



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 07:52 PM BST

PDB ID : 3V3N
Title : Crystal structure of TetX2 T280A: an adaptive mutant in complex with minocycline
Authors : Walkiewicz, K.; Shamoo, Y.
Deposited on : 2011-12-13
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

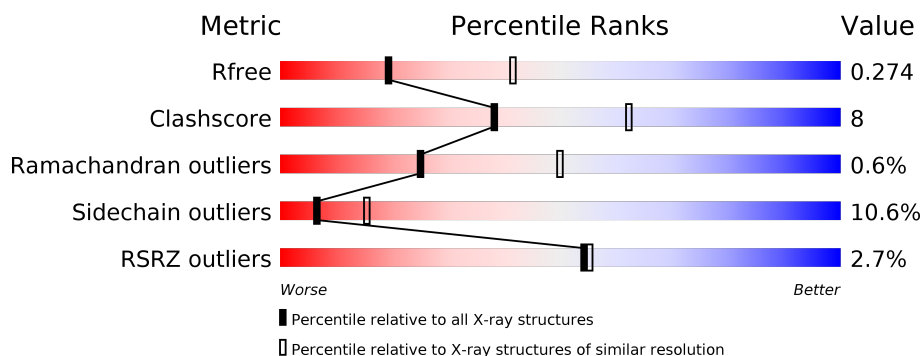
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	378	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>17%</div> <div>• •</div> </div> </div>
1	B	378	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>• •</div> </div> </div>
1	C	378	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>• •</div> </div> </div>
1	D	378	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>17%</div> <div>• •</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	B	2002	-	-	X	-
3	SO4	C	2002	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12093 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.

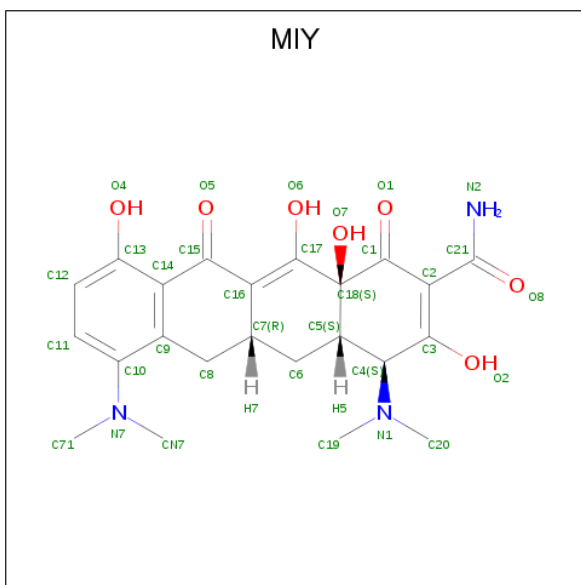
- Molecule 1 is a protein called TetX2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2879	1827	491	549	12			
1	B	368	Total	C	N	O	S	0	0	0
			2900	1840	497	551	12			
1	C	368	Total	C	N	O	S	0	0	0
			2894	1837	494	551	12			
1	D	367	Total	C	N	O	S	0	0	0
			2886	1833	492	549	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	LYS	GLU	ENGINEERED MUTATION	UNP Q93L51
A	266	LYS	GLU	ENGINEERED MUTATION	UNP Q93L51
A	280	ALA	THR	ENGINEERED MUTATION	UNP Q93L51
B	94	LYS	GLU	ENGINEERED MUTATION	UNP Q93L51
B	266	LYS	GLU	ENGINEERED MUTATION	UNP Q93L51
B	280	ALA	THR	ENGINEERED MUTATION	UNP Q93L51
C	94	LYS	GLU	ENGINEERED MUTATION	UNP Q93L51
C	266	LYS	GLU	ENGINEERED MUTATION	UNP Q93L51
C	280	ALA	THR	ENGINEERED MUTATION	UNP Q93L51
D	94	LYS	GLU	ENGINEERED MUTATION	UNP Q93L51
D	266	LYS	GLU	ENGINEERED MUTATION	UNP Q93L51
D	280	ALA	THR	ENGINEERED MUTATION	UNP Q93L51

- Molecule 2 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 (three-letter code: MIY) (formula: C₂₃H₂₇N₃O₇).



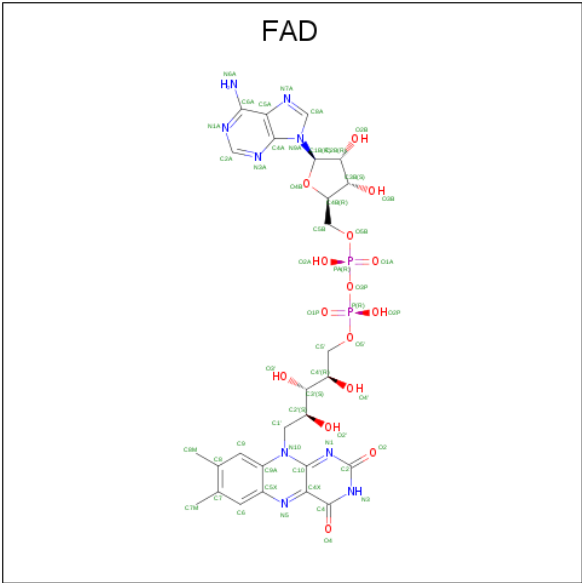
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 33	C 23	N 3	O 7	0	0
2	B	1	Total 33	C 23	N 3	O 7	0	0
2	C	1	Total 33	C 23	N 3	O 7	0	0
2	D	1	Total 33	C 23	N 3	O 7	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

Continued on next page...

Continued from previous page...

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

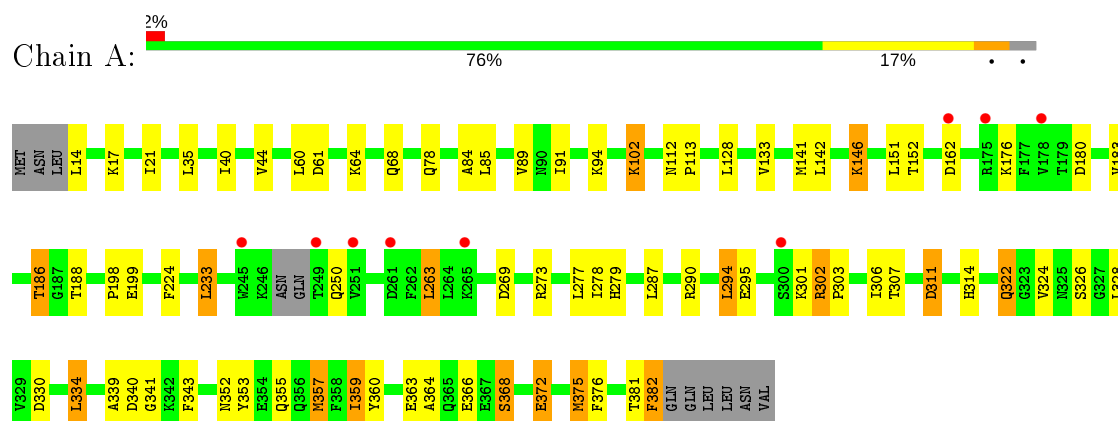
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	29	Total	O	0	0
			29	29		
5	B	50	Total	O	0	0
			50	50		
5	C	39	Total	O	0	0
			39	39		
5	D	32	Total	O	0	0
			32	32		

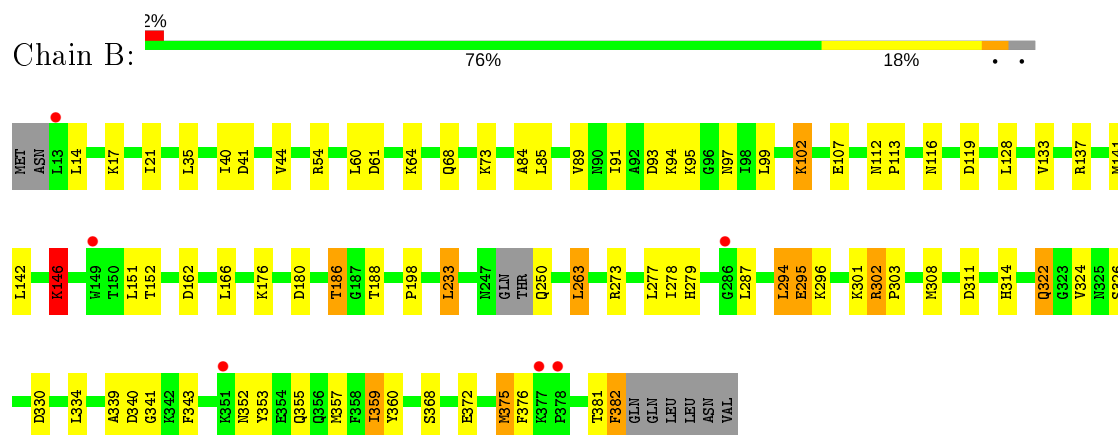
3 Residue-property plots [i](#)

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.

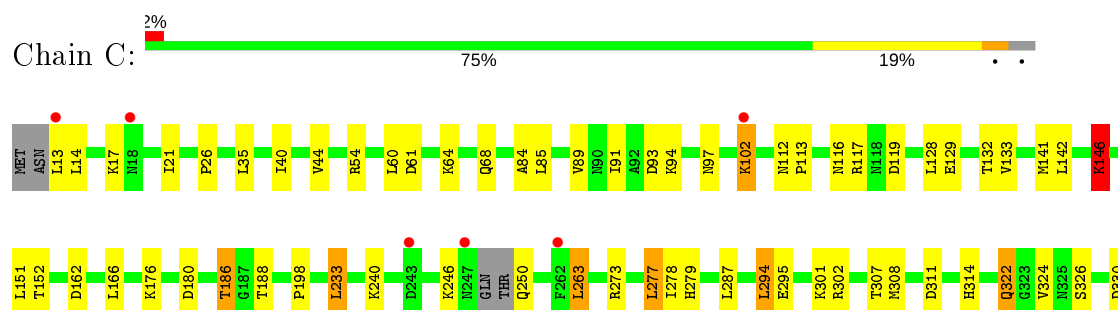
• Molecule 1: TetX2 protein

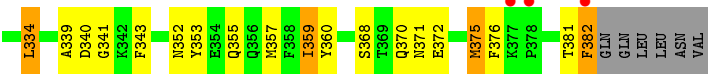


• Molecule 1: TetX2 protein

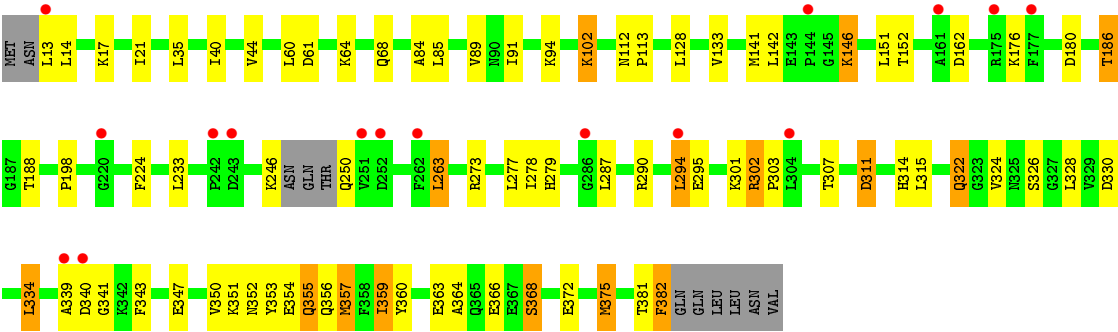
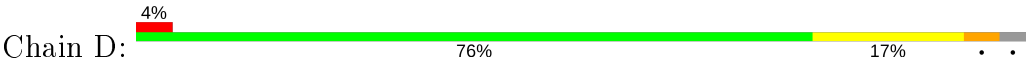


• Molecule 1: TetX2 protein





● 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	68.43 Å 80.10 Å 87.36 Å 111.11° 90.10° 93.01°	Depositor
Resolution (Å)	49.30 – 2.70 49.30 – 2.70	Depositor EDS
% Data completeness (in resolution range)	87.0 (49.30-2.70) 87.1 (49.30-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.57 (at 2.69 Å)	Xtriage
Refinement program	PHENIX 1.7.2 _869	Depositor
R, R_{free}	0.221 , 0.276 0.219 , 0.274	Depositor DCC
R_{free} test set	1997 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12093	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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	0.43	0/2937	0.57	0/3971
1	B	0.45	0/2958	0.58	0/3997
1	C	0.44	0/2952	0.58	1/3990 (0.0%)
1	D	0.43	0/2944	0.57	0/3979
All	All	0.44	0/11791	0.58	1/15937 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	13	LEU	CA-CB-CG	5.02	126.84	115.30

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	2879	0	2828	39	0
1	B	2900	0	2865	40	0
1	C	2894	0	2854	43	0
1	D	2886	0	2848	43	0
2	A	33	0	25	3	0
2	B	33	0	25	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	33	0	25	3	0
2	D	33	0	25	6	0
3	A	10	0	0	0	0
3	B	10	0	0	3	0
3	C	10	0	0	3	0
3	D	10	0	0	0	0
4	A	53	0	31	3	0
4	B	53	0	31	3	0
4	C	53	0	31	3	0
4	D	53	0	31	3	0
5	A	29	0	0	4	0
5	B	50	0	0	3	0
5	C	39	0	0	4	0
5	D	32	0	0	3	0
All	All	12093	0	11619	179	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 8.

