



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:35 PM UTC

PDB ID : 2GH5 / pdb_00002gh5
Title : Crystal Structure of human Glutathione Reductase complexed with a Fluoro-Analogue of the Menadione Derivative M5
Authors : Fritz-Wolf, K.; Winzer, A.; Bauer, H.; Schirmer, H.; Davioud-Charvet, E.
Deposited on : 2006-03-25
Resolution : 1.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

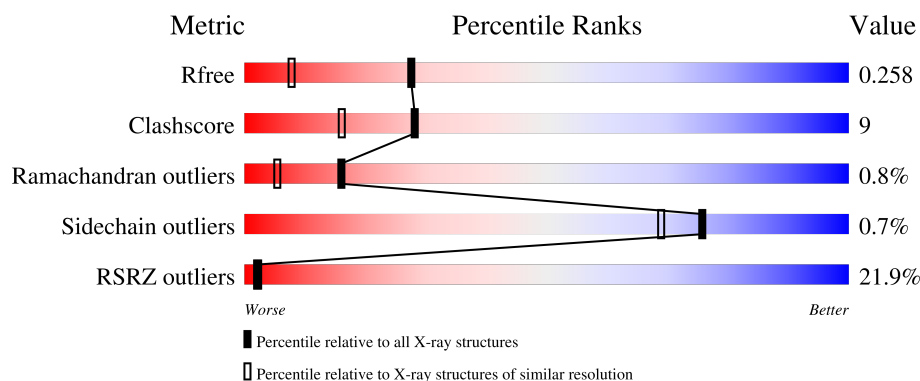
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	478	17% 79% 17% ..
1	B	478	25% 77% 18% ..

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
5	GOL	A	808	-	X	-	-
5	GOL	A	809	-	X	-	-
5	GOL	A	810	-	X	-	-
5	GOL	A	813	-	X	-	-
5	GOL	A	817	-	X	-	-
5	GOL	B	801	-	X	-	-
5	GOL	B	802	-	X	-	-
5	GOL	B	803	-	X	-	-
5	GOL	B	805	-	X	-	-
5	GOL	B	806	-	X	-	-
5	GOL	B	811	-	X	-	-
5	GOL	B	812	-	X	-	-

2 Entry composition [i](#)

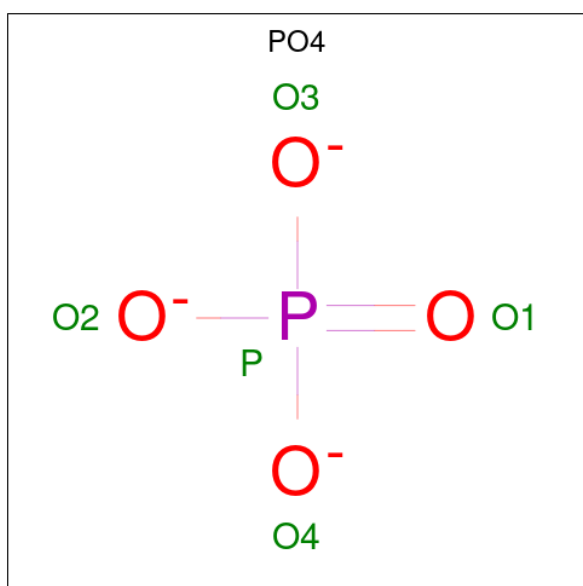
There are 6 unique types of molecules in this entry. The entry contains 7941 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 glutathione reductase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3499	2212	603	660	24			
1	B	461	Total	C	N	O	S	0	0	0
			3499	2212	603	660	24			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

