



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:04 AM UTC

PDB ID : 3FST / pdb_00003fst
Title : Crystal Structure of Escherichia coli Methylenetetrahydrofolate Reductase
Mutant Phe223Leu at pH 7.4
Authors : Tanner, J.J.
Deposited on : 2009-01-12
Resolution : 1.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

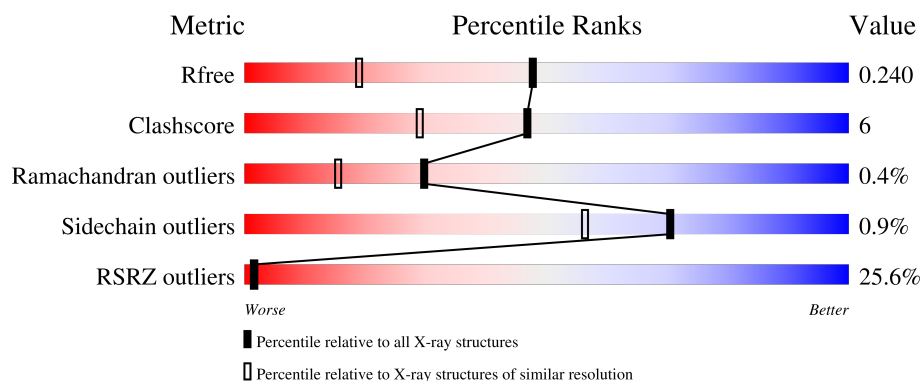
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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

Mol	Chain	Length	Quality of chain
1	A	304	10% 83% 11% 6%
1	C	304	3% 78% 9% 13%
1	E	304	57% 79% 11% 10%

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
3	MRY	C	5321[A]	-	-	X	-
3	MRY	C	5321[B]	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7104 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 5,10-methylenetetrahydrofolate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	15	0
			2297	1459	402	423	13			
1	C	265	Total	C	N	O	S	0	12	0
			2099	1337	358	393	11			
1	E	274	Total	C	N	O	S	0	7	0
			2062	1310	358	382	12			

There are 27 discrepancies between the modelled and reference sequences:

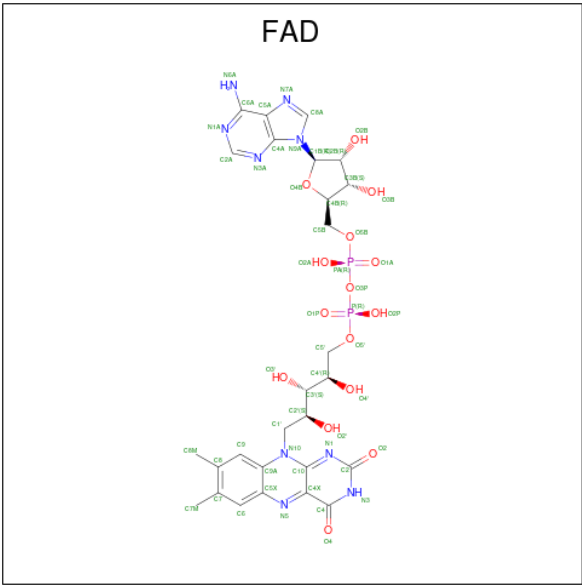
Chain	Residue	Modelled	Actual	Comment	Reference
A	223	LEU	PHE	engineered mutation	UNP P0AEZ1
A	297	LEU	-	expression tag	UNP P0AEZ1
A	298	GLU	-	expression tag	UNP P0AEZ1
A	299	HIS	-	expression tag	UNP P0AEZ1
A	300	HIS	-	expression tag	UNP P0AEZ1
A	301	HIS	-	expression tag	UNP P0AEZ1
A	302	HIS	-	expression tag	UNP P0AEZ1
A	303	HIS	-	expression tag	UNP P0AEZ1
A	304	HIS	-	expression tag	UNP P0AEZ1
C	223	LEU	PHE	engineered mutation	UNP P0AEZ1
C	297	LEU	-	expression tag	UNP P0AEZ1
C	298	GLU	-	expression tag	UNP P0AEZ1
C	299	HIS	-	expression tag	UNP P0AEZ1
C	300	HIS	-	expression tag	UNP P0AEZ1
C	301	HIS	-	expression tag	UNP P0AEZ1
C	302	HIS	-	expression tag	UNP P0AEZ1
C	303	HIS	-	expression tag	UNP P0AEZ1
C	304	HIS	-	expression tag	UNP P0AEZ1
E	223	LEU	PHE	engineered mutation	UNP P0AEZ1
E	297	LEU	-	expression tag	UNP P0AEZ1
E	298	GLU	-	expression tag	UNP P0AEZ1
E	299	HIS	-	expression tag	UNP P0AEZ1
E	300	HIS	-	expression tag	UNP P0AEZ1

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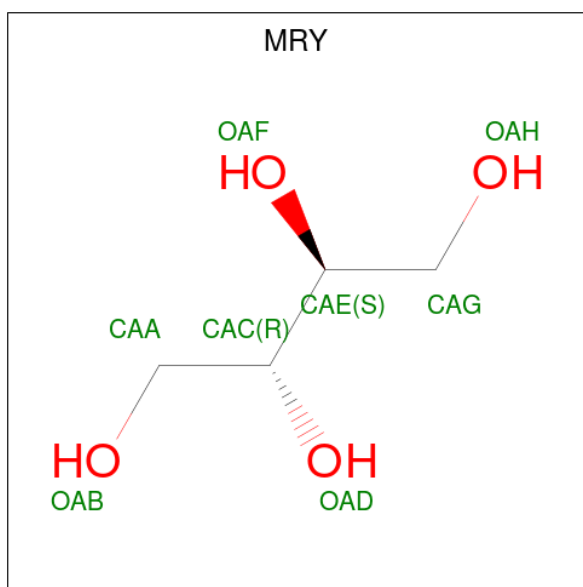
Chain	Residue	Modelled	Actual	Comment	Reference
E	301	HIS	-	expression tag	UNP P0AEZ1
E	302	HIS	-	expression tag	UNP P0AEZ1
E	303	HIS	-	expression tag	UNP P0AEZ1
E	304	HIS	-	expression tag	UNP P0AEZ1

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



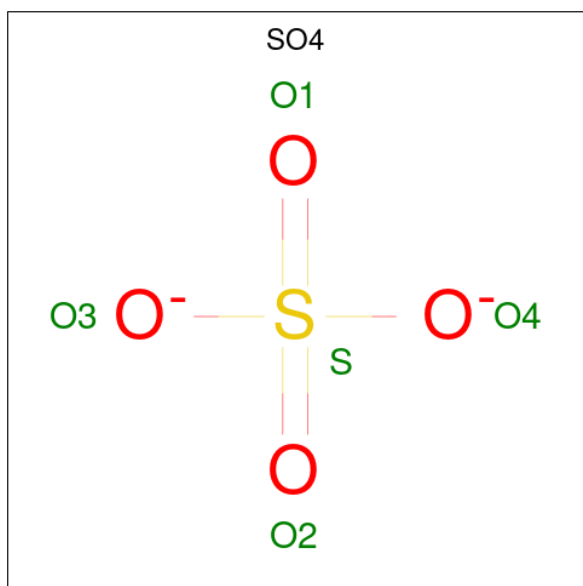
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is MESO-ERYTHRITOL (CCD ID: MRY) (formula: C₄H₁₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	1
			16	8	8		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

