W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 23, 2024 – 04:27 AM EDT

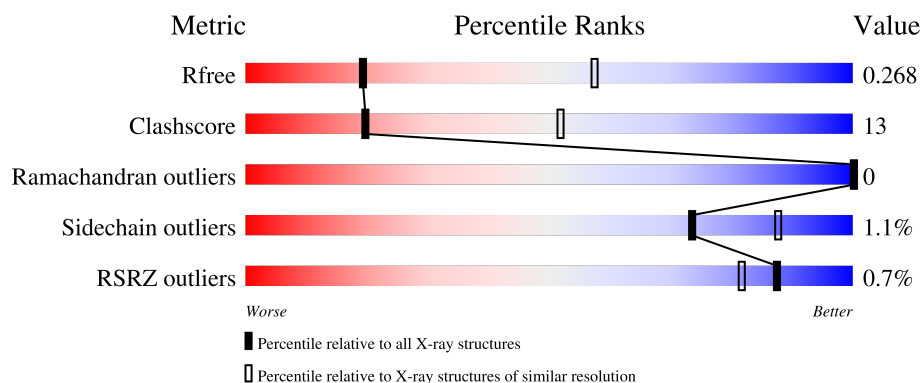|		
PDB ID	:	6RKF
Title	:	Structure of human DASPO
Authors	:	Chaves-Sanjuan, A.; Nardini, M.
Deposited on	:	2019-04-30
Resolution	:	3.22 Å(reported)

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 3.22 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	Percentile Ranks	Value
Rfree		0.268
Clashscore		13
Ramachandran outliers		0
Sidechain outliers		1.1%
RSRZ outliers		0.7%

Worse   *Better*

▌ Percentile relative to all X-ray structures

◻ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

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 <=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	350	67% 28% •
1	B	350	69% 26% 5%
1	C	350	74% 21% •
1	D	350	73% 21% 5%
1	E	350	67% 28% • 5%

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Mol	Chain	Length	Quality of chain
1	F	350	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16135 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 D-aspartate oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2604	1658	464	472	10			
1	B	334	Total	C	N	O	S	0	0	0
			2596	1653	463	471	9			
1	C	335	Total	C	N	O	S	0	0	0
			2604	1658	464	472	10			
1	D	333	Total	C	N	O	S	0	0	0
			2588	1649	462	468	9			
1	E	333	Total	C	N	O	S	0	0	0
			2588	1649	462	468	9			
1	F	333	Total	C	N	O	S	0	0	0
			2588	1649	462	468	9			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	initiating methionine	UNP Q99489
A	-7	HIS	-	expression tag	UNP Q99489
A	-6	HIS	-	expression tag	UNP Q99489
A	-5	HIS	-	expression tag	UNP Q99489
A	-4	HIS	-	expression tag	UNP Q99489
A	-3	HIS	-	expression tag	UNP Q99489
A	-2	HIS	-	expression tag	UNP Q99489
A	-1	ALA	-	expression tag	UNP Q99489
A	0	SER	-	expression tag	UNP Q99489
A	141	TYR	CYS	engineered mutation	UNP Q99489
A	143	GLY	CYS	engineered mutation	UNP Q99489
B	-8	MET	-	initiating methionine	UNP Q99489
B	-7	HIS	-	expression tag	UNP Q99489
B	-6	HIS	-	expression tag	UNP Q99489
B	-5	HIS	-	expression tag	UNP Q99489
B	-4	HIS	-	expression tag	UNP Q99489
B	-3	HIS	-	expression tag	UNP Q99489

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP Q99489
B	-1	ALA	-	expression tag	UNP Q99489
B	0	SER	-	expression tag	UNP Q99489
B	141	TYR	CYS	engineered mutation	UNP Q99489
B	143	GLY	CYS	engineered mutation	UNP Q99489
C	-8	MET	-	initiating methionine	UNP Q99489
C	-7	HIS	-	expression tag	UNP Q99489
C	-6	HIS	-	expression tag	UNP Q99489
C	-5	HIS	-	expression tag	UNP Q99489
C	-4	HIS	-	expression tag	UNP Q99489
C	-3	HIS	-	expression tag	UNP Q99489
C	-2	HIS	-	expression tag	UNP Q99489
C	-1	ALA	-	expression tag	UNP Q99489
C	0	SER	-	expression tag	UNP Q99489
C	141	TYR	CYS	engineered mutation	UNP Q99489
C	143	GLY	CYS	engineered mutation	UNP Q99489
D	-8	MET	-	initiating methionine	UNP Q99489
D	-7	HIS	-	expression tag	UNP Q99489
D	-6	HIS	-	expression tag	UNP Q99489
D	-5	HIS	-	expression tag	UNP Q99489
D	-4	HIS	-	expression tag	UNP Q99489
D	-3	HIS	-	expression tag	UNP Q99489
D	-2	HIS	-	expression tag	UNP Q99489
D	-1	ALA	-	expression tag	UNP Q99489
D	0	SER	-	expression tag	UNP Q99489
D	141	TYR	CYS	engineered mutation	UNP Q99489
D	143	GLY	CYS	engineered mutation	UNP Q99489
E	-8	MET	-	initiating methionine	UNP Q99489
E	-7	HIS	-	expression tag	UNP Q99489
E	-6	HIS	-	expression tag	UNP Q99489
E	-5	HIS	-	expression tag	UNP Q99489
E	-4	HIS	-	expression tag	UNP Q99489
E	-3	HIS	-	expression tag	UNP Q99489
E	-2	HIS	-	expression tag	UNP Q99489
E	-1	ALA	-	expression tag	UNP Q99489
E	0	SER	-	expression tag	UNP Q99489
E	141	TYR	CYS	engineered mutation	UNP Q99489
E	143	GLY	CYS	engineered mutation	UNP Q99489
F	-8	MET	-	initiating methionine	UNP Q99489
F	-7	HIS	-	expression tag	UNP Q99489
F	-6	HIS	-	expression tag	UNP Q99489
F	-5	HIS	-	expression tag	UNP Q99489

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| Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	HIS	-	expression tag	UNP Q99489
F	-3	HIS	-	expression tag	UNP Q99489
F	-2	HIS	-	expression tag	UNP Q99489
F	-1	ALA	-	expression tag	UNP Q99489
F	0	SER	-	expression tag	UNP Q99489
F	141	TYR	CYS	engineered mutation	UNP Q99489
F	143	GLY	CYS	engineered mutation	UNP Q99489

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

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL
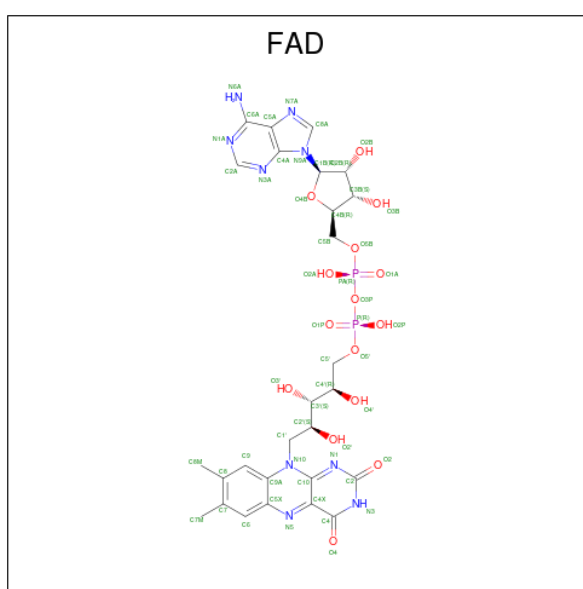
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	E	1	Total 6	C 3	O 3	0	0
3	F	1	Total 6	C 3	O 3	0	0

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).