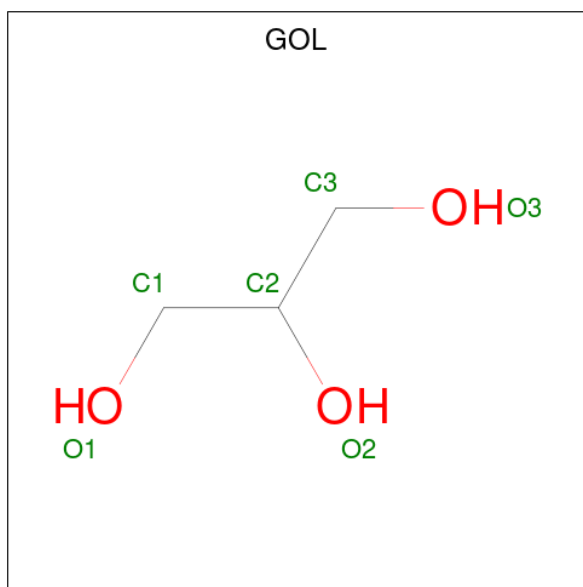
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- Chemical structure of ELI (Ergometrine) showing atom numbering. The structure consists of a benzene ring fused to a six-membered ring, which is further fused to a five-membered ring. The five-membered ring has a carboxylic acid group (-COOH) and a side chain. The side chain consists of a three-carbon chain ending in a hydroxyl group (-OH). The atoms are numbered: C1-C6 for the benzene ring, C7-C14 for the fused rings, and C15-C18 for the side chain. The carboxylic acid group is labeled O15 and H16.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	17	4		
3	B	1	Total	C	O	0	0
			21	17	4		

- # FAD

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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	350	Total	O	0	0
			350	350		
6	B	353	Total	O	0	0
			353	353		

- Molecule 1: glutathione reductase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.70Å 63.60Å 103.99Å 90.00° 101.12° 90.00°	Depositor
Resolution (Å)	19.74 – 1.70 19.74 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.74-1.70) 98.9 (19.74-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 1.70Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.256 0.225 , 0.258	Depositor DCC
R_{free} test set	5908 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7941	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 77.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.6982e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PO4, ELI, GOL, 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	0.35	0/3566	0.83	5/4824 (0.1%)
1	B	0.36	0/3566	0.81	4/4824 (0.1%)
All	All	0.35	0/7132	0.82	9/9648 (0.1%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	444	LEU	N-CA-C	8.19	120.29	111.36
1	B	444	LEU	N-CA-C	8.19	120.28	111.36
1	A	213	THR	N-CA-C	6.15	119.49	109.59
1	B	213	THR	N-CA-C	5.82	118.96	109.59
1	A	383	THR	N-CA-C	-5.65	103.24	110.53

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	3499	0	3537	60	0
1	B	3499	0	3537	71	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	21	0	14	5	0
3	B	21	0	14	2	0
4	A	53	0	31	0	0
4	B	53	0	31	1	0
5	A	30	0	20	1	0
5	B	42	0	28	0	0
6	A	350	0	0	5	0
6	B	353	0	0	11	0
All	All	7941	0	7212	128	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 9.

The worst 5 of 128 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:130:ALA:HB1	1:B:140:ILE:HD11	1.51	0.92
1:A:169:PRO:HG2	1:A:253:GLU:HG3	1.63	0.80
1:B:133:THR:HG22	1:B:134:SER:H	1.50	0.77
1:B:352:ARG:HA	6:B:6024:HOH:O	1.85	0.77
1:A:33:LEU:HD13	1:A:114:TYR:CE2	2.21	0.76

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	459/478 (96%)	439 (96%)	17 (4%)	3 (1%)	18	7
1	B	459/478 (96%)	432 (94%)	23 (5%)	4 (1%)	14	4
All	All	918/956 (96%)	871 (95%)	40 (4%)	7 (1%)	16	5

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	134	SER
1	A	91	GLU
1	B	135	ASP
1	A	144	GLY
1	B	358	GLU

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	382/393 (97%)	379 (99%)	3 (1%)	73	65
1	B	382/393 (97%)	380 (100%)	2 (0%)	81	76
All	All	764/786 (97%)	759 (99%)	5 (1%)	76	69

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	HIS
1	A	127	ARG
1	A	426	LYS
1	B	145	LYS
1	B	202	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	366	ASN
1	B	365	ASN
1	B	111	ASN
1	B	351	HIS
1	B	52	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