All (179) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:GLU:HG3	1:D:359:ILE:HD11	1.51	0.90
1:C:322:GLN:O	5:C:2139:HOH:O	1.89	0.88
1:A:322:GLN:O	5:A:2129:HOH:O	2.07	0.72
1:B:322:GLN:O	5:B:2149:HOH:O	2.11	0.69
1:C:84:ALA:HB1	1:C:113:PRO:HB2	1.74	0.68
1:D:322:GLN:O	5:D:2132:HOH:O	2.11	0.67
1:B:84:ALA:HB1	1:B:113:PRO:HB2	1.75	0.67
1:B:54:ARG:NH1	3:B:2002:SO4:O2	2.31	0.64
1:C:54:ARG:NH1	3:C:2002:SO4:O1	2.31	0.63
1:A:21:ILE:HB	1:A:44:VAL:HG22	1.81	0.61
1:C:314:HIS:NE2	1:C:330:ASP:OD2	2.33	0.60
1:A:343:PHE:HZ	1:A:352:ASN:HD22	1.48	0.60
1:A:263:LEU:HB3	1:A:278:ILE:HD13	1.83	0.59
1:D:84:ALA:HB1	1:D:113:PRO:HB2	1.83	0.59
1:A:78:GLN:HB3	5:A:2116:HOH:O	2.01	0.59
1:B:314:HIS:NE2	1:B:330:ASP:OD2	2.34	0.59
1:A:84:ALA:HB1	1:A:113:PRO:HB2	1.83	0.58
1:A:314:HIS:NE2	1:A:330:ASP:OD2	2.33	0.58
1:B:21:ILE:HB	1:B:44:VAL:HG22	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ASP:OD1	5:B:2126:HOH:O	2.16	0.58
1:D:263:LEU:HB3	1:D:278:ILE:HD13	1.85	0.58
1:C:21:ILE:HB	1:C:44:VAL:HG22	1.85	0.57
1:D:314:HIS:NE2	1:D:330:ASP:OD2	2.34	0.57
1:C:343:PHE:HZ	1:C:352:ASN:HD22	1.51	0.56
1:D:21:ILE:HB	1:D:44:VAL:HG22	1.88	0.56
1:A:269:ASP:HB2	5:A:2125:HOH:O	2.04	0.56
1:A:339:ALA:O	1:A:341:GLY:N	2.39	0.56
2:A:2001:MIY:O6	4:A:2004:FAD:O4	2.24	0.56
1:D:339:ALA:O	1:D:341:GLY:N	2.40	0.55
1:B:343:PHE:HZ	1:B:352:ASN:HD22	1.54	0.55
1:B:91:ILE:HD13	1:B:382:PHE:HB3	1.89	0.55
1:B:95:LYS:HE3	1:C:370:GLN:HG2	1.88	0.55
1:D:343:PHE:HZ	1:D:352:ASN:HD22	1.53	0.55
1:B:64:LYS:HA	1:B:68:GLN:HB2	1.88	0.55
1:C:91:ILE:HD13	1:C:382:PHE:HB3	1.90	0.54
1:A:198:PRO:HB3	1:A:233:LEU:HB2	1.90	0.54
1:C:339:ALA:O	1:C:341:GLY:N	2.40	0.54
1:B:339:ALA:O	1:B:341:GLY:N	2.40	0.54
1:D:198:PRO:HB3	1:D:233:LEU:HB2	1.90	0.54
1:A:64:LYS:HA	1:A:68:GLN:HB2	1.90	0.54
1:D:64:LYS:HA	1:D:68:GLN:HB2	1.90	0.54
1:B:263:LEU:HB3	1:B:278:ILE:HD13	1.90	0.53
1:C:54:ARG:NH1	3:C:2002:SO4:S	2.82	0.53
4:C:2004:FAD:H2'	4:C:2004:FAD:N1	2.22	0.53
1:C:186:THR:HG22	1:C:188:THR:H	1.74	0.52
1:C:54:ARG:NH1	3:C:2002:SO4:O3	2.42	0.52
1:A:60:LEU:HD13	1:A:324:VAL:HG21	1.90	0.52
4:D:2004:FAD:N1	4:D:2004:FAD:H2'	2.23	0.52
1:C:64:LYS:HA	1:C:68:GLN:HB2	1.90	0.52
1:C:198:PRO:HB3	1:C:233:LEU:HB2	1.92	0.52
1:D:91:ILE:HD13	1:D:382:PHE:HB3	1.92	0.52
1:B:180:ASP:N	1:B:180:ASP:OD1	2.42	0.51
1:C:263:LEU:HB3	1:C:278:ILE:HD13	1.93	0.51
1:D:61:ASP:HB2	1:D:112:ASN:HB2	1.92	0.50
1:A:61:ASP:HB2	1:A:112:ASN:HB2	1.92	0.50
1:D:186:THR:HG22	1:D:188:THR:H	1.75	0.50
1:B:60:LEU:HD13	1:B:324:VAL:HG21	1.93	0.50
1:A:180:ASP:OD1	1:A:180:ASP:N	2.42	0.50
1:D:186:THR:N	5:D:2102:HOH:O	2.45	0.50
1:A:186:THR:N	5:A:2102:HOH:O	2.40	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:MET:HB3	1:A:152:THR:HB	1.94	0.49
1:C:102:LYS:HB2	1:C:102:LYS:NZ	2.27	0.49
1:C:60:LEU:HD13	1:C:324:VAL:HG21	1.94	0.49
1:B:186:THR:HG22	1:B:188:THR:H	1.78	0.49
1:A:186:THR:HG22	1:A:188:THR:H	1.77	0.49
1:C:180:ASP:OD1	1:C:180:ASP:N	2.43	0.49
1:D:60:LEU:HD13	1:D:324:VAL:HG21	1.93	0.49
1:D:141:MET:HB3	1:D:152:THR:HB	1.95	0.48
1:B:198:PRO:HB3	1:B:233:LEU:HB2	1.95	0.48
1:A:343:PHE:HZ	1:A:352:ASN:ND2	2.09	0.48
1:B:61:ASP:HB2	1:B:112:ASN:HB2	1.93	0.48
1:C:343:PHE:HZ	1:C:352:ASN:ND2	2.11	0.48
1:A:91:ILE:HD13	1:A:382:PHE:HB3	1.95	0.48
1:C:166:LEU:HB2	1:C:308:MET:HG2	1.97	0.47
1:C:117:ARG:NH2	4:C:2004:FAD:O2'	2.32	0.47
1:B:141:MET:HB3	1:B:152:THR:HB	1.96	0.47
1:D:343:PHE:HZ	1:D:352:ASN:ND2	2.11	0.47
2:B:2001:MIY:O5	2:B:2001:MIY:O6	2.32	0.47
2:D:2001:MIY:H193	2:D:2001:MIY:O2	2.13	0.47
1:A:142:LEU:CD2	1:A:151:LEU:HD23	2.45	0.47
1:C:61:ASP:HB2	1:C:112:ASN:HB2	1.95	0.47
1:D:180:ASP:N	1:D:180:ASP:OD1	2.45	0.47
1:C:359:ILE:HG12	1:C:360:TYR:N	2.30	0.47
1:D:142:LEU:CD2	1:D:151:LEU:HD23	2.45	0.47
1:D:357:MET:HG2	5:D:2131:HOH:O	2.15	0.47
1:A:35:LEU:HD22	1:A:40:ILE:HD12	1.96	0.46
1:A:294:LEU:HD21	1:A:314:HIS:HB3	1.96	0.46
1:C:141:MET:HB3	1:C:152:THR:HB	1.97	0.46
1:D:102:LYS:HB2	1:D:102:LYS:NZ	2.30	0.46
4:A:2004:FAD:H2'	4:A:2004:FAD:N1	2.30	0.46
4:B:2004:FAD:N1	4:B:2004:FAD:H2'	2.29	0.46
1:A:302:ARG:NH2	1:A:306:ILE:O	2.48	0.46
1:B:54:ARG:NH1	3:B:2002:SO4:S	2.89	0.46
2:C:2001:MIY:O2	2:C:2001:MIY:O8	2.33	0.46
1:B:294:LEU:HD21	1:B:314:HIS:HB3	1.98	0.45
1:A:102:LYS:NZ	1:A:102:LYS:HB2	2.31	0.45
1:A:44:VAL:HB	1:A:133:VAL:HG22	1.99	0.45
1:B:295:GLU:HB2	1:B:296:LYS:H	1.57	0.45
1:D:357:MET:HA	1:D:360:TYR:CE2	2.51	0.45
4:B:2004:FAD:H9	4:B:2004:FAD:H1'1	1.80	0.45
1:C:26:PRO:HG3	5:C:2118:HOH:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:311:ASP:HB2	4:D:2004:FAD:O2P	2.17	0.45
1:D:359:ILE:HG12	1:D:360:TYR:N	2.32	0.45
1:D:224:PHE:CD1	2:D:2001:MIY:H4	2.50	0.45
1:D:307:THR:HG21	1:D:334:LEU:HD11	1.98	0.45
1:D:35:LEU:HD22	1:D:40:ILE:HD12	1.98	0.45
1:A:302:ARG:HA	1:A:303:PRO:HD3	1.80	0.45
1:B:372:GLU:O	1:B:376:PHE:HD2	2.00	0.45
1:C:116:ASN:HB3	1:C:119:ASP:OD2	2.16	0.45
1:D:328:LEU:HA	1:D:328:LEU:HD23	1.82	0.45
1:B:146:LYS:H	1:B:146:LYS:HG3	1.52	0.44
1:A:328:LEU:HD23	1:A:328:LEU:HA	1.83	0.44
1:B:343:PHE:HZ	1:B:352:ASN:ND2	2.15	0.44
1:B:102:LYS:NZ	1:B:102:LYS:HB2	2.31	0.44
2:D:2001:MIY:H5	2:D:2001:MIY:H203	1.70	0.44
1:D:302:ARG:HA	1:D:303:PRO:HD3	1.80	0.44
1:D:375:MET:HG2	1:D:375:MET:H	1.50	0.44
1:B:17:LYS:HB3	1:B:162:ASP:CG	2.38	0.44
1:C:186:THR:N	5:C:2102:HOH:O	2.47	0.44
2:D:2001:MIY:O6	4:D:2004:FAD:O4	2.36	0.44
2:B:2001:MIY:O6	4:B:2004:FAD:O4	2.36	0.44
1:C:17:LYS:HB3	1:C:162:ASP:CG	2.38	0.44
1:C:93:ASP:OD2	1:C:97:ASN:ND2	2.50	0.43
1:D:294:LEU:HD21	1:D:314:HIS:HB3	1.99	0.43
1:B:166:LEU:HB2	1:B:308:MET:HG2	2.01	0.43
1:D:290:ARG:HB2	1:D:315:LEU:HD21	2.00	0.43
1:C:142:LEU:HD23	1:C:142:LEU:HA	1.83	0.43
2:A:2001:MIY:O5	2:A:2001:MIY:O6	2.33	0.43
2:D:2001:MIY:O5	2:D:2001:MIY:O6	2.37	0.43
1:A:359:ILE:HG12	1:A:360:TYR:N	2.34	0.43
1:B:359:ILE:HG12	1:B:360:TYR:N	2.34	0.43
1:B:302:ARG:HA	1:B:303:PRO:HD3	1.81	0.43
1:C:263:LEU:HA	1:C:263:LEU:HD12	1.81	0.43
1:B:116:ASN:HB3	1:B:119:ASP:OD2	2.19	0.43
1:D:356:GLN:HA	1:D:359:ILE:HD13	2.01	0.43
1:A:363:GLU:O	1:A:366:GLU:HB2	2.19	0.42
1:B:107:GLU:HG3	1:D:359:ILE:CD1	2.35	0.42
1:B:375:MET:H	1:B:375:MET:HG2	1.51	0.42
2:C:2001:MIY:H192	4:C:2004:FAD:H6	2.00	0.42
1:B:44:VAL:HB	1:B:133:VAL:HG22	2.02	0.42
1:C:372:GLU:O	1:C:376:PHE:HD2	2.02	0.42
1:A:364:ALA:O	1:A:368:SER:OG	2.37	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:LYS:HG3	1:C:146:LYS:H	1.54	0.42
1:C:307:THR:HG21	1:C:334:LEU:HD11	2.00	0.42
1:A:311:ASP:OD1	4:A:2004:FAD:O3'	2.28	0.42
1:A:375:MET:H	1:A:375:MET:HG2	1.52	0.42
1:D:351:LYS:HE2	1:D:355:GLN:OE1	2.19	0.42
1:A:224:PHE:CD1	2:A:2001:MIY:H4	2.54	0.42
1:D:64:LYS:H	1:D:64:LYS:HG2	1.62	0.42
1:B:137:ARG:NH1	3:B:2003:SO4:O3	2.44	0.42
1:B:142:LEU:CD2	1:B:151:LEU:HD23	2.49	0.42
1:C:44:VAL:HB	1:C:133:VAL:HG22	2.02	0.42
1:C:240:LYS:HG3	5:C:2111:HOH:O	2.19	0.42
1:C:35:LEU:HD22	1:C:40:ILE:HD12	2.01	0.41
2:C:2001:MIY:H712	2:C:2001:MIY:H11	1.81	0.41
1:D:364:ALA:O	1:D:368:SER:OG	2.39	0.41
1:B:35:LEU:HD22	1:B:40:ILE:HD12	2.01	0.41
1:C:294:LEU:HD21	1:C:314:HIS:HB3	2.02	0.41
1:C:84:ALA:CB	1:C:113:PRO:HB2	2.46	0.41
1:D:44:VAL:HB	1:D:133:VAL:HG22	2.03	0.41
1:A:307:THR:HG21	1:A:334:LEU:HD11	2.02	0.41
1:A:357:MET:HA	1:A:360:TYR:CE2	2.55	0.41
1:A:372:GLU:O	1:A:376:PHE:HD2	2.03	0.41
1:D:17:LYS:HB3	1:D:162:ASP:CG	2.40	0.41
1:A:183:VAL:HG11	1:A:290:ARG:HD3	2.03	0.41
1:C:129:GLU:O	1:C:132:THR:OG1	2.28	0.41
1:C:142:LEU:CD2	1:C:151:LEU:HD23	2.50	0.41
1:D:350:VAL:O	1:D:354:GLU:HG3	2.21	0.41
1:D:363:GLU:O	1:D:366:GLU:HB2	2.21	0.41
1:C:233:LEU:HD22	1:C:277:LEU:HD21	2.03	0.40
1:D:347:GLU:N	1:D:347:GLU:OE1	2.52	0.40
1:D:357:MET:HA	1:D:360:TYR:CZ	2.56	0.40
1:A:17:LYS:HB3	1:A:162:ASP:CG	2.41	0.40
1:B:84:ALA:CB	1:B:113:PRO:HB2	2.46	0.40
1:B:73:LYS:NZ	5:B:2116:HOH:O	2.54	0.40
1:A:199:GLU:OE1	1:A:199:GLU:N	2.30	0.40
1:B:93:ASP:OD2	1:B:97:ASN:ND2	2.51	0.40
1:C:375:MET:H	1:C:375:MET:HG2	1.51	0.40
2:D:2001:MIY:H712	2:D:2001:MIY:H11	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	363/378 (96%)	335 (92%)	26 (7%)	2 (1%)	25	50
1	B	364/378 (96%)	334 (92%)	28 (8%)	2 (0%)	29	54
1	C	364/378 (96%)	334 (92%)	27 (7%)	3 (1%)	19	43
1	D	363/378 (96%)	334 (92%)	27 (7%)	2 (1%)	25	50
All	All	1454/1512 (96%)	1337 (92%)	108 (7%)	9 (1%)	25	50

