wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 16, 2023 – 06:20 PM EDT

PDB ID	:	2F1O
Title	:	Crystal Structure of NQO1 with Dicoumarol
Authors	:	Shaul, Y.; Asher, G.; Dym, O.; Tsvetkov, P.; Adler, J.; Israel Structural Proteomics Center (ISPC)
Deposited on	:	2005-11-15
Resolution	:	2.75 Å(reported)

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

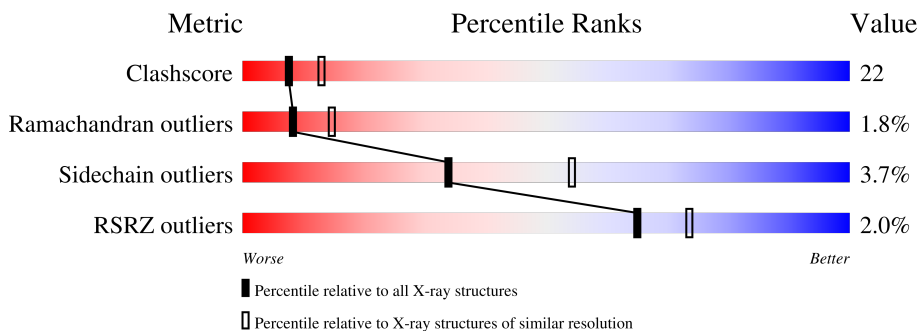|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1   Overall quality at a glance   ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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
Clashscore		22
Ramachandran outliers		1.8%
Sidechain outliers		3.7%
RSRZ outliers		2.0%

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))
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	273	59% 38%
1	B	273	53% 45%
1	C	273	59% 38%
1	D	273	58% 40%
1	E	273	63% 34%
1	F	273	55% 45%

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Mol	Chain	Length	Quality of chain
1	G	273	4% 60% 38%
1	H	273	3% 51% 45%

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	DTC	A	2280	X	-	-	-
2	DTC	B	3280	X	-	-	-
2	DTC	C	280	X	-	-	-
2	DTC	D	1280	X	-	-	-
2	DTC	E	4280	X	-	-	-
2	DTC	E	5280	X	-	-	-
2	DTC	G	7280	X	-	-	-
2	DTC	H	6280	X	-	-	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 18146 atoms, of which 0 are hydrogens and 0 are deuteriums.
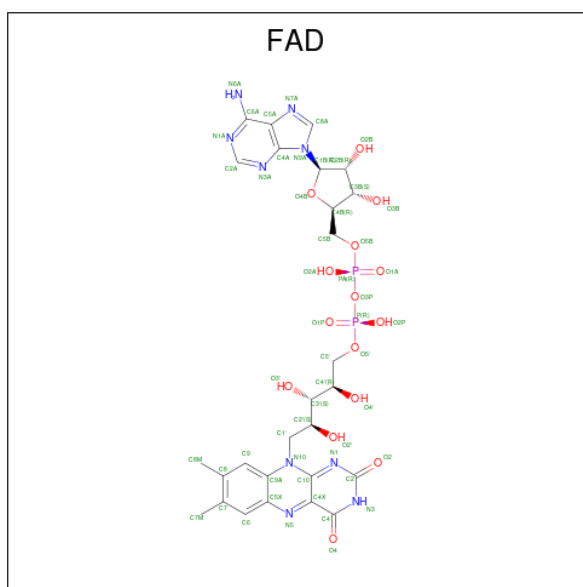
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NAD(P)H dehydrogenase [quinone] 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2175	1414	365	389	7			
1	B	273	Total	C	N	O	S	0	0	0
			2175	1414	365	389	7			
1	C	273	Total	C	N	O	S	0	0	0
			2175	1414	365	389	7			
1	D	273	Total	C	N	O	S	0	0	0
			2175	1414	365	389	7			
1	E	273	Total	C	N	O	S	0	0	0
			2175	1414	365	389	7			
1	F	273	Total	C	N	O	S	0	0	0
			2175	1414	365	389	7			
1	G	273	Total	C	N	O	S	0	0	0
			2175	1414	365	389	7			
1	H	273	Total	C	N	O	S	0	0	0
			2175	1414	365	389	7			

- Molecule 2 is BISHYDROXY[2H-1-BENZOPYRAN-2-ONE,1,2-BENZOPYRONE] (three-letter code: DTC) (formula: $C_{19}H_{12}O_6$).

DTC

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 25	C 19	O 6	0	0
2	B	1	Total 25	C 19	O 6	0	0
2	C	1	Total 25	C 19	O 6	0	0
2	D	1	Total 25	C 19	O 6	0	0
2	E	1	Total 25	C 19	O 6	0	0
2	E	1	Total 25	C 19	O 6	0	0
2	G	1	Total 25	C 19	O 6	0	0
2	H	1	Total 25	C 19	O 6	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

FAD

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total	O	0	0
			19	19		
4	B	23	Total	O	0	0
			23	23		
4	C	23	Total	O	0	0
			23	23		
4	D	13	Total	O	0	0
			13	13		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	18	Total 18	O 18	0	0
4	F	10	Total 10	O 10	0	0
4	G	8	Total 8	O 8	0	0
4	H	8	Total 8	O 8	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: NAD(P)H dehydrogenase [quinone] 1
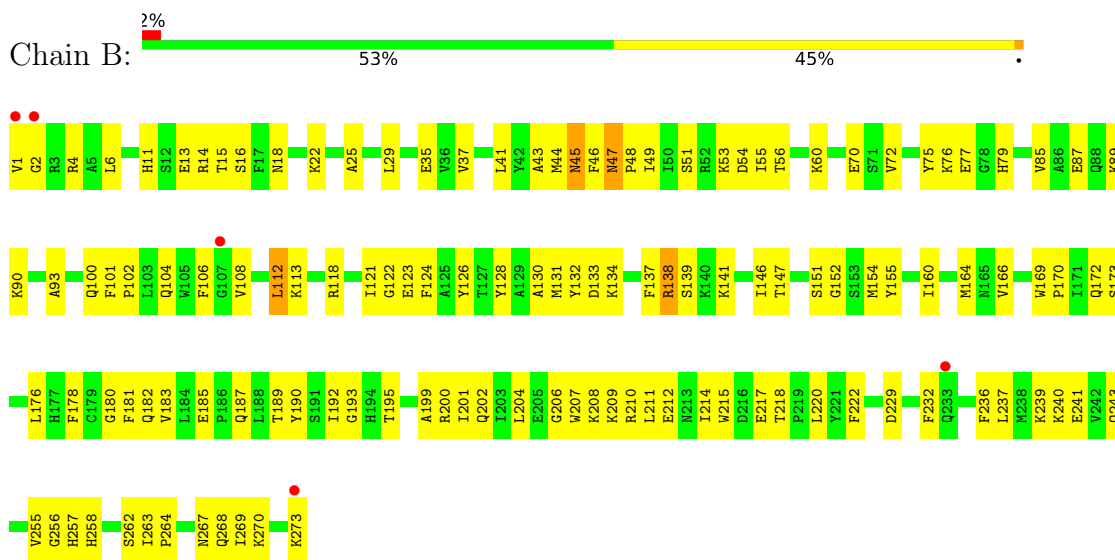
- Molecule 1: NAD(P)H dehydrogenase [quinone] 1

