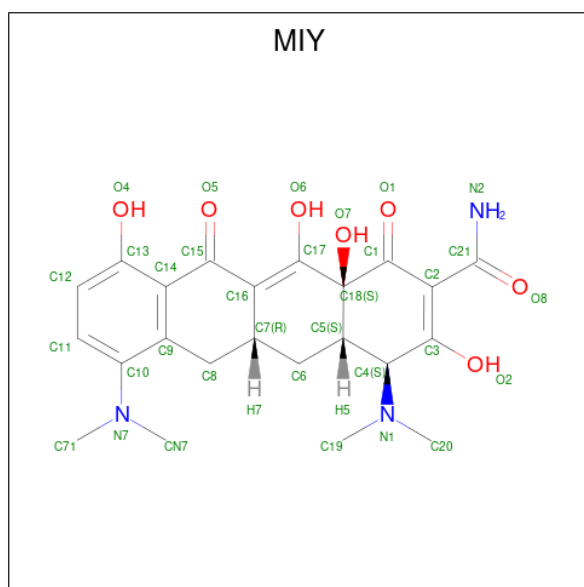
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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

- Molecule 3 is (4S,4AS,5AR,12AS)-4,7-BIS(DIMETHYLAMINO)-3,10,12,12A-TETRAHYDROXY-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (CCD ID: MIY) (formula: $C_{23}H_{27}N_3O_7$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O		0	0
			33	23	3	7			
3	A	1	Total	C	N	O		0	0
			33	23	3	7			
3	B	1	Total	C	N	O		0	0
			33	23	3	7			
3	C	1	Total	C	N	O		0	0
			33	23	3	7			
3	C	1	Total	C	N	O		0	0
			33	23	3	7			
3	D	1	Total	C	N	O		0	0
			33	23	3	7			
3	D	1	Total	C	N	O		0	0
			33	23	3	7			
3	D	1	Total	C	N	O		0	0
			33	23	3	7			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	203	Total	O	0	0
			203	203		
5	B	189	Total	O	0	0
			189	189		

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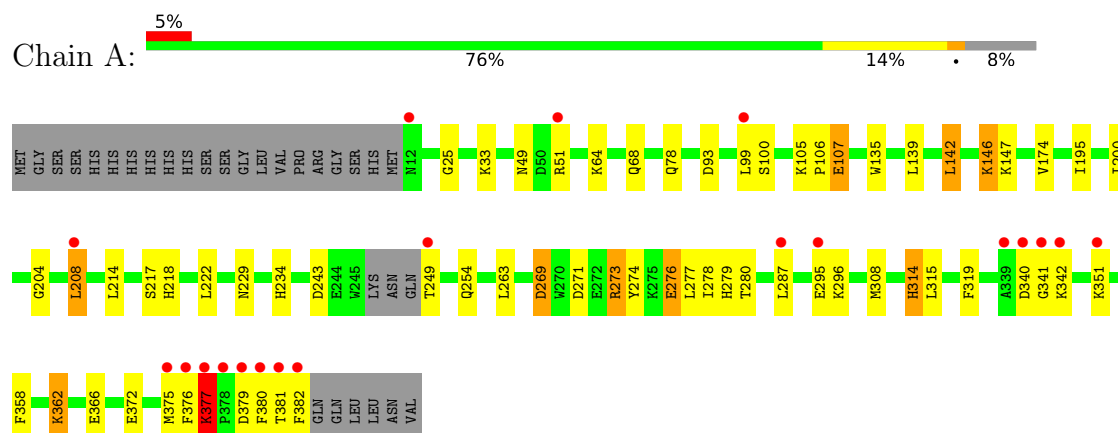
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	134	Total 134	O 134	0	0
5	D	114	Total 114	O 114	0	0

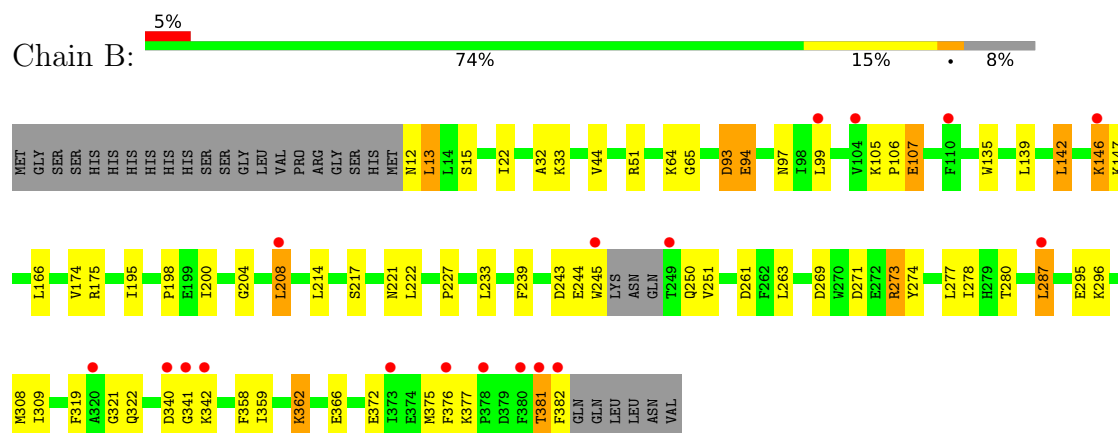
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

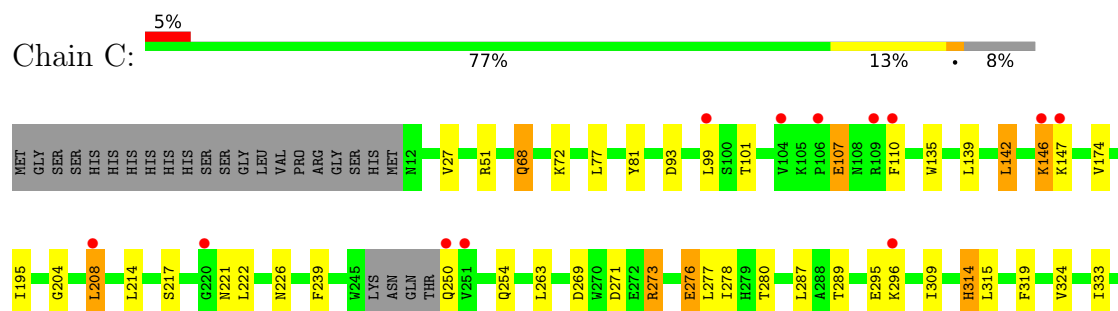
• Molecule 1: TETX2 PROTEIN

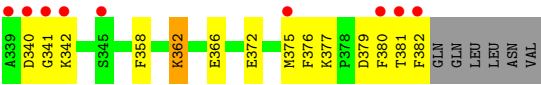


• Molecule 1: TETX2 PROTEIN

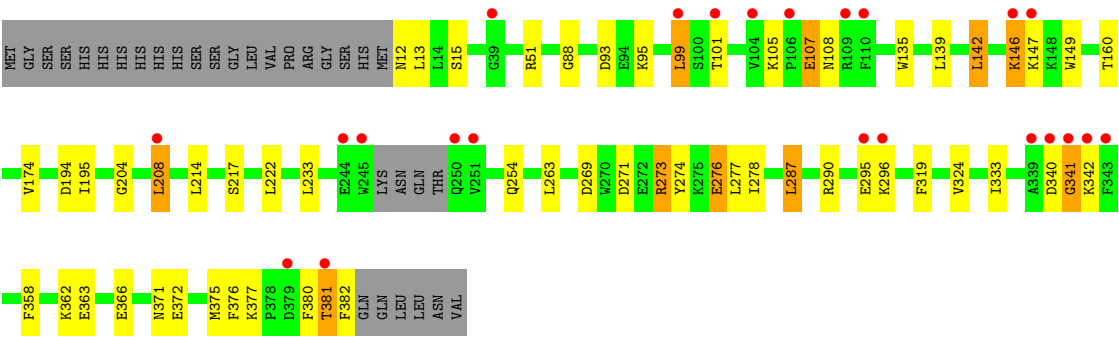
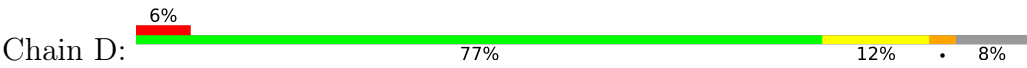


• Molecule 1: TETX2 PROTEIN





● Molecule 1: TETX2 PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	68.88Å 80.33Å 86.63Å 110.82° 90.27° 93.39°	Depositor
Resolution (Å)	80.94 – 2.18 80.94 – 2.18	Depositor EDS
% Data completeness (in resolution range)	95.5 (80.94-2.18) 95.6 (80.94-2.18)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.185 , 0.235 0.188 , 0.239	Depositor DCC
R_{free} test set	4301 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12662	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 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MIY, SO4, FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.19	9/2944 (0.3%)	1.13	6/3988 (0.2%)
1	B	1.20	4/2941 (0.1%)	1.15	8/3983 (0.2%)
1	C	1.06	4/2926 (0.1%)	1.07	3/3965 (0.1%)
1	D	1.08	3/2917 (0.1%)	1.09	7/3954 (0.2%)
All	All	1.13	20/11728 (0.2%)	1.11	24/15890 (0.2%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	GLN	CD-NE2	-7.13	1.18	1.33
1	A	314	HIS	CE1-NE2	6.86	1.39	1.32
1	D	371	ASN	CG-ND2	-6.85	1.18	1.33
1	B	198	PRO	C-O	6.58	1.31	1.24
1	C	226	ASN	C-O	-6.31	1.19	1.25
1	A	234	HIS	CG-CD2	6.19	1.42	1.35
1	C	68	GLN	CD-NE2	-5.97	1.20	1.33
1	A	234	HIS	CE1-NE2	5.72	1.38	1.32
1	B	33	LYS	N-CA	-5.66	1.39	1.46
1	A	78	GLN	CD-OE1	-5.65	1.12	1.23
1	C	289	THR	C-O	5.60	1.30	1.23
1	A	314	HIS	CG-CD2	5.56	1.42	1.35
1	B	93	ASP	CG-OD1	-5.53	1.14	1.25
1	D	290	ARG	C-O	-5.46	1.17	1.23
1	A	308	MET	N-CA	5.44	1.52	1.46
1	B	94	GLU	CD-OE2	-5.21	1.15	1.25
1	D	371	ASN	CG-OD1	-5.21	1.13	1.23
1	A	68	GLN	CD-NE2	-5.13	1.22	1.33
1	C	314	HIS	CD2-NE2	-5.11	1.32	1.37
1	A	279	HIS	CG-CD2	5.01	1.41	1.35

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	377	LYS	CA-C-N	7.16	128.78	119.84
1	B	377	LYS	C-N-CA	7.16	128.78	119.84
1	A	377	LYS	CA-C-N	7.13	128.75	119.84
1	A	377	LYS	C-N-CA	7.13	128.75	119.84
1	B	93	ASP	OD1-CG-OD2	-6.78	106.64	122.90
1	A	276	GLU	N-CA-C	-6.67	104.08	111.82
1	D	377	LYS	CA-C-N	6.62	128.12	119.84
1	D	377	LYS	C-N-CA	6.62	128.12	119.84
1	C	377	LYS	CA-C-N	6.26	127.67	119.84
1	C	377	LYS	C-N-CA	6.26	127.67	119.84
1	B	175	ARG	NE-CZ-NH2	-6.26	113.57	119.20
1	B	287	LEU	CA-CB-CG	6.12	137.72	116.30
1	B	200	ILE	N-CA-C	-5.82	106.80	111.81
1	D	88	GLY	N-CA-C	-5.82	103.61	112.51
1	A	200	ILE	N-CA-C	-5.78	106.84	111.81
1	B	15	SER	N-CA-C	5.63	117.86	111.11
1	D	287	LEU	N-CA-C	5.58	118.56	108.69
1	A	49	ASN	N-CA-C	5.42	117.88	111.33
1	D	15	SER	N-CA-C	5.41	117.60	111.11
1	D	287	LEU	CA-CB-CG	5.33	134.94	116.30
1	B	94	GLU	OE1-CD-OE2	-5.32	110.13	122.90
1	A	25	GLY	N-CA-C	-5.27	105.85	112.23
1	D	276	GLU	N-CA-C	-5.16	105.78	111.71
1	C	276	GLU	N-CA-C	-5.05	105.96	111.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2886	0	2800	46	0
1	B	2883	0	2797	54	0
1	C	2868	0	2771	42	0
1	D	2859	0	2761	43	0
2	A	53	0	31	4	0
2	B	53	0	31	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	53	0	31	2	0
2	D	53	0	31	3	0
3	A	66	0	48	3	0
3	B	33	0	24	2	0
3	C	66	0	49	7	0
3	D	99	0	73	7	0
4	A	5	0	0	0	0
4	B	15	0	0	0	0
4	C	15	0	0	0	0
4	D	15	0	0	0	0
5	A	203	0	0	7	0
5	B	189	0	0	10	0
5	C	134	0	0	2	0
5	D	114	0	0	3	0
All	All	12662	0	11447	202	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 9.

