



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:36 AM UTC

PDB ID : 4A6N / pdb_00004a6n
Title : STRUCTURE OF THE TETRACYCLINE DEGRADING MONOOXYGENASE TETX IN COMPLEX WITH TIGECYCLINE
Authors : Volkers, G.; Palm, G.J.; Weiss, M.S.; Hinrichs, W.
Deposited on : 2011-11-07
Resolution : 2.30 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

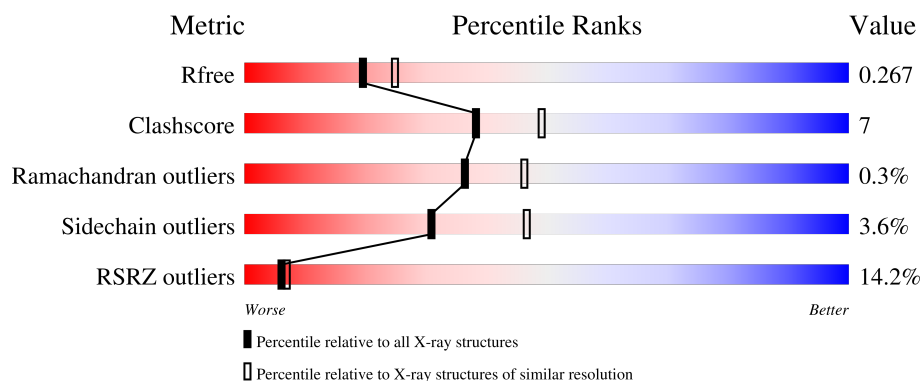
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	11% 77% 15% • 8%
2	B	398	11% 76% 16% • 8%
2	C	398	15% 78% 14% 8%
2	D	398	16% 78% 14% 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12141 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	1827	490	557	12			

There are 21 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
A	272	LYS	GLU	conflict	UNP Q93L51

- Molecule 2 is a protein called TETX2 PROTEIN.

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

There are 60 discrepancies between the modelled and reference sequences:

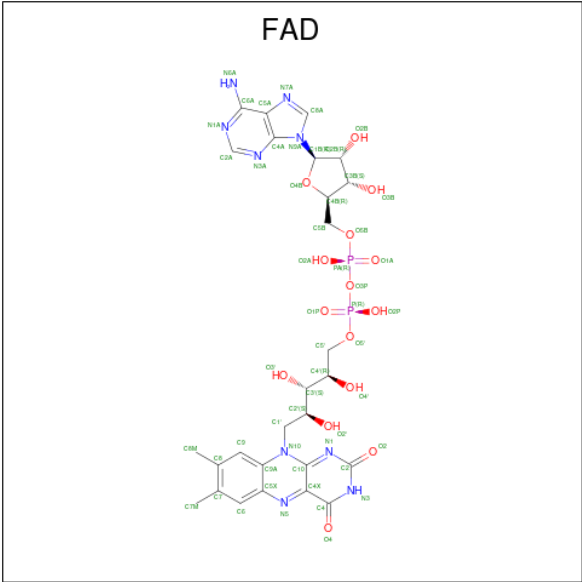
Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	MET	-	expression tag	UNP Q93L51
B	-8	GLY	-	expression tag	UNP Q93L51
B	-7	SER	-	expression tag	UNP Q93L51
B	-6	SER	-	expression tag	UNP Q93L51
B	-5	HIS	-	expression tag	UNP Q93L51
B	-4	HIS	-	expression tag	UNP Q93L51
B	-3	HIS	-	expression tag	UNP Q93L51
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

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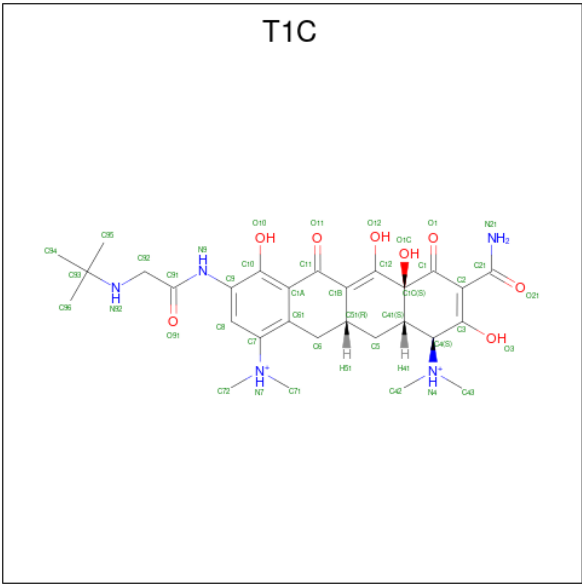
Chain	Residue	Modelled	Actual	Comment	Reference
C	4	LEU	-	expression tag	UNP Q93L51
C	5	VAL	-	expression tag	UNP Q93L51
C	6	PRO	-	expression tag	UNP Q93L51
C	7	ARG	-	expression tag	UNP Q93L51
C	8	GLY	-	expression tag	UNP Q93L51
C	9	SER	-	expression tag	UNP Q93L51
C	10	HIS	-	expression tag	UNP Q93L51
D	-9	MET	-	expression tag	UNP Q93L51
D	-8	GLY	-	expression tag	UNP Q93L51
D	-7	SER	-	expression tag	UNP Q93L51
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 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



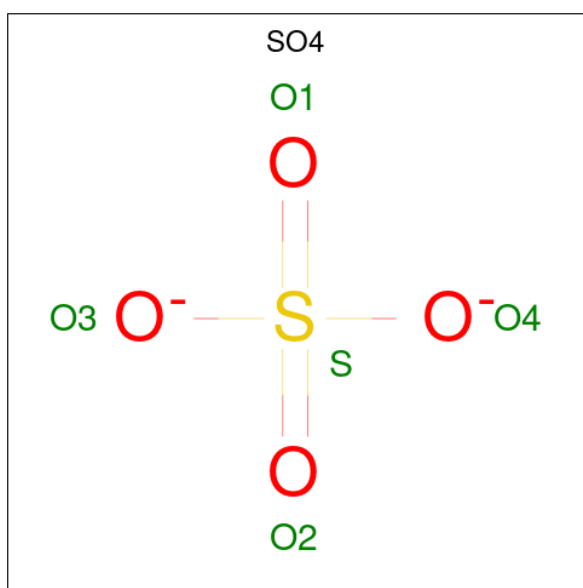
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	D	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 4 is TIGECYCLINE (CCD ID: T1C) (formula: C₂₉H₄₁N₅O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			42	29	5	8		
4	B	1	Total	C	N	O	0	0
			42	29	5	8		
4	C	1	Total	C	N	O	0	0
			42	29	5	8		
4	D	1	Total	C	N	O	0	0
			42	29	5	8		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

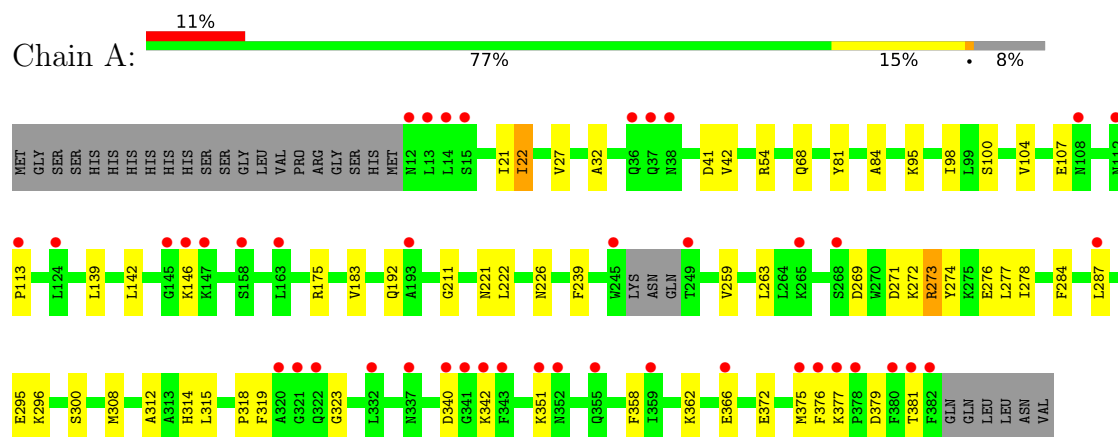
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	61	Total	O	0	0
			61	61		
6	B	68	Total	O	0	0
			68	68		
6	C	35	Total	O	0	0
			35	35		
6	D	46	Total	O	0	0
			46	46		

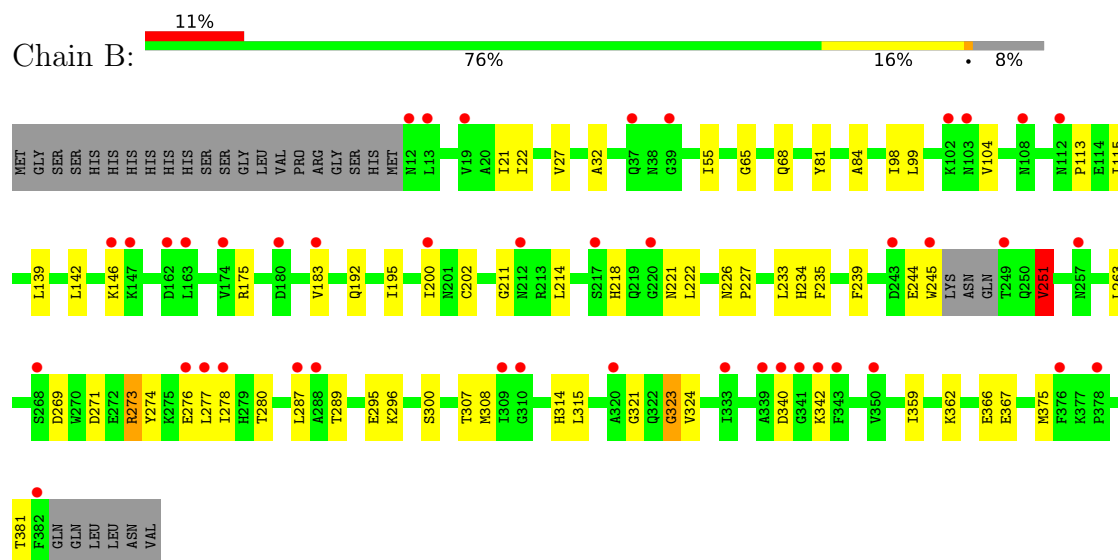
3 Residue-property plots [i](#)

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.