- Molecule 1: NAD(P)H dehydrogenase [quinone] 1

• Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain D:

• Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain E:

• Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain F:

I263 P264 T265 D266 N267 Q268 I269 K270 A271 R272 K273

• Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain G:

• Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain H:
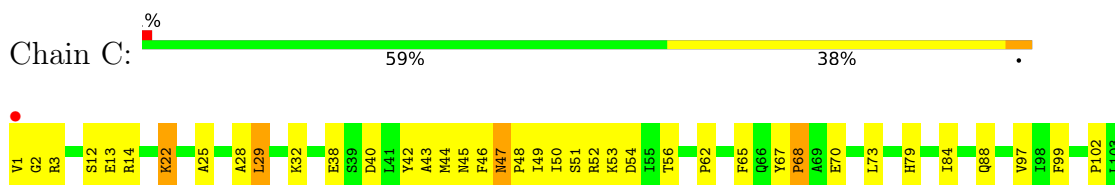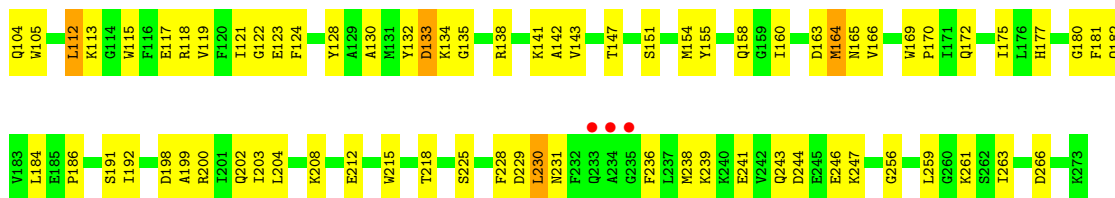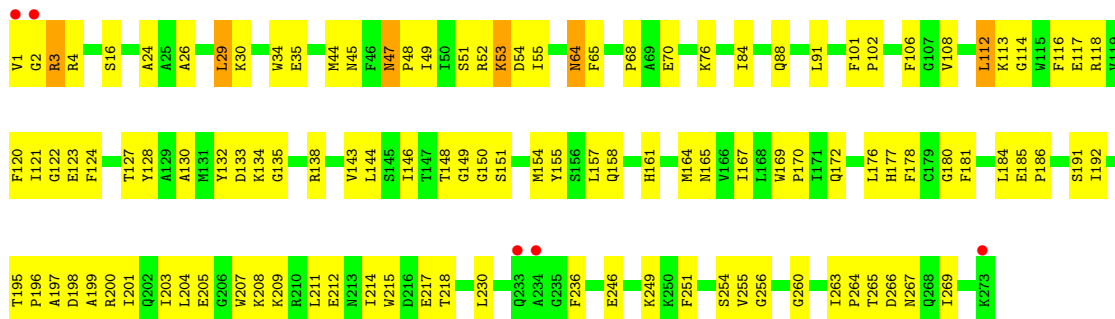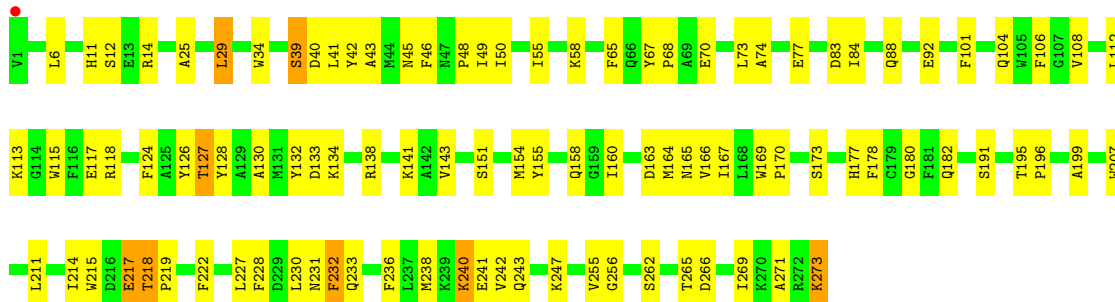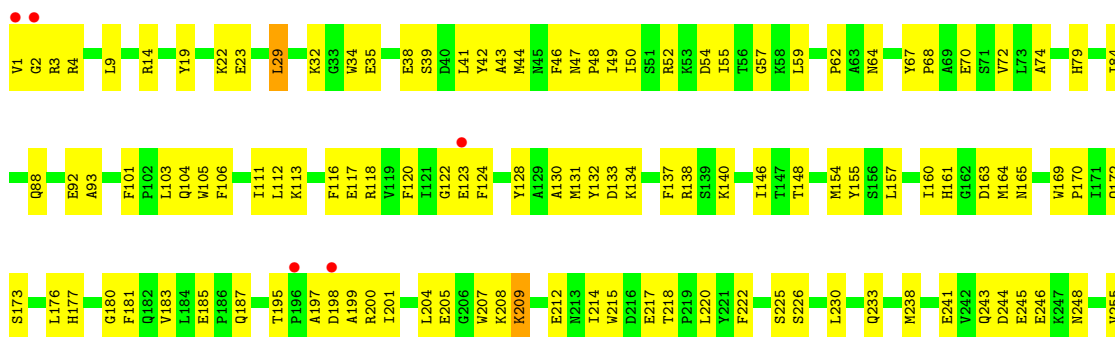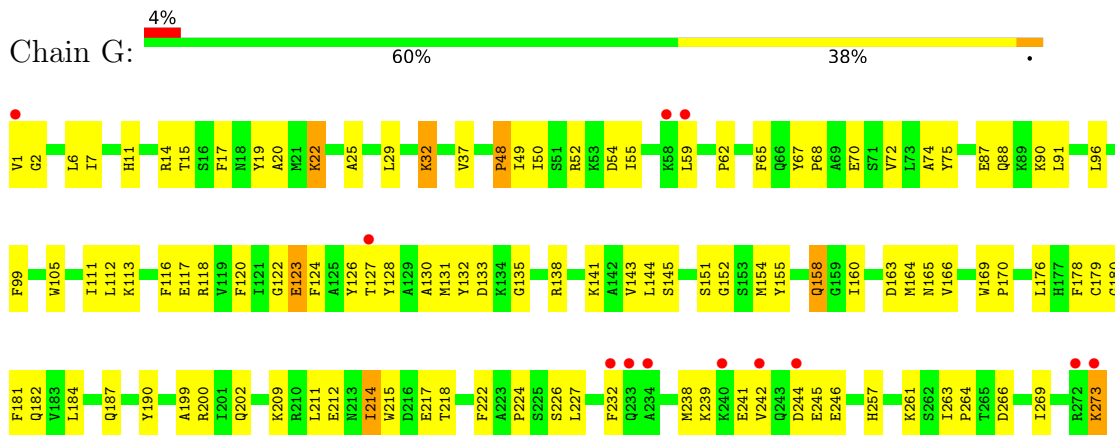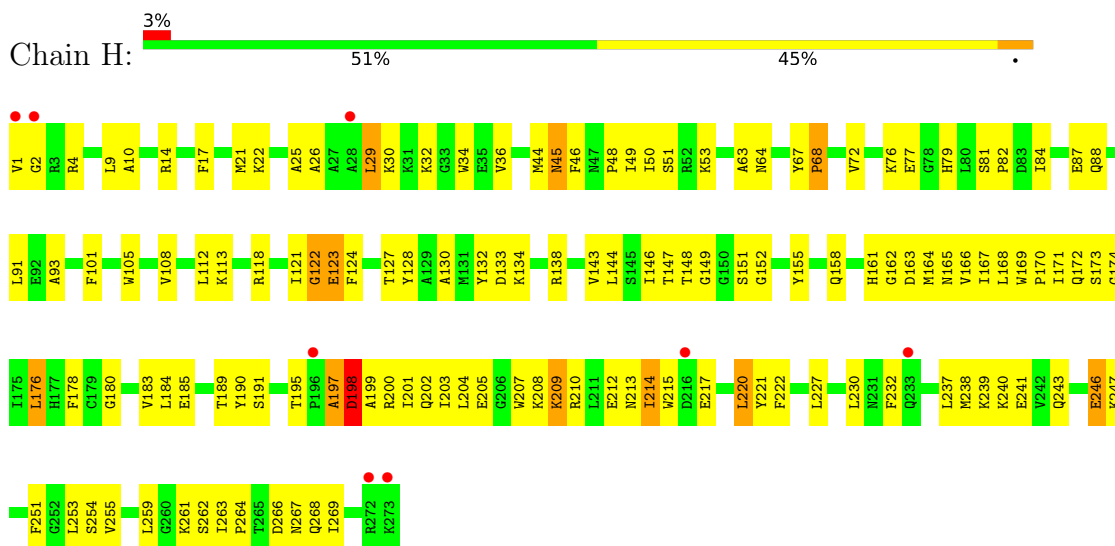
4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	76.24Å 86.19Å 100.56Å 91.14° 107.91° 93.17°	Depositor
Resolution (Å)	38.66 – 2.75 38.66 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (38.66-2.75) 95.1 (38.66-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.282 0.220 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	37.6	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 38.2	EDS
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	18146	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 11.12% 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: DTC, 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	0.41	0/2233	0.65	0/3015
1	B	0.42	0/2233	0.67	0/3015
1	C	0.41	0/2233	0.64	1/3015 (0.0%)
1	D	0.40	0/2233	0.66	0/3015
1	E	0.45	0/2233	0.65	1/3015 (0.0%)
1	F	0.41	0/2233	0.62	0/3015
1	G	0.40	0/2233	0.64	0/3015
1	H	0.41	0/2233	0.64	0/3015
All	All	0.41	0/17864	0.65	2/24120 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	182	GLN	N-CA-C	-5.24	96.86	111.00
1	C	182	GLN	N-CA-C	-5.19	96.98	111.00