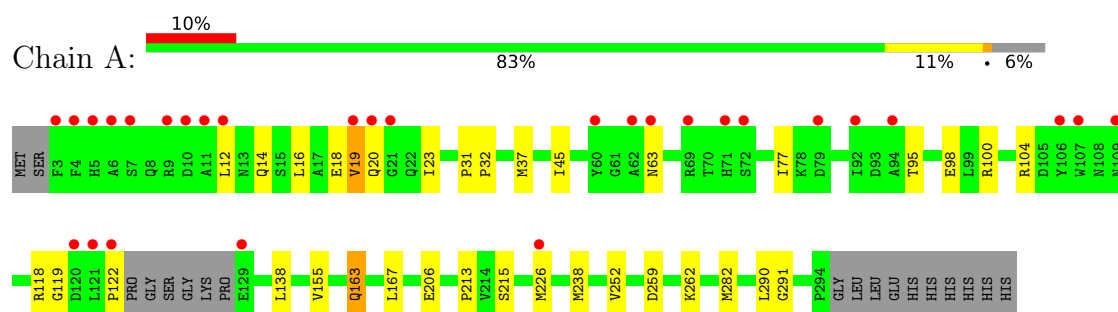
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	184	Total 184	O 184	0	0
5	C	207	Total 207	O 207	0	0
5	E	65	Total 65	O 65	0	0

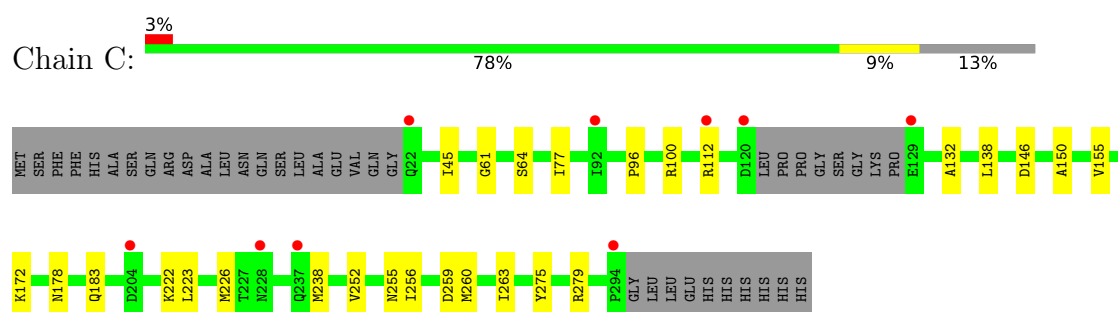
3 Residue-property plots [i](#)

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.

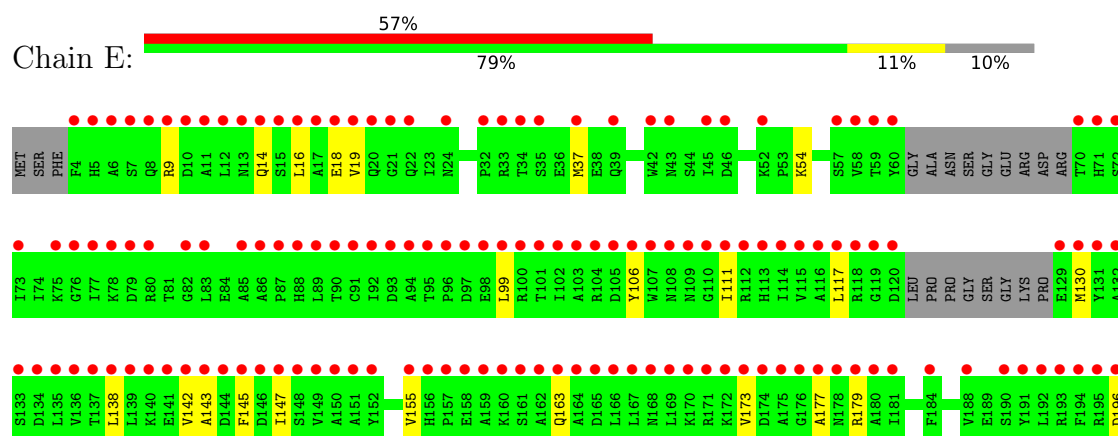
- Molecule 1: 5,10-methylenetetrahydrofolate reductase

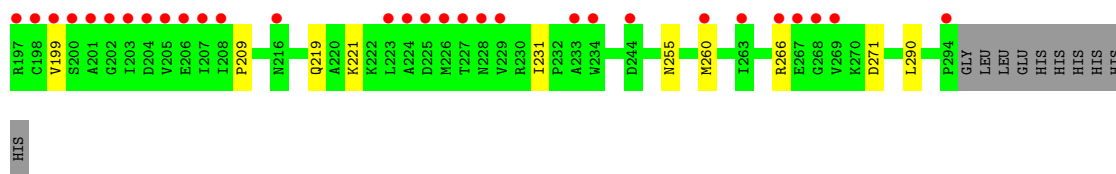


- Molecule 1: 5,10-methylenetetrahydrofolate reductase



- Molecule 1: 5,10-methylenetetrahydrofolate reductase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	103.06Å 128.16Å 98.31Å 90.00° 121.97° 90.00°	Depositor
Resolution (Å)	32.14 – 1.65 32.14 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.5 (32.14-1.65) 99.5 (32.14-1.65)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 1.65Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.210 , 0.228 0.227 , 0.240	Depositor DCC
R_{free} test set	6477 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7104	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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: SO4, MRY, 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	0.44	0/2386	0.69	0/3231
1	C	0.47	0/2179	0.72	0/2957
1	E	0.37	0/2119	0.69	0/2881
All	All	0.43	0/6684	0.70	0/9069

There are no bond length outliers.

There are no bond angle outliers.

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	2297	0	2295	24	0
1	C	2099	0	2074	23	0
1	E	2062	0	1976	29	0
2	A	53	0	29	0	0
2	C	53	0	30	2	0
2	E	53	0	28	2	0
3	C	16	0	20	7	0
4	E	15	0	0	0	0
5	A	184	0	0	3	0
5	C	207	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	65	0	0	2	0
All	All	7104	0	6452	74	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 6.