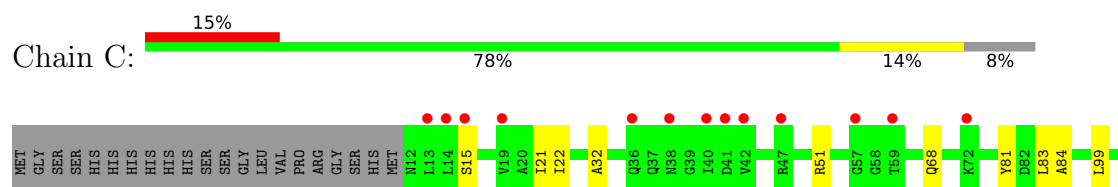
• Molecule 1: TETX2 PROTEIN

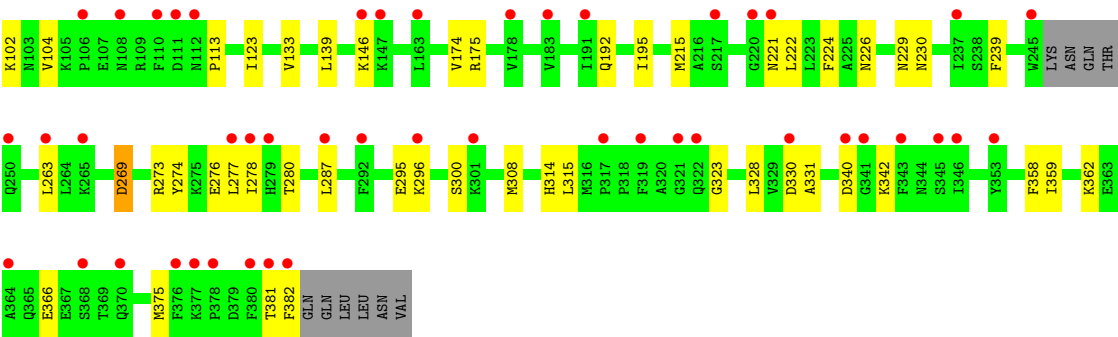


• Molecule 2: TETX2 PROTEIN

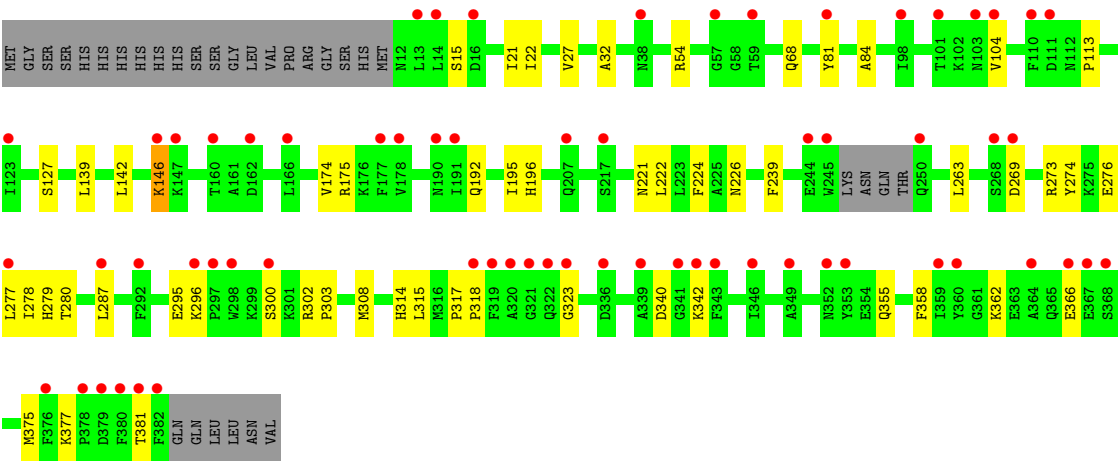
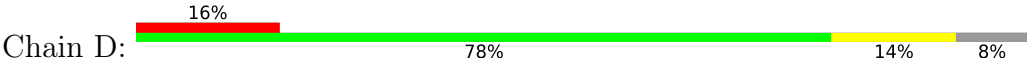


• Molecule 2: TETX2 PROTEIN





● Molecule 2: 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 80.79Å 87.65Å 110.84° 89.84° 93.63°	Depositor
Resolution (Å)	81.90 – 2.30 81.90 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.0 (81.90-2.30) 96.0 (81.90-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.218 , 0.260 0.227 , 0.267	Depositor DCC
R_{free} test set	3769 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.0	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	0.93	EDS
Total number of atoms	12141	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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: FAD, SO4, T1C

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	1.16	6/2944 (0.2%)	1.05	0/3987
2	B	1.15	9/2941 (0.3%)	1.06	2/3983 (0.1%)
2	C	0.97	0/2926	0.97	1/3965 (0.0%)
2	D	0.97	0/2917	0.99	6/3954 (0.2%)
All	All	1.07	15/11728 (0.1%)	1.02	9/15889 (0.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	289	THR	C-O	6.10	1.31	1.23
2	B	235	PHE	N-CA	6.07	1.53	1.45
1	A	183	VAL	N-CA	-6.00	1.39	1.46
1	A	27	VAL	C-O	-5.99	1.17	1.24
1	A	98	ILE	C-O	-5.92	1.18	1.24
2	B	218	HIS	CG-CD2	5.89	1.42	1.35
2	B	98	ILE	C-O	-5.67	1.18	1.23
1	A	211	GLY	C-O	-5.67	1.16	1.24
2	B	234	HIS	ND1-CE1	5.66	1.38	1.32
1	A	42	VAL	C-O	-5.58	1.18	1.24
2	B	202	CYS	CA-C	5.44	1.59	1.52
2	B	55	ILE	C-O	-5.33	1.18	1.24
1	A	312	ALA	N-CA	5.29	1.52	1.46
2	B	183	VAL	C-O	-5.28	1.18	1.24
2	B	211	GLY	C-O	-5.19	1.16	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	377	LYS	CA-C-N	6.55	128.03	119.84
2	D	377	LYS	C-N-CA	6.55	128.03	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	251	VAL	CG1-CB-CG2	6.42	124.92	110.80
2	D	27	VAL	N-CA-C	5.41	115.61	110.42
2	D	15	SER	N-CA-C	5.32	117.49	111.11
2	C	15	SER	N-CA-C	5.27	117.43	111.11
2	D	317	PRO	O-C-N	5.18	123.69	121.31
2	D	355	GLN	N-CA-C	5.17	116.60	111.07
2	B	307	THR	N-CA-C	5.02	115.66	108.74

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	2807	34	0
2	B	2883	0	2797	38	0
2	C	2868	0	2771	33	0
2	D	2859	0	2761	34	0
3	A	53	0	31	4	0
3	B	53	0	31	7	0
3	C	53	0	31	0	0
3	D	53	0	31	1	0
4	A	42	0	39	11	0
4	B	42	0	39	6	0
4	C	42	0	40	5	0
4	D	42	0	38	15	0
5	A	10	0	0	0	0
5	B	20	0	0	0	0
5	C	10	0	0	0	0
5	D	15	0	0	0	0
6	A	61	0	0	0	0
6	B	68	0	0	2	0
6	C	35	0	0	4	0
6	D	46	0	0	5	0
All	All	12141	0	11416	161	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 7.

All (161) 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)
2:C:269:ASP:HB2	6:C:2030:HOH:O	1.59	1.02
2:D:279:HIS:CE1	6:D:2037:HOH:O	2.13	0.98
4:D:392:T1C:C72	4:D:392:T1C:H62C	2.03	0.87
4:D:392:T1C:H422	4:D:392:T1C:O3	1.81	0.81
4:D:392:T1C:H62C	4:D:392:T1C:H722	1.62	0.80
3:A:389:FAD:C7M	4:A:392:T1C:H421	2.19	0.72
3:B:389:FAD:H6	4:B:392:T1C:H433	1.71	0.72
2:D:146:LYS:HG3	6:D:2021:HOH:O	1.90	0.71
4:D:392:T1C:C72	4:D:392:T1C:C6	2.69	0.70
2:B:263:LEU:HB3	2:B:278:ILE:HD13	1.75	0.69
3:A:389:FAD:HM72	4:A:392:T1C:H421	1.75	0.66
4:A:392:T1C:C6	4:A:392:T1C:H712	2.25	0.66
2:C:133:VAL:O	6:C:2016:HOH:O	2.14	0.65
2:D:263:LEU:HB3	2:D:278:ILE:HD13	1.77	0.64
4:D:392:T1C:H62C	4:D:392:T1C:H723	1.79	0.64
4:D:392:T1C:C6	4:D:392:T1C:H723	2.28	0.64
2:C:263:LEU:HB3	2:C:278:ILE:HD13	1.81	0.61
2:B:323:GLY:HA3	3:B:389:FAD:H1'2	1.82	0.60
4:B:392:T1C:O11	4:B:392:T1C:O12	2.12	0.60
2:D:21:ILE:HD12	2:D:32:ALA:HB2	1.82	0.60
3:B:389:FAD:H6	4:B:392:T1C:C43	2.32	0.60
2:D:146:LYS:CG	6:D:2021:HOH:O	2.48	0.60
1:A:222:LEU:CD2	1:A:375:MET:HE3	2.32	0.59
2:D:318:PRO:HG2	4:D:392:T1C:H431	1.84	0.59
1:A:263:LEU:HB3	1:A:278:ILE:HD13	1.85	0.59
4:C:392:T1C:H432	4:C:392:T1C:O3	2.01	0.59
2:C:222:LEU:CD2	2:C:375:MET:HE3	2.35	0.57
2:D:222:LEU:CD2	2:D:375:MET:HE3	2.35	0.56
2:B:324:VAL:HG12	3:B:389:FAD:O2	2.06	0.56
2:D:375:MET:SD	4:D:392:T1C:H721	2.46	0.56
3:B:389:FAD:C6	4:B:392:T1C:C43	2.84	0.56
4:A:392:T1C:O3	4:A:392:T1C:C42	2.54	0.56
2:D:84:ALA:HB1	2:D:113:PRO:HB2	1.86	0.55
1:A:222:LEU:HD23	1:A:375:MET:HE3	1.89	0.55
2:C:362:LYS:O	2:C:366:GLU:HG2	2.06	0.55
2:C:382:PHE:C	6:C:2035:HOH:O	2.49	0.55
1:A:95:LYS:NZ	2:B:367:GLU:HA	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:68:GLN:NE2	2:C:81:TYR:OH	2.39	0.54
2:D:222:LEU:HD23	2:D:375:MET:HE3	1.89	0.54
2:D:68:GLN:NE2	2:D:81:TYR:OH	2.41	0.53
2:D:22:ILE:HD13	2:D:22:ILE:N	2.24	0.53
2:B:222:LEU:HD23	2:B:375:MET:HE3	1.91	0.53
2:B:222:LEU:CD2	2:B:375:MET:HE3	2.39	0.53
2:C:84:ALA:HB1	2:C:113:PRO:HB2	1.90	0.53
2:D:362:LYS:O	2:D:366:GLU:HG2	2.09	0.52
1:A:362:LYS:O	1:A:366:GLU:HG2	2.10	0.52
2:B:323:GLY:N	6:B:2061:HOH:O	2.18	0.52
2:B:68:GLN:NE2	2:B:81:TYR:OH	2.42	0.52
2:C:222:LEU:HD23	2:C:375:MET:HE3	1.91	0.52
1:A:107:GLU:HG2	2:C:359:ILE:HD13	1.92	0.51
2:C:221:ASN:HD22	2:C:239:PHE:HB3	1.76	0.51
2:D:279:HIS:HE1	6:D:2037:HOH:O	1.71	0.51
2:B:362:LYS:O	2:B:366:GLU:HG2	2.11	0.50
1:A:379:ASP:HB3	2:B:65:GLY:HA3	1.94	0.50
1:A:314:HIS:O	1:A:315:LEU:C	2.55	0.50
2:C:226:ASN:OD1	2:C:226:ASN:C	2.55	0.50
2:B:221:ASN:HD22	2:B:239:PHE:HB3	1.77	0.50
2:D:22:ILE:HG13	2:D:139:LEU:HD22	1.94	0.49
1:A:318:PRO:HG2	4:A:392:T1C:H431	1.93	0.49
2:D:318:PRO:HG2	4:D:392:T1C:C43	2.42	0.49
1:A:100:SER:HB2	2:B:359:ILE:HG12	1.95	0.49
1:A:84:ALA:HB1	1:A:113:PRO:HB2	1.94	0.49
2:C:224:PHE:HB2	4:C:392:T1C:O3	2.12	0.48
2:B:245:TRP:CZ2	2:B:251:VAL:HG13	2.49	0.48
2:C:21:ILE:HD12	2:C:32:ALA:HB2	1.95	0.48
2:C:195:ILE:HD12	2:C:277:LEU:HD12	1.96	0.48
3:A:389:FAD:HM71	4:A:392:T1C:H421	1.95	0.48
1:A:22:ILE:HD13	1:A:22:ILE:N	2.29	0.47
1:A:68:GLN:NE2	1:A:81:TYR:OH	2.47	0.47
2:B:139:LEU:HD21	2:B:142:LEU:HD13	1.94	0.47
2:B:214:LEU:C	2:B:214:LEU:HD23	2.39	0.47
1:A:274:TYR:O	1:A:277:LEU:HB3	2.14	0.47
1:A:21:ILE:HD12	1:A:32:ALA:HB2	1.96	0.47
2:B:295:GLU:HG3	2:B:296:LYS:HG2	1.97	0.47
2:C:295:GLU:HG3	2:C:296:LYS:HG2	1.97	0.47
2:D:295:GLU:HG3	2:D:296:LYS:HG2	1.97	0.47
1:A:95:LYS:NZ	2:B:367:GLU:HG3	2.29	0.47
1:A:226:ASN:C	1:A:226:ASN:OD1	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:GLU:O	1:A:376:PHE:HD2	1.97	0.47
2:D:226:ASN:OD1	2:D:226:ASN:C	2.56	0.47
2:B:84:ALA:HB1	2:B:113:PRO:HB2	1.97	0.46
2:C:328:LEU:O	2:C:331:ALA:HB3	2.15	0.46
4:C:392:T1C:H41	4:C:392:T1C:H423	1.73	0.46
2:B:27:VAL:HG23	3:B:389:FAD:P	2.55	0.46
2:B:274:TYR:O	2:B:277:LEU:HB3	2.16	0.46
4:D:392:T1C:O3	4:D:392:T1C:C42	2.56	0.46
2:B:21:ILE:HD12	2:B:32:ALA:HB2	1.98	0.46
2:D:195:ILE:HD13	2:D:280:THR:CG2	2.46	0.46
1:A:221:ASN:HD22	1:A:239:PHE:HB3	1.81	0.46
1:A:22:ILE:HG13	1:A:139:LEU:HD22	1.99	0.46
2:D:196:HIS:CE1	6:D:2034:HOH:O	2.68	0.46
2:D:358:PHE:O	2:D:362:LYS:HB2	2.17	0.45
1:A:375:MET:SD	4:A:392:T1C:H721	2.56	0.45
2:B:340:ASP:HB2	2:B:342:LYS:HB2	1.97	0.45
2:D:221:ASN:HD22	2:D:239:PHE:HB3	1.82	0.45
2:D:139:LEU:HD23	2:D:174:VAL:HG11	1.99	0.45
4:D:392:T1C:H951	4:D:392:T1C:H922	1.80	0.45
1:A:295:GLU:HG3	1:A:296:LYS:HG2	1.99	0.45
2:B:244:GLU:H	2:B:244:GLU:CD	2.24	0.45
2:B:314:HIS:O	2:B:315:LEU:C	2.60	0.45
2:B:321:GLY:HA2	6:B:2060:HOH:O	2.16	0.45
1:A:379:ASP:CB	2:B:65:GLY:HA3	2.47	0.45
2:C:195:ILE:HD13	2:C:280:THR:CG2	2.47	0.45
2:C:229:ASN:O	2:C:230:ASN:C	2.61	0.45
2:C:274:TYR:O	2:C:277:LEU:HB3	2.17	0.44
2:B:227:PRO:HA	2:B:233:LEU:HD12	2.00	0.44
2:D:340:ASP:HB2	2:D:342:LYS:HB2	1.99	0.44
4:D:392:T1C:O10	4:D:392:T1C:O11	2.31	0.44
2:B:22:ILE:HG13	2:B:139:LEU:HD22	1.99	0.44
2:C:358:PHE:O	2:C:362:LYS:HB2	2.18	0.44
3:D:389:FAD:N1	3:D:389:FAD:H2'	2.32	0.44
4:D:392:T1C:O11	4:D:392:T1C:O12	2.32	0.44
4:A:392:T1C:H712	4:A:392:T1C:H62C	1.99	0.44
2:C:139:LEU:HD23	2:C:174:VAL:HG11	1.99	0.44
3:B:389:FAD:HM72	4:B:392:T1C:H431	1.99	0.44
2:D:139:LEU:HD21	2:D:142:LEU:HD13	1.99	0.44
1:A:142:LEU:HD12	1:A:142:LEU:HA	1.87	0.43
1:A:340:ASP:HB2	1:A:342:LYS:HB2	1.99	0.43
2:D:274:TYR:O	2:D:277:LEU:HB3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:375:MET:SD	4:D:392:T1C:C72	3.07	0.43
1:A:319:PHE:CD1	1:A:375:MET:HE1	2.53	0.43
2:B:175:ARG:HG2	2:B:308:MET:SD	2.59	0.42
4:B:392:T1C:H41	4:B:392:T1C:H423	1.74	0.42
2:C:340:ASP:HB2	2:C:342:LYS:HB2	2.00	0.42
2:C:314:HIS:NE2	2:C:330:ASP:OD2	2.44	0.42
3:A:389:FAD:H9	3:A:389:FAD:H1'1	1.76	0.42
2:B:226:ASN:OD1	2:B:226:ASN:C	2.62	0.42
2:B:340:ASP:CB	2:B:342:LYS:HB2	2.49	0.42
2:D:175:ARG:HG2	2:D:308:MET:SD	2.60	0.42
1:A:139:LEU:HD21	1:A:142:LEU:HD13	2.01	0.42
1:A:340:ASP:CB	1:A:342:LYS:HB2	2.49	0.42
2:C:382:PHE:CE1	4:C:392:T1C:H711	2.55	0.42
2:C:83:LEU:HD22	2:C:123:ILE:HD11	2.02	0.41
4:A:392:T1C:O11	4:A:392:T1C:O12	2.37	0.41
2:B:195:ILE:HD13	2:B:280:THR:CG2	2.51	0.41
2:C:51:ARG:HG2	6:C:2005:HOH:O	2.20	0.41
2:D:314:HIS:O	2:D:315:LEU:C	2.63	0.41
2:C:215:MET:SD	4:C:392:T1C:H712	2.60	0.41
4:A:392:T1C:C6	4:A:392:T1C:C71	2.95	0.41
2:B:221:ASN:ND2	2:B:239:PHE:HB3	2.36	0.41
2:C:314:HIS:O	2:C:315:LEU:C	2.62	0.41
2:D:195:ILE:HD12	2:D:277:LEU:HD12	2.03	0.41
1:A:41:ASP:OD1	1:A:41:ASP:C	2.63	0.41
2:C:22:ILE:HG13	2:C:139:LEU:HD22	2.03	0.41
1:A:54:ARG:CZ	2:D:54:ARG:CZ	2.98	0.41
4:A:392:T1C:O3	4:A:392:T1C:H423	2.20	0.41
2:D:340:ASP:CB	2:D:342:LYS:HB2	2.50	0.41
2:B:115:ILE:O	2:B:115:ILE:HG23	2.20	0.41
2:B:142:LEU:HD12	2:B:142:LEU:HA	1.89	0.41
2:C:195:ILE:CD1	2:C:277:LEU:HD12	2.50	0.41
2:B:200:ILE:HD13	2:B:200:ILE:HA	1.82	0.41
2:D:224:PHE:CD2	4:D:392:T1C:H51C	2.55	0.41
2:C:22:ILE:N	2:C:22:ILE:HD13	2.36	0.40
1:A:259:VAL:HG11	1:A:284:PHE:CG	2.57	0.40
2:B:271:ASP:OD2	2:B:273:ARG:HD3	2.21	0.40
1:A:175:ARG:HG2	1:A:308:MET:SD	2.62	0.40
1:A:271:ASP:OD2	1:A:273:ARG:HD3	2.22	0.40
1:A:358:PHE:O	1:A:362:LYS:HB2	2.20	0.40
2:B:22:ILE:N	2:B:22:ILE:HD13	2.35	0.40
2:D:302:ARG:HA	2:D:303:PRO:HD3	1.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:175:ARG:HG2	2:C:308:MET:SD	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	351 (96%)	12 (3%)	1 (0%)	36	46
2	B	364/398 (92%)	350 (96%)	13 (4%)	1 (0%)	36	46
2	C	363/398 (91%)	348 (96%)	14 (4%)	1 (0%)	36	46
2	D	363/398 (91%)	348 (96%)	14 (4%)	1 (0%)	36	46
All	All	1454/1592 (91%)	1397 (96%)	53 (4%)	4 (0%)	36	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	323	GLY
1	A	323	GLY
2	D	323	GLY
2	C	323	GLY