TRS
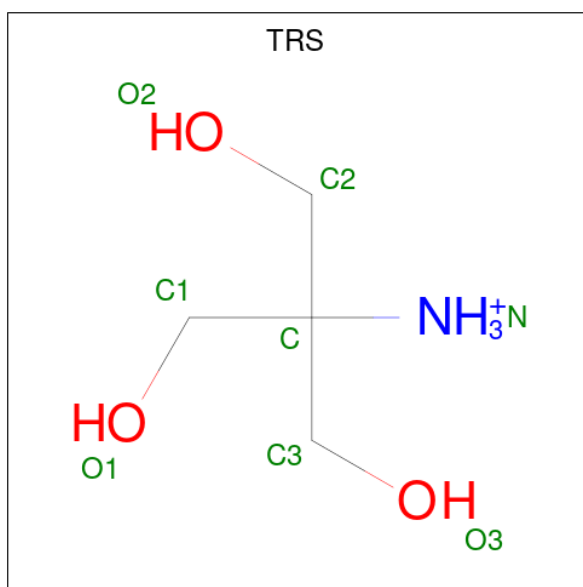
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 8	C 4	N 1	O 3	0	0
4	C	1	Total 8	C 4	N 1	O 3	0	0
4	F	1	Total 8	C 4	N 1	O 3	0	0

• Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

PO4
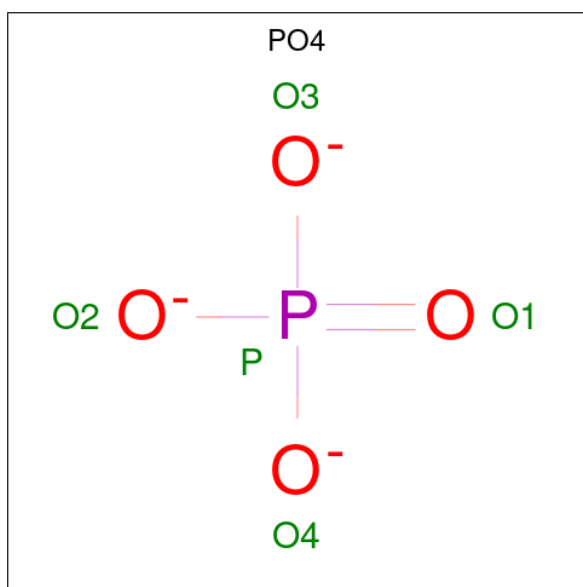
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 5	O 4	P 1	0	0

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	35	Total 35	O 35	0	0
6	B	35	Total 35	O 35	0	0
6	C	25	Total 25	O 25	0	0
6	D	27	Total 27	O 27	0	0
6	E	26	Total 26	O 26	0	0
6	F	31	Total 31	O 31	0	0

3 Residue-property plots ⓘ

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.
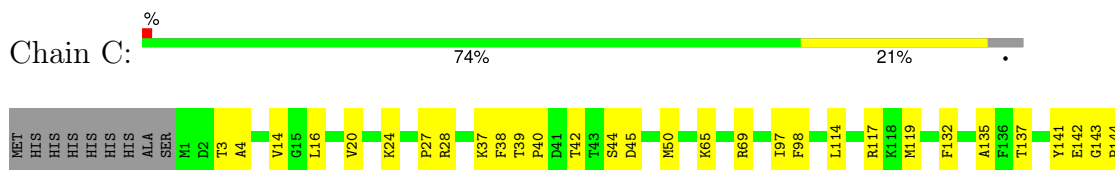
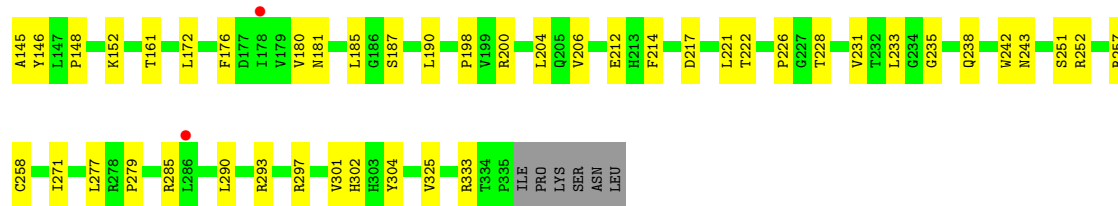- Molecule 1: D-aspartate oxidase
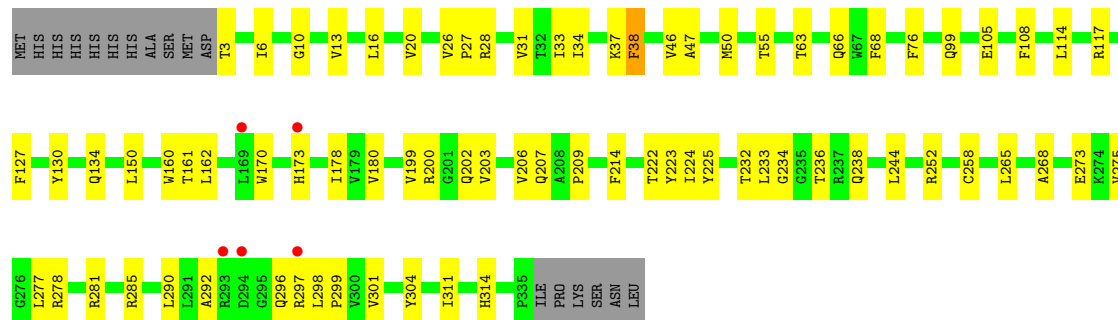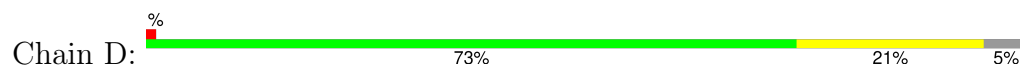
Chain A:

- Molecule 1: D-aspartate oxidase

Chain B:

- Molecule 1: D-aspartate oxidase

Chain C:

A145 Y146 L447 P148 K152 T161 L172 L177 F176 D177 I178 V179 V180 N181 L185 G186 S187 L190 P198 V199 R200 L204 Q205 V206 E212 H213 F214 D217 L221 T222 P226 G227 T228 V231 L233 G234 G235 Q238 W242 N243 S251 R252 R257

C258 I271 L277 R278 P279 R285 L286 L290 R293 R297 V301 H302 H303 Y304 V325 R333 T334 P335 ILE PRO LYS ASN LEU

• Molecule 1: D-aspartate oxidase

Chain D:

%

73%   21%   5%

MET HIS HIS HIS HIS HIS ALA SER MET ASP T3 I6 G10 V13 L16 V20 V26 P27 R28 V31 T32 I33 I34 K37 F38 V46 A47 M50 T55 T63 Q66 W67 F68 F76 Q99 E105 F108 L114 R117

F127 Y130 Q134 L150 W160 T161 L162 L169 W170 H173 I178 V179 V180 V199 R200 G201 Q202 V203 V206 Q207 A208 P209 F214 T222 Y223 I224 Y225 T232 L233 G234 G235 R237 Q238 L244 R252 C258 L265 A268 E273 K274 V275

G276 L277 R278 R281 R285 L290 L291 A292 R293 D294 G295 Q296 R297 L298 P299 V300 V301 Y304 I311 H314 P335 ILE PRO LYS SER ASN LEU

• Molecule 1: D-aspartate oxidase

Chain E:

