



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:59 AM UTC

PDB ID : 4KAS / pdb_00004kas
Title : Crystal structure of FDTS from *T. maritima* mutant (H53D) with FAD and dUMP
Authors : Mathews, I.I.
Deposited on : 2013-04-22
Resolution : 1.85 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

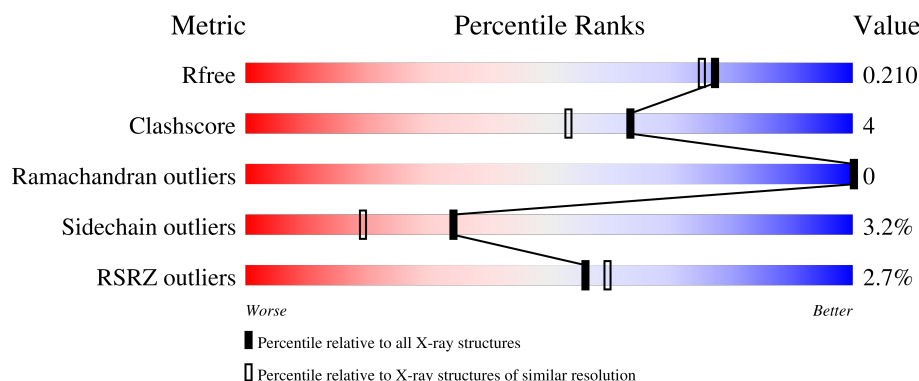
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	232	2% 81% 10% 8%
1	B	232	3% 84% 9% 6%
1	C	232	5% 84% 9% 6%
1	D	232	0% 83% 9% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DU	C	302	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7919 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 Thymidylate synthase ThyX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	4	0
			1820	1180	315	320	5			
1	B	217	Total	C	N	O	S	0	1	0
			1828	1186	312	325	5			
1	C	218	Total	C	N	O	S	0	15	0
			1953	1265	336	347	5			
1	D	214	Total	C	N	O	S	0	3	0
			1816	1181	310	320	5			

There are 52 discrepancies between the modelled and reference sequences:

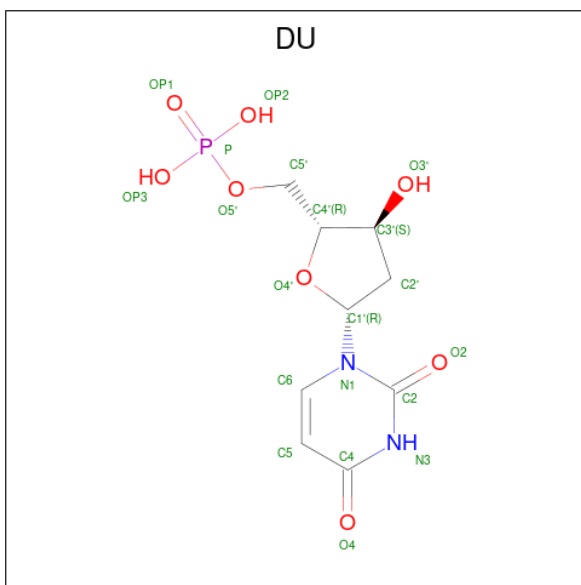
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP Q9WYT0
A	-10	GLY	-	expression tag	UNP Q9WYT0
A	-9	SER	-	expression tag	UNP Q9WYT0
A	-8	ASP	-	expression tag	UNP Q9WYT0
A	-7	LYS	-	expression tag	UNP Q9WYT0
A	-6	ILE	-	expression tag	UNP Q9WYT0
A	-5	HIS	-	expression tag	UNP Q9WYT0
A	-4	HIS	-	expression tag	UNP Q9WYT0
A	-3	HIS	-	expression tag	UNP Q9WYT0
A	-2	HIS	-	expression tag	UNP Q9WYT0
A	-1	HIS	-	expression tag	UNP Q9WYT0
A	0	HIS	-	expression tag	UNP Q9WYT0
A	53	ASP	HIS	engineered mutation	UNP Q9WYT0
B	-11	MET	-	engineered mutation	UNP Q9WYT0
B	-10	GLY	-	expression tag	UNP Q9WYT0
B	-9	SER	-	expression tag	UNP Q9WYT0
B	-8	ASP	-	expression tag	UNP Q9WYT0
B	-7	LYS	-	expression tag	UNP Q9WYT0
B	-6	ILE	-	expression tag	UNP Q9WYT0
B	-5	HIS	-	expression tag	UNP Q9WYT0
B	-4	HIS	-	expression tag	UNP Q9WYT0

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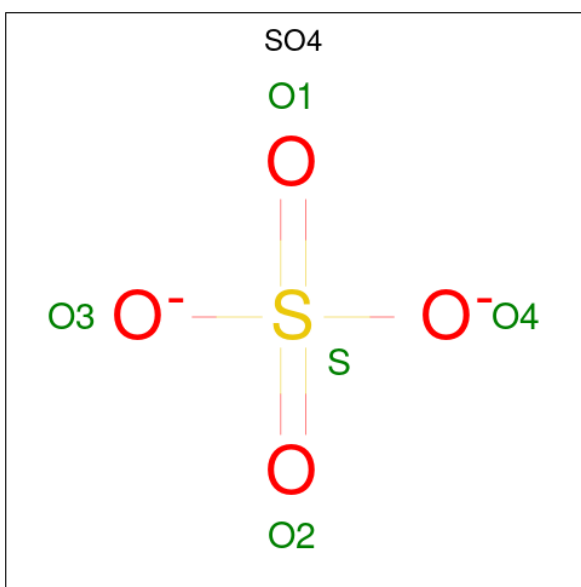
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	expression tag	UNP Q9WYT0
B	-2	HIS	-	expression tag	UNP Q9WYT0
B	-1	HIS	-	expression tag	UNP Q9WYT0
B	0	HIS	-	expression tag	UNP Q9WYT0
B	53	ASP	HIS	engineered mutation	UNP Q9WYT0
C	-11	MET	-	initiating methionine	UNP Q9WYT0
C	-10	GLY	-	expression tag	UNP Q9WYT0
C	-9	SER	-	expression tag	UNP Q9WYT0
C	-8	ASP	-	expression tag	UNP Q9WYT0
C	-7	LYS	-	expression tag	UNP Q9WYT0
C	-6	ILE	-	expression tag	UNP Q9WYT0
C	-5	HIS	-	expression tag	UNP Q9WYT0
C	-4	HIS	-	expression tag	UNP Q9WYT0
C	-3	HIS	-	expression tag	UNP Q9WYT0
C	-2	HIS	-	expression tag	UNP Q9WYT0
C	-1	HIS	-	expression tag	UNP Q9WYT0
C	0	HIS	-	expression tag	UNP Q9WYT0
C	53	ASP	HIS	engineered mutation	UNP Q9WYT0
D	-11	MET	-	initiating methionine	UNP Q9WYT0
D	-10	GLY	-	expression tag	UNP Q9WYT0
D	-9	SER	-	expression tag	UNP Q9WYT0
D	-8	ASP	-	expression tag	UNP Q9WYT0
D	-7	LYS	-	expression tag	UNP Q9WYT0
D	-6	ILE	-	expression tag	UNP Q9WYT0
D	-5	HIS	-	expression tag	UNP Q9WYT0
D	-4	HIS	-	expression tag	UNP Q9WYT0
D	-3	HIS	-	expression tag	UNP Q9WYT0
D	-2	HIS	-	expression tag	UNP Q9WYT0
D	-1	HIS	-	expression tag	UNP Q9WYT0
D	0	HIS	-	expression tag	UNP Q9WYT0
D	53	ASP	HIS	engineered mutation	UNP Q9WYT0

- Molecule 2 is 2'-DEOXYURIDINE-5'-MONOPHOSPHATE (CCD ID: DU) (formula: $C_9H_{13}N_2O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



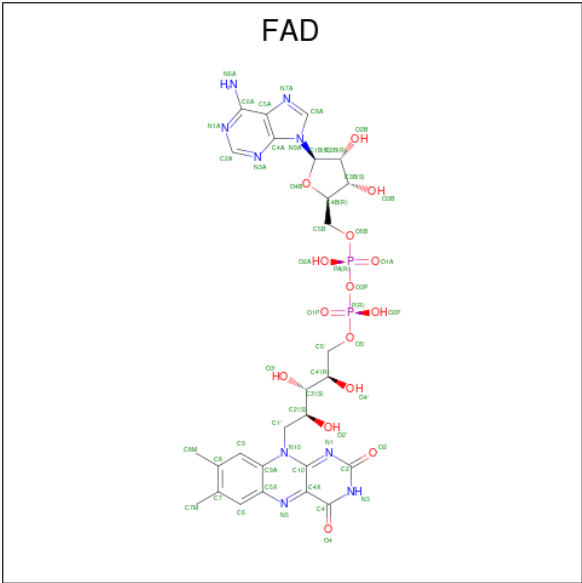
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O S	0	0
			5	4 1		

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

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).