5.3.2 Protein sidechains [i](#)

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%)	299 (96%)	13 (4%)	26	40
2	B	310/345 (90%)	299 (96%)	11 (4%)	32	48
2	C	307/345 (89%)	296 (96%)	11 (4%)	31	47
2	D	305/345 (88%)	295 (97%)	10 (3%)	33	50
All	All	1234/1380 (89%)	1189 (96%)	45 (4%)	31	47

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ILE
1	A	104	VAL
1	A	146	LYS
1	A	192	GLN
1	A	269	ASP
1	A	272	LYS
1	A	273	ARG
1	A	276	GLU
1	A	287	LEU
1	A	300	SER
1	A	351	LYS
1	A	377	LYS
1	A	381	THR
2	B	99	LEU
2	B	104	VAL
2	B	146	LYS
2	B	192	GLN
2	B	251	VAL
2	B	269	ASP
2	B	273	ARG
2	B	276	GLU
2	B	287	LEU
2	B	300	SER
2	B	381	THR
2	C	99	LEU
2	C	102	LYS
2	C	104	VAL
2	C	146	LYS
2	C	192	GLN
2	C	269	ASP
2	C	273	ARG
2	C	276	GLU
2	C	287	LEU

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Mol	Chain	Res	Type
2	C	300	SER
2	C	381	THR
2	D	104	VAL
2	D	127	SER
2	D	146	LYS
2	D	192	GLN
2	D	269	ASP
2	D	273	ARG
2	D	276	GLU
2	D	287	LEU
2	D	300	SER
2	D	381	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	49	ASN
1	A	68	GLN
1	A	130	ASN
1	A	221	ASN
1	A	356	GLN
1	A	371	ASN
2	B	38	ASN
2	B	49	ASN
2	B	68	GLN
2	B	130	ASN
2	B	192	GLN
2	B	221	ASN
2	B	250	GLN
2	B	356	GLN
2	B	371	ASN
2	C	38	ASN
2	C	49	ASN
2	C	68	GLN
2	C	130	ASN
2	C	221	ASN
2	C	356	GLN
2	C	371	ASN
2	D	38	ASN
2	D	49	ASN
2	D	68	GLN

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Mol	Chain	Res	Type
2	D	130	ASN
2	D	192	GLN
2	D	221	ASN
2	D	371	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

19 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	$\# Z > 2$
5	SO4	A	1384	-	4,4,4	0.56	0	6,6,6	0.44	0
3	FAD	C	389	-	58,58,58	2.02	10 (17%)	85,89,89	2.07	22 (25%)
5	SO4	B	1384	-	4,4,4	0.49	0	6,6,6	0.31	0
3	FAD	B	389	-	58,58,58	3.13	14 (24%)	85,89,89	2.01	21 (24%)
3	FAD	A	389	-	58,58,58	2.12	14 (24%)	85,89,89	1.81	20 (23%)
5	SO4	A	1383	-	4,4,4	0.40	0	6,6,6	0.33	0
4	T1C	B	392	-	45,45,45	2.12	11 (24%)	56,72,72	2.08	15 (26%)
5	SO4	D	1384	-	4,4,4	0.47	0	6,6,6	0.32	0
5	SO4	D	1385	-	4,4,4	0.50	0	6,6,6	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	C	1383	-	4,4,4	0.63	0	6,6,6	0.33	0
5	SO4	B	1385	-	4,4,4	0.45	0	6,6,6	0.26	0
5	SO4	C	1384	-	4,4,4	0.52	0	6,6,6	0.31	0
4	T1C	D	392	-	45,45,45	2.02	11 (24%)	56,72,72	1.83	13 (23%)
4	T1C	A	392	-	45,45,45	2.10	12 (26%)	56,72,72	1.77	11 (19%)
4	T1C	C	392	-	45,45,45	1.99	11 (24%)	56,72,72	1.72	10 (17%)
5	SO4	B	1383	-	4,4,4	0.41	0	6,6,6	0.36	0
3	FAD	D	389	-	58,58,58	1.76	13 (22%)	85,89,89	1.98	24 (28%)
5	SO4	D	1383	-	4,4,4	0.45	0	6,6,6	0.16	0
5	SO4	B	1386	-	4,4,4	0.52	0	6,6,6	0.27	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	T1C	A	392	-	-	3/22/80/80	0/4/4/4
3	FAD	C	389	-	-	1/34/50/50	0/6/6/6
3	FAD	B	389	-	-	2/34/50/50	0/6/6/6
4	T1C	C	392	-	-	4/22/80/80	0/4/4/4
4	T1C	B	392	-	-	0/22/80/80	0/4/4/4
3	FAD	D	389	-	-	5/34/50/50	0/6/6/6
4	T1C	D	392	-	-	7/22/80/80	0/4/4/4
3	FAD	A	389	-	-	1/34/50/50	0/6/6/6