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	2175	0	2179	94	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2175	0	2179	125	0
1	C	2175	0	2179	100	0
1	D	2175	0	2179	116	0
1	E	2175	0	2179	76	0
1	F	2175	0	2179	110	0
1	G	2175	0	2179	97	0
1	H	2175	0	2179	129	0
2	A	25	0	10	1	0
2	B	25	0	10	1	0
2	C	25	0	10	2	0
2	D	25	0	10	1	0
2	E	50	0	20	3	0
2	G	25	0	10	5	0
2	H	25	0	10	3	0
3	A	53	0	31	4	0
3	B	53	0	31	5	0
3	C	53	0	31	6	0
3	D	53	0	31	4	0
3	E	53	0	31	2	0
3	F	53	0	31	2	0
3	G	53	0	31	2	0
3	H	53	0	31	5	0
4	A	19	0	0	1	0
4	B	23	0	0	2	0
4	C	23	0	0	4	0
4	D	13	0	0	1	0
4	E	18	0	0	1	0
4	F	10	0	0	2	0
4	G	8	0	0	0	0
4	H	8	0	0	2	0
All	All	18146	0	17760	788	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 22.

The worst 5 of 788 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:VAL:HG23	1:B:267:ASN:HD22	1.05	1.17
1:D:151:SER:H	1:D:154:MET:HE3	1.07	1.15
1:D:47:ASN:HD22	1:D:48:PRO:N	1.51	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:PRO:HG3	1:C:49:ILE:HD11	1.37	1.06
1:G:1:VAL:HG12	1:G:2:GLY:H	1.17	1.06

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	271/273 (99%)	247 (91%)	21 (8%)	3 (1%)	14	25
1	B	271/273 (99%)	246 (91%)	21 (8%)	4 (2%)	10	18
1	C	271/273 (99%)	246 (91%)	18 (7%)	7 (3%)	5	8
1	D	271/273 (99%)	239 (88%)	29 (11%)	3 (1%)	14	25
1	E	271/273 (99%)	242 (89%)	23 (8%)	6 (2%)	6	11
1	F	271/273 (99%)	241 (89%)	29 (11%)	1 (0%)	34	53
1	G	271/273 (99%)	245 (90%)	21 (8%)	5 (2%)	8	15
1	H	271/273 (99%)	235 (87%)	25 (9%)	11 (4%)	3	3
All	All	2168/2184 (99%)	1941 (90%)	187 (9%)	40 (2%)	8	15

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	133	ASP
1	C	230	LEU
1	H	63	ALA
1	H	133	ASP
1	H	197	ALA

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	227/227 (100%)	219 (96%)	8 (4%)	36	56
1	B	227/227 (100%)	221 (97%)	6 (3%)	46	66
1	C	227/227 (100%)	222 (98%)	5 (2%)	52	70
1	D	227/227 (100%)	220 (97%)	7 (3%)	40	60
1	E	227/227 (100%)	214 (94%)	13 (6%)	20	36
1	F	227/227 (100%)	220 (97%)	7 (3%)	40	60
1	G	227/227 (100%)	218 (96%)	9 (4%)	31	51
1	H	227/227 (100%)	214 (94%)	13 (6%)	20	36
All	All	1816/1816 (100%)	1748 (96%)	68 (4%)	34	54

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	81	SER
1	H	91	LEU
1	H	232	PHE
1	D	112	LEU
1	D	91	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	47	ASN
1	G	45	ASN
1	F	64	ASN
1	F	161	HIS
1	G	177	HIS

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	DTC	G	7280	-	28,28,28	5.04	22 (78%)	36,41,41	1.55	9 (25%)
3	FAD	F	5301	-	53,58,58	11.82	17 (32%)	68,89,89	2.44	12 (17%)
2	DTC	D	1280	-	28,28,28	5.05	21 (75%)	36,41,41	1.58	9 (25%)
3	FAD	H	7301	-	53,58,58	11.42	15 (28%)	68,89,89	2.48	10 (14%)
3	FAD	C	2301	-	53,58,58	12.26	16 (30%)	68,89,89	2.42	12 (17%)
3	FAD	E	4301	-	53,58,58	12.88	13 (24%)	68,89,89	2.51	13 (19%)
2	DTC	B	3280	-	28,28,28	4.96	21 (75%)	36,41,41	1.61	11 (30%)
3	FAD	B	1301	-	53,58,58	12.17	16 (30%)	68,89,89	2.46	13 (19%)
3	FAD	G	6301	-	53,58,58	11.57	18 (33%)	68,89,89	2.46	13 (19%)
2	DTC	H	6280	-	28,28,28	5.01	22 (78%)	36,41,41	1.57	8 (22%)
3	FAD	D	3301	-	53,58,58	12.04	16 (30%)	68,89,89	2.43	14 (20%)
2	DTC	A	2280	-	28,28,28	4.98	22 (78%)	36,41,41	1.54	8 (22%)
2	DTC	C	280	-	28,28,28	5.07	22 (78%)	36,41,41	1.52	8 (22%)
2	DTC	E	4280	-	28,28,28	5.03	22 (78%)	36,41,41	1.50	8 (22%)
2	DTC	E	5280	-	28,28,28	4.98	22 (78%)	36,41,41	1.61	9 (25%)
3	FAD	A	301	-	53,58,58	11.67	18 (33%)	68,89,89	2.48	13 (19%)