All (202) 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:A:269:ASP:HB2	5:A:2163:HOH:O	1.28	1.29
1:A:218:HIS:HD2	5:A:2063:HOH:O	1.43	0.99
1:B:381:THR:HA	5:B:2185:HOH:O	1.64	0.96
1:D:12:ASN:HD21	1:D:341:GLY:CA	1.83	0.92
1:D:12:ASN:HD21	1:D:341:GLY:HA2	1.35	0.91
1:C:333:ILE:HD11	3:C:392:MIY:HN73	1.52	0.91
3:D:392:MIY:O2	3:D:392:MIY:H192	1.70	0.89
1:D:146:LYS:HE2	1:D:147:LYS:H	1.45	0.81
1:A:269:ASP:CB	5:A:2163:HOH:O	2.02	0.80
1:D:139:LEU:HD21	1:D:142:LEU:HD13	1.64	0.79
1:C:139:LEU:HD21	1:C:142:LEU:HD13	1.65	0.78
1:C:146:LYS:HE2	1:C:147:LYS:H	1.50	0.77
1:A:379:ASP:HB3	1:B:65:GLY:O	1.87	0.75
1:B:146:LYS:HE2	1:B:147:LYS:H	1.53	0.74
1:B:174:VAL:HG22	1:B:174:VAL:O	1.87	0.73
1:B:244:GLU:H	1:B:244:GLU:CD	1.96	0.73
1:A:146:LYS:HE2	1:A:147:LYS:H	1.53	0.73
1:D:340:ASP:C	1:D:342:LYS:H	1.97	0.72
1:B:222:LEU:HD22	1:B:375:MET:HE3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:LYS:O	1:A:366:GLU:HG2	1.90	0.71
1:D:222:LEU:HD22	1:D:375:MET:HE3	1.72	0.71
1:C:250:GLN:N	5:C:2103:HOH:O	2.24	0.70
1:B:340:ASP:C	1:B:342:LYS:H	1.98	0.70
1:C:222:LEU:HD22	1:C:375:MET:HE3	1.74	0.70
1:C:340:ASP:C	1:C:342:LYS:H	2.00	0.70
1:A:340:ASP:C	1:A:342:LYS:H	1.99	0.70
1:B:322:GLN:OE1	5:B:2176:HOH:O	2.09	0.69
1:C:174:VAL:HG22	1:C:174:VAL:O	1.92	0.69
1:C:362:LYS:O	1:C:366:GLU:HG2	1.92	0.69
1:D:319:PHE:CD1	1:D:375:MET:HE1	2.27	0.68
1:C:333:ILE:HD11	3:C:392:MIY:CN7	2.23	0.68
1:D:93:ASP:HB3	1:D:99:LEU:HD11	1.75	0.68
1:B:321:GLY:O	5:B:2174:HOH:O	2.10	0.68
1:A:99:LEU:HB3	1:B:359:ILE:HG23	1.75	0.67
1:A:99:LEU:HD22	1:B:359:ILE:O	1.94	0.67
1:D:362:LYS:O	1:D:366:GLU:HG2	1.94	0.67
1:D:51:ARG:HG2	5:D:2017:HOH:O	1.94	0.67
1:A:372:GLU:O	1:A:376:PHE:HD2	1.79	0.66
1:B:139:LEU:HD21	1:B:142:LEU:HD13	1.79	0.65
1:C:208:LEU:HD12	1:C:214:LEU:HD11	1.79	0.65
1:D:174:VAL:O	1:D:174:VAL:HG22	1.96	0.65
3:D:392:MIY:O2	3:D:392:MIY:C19	2.43	0.65
1:D:271:ASP:OD1	1:D:273:ARG:HD3	1.97	0.65
1:A:174:VAL:O	1:A:174:VAL:HG22	1.97	0.64
1:C:295:GLU:HG3	1:C:296:LYS:HG2	1.79	0.64
1:C:93:ASP:HB3	1:C:99:LEU:HD21	1.81	0.63
3:D:393:MIY:C8	3:D:393:MIY:H712	2.30	0.62
1:A:263:LEU:HB3	1:A:278:ILE:HD13	1.82	0.62
1:B:263:LEU:HB3	1:B:278:ILE:HD13	1.81	0.62
1:C:217:SER:HB2	1:C:382:PHE:CE2	2.35	0.62
1:B:319:PHE:CD1	1:B:375:MET:HE1	2.34	0.62
1:A:319:PHE:CD1	1:A:375:MET:HE1	2.35	0.62
1:C:319:PHE:CD1	1:C:375:MET:HE1	2.35	0.61
1:D:208:LEU:HD12	1:D:214:LEU:HD11	1.83	0.61
1:B:271:ASP:OD1	1:B:273:ARG:HD3	2.01	0.61
1:D:381:THR:HG23	5:D:2110:HOH:O	2.01	0.61
1:D:358:PHE:O	1:D:362:LYS:HB2	2.01	0.60
2:D:389:FAD:N1	2:D:389:FAD:H2'	2.15	0.60
1:A:358:PHE:O	1:A:362:LYS:HB2	2.00	0.60
1:D:12:ASN:ND2	1:D:341:GLY:CA	2.62	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LEU:HD21	1:A:142:LEU:HD13	1.84	0.59
1:C:271:ASP:OD1	1:C:273:ARG:HD3	2.02	0.59
1:B:358:PHE:O	1:B:362:LYS:HB2	2.01	0.59
1:A:195:ILE:HD12	1:A:277:LEU:HD12	1.85	0.58
1:B:142:LEU:HD22	1:B:174:VAL:CG2	2.34	0.58
1:A:271:ASP:OD1	1:A:273:ARG:HD3	2.03	0.58
2:B:389:FAD:H2'	2:B:389:FAD:N1	2.19	0.58
1:C:195:ILE:HD12	1:C:277:LEU:HD12	1.86	0.57
1:D:217:SER:HB2	1:D:382:PHE:CE2	2.39	0.57
1:B:217:SER:HB2	1:B:382:PHE:CE2	2.39	0.57
1:A:379:ASP:CG	1:A:379:ASP:O	2.47	0.56
1:B:372:GLU:O	1:B:376:PHE:HD2	1.88	0.56
2:C:389:FAD:H2'	2:C:389:FAD:N1	2.19	0.56
1:C:358:PHE:O	1:C:362:LYS:HB2	2.05	0.56
1:D:295:GLU:HG3	1:D:296:LYS:HG2	1.87	0.56
1:A:222:LEU:HD22	1:A:375:MET:HE3	1.88	0.55
1:B:208:LEU:HD12	1:B:214:LEU:HD11	1.87	0.55
1:B:243:ASP:CB	5:B:2147:HOH:O	2.55	0.55
1:C:333:ILE:CD1	3:C:392:MIY:HN73	2.32	0.55
1:A:274:TYR:O	1:A:277:LEU:HB3	2.07	0.55
1:B:64:LYS:NZ	5:B:2037:HOH:O	2.40	0.55
1:A:93:ASP:HB3	1:A:99:LEU:HD11	1.89	0.54
1:B:243:ASP:HA	5:B:2147:HOH:O	2.05	0.54
1:D:319:PHE:CE1	1:D:375:MET:HE1	2.43	0.54
1:B:295:GLU:HG3	1:B:296:LYS:HG2	1.89	0.54
1:B:340:ASP:C	1:B:342:LYS:N	2.66	0.54
3:C:392:MIY:O5	3:C:392:MIY:O6	2.24	0.54
1:A:64:LYS:NZ	5:A:2039:HOH:O	2.41	0.53
1:D:340:ASP:C	1:D:342:LYS:N	2.66	0.53
1:A:33:LYS:NZ	5:A:2006:HOH:O	2.41	0.53
1:A:204:GLY:HA3	1:A:273:ARG:HG2	1.91	0.53
1:A:295:GLU:HG3	1:A:296:LYS:HG2	1.90	0.53
1:D:105:LYS:HD2	1:D:108:ASN:ND2	2.24	0.53
1:A:142:LEU:HD22	1:A:174:VAL:CG2	2.39	0.52
1:D:12:ASN:CG	1:D:13:LEU:H	2.17	0.52
1:A:340:ASP:C	1:A:342:LYS:N	2.68	0.52
1:C:204:GLY:HA3	1:C:273:ARG:HG2	1.92	0.52
1:C:340:ASP:C	1:C:342:LYS:N	2.68	0.52
1:B:274:TYR:O	1:B:277:LEU:HB3	2.09	0.52
1:A:217:SER:HB2	1:A:382:PHE:CE1	2.45	0.51
1:C:324:VAL:HG12	2:C:389:FAD:O2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:392:MIY:HN72	3:C:392:MIY:N2	2.26	0.50
1:A:229:ASN:ND2	5:A:2028:HOH:O	2.39	0.50
3:D:393:MIY:H712	3:D:393:MIY:H81	1.94	0.50
1:B:362:LYS:O	1:B:366:GLU:HG2	2.11	0.49
1:A:100:SER:HB2	1:B:359:ILE:HG12	1.94	0.49
1:D:274:TYR:O	1:D:277:LEU:HB3	2.11	0.49
1:A:377:LYS:HB2	1:A:377:LYS:NZ	2.28	0.49
2:A:389:FAD:H2'	2:A:389:FAD:N1	2.28	0.49
1:D:204:GLY:HA3	1:D:273:ARG:HG2	1.95	0.49
1:B:245:TRP:O	5:B:2148:HOH:O	2.20	0.48
1:A:314:HIS:O	1:A:315:LEU:C	2.56	0.48
1:A:208:LEU:HD12	1:A:214:LEU:HD11	1.96	0.48
1:C:174:VAL:O	1:C:174:VAL:CG2	2.60	0.48
1:B:166:LEU:HB2	1:B:308:MET:HG2	1.96	0.48
1:C:72:LYS:CG	1:C:77:LEU:HD22	2.44	0.48
1:C:195:ILE:HD13	1:C:280:THR:CG2	2.44	0.47
1:D:208:LEU:HD23	1:D:273:ARG:NH2	2.29	0.47
1:D:324:VAL:HG12	2:D:389:FAD:O2	2.14	0.47
1:B:195:ILE:HD12	1:B:277:LEU:HD12	1.97	0.47
1:A:319:PHE:CE1	1:A:375:MET:HE1	2.50	0.47
1:B:93:ASP:HB3	1:B:99:LEU:HD21	1.96	0.47
1:A:380:PHE:CZ	1:A:382:PHE:HA	2.49	0.47
1:D:263:LEU:HB3	1:D:278:ILE:HD13	1.97	0.47
1:B:51:ARG:HB3	1:B:135:TRP:CZ2	2.50	0.47
1:B:204:GLY:HA3	1:B:273:ARG:HG2	1.97	0.47
1:D:95:LYS:HE3	5:D:2037:HOH:O	2.15	0.46
1:D:195:ILE:HD12	1:D:277:LEU:HD12	1.96	0.46
1:C:342:LYS:HG3	5:C:2123:HOH:O	2.15	0.46
1:C:222:LEU:N	1:C:222:LEU:HD12	2.31	0.46
1:B:243:ASP:CA	5:B:2147:HOH:O	2.63	0.46
1:C:380:PHE:CZ	1:C:382:PHE:HA	2.51	0.46
1:C:208:LEU:HD12	1:C:214:LEU:CD1	2.46	0.46
1:C:51:ARG:HB3	1:C:135:TRP:CZ2	2.51	0.45
3:D:393:MIY:O5	3:D:393:MIY:O6	2.33	0.45
1:B:93:ASP:OD1	1:B:97:ASN:HB2	2.16	0.45
1:A:375:MET:HE2	1:A:376:PHE:CE2	2.51	0.45
1:C:107:GLU:H	1:C:107:GLU:HG3	1.34	0.45
1:D:208:LEU:HD12	1:D:214:LEU:CD1	2.46	0.45
1:D:333:ILE:HD11	3:D:393:MIY:H713	1.98	0.45
1:D:51:ARG:HB3	1:D:135:TRP:CZ2	2.52	0.45
1:D:107:GLU:H	1:D:107:GLU:HG3	1.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:391:MIY:H5	3:C:391:MIY:H203	1.77	0.44
1:D:372:GLU:O	1:D:376:PHE:HD2	2.00	0.44
1:B:174:VAL:O	1:B:174:VAL:CG2	2.57	0.44
1:B:261:ASP:OD1	5:B:2151:HOH:O	2.21	0.44
2:B:389:FAD:H1'1	2:B:389:FAD:H9	1.75	0.44
1:A:105:LYS:O	1:A:106:PRO:C	2.60	0.44
1:B:227:PRO:HA	1:B:233:LEU:HD12	2.00	0.44
1:B:105:LYS:O	1:B:106:PRO:C	2.61	0.44
1:A:195:ILE:HD13	1:A:280:THR:CG2	2.48	0.44
1:C:27:VAL:HG12	1:C:309:ILE:HD12	2.00	0.43
3:B:391:MIY:O5	3:B:391:MIY:O6	2.35	0.43
1:C:263:LEU:HB3	1:C:278:ILE:HD13	2.00	0.43
3:A:391:MIY:O5	3:A:391:MIY:O6	2.35	0.43
1:B:107:GLU:H	1:B:107:GLU:HG3	1.31	0.43
1:B:244:GLU:CD	1:B:244:GLU:N	2.71	0.43
1:B:22:ILE:HG13	1:B:139:LEU:HD22	2.00	0.43
1:B:208:LEU:HD12	1:B:214:LEU:CD1	2.49	0.43
1:C:208:LEU:HD23	1:C:273:ARG:NH2	2.34	0.43
1:C:221:ASN:HD22	1:C:239:PHE:HB3	1.84	0.43
1:B:146:LYS:H	1:B:146:LYS:HG3	1.38	0.43
1:C:72:LYS:HG3	1:C:77:LEU:HD22	2.00	0.43
2:D:389:FAD:H9	2:D:389:FAD:H1'1	1.79	0.43
2:A:389:FAD:H6	3:A:391:MIY:C19	2.48	0.43
1:D:142:LEU:HD12	1:D:142:LEU:HA	1.88	0.43
3:B:391:MIY:H203	3:B:391:MIY:H5	1.74	0.42
1:B:195:ILE:HD13	1:B:280:THR:CG2	2.49	0.42
1:B:245:TRP:HA	1:B:250:GLN:HE21	1.85	0.42
1:C:110:PHE:CD1	1:C:110:PHE:N	2.88	0.42
1:A:51:ARG:HB3	1:A:135:TRP:CZ2	2.54	0.42
1:D:174:VAL:O	1:D:174:VAL:CG2	2.67	0.42
1:C:254:GLN:HE21	1:C:254:GLN:HB3	1.72	0.42
1:B:221:ASN:HD22	1:B:239:PHE:HB3	1.84	0.42
1:A:195:ILE:CD1	1:A:277:LEU:HD12	2.48	0.42
1:A:218:HIS:HE1	1:A:269:ASP:OD2	2.02	0.42
1:C:372:GLU:O	1:C:376:PHE:HD2	2.02	0.42
1:D:254:GLN:HE21	1:D:254:GLN:HB3	1.73	0.42
1:A:142:LEU:HD22	1:A:174:VAL:HG22	2.02	0.42
1:C:319:PHE:CE1	1:C:375:MET:HE1	2.55	0.42
1:A:107:GLU:H	1:A:107:GLU:HG3	1.20	0.42
1:D:363:GLU:OE1	3:D:393:MIY:O6	2.37	0.41
1:D:380:PHE:CZ	1:D:382:PHE:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:LEU:H	1:B:13:LEU:HG	1.72	0.41
1:D:149:TRP:O	1:D:160:THR:HA	2.20	0.41
1:C:142:LEU:HD12	1:C:142:LEU:HA	1.88	0.41
1:A:379:ASP:HB3	1:B:65:GLY:C	2.46	0.41
1:C:68:GLN:NE2	1:C:81:TYR:OH	2.53	0.41
2:A:389:FAD:H9	5:A:2185:HOH:O	2.21	0.41
1:B:244:GLU:O	1:B:250:GLN:HG2	2.20	0.41
1:D:295:GLU:HG3	1:D:296:LYS:H	1.85	0.41
1:A:362:LYS:O	1:A:366:GLU:CG	2.65	0.41
1:D:263:LEU:HA	1:D:263:LEU:HD23	1.87	0.41
2:B:389:FAD:H9	5:B:2170:HOH:O	2.21	0.41
1:C:314:HIS:O	1:C:315:LEU:C	2.64	0.41
1:B:94:GLU:OE1	1:B:94:GLU:N	2.52	0.40
1:D:194:ASP:HA	1:D:233:LEU:O	2.21	0.40
3:C:392:MIY:H203	3:C:392:MIY:H5	1.68	0.40
1:A:375:MET:CE	1:A:376:PHE:CE2	3.05	0.40
2:A:389:FAD:H9	2:A:389:FAD:H1'1	1.81	0.40
1:B:32:ALA:HB2	1:B:44:VAL:CG2	2.51	0.40
1:B:309:ILE:HD13	1:B:309:ILE:HG21	1.91	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	364/398 (92%)	352 (97%)	11 (3%)	1 (0%)	36	39
1	B	364/398 (92%)	350 (96%)	12 (3%)	2 (0%)	24	25
1	C	363/398 (91%)	348 (96%)	14 (4%)	1 (0%)	36	39
1	D	363/398 (91%)	348 (96%)	14 (4%)	1 (0%)	36	39
All	All	1454/1592 (91%)	1398 (96%)	51 (4%)	5 (0%)	36	39

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	13	LEU
1	A	341	GLY
1	B	341	GLY
1	D	341	GLY
1	C	341	GLY

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	312/345 (90%)	297 (95%)	15 (5%)	23	27
1	B	310/345 (90%)	299 (96%)	11 (4%)	32	40
1	C	307/345 (89%)	295 (96%)	12 (4%)	28	36
1	D	305/345 (88%)	294 (96%)	11 (4%)	31	39
All	All	1234/1380 (89%)	1185 (96%)	49 (4%)	28	35

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	GLU
1	A	142	LEU
1	A	146	LYS
1	A	208	LEU
1	A	243	ASP
1	A	249	THR
1	A	254	GLN
1	A	269	ASP
1	A	273	ARG
1	A	276	GLU
1	A	287	LEU
1	A	351	LYS
1	A	362	LYS
1	A	377	LYS
1	A	381	THR

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Mol	Chain	Res	Type
1	B	12	ASN
1	B	107	GLU
1	B	142	LEU
1	B	146	LYS
1	B	208	LEU
1	B	251	VAL
1	B	269	ASP
1	B	273	ARG
1	B	287	LEU
1	B	362	LYS
1	B	381	THR
1	C	101	THR
1	C	107	GLU
1	C	142	LEU
1	C	146	LYS
1	C	208	LEU
1	C	269	ASP
1	C	273	ARG
1	C	276	GLU
1	C	287	LEU
1	C	362	LYS
1	C	379	ASP
1	C	381	THR
1	D	99	LEU
1	D	101	THR
1	D	107	GLU
1	D	142	LEU
1	D	146	LYS
1	D	208	LEU
1	D	269	ASP
1	D	273	ARG
1	D	276	GLU
1	D	287	LEU
1	D	381	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	68	GLN
1	A	78	GLN
1	A	130	ASN