20 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	FAD	A	479	-	58,58,58	1.65	10 (17%)	85,89,89	1.12	5 (5%)
5	GOL	B	805	-	5,5,5	4.78	5 (100%)	5,5,5	6.08	3 (60%)
5	GOL	B	803	-	5,5,5	4.78	5 (100%)	5,5,5	6.13	3 (60%)
2	PO4	A	5706	-	4,4,4	1.80	0	6,6,6	0.46	0
5	GOL	A	817	-	5,5,5	4.78	5 (100%)	5,5,5	6.12	3 (60%)
5	GOL	A	813	-	5,5,5	4.79	5 (100%)	5,5,5	6.11	3 (60%)
2	PO4	B	5705	-	4,4,4	1.79	1 (25%)	6,6,6	0.47	0
3	ELI	B	958	1	22,22,22	5.16	13 (59%)	27,30,30	3.80	6 (22%)
5	GOL	B	811	-	5,5,5	4.77	5 (100%)	5,5,5	6.14	3 (60%)
5	GOL	B	806	-	5,5,5	4.77	5 (100%)	5,5,5	6.11	3 (60%)
2	PO4	B	5704	-	4,4,4	1.74	1 (25%)	6,6,6	0.45	0
5	GOL	A	809	-	5,5,5	4.77	5 (100%)	5,5,5	6.12	3 (60%)
5	GOL	A	810	-	5,5,5	4.75	5 (100%)	5,5,5	6.12	3 (60%)
5	GOL	B	801	-	5,5,5	4.77	5 (100%)	5,5,5	6.09	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FAD	B	479	-	58,58,58	1.68	8 (13%)	85,89,89	1.22	9 (10%)
2	PO4	A	5703	-	4,4,4	1.74	0	6,6,6	0.46	0
3	ELI	A	958	1	22,22,22	5.50	17 (77%)	27,30,30	3.18	6 (22%)
5	GOL	B	802	-	5,5,5	4.80	5 (100%)	5,5,5	6.12	3 (60%)
5	GOL	A	808	-	5,5,5	4.77	5 (100%)	5,5,5	6.11	3 (60%)
5	GOL	B	812	-	5,5,5	4.78	5 (100%)	5,5,5	6.11	3 (60%)

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
5	GOL	B	801	-	-	2/4/4/4	-
4	FAD	B	479	-	-	3/34/50/50	0/6/6/6
3	ELI	B	958	1	-	5/8/28/28	0/2/2/2
5	GOL	A	817	-	-	4/4/4/4	-
5	GOL	B	811	-	-	4/4/4/4	-
5	GOL	B	806	-	-	2/4/4/4	-
5	GOL	A	813	-	-	3/4/4/4	-
4	FAD	A	479	-	-	3/34/50/50	0/6/6/6
3	ELI	A	958	1	-	1/8/28/28	0/2/2/2
5	GOL	B	805	-	-	3/4/4/4	-
5	GOL	B	802	-	-	2/4/4/4	-
5	GOL	B	803	-	-	2/4/4/4	-
5	GOL	A	809	-	-	2/4/4/4	-
5	GOL	A	808	-	-	2/4/4/4	-
5	GOL	A	810	-	-	4/4/4/4	-
5	GOL	B	812	-	-	2/4/4/4	-

The worst 5 of 110 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	958	ELI	C4-C3	12.13	1.60	1.40
3	B	958	ELI	C4-C3	10.19	1.57	1.40
3	A	958	ELI	C15-C14	8.51	1.50	1.35
3	B	958	ELI	C5-C4	8.17	1.52	1.39
5	B	812	GOL	C3-C2	-8.11	1.20	1.51

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	958	ELI	C20-C19-C18	16.18	172.57	113.13
3	A	958	ELI	C20-C19-C18	13.03	160.99	113.13
5	B	803	GOL	O3-C3-C2	11.13	160.47	110.38
5	B	811	GOL	O3-C3-C2	11.12	160.44	110.38
5	B	802	GOL	O3-C3-C2	11.11	160.38	110.38

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	479	FAD	PA-O3P-P-O5'
4	B	479	FAD	PA-O3P-P-O5'
5	A	808	GOL	C1-C2-C3-O3
5	A	809	GOL	O1-C1-C2-C3
5	A	813	GOL	C1-C2-C3-O3