All (74) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:ASN:HD22	1:E:255:ASN:HD22	1.16	0.86
3:C:5321[B]:MRY:HAG2	5:C:394:HOH:O	1.88	0.72
1:E:117:LEU:HD13	2:E:397:FAD:C4X	2.21	0.71
1:C:255:ASN:HD22	1:E:255:ASN:ND2	1.88	0.70
3:C:5321[A]:MRY:HAA2	5:C:459:HOH:O	1.92	0.69
1:C:275:TYR:CE1	3:C:5321[B]:MRY:HAC	2.28	0.69
1:A:163:GLN:HE21	1:A:163:GLN:H	1.44	0.66
1:A:118[A]:ARG:NE	1:A:119:GLY:O	2.28	0.65
1:C:238:MET:HG3	1:C:252[A]:VAL:HG11	1.78	0.65
1:A:238[A]:MET:HG3	1:A:252[A]:VAL:HG11	1.78	0.64
3:C:5321[B]:MRY:HAA1	5:C:459:HOH:O	1.98	0.63
1:C:275:TYR:CE1	3:C:5321[A]:MRY:HAC	2.34	0.61
1:A:12[A]:LEU:HG	1:A:262:LYS:HG2	1.83	0.61
1:A:238[A]:MET:HG3	1:A:252[A]:VAL:CG1	2.32	0.58
1:E:54:LYS:HD3	1:E:179:ARG:NH1	2.19	0.57
1:A:238[B]:MET:HA	1:A:238[B]:MET:CE	2.34	0.57
1:E:16:LEU:O	1:E:19:VAL:HG22	2.06	0.56
1:C:238:MET:HG3	1:C:252[A]:VAL:CG1	2.37	0.55
3:C:5321[A]:MRY:HAG2	5:C:394:HOH:O	2.04	0.55
1:E:145:PHE:HB2	1:E:147:ILE:HD11	1.88	0.55
1:A:45:ILE:HD13	1:A:77:ILE:HG12	1.90	0.53
1:C:222:LYS:O	1:C:226:MET:HG3	2.09	0.53
1:C:223:LEU:HA	1:C:226:MET:HE2	1.91	0.52
1:E:221:LYS:HA	1:E:231[A]:ILE:HD11	1.91	0.52
1:A:20:GLN:HG2	1:A:291:GLY:HA3	1.91	0.52
1:A:163:GLN:H	1:A:163:GLN:NE2	2.09	0.51
1:E:138:LEU:O	1:E:142:VAL:HG23	2.11	0.51
1:A:226:MET:HG3	5:A:458:HOH:O	2.10	0.51
1:C:150:ALA:HB1	2:C:396:FAD:HM81	1.94	0.50
1:E:54:LYS:HD3	1:E:179:ARG:HH11	1.77	0.50
1:A:138:LEU:C	1:A:138:LEU:HD23	2.37	0.49
1:E:196:ASP:O	1:E:199:VAL:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45[A]:ILE:HD13	1:C:77:ILE:HG12	1.95	0.49
1:C:183:GLN:OE1	3:C:5321[A]:MRY:HAA1	2.11	0.49
1:A:282[A]:MET:HG3	5:A:318:HOH:O	2.13	0.48
1:A:213:PRO:HB2	1:A:282[B]:MET:HE3	1.95	0.48
1:C:138:LEU:C	1:C:138:LEU:HD23	2.38	0.48
1:C:263:ILE:HD11	1:E:9:ARG:CD	2.43	0.48
1:E:106:TYR:HB3	1:E:111:ILE:HB	1.94	0.48
1:A:238[B]:MET:HA	1:A:238[B]:MET:HE3	1.95	0.47
1:C:96:PRO:O	1:C:100[A]:ARG:HG3	2.13	0.47
1:C:263:ILE:CD1	1:E:9:ARG:HD3	2.45	0.47
1:A:14:GLN:O	1:A:18:GLU:HG3	2.15	0.47
1:C:263:ILE:HD12	1:E:9:ARG:HD3	1.97	0.46
1:A:19:VAL:HG13	1:A:23:ILE:HG12	1.98	0.46
1:A:100:ARG:O	1:A:104[B]:ARG:HG3	2.15	0.46
2:C:396:FAD:H9	2:C:396:FAD:H1'2	1.70	0.46
1:E:99:LEU:HD12	1:E:130:MET:HE1	1.98	0.45
1:E:219:GLN:HG3	5:E:448:HOH:O	2.17	0.45
1:E:37:MET:HG2	5:E:393:HOH:O	2.18	0.44
1:E:260:MET:HE2	1:E:260:MET:HB3	1.76	0.44
1:C:256:ILE:O	1:C:260:MET:HG3	2.18	0.44
1:E:14:GLN:O	1:E:18:GLU:HG3	2.18	0.44
1:E:117:LEU:HA	2:E:397:FAD:O1P	2.18	0.43
1:E:138:LEU:C	1:E:138:LEU:HD23	2.43	0.43
1:E:209:PRO:HD2	1:E:271:ASP:O	2.19	0.43
1:E:266:ARG:HD2	1:E:266:ARG:HA	1.86	0.43
1:C:263:ILE:CD1	1:E:9:ARG:CD	2.97	0.42
1:E:16:LEU:HD11	1:E:290:LEU:HD23	2.01	0.42
1:E:143:ALA:HB3	1:E:145:PHE:CE1	2.55	0.42
1:A:215:SER:HB3	1:A:282[B]:MET:HE2	2.02	0.42
1:C:263:ILE:HD11	1:E:9:ARG:HD2	2.01	0.42
1:A:167:LEU:HD23	1:A:167:LEU:HA	1.91	0.41
1:C:112:ARG:HG2	1:C:112:ARG:HH11	1.85	0.41
1:A:31:PRO:HA	1:A:32:PRO:HD3	1.89	0.41
1:C:132:ALA:HB3	1:C:172:LYS:HD3	2.03	0.41
1:E:163:GLN:HA	1:E:163:GLN:NE2	2.36	0.41
1:A:16:LEU:HD11	1:A:290:LEU:HD23	2.03	0.41
1:E:173:VAL:HA	1:E:177:ALA:HB3	2.02	0.41
1:C:61:GLY:HA3	1:C:64:SER:OG	2.21	0.40
1:C:146[A]:ASP:OD2	1:C:178:ASN:OD1	2.39	0.40
1:A:95:THR:OG1	1:A:98:GLU:HG3	2.21	0.40
1:A:37:MET:HG2	5:A:417:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ASN:ND2	1:A:122:PRO:HA	2.37	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	297/304 (98%)	295 (99%)	1 (0%)	1 (0%)	36	21
1	C	274/304 (90%)	271 (99%)	2 (1%)	1 (0%)	30	15
1	E	275/304 (90%)	269 (98%)	5 (2%)	1 (0%)	30	15
All	All	846/912 (93%)	835 (99%)	8 (1%)	3 (0%)	30	15

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	155	VAL
1	A	155	VAL
1	E	155	VAL

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	247/258 (96%)	242 (98%)	5 (2%)	48	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	225/258 (87%)	223 (99%)	2 (1%)	70	56
1	E	205/258 (80%)	205 (100%)	0	100	100
All	All	677/774 (88%)	670 (99%)	7 (1%)	70	52

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	VAL
1	A	163	GLN
1	A	206	GLU
1	A	259[A]	ASP
1	A	259[B]	ASP
1	C	259	ASP
1	C	279	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	63	ASN
1	A	163	GLN
1	C	24	ASN
1	C	178	ASN
1	E	14	GLN
1	E	20	GLN
1	E	163	GLN
1	E	228	ASN
1	E	237	GLN
1	E	255	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	E	305	-	4,4,4	0.24	0	6,6,6	0.06	0
3	MRY	C	5321[A]	-	7,7,7	0.86	0	8,8,8	1.23	1 (12%)
2	FAD	E	397	-	58,58,58	4.48	39 (67%)	85,89,89	1.85	21 (24%)
4	SO4	E	306	-	4,4,4	0.28	0	6,6,6	0.30	0
2	FAD	C	396	-	58,58,58	3.68	33 (56%)	85,89,89	1.76	17 (20%)
2	FAD	A	395	-	58,58,58	4.01	34 (58%)	85,89,89	1.68	16 (18%)
4	SO4	E	307	-	4,4,4	0.24	0	6,6,6	0.09	0
3	MRY	C	5321[B]	-	7,7,7	0.79	0	8,8,8	2.05	3 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MRY	C	5321[A]	-	-	6/8/8/8	-
2	FAD	E	397	-	-	2/34/50/50	0/6/6/6
2	FAD	C	396	-	-	3/34/50/50	0/6/6/6
2	FAD	A	395	-	-	4/34/50/50	0/6/6/6
3	MRY	C	5321[B]	-	-	8/8/8/8	-