%

67%   28%   • 5%

MET HIS HIS HIS HIS HIS ALA SER MET ASP T3 V8 V9 G10 A11 G12 V13 V14 T18 A19 I22 S23 I33 I34 S35 D36 K37 F38 T39 P40 D41 T42 T43 S44 P60 I61 H62 W67 F68 T71 L75 F76 A84 L91 Q99 P102

E105 V112 M119 K126 V130 G133 T137 T138 L139 K140 Y141 Y146 L147 P148 E151 I154 S157 T161 R165 W170 H173 V180 N181 G186 S187 R188 K195 I196 R200 G201 Q202 V203 L204 Q205 V206 G220 T232 L233 G234 G235

T236 R237 Q238 D247 A248 E249 N250 E253 I254 L255 C259 E262 P263 I271 R272 E273 R278 R281 L286 Q287 T288 R293 D294 G295 Q296 V301 H302 H303 Y304 G305 H306 G307 S308 G309 G310 I311 S312 V313 H314 W315 L319 E320 A321 V325 V329 R333

T334 P335 ILE PRO LYS SER ASN LEU

• Molecule 1: D-aspartate oxidase

Chain F:

%

70%   25%   • 5%

MET HIS HIS HIS HIS HIS ALA SER MET ASP T3 V8 V9 G10 V13 V14 A19 I22 V26 P27 R28 F38 T39 H54 T55 Y56 H62 Q66 R69 L91 W95 Q96 I97 F98 Q99 S100 T101 E105 V112 R117 K118 M119 L124

K125 K126 F127 Y130 V131 F132 G133 Q134 A135 L139 K140 Y141 E142 G143 P144 L147 P148 W149 L150 E151 I154 R153 I154 K155 T163 R164 R165 I166 L172 F176 N181 C182 Q202 V203 V206 I215 R216 L221 T228 T232 L233 G234 G235 T236 R237 W242

N243 L244 S245 P246 E253 I254 R257 C258 L261 E262 P263 S264 L265 E273 K274 V275 G276 L277 V284 R285 L286 L290 L291 A292 R297 V301 H302 H303 I311 H314 V325 P335 ILE PRO LYS SER ASN LEU

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	114.40Å 159.72Å 288.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.00 – 3.22 93.00 – 3.22	Depositor EDS
% Data completeness (in resolution range)	53.4 (93.00-3.22) 53.4 (93.00-3.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.96 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.15_3448: ???)	Depositor
R, R_{free}	0.231 , 0.271 0.232 , 0.268	Depositor DCC
R_{free} test set	1203 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å^2)	51.5	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.8	EDS
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	16135	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: FAD, TRS, GOL, PO4

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	0.28	0/2675	0.48	0/3643
1	B	0.29	0/2667	0.48	0/3633
1	C	0.27	0/2675	0.47	0/3643
1	D	0.27	0/2659	0.46	0/3622
1	E	0.28	0/2659	0.47	0/3622
1	F	0.30	0/2659	0.49	0/3622
All	All	0.28	0/15994	0.48	0/21785

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 ⓘ

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	2604	0	2575	75	0
1	B	2596	0	2563	62	0
1	C	2604	0	2575	56	0
1	D	2588	0	2559	56	0
1	E	2588	0	2559	75	0
1	F	2588	0	2559	86	0
2	A	53	0	31	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	0	31	5	0
2	C	53	0	31	2	0
2	D	53	0	31	3	0
2	E	53	0	31	6	0
2	F	53	0	31	1	0
3	A	6	0	8	0	0
3	B	6	0	8	1	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
3	E	6	0	8	0	0
3	F	6	0	8	1	0
4	A	8	0	12	1	0
4	C	8	0	12	1	0
4	F	8	0	12	1	0
5	A	5	0	0	0	0
5	F	5	0	0	0	0
6	A	35	0	0	0	0
6	B	35	0	0	0	0
6	C	25	0	0	0	0
6	D	27	0	0	0	0
6	E	26	0	0	0	0
6	F	31	0	0	0	0
All	All	16135	0	15660	402	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 13.

The worst 5 of 402 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:E:38:PHE:CZ	1:E:161:THR:HG21	1.94	1.01
1:E:39:THR:HG21	1:E:148:PRO:HG3	1.44	0.96
1:F:119:MET:HE3	1:F:133:GLY:HA3	1.57	0.87
1:F:9:VAL:HG12	1:F:181:ASN:HA	1.56	0.87
1:F:290:LEU:HD21	1:F:297:ARG:HD2	1.58	0.83

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/350 (95%)	308 (92%)	25 (8%)	0	100	100
1	B	332/350 (95%)	313 (94%)	19 (6%)	0	100	100
1	C	333/350 (95%)	308 (92%)	25 (8%)	0	100	100
1	D	331/350 (95%)	312 (94%)	19 (6%)	0	100	100
1	E	331/350 (95%)	310 (94%)	21 (6%)	0	100	100
1	F	331/350 (95%)	307 (93%)	24 (7%)	0	100	100
All	All	1991/2100 (95%)	1858 (93%)	133 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	278/292 (95%)	273 (98%)	5 (2%)	59	81
1	B	277/292 (95%)	275 (99%)	2 (1%)	84	93
1	C	278/292 (95%)	278 (100%)	0	100	100
1	D	276/292 (94%)	273 (99%)	3 (1%)	73	88
1	E	276/292 (94%)	270 (98%)	6 (2%)	52	78
1	F	276/292 (94%)	273 (99%)	3 (1%)	73	88
All	All	1661/1752 (95%)	1642 (99%)	19 (1%)	73	88

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	259	CYS
1	F	127	PHE
1	F	141	TYR
1	F	95	TRP
1	D	68	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	189	GLN
1	F	189	GLN
1	E	207	GLN
1	F	62	HIS
1	F	243	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

17 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	FAD	E	401	-	54,58,58	0.50	0	71,89,89	0.47	1 (1%)
4	TRS	A	403	-	7,7,7	0.34	0	9,9,9	0.34	0
5	PO4	F	404	-	4,4,4	0.93	0	6,6,6	0.47	0
2	FAD	D	401	-	54,58,58	0.52	0	71,89,89	0.47	1 (1%)
3	GOL	A	402	-	5,5,5	0.93	0	5,5,5	1.07	0
3	GOL	D	402	-	5,5,5	0.96	0	5,5,5	1.08	0
2	FAD	C	401	-	54,58,58	0.51	0	71,89,89	0.45	1 (1%)
3	GOL	F	403	-	5,5,5	0.89	0	5,5,5	1.10	0
4	TRS	F	402	-	7,7,7	0.34	0	9,9,9	0.27	0
3	GOL	B	402	-	5,5,5	0.10	0	5,5,5	0.28	0
2	FAD	F	401	-	54,58,58	0.50	0	71,89,89	0.46	1 (1%)
3	GOL	C	403	-	5,5,5	0.10	0	5,5,5	0.26	0
5	PO4	A	404	-	4,4,4	0.95	0	6,6,6	0.45	0
4	TRS	C	402	-	7,7,7	0.36	0	9,9,9	0.38	0
3	GOL	E	402	-	5,5,5	0.96	0	5,5,5	1.08	0
2	FAD	B	401	-	54,58,58	0.53	0	71,89,89	0.49	1 (1%)
2	FAD	A	401	-	54,58,58	0.50	0	71,89,89	0.46	1 (1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	E	401	-	-	11/30/50/50	0/6/6/6
4	TRS	A	403	-	-	0/9/9/9	-
2	FAD	D	401	-	-	5/30/50/50	0/6/6/6
3	GOL	A	402	-	-	0/4/4/4	-
3	GOL	D	402	-	-	0/4/4/4	-
2	FAD	C	401	-	-	5/30/50/50	0/6/6/6
3	GOL	F	403	-	-	0/4/4/4	-
4	TRS	F	402	-	-	0/9/9/9	-
3	GOL	B	402	-	-	0/4/4/4	-
2	FAD	F	401	-	-	2/30/50/50	0/6/6/6
3	GOL	C	403	-	-	0/4/4/4	-
4	TRS	C	402	-	-	0/9/9/9	-
3	GOL	E	402	-	-	0/4/4/4	-
2	FAD	B	401	-	-	1/30/50/50	0/6/6/6
2	FAD	A	401	-	-	17/30/50/50	0/6/6/6