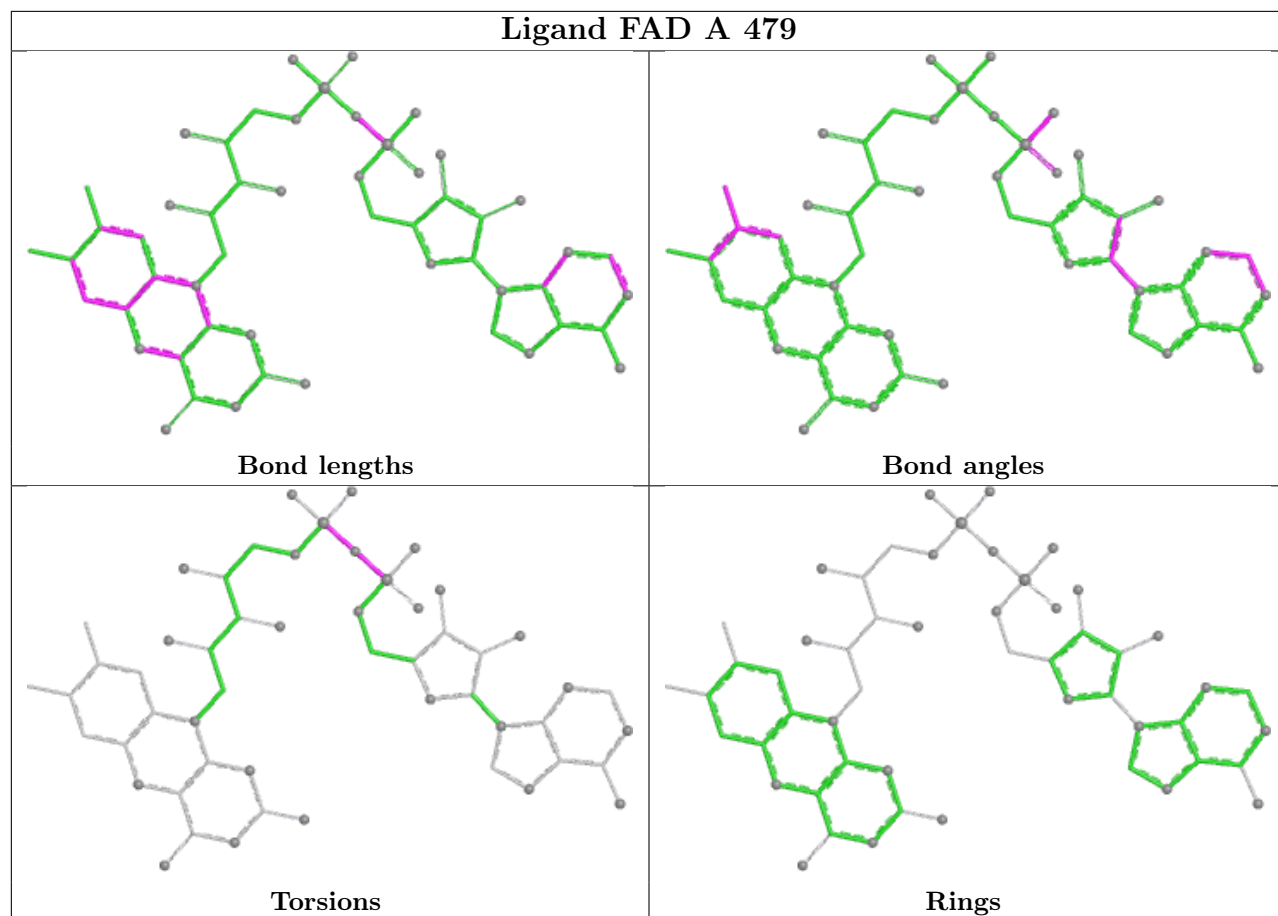
There are no ring outliers.