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	DTC	G	7280	-	2/2/6/6	2/4/36/36	0/4/4/4
3	FAD	F	5301	-	-	4/30/50/50	0/6/6/6
2	DTC	D	1280	-	2/2/6/6	2/4/36/36	0/4/4/4
3	FAD	H	7301	-	-	7/30/50/50	0/6/6/6
3	FAD	C	2301	-	-	5/30/50/50	0/6/6/6
3	FAD	E	4301	-	-	6/30/50/50	0/6/6/6
2	DTC	B	3280	-	2/2/6/6	1/4/36/36	0/4/4/4
3	FAD	B	1301	-	-	4/30/50/50	0/6/6/6
3	FAD	G	6301	-	-	6/30/50/50	0/6/6/6
2	DTC	H	6280	-	2/2/6/6	2/4/36/36	0/4/4/4
3	FAD	D	3301	-	-	7/30/50/50	0/6/6/6
2	DTC	A	2280	-	2/2/6/6	2/4/36/36	0/4/4/4
2	DTC	C	280	-	2/2/6/6	2/4/36/36	0/4/4/4
2	DTC	E	4280	-	2/2/6/6	2/4/36/36	0/4/4/4
2	DTC	E	5280	-	2/2/6/6	2/4/36/36	0/4/4/4
3	FAD	A	301	-	-	3/30/50/50	0/6/6/6

The worst 5 of 303 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4301	FAD	PA-O2A	92.90	5.91	1.55
3	C	2301	FAD	PA-O2A	88.30	5.69	1.55
3	B	1301	FAD	PA-O2A	87.65	5.66	1.55
3	D	3301	FAD	PA-O2A	86.76	5.62	1.55
3	F	5301	FAD	PA-O2A	85.05	5.54	1.55

The worst 5 of 170 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	4301	FAD	O2A-PA-O5B	-14.92	38.45	107.75
3	C	2301	FAD	O2A-PA-O5B	-14.28	41.43	107.75
3	B	1301	FAD	O2A-PA-O5B	-14.03	42.59	107.75
3	D	3301	FAD	O2A-PA-O5B	-13.90	43.20	107.75
3	F	5301	FAD	O2A-PA-O5B	-13.82	43.58	107.75

5 of 16 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2280	DTC	C13
2	A	2280	DTC	C7
2	B	3280	DTC	C13
2	B	3280	DTC	C7
2	C	280	DTC	C13

5 of 57 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2280	DTC	C13-C15-C7-C8
2	B	3280	DTC	C13-C15-C7-C8
2	C	280	DTC	C13-C15-C7-C8
2	C	280	DTC	C12-C13-C15-C7
2	D	1280	DTC	C13-C15-C7-C8

There are no ring outliers.

16 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	7280	DTC	5	0
3	F	5301	FAD	2	0
2	D	1280	DTC	1	0
3	H	7301	FAD	5	0
3	C	2301	FAD	6	0
3	E	4301	FAD	2	0
2	B	3280	DTC	1	0
3	B	1301	FAD	5	0
3	G	6301	FAD	2	0
2	H	6280	DTC	3	0
3	D	3301	FAD	4	0
2	A	2280	DTC	1	0
2	C	280	DTC	2	0
2	E	4280	DTC	1	0
2	E	5280	DTC	2	0
3	A	301	FAD	4	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 DTC G 7280

Ligand FAD F 5301

Bond lengths

Bond angles

Torsions

Rings

Ligand DTC D 1280

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD H 7301

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD C 2301

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD E 4301

Bond lengths

Bond angles

Torsions

Rings

Ligand DTC B 3280

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD B 1301

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD G 6301

Bond lengths

Bond angles

Torsions

Rings

Ligand DTC H 6280

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD D 3301

Bond lengths

Bond angles

Torsions

Rings

Ligand DTC A 2280

Bond lengths

Bond angles

Torsions

Rings

Ligand DTC C 280

Bond lengths

Bond angles

Torsions

Rings

Ligand DTC E 4280

Bond lengths

Bond angles

Torsions

Rings

Ligand DTC E 5280

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD A 301

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	273/273 (100%)	-0.12	4 (1%)	73	81	13, 31, 50, 78	0
1	B	273/273 (100%)	-0.20	5 (1%)	68	76	14, 29, 47, 74	0
1	C	273/273 (100%)	-0.18	4 (1%)	73	81	12, 28, 53, 71	0
1	D	273/273 (100%)	-0.11	5 (1%)	68	76	13, 33, 52, 80	0
1	E	273/273 (100%)	-0.22	1 (0%)	92	95	11, 27, 52, 69	0
1	F	273/273 (100%)	-0.12	5 (1%)	68	76	15, 32, 53, 68	0
1	G	273/273 (100%)	-0.02	12 (4%)	34	41	15, 35, 65, 81	0
1	H	273/273 (100%)	0.15	8 (2%)	51	61	18, 41, 70, 82	0
All	All	2184/2184 (100%)	-0.10	44 (2%)	65	73	11, 32, 58, 82	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	VAL	9.6
1	E	1	VAL	8.3
1	A	1	VAL	7.0
1	B	1	VAL	6.1
1	D	273	LYS	4.6