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Mol	Chain	Res	Type
1	A	218	HIS
1	A	221	ASN
1	A	254	GLN
1	A	279	HIS
1	A	356	GLN
1	A	370	GLN
1	A	371	ASN
1	B	38	ASN
1	B	49	ASN
1	B	108	ASN
1	B	130	ASN
1	B	190	ASN
1	B	218	HIS
1	B	221	ASN
1	B	254	GLN
1	B	279	HIS
1	B	356	GLN
1	B	370	GLN
1	B	371	ASN
1	C	38	ASN
1	C	49	ASN
1	C	68	GLN
1	C	78	GLN
1	C	130	ASN
1	C	218	HIS
1	C	221	ASN
1	C	254	GLN
1	C	279	HIS
1	C	371	ASN
1	D	12	ASN
1	D	38	ASN
1	D	49	ASN
1	D	108	ASN
1	D	130	ASN
1	D	221	ASN
1	D	254	GLN
1	D	279	HIS

5.3.3 RNA ⓘ

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](#)

22 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	SO4	B	1384	-	4,4,4	0.45	0	6,6,6	0.21	0
3	MIY	A	391	-	36,36,36	1.51	6 (16%)	42,58,58	1.71	10 (23%)
2	FAD	D	389	-	58,58,58	1.35	7 (12%)	85,89,89	2.31	21 (24%)
4	SO4	C	1384	-	4,4,4	0.47	0	6,6,6	0.37	0
3	MIY	A	392	-	36,36,36	1.30	4 (11%)	42,58,58	2.16	13 (30%)
4	SO4	B	1385	-	4,4,4	0.52	0	6,6,6	0.24	0
3	MIY	D	391	-	36,36,36	1.14	2 (5%)	42,58,58	1.89	10 (23%)
4	SO4	D	1384	-	4,4,4	0.42	0	6,6,6	0.25	0
4	SO4	C	1383	-	4,4,4	0.65	0	6,6,6	0.23	0
4	SO4	D	1383	-	4,4,4	0.66	0	6,6,6	0.30	0
2	FAD	C	389	-	58,58,58	1.43	9 (15%)	85,89,89	2.35	20 (23%)
2	FAD	A	389	-	58,58,58	1.38	6 (10%)	85,89,89	1.74	18 (21%)
3	MIY	C	392	-	36,36,36	1.58	8 (22%)	42,58,58	2.23	11 (26%)
2	FAD	B	389	-	58,58,58	1.48	9 (15%)	85,89,89	2.32	21 (24%)
3	MIY	C	391	-	36,36,36	1.21	1 (2%)	42,58,58	1.89	13 (30%)
4	SO4	C	1385	-	4,4,4	0.41	0	6,6,6	0.22	0
4	SO4	A	1383	-	4,4,4	0.47	0	6,6,6	0.20	0
3	MIY	B	391	-	36,36,36	1.41	7 (19%)	42,58,58	1.67	12 (28%)
4	SO4	B	1383	-	4,4,4	0.53	0	6,6,6	0.39	0
3	MIY	D	392	-	36,36,36	1.39	6 (16%)	42,58,58	2.35	15 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	D	1385	-	4,4,4	0.52	0	6,6,6	0.28	0
3	MIY	D	393	-	36,36,36	1.12	3 (8%)	42,58,58	2.48	16 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MIY	B	391	-	-	0/12/70/70	0/4/4/4
2	FAD	C	389	-	-	4/34/50/50	0/6/6/6
3	MIY	D	391	-	-	0/12/70/70	0/4/4/4
2	FAD	A	389	-	-	5/34/50/50	0/6/6/6
3	MIY	C	392	-	-	1/12/70/70	0/4/4/4
3	MIY	A	391	-	-	0/12/70/70	0/4/4/4
2	FAD	B	389	-	-	5/34/50/50	0/6/6/6
2	FAD	D	389	-	-	3/34/50/50	0/6/6/6
3	MIY	C	391	-	-	0/12/70/70	0/4/4/4
3	MIY	D	392	-	-	1/12/70/70	0/4/4/4
3	MIY	A	392	-	-	0/12/70/70	0/4/4/4
3	MIY	D	393	-	-	1/12/70/70	0/4/4/4

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	392	MIY	C18-C5	4.68	1.57	1.53
2	A	389	FAD	PA-O3P	4.63	1.64	1.59
2	C	389	FAD	C4X-N5	4.44	1.40	1.30
2	D	389	FAD	C4X-N5	4.26	1.39	1.30
2	B	389	FAD	C4X-N5	4.25	1.39	1.30
2	A	389	FAD	C4X-N5	4.20	1.39	1.30
2	D	389	FAD	C10-N1	4.02	1.41	1.33
3	A	391	MIY	C18-C5	3.97	1.56	1.53
2	C	389	FAD	C10-N1	3.86	1.41	1.33
2	C	389	FAD	C2A-N1A	3.80	1.40	1.33
3	C	392	MIY	C16-C17	-3.77	1.31	1.36
2	D	389	FAD	O5'-C5'	-3.75	1.30	1.44
2	B	389	FAD	PA-O3P	3.72	1.63	1.59
3	C	392	MIY	C18-C5	3.68	1.56	1.53
2	B	389	FAD	O5'-C5'	-3.67	1.30	1.44
3	B	391	MIY	C5-C4	-3.58	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	389	FAD	O5'-C5'	-3.42	1.31	1.44
3	A	391	MIY	C6-C5	-3.39	1.48	1.53
3	C	391	MIY	C5-C4	-3.03	1.52	1.54
2	B	389	FAD	C10-N1	3.01	1.39	1.33
3	D	391	MIY	C18-C5	2.99	1.55	1.53
3	D	393	MIY	O5-C15	2.93	1.29	1.23
3	A	391	MIY	C5-C4	-2.84	1.52	1.54
2	B	389	FAD	C2A-N1A	2.80	1.38	1.33
2	B	389	FAD	O4'-C4'	2.78	1.49	1.43
2	C	389	FAD	P-O3P	2.75	1.62	1.59
2	B	389	FAD	P-O3P	-2.75	1.56	1.59
2	A	389	FAD	O5'-C5'	-2.75	1.34	1.44
3	D	392	MIY	O7-C18	2.73	1.46	1.42
3	D	392	MIY	C14-C13	-2.67	1.37	1.41
2	A	389	FAD	P-O3P	-2.67	1.56	1.59
3	A	391	MIY	C18-C1	-2.66	1.51	1.55
3	C	392	MIY	O5-C15	2.66	1.28	1.23
2	D	389	FAD	C2A-N1A	2.65	1.38	1.33
3	B	391	MIY	C18-C5	2.64	1.55	1.53
2	B	389	FAD	C8A-N7A	2.63	1.36	1.31
2	A	389	FAD	O4B-C4B	-2.62	1.39	1.45
3	C	392	MIY	C5-C4	2.62	1.57	1.54
3	D	392	MIY	C18-C1	-2.60	1.51	1.55
3	C	392	MIY	C18-C17	2.52	1.54	1.52
3	D	392	MIY	C4-C3	2.47	1.56	1.51
3	A	392	MIY	C7-C16	2.43	1.54	1.51
3	B	391	MIY	C18-C1	-2.42	1.51	1.55
3	D	392	MIY	C14-C15	2.39	1.52	1.46
3	B	391	MIY	C11-C10	2.38	1.43	1.39
3	D	391	MIY	C6-C5	-2.37	1.49	1.53
3	A	391	MIY	C14-C15	2.36	1.52	1.46
3	A	392	MIY	O5-C15	2.31	1.28	1.23
3	A	392	MIY	C14-C15	2.30	1.52	1.46
3	B	391	MIY	C10-C9	2.26	1.43	1.40
3	C	392	MIY	C4-C3	2.26	1.56	1.51
2	D	389	FAD	C8A-N7A	2.23	1.36	1.31
2	D	389	FAD	O2'-C2'	-2.21	1.38	1.43
2	C	389	FAD	O2'-C2'	-2.17	1.38	1.43
3	D	392	MIY	O1-C1	2.17	1.26	1.22
3	D	393	MIY	C14-C9	2.16	1.44	1.40
2	C	389	FAD	C8A-N7A	2.16	1.35	1.31
3	A	391	MIY	C11-C10	2.15	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	389	FAD	C4X-C4	-2.15	1.36	1.44
2	C	389	FAD	C2A-N3A	2.15	1.37	1.33
3	D	393	MIY	O1-C1	2.15	1.26	1.22
3	C	392	MIY	O7-C18	2.14	1.45	1.42
3	C	392	MIY	C19-N1	2.10	1.53	1.46
2	C	389	FAD	C4A-N3A	2.05	1.38	1.34
2	D	389	FAD	C2A-N3A	2.04	1.37	1.33
3	B	391	MIY	C14-C15	2.03	1.51	1.46
2	A	389	FAD	O2-C2	-2.00	1.20	1.24
3	B	391	MIY	C8-C9	2.00	1.54	1.51

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	389	FAD	C5'-C4'-C3'	-13.80	86.19	112.22
2	C	389	FAD	C5'-C4'-C3'	-13.39	86.95	112.22
2	B	389	FAD	C5'-C4'-C3'	-13.04	87.62	112.22
3	D	393	MIY	C9-C10-N7	8.96	129.57	118.87
2	D	389	FAD	N3A-C2A-N1A	-7.53	117.18	128.58
2	A	389	FAD	N3A-C2A-N1A	-6.90	118.14	128.58
2	C	389	FAD	N3A-C2A-N1A	-6.73	118.39	128.58
3	C	392	MIY	C20-N1-C4	-6.65	98.95	114.10
2	B	389	FAD	N3A-C2A-N1A	-6.50	118.74	128.58
3	D	391	MIY	C20-N1-C4	-5.92	100.63	114.10
3	C	391	MIY	C20-N1-C4	-5.83	100.83	114.10
3	D	393	MIY	C11-C10-N7	-5.78	113.70	121.65
3	C	392	MIY	O6-C17-C18	5.60	121.47	113.37
2	C	389	FAD	N9A-C8A-N7A	-5.49	106.15	113.94
2	C	389	FAD	C4A-N9A-C8A	5.38	111.39	105.74
3	D	392	MIY	C18-C5-C4	5.26	118.83	111.64
3	A	392	MIY	C5-C18-C1	-5.25	105.03	111.05
3	A	392	MIY	C7-C6-C5	-5.13	101.64	110.38
3	D	392	MIY	C21-C2-C1	-5.12	114.91	120.97
2	B	389	FAD	N9A-C8A-N7A	-5.05	106.77	113.94
2	A	389	FAD	N9A-C8A-N7A	-4.85	107.05	113.94
2	D	389	FAD	N9A-C8A-N7A	-4.84	107.07	113.94
3	D	392	MIY	C6-C5-C4	-4.68	106.97	113.73
3	C	392	MIY	O6-C17-C16	-4.58	114.63	123.52
2	B	389	FAD	O4-C4-C4X	-4.52	114.59	126.53
3	D	392	MIY	C20-N1-C4	-4.50	103.85	114.10
3	A	392	MIY	C1-C18-C17	-4.44	104.69	109.88
3	A	392	MIY	C20-N1-C4	-4.31	104.29	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	391	MIY	C20-N1-C4	-4.30	104.30	114.10
2	D	389	FAD	C4A-N9A-C8A	4.16	110.11	105.74
3	D	392	MIY	O8-C21-N2	-4.13	113.63	122.89
3	A	391	MIY	C20-N1-C4	-4.11	104.73	114.10
3	C	392	MIY	C1-C18-C17	-4.09	105.09	109.88
3	D	391	MIY	C6-C5-C4	-4.01	107.94	113.73
3	D	391	MIY	O8-C21-N2	-4.01	113.91	122.89
2	B	389	FAD	C5A-C4A-N3A	-4.00	121.21	126.72
2	A	389	FAD	C5X-C9A-N10	3.96	121.55	117.97
3	C	392	MIY	C19-N1-C4	3.95	123.10	114.10
3	D	392	MIY	C5-C18-C1	-3.92	106.55	111.05
3	A	391	MIY	O8-C21-N2	-3.86	114.23	122.89
2	B	389	FAD	C2A-N3A-C4A	3.81	121.14	111.83
3	D	393	MIY	C20-N1-C4	-3.78	105.49	114.10
3	D	393	MIY	C13-C14-C15	-3.75	115.89	121.45
3	D	392	MIY	C11-C12-C13	-3.75	116.75	120.50
2	B	389	FAD	C5A-N7A-C8A	3.68	109.23	103.45
2	D	389	FAD	C2A-N3A-C4A	3.63	120.70	111.83
2	B	389	FAD	O5'-P-O1P	-3.58	94.74	108.94
3	D	393	MIY	C13-C14-C9	3.58	122.87	119.03
2	A	389	FAD	C2A-N3A-C4A	3.57	120.54	111.83
2	C	389	FAD	C5X-C9A-N10	3.56	121.19	117.97
3	C	391	MIY	C6-C5-C4	-3.55	108.61	113.73
3	A	392	MIY	O6-C17-C18	3.54	118.50	113.37
3	D	392	MIY	O7-C18-C5	3.52	117.08	109.30
3	A	391	MIY	C7-C6-C5	-3.48	104.44	110.38
3	C	391	MIY	C13-C14-C9	3.48	122.77	119.03
3	D	392	MIY	C71-N7-C10	-3.45	104.47	115.16
3	D	393	MIY	C1-C18-C17	-3.45	105.84	109.88
3	C	391	MIY	O8-C21-N2	-3.44	115.18	122.89
3	D	393	MIY	O8-C21-N2	-3.32	115.45	122.89
2	B	389	FAD	O4-C4-N3	3.31	126.35	120.11
2	A	389	FAD	C5A-N7A-C8A	3.28	108.61	103.45
2	A	389	FAD	C4A-N9A-C8A	3.25	109.16	105.74
3	A	392	MIY	O7-C18-C5	3.25	116.49	109.30
3	D	391	MIY	C7-C6-C5	-3.20	104.92	110.38
3	A	392	MIY	C2-C21-N2	3.16	125.09	118.64
3	C	392	MIY	O2-C3-C2	-3.15	117.67	122.93
3	B	391	MIY	O8-C21-N2	-3.14	115.85	122.89
2	D	389	FAD	C5X-C9A-N10	3.12	120.79	117.97
3	D	392	MIY	C1-C18-C17	-3.11	106.24	109.88
2	A	389	FAD	C5A-C4A-N3A	-3.11	122.44	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	389	FAD	O4'-C4'-C3'	3.06	116.41	109.25
3	D	391	MIY	C2-C21-N2	3.05	124.87	118.64
2	C	389	FAD	C5A-N7A-C8A	3.05	108.25	103.45
3	B	391	MIY	C7-C6-C5	-3.01	105.25	110.38
2	A	389	FAD	O4-C4-C4X	-2.97	118.69	126.53
3	A	392	MIY	C21-C2-C1	-2.95	117.47	120.97
2	B	389	FAD	C4A-N9A-C8A	2.94	108.83	105.74
3	A	391	MIY	O7-C18-C17	-2.94	105.44	110.14
3	C	391	MIY	C7-C6-C5	-2.93	105.39	110.38
3	C	392	MIY	C8-C9-C14	2.93	123.10	118.13
3	D	392	MIY	C2-C21-N2	2.92	124.59	118.64
3	D	393	MIY	C11-C10-C9	-2.91	116.61	120.59
2	C	389	FAD	C9A-C5X-N5	-2.88	119.39	122.45
2	C	389	FAD	C2A-N3A-C4A	2.87	118.85	111.83
3	C	392	MIY	O8-C21-N2	-2.84	116.53	122.89
2	D	389	FAD	C4-N3-C2	-2.81	120.66	125.64
2	A	389	FAD	C4-N3-C2	-2.81	120.66	125.64
3	C	391	MIY	C6-C7-C16	-2.78	104.25	110.28
2	B	389	FAD	O2-C2-N1	-2.77	117.19	121.80
2	D	389	FAD	O4-C4-C4X	-2.76	119.25	126.53
3	B	391	MIY	C71-N7-CN7	-2.76	107.33	116.18
2	C	389	FAD	C2A-N1A-C6A	2.75	123.25	118.73
2	C	389	FAD	C4-N3-C2	-2.75	120.76	125.64
2	D	389	FAD	C5A-N7A-C8A	2.74	107.76	103.45
3	C	392	MIY	C2-C21-N2	2.73	124.20	118.64
3	A	392	MIY	O8-C21-N2	-2.73	116.78	122.89
2	A	389	FAD	C4X-C10-N10	2.72	120.38	116.48
2	C	389	FAD	N3A-C4A-N9A	2.72	131.78	127.17
2	D	389	FAD	O2-C2-N1	-2.70	117.32	121.80
3	D	393	MIY	C12-C11-C10	2.70	124.51	119.10
3	D	392	MIY	O2-C3-C2	-2.67	118.47	122.93
3	D	393	MIY	C2-C21-N2	2.66	124.07	118.64
3	B	391	MIY	C6-C5-C4	-2.66	109.89	113.73
3	B	391	MIY	C1-C18-C17	-2.66	106.77	109.88
3	B	391	MIY	O6-C17-C18	2.65	117.20	113.37
2	B	389	FAD	N3A-C4A-N9A	2.64	131.65	127.17
3	D	391	MIY	O7-C18-C17	-2.63	105.93	110.14
3	A	391	MIY	C6-C5-C4	-2.63	109.94	113.73
2	A	389	FAD	O2-C2-N1	-2.62	117.44	121.80
3	B	391	MIY	C6-C7-C16	-2.60	104.64	110.28
3	D	393	MIY	C19-N1-C4	2.58	119.97	114.10
3	D	393	MIY	C15-C16-C17	-2.57	116.77	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	389	FAD	N3A-C4A-N9A	2.51	131.43	127.17
2	C	389	FAD	C4X-C4-N3	2.50	119.61	113.25
2	A	389	FAD	O4'-C4'-C3'	2.50	115.09	109.25
2	B	389	FAD	C4-N3-C2	-2.47	121.26	125.64
3	A	391	MIY	C21-C2-C1	-2.47	118.05	120.97
3	C	392	MIY	C5-C18-C1	-2.46	108.23	111.05
3	A	392	MIY	O1-C1-C18	2.46	123.80	119.11
3	C	391	MIY	C13-C14-C15	-2.46	117.81	121.45
2	C	389	FAD	O3B-C3B-C4B	-2.45	104.03	111.08
2	C	389	FAD	C5A-C4A-N3A	-2.45	123.35	126.72
3	A	391	MIY	C71-N7-CN7	-2.44	108.34	116.18
2	D	389	FAD	C5A-C4A-N3A	-2.43	123.37	126.72
2	D	389	FAD	O4'-C4'-C3'	2.40	114.87	109.25
2	D	389	FAD	C4X-C4-N3	2.38	119.32	113.25
3	C	391	MIY	O6-C17-C18	2.37	116.81	113.37
3	A	391	MIY	C6-C7-C16	-2.37	105.15	110.28
2	C	389	FAD	O5'-P-O1P	-2.34	99.66	108.94
3	B	391	MIY	O6-C17-C16	-2.33	119.01	123.52
2	A	389	FAD	C2A-N1A-C6A	2.29	122.49	118.73
3	B	391	MIY	C21-C2-C1	-2.27	118.28	120.97
3	C	391	MIY	C71-N7-CN7	-2.26	108.91	116.18
3	D	391	MIY	C6-C7-C16	-2.26	105.38	110.28
3	A	391	MIY	O6-C17-C18	2.26	116.63	113.37
2	B	389	FAD	O5B-C5B-C4B	-2.25	101.33	108.99
3	C	391	MIY	O7-C18-C17	-2.24	106.55	110.14
2	B	389	FAD	C4X-C4-N3	2.24	118.97	113.25
3	D	393	MIY	O1-C1-C18	2.24	123.38	119.11
2	D	389	FAD	N3A-C4A-N9A	2.23	130.97	127.17
2	B	389	FAD	C4A-C5A-N7A	-2.21	108.05	110.58
2	B	389	FAD	C5X-C9A-N10	2.20	119.96	117.97
2	D	389	FAD	C2A-N1A-C6A	2.20	122.34	118.73
2	D	389	FAD	O2'-C2'-C3'	2.18	114.35	109.25
2	C	389	FAD	O4B-C4B-C3B	2.18	109.48	105.15
2	C	389	FAD	C8M-C8-C7	2.17	125.20	120.76
3	D	391	MIY	C13-C14-C9	2.17	121.36	119.03
3	D	393	MIY	O2-C3-C2	-2.17	119.31	122.93
3	D	391	MIY	O6-C17-C18	2.16	116.50	113.37
2	B	389	FAD	O5'-C5'-C4'	2.16	115.12	109.36
3	C	392	MIY	CN7-N7-C10	-2.15	108.49	115.16
2	D	389	FAD	C7M-C7-C6	-2.15	115.78	119.57
2	D	389	FAD	C4A-N9A-C1B	-2.15	121.60	126.63
2	A	389	FAD	C4X-C4-N3	2.15	118.72	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	392	MIY	C8-C9-C14	2.14	121.76	118.13
3	C	391	MIY	O6-C17-C16	-2.13	119.39	123.52
3	D	392	MIY	C11-C10-N7	-2.12	118.73	121.65
2	B	389	FAD	O2A-PA-O3P	-2.12	101.54	107.27
2	A	389	FAD	O5'-C5'-C4'	2.11	114.99	109.36
3	D	391	MIY	C15-C16-C17	2.10	120.46	118.80
2	C	389	FAD	C4A-N9A-C1B	-2.10	121.72	126.63
3	A	391	MIY	C2-C21-N2	2.10	122.92	118.64
2	A	389	FAD	O5'-P-O1P	2.09	117.23	108.94
3	A	392	MIY	C9-C8-C7	2.08	115.88	113.12
2	B	389	FAD	O2-C2-N3	2.08	122.57	118.58
2	D	389	FAD	C9-C9A-N10	-2.08	119.06	121.85
3	B	391	MIY	C2-C21-N2	2.07	122.87	118.64
2	D	389	FAD	C4X-C10-N10	2.07	119.44	116.48
3	D	392	MIY	O7-C18-C17	2.06	113.43	110.14
3	D	392	MIY	C13-C14-C15	-2.05	118.41	121.45
2	B	389	FAD	C9A-C5X-N5	-2.05	120.28	122.45
2	C	389	FAD	C8M-C8-C9	-2.03	115.99	119.57
3	D	393	MIY	C71-N7-CN7	-2.03	109.66	116.18
3	D	393	MIY	C6-C7-C16	-2.03	105.88	110.28
2	D	389	FAD	O2B-C2B-C1B	-2.03	103.12	110.10
3	C	391	MIY	C19-N1-C4	-2.03	109.49	114.10
3	C	391	MIY	C12-C13-C14	-2.03	117.57	120.15
3	A	392	MIY	C6-C5-C4	-2.02	110.81	113.73
2	A	389	FAD	C9-C9A-N10	-2.01	119.15	121.85
3	B	391	MIY	O7-C18-C5	2.01	113.74	109.30