4 monomers are involved in 9 short contacts:

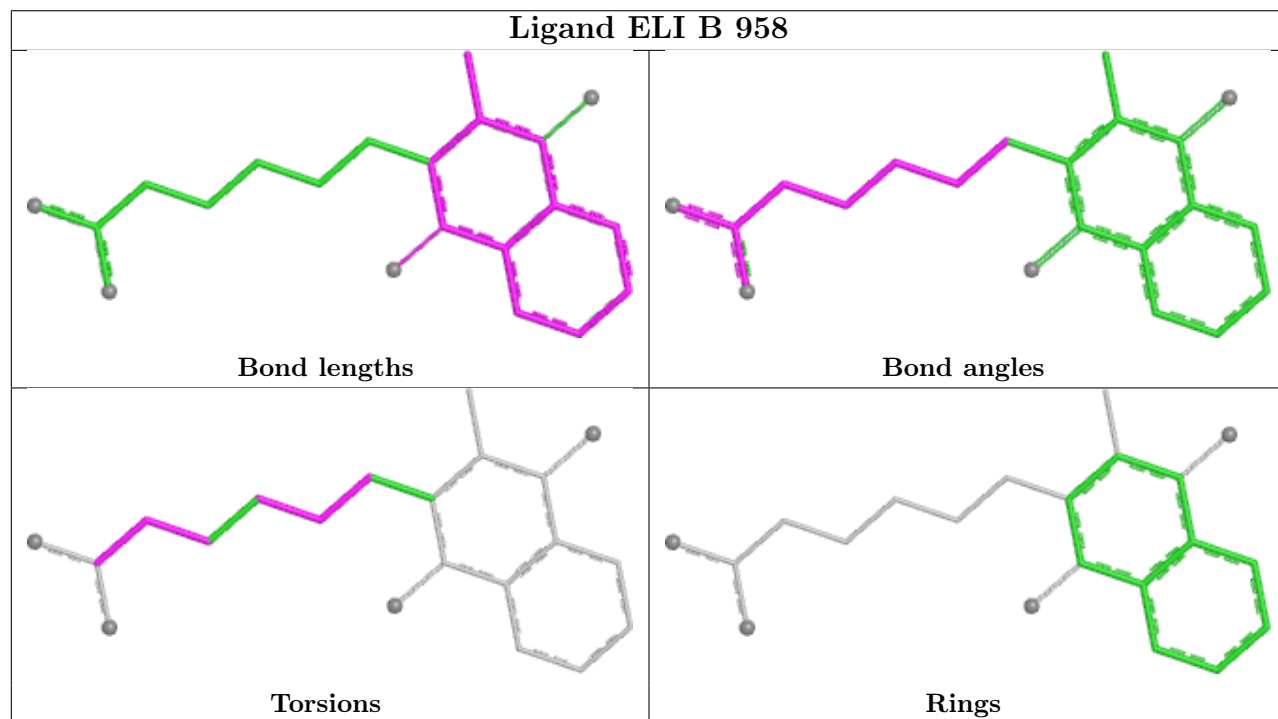
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	817	GOL	1	0
3	B	958	ELI	2	0
4	B	479	FAD	1	0
3	A	958	ELI	5	0