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	397	FAD	O2'-C2'	-12.82	1.16	1.43
2	A	395	FAD	O2'-C2'	-12.55	1.17	1.43
2	C	396	FAD	O2'-C2'	-11.76	1.18	1.43
2	E	397	FAD	C9-C8	9.17	1.52	1.39
2	E	397	FAD	C2A-N1A	8.67	1.49	1.33
2	A	395	FAD	C2A-N1A	8.44	1.48	1.33
2	E	397	FAD	C2A-N3A	8.35	1.48	1.33
2	C	396	FAD	C9-C8	8.08	1.50	1.39
2	E	397	FAD	C9-C9A	8.03	1.52	1.39
2	E	397	FAD	C8A-N7A	7.98	1.47	1.31
2	A	395	FAD	C9-C9A	7.60	1.51	1.39
2	E	397	FAD	C6-C7	7.46	1.49	1.39
2	A	395	FAD	C6-C7	7.39	1.49	1.39
2	E	397	FAD	C6-C5X	7.39	1.51	1.40
2	C	396	FAD	C9-C9A	7.38	1.51	1.39
2	A	395	FAD	C2A-N3A	7.32	1.46	1.33
2	A	395	FAD	C6-C5X	7.27	1.51	1.40
2	E	397	FAD	C4X-N5	7.15	1.46	1.30
2	A	395	FAD	C9-C8	7.14	1.49	1.39
2	C	396	FAD	C2A-N1A	7.04	1.46	1.33
2	A	395	FAD	C9A-C5X	6.91	1.52	1.41
2	C	396	FAD	C6-C7	6.81	1.48	1.39
2	E	397	FAD	O4-C4	6.80	1.36	1.23
2	C	396	FAD	C2A-N3A	6.78	1.46	1.33
2	E	397	FAD	C4A-N3A	6.34	1.46	1.34
2	A	395	FAD	C8A-N7A	6.13	1.43	1.31
2	E	397	FAD	C8A-N9A	5.97	1.47	1.37
2	E	397	FAD	O2-C2	5.87	1.36	1.24
2	A	395	FAD	C4A-N3A	5.79	1.45	1.34
2	A	395	FAD	C4X-N5	5.67	1.43	1.30
2	C	396	FAD	C6-C5X	5.58	1.48	1.40
2	C	396	FAD	C8A-N7A	5.57	1.42	1.31
2	E	397	FAD	C9A-C5X	5.42	1.49	1.41
2	C	396	FAD	C4X-N5	5.33	1.42	1.30
2	A	395	FAD	C8-C7	5.14	1.53	1.40
2	C	396	FAD	C9A-C5X	5.13	1.49	1.41
2	C	396	FAD	C4A-N3A	5.00	1.43	1.34
2	C	396	FAD	C8-C7	4.98	1.52	1.40
2	A	395	FAD	O4-C4	4.92	1.32	1.23
2	E	397	FAD	C8-C7	4.91	1.52	1.40
2	A	395	FAD	O2-C2	4.89	1.34	1.24
2	C	396	FAD	C8A-N9A	4.76	1.45	1.37
2	C	396	FAD	O4-C4	4.54	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	397	FAD	C10-N1	4.45	1.42	1.33
2	E	397	FAD	P-O3P	4.40	1.64	1.59
2	A	395	FAD	C8A-N9A	4.40	1.45	1.37
2	E	397	FAD	C2-N1	4.38	1.46	1.36
2	C	396	FAD	O2-C2	4.33	1.32	1.24
2	E	397	FAD	C5A-N7A	4.21	1.46	1.39
2	E	397	FAD	C5A-C4A	4.16	1.46	1.39
2	A	395	FAD	C2-N1	4.15	1.46	1.36
2	E	397	FAD	PA-O1A	4.10	1.65	1.50
2	E	397	FAD	P-O2P	-4.08	1.36	1.55
2	C	396	FAD	C2-N1	3.78	1.45	1.36
2	A	395	FAD	C5A-C4A	3.69	1.45	1.39
2	A	395	FAD	PA-O2A	-3.65	1.38	1.55
2	C	396	FAD	PA-O2A	-3.64	1.38	1.55
2	A	395	FAD	C6A-N6A	3.57	1.43	1.34
2	A	395	FAD	P-O2P	-3.57	1.38	1.55
2	E	397	FAD	C6A-N6A	3.43	1.43	1.34
2	C	396	FAD	C5A-C4A	3.19	1.44	1.39
2	E	397	FAD	C6A-N1A	3.19	1.44	1.35
2	E	397	FAD	C10-N10	3.17	1.44	1.37
2	A	395	FAD	C10-N1	3.14	1.39	1.33
2	A	395	FAD	C5X-N5	3.14	1.45	1.39
2	C	396	FAD	C6A-N6A	3.05	1.42	1.34
2	C	396	FAD	P-O2P	-3.05	1.41	1.55
2	E	397	FAD	PA-O2A	-3.05	1.41	1.55
2	A	395	FAD	O4'-C4'	-2.94	1.37	1.43
2	C	396	FAD	C10-N1	2.87	1.39	1.33
2	A	395	FAD	P-O3P	2.86	1.62	1.59
2	E	397	FAD	C4A-N9A	2.82	1.43	1.37
2	C	396	FAD	C2-N3	2.80	1.45	1.39
2	E	397	FAD	C5'-C4'	2.74	1.55	1.51
2	A	395	FAD	C5A-C6A	2.70	1.48	1.41
2	A	395	FAD	C5A-N7A	2.70	1.44	1.39
2	E	397	FAD	O4'-C4'	-2.69	1.37	1.43
2	E	397	FAD	C5X-N5	2.63	1.44	1.39
2	E	397	FAD	C4-N3	2.62	1.43	1.38
2	E	397	FAD	C5A-C6A	2.60	1.48	1.41
2	C	396	FAD	C10-N10	2.57	1.42	1.37
2	C	396	FAD	C5A-N7A	2.57	1.43	1.39
2	A	395	FAD	O3B-C3B	-2.55	1.36	1.43
2	E	397	FAD	O3B-C3B	-2.53	1.36	1.43
2	A	395	FAD	C10-N10	2.52	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	397	FAD	O3'-C3'	-2.48	1.36	1.43
2	A	395	FAD	O5'-C5'	-2.47	1.35	1.44
2	A	395	FAD	C6A-N1A	2.41	1.42	1.35
2	C	396	FAD	P-O1P	2.40	1.59	1.50
2	E	397	FAD	C9A-N10	2.39	1.45	1.41
2	C	396	FAD	C5A-C6A	2.39	1.47	1.41
2	A	395	FAD	C2-N3	2.38	1.44	1.39
2	C	396	FAD	C6A-N1A	2.37	1.42	1.35
2	C	396	FAD	C4-N3	2.35	1.43	1.38
2	E	397	FAD	C2-N3	2.32	1.44	1.39
2	E	397	FAD	P-O1P	2.28	1.58	1.50
2	A	395	FAD	C1B-N9A	-2.17	1.40	1.46
2	E	397	FAD	C1'-N10	-2.16	1.42	1.47
2	C	396	FAD	PA-O3P	-2.16	1.57	1.59
2	A	395	FAD	O5B-C5B	-2.15	1.36	1.44
2	A	395	FAD	PA-O1A	2.09	1.58	1.50
2	C	396	FAD	P-O3P	2.09	1.61	1.59
2	C	396	FAD	PA-O1A	2.08	1.58	1.50
2	C	396	FAD	C1'-N10	-2.08	1.42	1.47
2	C	396	FAD	O5'-C5'	-2.03	1.36	1.44
2	E	397	FAD	O5B-C5B	-2.00	1.37	1.44