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	ASP
1	B	340	ASP
1	C	340	ASP
1	D	340	ASP
1	A	146	LYS
1	C	146	LYS
1	D	146	LYS
1	B	146	LYS
1	C	246	LYS

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	311/327 (95%)	278 (89%)	33 (11%)	6	15
1	B	315/327 (96%)	282 (90%)	33 (10%)	7	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	314/327 (96%)	281 (90%)	33 (10%)	7	16
1	D	313/327 (96%)	279 (89%)	34 (11%)	6	14
All	All	1253/1308 (96%)	1120 (89%)	133 (11%)	6	15

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	85	LEU
1	A	89	VAL
1	A	94	LYS
1	A	102	LYS
1	A	128	LEU
1	A	146	LYS
1	A	176	LYS
1	A	186	THR
1	A	233	LEU
1	A	250	GLN
1	A	263	LEU
1	A	273	ARG
1	A	277	LEU
1	A	279	HIS
1	A	287	LEU
1	A	294	LEU
1	A	295	GLU
1	A	301	LYS
1	A	302	ARG
1	A	311	ASP
1	A	322	GLN
1	A	326	SER
1	A	334	LEU
1	A	353	TYR
1	A	355	GLN
1	A	357	MET
1	A	359	ILE
1	A	368	SER
1	A	372	GLU
1	A	375	MET
1	A	381	THR
1	A	382	PHE
1	B	14	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	85	LEU
1	B	89	VAL
1	B	94	LYS
1	B	99	LEU
1	B	102	LYS
1	B	128	LEU
1	B	146	LYS
1	B	176	LYS
1	B	186	THR
1	B	233	LEU
1	B	250	GLN
1	B	263	LEU
1	B	273	ARG
1	B	277	LEU
1	B	279	HIS
1	B	287	LEU
1	B	294	LEU
1	B	295	GLU
1	B	301	LYS
1	B	302	ARG
1	B	311	ASP
1	B	322	GLN
1	B	326	SER
1	B	334	LEU
1	B	353	TYR
1	B	355	GLN
1	B	357	MET
1	B	359	ILE
1	B	368	SER
1	B	375	MET
1	B	381	THR
1	B	382	PHE
1	C	14	LEU
1	C	85	LEU
1	C	89	VAL
1	C	94	LYS
1	C	102	LYS
1	C	128	LEU
1	C	146	LYS
1	C	176	LYS
1	C	186	THR
1	C	233	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	250	GLN
1	C	263	LEU
1	C	273	ARG
1	C	277	LEU
1	C	279	HIS
1	C	287	LEU
1	C	294	LEU
1	C	295	GLU
1	C	301	LYS
1	C	302	ARG
1	C	311	ASP
1	C	322	GLN
1	C	326	SER
1	C	334	LEU
1	C	353	TYR
1	C	355	GLN
1	C	357	MET
1	C	359	ILE
1	C	368	SER
1	C	371	ASN
1	C	375	MET
1	C	381	THR
1	C	382	PHE
1	D	13	LEU
1	D	14	LEU
1	D	85	LEU
1	D	89	VAL
1	D	94	LYS
1	D	102	LYS
1	D	128	LEU
1	D	146	LYS
1	D	176	LYS
1	D	186	THR
1	D	246	LYS
1	D	250	GLN
1	D	263	LEU
1	D	273	ARG
1	D	277	LEU
1	D	279	HIS
1	D	287	LEU
1	D	294	LEU
1	D	295	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	301	LYS
1	D	302	ARG
1	D	311	ASP
1	D	322	GLN
1	D	326	SER
1	D	334	LEU
1	D	353	TYR
1	D	355	GLN
1	D	357	MET
1	D	359	ILE
1	D	368	SER
1	D	372	GLU
1	D	375	MET
1	D	381	THR
1	D	382	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	322	GLN
1	A	371	ASN
1	B	234	HIS
1	B	322	GLN
1	C	322	GLN
1	D	322	GLN
1	D	371	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

16 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
2	MIY	B	2001	-	35,36,36	2.12	8 (22%)	41,58,58	1.68	9 (21%)
2	MIY	A	2001	-	35,36,36	2.06	6 (17%)	41,58,58	1.51	4 (9%)
4	FAD	D	2004	-	51,58,58	1.79	5 (9%)	60,89,89	2.04	14 (23%)
2	MIY	D	2001	-	35,36,36	1.89	5 (14%)	41,58,58	1.70	8 (19%)
4	FAD	B	2004	-	51,58,58	1.82	8 (15%)	60,89,89	2.30	15 (25%)
3	SO4	A	2003	-	4,4,4	0.21	0	6,6,6	0.16	0
3	SO4	C	2003	-	4,4,4	0.13	0	6,6,6	0.19	0
3	SO4	D	2002	-	4,4,4	0.15	0	6,6,6	0.21	0
3	SO4	C	2002	-	4,4,4	0.13	0	6,6,6	0.25	0
3	SO4	B	2002	-	4,4,4	0.16	0	6,6,6	0.12	0
3	SO4	A	2002	-	4,4,4	0.16	0	6,6,6	0.15	0
3	SO4	B	2003	-	4,4,4	0.10	0	6,6,6	0.43	0
3	SO4	D	2003	-	4,4,4	0.14	0	6,6,6	0.12	0
4	FAD	A	2004	-	51,58,58	1.76	6 (11%)	60,89,89	2.02	11 (18%)
4	FAD	C	2004	-	51,58,58	1.83	6 (11%)	60,89,89	2.28	18 (30%)
2	MIY	C	2001	-	35,36,36	2.04	5 (14%)	41,58,58	1.58	10 (24%)

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
2	MIY	B	2001	-	-	2/12/70/70	0/4/4/4
2	MIY	A	2001	-	-	0/12/70/70	0/4/4/4
4	FAD	D	2004	-	-	10/30/50/50	0/6/6/6
2	MIY	D	2001	-	-	5/12/70/70	0/4/4/4
4	FAD	B	2004	-	-	7/30/50/50	0/6/6/6
4	FAD	A	2004	-	-	7/30/50/50	0/6/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FAD	C	2004	-	-	4/30/50/50	0/6/6/6
2	MIY	C	2001	-	-	1/12/70/70	0/4/4/4