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	389	FAD	PA-O3P	18.61	1.79	1.59
3	A	389	FAD	PA-O3P	9.85	1.70	1.59
3	C	389	FAD	P-O3P	-7.12	1.51	1.59
3	B	389	FAD	P-O3P	-7.04	1.51	1.59
4	A	392	T1C	C2-C21	6.90	1.61	1.47
4	B	392	T1C	C1C-C12	6.47	1.57	1.52
3	C	389	FAD	PA-O3P	6.38	1.66	1.59
4	D	392	T1C	C41-C4	6.09	1.60	1.54
3	A	389	FAD	C9A-C5X	6.01	1.50	1.41
4	C	392	T1C	C2-C21	5.92	1.59	1.47
3	C	389	FAD	C9A-C5X	5.84	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	392	T1C	C2-C21	5.75	1.59	1.47
4	C	392	T1C	C41-C4	5.74	1.60	1.54
4	D	392	T1C	C2-C21	5.69	1.59	1.47
3	D	389	FAD	C9A-C5X	5.58	1.50	1.41
3	D	389	FAD	C5A-C4A	5.24	1.48	1.39
3	B	389	FAD	C9A-C5X	5.21	1.49	1.41
4	A	392	T1C	C1C-C41	-5.20	1.48	1.53
4	D	392	T1C	C1C-C12	4.71	1.56	1.52
3	B	389	FAD	C8A-N7A	4.54	1.40	1.31
3	C	389	FAD	C8-C7	4.37	1.51	1.40
4	C	392	T1C	C1C-C12	4.35	1.55	1.52
3	C	389	FAD	C8A-N7A	4.29	1.39	1.31
4	B	392	T1C	C6-C61	4.23	1.57	1.51
4	D	392	T1C	C6-C61	4.23	1.57	1.51
4	A	392	T1C	C6-C61	4.10	1.57	1.51
4	A	392	T1C	C41-C4	3.97	1.58	1.54
4	B	392	T1C	C41-C4	3.97	1.58	1.54
3	D	389	FAD	C8A-N7A	3.89	1.39	1.31
4	A	392	T1C	C1C-C12	3.87	1.55	1.52
3	D	389	FAD	PA-O3P	3.69	1.63	1.59
3	B	389	FAD	C5A-C4A	3.68	1.45	1.39
3	D	389	FAD	C8-C7	3.68	1.49	1.40
4	B	392	T1C	C1C-C41	-3.60	1.50	1.53
3	A	389	FAD	C8-C7	3.56	1.49	1.40
3	B	389	FAD	C2-N3	-3.51	1.31	1.39
3	C	389	FAD	C5A-C6A	3.49	1.50	1.41
4	C	392	T1C	C6-C61	3.39	1.56	1.51
4	C	392	T1C	C7-N7	-3.20	1.34	1.42
3	A	389	FAD	C4X-N5	3.20	1.37	1.30
3	A	389	FAD	P-O3P	-3.19	1.56	1.59
3	A	389	FAD	O4'-C4'	3.15	1.49	1.43
3	A	389	FAD	C4-N3	-3.15	1.33	1.38
4	B	392	T1C	C51-C1B	3.14	1.54	1.51
3	C	389	FAD	C5A-C4A	3.11	1.44	1.39
3	A	389	FAD	C5A-C4A	3.10	1.44	1.39
4	C	392	T1C	C9-N9	-2.96	1.35	1.41
4	B	392	T1C	C1B-C11	-2.96	1.40	1.46
3	B	389	FAD	C4-N3	-2.86	1.33	1.38
3	B	389	FAD	PA-O1A	-2.81	1.41	1.50
4	D	392	T1C	C9-N9	-2.79	1.36	1.41
4	C	392	T1C	C1B-C11	-2.77	1.40	1.46
3	C	389	FAD	C4A-N9A	-2.76	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	392	T1C	C1B-C12	2.73	1.39	1.36
4	D	392	T1C	C7-N7	-2.72	1.35	1.42
3	A	389	FAD	C8A-N7A	2.70	1.36	1.31
4	A	392	T1C	C9-N9	-2.69	1.36	1.41
3	A	389	FAD	C6-C5X	-2.68	1.35	1.40
4	A	392	T1C	C1C-C1	2.67	1.58	1.55
4	A	392	T1C	C7-N7	-2.65	1.35	1.42
4	B	392	T1C	C9-N9	-2.64	1.36	1.41
4	C	392	T1C	C1A-C11	-2.63	1.39	1.46
4	B	392	T1C	C4-C3	2.61	1.56	1.51
3	B	389	FAD	C5X-N5	-2.61	1.34	1.39
3	D	389	FAD	C4A-N9A	-2.60	1.32	1.37
3	D	389	FAD	C5A-C6A	2.60	1.48	1.41
4	D	392	T1C	C7-C61	2.59	1.43	1.40
3	B	389	FAD	C4X-N5	2.58	1.36	1.30
4	A	392	T1C	C1B-C12	2.58	1.39	1.36
4	B	392	T1C	O1C-C1C	2.57	1.46	1.42
3	A	389	FAD	C4'-C3'	-2.54	1.49	1.53
4	B	392	T1C	C7-N7	-2.54	1.35	1.42
4	D	392	T1C	C1B-C11	-2.53	1.41	1.46
4	D	392	T1C	C1B-C12	2.49	1.39	1.36
3	C	389	FAD	C4'-C3'	-2.46	1.49	1.53
3	D	389	FAD	C4'-C3'	-2.43	1.49	1.53
3	B	389	FAD	C1B-N9A	-2.39	1.39	1.46
4	D	392	T1C	C1A-C11	-2.35	1.40	1.46
3	B	389	FAD	O4B-C4B	-2.32	1.39	1.45
3	A	389	FAD	O4-C4	2.30	1.27	1.23
3	A	389	FAD	C5A-C6A	2.29	1.47	1.41
3	D	389	FAD	C4X-N5	2.28	1.35	1.30
4	A	392	T1C	C1B-C11	-2.28	1.41	1.46
4	A	392	T1C	C2-C1	-2.23	1.40	1.46
4	C	392	T1C	C1C-C1	2.23	1.58	1.55
3	C	389	FAD	C8M-C8	2.16	1.55	1.51
4	A	392	T1C	C4-C3	2.12	1.55	1.51
3	D	389	FAD	O4-C4	2.12	1.27	1.23
3	D	389	FAD	C4X-C10	2.09	1.50	1.44
3	B	389	FAD	C1'-C2'	2.08	1.55	1.52
4	C	392	T1C	C92-C91	2.08	1.58	1.52
3	D	389	FAD	O4B-C1B	2.08	1.46	1.42
3	A	389	FAD	C5'-C4'	2.07	1.54	1.51
4	D	392	T1C	C2-C1	-2.03	1.40	1.46
3	B	389	FAD	P-O1P	2.02	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	389	FAD	P-O3P	2.02	1.61	1.59

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	392	T1C	O12-C12-C1C	7.03	123.55	113.37
3	D	389	FAD	C5'-C4'-C3'	-7.02	98.97	112.22
4	C	392	T1C	C1C-C1-C2	6.35	125.83	115.75
3	C	389	FAD	C5A-C4A-N3A	-6.10	118.32	126.72
3	A	389	FAD	C5'-C4'-C3'	-5.73	101.40	112.22
3	B	389	FAD	N3A-C4A-N9A	5.61	136.71	127.17
3	B	389	FAD	C5A-C4A-N3A	-5.60	119.01	126.72
3	B	389	FAD	C4A-N9A-C8A	5.55	111.57	105.74
4	D	392	T1C	C1C-C1-C2	5.44	124.40	115.75
4	D	392	T1C	C61-C7-N7	5.33	125.23	118.87
3	C	389	FAD	O2-C2-N1	-5.18	113.19	121.80
4	B	392	T1C	C42-N4-C4	-5.15	102.37	114.10
3	B	389	FAD	O3P-P-O1P	-5.03	95.57	110.70
4	A	392	T1C	C43-N4-C4	-4.88	102.98	114.10
3	B	389	FAD	N9A-C8A-N7A	-4.81	107.11	113.94
3	C	389	FAD	N9A-C8A-N7A	-4.77	107.16	113.94
3	A	389	FAD	C5A-C4A-N3A	-4.72	120.22	126.72
3	C	389	FAD	C2A-N3A-C4A	4.68	123.25	111.83
4	A	392	T1C	C1C-C1-C2	4.65	123.13	115.75
3	D	389	FAD	C5A-C4A-N3A	-4.59	120.39	126.72
4	B	392	T1C	C41-C1C-C1	4.53	116.24	111.05
4	D	392	T1C	C8-C7-N7	-4.46	113.95	120.89
3	C	389	FAD	O3'-C3'-C4'	-4.40	98.93	108.93
3	C	389	FAD	N3A-C2A-N1A	-4.34	122.01	128.58
4	A	392	T1C	O1C-C1C-C12	-4.30	103.27	110.14
3	D	389	FAD	N3A-C2A-N1A	-4.23	122.17	128.58
4	C	392	T1C	O12-C12-C1C	4.22	119.48	113.37
3	C	389	FAD	C4A-N9A-C8A	4.22	110.17	105.74
3	D	389	FAD	N9A-C8A-N7A	-4.16	108.03	113.94
3	B	389	FAD	C5X-C9A-N10	4.11	121.68	117.97
3	A	389	FAD	O3P-PA-O1A	-4.03	98.58	110.70
3	C	389	FAD	N3A-C4A-N9A	4.02	134.00	127.17
4	B	392	T1C	C1C-C1-C2	3.98	122.08	115.75
3	A	389	FAD	N3A-C4A-N9A	3.93	133.86	127.17
4	A	392	T1C	C1-C1C-C12	3.81	114.34	109.88
3	D	389	FAD	O3'-C3'-C4'	-3.74	100.42	108.93
4	C	392	T1C	C42-N4-C4	-3.70	105.67	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	389	FAD	C4A-N9A-C8A	3.69	109.62	105.74
4	B	392	T1C	C21-C2-C1	-3.68	116.61	120.97
4	D	392	T1C	O12-C12-C1C	3.64	118.64	113.37
3	B	389	FAD	O4-C4-C4X	-3.56	117.15	126.53
4	B	392	T1C	O12-C12-C1B	-3.53	116.68	123.52
4	C	392	T1C	O12-C12-C1B	-3.48	116.77	123.52
4	A	392	T1C	O1-C1-C2	-3.47	115.89	123.23
3	D	389	FAD	C4A-C5A-N7A	-3.46	106.62	110.58
3	A	389	FAD	O4B-C1B-N9A	-3.46	101.45	108.09
3	C	389	FAD	C4-C4X-N5	3.45	122.97	118.21
3	D	389	FAD	C2A-N3A-C4A	3.44	120.23	111.83
3	D	389	FAD	O2-C2-N1	-3.41	116.14	121.80
3	B	389	FAD	C2A-N3A-C4A	3.37	120.06	111.83
4	D	392	T1C	O12-C12-C1B	-3.36	117.00	123.52
4	D	392	T1C	C8-C9-C10	-3.36	117.27	120.53
3	A	389	FAD	O4-C4-C4X	-3.31	117.80	126.53
3	C	389	FAD	C4A-C5A-N7A	-3.30	106.81	110.58
4	B	392	T1C	O1C-C1C-C12	-3.27	104.91	110.14
3	D	389	FAD	C5A-N7A-C8A	3.26	108.58	103.45
4	A	392	T1C	C21-C2-C1	-3.24	117.13	120.97
4	B	392	T1C	C1C-C12-C1B	-3.24	119.77	123.06
3	C	389	FAD	C4A-N9A-C1B	-3.23	119.08	126.63
3	A	389	FAD	O3B-C3B-C2B	-3.18	101.61	111.82
3	A	389	FAD	O2-C2-N1	-3.15	116.56	121.80
3	B	389	FAD	O5B-C5B-C4B	-3.15	98.27	108.99
3	D	389	FAD	N3A-C4A-N9A	3.14	132.50	127.17
3	A	389	FAD	C2A-N3A-C4A	3.13	119.47	111.83
4	C	392	T1C	O1-C1-C2	-3.12	116.64	123.23
3	B	389	FAD	N3A-C2A-N1A	-3.12	123.86	128.58
4	A	392	T1C	O12-C12-C1C	3.11	117.88	113.37
3	D	389	FAD	C4-C4X-N5	3.09	122.47	118.21
3	C	389	FAD	C5A-N7A-C8A	3.03	108.21	103.45
4	D	392	T1C	O1C-C1C-C12	-3.02	105.31	110.14
3	C	389	FAD	O5'-P-O1P	3.01	120.85	108.94
4	B	392	T1C	O11-C11-C1B	-3.00	115.92	121.14
3	A	389	FAD	N3A-C2A-N1A	-3.00	124.04	128.58
3	A	389	FAD	O4-C4-N3	2.96	125.67	120.11
3	D	389	FAD	C4A-N9A-C1B	-2.91	119.81	126.63
3	D	389	FAD	C2A-N1A-C6A	2.91	123.51	118.73
4	D	392	T1C	O1-C1-C2	-2.91	117.09	123.23
4	C	392	T1C	C8-C9-C10	-2.90	117.72	120.53
3	C	389	FAD	C2B-C1B-N9A	-2.89	106.13	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	389	FAD	O4-C4-C4X	-2.86	118.98	126.53
3	C	389	FAD	O2-C2-N3	2.83	124.01	118.58
4	C	392	T1C	O1C-C1C-C12	-2.83	105.62	110.14
3	D	389	FAD	C6A-C5A-N7A	2.80	137.49	132.09
3	A	389	FAD	C4A-N9A-C8A	2.80	108.68	105.74
3	D	389	FAD	O4'-C4'-C5'	2.80	116.16	109.99
4	B	392	T1C	C1-C1C-C12	2.79	113.15	109.88
3	C	389	FAD	C5'-C4'-C3'	-2.79	106.96	112.22
4	B	392	T1C	C11-C1B-C12	-2.73	116.64	118.80
4	C	392	T1C	C1-C1C-C12	-2.71	106.70	109.88
3	A	389	FAD	N9A-C8A-N7A	-2.71	110.10	113.94
3	C	389	FAD	O3P-P-O1P	-2.60	102.88	110.70
3	D	389	FAD	O3B-C3B-C2B	-2.56	103.60	111.82
4	A	392	T1C	C8-C9-C10	-2.54	118.06	120.53
4	D	392	T1C	C1A-C11-C1B	2.54	123.04	118.28
4	A	392	T1C	O11-C11-C1B	-2.54	116.73	121.14
3	B	389	FAD	C4X-C4-N3	2.54	119.71	113.25
3	B	389	FAD	O2P-P-O1P	2.53	124.22	112.44
3	D	389	FAD	O4-C4-C4X	-2.51	119.90	126.53
3	D	389	FAD	C4'-C3'-C2'	-2.50	109.41	113.57
3	B	389	FAD	C4-C4X-C10	-2.48	112.67	116.93
4	A	392	T1C	C1A-C11-C1B	2.48	122.92	118.28
3	B	389	FAD	C5A-N7A-C8A	2.43	107.27	103.45
3	D	389	FAD	O4-C4-N3	2.42	124.66	120.11
3	C	389	FAD	C6A-C5A-N7A	2.42	136.75	132.09
4	A	392	T1C	C5-C41-C4	2.41	117.22	113.73
3	B	389	FAD	C9A-N10-C10	-2.35	117.16	120.75
3	B	389	FAD	C1B-N9A-C8A	-2.35	121.88	127.09
4	D	392	T1C	O11-C11-C1A	-2.35	117.82	122.06
4	D	392	T1C	C43-N4-C4	-2.32	108.81	114.10
4	B	392	T1C	C8-C9-C10	-2.30	118.30	120.53
3	C	389	FAD	C9A-C5X-N5	-2.30	120.01	122.45
3	D	389	FAD	C2B-C3B-C4B	2.29	107.03	102.61
4	D	392	T1C	C42-N4-C4	-2.28	108.91	114.10
3	A	389	FAD	O2P-P-O3P	2.28	113.42	107.27
3	C	389	FAD	O4-C4-N3	2.27	124.39	120.11
3	A	389	FAD	O3'-C3'-C4'	-2.27	103.78	108.93
3	B	389	FAD	O3'-C3'-C2'	-2.26	103.78	108.93
3	B	389	FAD	C5X-N5-C4X	-2.24	114.47	118.09
3	C	389	FAD	O3P-PA-O1A	-2.23	103.98	110.70
4	B	392	T1C	O1C-C1C-C41	-2.23	104.38	109.30
3	D	389	FAD	O2P-P-O1P	-2.23	102.09	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	392	T1C	C1A-C11-C1B	2.23	122.45	118.28
3	B	389	FAD	O2A-PA-O3P	2.21	113.25	107.27
3	A	389	FAD	C6-C5X-N5	2.21	122.11	118.44
4	B	392	T1C	O1C-C1C-C1	-2.19	100.09	106.35
3	D	389	FAD	C7M-C7-C6	-2.19	115.71	119.57
4	C	392	T1C	O11-C11-C1A	-2.16	118.15	122.06
4	B	392	T1C	C72-N7-C71	-2.14	109.31	116.18
3	A	389	FAD	C4'-C3'-C2'	-2.14	110.01	113.57
3	B	389	FAD	C5B-C4B-C3B	-2.14	107.52	115.21
3	D	389	FAD	O2A-PA-O1A	2.14	122.38	112.44
3	B	389	FAD	O2P-P-O3P	2.12	113.01	107.27
3	A	389	FAD	O3P-P-O1P	-2.12	104.34	110.70
4	D	392	T1C	C72-N7-C71	-2.11	109.39	116.18
3	A	389	FAD	C8M-C8-C7	2.09	125.03	120.76
3	A	389	FAD	O4'-C4'-C3'	2.03	114.00	109.25