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	397	FAD	N3A-C2A-N1A	-7.24	117.63	128.58
2	C	396	FAD	N3A-C2A-N1A	-6.95	118.06	128.58
2	A	395	FAD	N3A-C2A-N1A	-5.85	119.73	128.58
2	C	396	FAD	C5X-C9A-N10	5.13	122.61	117.97
2	E	397	FAD	C4X-C10-N10	4.66	123.16	116.48
3	C	5321[B]	MRY	CAA-CAC-CAE	-4.55	103.74	113.00
2	C	396	FAD	N9A-C8A-N7A	-4.09	108.14	113.94
2	E	397	FAD	N9A-C8A-N7A	-4.03	108.22	113.94
2	A	395	FAD	N9A-C8A-N7A	-3.70	108.69	113.94
2	E	397	FAD	C7M-C7-C6	-3.63	113.17	119.57
2	A	395	FAD	C4X-C10-N10	3.59	121.62	116.48
2	A	395	FAD	C4A-N9A-C8A	3.52	109.43	105.74
2	C	396	FAD	O2A-PA-O3P	3.44	116.58	107.27
2	C	396	FAD	C9-C9A-N10	-3.40	117.28	121.85
2	A	395	FAD	O4B-C1B-N9A	-3.37	101.61	108.09
2	A	395	FAD	O2'-C2'-C3'	3.36	117.11	109.25
2	A	395	FAD	O4-C4-C4X	-3.33	117.73	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	396	FAD	C5A-C4A-N3A	-3.20	122.30	126.72
2	E	397	FAD	O4B-C1B-N9A	-3.19	101.97	108.09
2	A	395	FAD	C2A-N1A-C6A	3.16	123.92	118.73
2	C	396	FAD	C4A-N9A-C8A	3.16	109.06	105.74
2	E	397	FAD	C5A-C4A-N3A	-3.08	122.47	126.72
2	A	395	FAD	O2A-PA-O3P	3.08	115.61	107.27
2	E	397	FAD	C2A-N3A-C4A	3.08	119.36	111.83
2	E	397	FAD	C4A-N9A-C8A	3.08	108.97	105.74
2	C	396	FAD	C2A-N3A-C4A	3.07	119.33	111.83
2	A	395	FAD	C5X-C9A-N10	3.02	120.70	117.97
2	E	397	FAD	C9-C9A-N10	-2.99	117.84	121.85
2	E	397	FAD	O2P-P-O1P	2.81	125.51	112.44
2	E	397	FAD	C4-N3-C2	-2.76	120.75	125.64
2	A	395	FAD	C9-C9A-N10	-2.74	118.16	121.85
2	C	396	FAD	C2A-N1A-C6A	2.61	123.02	118.73
2	C	396	FAD	O3'-C3'-C2'	2.60	114.85	108.93
2	C	396	FAD	C6-C5X-C9A	2.60	122.62	119.05
2	E	397	FAD	O4'-C4'-C3'	-2.57	103.24	109.25
2	E	397	FAD	O4'-C4'-C5'	-2.54	104.39	109.99
2	A	395	FAD	O3P-PA-O1A	-2.52	103.11	110.70
3	C	5321[A]	MRY	CAA-CAC-CAE	-2.50	107.91	113.00
2	C	396	FAD	C9A-C5X-N5	-2.47	119.84	122.45
2	E	397	FAD	C4-C4X-C10	2.42	121.09	116.93
2	A	395	FAD	O4-C4-N3	2.37	124.57	120.11
3	C	5321[B]	MRY	OAD-CAC-CAE	2.35	114.50	109.57
2	A	395	FAD	C4A-N9A-C1B	-2.34	121.16	126.63
2	E	397	FAD	C9A-N10-C10	-2.33	117.20	120.75
2	C	396	FAD	O2'-C2'-C3'	2.28	114.59	109.25
2	C	396	FAD	C1'-C2'-C3'	-2.24	103.58	109.66
2	A	395	FAD	C9A-N10-C10	-2.22	117.36	120.75
2	E	397	FAD	C2A-N1A-C6A	2.22	122.37	118.73
2	C	396	FAD	N3A-C4A-N9A	2.19	130.89	127.17
2	C	396	FAD	O2-C2-N1	-2.18	118.17	121.80
2	E	397	FAD	C6-C7-C8	2.18	122.89	119.69
2	E	397	FAD	C5B-C4B-C3B	-2.15	107.47	115.21
2	E	397	FAD	O3P-PA-O1A	-2.10	104.40	110.70
3	C	5321[B]	MRY	OAB-CAA-CAC	-2.09	106.76	111.16
2	E	397	FAD	N3A-C4A-N9A	2.06	130.67	127.17
2	A	395	FAD	N6A-C6A-N1A	2.05	122.95	118.38
2	C	396	FAD	O3P-PA-O1A	-2.03	104.59	110.70
2	E	397	FAD	C10-C4X-N5	-2.03	120.67	124.81

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	397	FAD	C5B-O5B-PA-O1A
2	E	397	FAD	C5B-O5B-PA-O3P
3	C	5321[A]	MRY	CAA-CAC-CAE-OAF
3	C	5321[A]	MRY	OAD-CAC-CAE-OAF
3	C	5321[A]	MRY	OAD-CAC-CAE-CAG
3	C	5321[A]	MRY	CAC-CAE-CAG-OAH
3	C	5321[A]	MRY	OAF-CAE-CAG-OAH
3	C	5321[B]	MRY	OAB-CAA-CAC-CAE
3	C	5321[B]	MRY	OAD-CAC-CAE-OAF
3	C	5321[B]	MRY	OAD-CAC-CAE-CAG
3	C	5321[B]	MRY	CAC-CAE-CAG-OAH
3	C	5321[B]	MRY	OAF-CAE-CAG-OAH
3	C	5321[B]	MRY	OAB-CAA-CAC-OAD
2	C	396	FAD	P-O3P-PA-O1A
3	C	5321[A]	MRY	CAA-CAC-CAE-CAG
3	C	5321[B]	MRY	CAA-CAC-CAE-CAG
2	A	395	FAD	C5B-O5B-PA-O1A
2	C	396	FAD	C5B-O5B-PA-O1A
2	A	395	FAD	P-O3P-PA-O1A
2	C	396	FAD	P-O3P-PA-O2A
3	C	5321[B]	MRY	CAA-CAC-CAE-OAF
2	A	395	FAD	C2B-C1B-N9A-C8A
2	A	395	FAD	P-O3P-PA-O2A