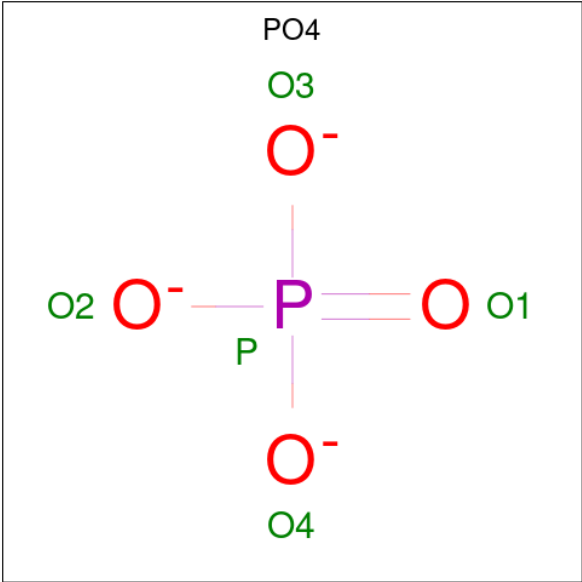


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

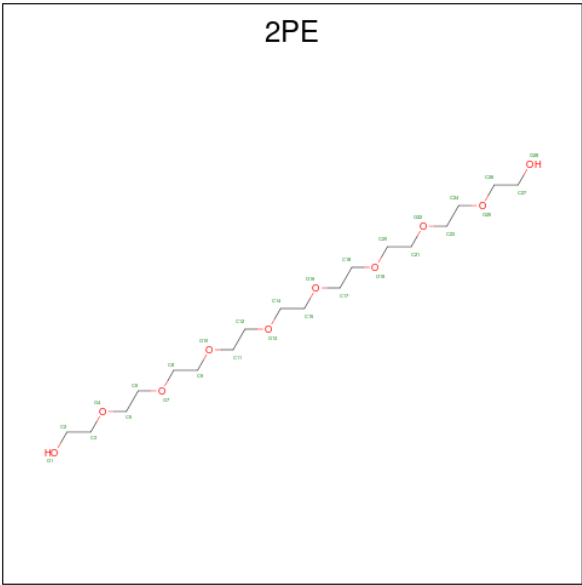
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Cl	0	0
			1	1		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 7 is NONAETHYLENE GLYCOL (CCD ID: 2PE) (formula: C₁₈H₃₈O₁₀).

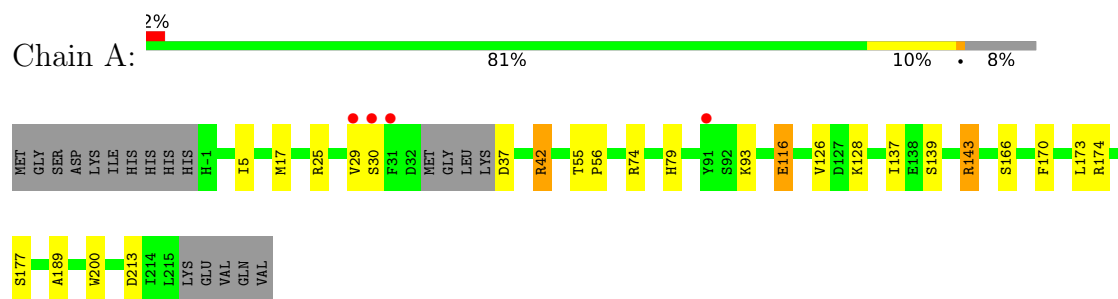


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	71	Total 72	O 72	0	1
8	B	58	Total 58	O 58	0	0
8	C	98	Total 99	O 99	0	1
8	D	78	Total 78	O 78	0	0

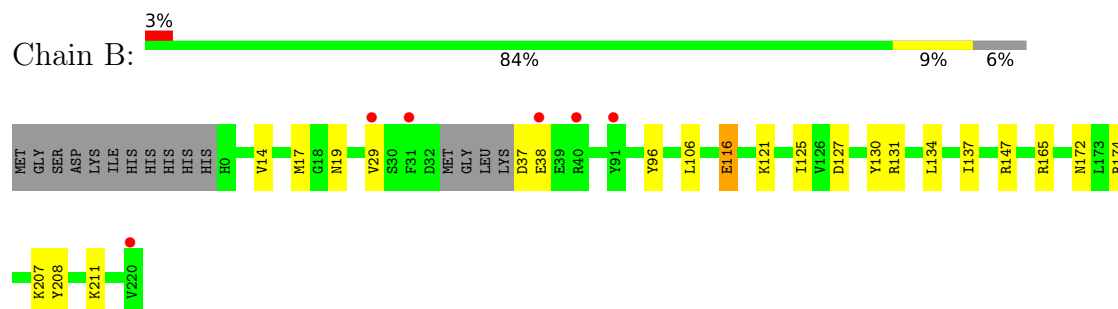
3 Residue-property plots [i](#)

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

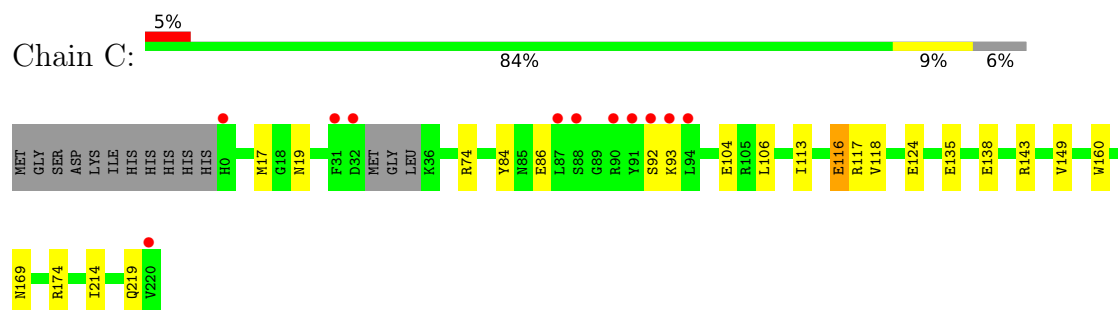
- Molecule 1: Thymidylate synthase ThyX



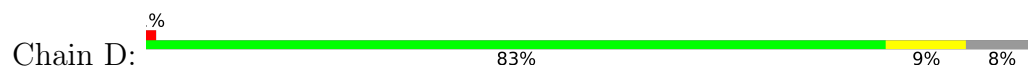
- Molecule 1: Thymidylate synthase ThyX

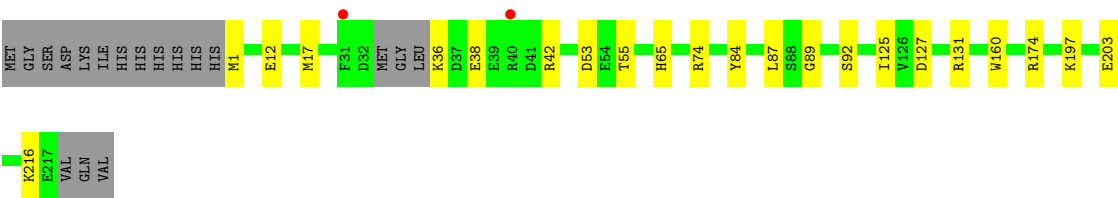


- Molecule 1: Thymidylate synthase ThyX



- Molecule 1: Thymidylate synthase ThyX





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.37Å 116.67Å 141.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.29 – 1.85 38.29 – 1.85	Depositor EDS
% Data completeness (in resolution range)	93.4 (38.29-1.85) 93.5 (38.29-1.85)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 1.85Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.170 , 0.211 (Not available) , 0.210	Depositor DCC
R_{free} test set	3632 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7919	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, CL, 2PE, FAD, SO4

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	0.96	0/1874	1.03	2/2534 (0.1%)
1	B	0.96	0/1876	1.02	1/2536 (0.0%)
1	C	0.99	0/2009	1.01	5/2711 (0.2%)
1	D	1.00	2/1870 (0.1%)	0.97	0/2526
All	All	0.98	2/7629 (0.0%)	1.01	8/10307 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	87	LEU	CA-C	-5.57	1.45	1.52
1	D	89	GLY	C-O	-5.17	1.18	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	214	ILE	N-CA-C	7.77	118.55	110.62
1	A	137	ILE	CB-CA-C	-6.87	103.18	111.97
1	A	30	SER	N-CA-C	5.86	117.67	111.28
1	C	113	ILE	CA-C-N	-5.67	115.52	119.66
1	C	113	ILE	C-N-CA	-5.67	115.52	119.66
1	C	219	GLN	CA-C-N	5.42	131.45	121.70
1	C	219	GLN	C-N-CA	5.42	131.45	121.70
1	B	14	VAL	CB-CA-C	-5.21	105.37	111.94

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	1820	0	1792	20	0
1	B	1828	0	1811	13	0
1	C	1953	0	1945	16	0
1	D	1816	0	1813	17	0
2	A	20	0	11	1	0
2	B	20	0	11	1	0
2	C	20	0	11	7	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	C	53	0	31	2	0
4	D	53	0	31	4	0
5	C	1	0	0	0	0
6	D	5	0	0	0	0
7	D	13	0	17	0	0
8	A	72	0	0	1	0
8	B	58	0	0	1	0
8	C	99	0	0	3	0
8	D	78	0	0	5	0
All	All	7919	0	7473	60	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 4.