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	392	T1C	C41-C4-N4-C42
4	D	392	T1C	C94-C93-N92-C92
4	D	392	T1C	C95-C93-N92-C92
4	D	392	T1C	C41-C4-N4-C43
4	D	392	T1C	C96-C93-N92-C92
4	D	392	T1C	C61-C7-N7-C72
4	D	392	T1C	C8-C7-N7-C72
4	C	392	T1C	C96-C93-N92-C92
3	C	389	FAD	PA-O3P-P-O5'
3	D	389	FAD	PA-O3P-P-O5'
4	A	392	T1C	C3-C4-N4-C43
4	A	392	T1C	C3-C4-N4-C42
4	C	392	T1C	C95-C93-N92-C92
4	A	392	T1C	C91-C92-N92-C93
4	D	392	T1C	C91-C92-N92-C93
3	D	389	FAD	P-O3P-PA-O2A
4	C	392	T1C	C94-C93-N92-C92
3	D	389	FAD	C2B-C1B-N9A-C8A
3	D	389	FAD	P-O3P-PA-O1A
3	B	389	FAD	O2'-C2'-C3'-C4'
3	B	389	FAD	C2B-C1B-N9A-C8A
3	D	389	FAD	O4B-C4B-C5B-O5B

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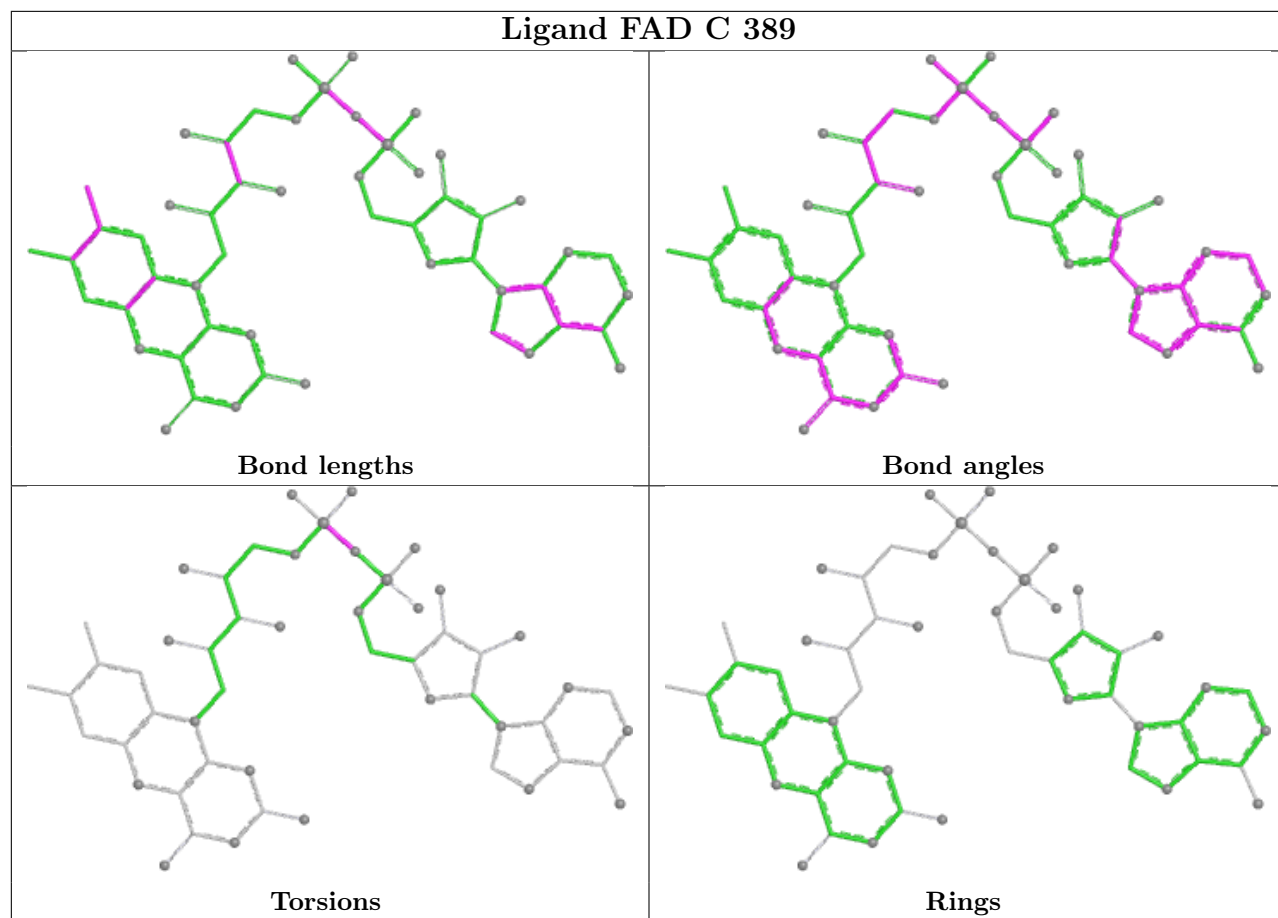
Mol	Chain	Res	Type	Atoms
3	A	389	FAD	C2B-C1B-N9A-C8A

There are no ring outliers.

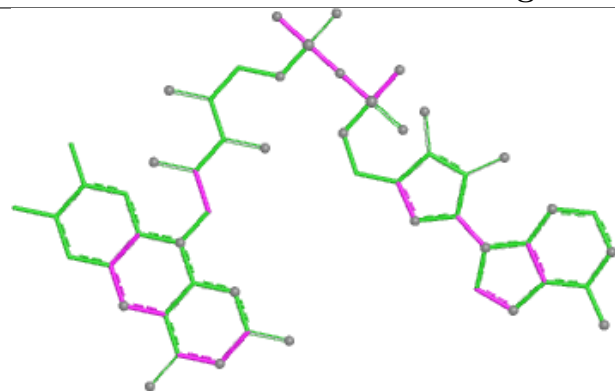
7 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	389	FAD	7	0
3	A	389	FAD	4	0
4	B	392	T1C	6	0
4	D	392	T1C	15	0
4	A	392	T1C	11	0
4	C	392	T1C	5	0
3	D	389	FAD	1	0

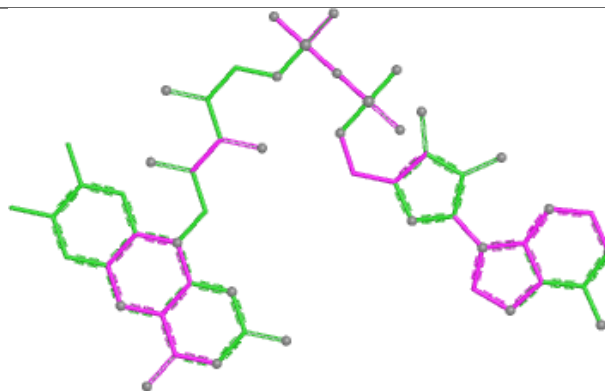
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