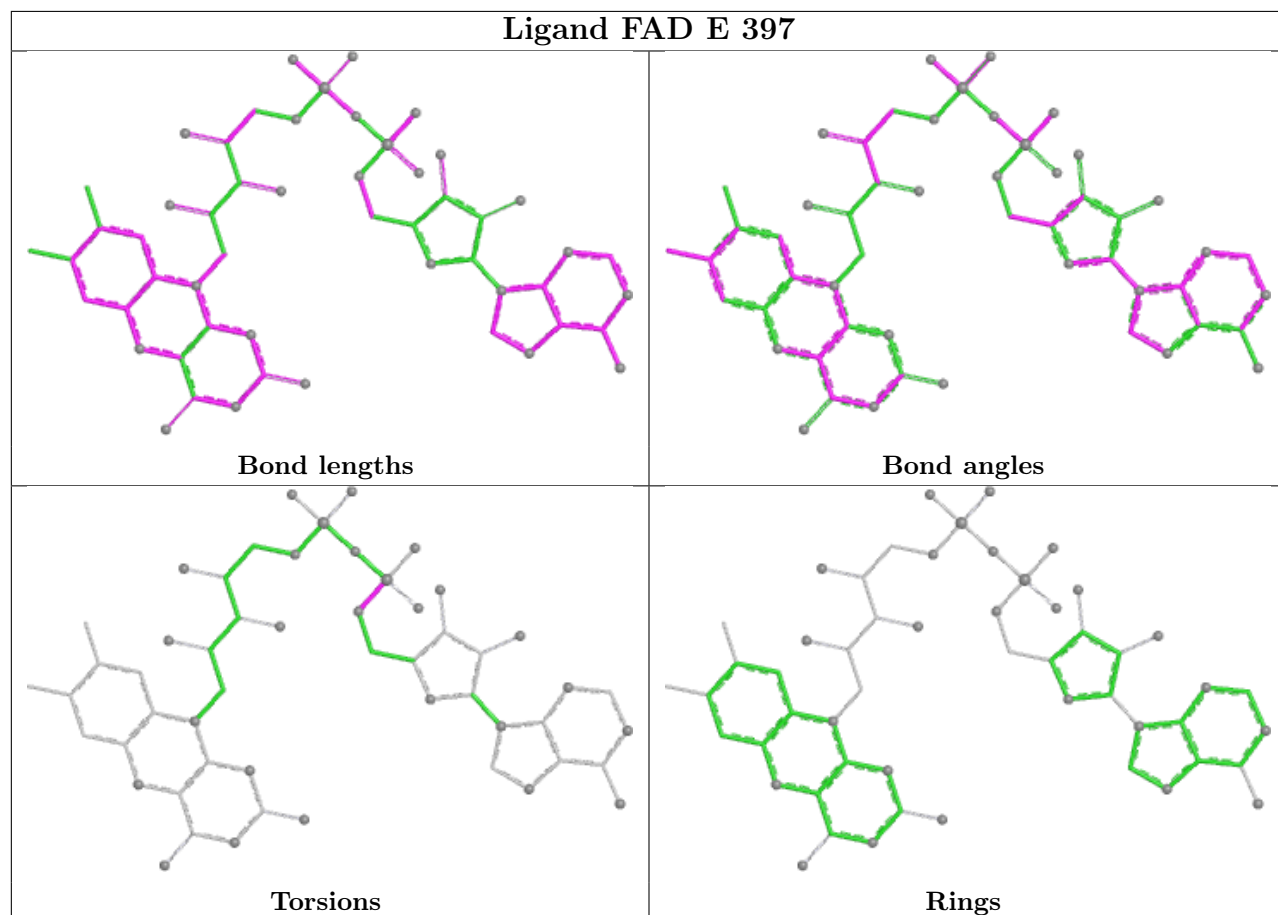
There are no ring outliers.

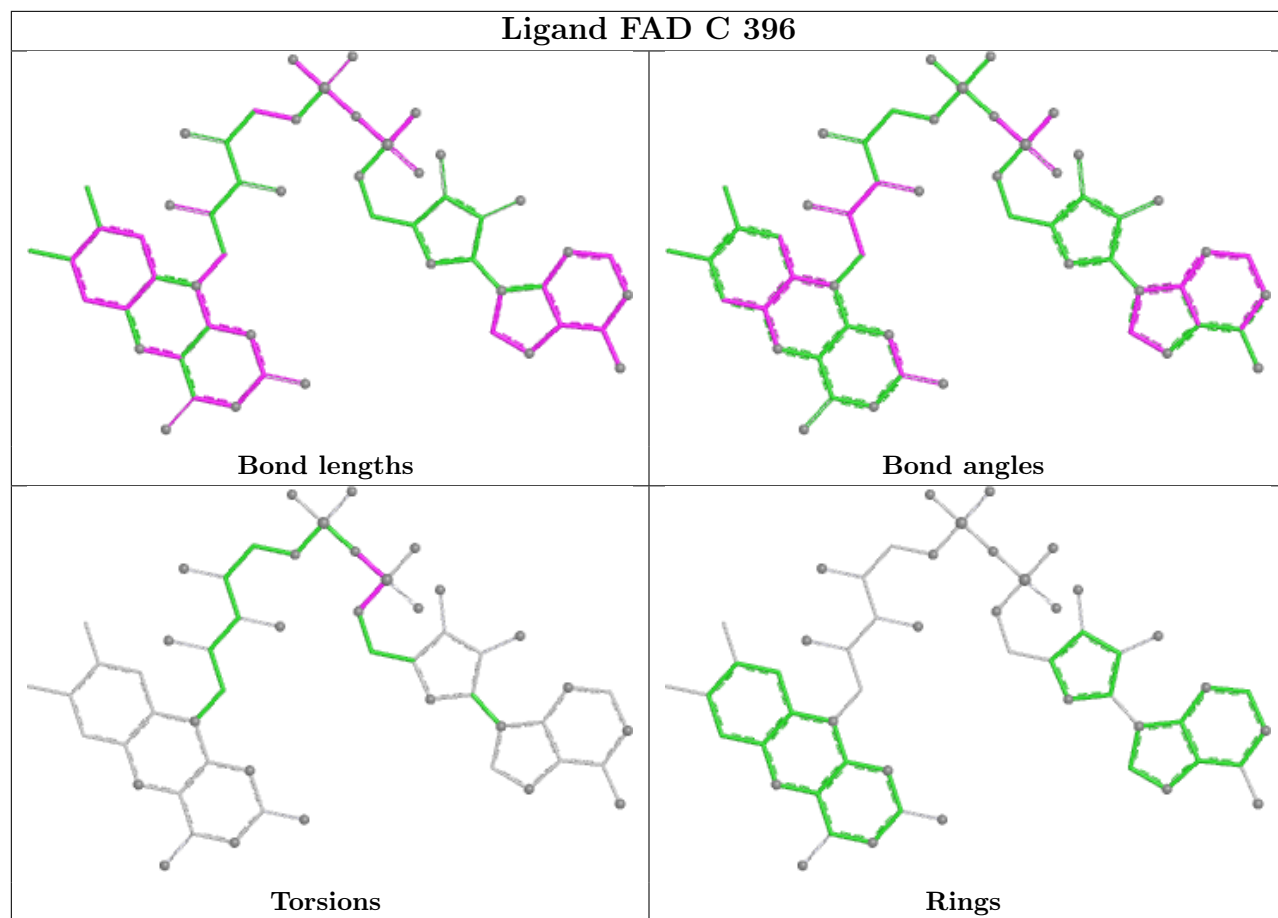
4 monomers are involved in 11 short contacts:

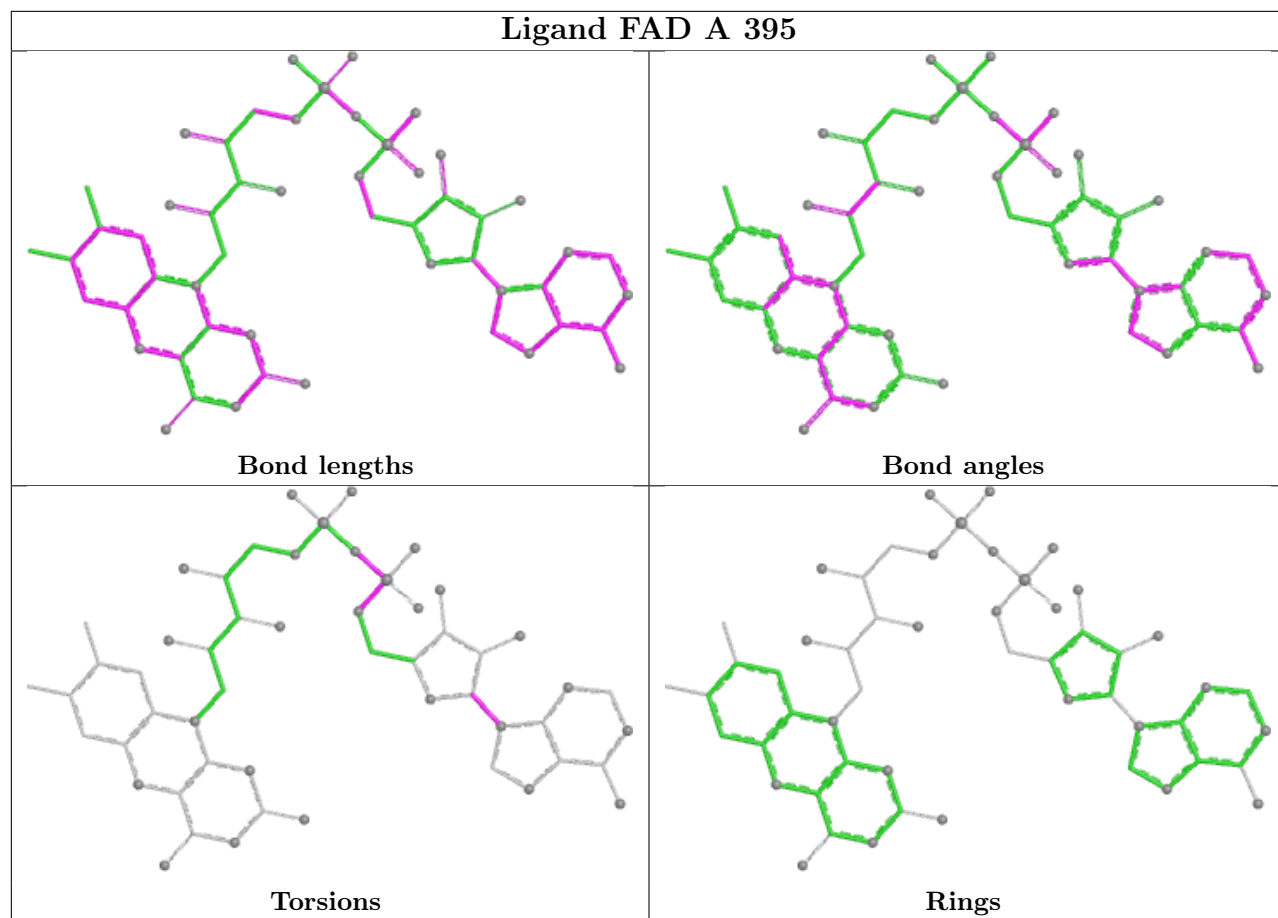
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	5321[A]	MRY	4	0
2	E	397	FAD	2	0
2	C	396	FAD	2	0
3	C	5321[B]	MRY	3	0

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.







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	286/304 (94%)	0.69	29 (10%)	12 13	11, 26, 45, 65	15 (5%)
1	C	265/304 (87%)	0.22	9 (3%)	48 52	12, 22, 37, 48	12 (4%)
1	E	274/304 (90%)	3.49	173 (63%)	0 0	15, 43, 131, 325	7 (2%)
All	All	825/912 (90%)	1.47	211 (25%)	1 1	11, 28, 64, 325	34 (4%)

All (211) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	107	TRP	26.5
1	E	102	ILE	17.7
1	E	111	ILE	16.2
1	E	103	ALA	13.9
1	E	106	TYR	13.0
1	E	97	ASP	12.0
1	E	143	ALA	11.6
1	E	141	GLU	11.4
1	E	101	THR	11.1
1	E	108	ASN	11.1
1	E	142	VAL	10.6
1	E	78	LYS	10.5
1	E	94	ALA	10.3
1	E	100	ARG	10.0
1	E	110	GLY	9.3
1	E	96	PRO	9.3
1	E	92	ILE	9.1
1	E	98	GLU	8.3
1	E	21	GLY	8.2
1	E	95	THR	8.0
1	E	19	VAL	7.5
1	E	93	ASP	7.4
1	A	4	PHE	7.4

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Mol	Chain	Res	Type	RSRZ
1	E	105	ASP	7.4
1	E	4	PHE	7.3
1	E	167	LEU	7.3
1	E	104	ARG	7.1
1	E	140	LYS	7.0
1	E	71	HIS	6.9
1	E	72	SER	6.8
1	E	109	ASN	6.8
1	E	112	ARG	6.8
1	E	11	ALA	6.4
1	E	136	VAL	6.4
1	E	159	ALA	6.4
1	E	139	LEU	6.2
1	E	147	ILE	6.0
1	E	6	ALA	6.0
1	E	131	TYR	6.0
1	E	99	LEU	5.9
1	E	137	THR	5.7
1	E	145	PHE	5.7
1	E	17	ALA	5.7
1	E	173	VAL	5.6
1	E	91	CYS	5.4
1	E	138	LEU	5.4
1	E	155	VAL	5.4
1	C	92	ILE	5.3
1	E	133	SER	5.3
1	E	200	SER	5.3
1	E	5	HIS	5.2
1	E	160	LYS	5.2
1	E	115	VAL	5.2
1	E	199	VAL	5.2
1	A	62	ALA	5.2
1	E	168	ASN	5.1
1	E	202	GLY	5.1
1	E	203	ILE	5.0
1	E	129	GLU	4.9
1	E	79	ASP	4.9
1	E	135	LEU	4.9
1	E	114	ILE	4.9
1	E	198	CYS	4.8
1	E	201	ALA	4.7
1	E	12	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	E	177	ALA	4.7
1	E	7	SER	4.7
1	E	120	ASP	4.6
1	E	178	ASN	4.6
1	E	194	PHE	4.5
1	A	3	PHE	4.5
1	E	152	TYR	4.5
1	A	122	PRO	4.5
1	E	161	SER	4.5
1	A	6	ALA	4.5
1	E	204	ASP	4.4
1	E	162	ALA	4.3
1	E	169	LEU	4.3
1	E	176	GLY	4.3
1	E	164	ALA	4.2
1	E	166	LEU	4.2
1	A	129	GLU	4.2
1	E	73	ILE	4.2
1	E	205	VAL	4.1
1	E	157	PRO	4.1
1	E	174	ASP	4.1
1	E	149	VAL	4.0
1	E	130	MET	4.0
1	E	70	THR	4.0
1	E	268	GLY	4.0
1	E	228	ASN	4.0
1	E	80	ARG	3.9
1	E	89	LEU	3.9
1	E	134	ASP	3.9
1	E	119	GLY	3.9
1	E	33	ARG	3.9
1	E	18	GLU	3.9
1	E	229	VAL	3.8
1	E	170	LYS	3.8
1	E	179	ARG	3.8
1	E	193	ARG	3.8
1	E	15[A]	SER	3.8
1	A	121	LEU	3.7
1	E	175	ALA	3.7
1	A	19	VAL	3.7
1	E	150	ALA	3.7
1	E	42	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	60	TYR	3.7
1	E	117	LEU	3.6
1	E	144	ASP	3.6
1	C	22	GLN	3.6
1	C	120	ASP	3.6
1	E	85	ALA	3.6
1	E	163	GLN	3.5
1	E	206	GLU	3.5
1	A	226	MET	3.5
1	E	151	ALA	3.5
1	E	16	LEU	3.5
1	E	39	GLN	3.5
1	E	156	HIS	3.4
1	E	158	GLU	3.4
1	E	59	THR	3.4
1	E	172	LYS	3.4
1	E	192	LEU	3.3
1	E	24	ASN	3.3
1	E	208	ILE	3.2
1	E	116	ALA	3.2
1	E	269	VAL	3.2
1	E	57	SER	3.1
1	E	86	ALA	3.1
1	E	180	ALA	3.1
1	E	184	PHE	3.1
1	E	188	VAL	3.1
1	E	171	ARG	3.1
1	E	58	VAL	3.0
1	E	20	GLN	3.0
1	E	118	ARG	3.0
1	E	90	THR	3.0
1	E	266	ARG	3.0
1	E	267	GLU	3.0
1	A	106	TYR	3.0
1	E	165	ASP	3.0
1	E	263	ILE	2.9
1	E	190	SER	2.9
1	E	191	TYR	2.9
1	E	8	GLN	2.9
1	E	207	ILE	2.9
1	E	14	GLN	2.8
1	A	10	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	46	ASP	2.8
1	E	35	SER	2.8
1	E	148	SER	2.8
1	E	22	GLN	2.8
1	E	195[A]	ARG	2.8
1	A	12[A]	LEU	2.8
1	A	5	HIS	2.8
1	A	9	ARG	2.7
1	E	88	HIS	2.7
1	E	294	PRO	2.7
1	C	129	GLU	2.7
1	E	132	ALA	2.7
1	E	224	ALA	2.7
1	E	113	HIS	2.7
1	E	225	ASP	2.7
1	E	233	ALA	2.7
1	E	223	LEU	2.6
1	E	9	ARG	2.6
1	E	227	THR	2.6
1	E	13	ASN	2.6
1	E	216	ASN	2.6
1	A	21	GLY	2.6
1	E	181	ILE	2.5
1	E	10	ASP	2.5
1	E	146	ASP	2.5
1	C	237	GLN	2.5
1	A	107	TRP	2.5
1	E	75	LYS	2.5
1	A	11	ALA	2.5
1	A	92	ILE	2.5
1	E	77	ILE	2.5
1	C	294	PRO	2.4
1	A	60	TYR	2.4
1	E	197	ARG	2.4
1	E	260	MET	2.4
1	E	34	THR	2.3
1	E	196	ASP	2.3
1	E	37	MET	2.3
1	E	226	MET	2.3
1	E	83	LEU	2.3
1	E	234	TRP	2.3
1	E	87	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	45	ILE	2.3
1	A	94	ALA	2.2
1	A	109	ASN	2.2
1	C	112	ARG	2.2
1	C	228	ASN	2.2
1	E	82	GLY	2.2
1	A	71	HIS	2.2
1	A	63	ASN	2.2
1	A	7	SER	2.2
1	A	79	ASP	2.1
1	C	204	ASP	2.1
1	E	76	GLY	2.1
1	A	72	SER	2.1
1	E	43	ASN	2.1
1	E	52	LYS	2.1
1	A	69	ARG	2.1
1	A	20	GLN	2.0
1	A	120	ASP	2.0
1	E	244	ASP	2.0
1	E	32	PRO	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	MRY	C	5321[A]	8/8	0.82	0.14	26,34,42,47	8
3	MRY	C	5321[B]	8/8	0.82	0.14	24,34,43,46	8
4	SO4	E	305	5/5	0.85	0.11	49,58,61,64	0