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	389	FAD	C5'-O5'-P-O2P
2	A	389	FAD	C5'-O5'-P-O3P
2	B	389	FAD	C5'-O5'-P-O2P
2	B	389	FAD	C5'-O5'-P-O3P
2	C	389	FAD	C2'-C1'-N10-C10
2	C	389	FAD	C5'-O5'-P-O2P
2	C	389	FAD	C5'-O5'-P-O3P
2	D	389	FAD	C2'-C1'-N10-C10
2	D	389	FAD	C5'-O5'-P-O2P
2	A	389	FAD	C2'-C1'-N10-C10
2	B	389	FAD	C2'-C1'-N10-C10

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Mol	Chain	Res	Type	Atoms
2	D	389	FAD	C5'-O5'-P-O3P
3	C	392	MIY	C1-C2-C21-N2
2	A	389	FAD	C2B-C1B-N9A-C8A
2	A	389	FAD	O4B-C4B-C5B-O5B
3	D	392	MIY	C5-C4-N1-C19
3	D	393	MIY	C9-C10-N7-C71
2	B	389	FAD	C2B-C1B-N9A-C8A
2	C	389	FAD	C2B-C1B-N9A-C8A
2	B	389	FAD	O4B-C4B-C5B-O5B

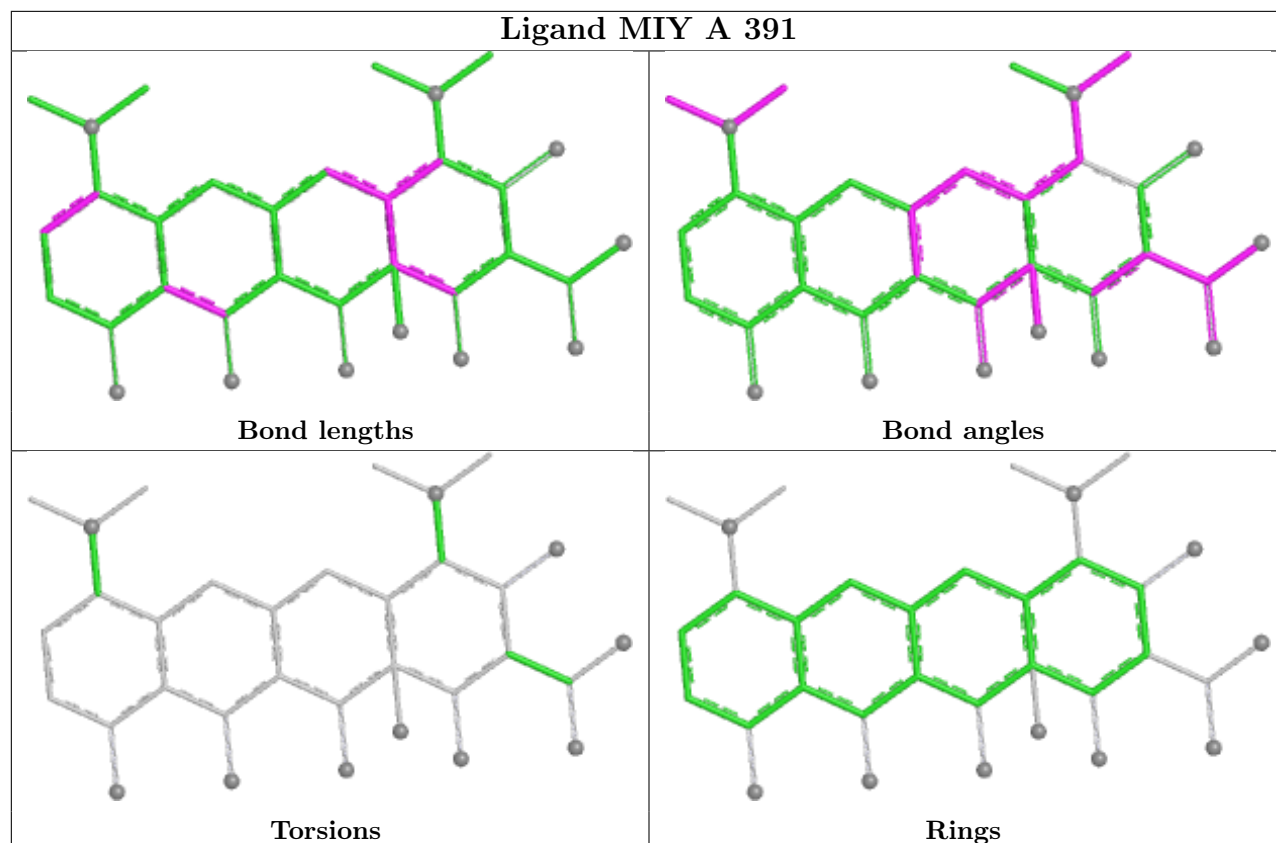
There are no ring outliers.

11 monomers are involved in 29 short contacts:

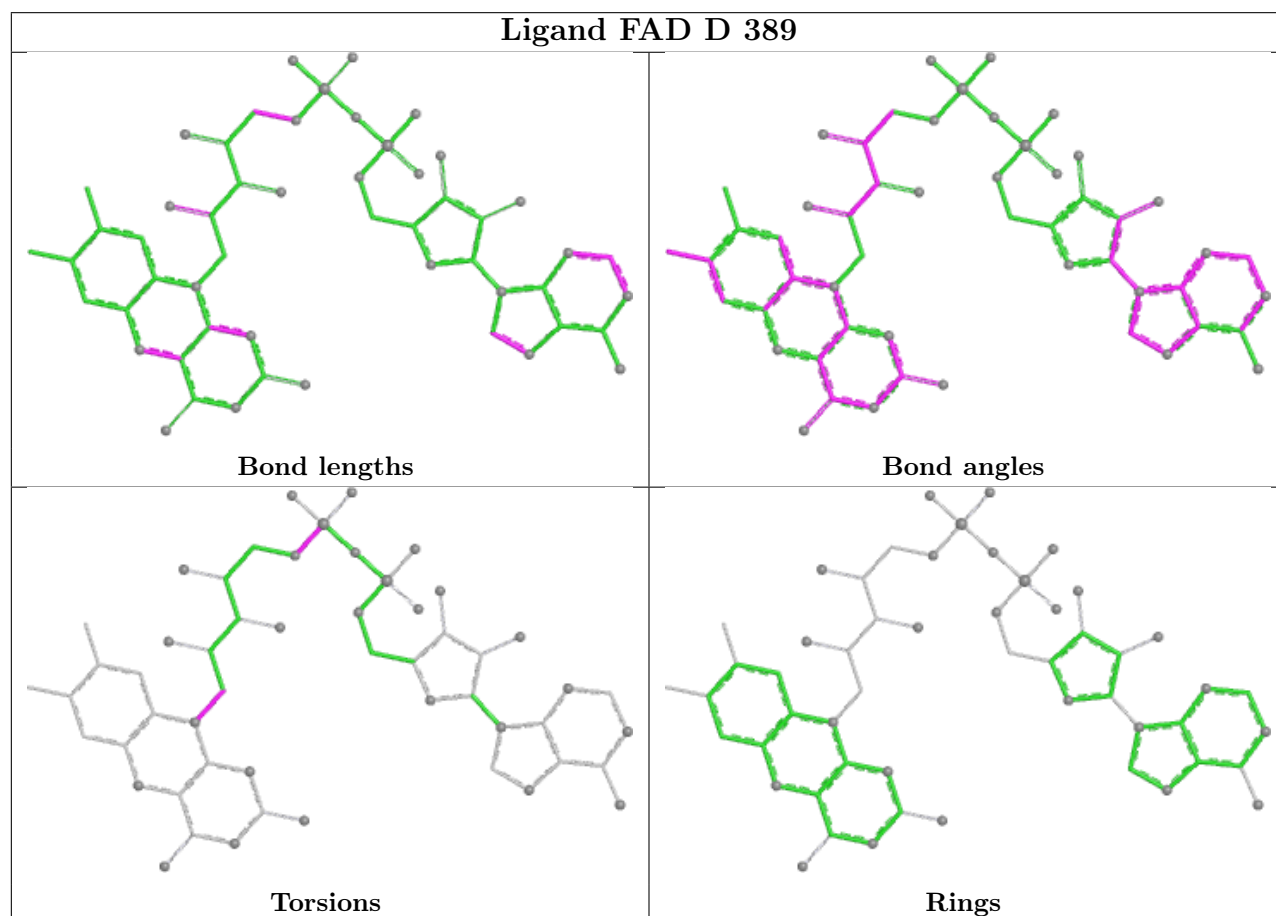
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	391	MIY	2	0
2	D	389	FAD	3	0
3	A	392	MIY	1	0
2	C	389	FAD	2	0
2	A	389	FAD	4	0
3	C	392	MIY	6	0
2	B	389	FAD	3	0
3	C	391	MIY	1	0
3	B	391	MIY	2	0
3	D	392	MIY	2	0
3	D	393	MIY	5	0

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.