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2004	FAD	C4X-C10	9.24	1.48	1.38
4	D	2004	FAD	C4X-C10	9.08	1.47	1.38
4	A	2004	FAD	C4X-C10	8.91	1.47	1.38
4	B	2004	FAD	C4X-C10	8.81	1.47	1.38
2	C	2001	MIY	C10-C9	7.86	1.50	1.40
2	A	2001	MIY	C10-C9	7.46	1.50	1.40
2	B	2001	MIY	C10-C9	7.24	1.49	1.40
2	D	2001	MIY	C10-C9	6.80	1.49	1.40
2	A	2001	MIY	C14-C13	5.58	1.50	1.41
2	B	2001	MIY	C14-C13	5.11	1.49	1.41
2	D	2001	MIY	C14-C13	4.99	1.49	1.41
2	C	2001	MIY	C14-C13	4.86	1.49	1.41
2	A	2001	MIY	C14-C9	4.56	1.48	1.40
2	C	2001	MIY	C14-C9	4.42	1.48	1.40
2	B	2001	MIY	C18-C1	-4.39	1.49	1.55
2	B	2001	MIY	C14-C9	4.32	1.48	1.40
4	C	2004	FAD	C9A-C5X	4.24	1.51	1.42
4	B	2004	FAD	C9A-C5X	4.24	1.51	1.42
2	D	2001	MIY	C14-C9	4.21	1.48	1.40
2	A	2001	MIY	C18-C1	-4.09	1.49	1.55
4	A	2004	FAD	C9A-C5X	3.85	1.50	1.42
4	D	2004	FAD	C4-C4X	3.83	1.48	1.41
2	D	2001	MIY	C18-C1	-3.82	1.50	1.55
2	C	2001	MIY	C18-C1	-3.76	1.50	1.55
4	D	2004	FAD	C9A-C5X	3.63	1.49	1.42
4	B	2004	FAD	C4-C4X	3.34	1.47	1.41
4	D	2004	FAD	C8-C7	3.24	1.49	1.40
4	A	2004	FAD	C8-C7	3.22	1.48	1.40
2	B	2001	MIY	C16-C17	-3.15	1.32	1.36
4	B	2004	FAD	C8-C7	3.07	1.48	1.40
4	C	2004	FAD	C9A-N10	3.02	1.42	1.38
2	A	2001	MIY	C2-C3	-2.85	1.33	1.40
4	A	2004	FAD	C4-C4X	2.83	1.46	1.41
2	D	2001	MIY	C2-C3	-2.72	1.33	1.40
2	C	2001	MIY	C2-C3	-2.61	1.33	1.40
2	B	2001	MIY	C18-C17	-2.51	1.49	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2004	FAD	C8-C7	2.46	1.47	1.40
2	B	2001	MIY	C2-C3	-2.36	1.34	1.40
4	A	2004	FAD	C9A-N10	2.34	1.41	1.38
4	B	2004	FAD	C9A-N10	2.32	1.41	1.38
4	C	2004	FAD	C5A-C4A	2.26	1.46	1.40
4	D	2004	FAD	C5A-C4A	2.25	1.46	1.40
4	C	2004	FAD	C2-N3	-2.20	1.33	1.38
4	B	2004	FAD	C4X-N5	2.16	1.36	1.33
4	A	2004	FAD	C5A-C4A	2.12	1.46	1.40
2	A	2001	MIY	C16-C17	-2.09	1.33	1.36
2	B	2001	MIY	C7-C16	-2.06	1.49	1.51
4	B	2004	FAD	C2A-N3A	2.04	1.35	1.32
4	B	2004	FAD	C5A-C4A	2.01	1.46	1.40

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2004	FAD	C4-N3-C2	9.41	123.08	115.14
4	B	2004	FAD	C4-N3-C2	9.10	122.83	115.14
4	D	2004	FAD	C4-N3-C2	8.26	122.11	115.14
4	B	2004	FAD	C4-C4X-C10	-8.07	114.61	119.95
4	A	2004	FAD	C4-N3-C2	8.00	121.89	115.14
4	D	2004	FAD	C4-C4X-C10	-6.38	115.73	119.95
4	C	2004	FAD	C4-C4X-C10	-5.24	116.48	119.95
4	A	2004	FAD	C5'-C4'-C3'	-4.95	102.65	112.20
2	D	2001	MIY	C1-C18-C17	-4.88	104.17	109.88
4	C	2004	FAD	C5'-C4'-C3'	-4.83	102.87	112.20
4	A	2004	FAD	C4-C4X-C10	-4.73	116.82	119.95
4	B	2004	FAD	C5'-C4'-C3'	-4.54	103.44	112.20
2	A	2001	MIY	O6-C17-C16	-4.37	117.92	123.90
2	D	2001	MIY	O6-C17-C16	-4.27	118.05	123.90
4	B	2004	FAD	C1'-N10-C9A	4.14	121.55	118.29
4	B	2004	FAD	C4-C4X-N5	3.94	123.11	118.60
4	C	2004	FAD	O4'-C4'-C5'	3.88	118.63	109.92
4	C	2004	FAD	N3A-C2A-N1A	-3.87	122.62	128.68
4	D	2004	FAD	C4X-N5-C5X	3.80	120.56	116.77
2	C	2001	MIY	O6-C17-C16	-3.77	118.73	123.90
4	D	2004	FAD	N3A-C2A-N1A	-3.69	122.91	128.68
4	A	2004	FAD	C1'-N10-C9A	3.67	121.18	118.29
2	C	2001	MIY	C18-C5-C4	3.65	116.63	111.64
4	A	2004	FAD	C4X-N5-C5X	3.65	120.41	116.77
4	C	2004	FAD	C1B-N9A-C4A	-3.63	120.27	126.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2004	FAD	N3A-C2A-N1A	-3.57	123.10	128.68
2	B	2001	MIY	C1-C18-C17	-3.52	105.76	109.88
4	B	2004	FAD	N3A-C2A-N1A	-3.44	123.31	128.68
2	A	2001	MIY	O6-C17-C18	3.40	118.29	113.37
2	B	2001	MIY	O6-C17-C16	-3.39	119.26	123.90
2	B	2001	MIY	C5-C18-C1	-3.36	107.19	111.05
2	C	2001	MIY	C1-C18-C17	-3.35	105.96	109.88
4	D	2004	FAD	C4-C4X-N5	3.30	122.37	118.60
4	C	2004	FAD	C10-C4X-N5	3.23	123.49	121.26
4	C	2004	FAD	C1'-N10-C10	3.22	121.29	118.41
4	B	2004	FAD	C4A-C5A-N7A	-3.16	106.11	109.40
4	B	2004	FAD	C4X-N5-C5X	3.14	119.91	116.77
2	B	2001	MIY	C11-C12-C13	3.13	123.72	120.50
4	C	2004	FAD	C4X-C4-N3	-3.12	119.17	123.43
4	A	2004	FAD	C4X-C4-N3	-3.09	119.21	123.43
2	B	2001	MIY	C18-C5-C4	3.03	115.78	111.64
4	D	2004	FAD	C4X-C4-N3	-3.00	119.33	123.43
4	A	2004	FAD	C9A-N10-C10	-2.98	118.00	121.91
4	D	2004	FAD	C5X-C9A-N10	2.98	119.87	117.72
4	C	2004	FAD	C1'-N10-C9A	2.95	120.61	118.29
4	D	2004	FAD	C1'-N10-C9A	2.92	120.59	118.29
4	C	2004	FAD	C9A-N10-C10	-2.91	118.10	121.91
2	D	2001	MIY	O6-C17-C18	2.87	117.52	113.37
4	C	2004	FAD	C4X-N5-C5X	2.86	119.63	116.77
4	C	2004	FAD	C5X-C9A-N10	2.85	119.78	117.72
2	B	2001	MIY	O6-C17-C18	2.81	117.44	113.37
2	C	2001	MIY	C71-N7-CN7	-2.75	107.26	116.12
2	A	2001	MIY	C71-N7-CN7	-2.74	107.30	116.12
4	C	2004	FAD	C4A-C5A-N7A	-2.72	106.57	109.40
4	A	2004	FAD	C1'-N10-C10	2.67	120.80	118.41
4	B	2004	FAD	C4X-C4-N3	-2.67	119.78	123.43
4	C	2004	FAD	O5'-C5'-C4'	2.61	116.32	109.36
4	D	2004	FAD	C1'-N10-C10	2.57	120.71	118.41
4	A	2004	FAD	C5X-C9A-N10	2.53	119.55	117.72
4	D	2004	FAD	C1B-N9A-C4A	-2.53	122.19	126.64
2	B	2001	MIY	C71-N7-CN7	-2.48	108.12	116.12
2	D	2001	MIY	C21-C2-C1	-2.48	118.03	120.97
4	D	2004	FAD	C9A-N10-C10	-2.48	118.66	121.91
2	C	2001	MIY	O6-C17-C18	2.46	116.92	113.37
4	D	2004	FAD	C2A-N1A-C6A	2.43	122.91	118.75
4	B	2004	FAD	P-O3P-PA	-2.41	124.55	132.83
4	B	2004	FAD	C1B-N9A-C4A	-2.41	122.41	126.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2001	MIY	C11-C12-C13	2.37	122.94	120.50
4	D	2004	FAD	C4'-C3'-C2'	-2.32	108.53	113.36
2	C	2001	MIY	C9-C10-N7	2.32	121.74	118.91
4	B	2004	FAD	C9A-N10-C10	-2.27	118.94	121.91
4	C	2004	FAD	C8M-C8-C7	-2.24	116.15	120.74
2	C	2001	MIY	O7-C18-C17	-2.22	106.59	110.14
4	C	2004	FAD	C2A-N1A-C6A	2.21	122.54	118.75
4	C	2004	FAD	C7M-C7-C8	-2.19	116.24	120.74
2	D	2001	MIY	O7-C18-C5	-2.18	107.42	110.09
2	D	2001	MIY	C11-C12-C13	2.17	122.73	120.50
2	D	2001	MIY	C18-C1-C2	2.16	119.18	115.75
4	B	2004	FAD	C7M-C7-C8	-2.16	116.32	120.74
4	B	2004	FAD	C5X-C9A-N10	2.15	119.27	117.72
4	A	2004	FAD	C5B-C4B-C3B	-2.15	107.14	115.18
2	C	2001	MIY	O2-C3-C2	-2.12	119.23	122.96
2	C	2001	MIY	O8-C21-C2	-2.11	117.05	120.67
4	B	2004	FAD	O4'-C4'-C5'	2.07	114.56	109.92
2	D	2001	MIY	C18-C5-C4	2.06	114.46	111.64
4	D	2004	FAD	C5'-C4'-C3'	-2.06	108.22	112.20
2	B	2001	MIY	C21-C2-C1	-2.05	118.54	120.97
2	A	2001	MIY	C71-N7-C10	-2.05	108.83	115.17
2	B	2001	MIY	C9-C10-N7	2.03	121.39	118.91

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2004	FAD	C2'-C1'-N10-C9A
4	D	2004	FAD	C3'-C4'-C5'-O5'
4	D	2004	FAD	O4'-C4'-C5'-O5'
4	D	2004	FAD	C5'-O5'-P-O1P
2	D	2001	MIY	C1-C2-C21-O8
2	D	2001	MIY	C3-C2-C21-O8
2	D	2001	MIY	C3-C2-C21-N2
2	D	2001	MIY	C5-C4-N1-C20
4	B	2004	FAD	C5B-O5B-PA-O1A
4	B	2004	FAD	O4'-C4'-C5'-O5'
4	A	2004	FAD	C5B-O5B-PA-O3P
4	A	2004	FAD	C3B-C4B-C5B-O5B
4	A	2004	FAD	C2'-C1'-N10-C9A
4	C	2004	FAD	C2'-C1'-N10-C9A
4	C	2004	FAD	C2'-C1'-N10-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	2001	MIY	C5-C4-N1-C20
4	B	2004	FAD	O4B-C4B-C5B-O5B
4	D	2004	FAD	O4B-C4B-C5B-O5B
4	B	2004	FAD	C3B-C4B-C5B-O5B
4	A	2004	FAD	O4B-C4B-C5B-O5B
4	C	2004	FAD	O4'-C4'-C5'-O5'
4	D	2004	FAD	C3B-C4B-C5B-O5B
4	D	2004	FAD	PA-O3P-P-O5'
4	A	2004	FAD	P-O3P-PA-O5B
4	B	2004	FAD	C5B-O5B-PA-O3P
4	D	2004	FAD	P-O3P-PA-O2A
2	B	2001	MIY	C3-C2-C21-N2
4	B	2004	FAD	C5B-O5B-PA-O2A
4	B	2004	FAD	C3'-C4'-C5'-O5'
4	A	2004	FAD	C5B-O5B-PA-O2A
2	D	2001	MIY	C1-C2-C21-N2
4	D	2004	FAD	P-O3P-PA-O1A
4	A	2004	FAD	O4'-C4'-C5'-O5'
4	D	2004	FAD	C5'-O5'-P-O3P
4	C	2004	FAD	O4B-C4B-C5B-O5B
2	B	2001	MIY	C5-C4-N1-C20