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	401	FAD	C5A-C6A-N6A	2.35	123.89	120.31
2	C	401	FAD	C5A-C6A-N6A	2.34	123.87	120.31
2	F	401	FAD	C5A-C6A-N6A	2.33	123.87	120.31
2	B	401	FAD	C5A-C6A-N6A	2.33	123.86	120.31
2	D	401	FAD	C5A-C6A-N6A	2.32	123.85	120.31

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	FAD	C5'-O5'-P-O1P
2	A	401	FAD	C5'-O5'-P-O2P
2	C	401	FAD	C5'-O5'-P-O1P
2	C	401	FAD	C5'-O5'-P-O3P
2	D	401	FAD	C5B-O5B-PA-O2A

There are no ring outliers.

11 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	FAD	6	0
4	A	403	TRS	1	0
2	D	401	FAD	3	0
2	C	401	FAD	2	0
3	F	403	GOL	1	0
4	F	402	TRS	1	0
3	B	402	GOL	1	0
2	F	401	FAD	1	0
4	C	402	TRS	1	0
2	B	401	FAD	5	0
2	A	401	FAD	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.
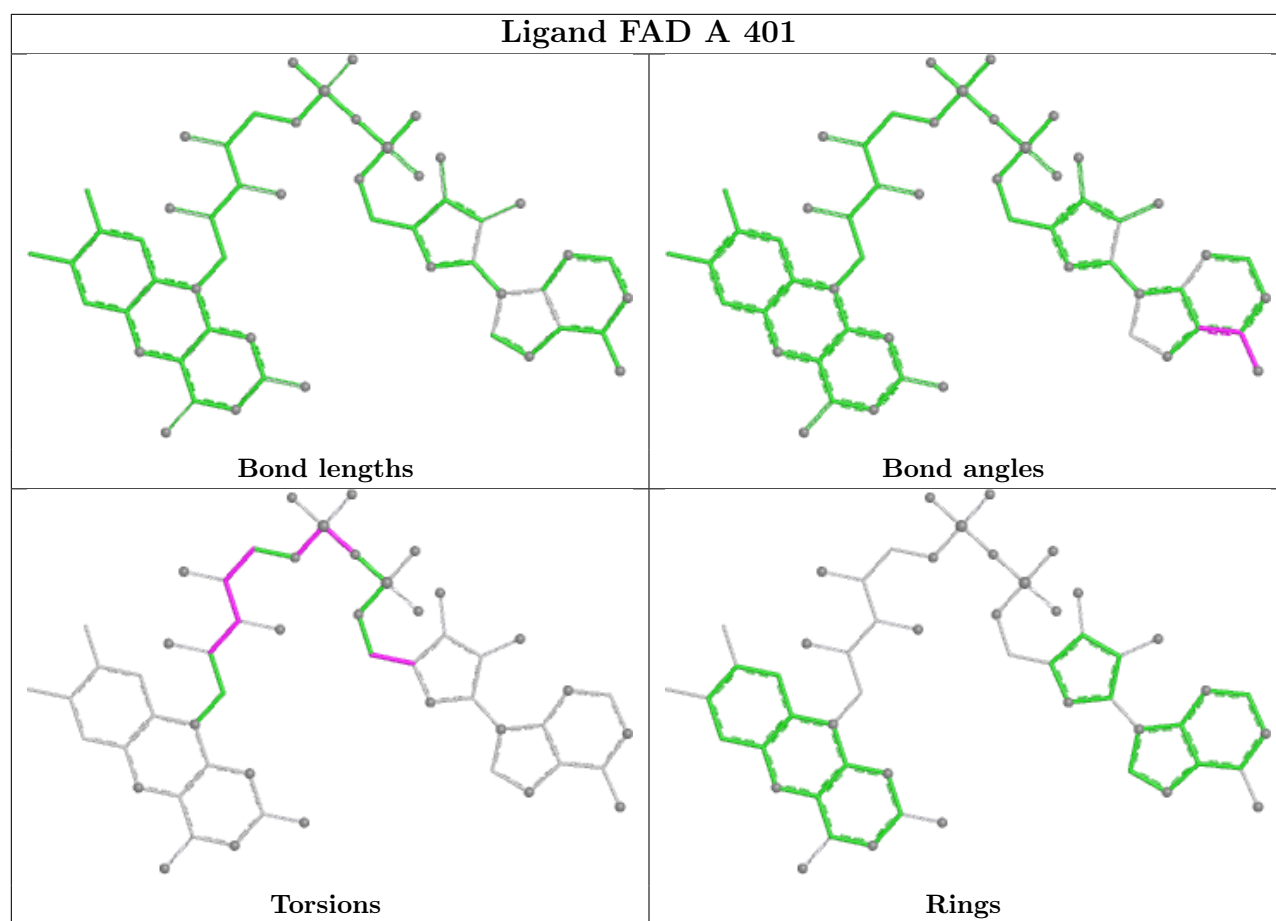
Ligand FAD E 401