All (60) 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:A:301:DU:H3	1:D:174:ARG:HH12	1.14	0.96
1:B:174:ARG:HH12	2:C:302:DU:H3	1.20	0.90
2:B:301:DU:H3	1:C:174:ARG:HH12	1.19	0.89
4:C:301:FAD:H51A	8:C:403:HOH:O	1.75	0.84
1:A:79[A]:HIS:HE1	1:A:166[A]:SER:OG	1.60	0.84
1:A:79[A]:HIS:CE1	1:A:166[A]:SER:OG	2.37	0.78
1:C:106:LEU:HD11	1:C:118:VAL:HG11	1.69	0.74
1:A:17:MET:HB2	1:B:17:MET:HB2	1.73	0.71
1:A:128:LYS:HG3	1:D:125:ILE:HD11	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:MET:HB2	1:D:17:MET:HB2	1.75	0.69
4:D:301:FAD:H51A	8:D:450:HOH:O	1.92	0.68
1:D:53:ASP:OD1	8:D:425:HOH:O	2.13	0.67
1:C:86[A]:GLU:OE1	2:C:302:DU:H4'	1.98	0.62
1:D:127:ASP:OD2	1:D:131:ARG:NH1	2.34	0.60
1:D:55:THR:HG23	8:D:425:HOH:O	2.01	0.60
1:B:165:ARG:CZ	4:D:301:FAD:H2B	2.36	0.55
1:A:74:ARG:HG2	1:D:74[A]:ARG:CD	2.37	0.55
4:D:301:FAD:N3A	8:D:415:HOH:O	2.34	0.54
1:A:5:ILE:HD11	1:A:189:ALA:HB2	1.90	0.53
1:A:170:PHE:CE1	1:A:174[B]:ARG:HD2	2.44	0.53
1:C:74[A]:ARG:NH1	8:C:450:HOH:O	2.42	0.52
1:B:96:TYR:OH	1:B:127:ASP:OD1	2.17	0.49
1:C:169[A]:ASN:ND2	4:C:301:FAD:H52A	2.27	0.49
1:B:125:ILE:HG21	1:C:149:VAL:HB	1.94	0.48
1:C:19:ASN:HB2	8:C:421:HOH:O	2.13	0.48
1:A:128:LYS:HG3	1:D:125:ILE:CD1	2.42	0.48
1:D:1:MET:HE1	1:D:197:LYS:HE2	1.94	0.48
1:B:116:GLU:H	1:B:116:GLU:CD	2.22	0.48
1:D:74[A]:ARG:NH1	8:D:427:HOH:O	2.46	0.47
1:A:143:ARG:HH11	1:A:143:ARG:CG	2.28	0.47
1:A:55:THR:OG1	1:A:56:PRO:HD3	2.14	0.46
1:D:12:GLU:HG2	1:D:65:HIS:HB3	1.97	0.46
1:A:79[B]:HIS:HE1	1:A:173:LEU:HD12	1.79	0.46
1:A:74:ARG:HG2	1:D:74[A]:ARG:HD2	1.98	0.45
1:B:37:ASP:OD1	1:B:38:GLU:N	2.50	0.45
1:B:130:TYR:CE2	1:B:134:LEU:HD11	2.52	0.45
1:A:37:ASP:OD1	1:A:37:ASP:C	2.61	0.44
1:C:86[A]:GLU:OE1	2:C:302:DU:O3'	2.26	0.44
4:D:301:FAD:O2P	4:D:301:FAD:H3B	2.18	0.43
1:A:79[B]:HIS:CE1	1:A:170:PHE:HA	2.53	0.43
1:C:86[A]:GLU:CD	2:C:302:DU:H4'	2.43	0.43
1:D:125:ILE:HD13	1:D:125:ILE:HA	1.87	0.43
1:A:116:GLU:H	1:A:116:GLU:CD	2.27	0.43
1:A:74:ARG:HG2	1:D:74[A]:ARG:HD3	2.01	0.42
1:A:74:ARG:CG	1:D:74[A]:ARG:HD3	2.49	0.42
1:B:127:ASP:O	1:B:131:ARG:HG3	2.20	0.42
1:D:84:TYR:CE2	1:D:160:TRP:CD1	3.07	0.42
1:B:207:LYS:HE2	1:B:208:TYR:OH	2.20	0.42
1:C:86[A]:GLU:OE1	2:C:302:DU:C4'	2.67	0.42
1:C:116:GLU:CD	1:C:116:GLU:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ARG:NE	8:A:454:HOH:O	2.47	0.41
1:B:172:ASN:ND2	1:B:211:LYS:HE3	2.35	0.41
1:A:42:ARG:HG3	1:A:200:TRP:CD2	2.55	0.41
1:A:177:SER:OG	1:A:213:ASP:OD2	2.33	0.41
1:D:216:LYS:HB2	1:D:216:LYS:HE3	1.88	0.41
1:C:84:TYR:CE2	1:C:160:TRP:CD1	3.09	0.41
1:C:86[A]:GLU:OE1	2:C:302:DU:C3'	2.69	0.41
1:C:86[A]:GLU:HB3	2:C:302:DU:H4'	2.02	0.41
1:B:121:LYS:NZ	1:C:135:GLU:OE2	2.50	0.40
1:B:19:ASN:HB2	8:B:426:HOH:O	2.21	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	213/232 (92%)	210 (99%)	3 (1%)	0	100	100
1	B	214/232 (92%)	210 (98%)	4 (2%)	0	100	100
1	C	229/232 (99%)	222 (97%)	7 (3%)	0	100	100
1	D	213/232 (92%)	209 (98%)	4 (2%)	0	100	100
All	All	869/928 (94%)	851 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	194/207 (94%)	187 (96%)	7 (4%)	31	16
1	B	195/207 (94%)	190 (97%)	5 (3%)	40	25
1	C	209/207 (101%)	199 (95%)	10 (5%)	23	8
1	D	194/207 (94%)	189 (97%)	5 (3%)	40	25
All	All	792/828 (96%)	765 (97%)	27 (3%)	34	17

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	42	ARG
1	A	93	LYS
1	A	116	GLU
1	A	126	VAL
1	A	139	SER
1	A	143	ARG
1	B	29	VAL
1	B	106	LEU
1	B	116	GLU
1	B	137	ILE
1	B	147	ARG
1	C	92[A]	SER
1	C	92[B]	SER
1	C	93[A]	LYS
1	C	93[B]	LYS
1	C	104	GLU
1	C	116	GLU
1	C	117	ARG
1	C	124	GLU
1	C	138	GLU
1	C	143	ARG
1	D	36	LYS
1	D	38	GLU
1	D	42	ARG
1	D	92	SER
1	D	203	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	75	GLN
1	B	185	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	302	-	4,4,4	1.21	1 (25%)	6,6,6	1.00	0
4	FAD	D	301	-	58,58,58	3.11	17 (29%)	85,89,89	2.01	24 (28%)
2	DU	C	302	-	21,21,21	1.22	3 (14%)	30,31,31	1.66	7 (23%)
2	DU	A	301	-	21,21,21	1.44	3 (14%)	30,31,31	1.44	4 (13%)
2	DU	B	301	-	21,21,21	1.20	4 (19%)	30,31,31	1.27	3 (10%)
3	SO4	B	302	-	4,4,4	1.41	1 (25%)	6,6,6	0.94	0
4	FAD	C	301	-	58,58,58	3.17	19 (32%)	85,89,89	1.90	21 (24%)
7	2PE	D	303	-	12,12,27	0.54	0	11,11,26	0.53	0
6	PO4	D	302	-	4,4,4	0.93	0	6,6,6	0.84	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	FAD	D	301	-	-	3/34/50/50	0/6/6/6
2	DU	C	302	-	-	0/10/22/22	0/2/2/2
2	DU	A	301	-	-	0/10/22/22	0/2/2/2
2	DU	B	301	-	-	0/10/22/22	0/2/2/2
7	2PE	D	303	-	-	2/10/10/25	-
4	FAD	C	301	-	-	7/34/50/50	0/6/6/6