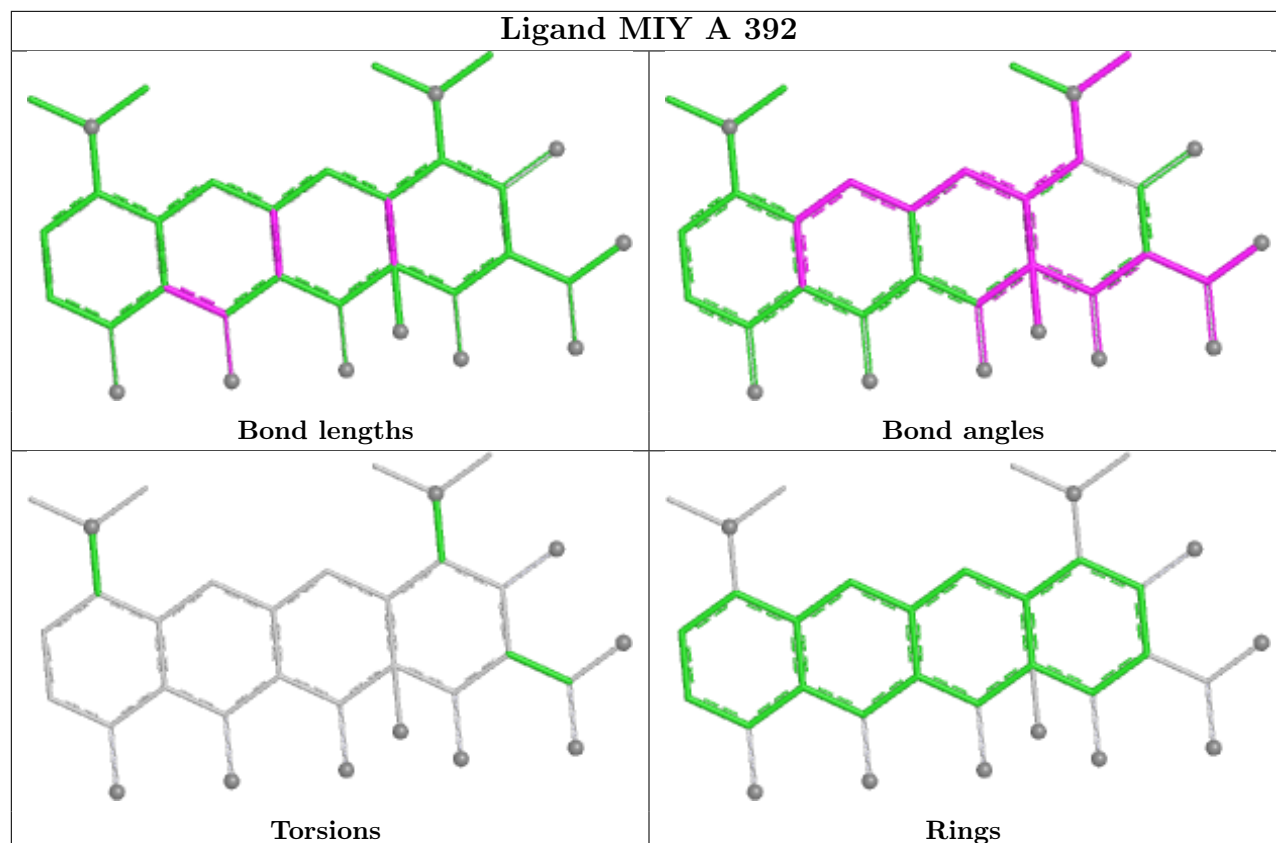
Ligand MIY A 391



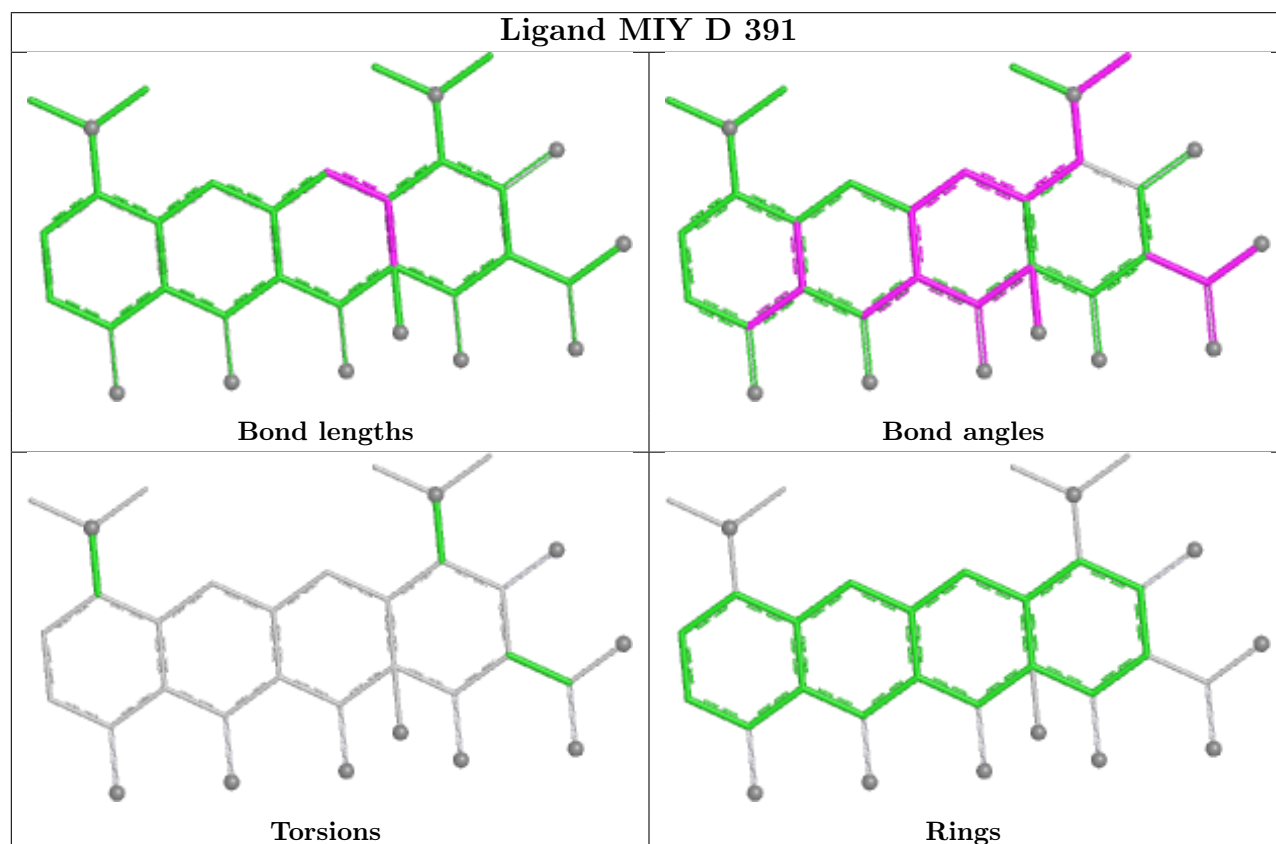
Ligand FAD D 389

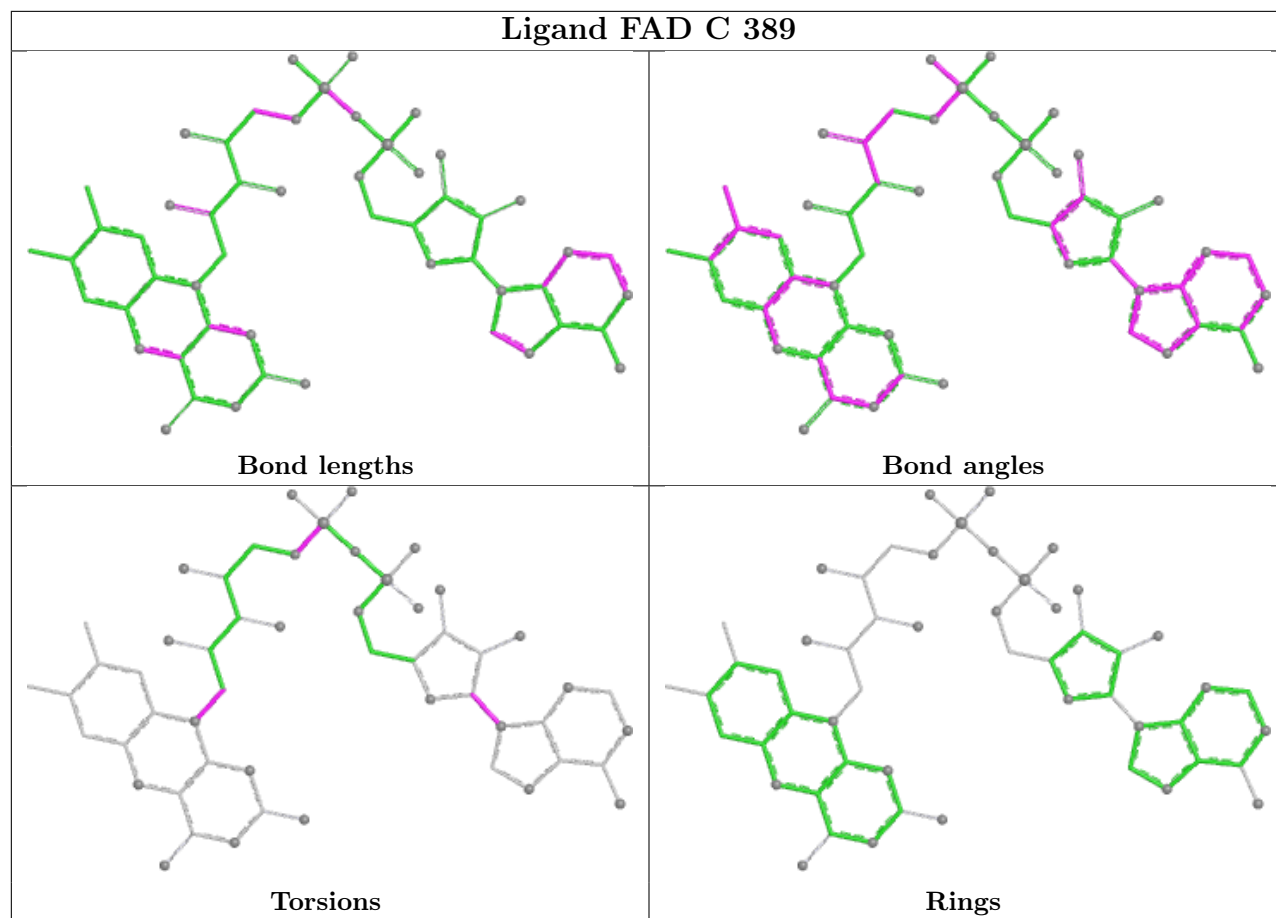


Ligand MIY A 392

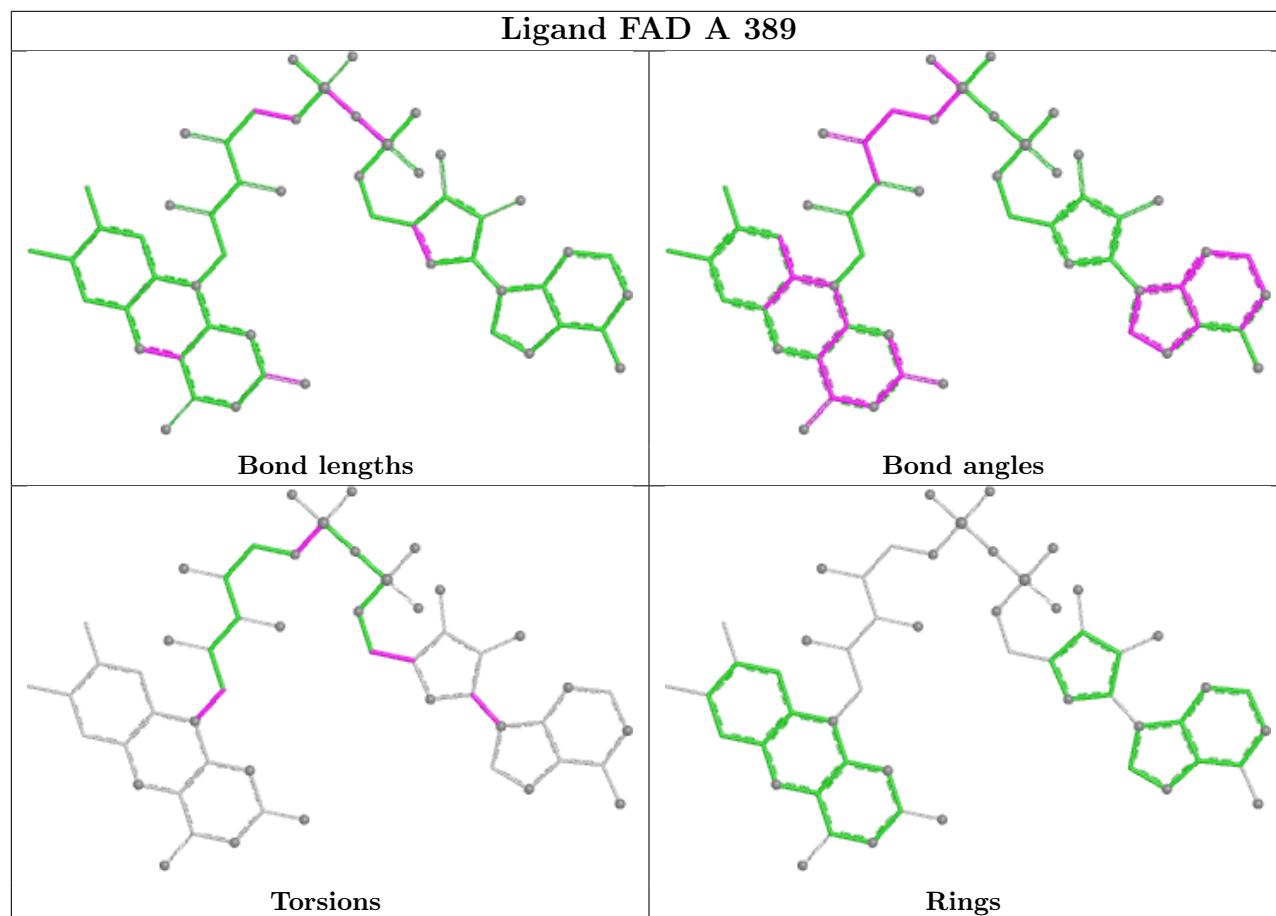


Ligand MIY D 391

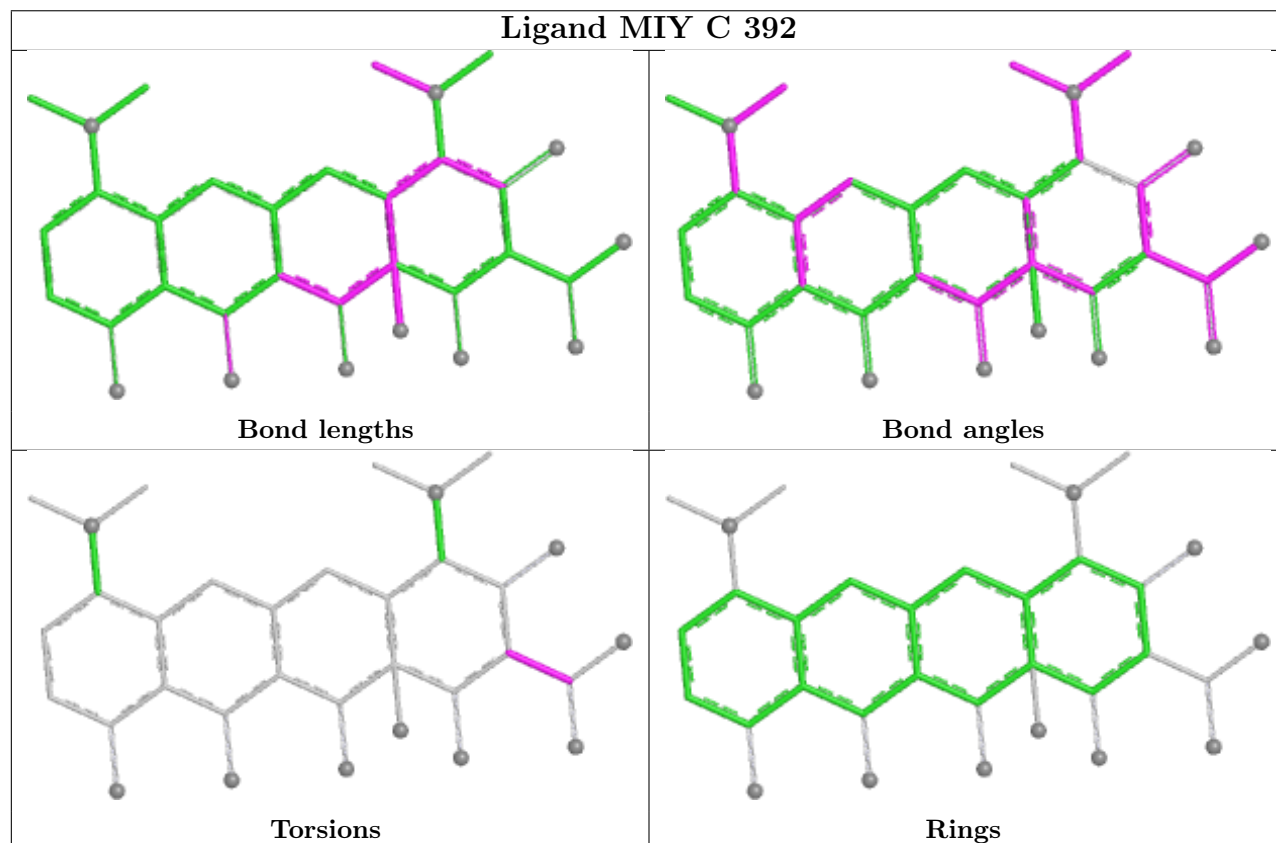