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(Å^2)	Q<0.9
2	DTC	G	7280	25/25	0.77	0.28	34,74,75,75	0
2	DTC	E	5280	25/25	0.79	0.27	34,74,75,75	0
2	DTC	B	3280	25/25	0.81	0.27	34,74,75,75	0
2	DTC	D	1280	25/25	0.81	0.31	34,74,75,75	0
2	DTC	C	280	25/25	0.83	0.28	34,74,75,75	0
2	DTC	H	6280	25/25	0.83	0.27	34,74,75,75	0
2	DTC	A	2280	25/25	0.84	0.28	34,74,75,75	0
2	DTC	E	4280	25/25	0.85	0.29	34,74,75,75	0
3	FAD	H	7301	53/53	0.87	0.18	25,45,53,55	0
3	FAD	A	301	53/53	0.90	0.17	25,34,42,42	0
3	FAD	F	5301	53/53	0.91	0.16	21,30,38,41	0
3	FAD	D	3301	53/53	0.92	0.16	19,28,38,39	0
3	FAD	B	1301	53/53	0.92	0.16	17,22,34,34	0
3	FAD	G	6301	53/53	0.92	0.16	20,28,34,37	0
3	FAD	C	2301	53/53	0.92	0.15	19,27,34,34	0
3	FAD	E	4301	53/53	0.93	0.14	14,23,34,34	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.
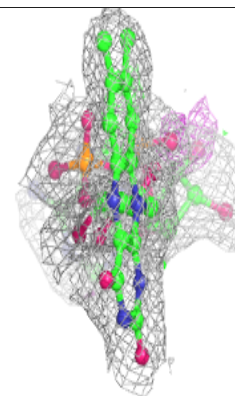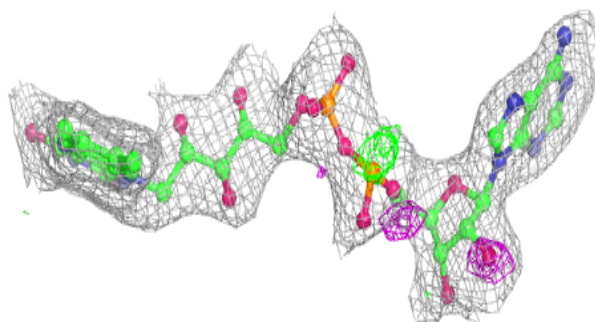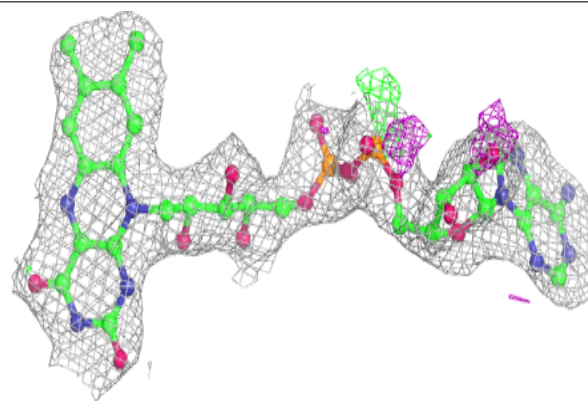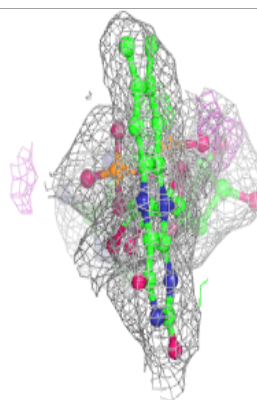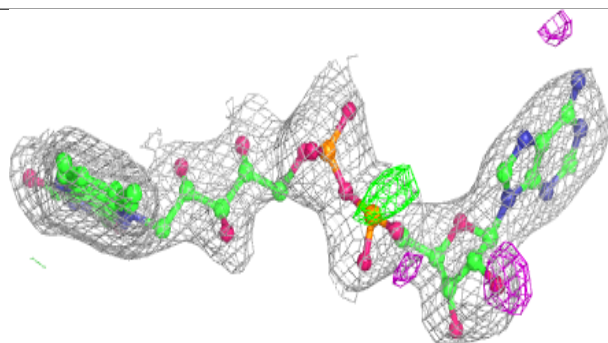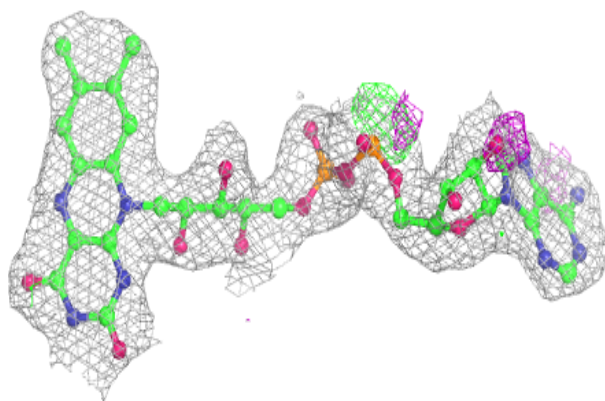
Electron density around DTC G 7280:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