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	301	FAD	C6-C7	9.28	1.52	1.39
4	D	301	FAD	C6-C5X	8.80	1.53	1.40
4	C	301	FAD	C6-C7	8.66	1.51	1.39
4	C	301	FAD	C6-C5X	8.45	1.52	1.40
4	C	301	FAD	C9A-C5X	7.74	1.53	1.41
4	D	301	FAD	C9A-C5X	7.43	1.53	1.41
4	D	301	FAD	C10-N1	6.92	1.47	1.33
4	C	301	FAD	C10-N1	6.69	1.46	1.33
4	D	301	FAD	C4X-N5	6.25	1.44	1.30
4	C	301	FAD	C4X-N5	6.24	1.44	1.30
4	C	301	FAD	C5A-C4A	6.22	1.50	1.39
4	D	301	FAD	C9-C9A	6.16	1.49	1.39
4	C	301	FAD	C9-C9A	6.14	1.49	1.39
4	D	301	FAD	C9A-N10	-5.90	1.30	1.41
4	C	301	FAD	C9A-N10	-5.74	1.31	1.41
4	D	301	FAD	C5A-C4A	5.43	1.48	1.39
4	D	301	FAD	C10-N10	5.20	1.48	1.37
4	C	301	FAD	P-O3P	5.11	1.65	1.59
4	C	301	FAD	C10-N10	4.87	1.47	1.37
4	C	301	FAD	C8-C7	4.66	1.52	1.40
4	D	301	FAD	C8-C7	4.37	1.51	1.40
4	C	301	FAD	PA-O1A	4.28	1.65	1.50
4	C	301	FAD	C8A-N7A	4.00	1.39	1.31
4	D	301	FAD	P-O3P	3.84	1.63	1.59
4	D	301	FAD	PA-O1A	3.83	1.64	1.50
4	C	301	FAD	C2-N1	-3.45	1.28	1.36
4	D	301	FAD	C2-N1	-3.32	1.29	1.36
2	A	301	DU	C6-C5	3.25	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	301	FAD	C5X-N5	3.19	1.45	1.39
4	D	301	FAD	C5X-N5	3.14	1.45	1.39
2	C	302	DU	C4-N3	-3.06	1.33	1.38
2	B	301	DU	C2-N3	-2.88	1.32	1.38
2	A	301	DU	O2-C2	2.81	1.28	1.23
4	D	301	FAD	C8A-N7A	2.78	1.37	1.31
4	C	301	FAD	C4X-C10	2.74	1.52	1.44
4	D	301	FAD	C4X-C10	2.68	1.52	1.44
4	C	301	FAD	PA-O3P	2.65	1.62	1.59
4	C	301	FAD	C9-C8	-2.56	1.36	1.39
4	C	301	FAD	C1B-N9A	2.50	1.53	1.46
2	C	302	DU	C6-C5	2.47	1.40	1.35
2	B	301	DU	C6-C5	2.47	1.40	1.35
3	B	302	SO4	O2-S	2.45	1.59	1.44
2	B	301	DU	O2-C2	2.25	1.27	1.23
4	D	301	FAD	C9-C8	-2.20	1.36	1.39
2	C	302	DU	C2-N3	-2.19	1.34	1.38
3	A	302	SO4	O1-S	2.09	1.57	1.44
2	B	301	DU	C4-N3	-2.07	1.35	1.38
2	A	301	DU	C5-C4	-2.04	1.39	1.43

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	301	FAD	C5A-C4A-N3A	-6.53	117.73	126.72
4	C	301	FAD	C5A-C4A-N3A	-5.84	118.67	126.72
4	D	301	FAD	N3A-C4A-N9A	4.65	135.08	127.17
4	C	301	FAD	C2B-C1B-N9A	4.61	124.77	113.30
4	D	301	FAD	O2A-PA-O3P	-4.45	95.23	107.27
2	C	302	DU	N3-C2-N1	4.39	120.61	114.89
4	C	301	FAD	C5X-C9A-N10	4.26	121.82	117.97
4	D	301	FAD	C4X-C10-N1	-4.26	114.15	124.59
4	D	301	FAD	C5X-C9A-N10	4.19	121.76	117.97
4	C	301	FAD	N3A-C2A-N1A	-4.11	122.36	128.58
4	D	301	FAD	N3A-C2A-N1A	-4.01	122.52	128.58
4	C	301	FAD	N3A-C4A-N9A	3.93	133.86	127.17
4	C	301	FAD	O2A-PA-O3P	-3.91	96.70	107.27
4	D	301	FAD	C2A-N3A-C4A	3.72	120.91	111.83
4	D	301	FAD	C4-C4X-N5	3.71	123.33	118.21
4	C	301	FAD	C4X-C10-N1	-3.66	115.61	124.59
4	C	301	FAD	C4-C4X-N5	3.55	123.11	118.21
4	C	301	FAD	C2A-N3A-C4A	3.51	120.40	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	DU	C5-C4-N3	3.48	119.68	114.80
2	A	301	DU	C5-C4-N3	3.44	119.62	114.80
4	D	301	FAD	C4A-C5A-N7A	-3.39	106.71	110.58
4	D	301	FAD	O5B-C5B-C4B	3.32	120.31	108.99
4	C	301	FAD	O2A-PA-O1A	3.19	127.28	112.44
4	C	301	FAD	O2-C2-N1	-3.16	116.55	121.80
4	C	301	FAD	C3B-C2B-C1B	3.05	107.23	101.46
4	D	301	FAD	O2A-PA-O1A	3.02	126.48	112.44
4	D	301	FAD	C4X-C10-N10	3.01	120.79	116.48
4	C	301	FAD	O4-C4-C4X	-2.94	118.76	126.53
2	C	302	DU	C5-C4-N3	2.93	118.90	114.80
4	D	301	FAD	O2-C2-N1	-2.92	116.96	121.80
2	A	301	DU	N3-C2-N1	2.90	118.67	114.89
4	C	301	FAD	C4X-C10-N10	2.88	120.61	116.48
2	C	302	DU	O2-C2-N1	-2.87	119.06	122.80
4	D	301	FAD	C3B-C2B-C1B	2.84	106.84	101.46
4	D	301	FAD	C10-C4X-N5	-2.82	119.04	124.81
2	A	301	DU	C4-N3-C2	-2.82	123.11	126.61
2	C	302	DU	C4-N3-C2	-2.82	123.12	126.61
4	D	301	FAD	O4-C4-C4X	-2.79	119.18	126.53
4	D	301	FAD	C10-N1-C2	2.72	122.74	116.85
4	C	301	FAD	C4A-C5A-N7A	-2.71	107.48	110.58
2	C	302	DU	C6-N1-C2	-2.68	117.74	121.00
2	A	301	DU	OP2-P-OP3	2.56	117.40	107.80
4	D	301	FAD	C9A-C9-C8	2.42	124.08	119.22
4	C	301	FAD	C10-C4X-N5	-2.36	120.00	124.81
4	C	301	FAD	C9A-C9-C8	2.33	123.92	119.22
4	C	301	FAD	C10-N1-C2	2.31	121.85	116.85
2	C	302	DU	OP3-P-O5'	-2.31	100.66	106.67
4	D	301	FAD	C9-C9A-C5X	-2.29	115.98	120.03
4	D	301	FAD	N3-C2-N1	2.27	124.32	119.50
4	D	301	FAD	C9-C8-C7	2.25	122.99	119.69
4	D	301	FAD	N10-C10-N1	2.22	125.05	118.51
2	C	302	DU	OP3-P-OP1	2.15	119.20	110.83
4	C	301	FAD	C9-C9A-C5X	-2.14	116.25	120.03
4	D	301	FAD	C4X-C4-N3	2.14	118.69	113.25
2	B	301	DU	O4-C4-C5	-2.14	121.48	125.16
4	C	301	FAD	N3-C2-N1	2.08	123.93	119.50
4	D	301	FAD	C5A-N7A-C8A	2.06	106.68	103.45
4	C	301	FAD	C5X-C6-C7	-2.05	117.03	120.83
2	B	301	DU	N3-C2-N1	2.03	117.54	114.89