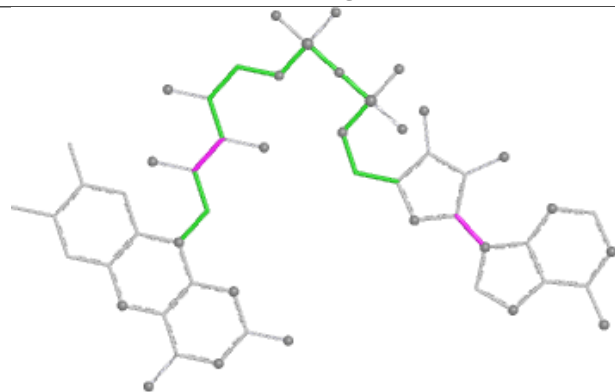
Ligand FAD B 389



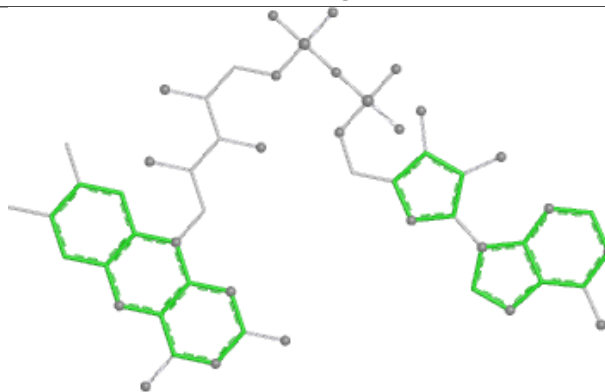
Bond lengths



Bond angles

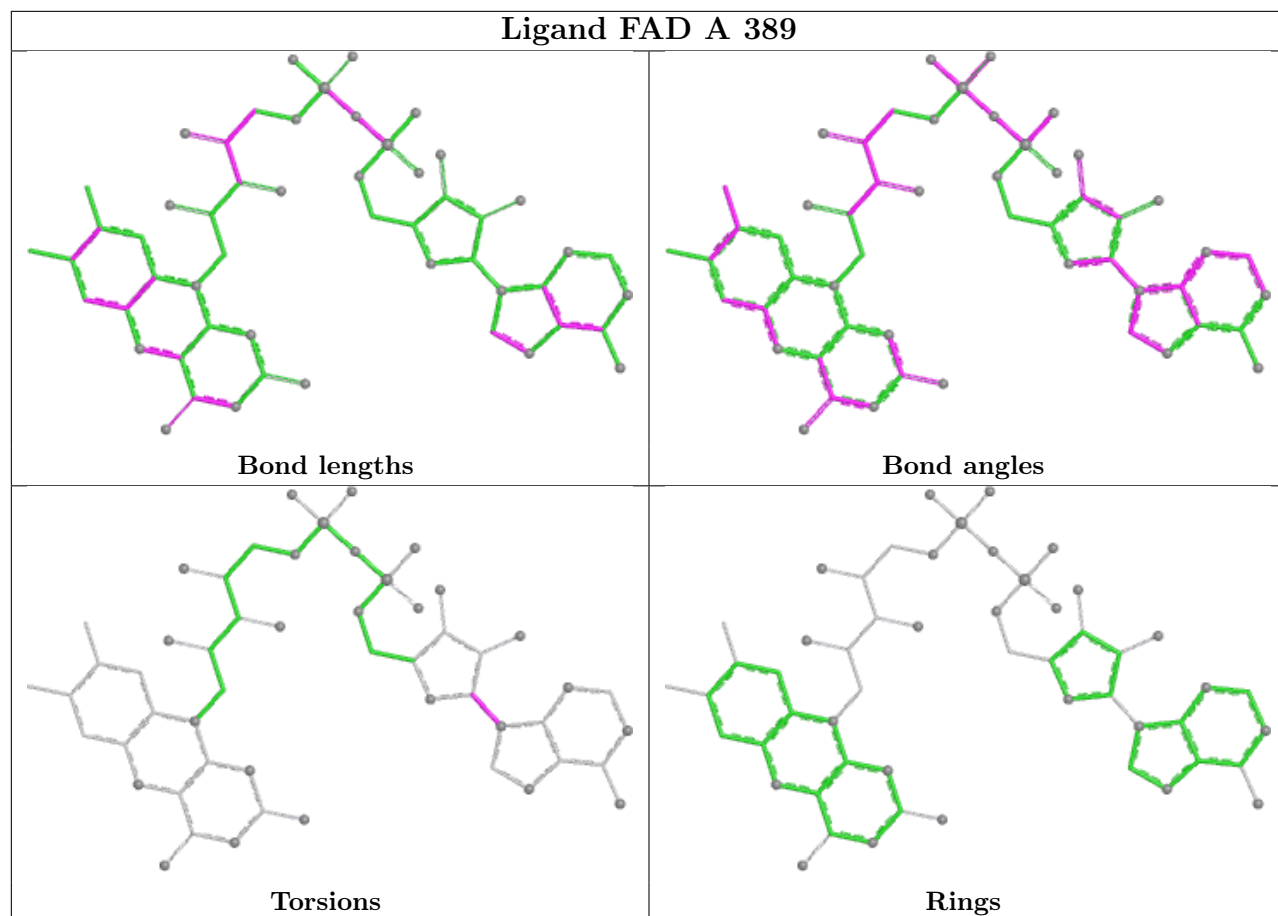


Torsions

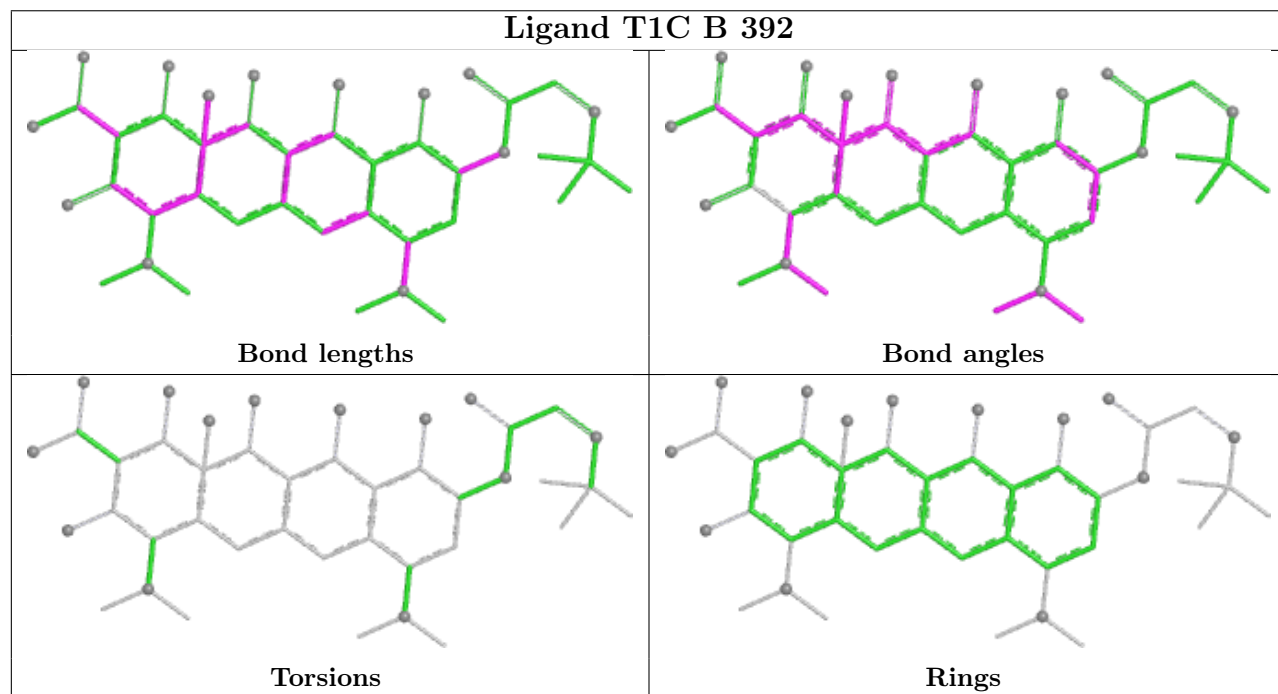


Rings

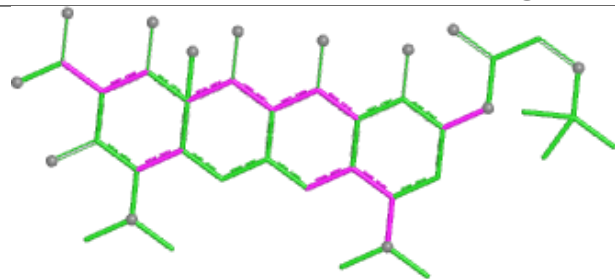
Ligand FAD A 389



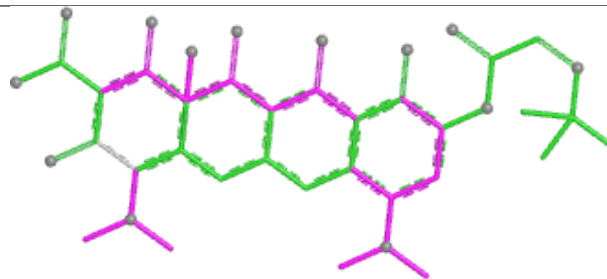
Ligand T1C B 392



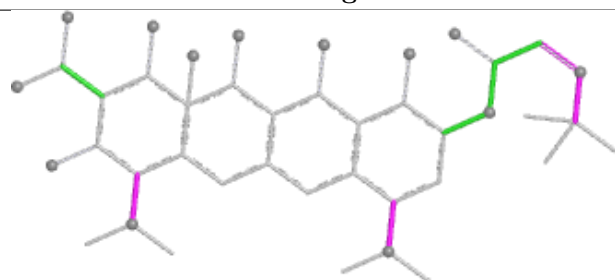
Ligand T1C D 392



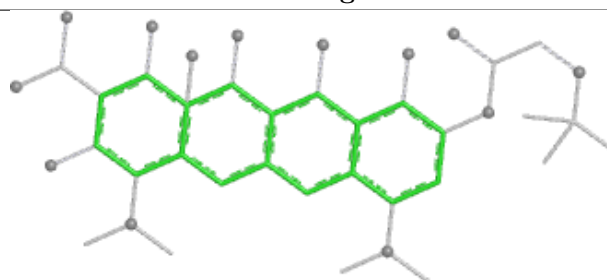
Bond lengths



Bond angles

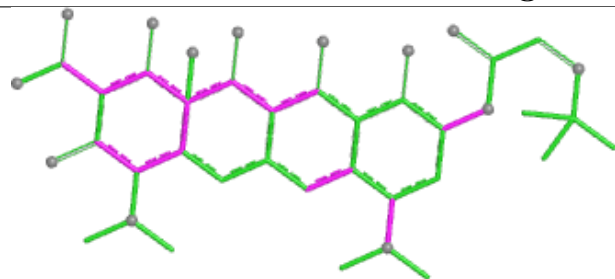


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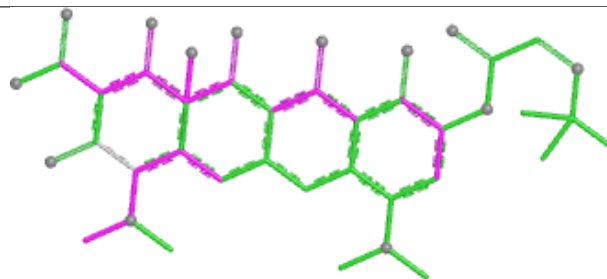