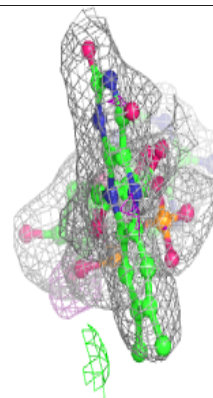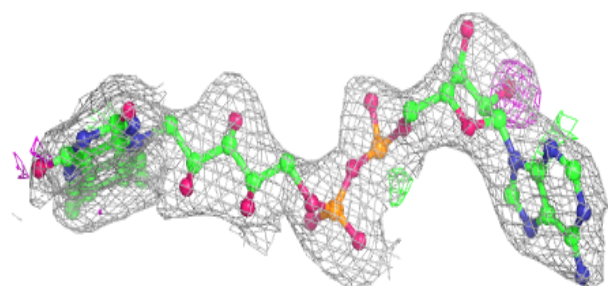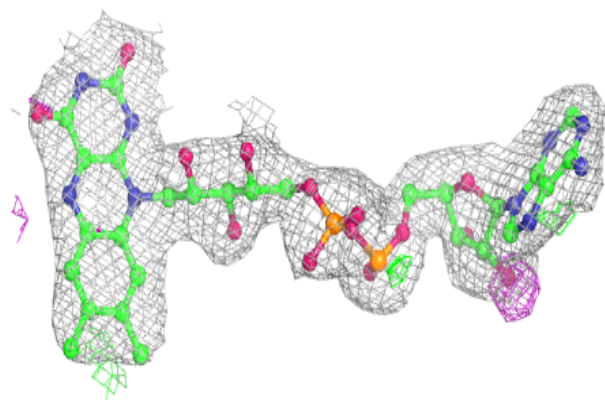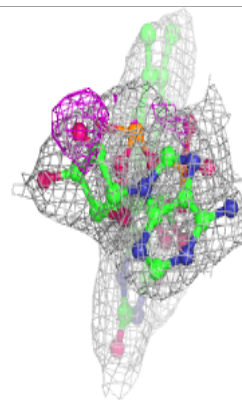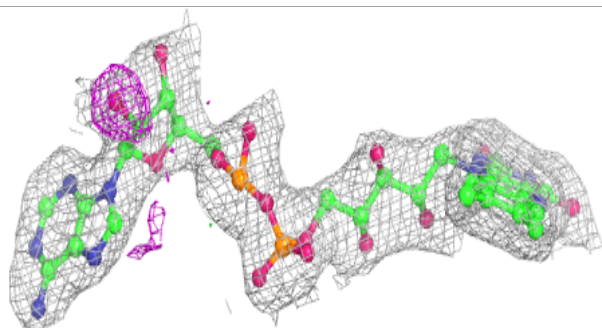and green (positive)
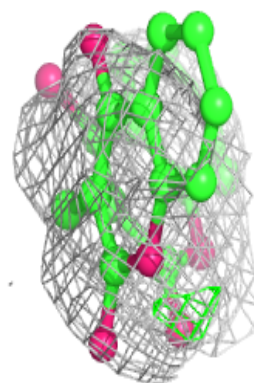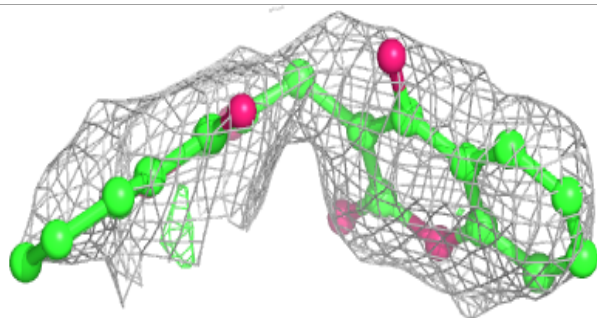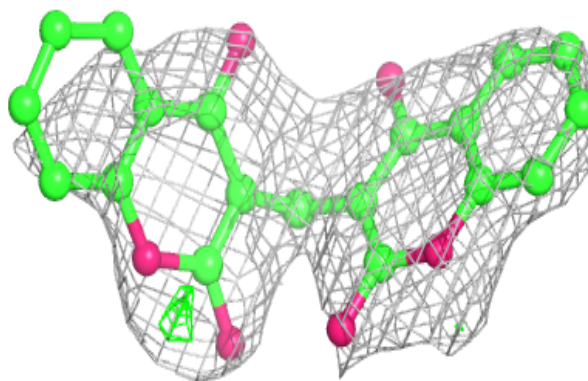
Electron density around DTC E 5280:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
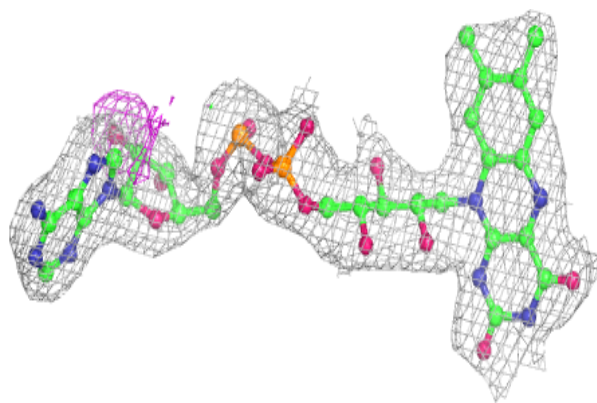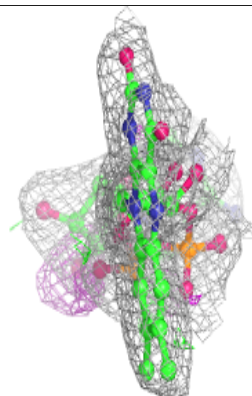and green (positive)
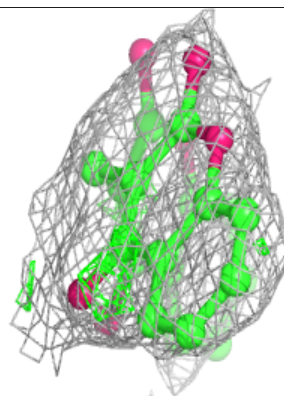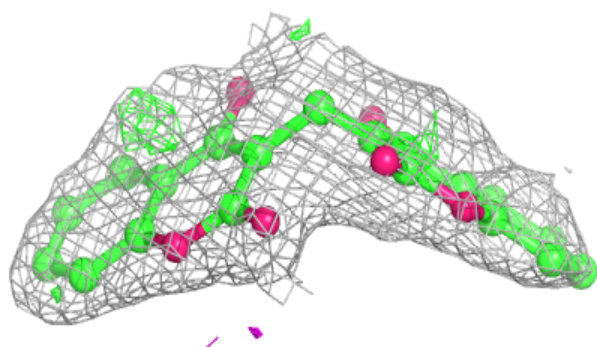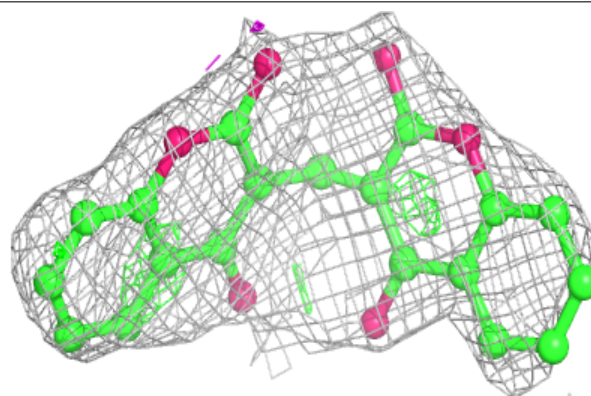
Electron density around DTC B 3280:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
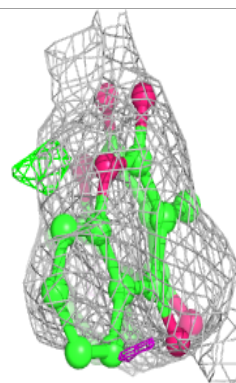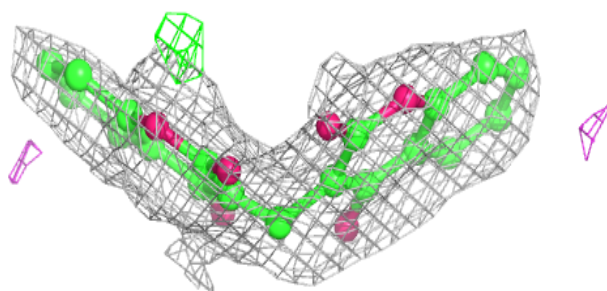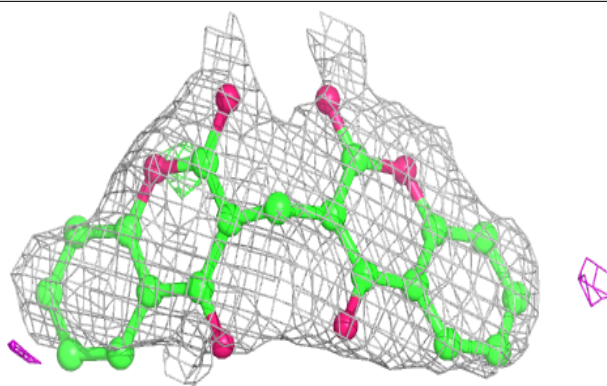
Electron density around DTC D 1280:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
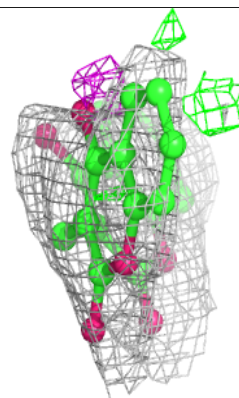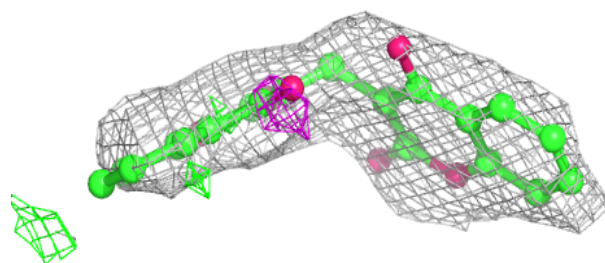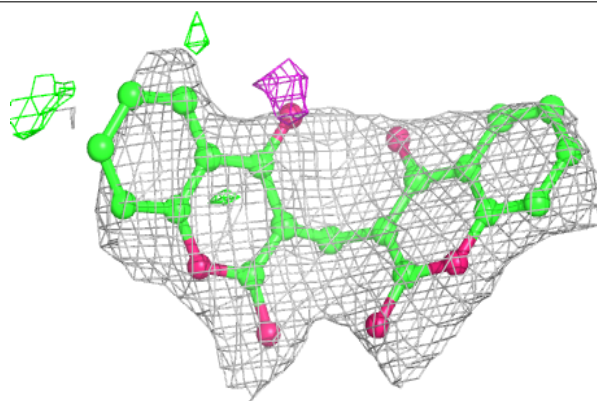
Electron density around DTC C 280:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