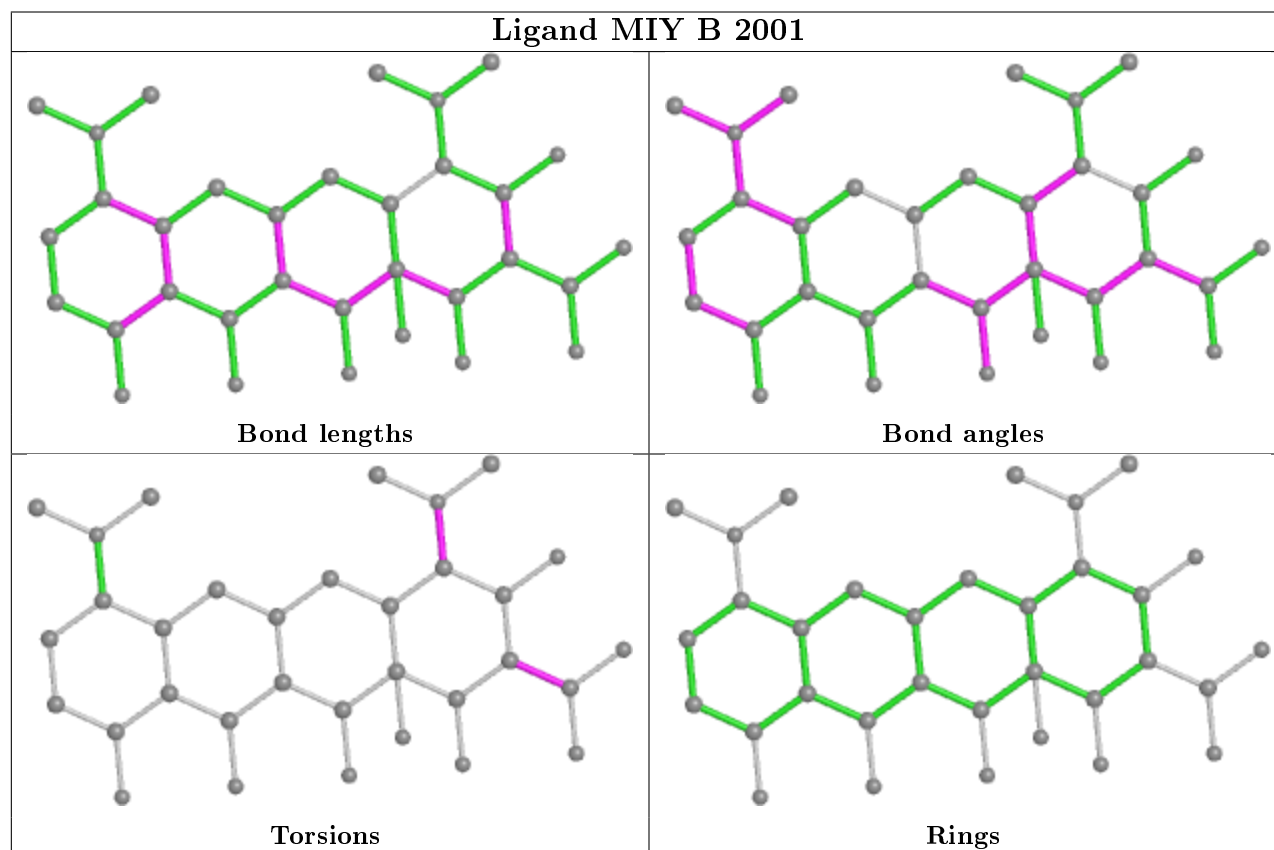
There are no ring outliers.

11 monomers are involved in 28 short contacts:

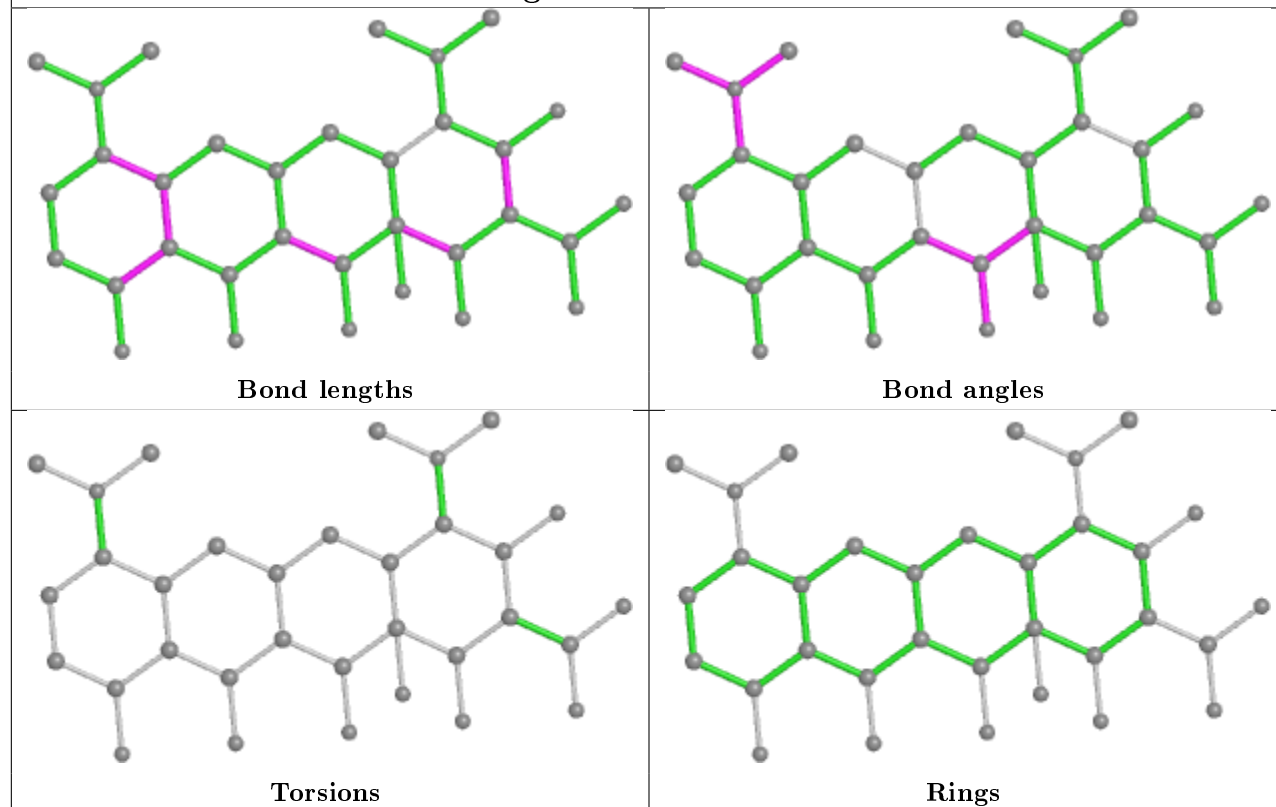
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	MIY	2	0
2	A	2001	MIY	3	0
4	D	2004	FAD	3	0
2	D	2001	MIY	6	0
4	B	2004	FAD	3	0
3	C	2002	SO4	3	0
3	B	2002	SO4	2	0
3	B	2003	SO4	1	0
4	A	2004	FAD	3	0
4	C	2004	FAD	3	0
2	C	2001	MIY	3	0

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

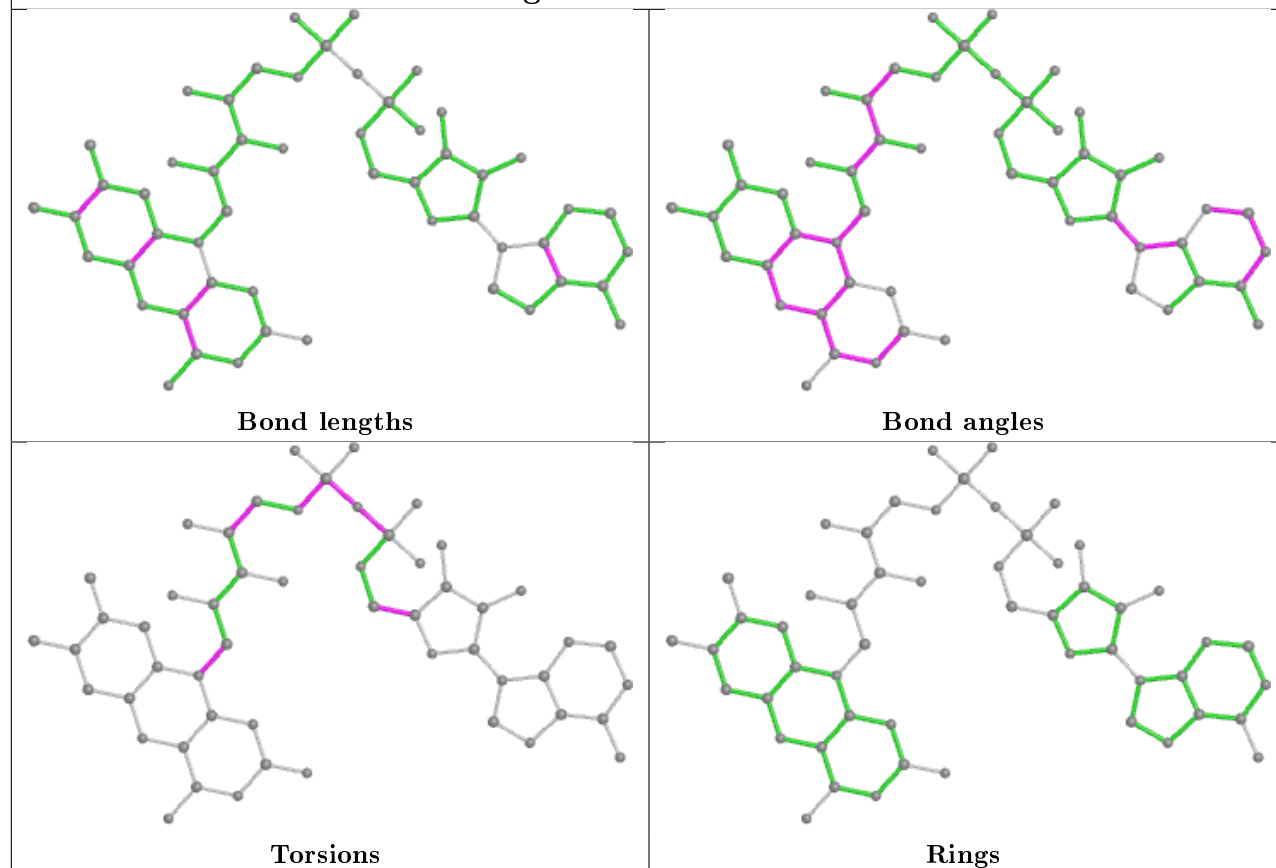
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.