Rings

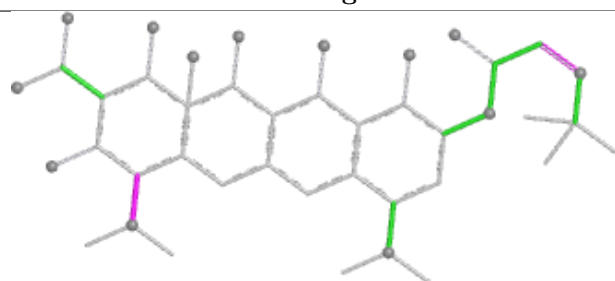
Ligand T1C A 392



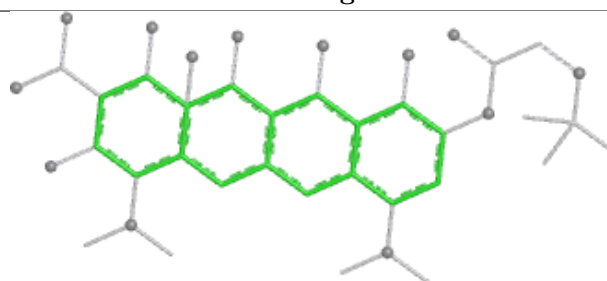
Bond lengths



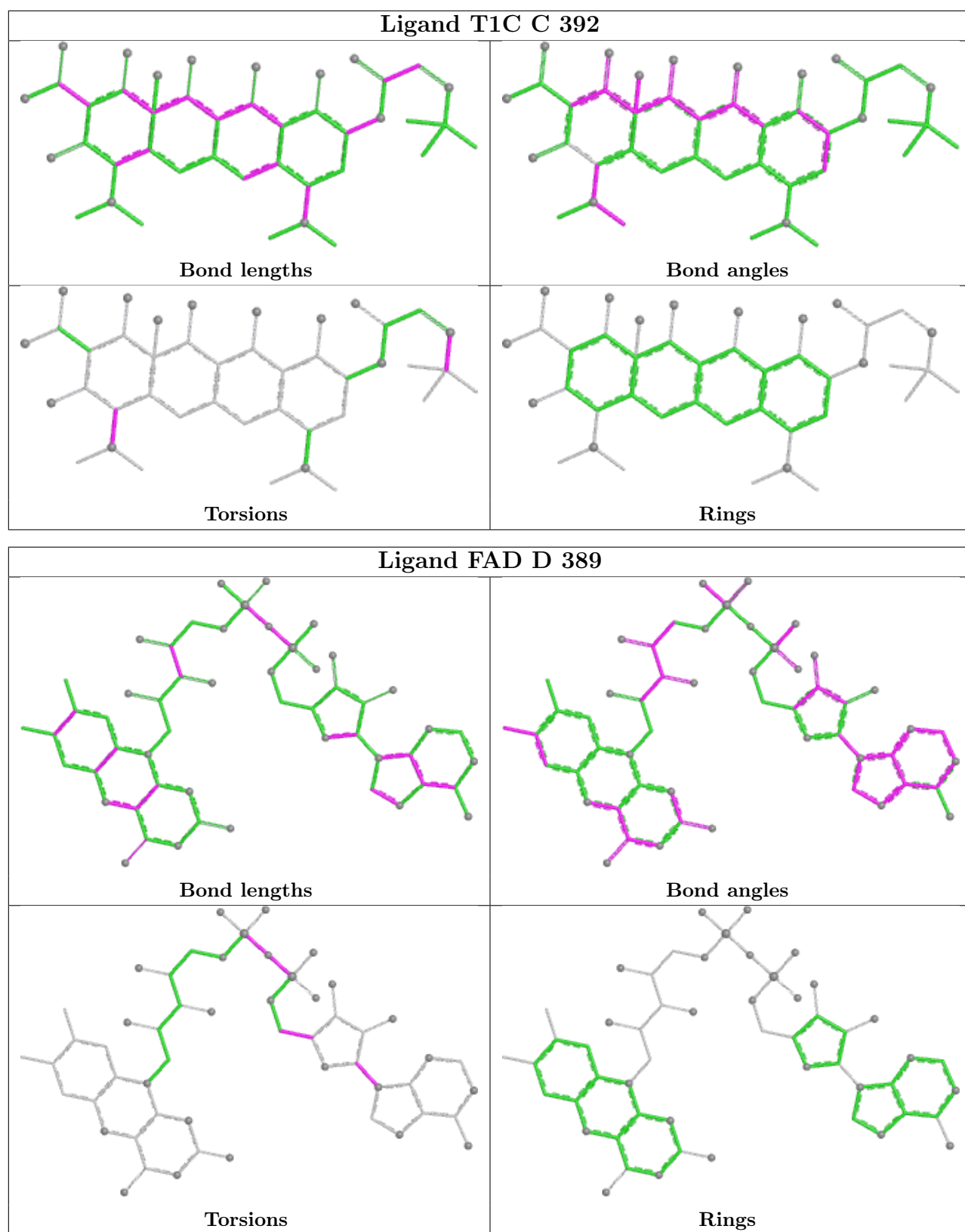
Bond angles



Torsions



Rings



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	368/398 (92%)	0.96	43 (11%) 9 10	43, 62, 96, 142	0
2	B	368/398 (92%)	0.95	43 (11%) 9 10	45, 63, 95, 130	0
2	C	367/398 (92%)	1.27	59 (16%) 4 5	53, 75, 111, 156	0
2	D	367/398 (92%)	1.27	64 (17%) 4 4	50, 75, 115, 144	0
All	All	1470/1592 (92%)	1.11	209 (14%) 6 7	43, 69, 108, 156	0

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	220	GLY	6.3
2	B	341	GLY	5.3
1	A	343	PHE	4.9
1	A	378	PRO	4.7
1	A	381	THR	4.4
2	D	110	PHE	4.4
1	A	376	PHE	4.3
2	C	42	VAL	4.2
1	A	341	GLY	4.2
2	C	341	GLY	4.2
2	D	147	LYS	4.2
2	D	250	GLN	4.1
1	A	145	GLY	3.8
2	D	378	PRO	3.7
2	B	343	PHE	3.7
2	C	13	LEU	3.7
2	C	217	SER	3.7
1	A	287	LEU	3.6
2	D	381	THR	3.6
2	C	287	LEU	3.5
2	D	339	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	12	ASN	3.5
1	A	322	GLN	3.5
2	C	378	PRO	3.5
1	A	268	SER	3.5
2	D	364	ALA	3.4
2	D	336	ASP	3.4
2	B	249	THR	3.3
2	D	379	ASP	3.3
1	A	249	THR	3.3
2	C	381	THR	3.2
2	C	57	GLY	3.2
2	C	250	GLN	3.2
2	B	174	VAL	3.1
2	C	191	ILE	3.1
2	D	191	ILE	3.1
2	C	146	LYS	3.1
2	C	376	PHE	3.1
2	D	353	TYR	3.1
2	B	376	PHE	3.1
2	B	268	SER	3.1
2	C	110	PHE	3.0
2	D	297	PRO	3.0
2	C	59	THR	3.0
1	A	355	GLN	3.0
2	B	333	ILE	3.0
1	A	382	PHE	3.0
2	D	59	THR	3.0
1	A	352	ASN	3.0
2	C	343	PHE	2.9
1	A	351	LYS	2.9
2	D	359	ILE	2.9
2	D	360	TYR	2.9
2	C	147	LYS	2.9
1	A	124	LEU	2.9
2	D	322	GLN	2.9
2	B	245	TRP	2.9
2	C	279	HIS	2.8
2	D	287	LEU	2.8
2	C	380	PHE	2.8
2	D	320	ALA	2.8
1	A	359	ILE	2.8
1	A	38	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	13	LEU	2.8
2	D	292	PHE	2.8
2	B	287	LEU	2.8
2	D	245	TRP	2.8
2	C	106	PRO	2.8
1	A	342	LYS	2.7
2	B	13	LEU	2.7
2	C	340	ASP	2.7
1	A	14	LEU	2.7
2	D	343	PHE	2.7
1	A	340	ASP	2.7
2	B	146	LYS	2.7
2	C	301	LYS	2.7
2	C	14	LEU	2.6
1	A	12	ASN	2.6
1	A	113	PRO	2.6
2	B	147	LYS	2.6
2	D	16	ASP	2.6
2	D	38	ASN	2.6
2	B	39	GLY	2.6
2	D	380	PHE	2.6
2	C	40	ILE	2.6
2	C	368	SER	2.6
2	D	268	SER	2.6
2	C	245	TRP	2.5
2	B	382	PHE	2.5
1	A	147	LYS	2.5
2	D	81	TYR	2.5
2	B	310	GLY	2.5
2	C	346	ILE	2.5
2	D	146	LYS	2.5
2	D	269	ASP	2.5
2	D	341	GLY	2.5
2	D	166	LEU	2.5
2	B	342	LYS	2.5
2	C	112	ASN	2.5
1	A	321	GLY	2.5
2	B	37	GLN	2.5
2	C	15	SER	2.4
2	B	278	ILE	2.4
1	A	13	LEU	2.4
2	D	277	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	377	LYS	2.4
2	C	296	LYS	2.4
2	B	378	PRO	2.4
2	C	292	PHE	2.4
1	A	146	LYS	2.4
2	D	349	ALA	2.4
2	D	319	PHE	2.4
2	C	47	ARG	2.4
2	D	207	GLN	2.4
1	A	108	ASN	2.4
2	B	340	ASP	2.4
2	B	339	ALA	2.4
2	C	265	LYS	2.4
2	D	368	SER	2.4
2	D	177	PHE	2.4
1	A	37	GLN	2.4
2	C	322	GLN	2.4
2	B	220	GLY	2.3
2	D	101	THR	2.3
1	A	158	SER	2.3
2	D	14	LEU	2.3
2	B	243	ASP	2.3
2	D	296	LYS	2.3
2	D	323	GLY	2.3
2	C	163	LEU	2.3
2	C	263	LEU	2.3
2	B	180	ASP	2.3
2	C	111	ASP	2.3
2	D	162	ASP	2.3
2	C	317	PRO	2.3
2	D	321	GLY	2.3
2	D	217	SER	2.3
2	C	36	GLN	2.3
2	B	19	VAL	2.3
2	C	19	VAL	2.3
2	C	178	VAL	2.3
2	D	57	GLY	2.3
2	C	377	LYS	2.3
1	A	163	LEU	2.2
2	B	183	VAL	2.3
2	C	183	VAL	2.3
1	A	337	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	38	ASN	2.2
2	C	108	ASN	2.2
2	C	330	ASP	2.2
1	A	375	MET	2.2
2	D	366	GLU	2.2
2	D	298	TRP	2.2
2	D	104	VAL	2.2
2	D	178	VAL	2.2
2	B	103	ASN	2.2
2	C	321	GLY	2.2
2	D	367	GLU	2.2
2	B	320	ALA	2.2
1	A	15	SER	2.2
2	D	123	ILE	2.2
2	D	382	PHE	2.2
1	A	366	GLU	2.2
1	A	320	ALA	2.2
2	B	288	ALA	2.2
2	C	364	ALA	2.2
2	B	217	SER	2.2
2	B	163	LEU	2.2
2	B	257	ASN	2.2
2	D	318	PRO	2.2
2	D	244	GLU	2.2
1	A	245	TRP	2.1
2	B	277	LEU	2.1
2	B	309	ILE	2.1
2	C	278	ILE	2.1
2	D	346	ILE	2.1
2	B	108	ASN	2.1
2	B	162	ASP	2.1
2	D	342	LYS	2.1
2	D	300	SER	2.1
2	C	72	LYS	2.1
2	D	111	ASP	2.1
1	A	380	PHE	2.1
2	D	376	PHE	2.1
1	A	193	ALA	2.1
2	B	102	LYS	2.1
1	A	332	LEU	2.1
2	B	200	ILE	2.1
2	C	221	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	237	ILE	2.1
2	C	353	TYR	2.1
2	D	103	ASN	2.1
1	A	36	GLN	2.1
2	C	382	PHE	2.1
2	D	160	THR	2.1
2	B	112	ASN	2.1
2	C	41	ASP	2.1
2	D	98	ILE	2.1
2	B	350	VAL	2.1
2	C	277	LEU	2.0
2	D	352	ASN	2.0
2	C	319	PHE	2.0
2	B	276	GLU	2.0
2	C	345	SER	2.0
2	C	370	GLN	2.0
1	A	112	ASN	2.0
2	B	212	ASN	2.0
2	D	190	ASN	2.0
1	A	265	LYS	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(Å ²)	Q<0.9
4	T1C	C	392	42/42	0.55	0.21	77,120,163,175	0
5	SO4	D	1383	5/5	0.62	0.10	117,119,129,130	0
5	SO4	B	1385	5/5	0.65	0.12	105,109,124,129	0

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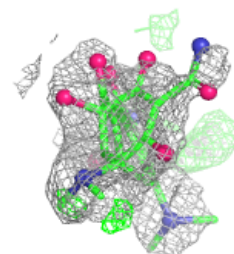
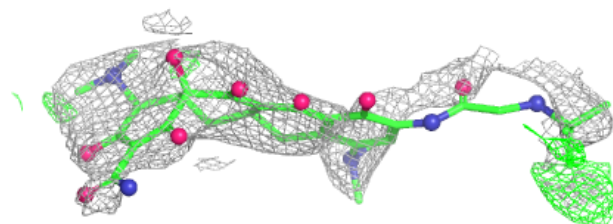
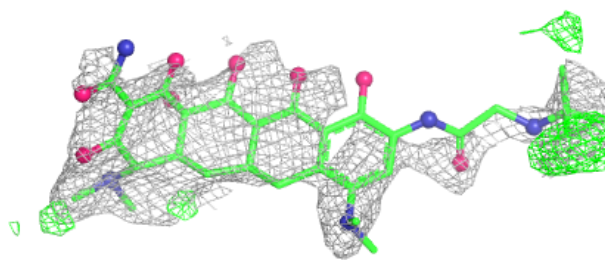
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	C	1383	5/5	0.66	0.13	99,100,115,129	0
5	SO4	A	1384	5/5	0.68	0.17	109,115,142,145	0
4	T1C	D	392	42/42	0.70	0.20	91,115,142,151	0
4	T1C	B	392	42/42	0.73	0.21	61,90,115,117	0
4	T1C	A	392	42/42	0.77	0.18	61,85,102,117	0
5	SO4	B	1386	5/5	0.78	0.09	80,96,107,108	0
5	SO4	B	1383	5/5	0.81	0.12	98,100,106,119	0
5	SO4	C	1384	5/5	0.82	0.09	90,97,107,118	0
5	SO4	D	1385	5/5	0.83	0.09	90,93,100,108	0
5	SO4	D	1384	5/5	0.85	0.11	88,88,92,98	0
5	SO4	B	1384	5/5	0.85	0.12	89,95,103,109	0
5	SO4	A	1383	5/5	0.87	0.10	94,96,104,108	0
3	FAD	B	389	53/53	0.92	0.12	33,45,58,72	0
3	FAD	C	389	53/53	0.93	0.10	36,50,62,73	0
3	FAD	D	389	53/53	0.94	0.10	39,50,61,69	0
3	FAD	A	389	53/53	0.95	0.09	30,43,53,65	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.