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	301	FAD	P-O3P-PA-O5B
4	C	301	FAD	C5'-O5'-P-O1P
4	D	301	FAD	P-O3P-PA-O5B
4	D	301	FAD	C5'-O5'-P-O1P
4	C	301	FAD	C2'-C3'-C4'-O4'
4	D	301	FAD	C2'-C3'-C4'-O4'
7	D	303	2PE	O10-C11-C12-O13
7	D	303	2PE	C5-C6-O7-C8
4	C	301	FAD	O3'-C3'-C4'-O4'
4	C	301	FAD	O3'-C3'-C4'-C5'
4	C	301	FAD	O4B-C4B-C5B-O5B
4	C	301	FAD	C2'-C3'-C4'-C5'

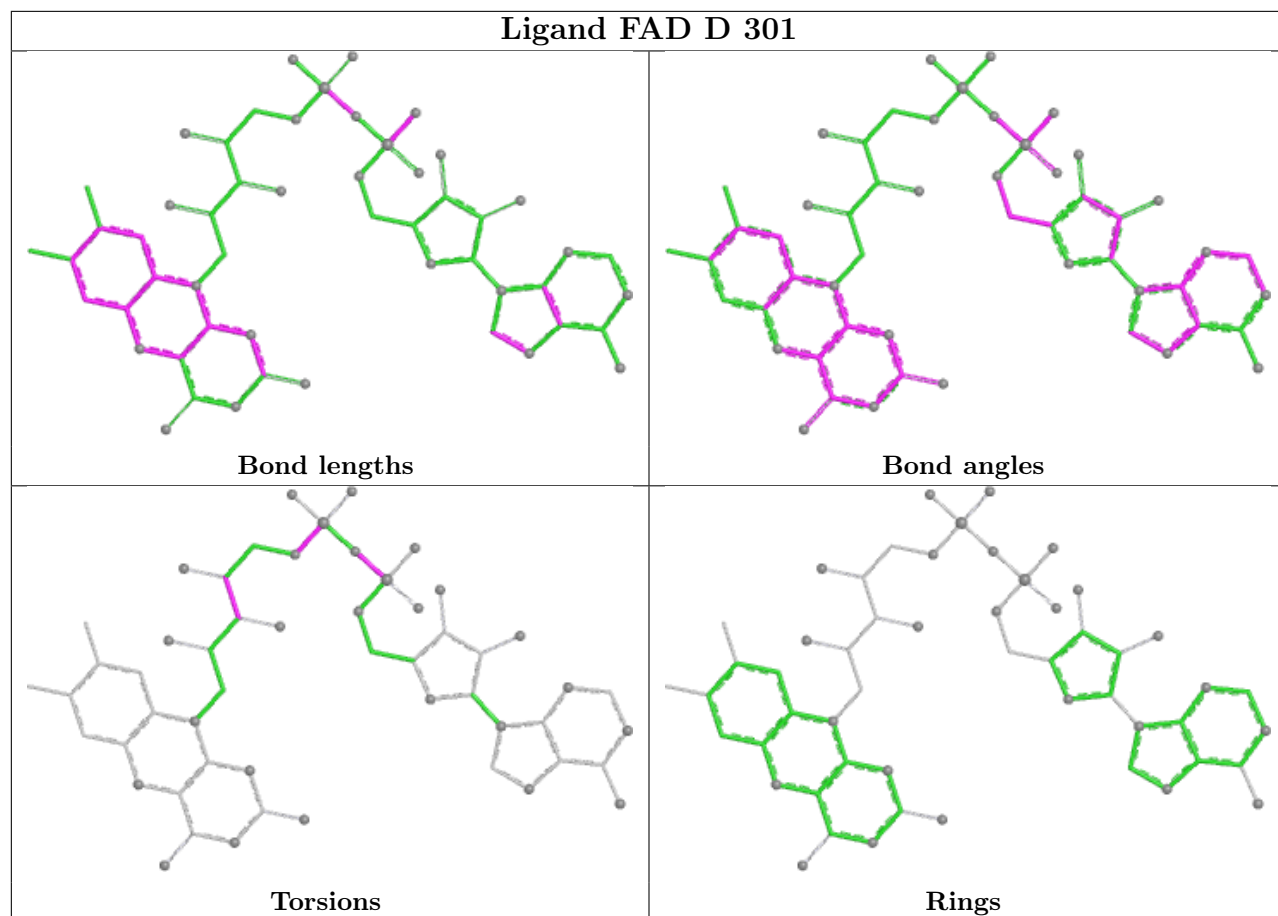
There are no ring outliers.

5 monomers are involved in 15 short contacts:

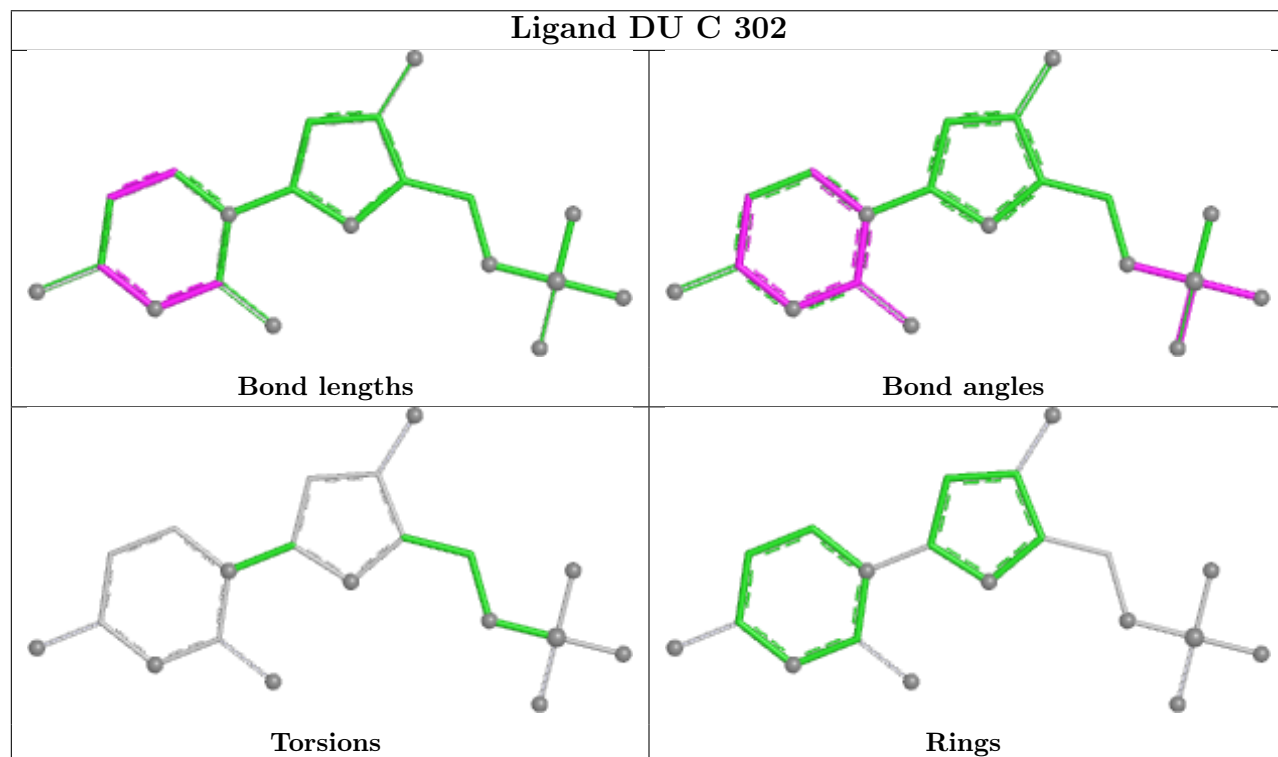
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	301	FAD	4	0
2	C	302	DU	7	0
2	A	301	DU	1	0
2	B	301	DU	1	0
4	C	301	FAD	2	0

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.