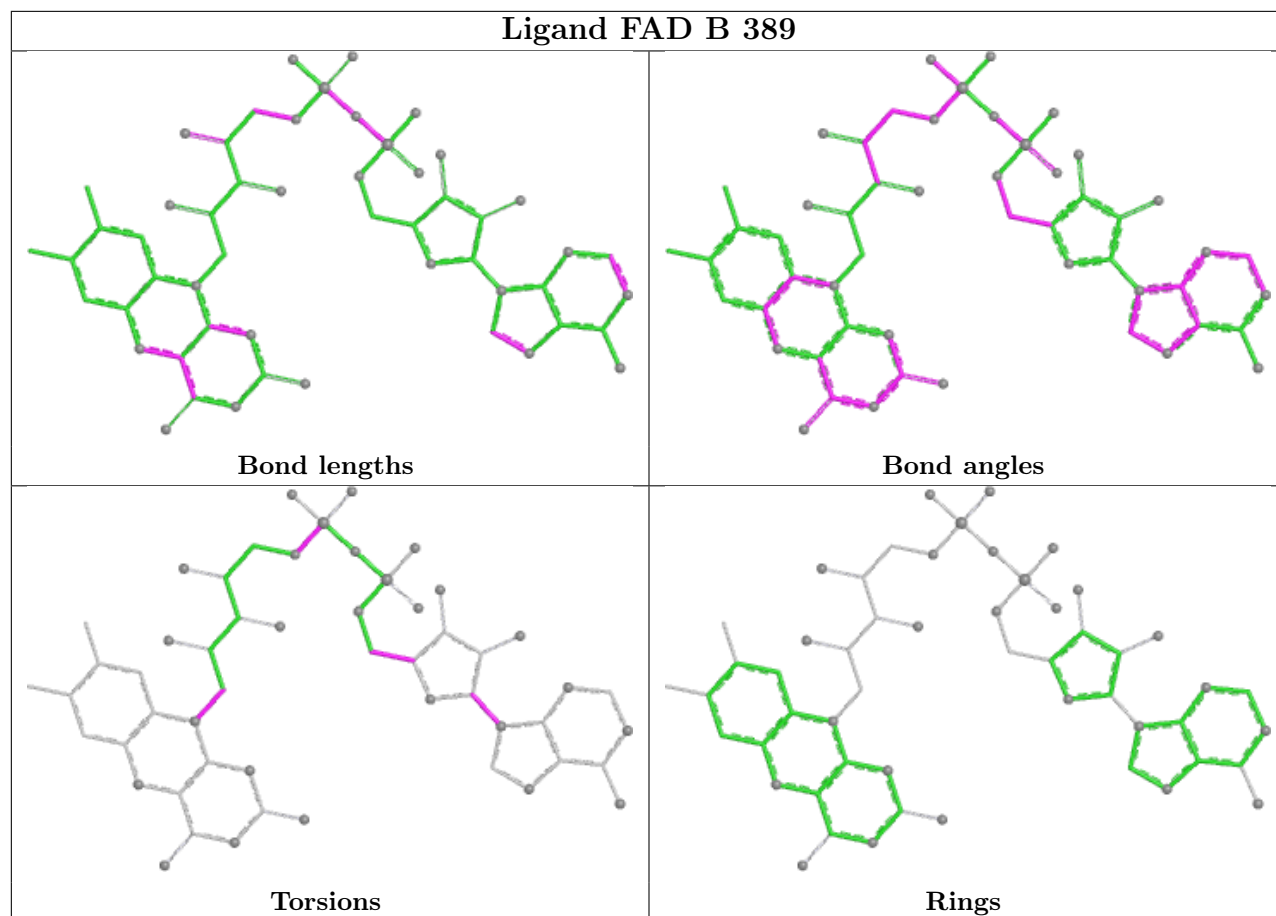
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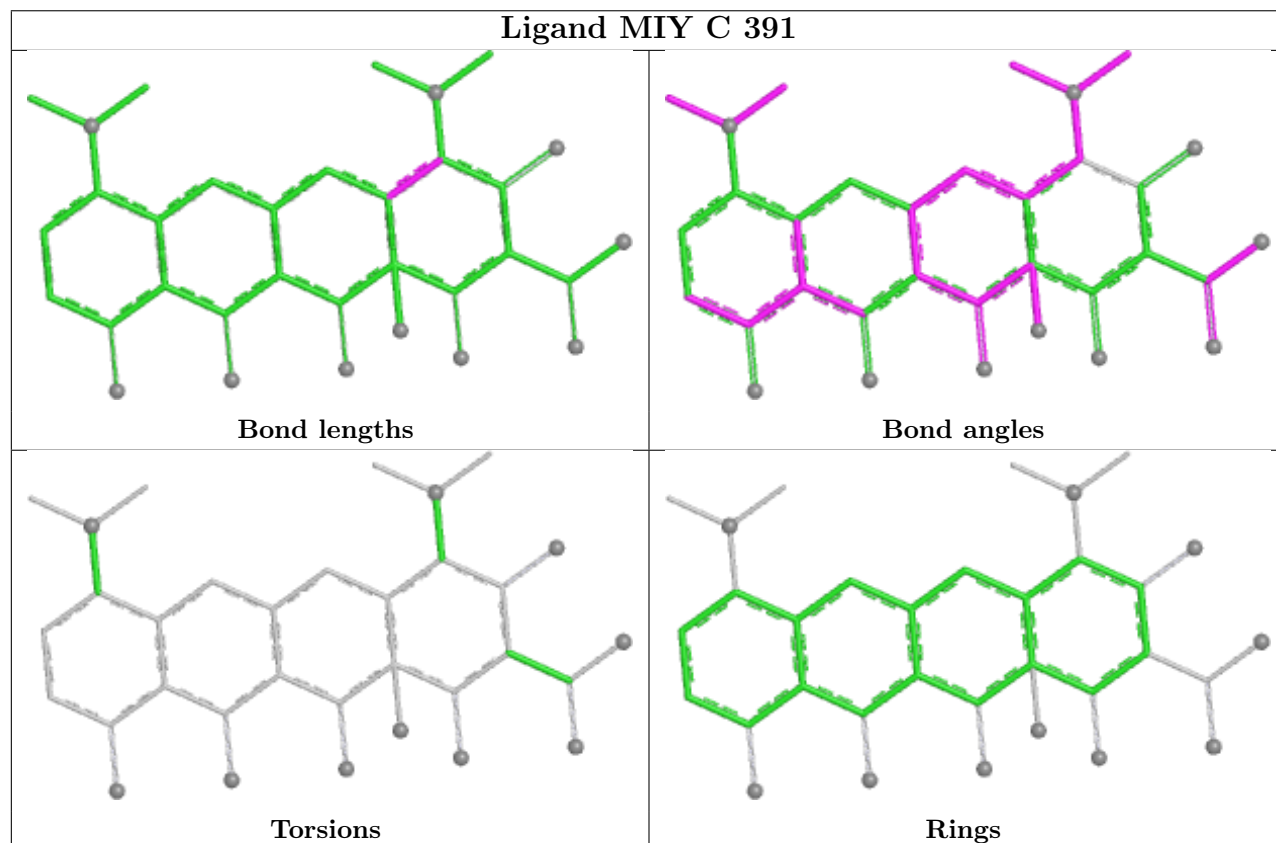
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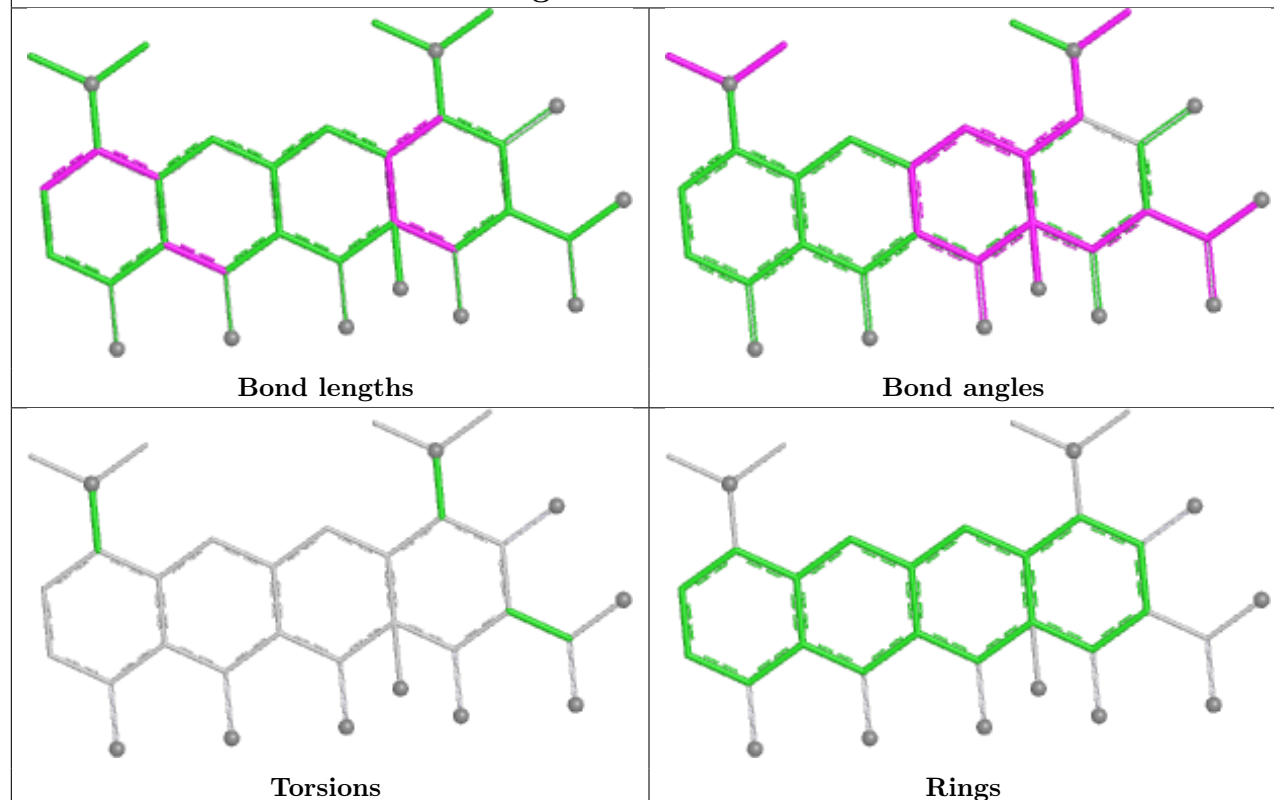
Ligand FAD B 389