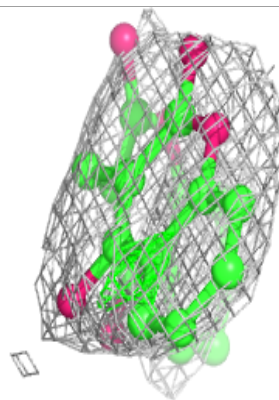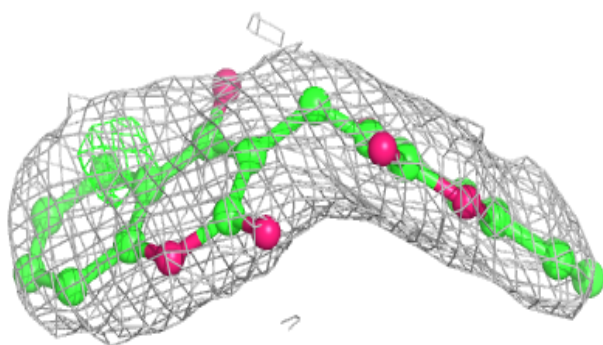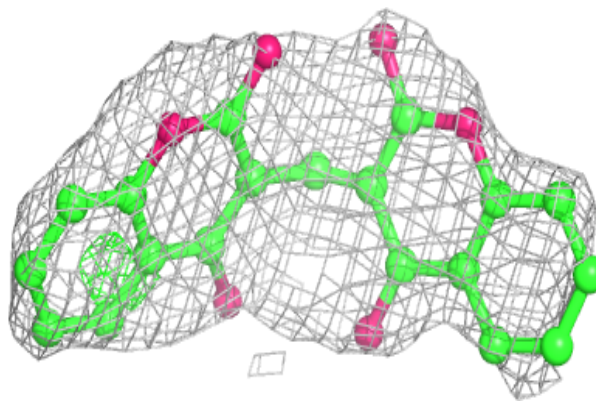
Electron density around DTC H 6280:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
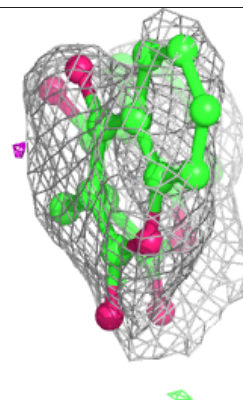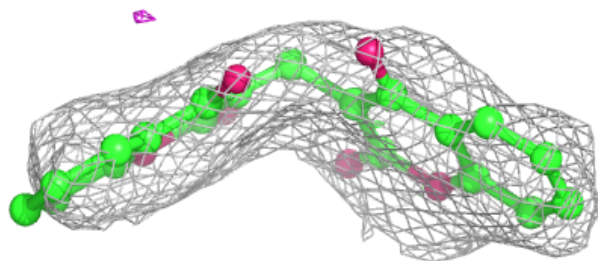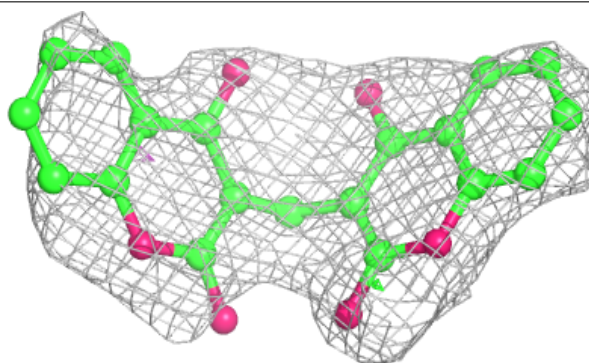
Electron density around DTC A 2280:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
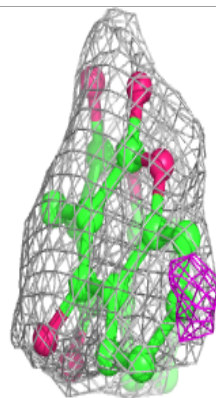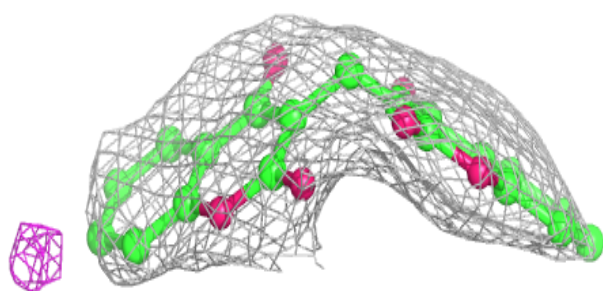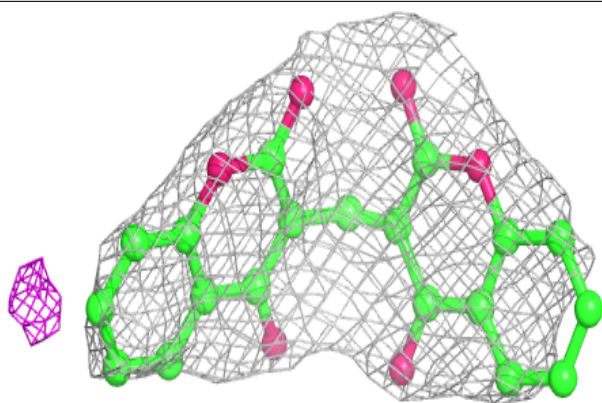
Electron density around DTC E 4280:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
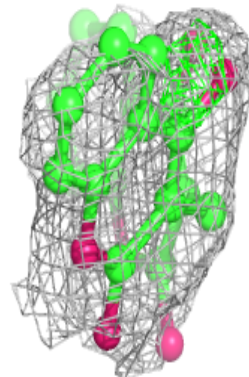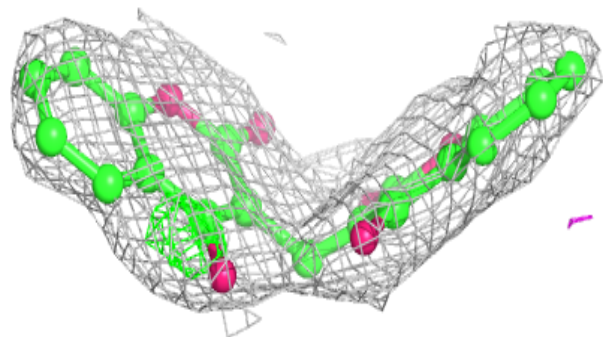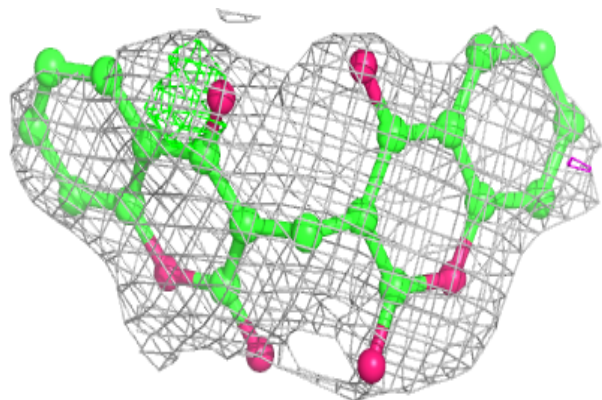
Electron density around FAD H 7301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
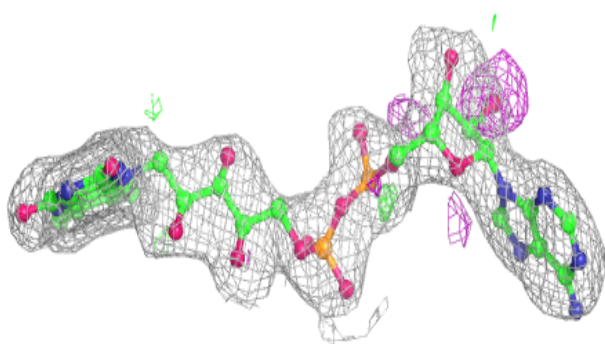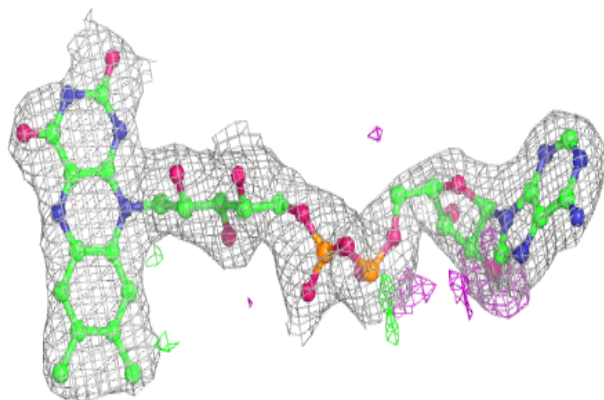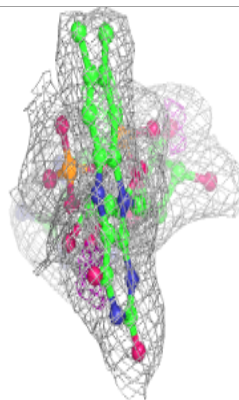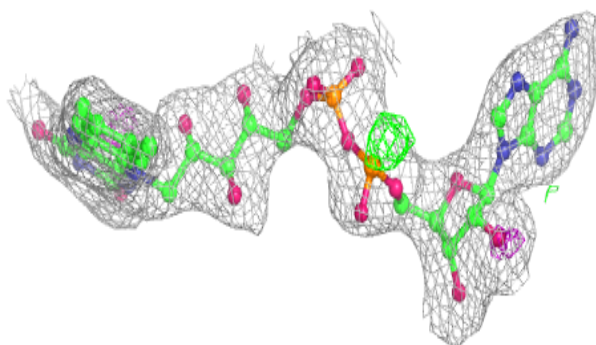mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
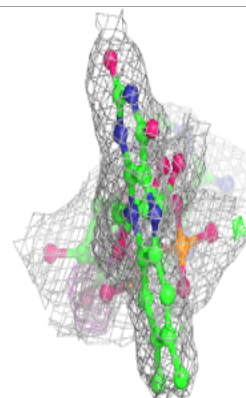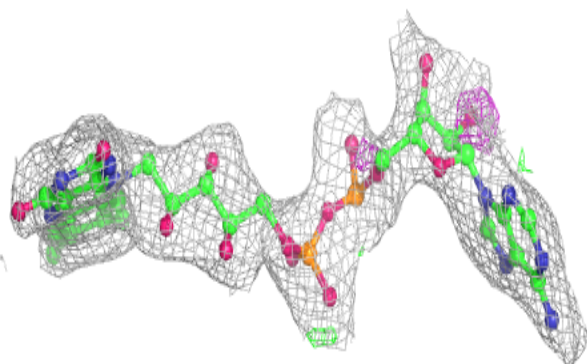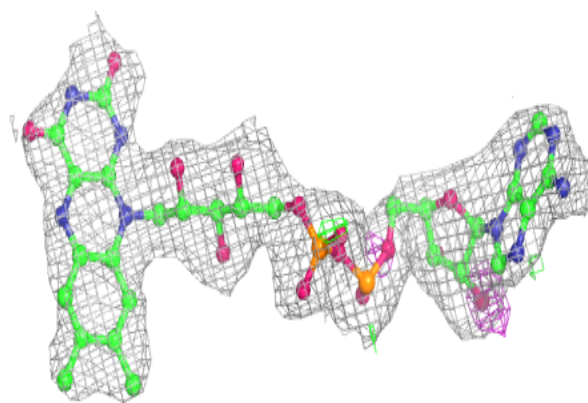
Electron density around FAD A 301:

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

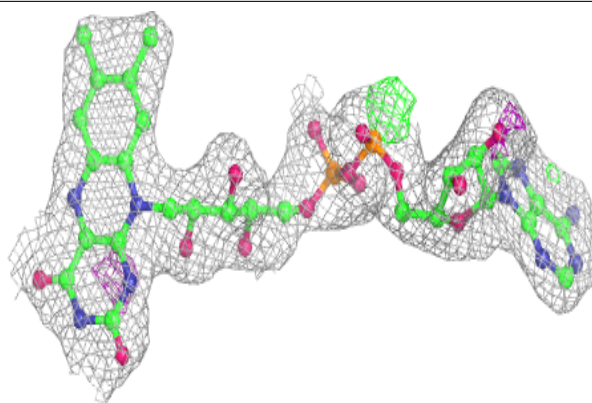**Electron density around FAD F 5301:**

$2mF_o$-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 3301:

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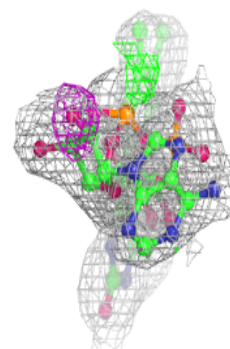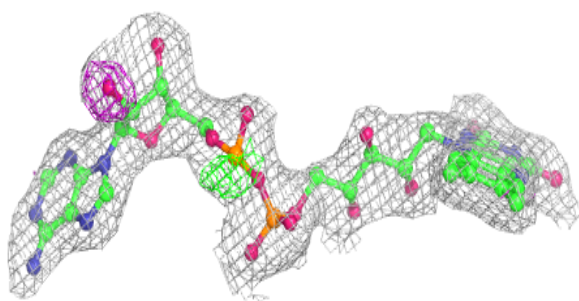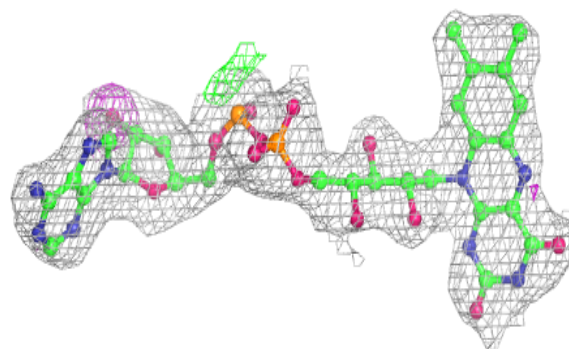and green (positive)

Electron density around FAD B 1301:

$2mF_o$-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 G 6301:

$2mF_o$-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 2301:

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

Electron density around FAD E 4301:

$2mF_o\text{-}DF_c$ (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.