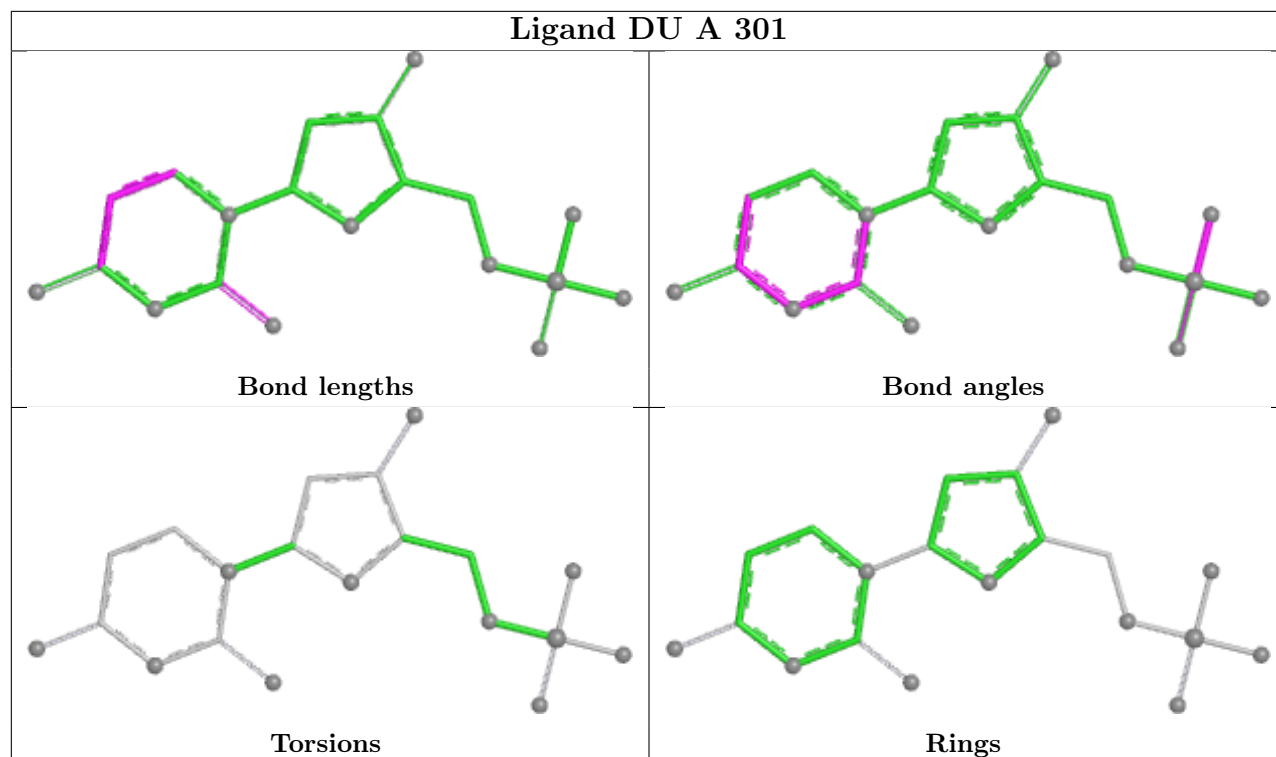
Ligand FAD D 301



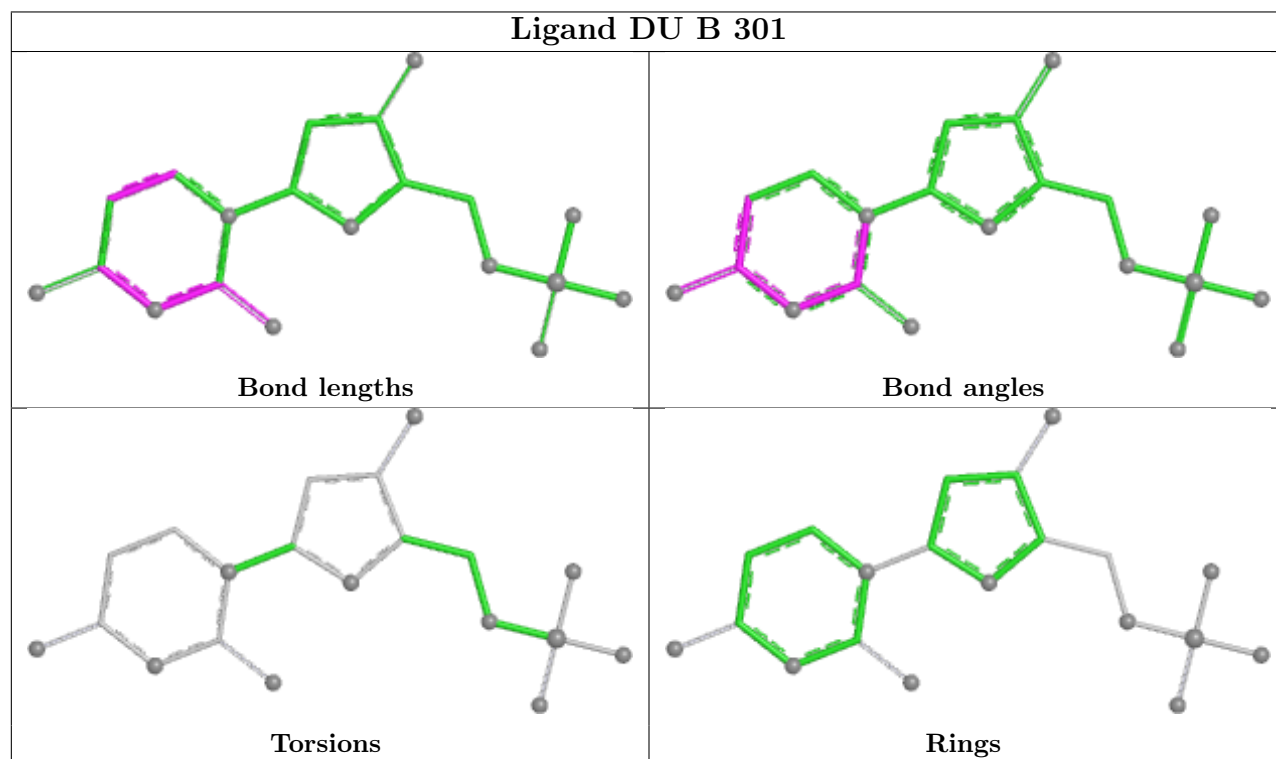
Ligand DU C 302

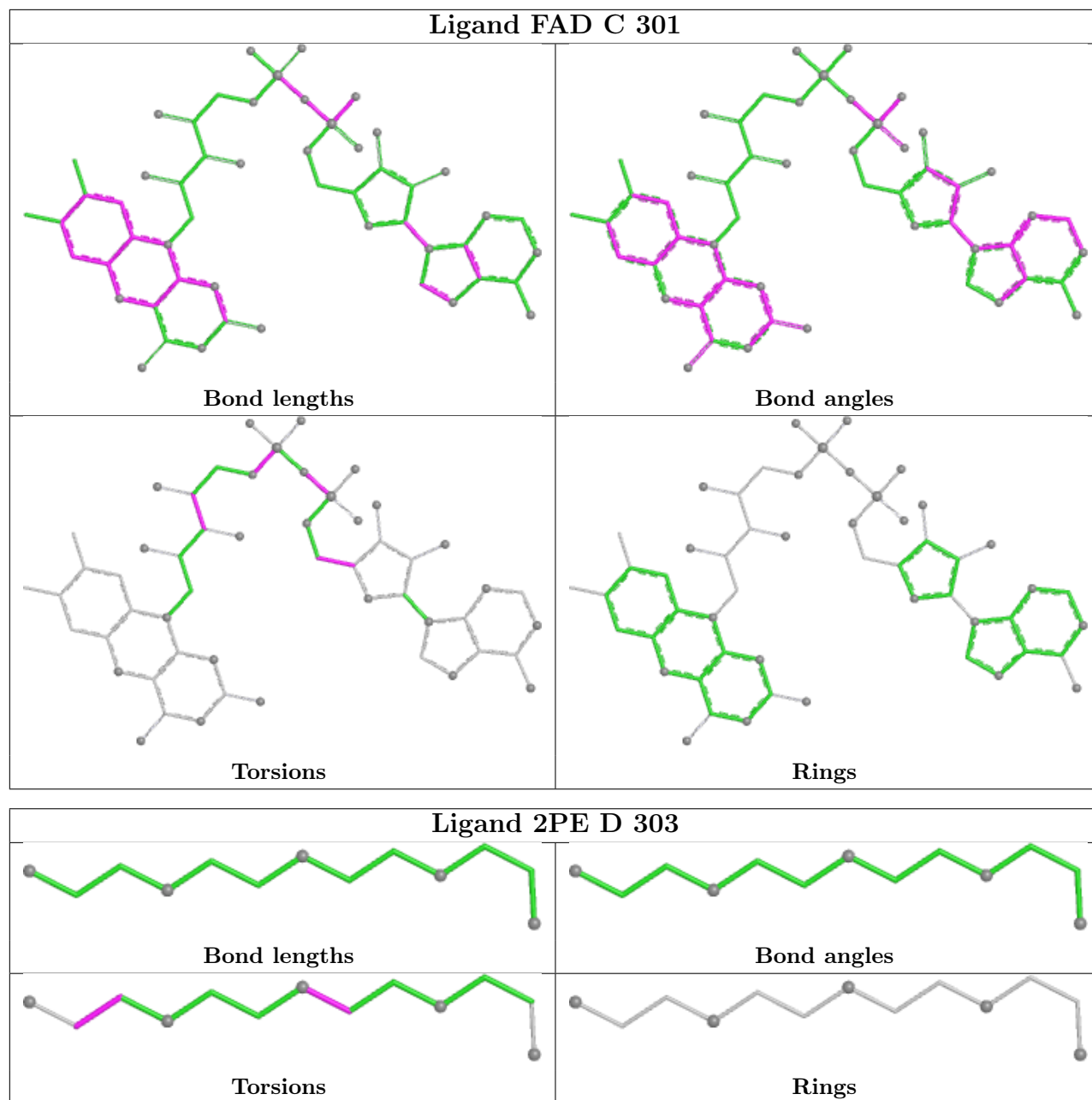


Ligand DU A 301



Ligand DU B 301





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	213/232 (91%)	0.04	4 (1%) 66 70	9, 28, 52, 75	4 (1%)
1	B	217/232 (93%)	0.09	6 (2%) 55 58	12, 30, 61, 75	1 (0%)
1	C	218/232 (93%)	0.01	11 (5%) 34 37	11, 24, 53, 67	15 (6%)
1	D	214/232 (92%)	-0.10	2 (0%) 81 84	11, 27, 56, 77	3 (1%)
All	All	862/928 (92%)	0.01	23 (2%) 56 59	9, 28, 56, 77	23 (2%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	91[A]	TYR	5.9
1	B	220	VAL	5.4
1	C	93[A]	LYS	4.6
1	C	90[A]	ARG	4.6
1	A	30	SER	3.7
1	C	92[A]	SER	3.6
1	A	29	VAL	3.5
1	C	220	VAL	3.3
1	B	31	PHE	3.1
1	A	91	TYR	3.1
1	A	31	PHE	3.1
1	C	94[A]	LEU	3.0
1	C	88[A]	SER	2.9
1	C	0	HIS	2.8
1	B	91	TYR	2.8
1	B	29	VAL	2.5
1	B	40	ARG	2.3
1	C	87[A]	LEU	2.3
1	C	31	PHE	2.3
1	B	38	GLU	2.3
1	D	31	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	40	ARG	2.2