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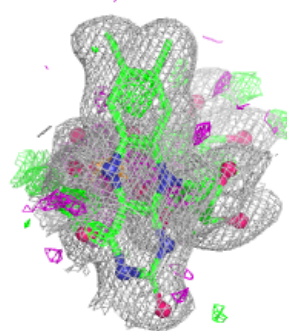
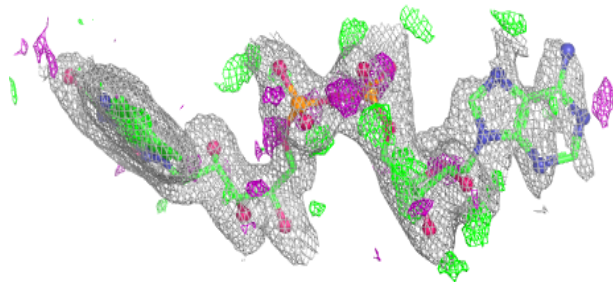
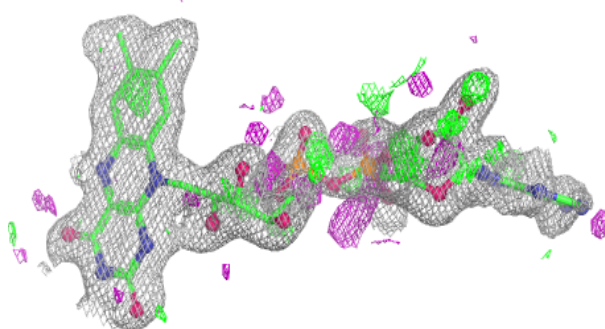
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	E	397	53/53	0.86	0.15	24,35,57,60	0
4	SO4	E	307	5/5	0.86	0.12	57,60,69,70	0
4	SO4	E	306	5/5	0.89	0.13	34,40,48,49	0
2	FAD	A	395	53/53	0.96	0.08	15,22,38,41	0
2	FAD	C	396	53/53	0.97	0.07	13,18,31,39	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.

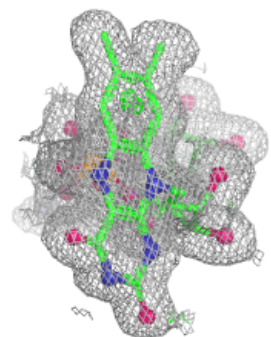
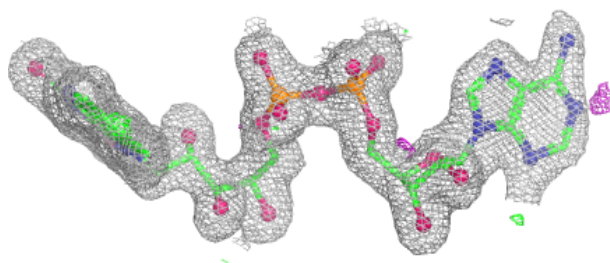
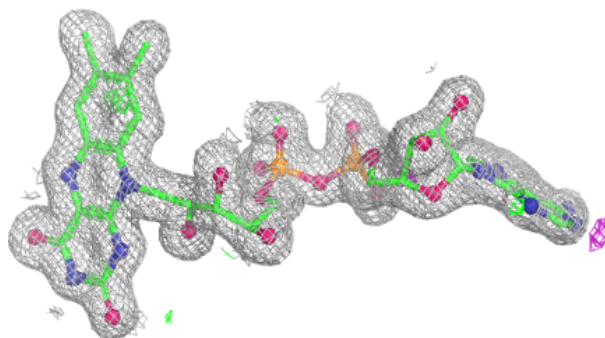
Electron density around FAD E 397:

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

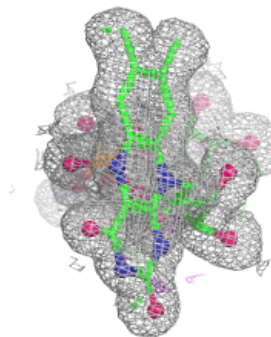
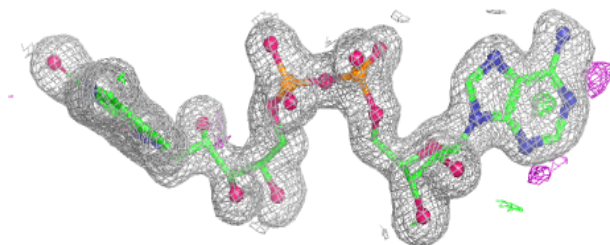
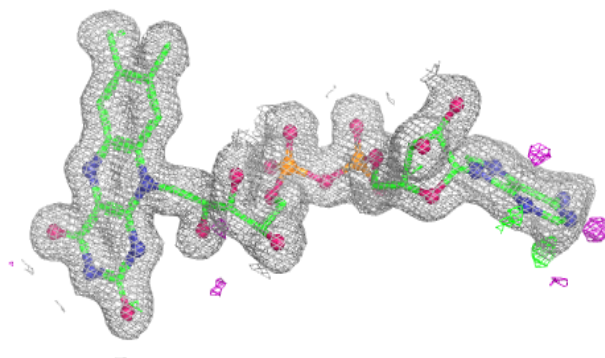


Electron density around FAD A 395:

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

**Electron density around FAD C 396:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.