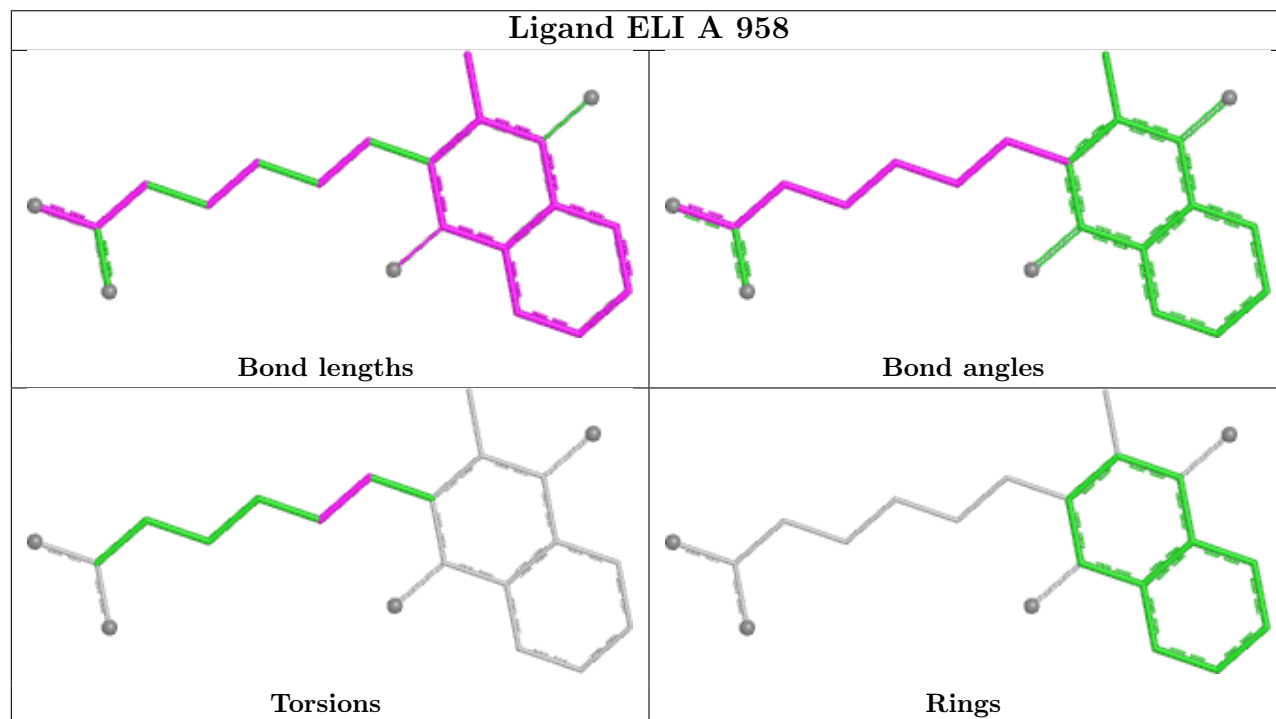
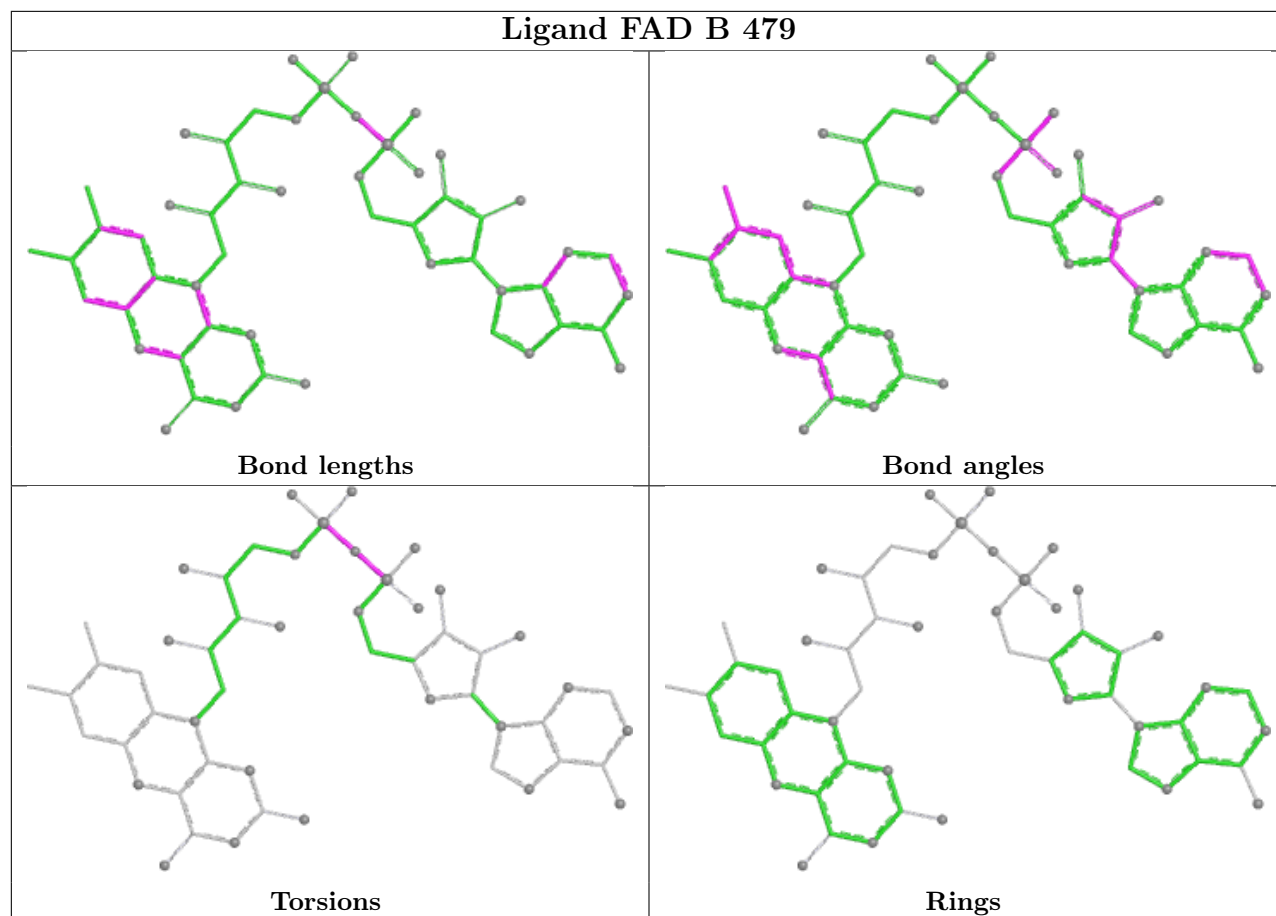
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand FAD A 479