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD D 401

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD C 401

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD F 401

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD A 401

Bond lengths

Bond angles

Torsions

Rings
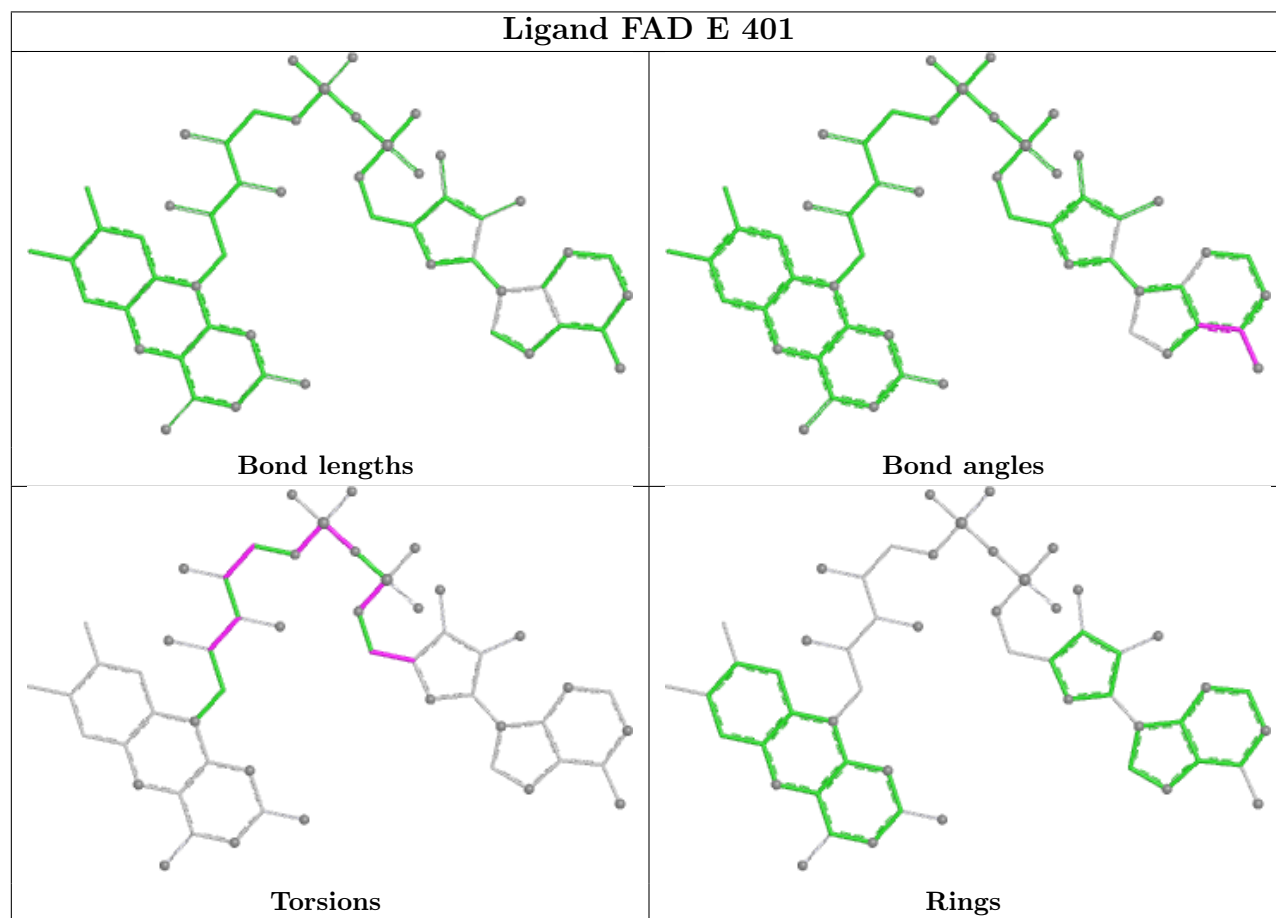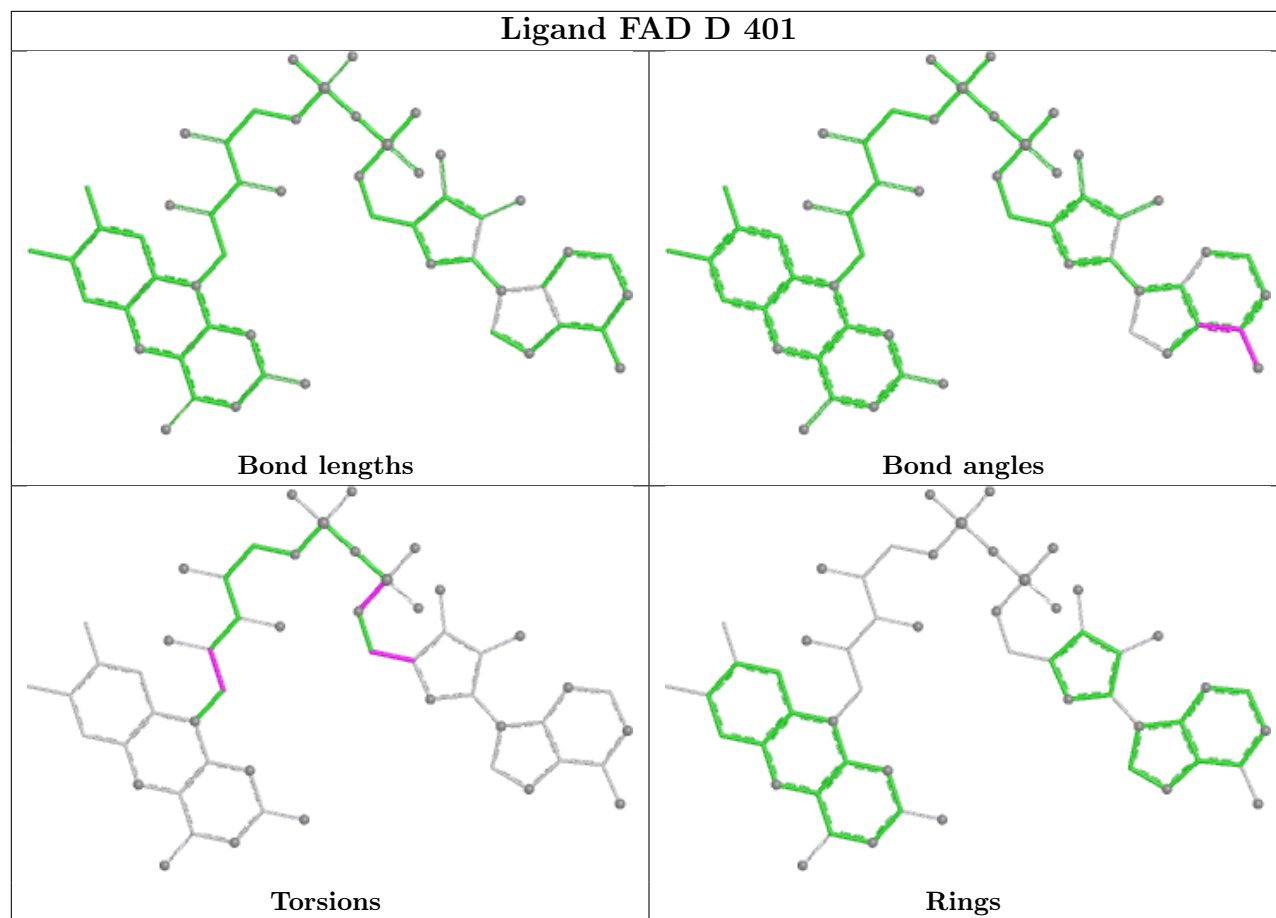