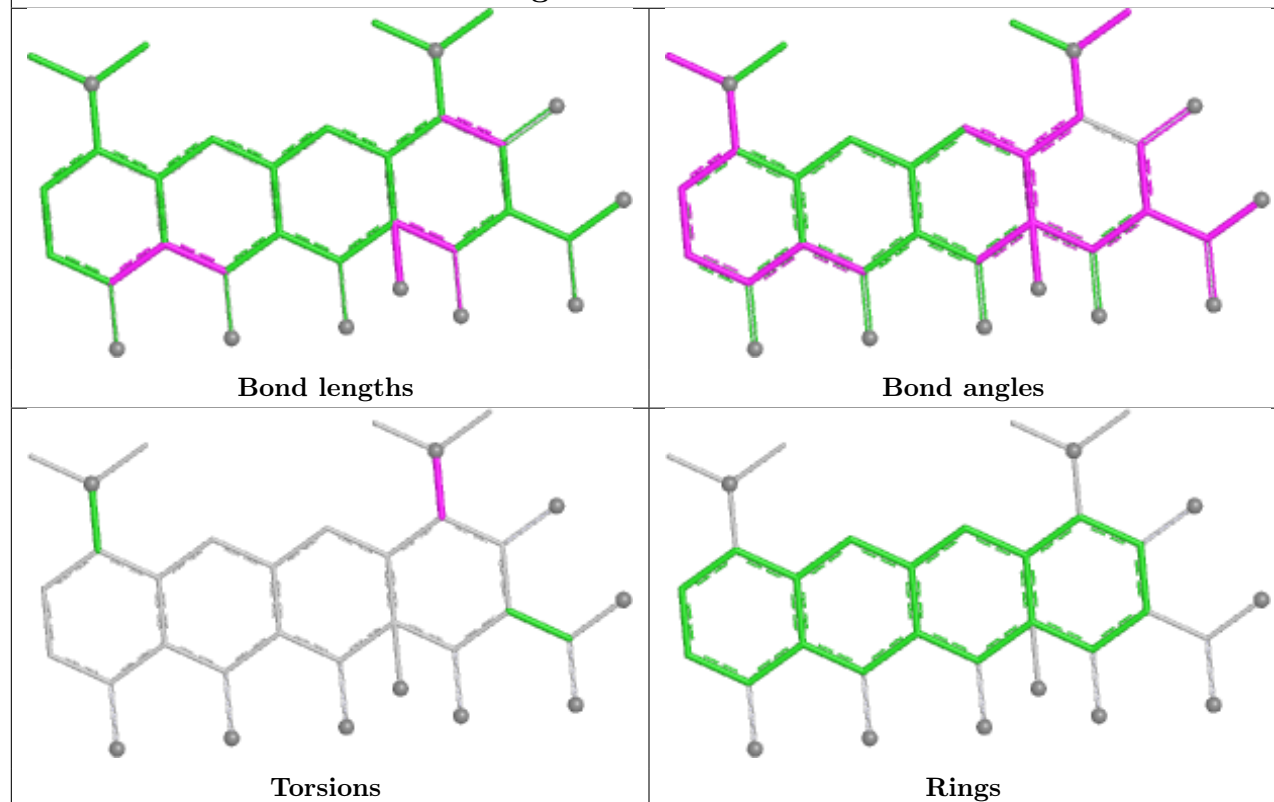
Ligand MIY C 391

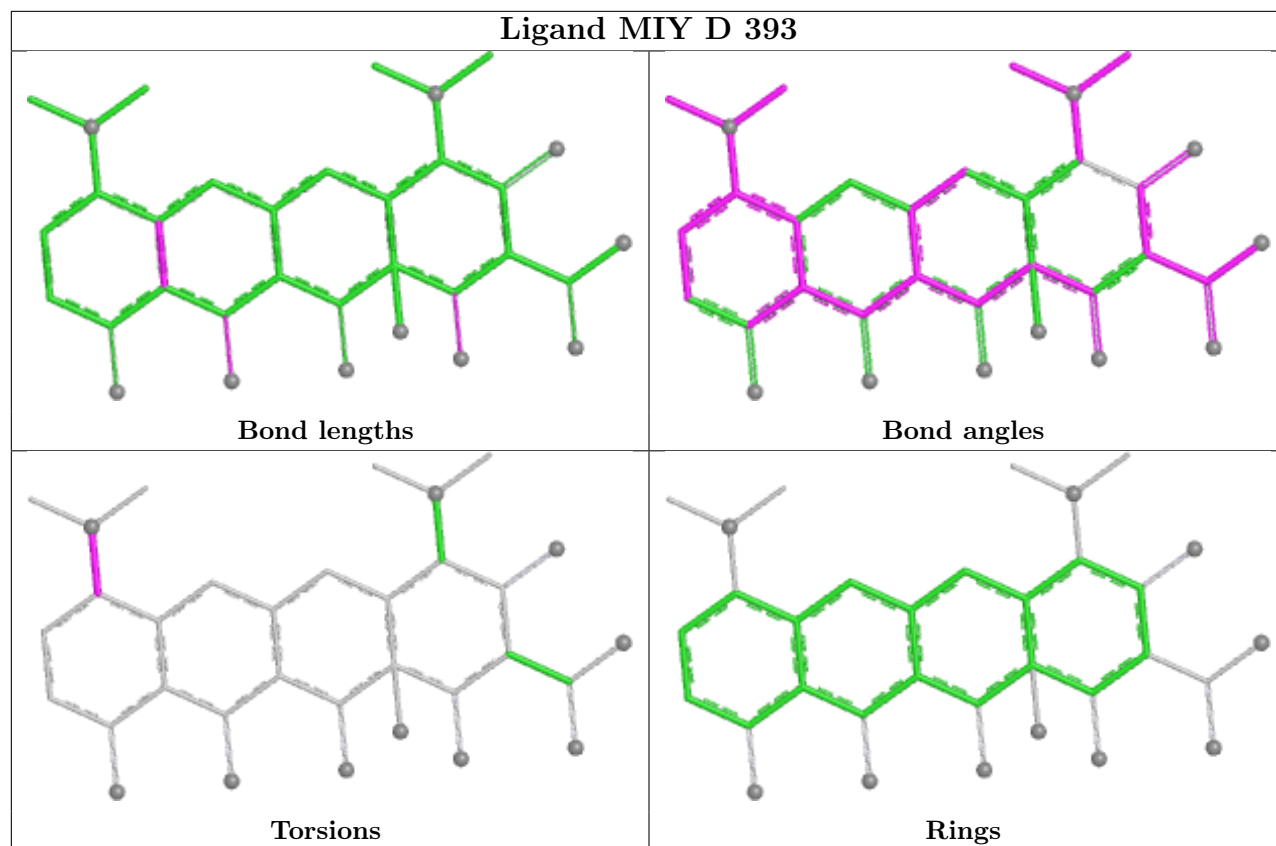


Ligand MIY B 391



Ligand MIY D 392





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	368/398 (92%)	0.36	20 (5%) 31 30	33, 47, 77, 124	0
1	B	368/398 (92%)	0.41	18 (4%) 35 34	32, 48, 80, 124	0
1	C	367/398 (92%)	0.53	21 (5%) 29 28	36, 53, 85, 119	0
1	D	367/398 (92%)	0.48	23 (6%) 26 25	33, 52, 84, 118	0
All	All	1470/1592 (92%)	0.44	82 (5%) 30 29	32, 50, 83, 124	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	381	THR	5.1
1	A	376	PHE	4.6
1	A	378	PRO	4.3
1	B	341	GLY	4.3
1	A	249	THR	4.3
1	A	382	PHE	4.2
1	A	380	PHE	4.2
1	A	341	GLY	4.2
1	B	249	THR	3.9
1	A	340	ASP	3.8
1	A	377	LYS	3.6
1	A	379	ASP	3.6
1	B	378	PRO	3.6
1	C	341	GLY	3.6
1	D	104	VAL	3.6
1	C	99	LEU	3.5
1	C	381	THR	3.4
1	D	341	GLY	3.3
1	D	146	LYS	3.1
1	D	342	LYS	3.1
1	B	340	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	109	ARG	3.1
1	C	109	ARG	3.1
1	B	381	THR	3.0
1	B	380	PHE	3.0
1	C	382	PHE	3.0
1	C	146	LYS	3.0
1	D	147	LYS	3.0
1	C	208	LEU	3.0
1	C	147	LYS	2.9
1	D	250	GLN	2.9
1	B	208	LEU	2.9
1	D	381	THR	2.9
1	B	382	PHE	2.8
1	D	110	PHE	2.8
1	A	342	LYS	2.7
1	B	320	ALA	2.7
1	A	287	LEU	2.7
1	C	340	ASP	2.7
1	C	250	GLN	2.6
1	B	342	LYS	2.6
1	A	339	ALA	2.6
1	D	99	LEU	2.6
1	C	380	PHE	2.6
1	C	110	PHE	2.5
1	D	295	GLU	2.5
1	A	351	LYS	2.5
1	B	376	PHE	2.5
1	D	245	TRP	2.5
1	B	104	VAL	2.5
1	A	99	LEU	2.5
1	B	373	ILE	2.4
1	C	104	VAL	2.4
1	D	340	ASP	2.4
1	A	375	MET	2.4
1	B	99	LEU	2.4
1	C	251	VAL	2.4
1	B	287	LEU	2.3
1	C	342	LYS	2.2
1	C	375	MET	2.2
1	D	379	ASP	2.2
1	D	339	ALA	2.2
1	D	296	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	343	PHE	2.2
1	B	245	TRP	2.2
1	C	220	GLY	2.1
1	C	339	ALA	2.1
1	A	51	ARG	2.1
1	C	296	LYS	2.1
1	C	106	PRO	2.1
1	D	106	PRO	2.1
1	D	39	GLY	2.1
1	D	251	VAL	2.1
1	D	244	GLU	2.1
1	B	110	PHE	2.1
1	A	12	ASN	2.1
1	C	345	SER	2.1
1	D	101	THR	2.0
1	B	146	LYS	2.0
1	A	295	GLU	2.0
1	A	208	LEU	2.0
1	D	208	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	B	1385	5/5	0.65	0.17	74,87,92,95	5
4	SO4	D	1385	5/5	0.68	0.13	81,86,93,98	5
4	SO4	C	1385	5/5	0.71	0.12	101,102,111,113	0
4	SO4	C	1383	5/5	0.79	0.12	81,85,105,109	0

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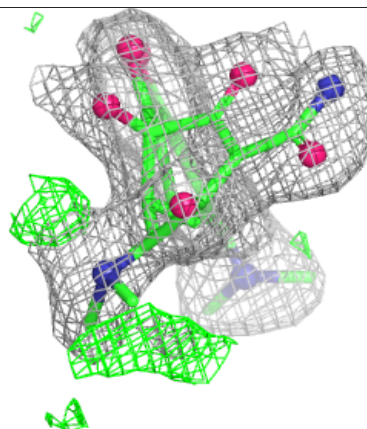
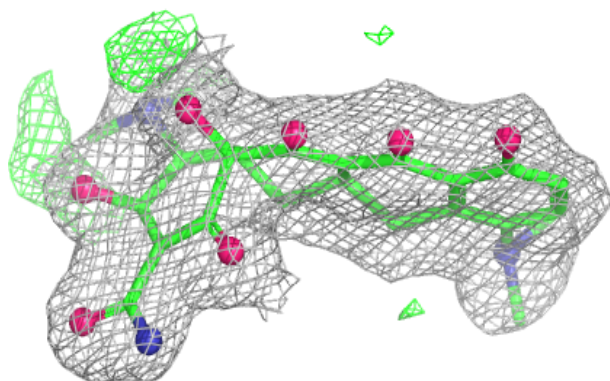
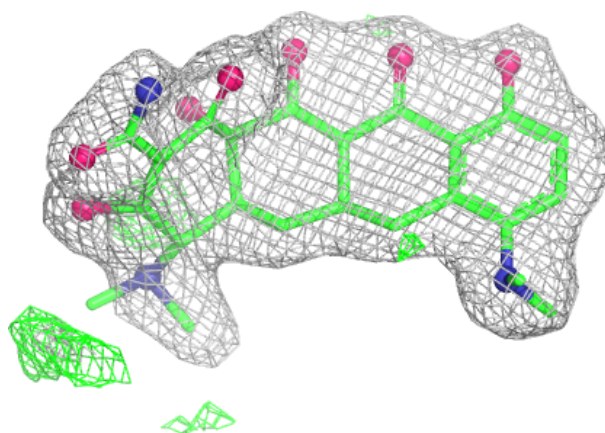
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	D	1383	5/5	0.80	0.11	72,93,95,102	0
4	SO4	B	1383	5/5	0.84	0.10	92,94,101,104	0
4	SO4	A	1383	5/5	0.87	0.07	86,88,91,92	0
4	SO4	C	1384	5/5	0.88	0.08	79,80,84,87	0
4	SO4	B	1384	5/5	0.90	0.08	80,81,83,96	0
3	MIY	D	392	33/33	0.91	0.09	38,45,54,69	0
3	MIY	B	391	33/33	0.92	0.11	32,47,62,71	0
3	MIY	C	392	33/33	0.93	0.09	42,52,55,62	0
3	MIY	A	392	33/33	0.93	0.09	42,50,55,56	0
3	MIY	D	393	33/33	0.93	0.09	42,50,54,60	0
3	MIY	D	391	33/33	0.94	0.09	38,55,64,71	0
4	SO4	D	1384	5/5	0.94	0.07	65,70,80,83	0
3	MIY	A	391	33/33	0.94	0.09	32,43,57,59	0
3	MIY	C	391	33/33	0.95	0.09	41,50,58,63	0
2	FAD	B	389	53/53	0.96	0.08	31,40,55,59	0
2	FAD	C	389	53/53	0.96	0.08	33,42,60,68	0
2	FAD	A	389	53/53	0.97	0.07	29,38,52,67	0
2	FAD	D	389	53/53	0.97	0.08	33,42,56,62	0

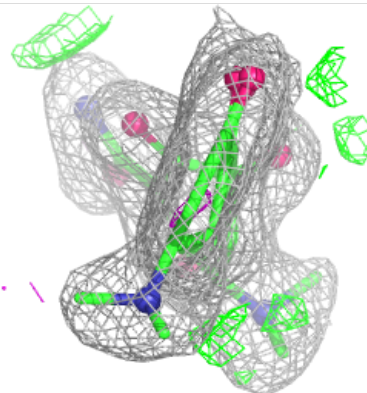
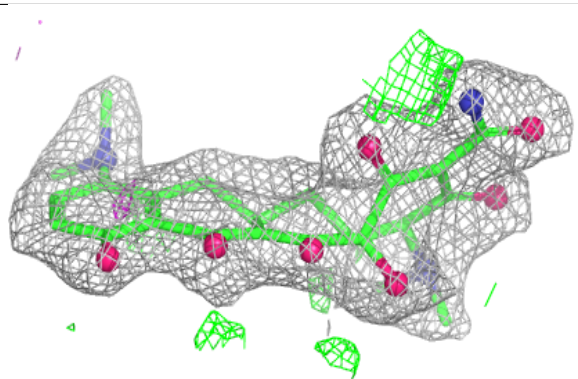
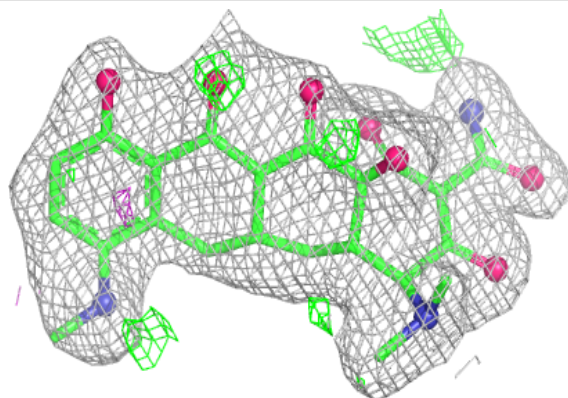
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MIY D 392:

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

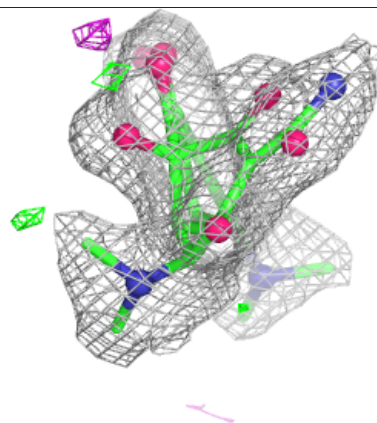
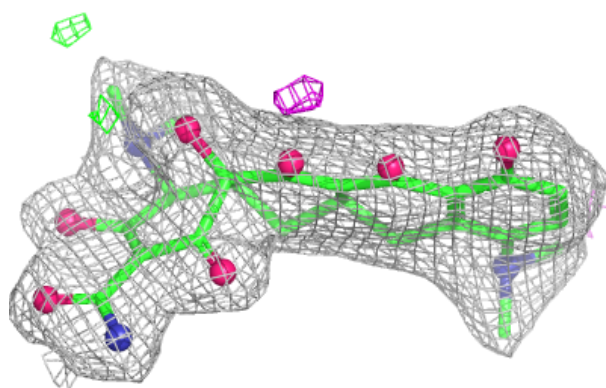
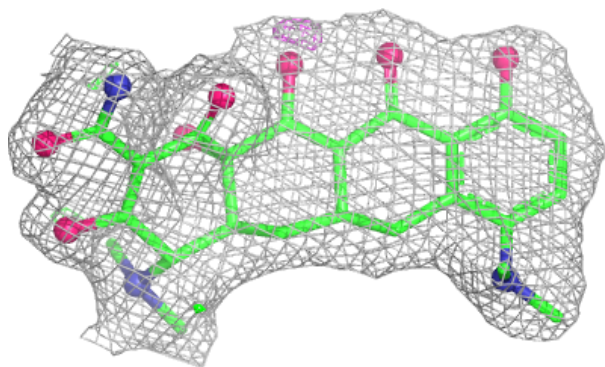
**Electron density around MIY B 391:**

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



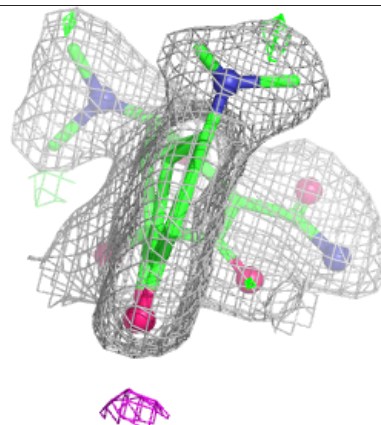
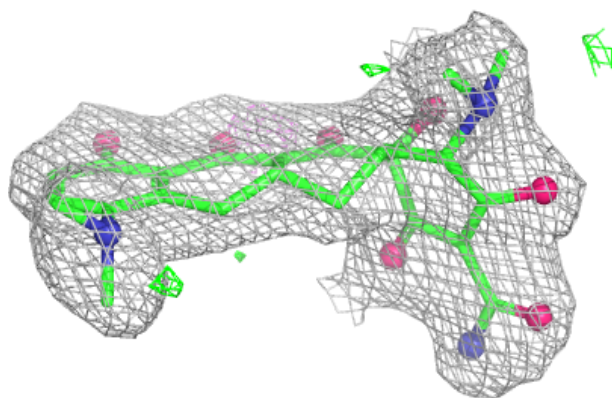
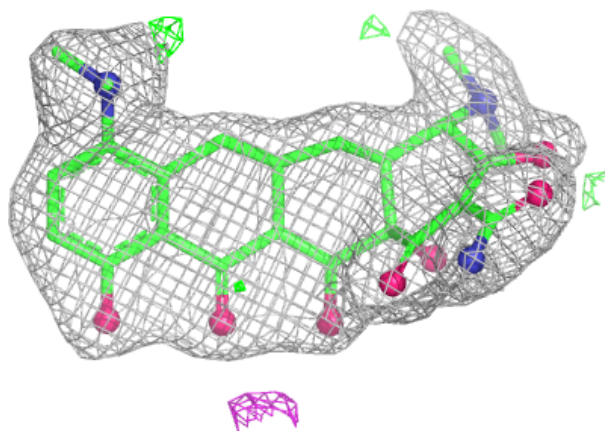
Electron density around MIY C 392:

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



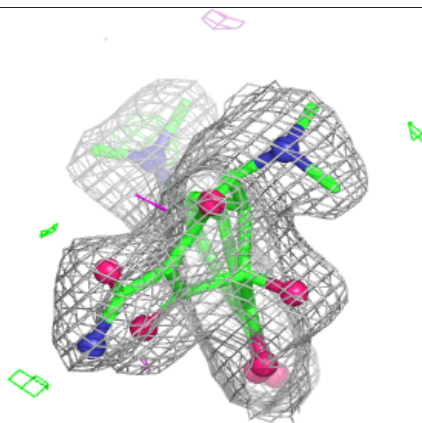
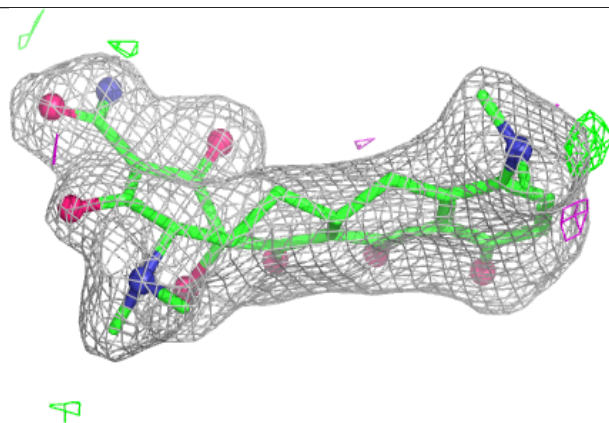
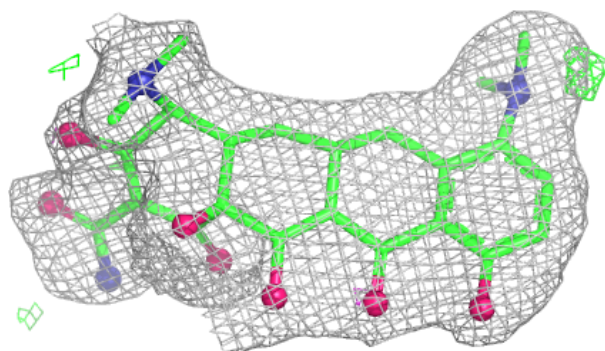
Electron density around MIY A 392:

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and green (positive)



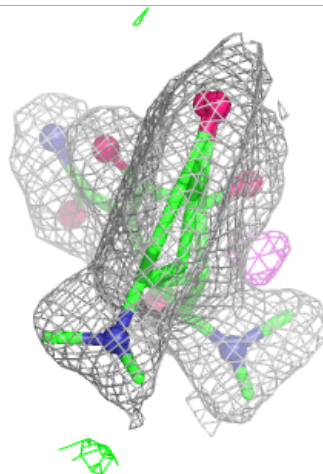
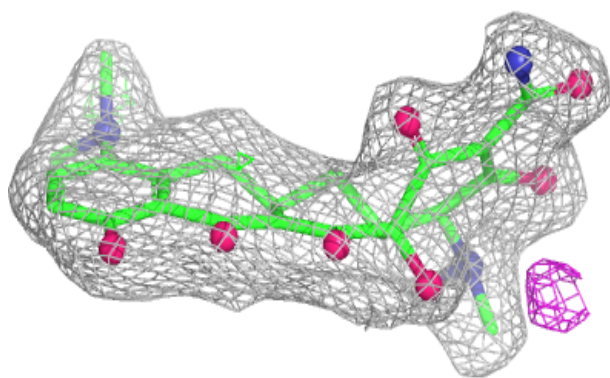
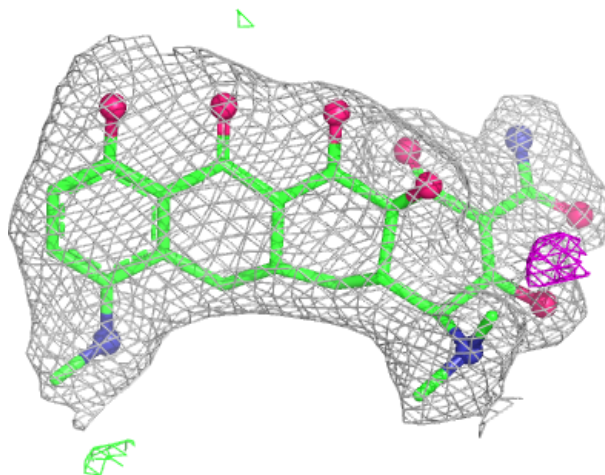
Electron density around MIY D 393:

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



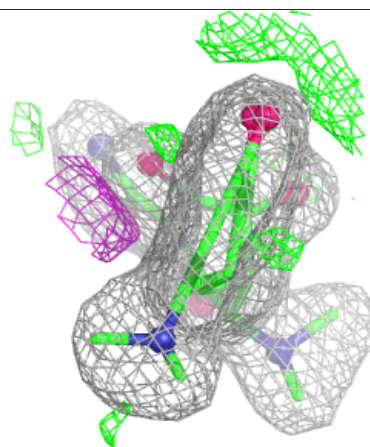
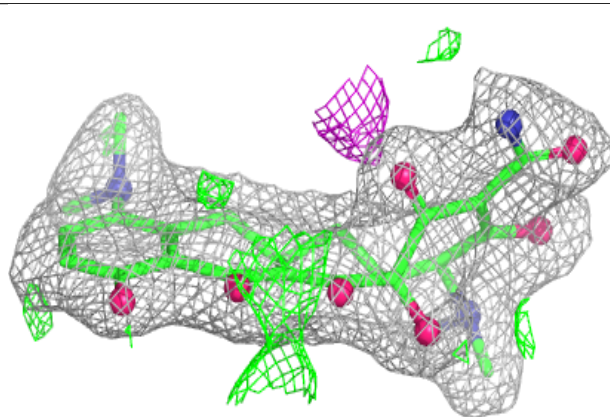
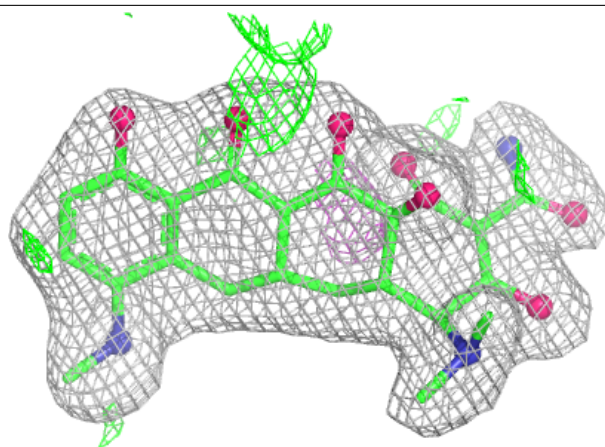
Electron density around MIY D 391:

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



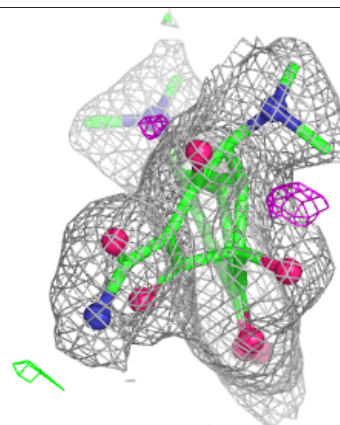
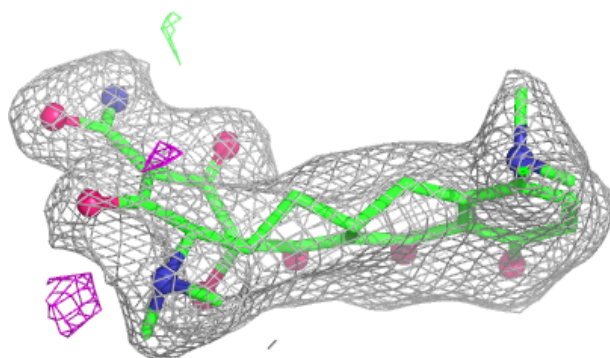
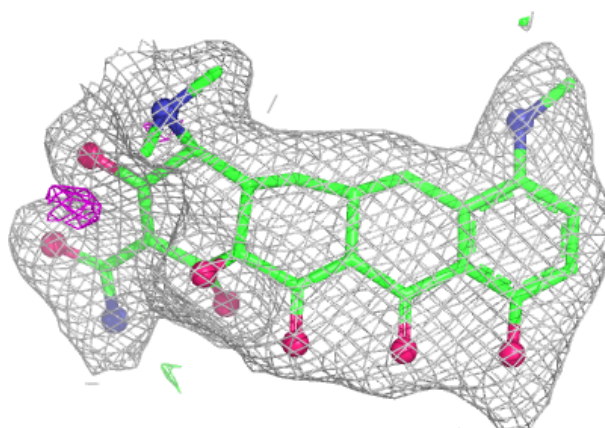
Electron density around MIY A 391:

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

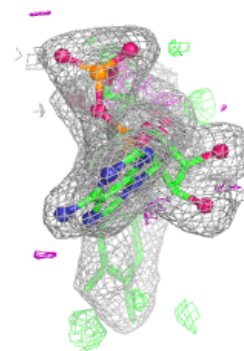
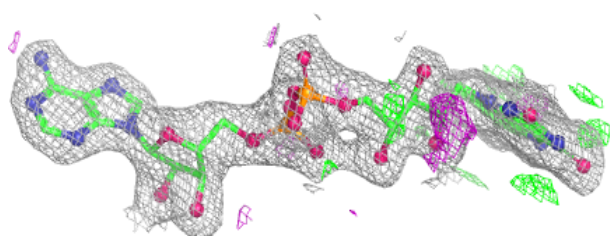
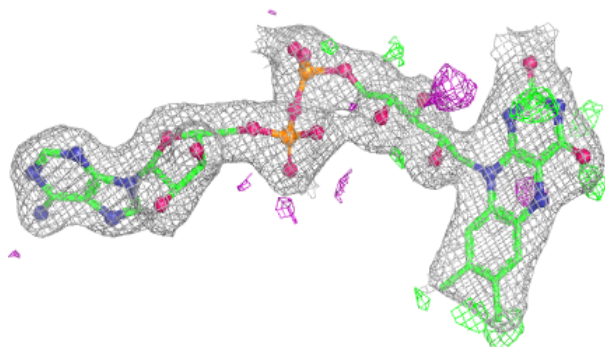


Electron density around MIY C 391:

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

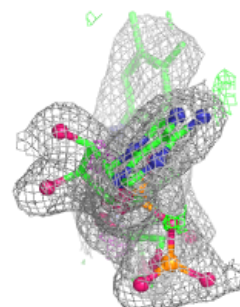
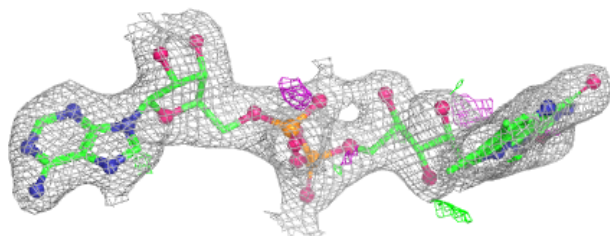
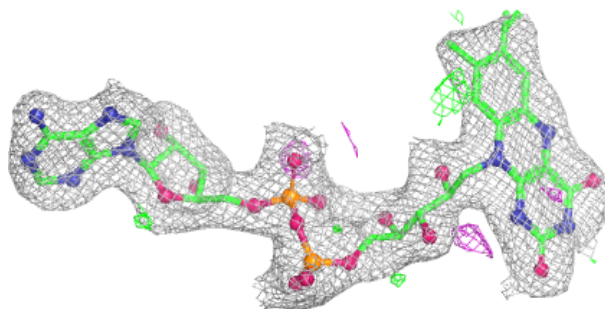
**Electron density around FAD B 389:**

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

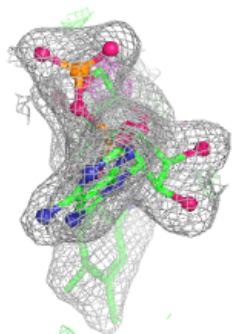
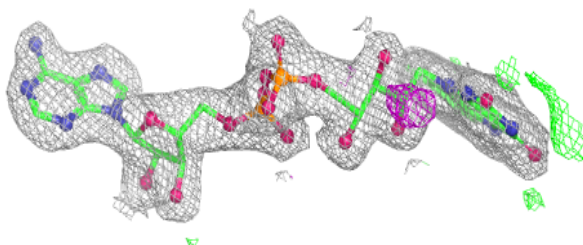
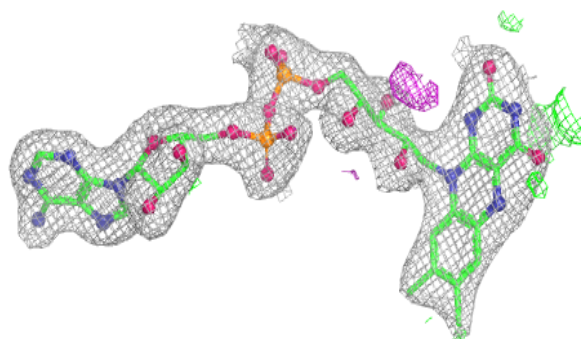


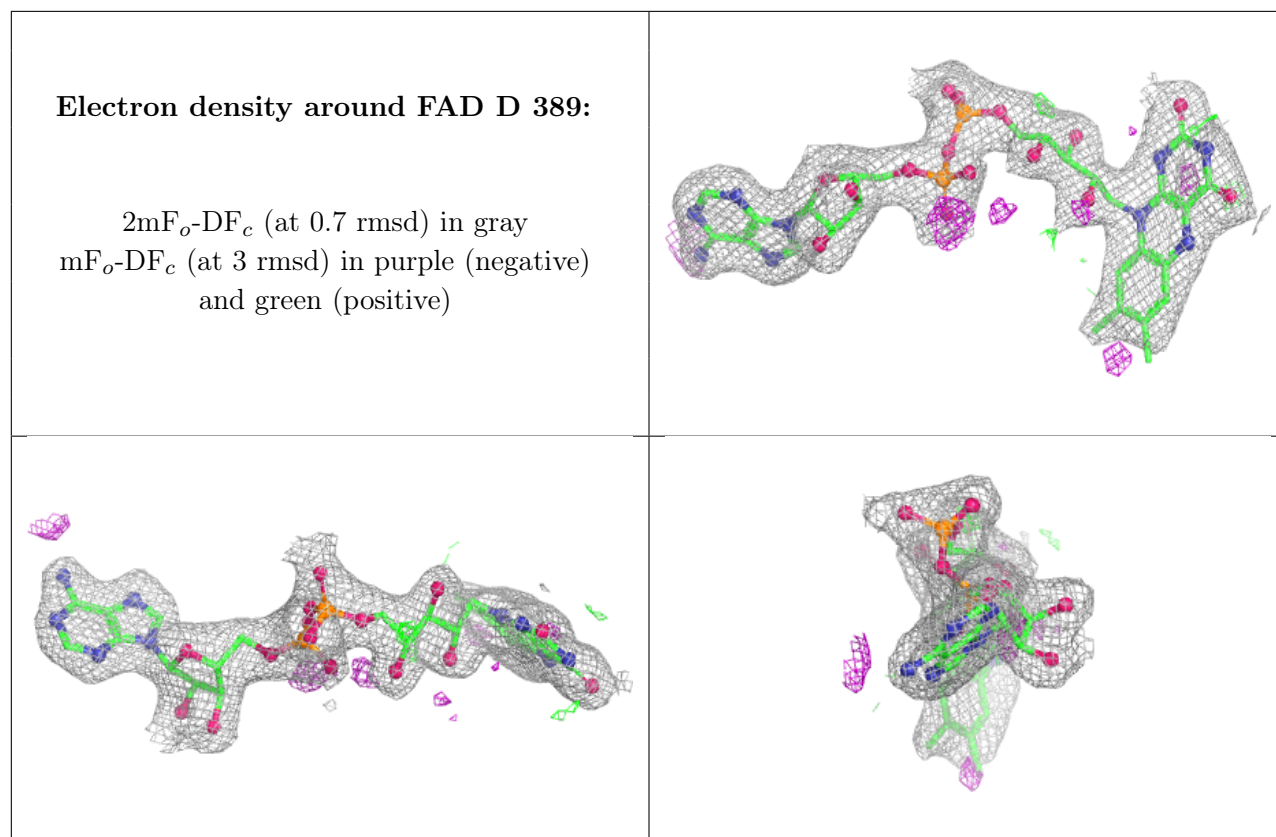
Electron density around FAD C 389:

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

**Electron density around FAD A 389:**

$2mF_o-DF_c$ (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.