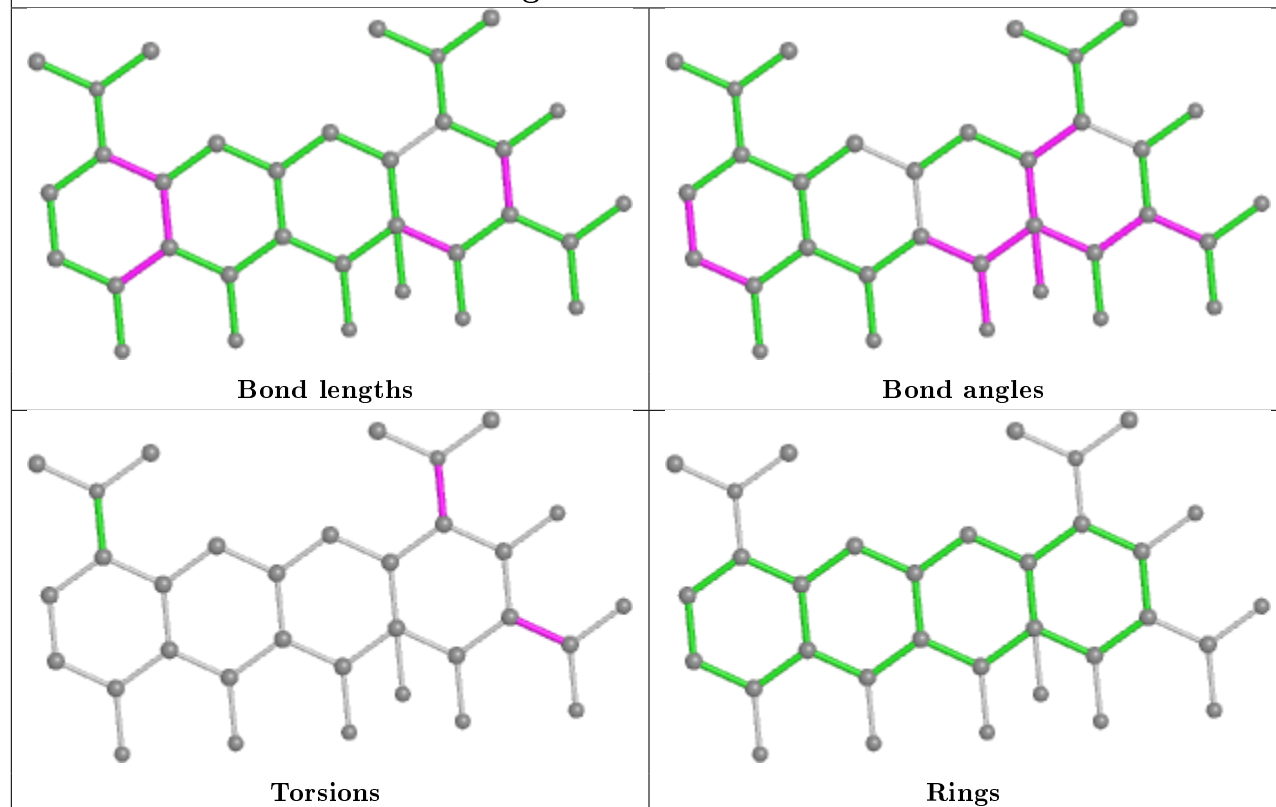
Ligand MIY A 2001



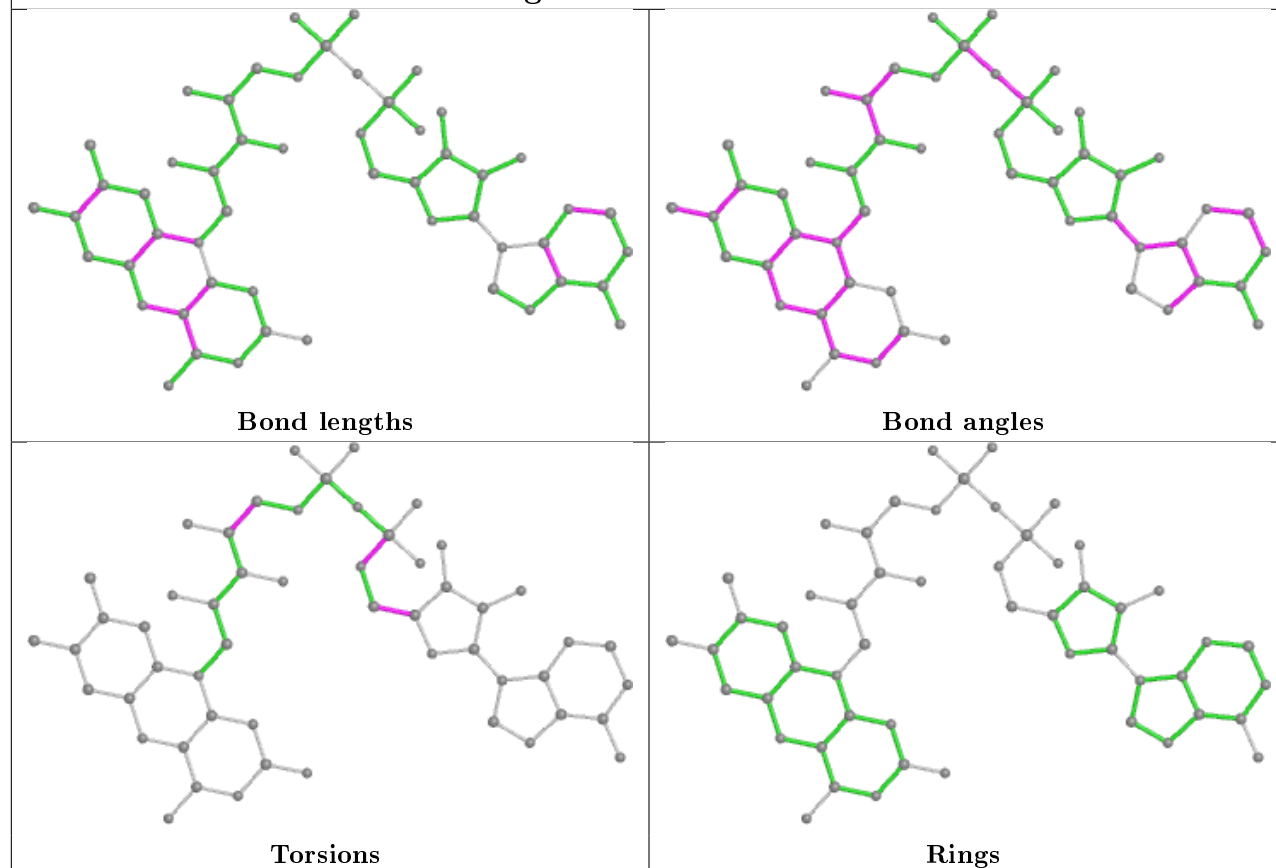
Ligand FAD D 2004

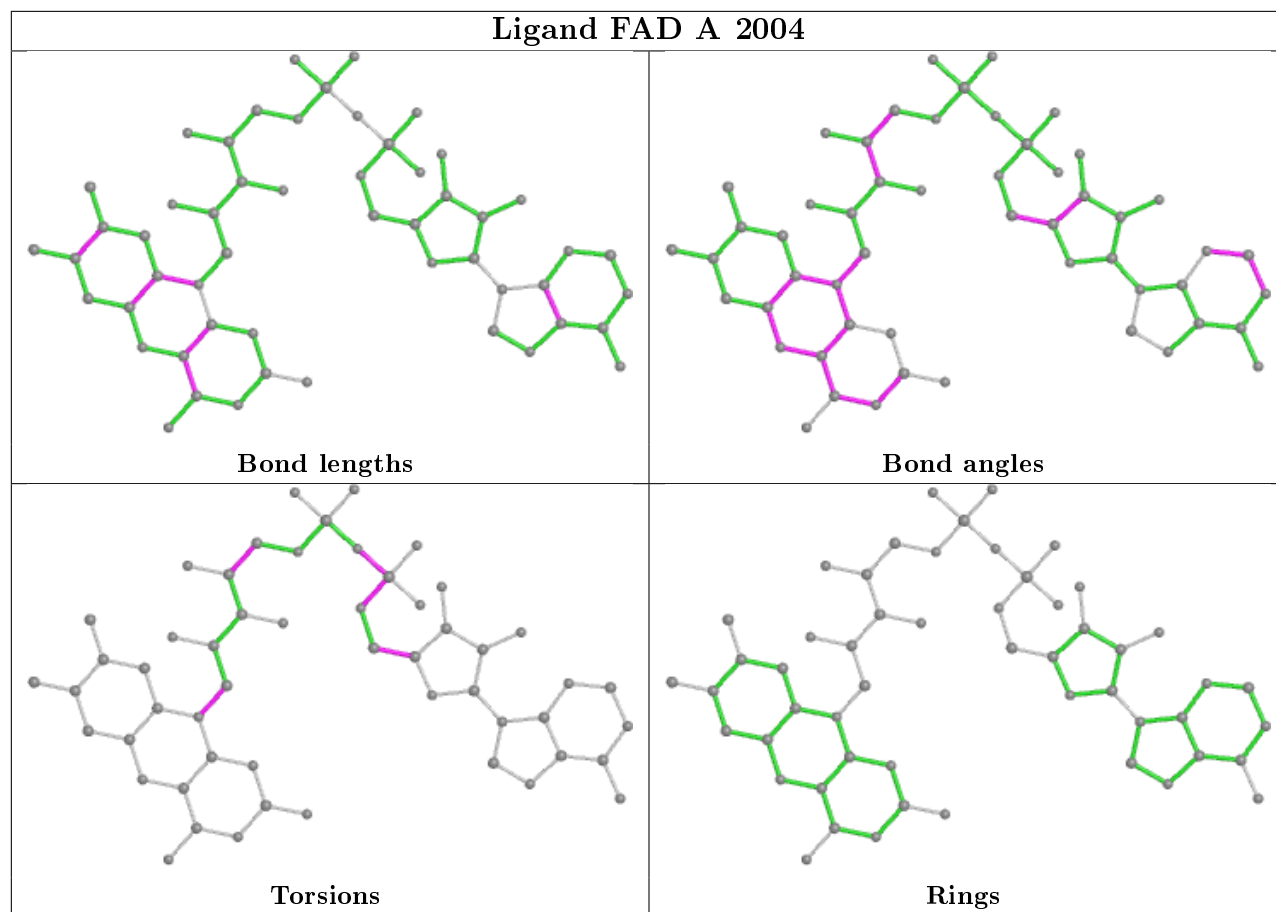


Ligand MIY D 2001

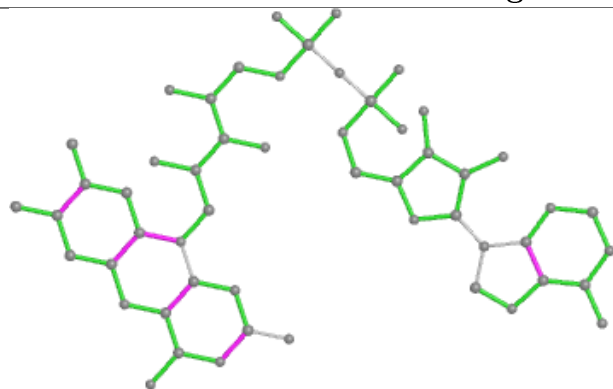


Ligand FAD B 2004

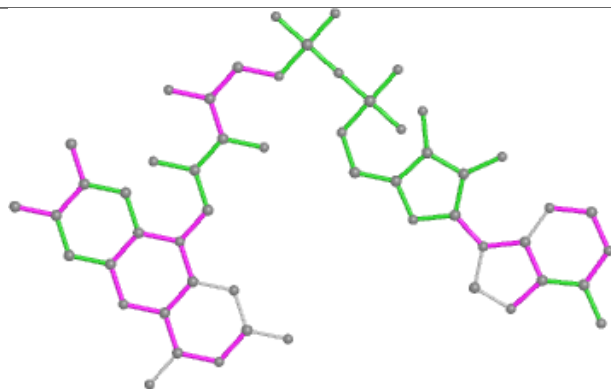




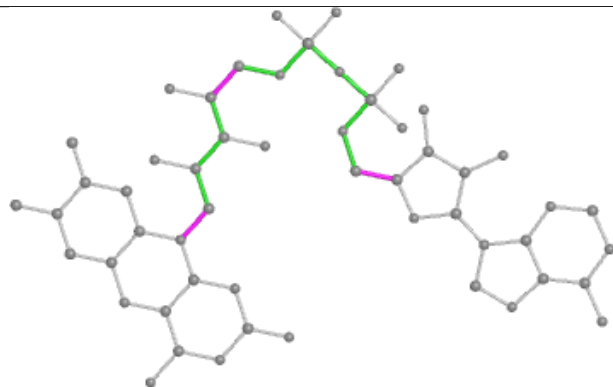
Ligand FAD C 2004



Bond lengths



Bond angles

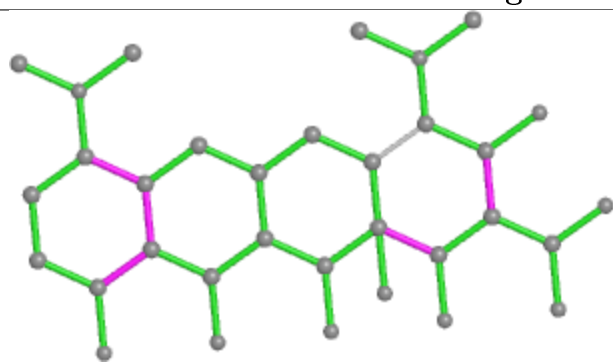


Torsions

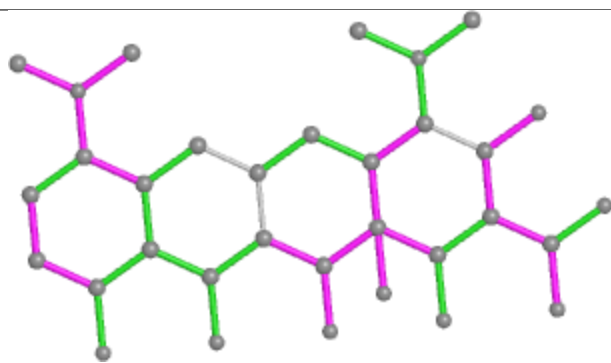


Rings

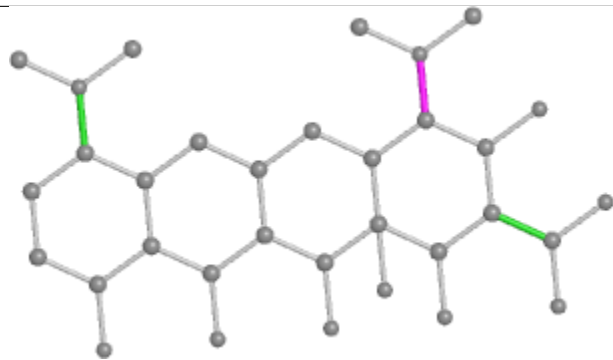
Ligand MIY C 2001



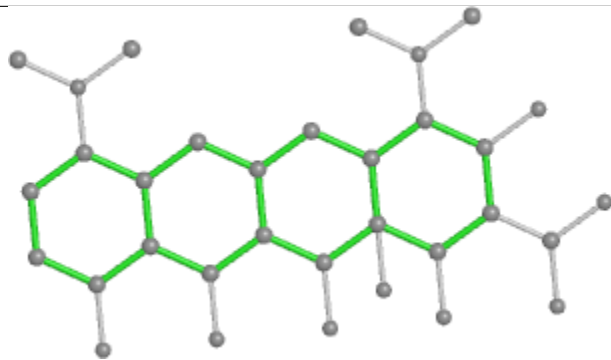
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	367/378 (97%)	0.13	9 (2%) 57 59	30, 49, 81, 110	0
1	B	368/378 (97%)	0.09	6 (1%) 72 74	28, 47, 81, 115	0
1	C	368/378 (97%)	0.18	9 (2%) 59 60	28, 48, 81, 115	0
1	D	367/378 (97%)	0.20	16 (4%) 34 33	30, 49, 82, 112	0
All	All	1470/1512 (97%)	0.15	40 (2%) 54 55	28, 48, 82, 115	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300	SER	4.9
1	C	378	PRO	4.8
1	C	247	ASN	3.9
1	B	13	LEU	3.6
1	D	220	GLY	3.6
1	C	382	PHE	3.5
1	B	378	PRO	3.4
1	D	340	ASP	3.3
1	D	262	PHE	2.9
1	C	243	ASP	2.8
1	D	175	ARG	2.8
1	A	251	VAL	2.8
1	C	262	PHE	2.8
1	D	13	LEU	2.6
1	D	304	LEU	2.6
1	D	144	PRO	2.6
1	D	286	GLY	2.6
1	C	377	LYS	2.5
1	D	252	ASP	2.4
1	D	161	ALA	2.4
1	A	261	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	245	TRP	2.4
1	C	13	LEU	2.4