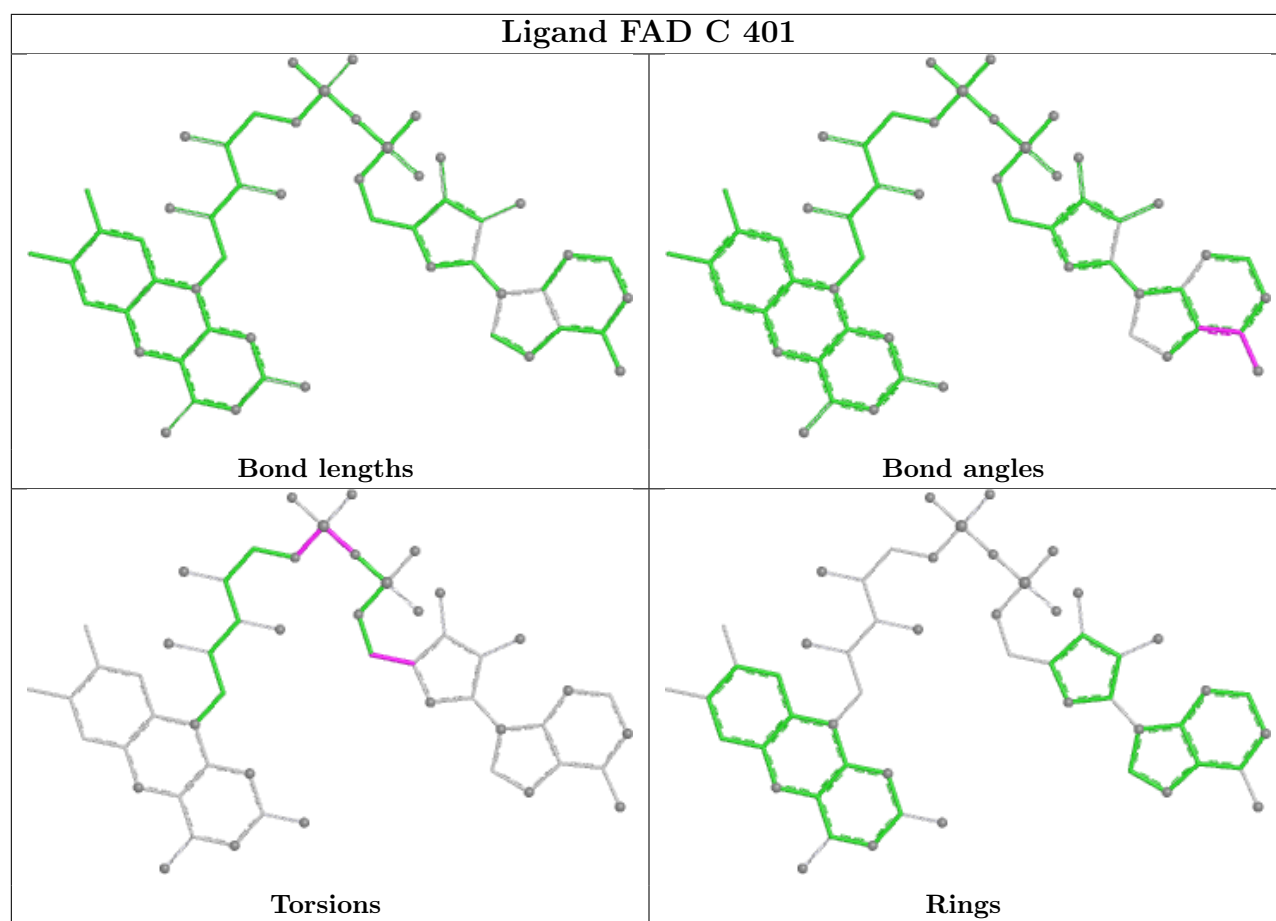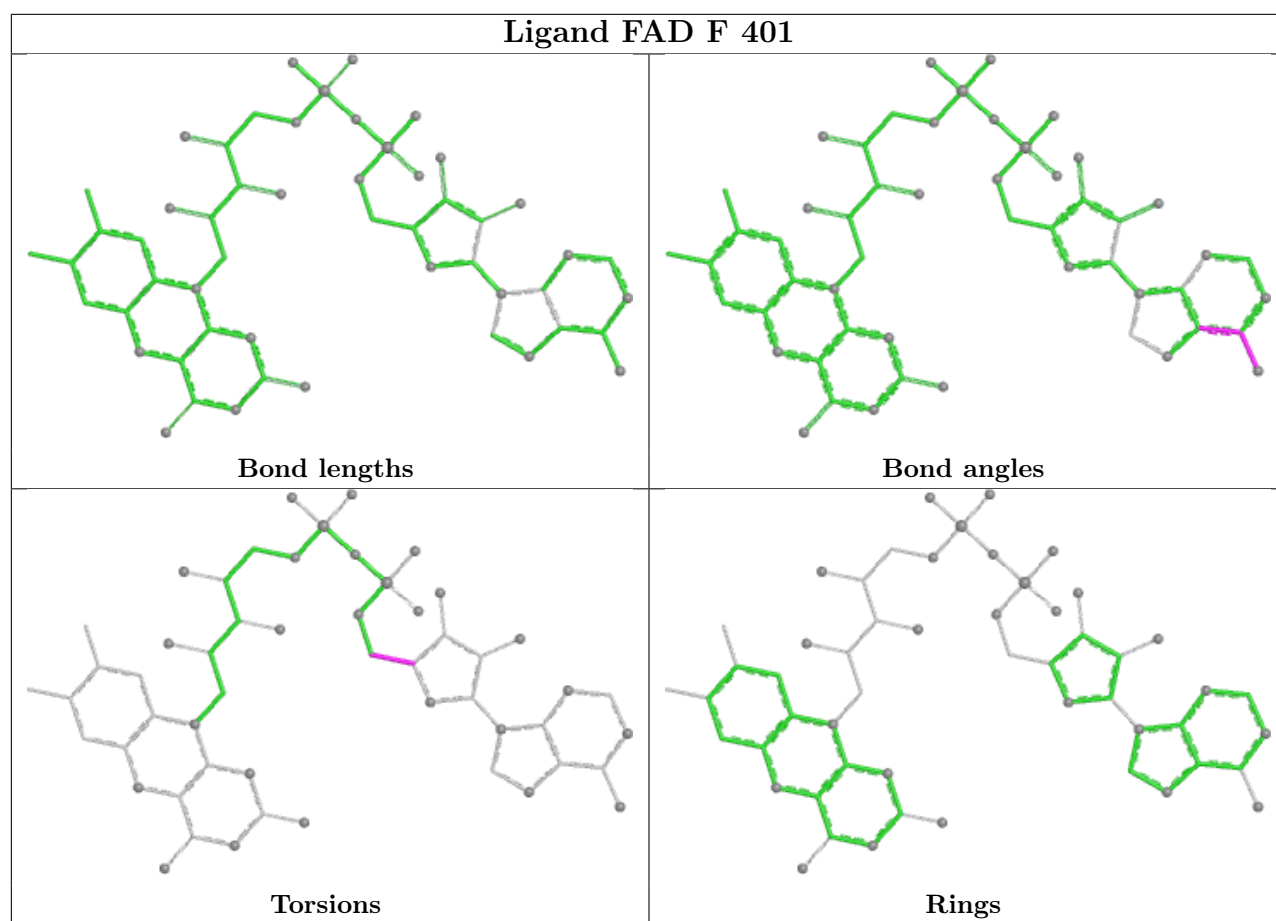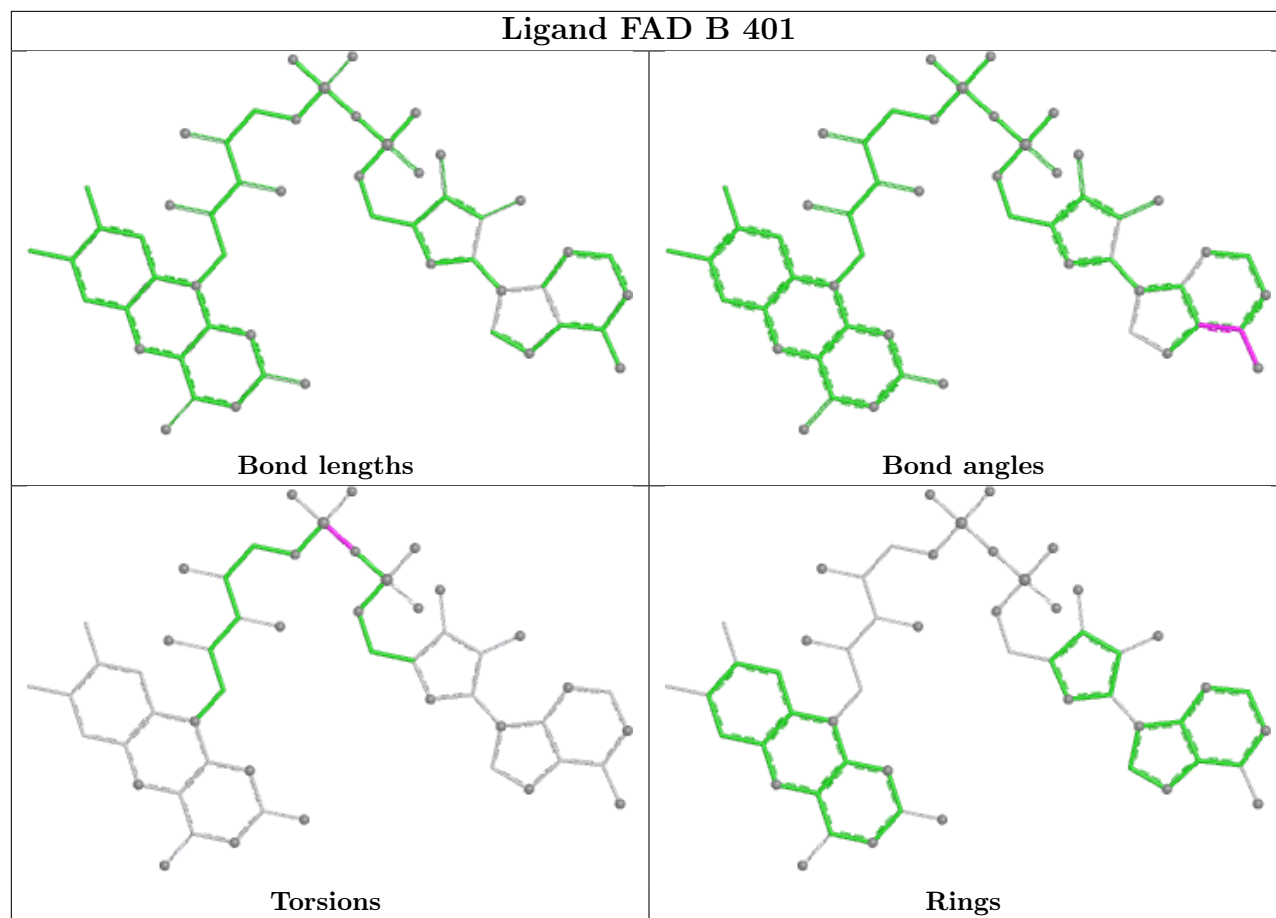
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	335/350 (95%)	-0.01	2 (0%)	89	84	13, 45, 81, 109	0
1	B	334/350 (95%)	0.01	2 (0%)	89	84	20, 46, 72, 108	0
1	C	335/350 (95%)	0.06	2 (0%)	89	84	16, 53, 86, 111	0
1	D	333/350 (95%)	0.08	5 (1%)	73	62	20, 57, 98, 131	0
1	E	333/350 (95%)	0.15	2 (0%)	89	84	25, 62, 97, 113	0
1	F	333/350 (95%)	0.05	2 (0%)	89	84	26, 52, 85, 111	0
All	All	2003/2100 (95%)	0.06	15 (0%)	87	82	13, 52, 90, 131	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	297	ARG	3.2
1	E	102	PRO	2.9
1	B	221	LEU	2.9
1	D	293	ARG	2.6
1	C	178	ILE	2.4