1	C	32	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

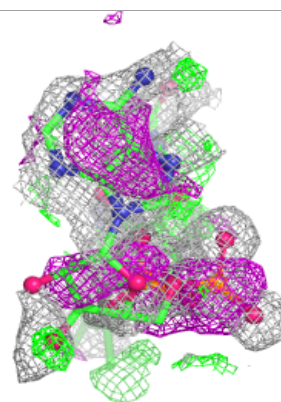
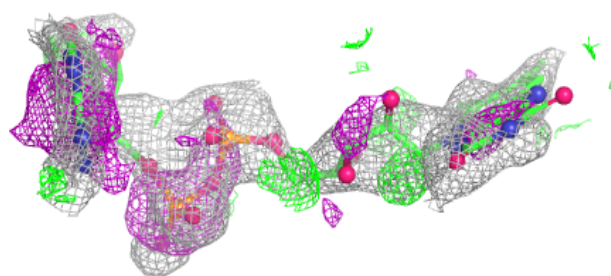
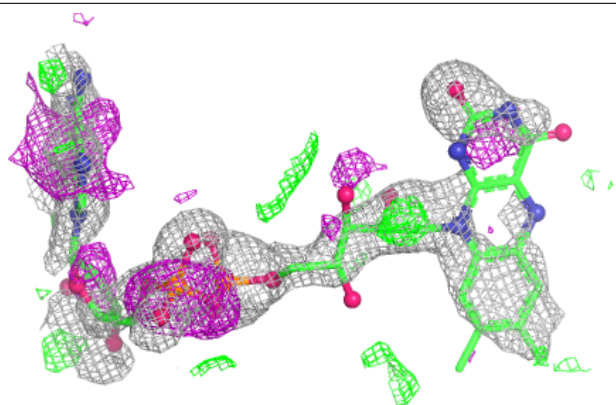
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	A	302	5/5	0.74	0.16	27,39,59,61	0
4	FAD	C	301	53/53	0.76	0.20	24,70,80,84	0
4	FAD	D	301	53/53	0.76	0.19	28,66,81,87	0
3	SO4	B	302	5/5	0.78	0.14	24,34,53,56	0
6	PO4	D	302	5/5	0.79	0.10	54,57,58,60	0
7	2PE	D	303	13/28	0.83	0.15	52,58,67,68	0
2	DU	C	302	20/20	0.87	0.11	34,39,45,45	0
5	CL	C	303	1/1	0.87	0.13	67,67,67,67	0
2	DU	A	301	20/20	0.97	0.05	20,24,26,27	0
2	DU	B	301	20/20	0.97	0.06	24,26,30,31	0

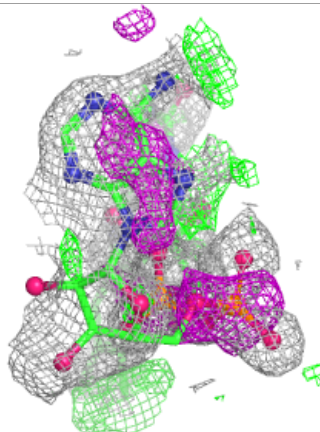
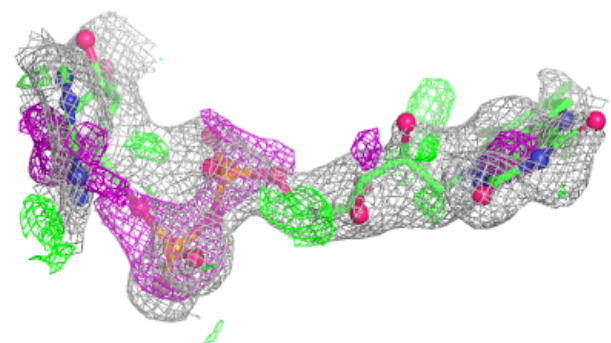
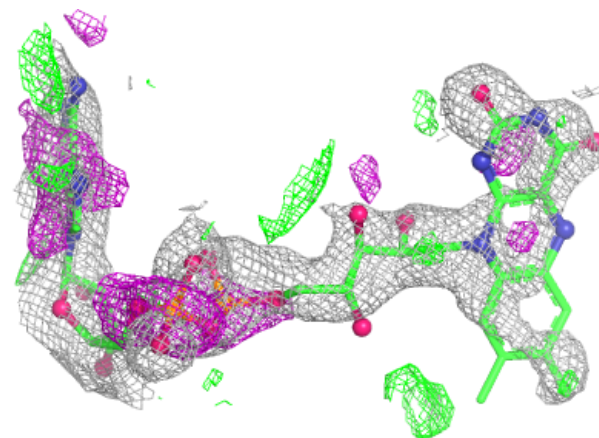
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD C 301:

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

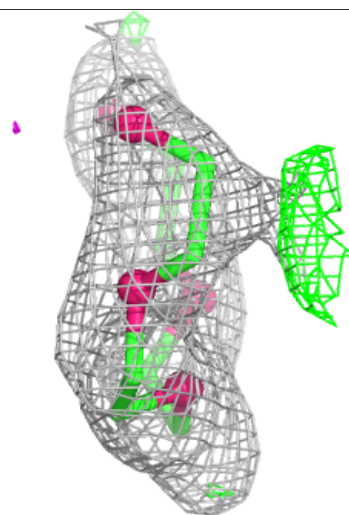
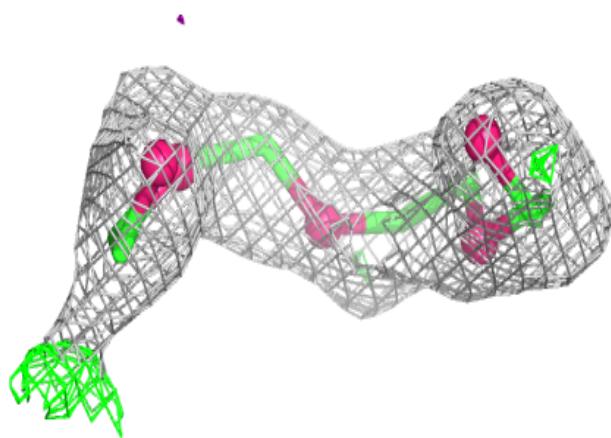
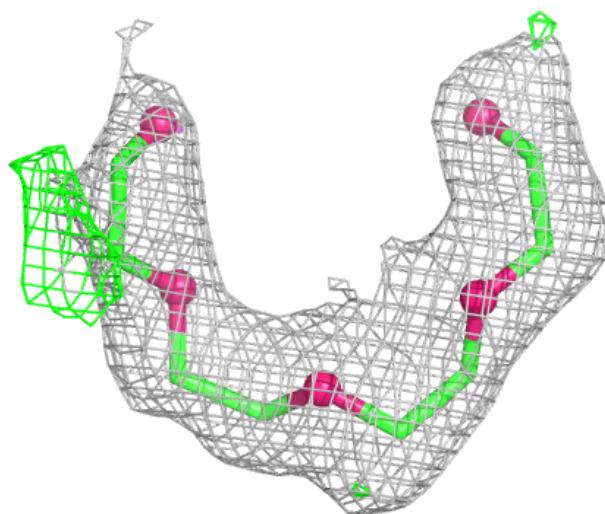
**Electron density around FAD D 301:**