1	D	251	VAL	2.4
1	D	242	PRO	2.3
1	B	351	LYS	2.3
1	B	377	LYS	2.3
1	C	102	LYS	2.2
1	A	178	VAL	2.2
1	B	286	GLY	2.2
1	A	249	THR	2.2
1	A	265	LYS	2.1
1	A	162	ASP	2.1
1	D	177	PHE	2.1
1	D	294	LEU	2.1
1	B	149	TRP	2.1
1	D	243	ASP	2.0
1	A	175	ARG	2.0
1	C	18	ASN	2.0
1	D	339	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.

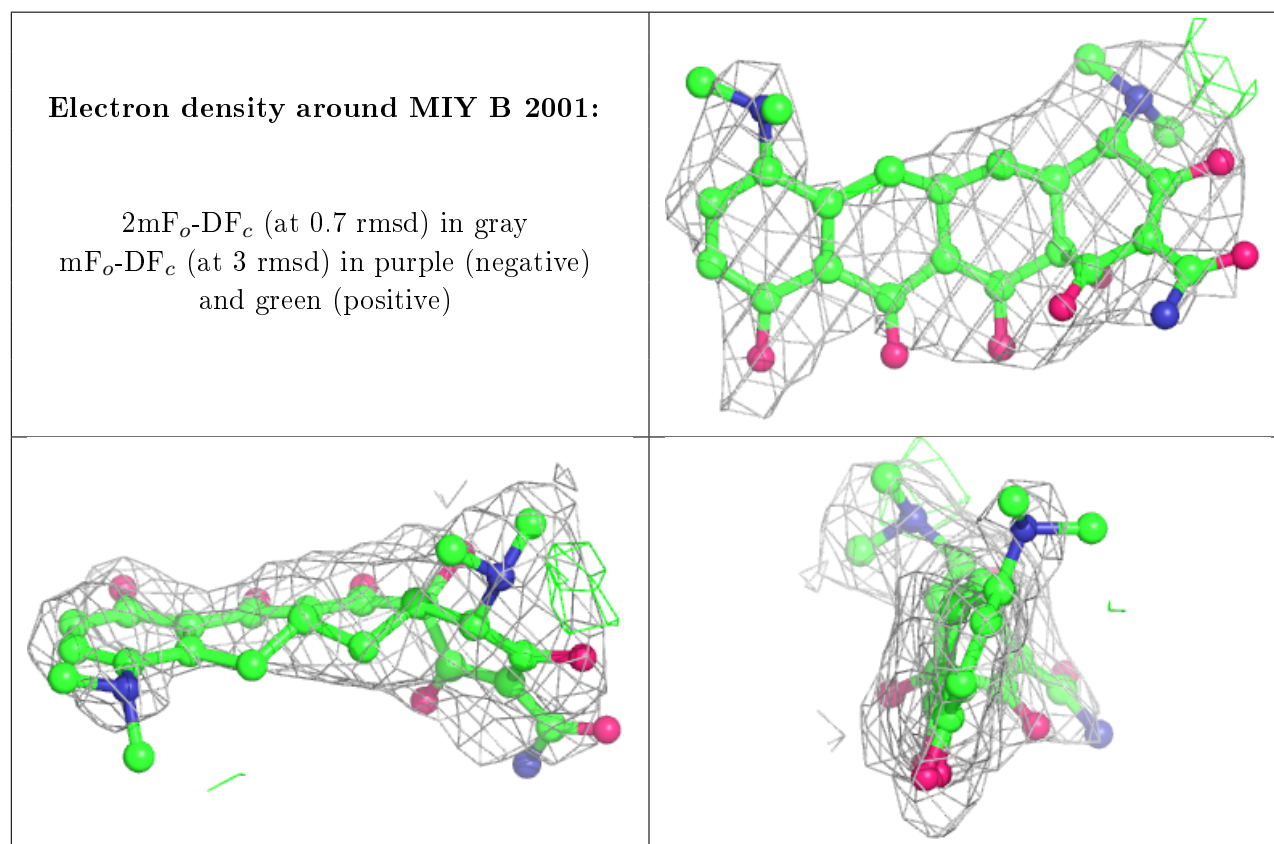
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MIY	B	2001	33/33	0.89	0.27	39,66,76,88	0
2	MIY	C	2001	33/33	0.89	0.29	48,73,86,91	0
2	MIY	D	2001	33/33	0.90	0.23	49,67,84,86	0
3	SO4	A	2003	5/5	0.91	0.15	67,69,77,107	0

Continued on next page...

Continued from previous page...

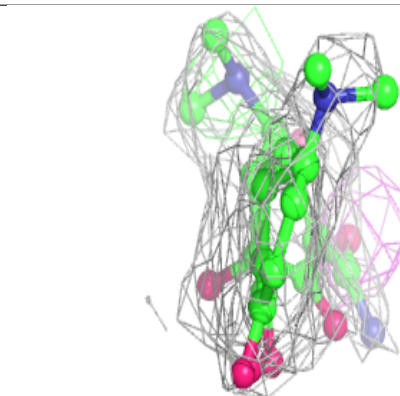
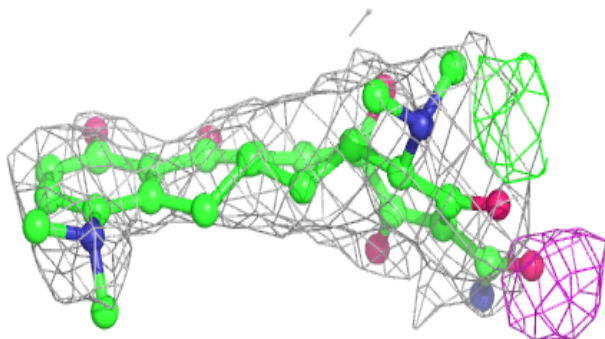
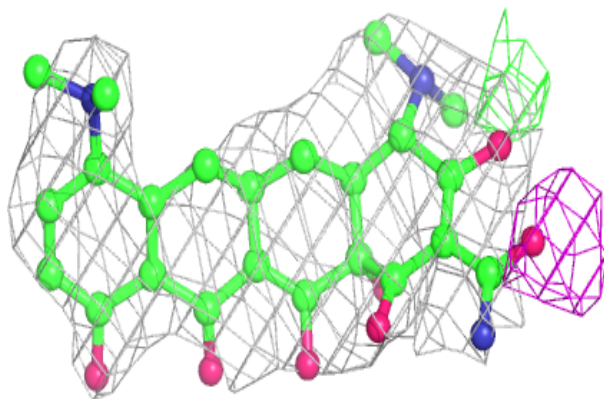
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MIY	A	2001	33/33	0.91	0.23	50,68,82,91	0
3	SO4	C	2002	5/5	0.93	0.11	46,71,95,105	0
3	SO4	D	2002	5/5	0.93	0.13	63,66,91,112	0
3	SO4	A	2002	5/5	0.94	0.18	63,65,86,98	0
3	SO4	B	2003	5/5	0.95	0.16	52,63,74,83	0
3	SO4	C	2003	5/5	0.96	0.20	43,52,87,90	0
4	FAD	C	2004	53/53	0.96	0.17	20,38,51,60	0
4	FAD	D	2004	53/53	0.96	0.15	25,41,59,71	0
3	SO4	D	2003	5/5	0.97	0.19	68,72,83,93	0
4	FAD	A	2004	53/53	0.97	0.16	24,38,65,74	0
4	FAD	B	2004	53/53	0.97	0.16	21,35,53,66	0
3	SO4	B	2002	5/5	0.97	0.11	68,74,87,90	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.