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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($\mathring{A}^2$)	Q<0.9
3	GOL	A	402	6/6	0.85	0.38	43,45,46,47	0
3	GOL	D	402	6/6	0.85	0.32	46,48,49,49	0
4	TRS	F	402	8/8	0.88	0.38	56,58,61,62	0
3	GOL	B	402	6/6	0.91	0.36	47,48,49,49	0
5	PO4	F	404	5/5	0.91	0.21	84,85,85,86	0
3	GOL	F	403	6/6	0.93	0.49	63,64,65,65	0
5	PO4	A	404	5/5	0.93	0.34	98,98,99,99	0
4	TRS	A	403	8/8	0.93	0.22	45,47,48,49	0
4	TRS	C	402	8/8	0.94	0.33	41,42,42,43	0
2	FAD	E	401	53/53	0.94	0.21	39,50,54,56	0
2	FAD	A	401	53/53	0.95	0.22	25,38,45,46	0
3	GOL	C	403	6/6	0.95	0.23	20,21,22,23	0
2	FAD	F	401	53/53	0.95	0.19	39,43,53,60	0
3	GOL	E	402	6/6	0.95	0.20	40,42,43,45	0
2	FAD	D	401	53/53	0.95	0.21	38,54,62,62	0
2	FAD	B	401	53/53	0.96	0.21	33,43,52,56	0
2	FAD	C	401	53/53	0.96	0.23	23,38,57,68	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 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
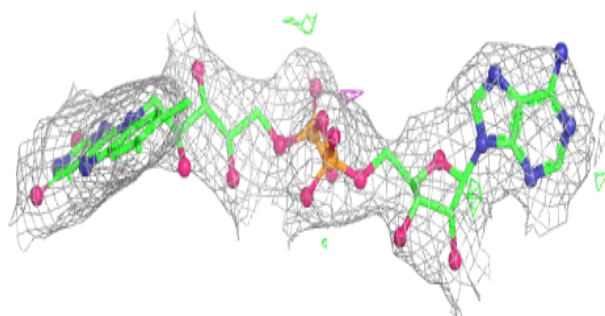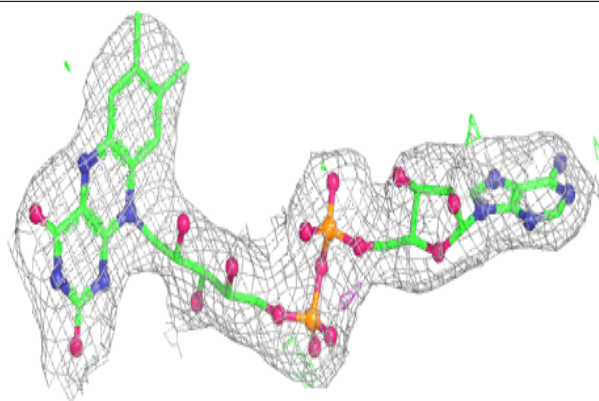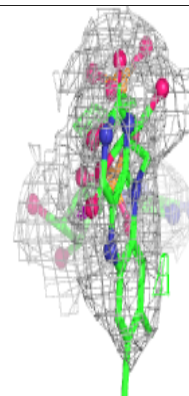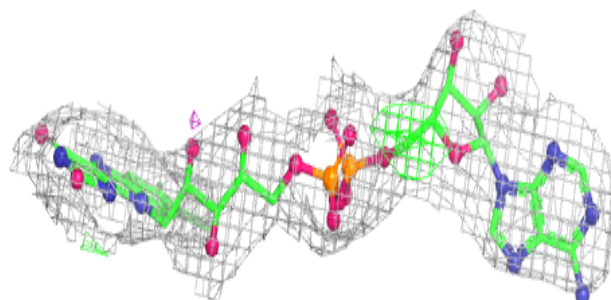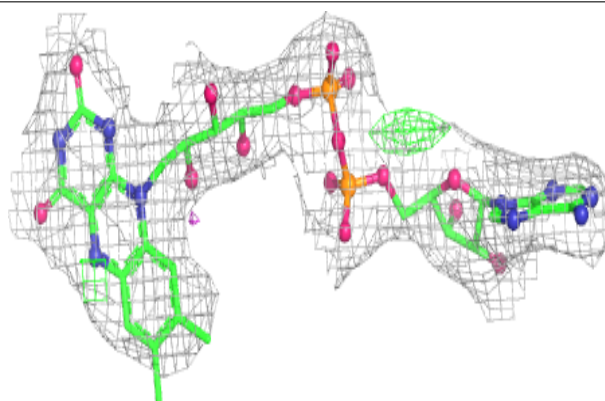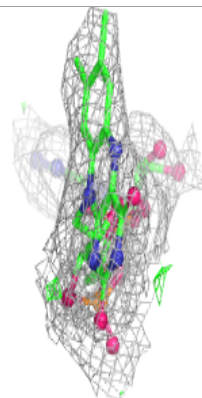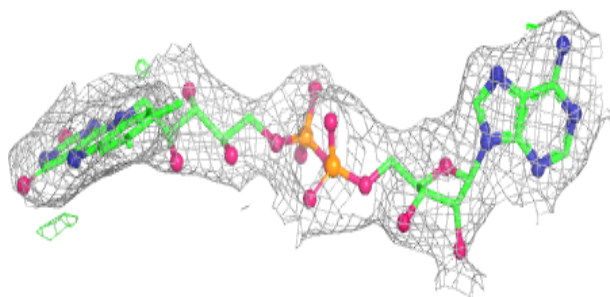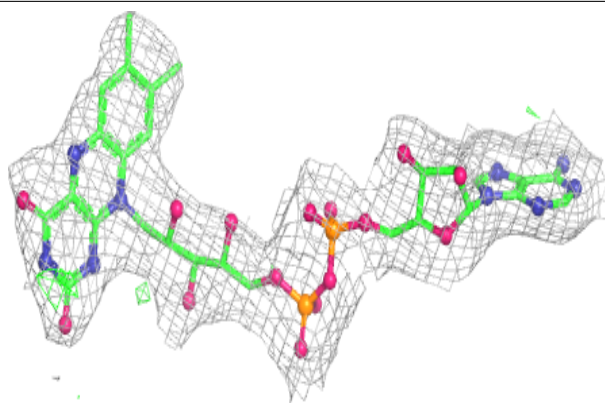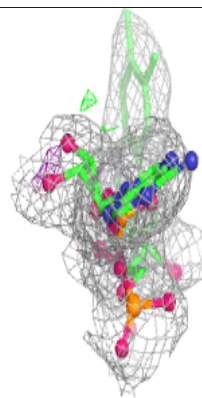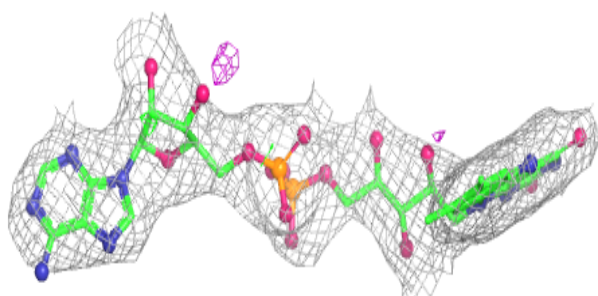mF_o-DF_c (at 3 rmsd) in purple (negative)
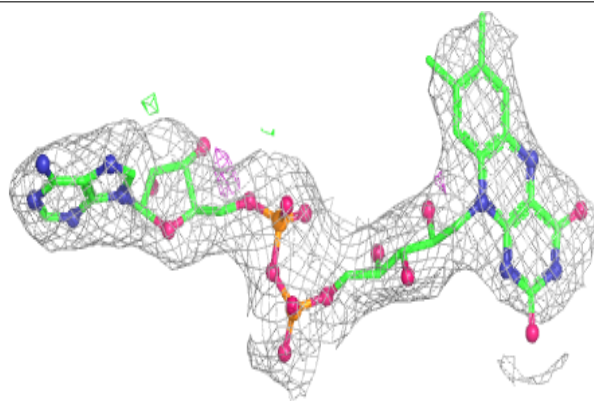and green (positive)
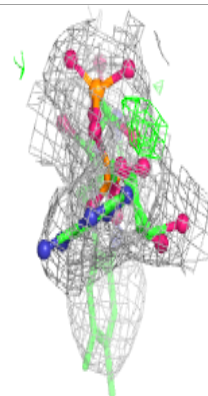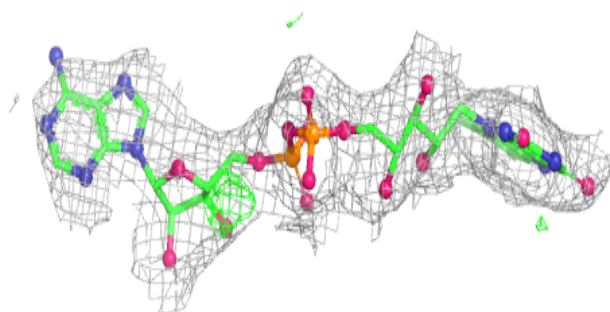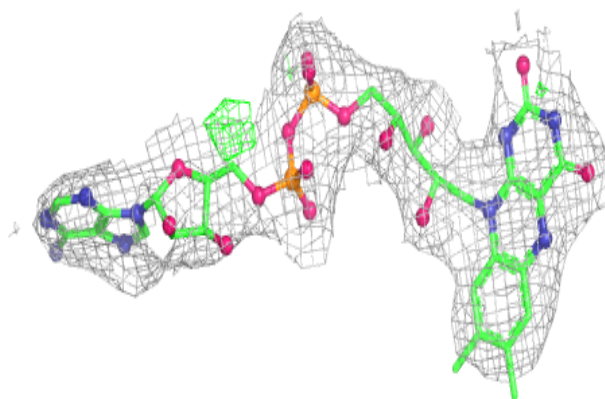
Electron density around FAD A 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
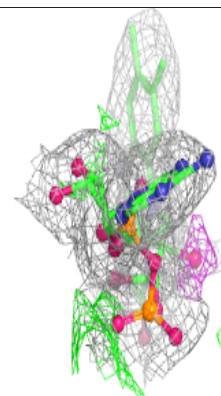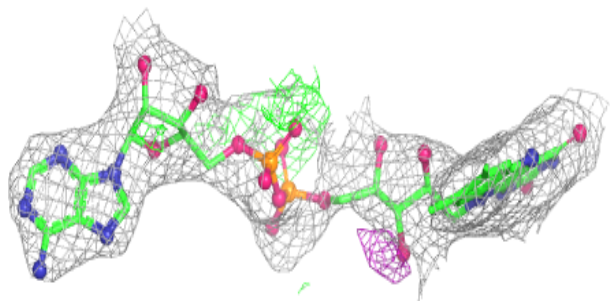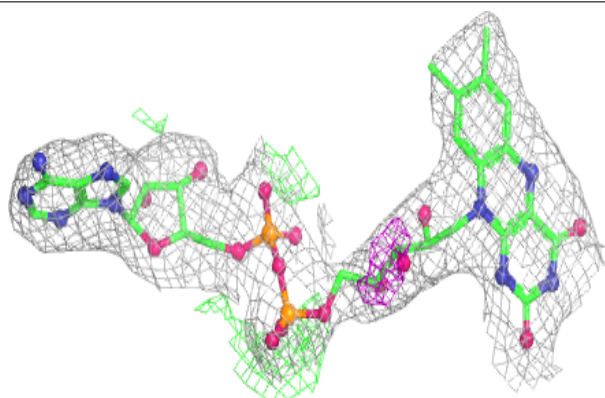
Electron density around FAD F 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
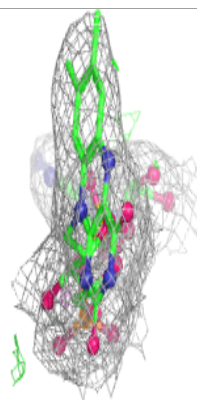
Electron density around FAD D 401:

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

Electron density around FAD B 401:

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

Electron density around FAD C 401:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.