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



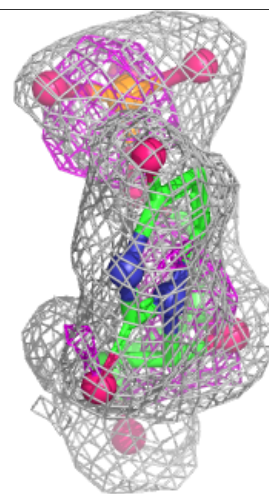
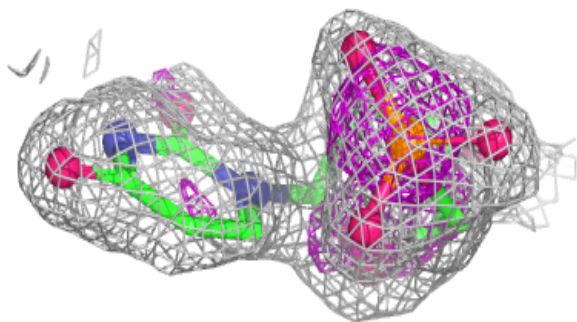
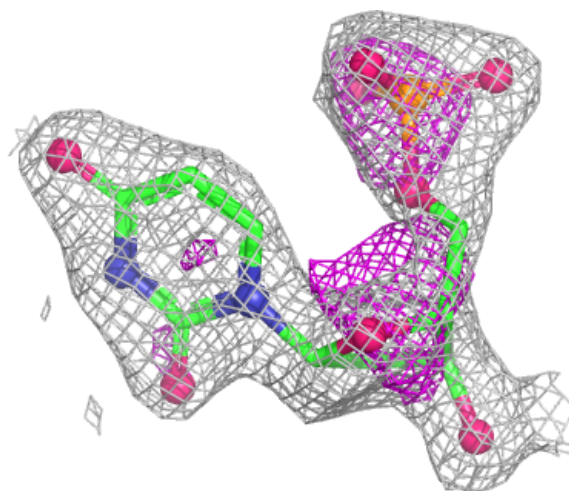
Electron density around 2PE D 303:

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



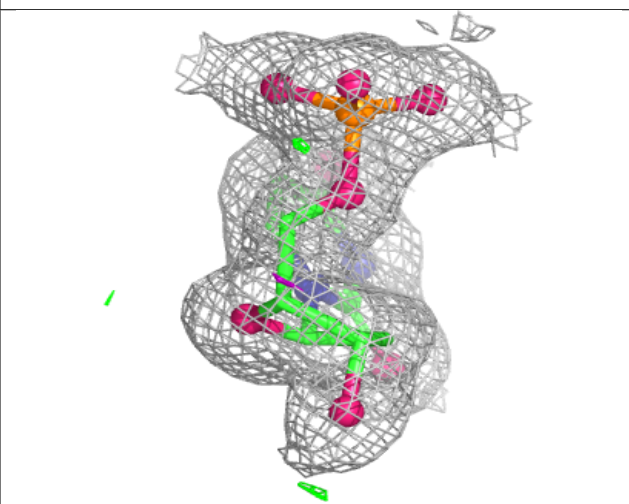
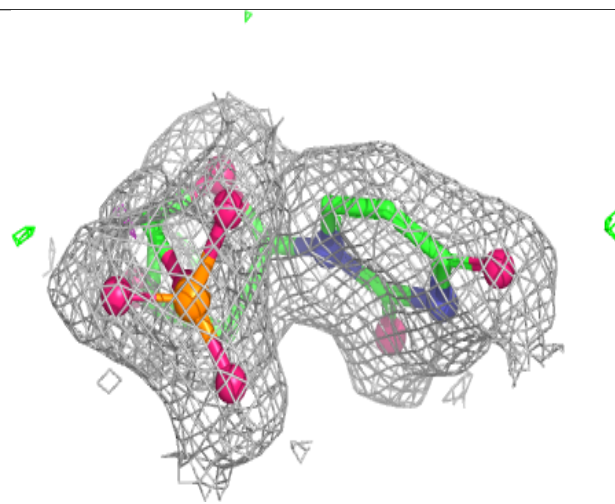
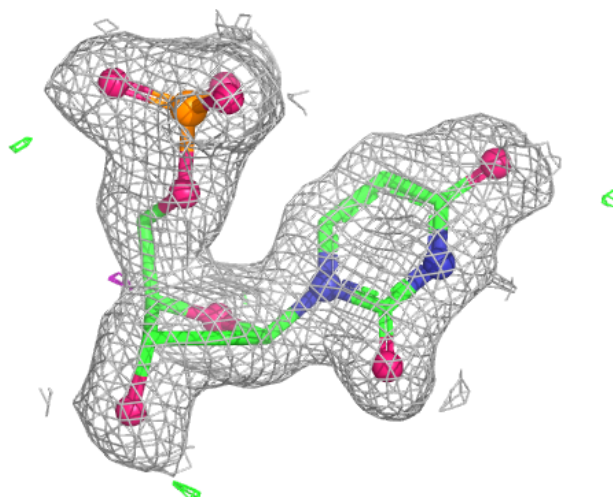
Electron density around DU C 302:

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



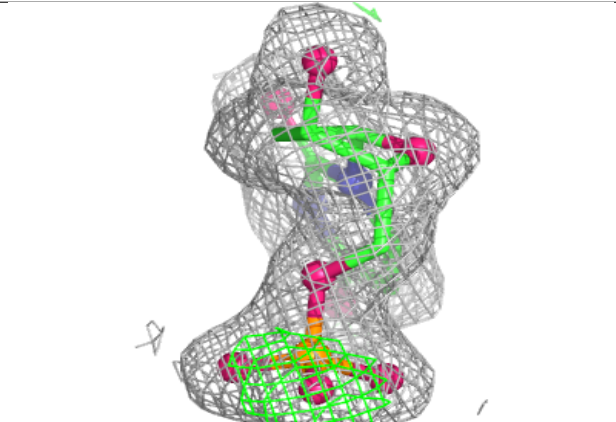
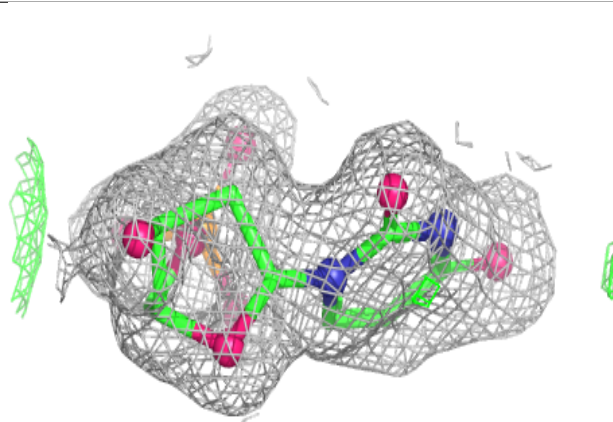
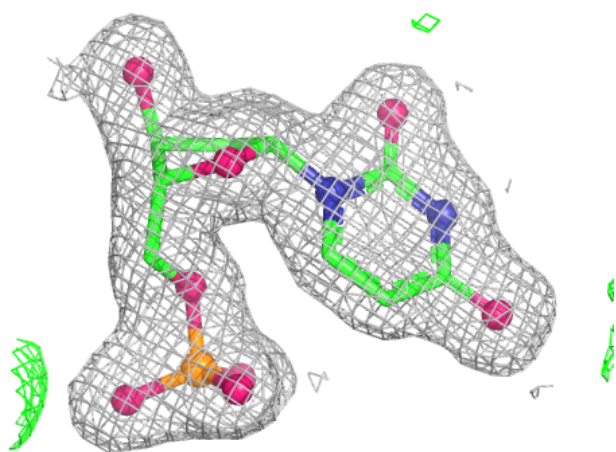
Electron density around DU A 301:

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



Electron density around DU B 301:

$2mF_o-DF_c$ (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.