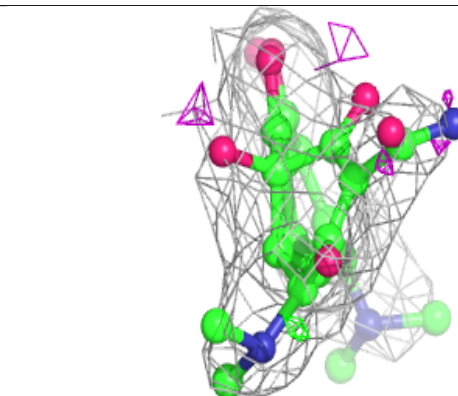
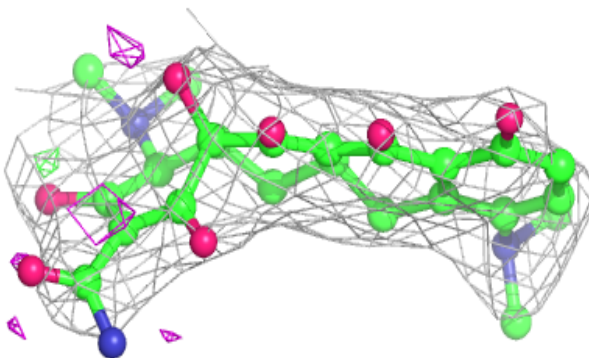
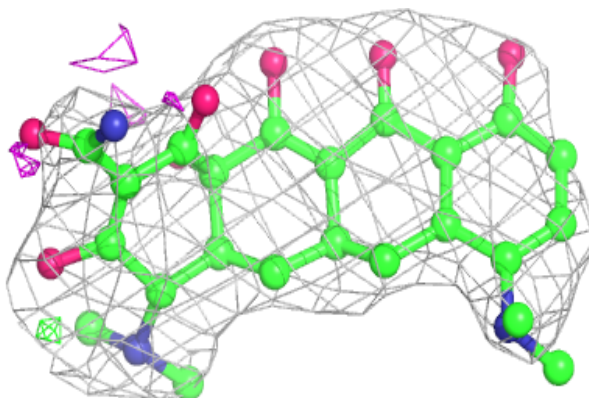


Electron density around MIY C 2001:

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

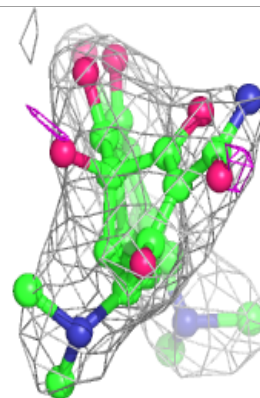
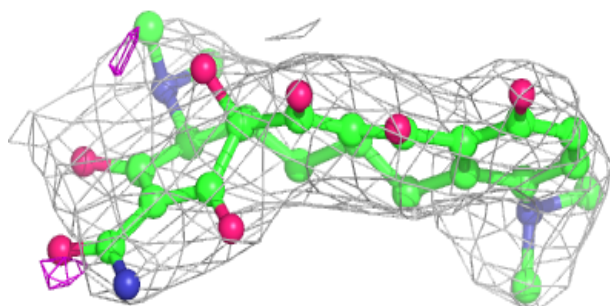
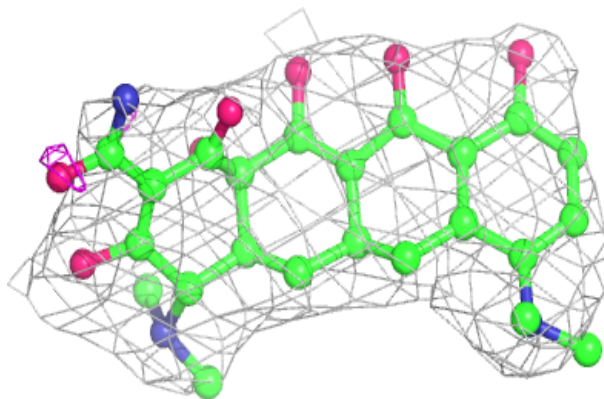
**Electron density around MIY D 2001:**

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

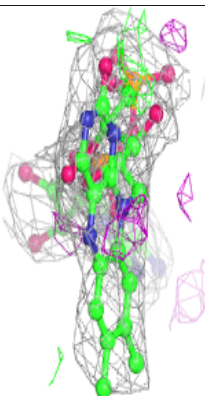
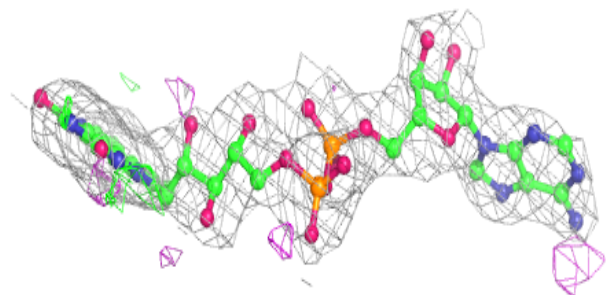
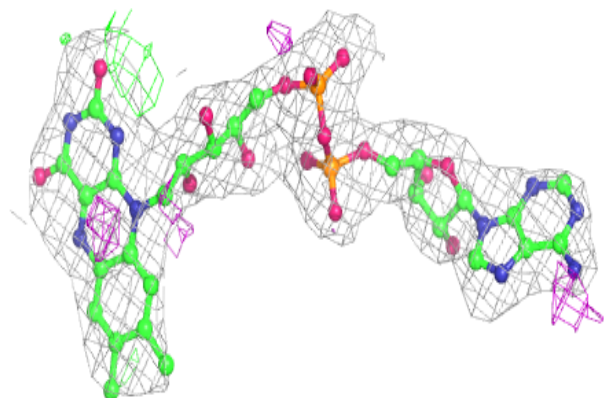


Electron density around MIY A 2001:

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

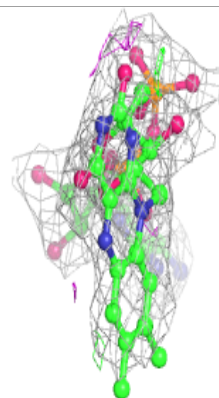
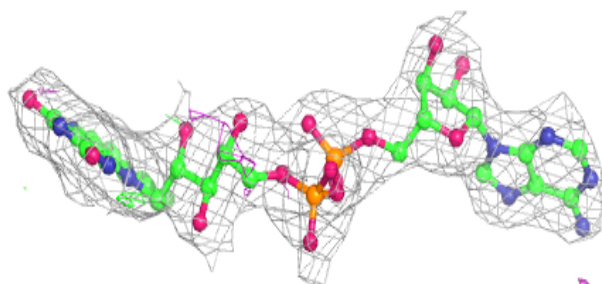
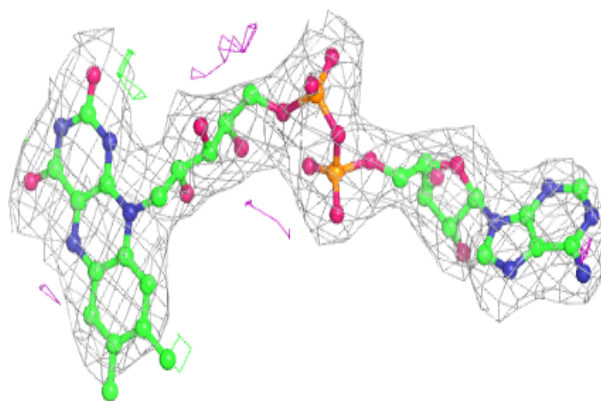
**Electron density around FAD C 2004:**

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

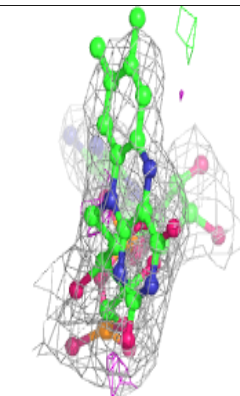
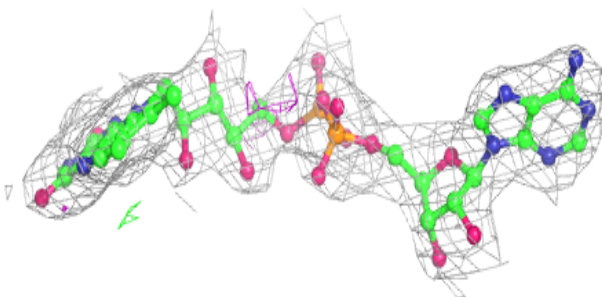
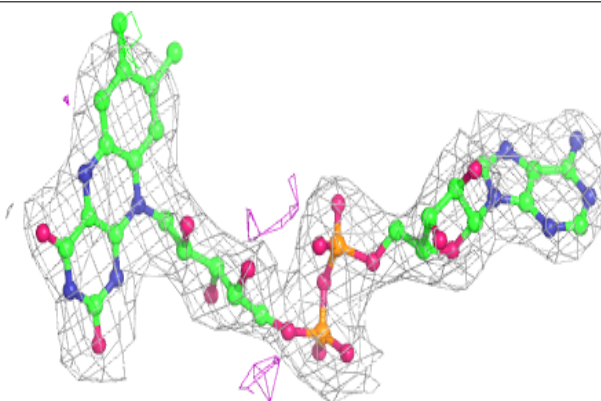


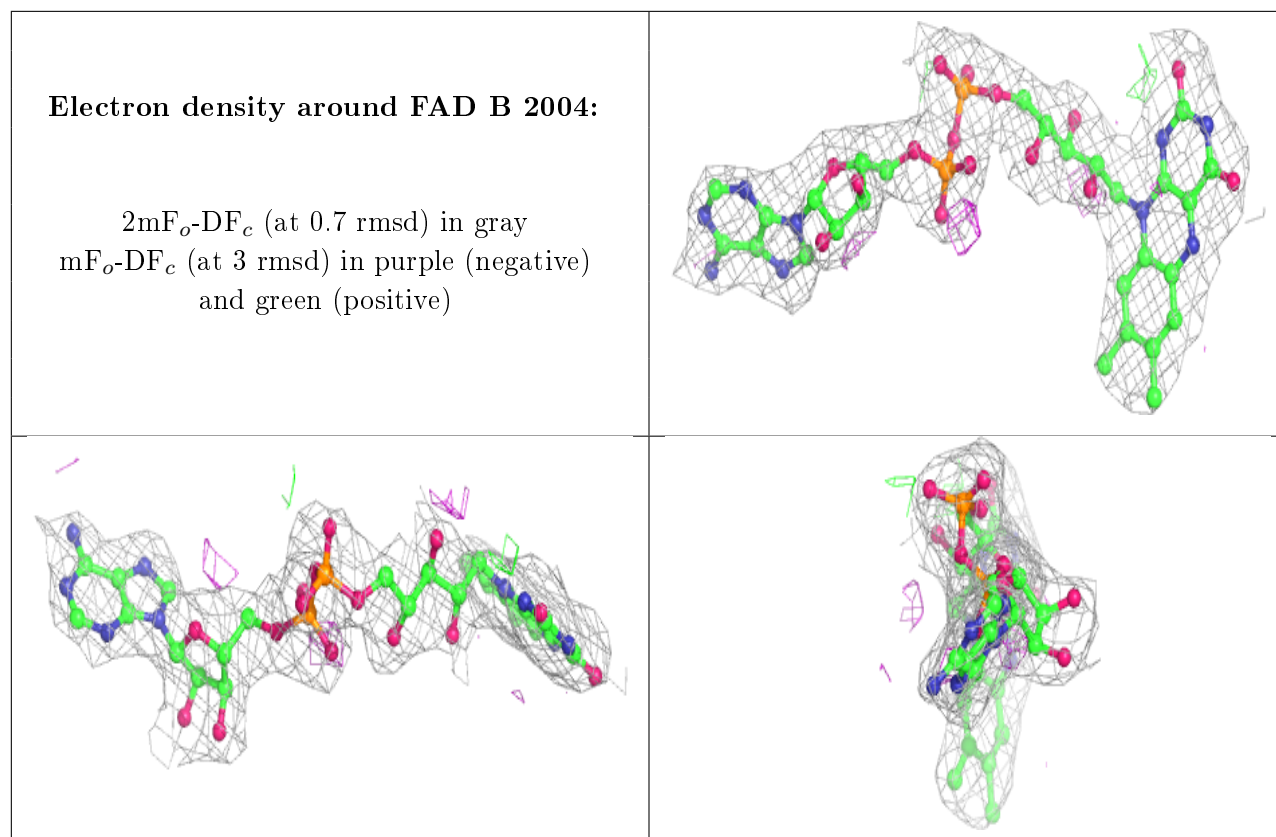
Electron density around FAD D 2004:

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

**Electron density around FAD A 2004:**

$2mF_o - DF_c$ (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.