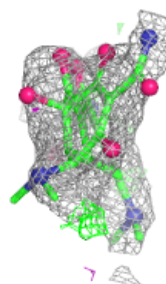
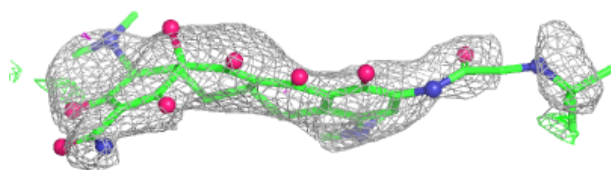
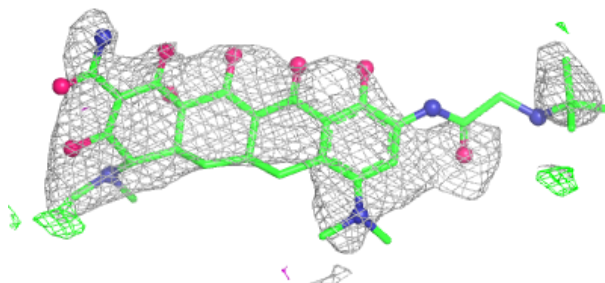
Electron density around T1C C 392:

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

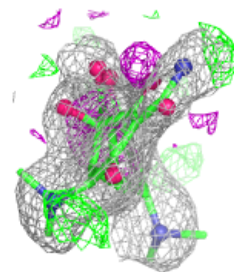
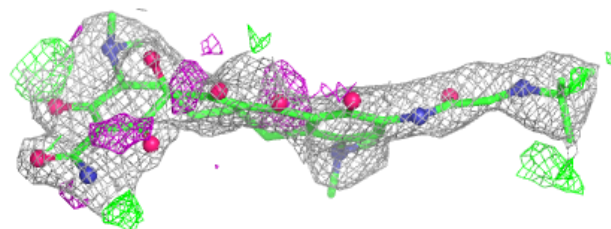
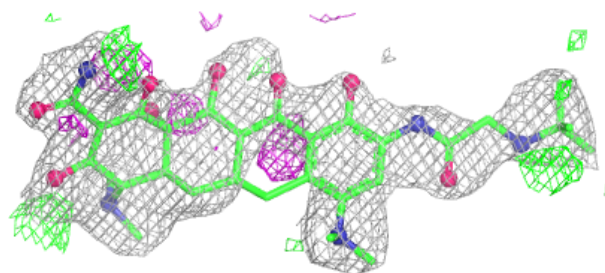


Electron density around T1C D 392:

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

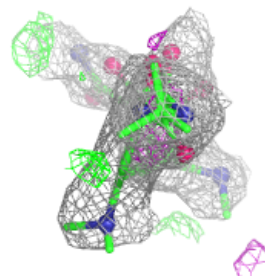
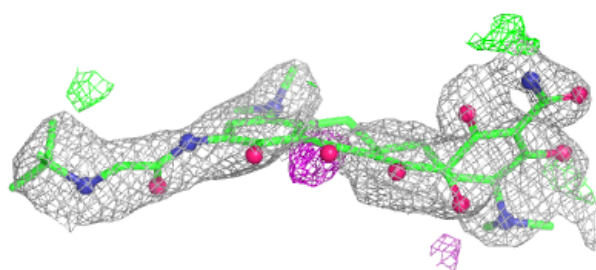
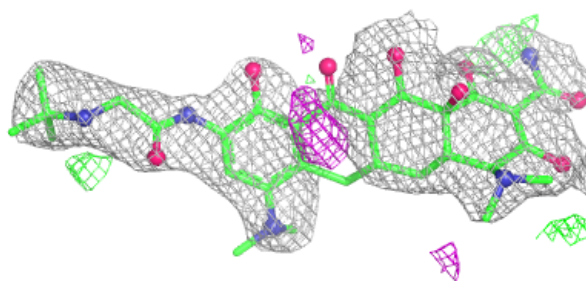
**Electron density around T1C B 392:**

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

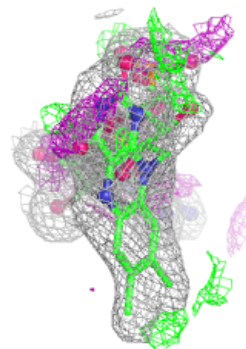
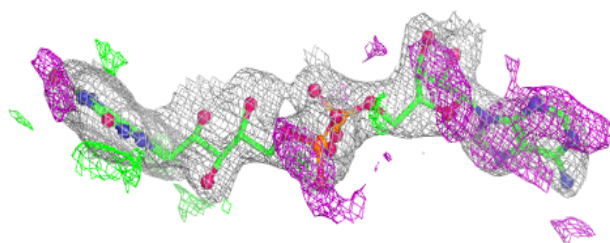
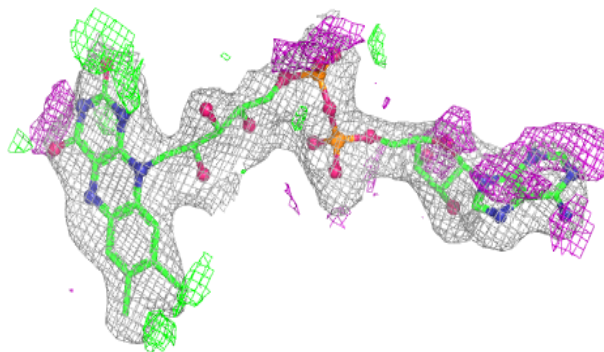


Electron density around T1C A 392:

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

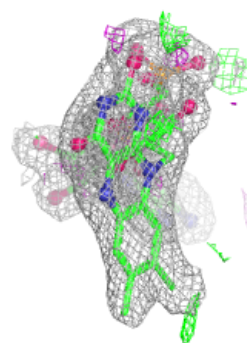
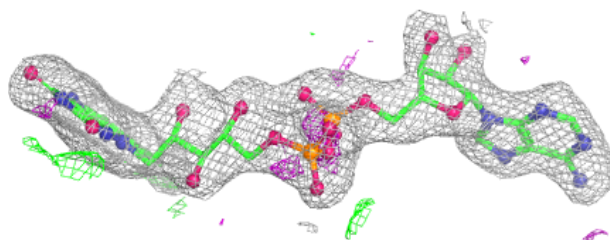
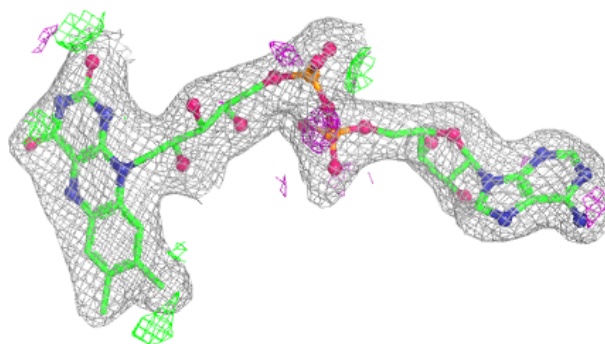
**Electron density around FAD B 389:**

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

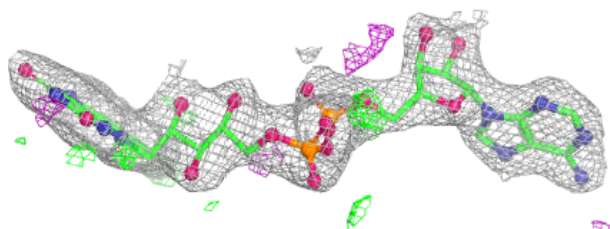
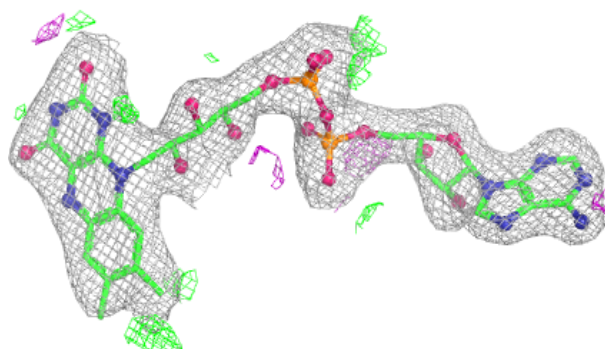


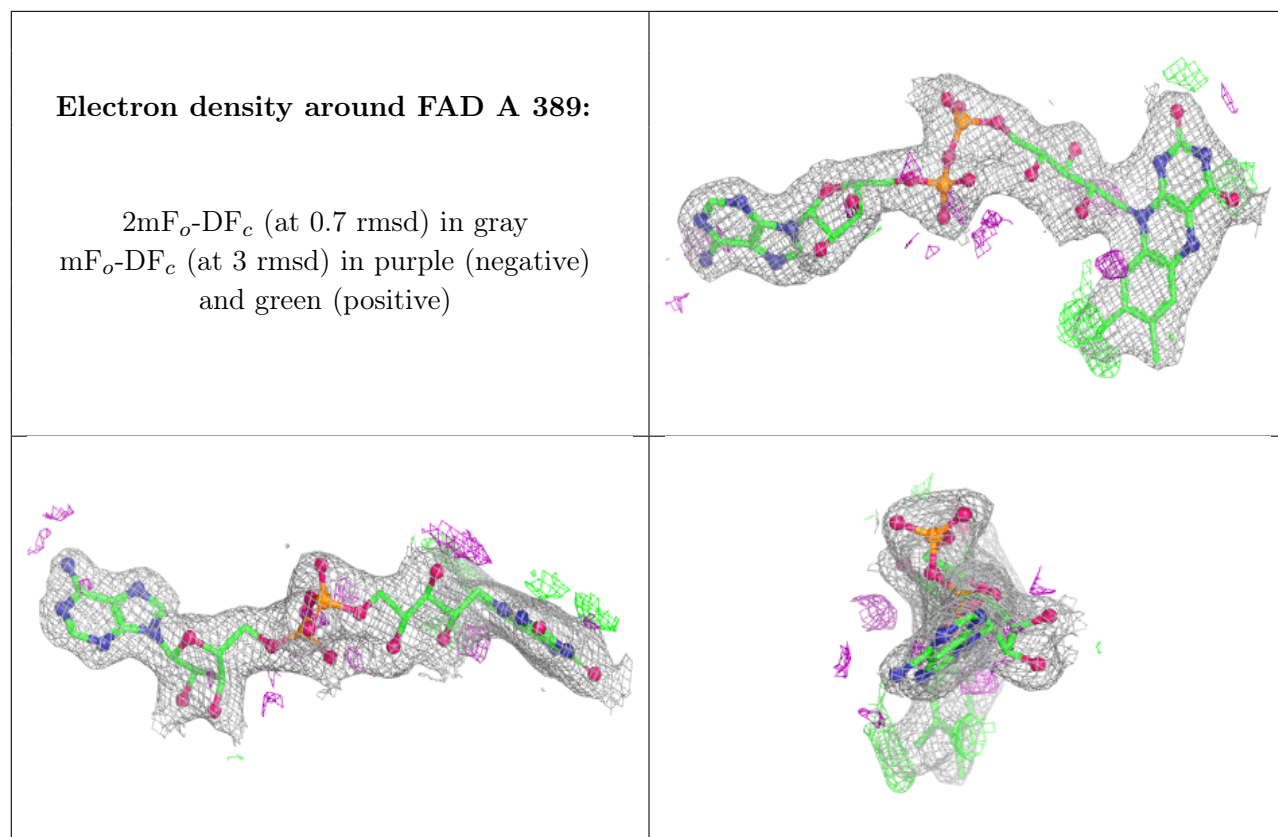
Electron density around FAD C 389:

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

**Electron density around FAD D 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.