Ligand ELI B 958





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	461/478 (96%)	0.91	83 (18%) 3 3	12, 25, 45, 62	0
1	B	461/478 (96%)	1.22	119 (25%) 1 1	13, 26, 62, 75	0
All	All	922/956 (96%)	1.07	202 (21%) 2 2	12, 25, 56, 75	0

The worst 5 of 202 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	92	GLY	7.7
1	B	354	PHE	7.3
1	A	78	PHE	7.0
1	B	21	TYR	6.8
1	B	350	ALA	6.7

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](#)

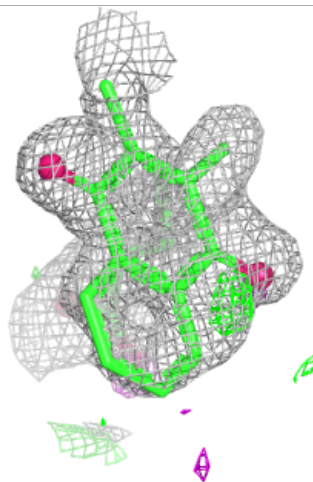
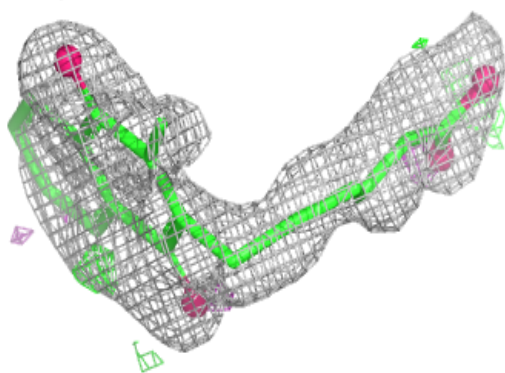
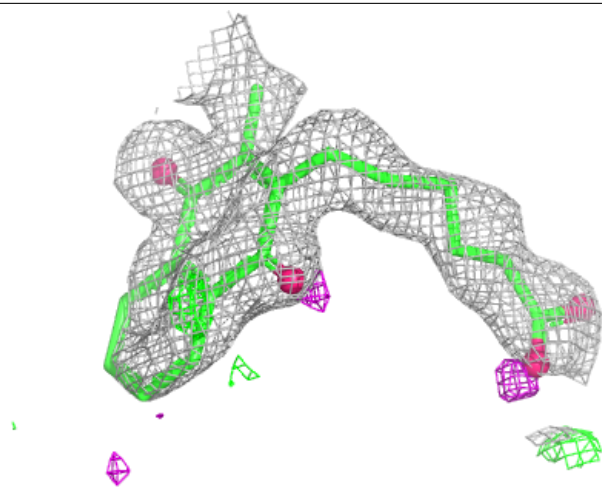
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	B	801	6/6	0.53	0.25	50,51,52,52	0
5	GOL	B	805	6/6	0.57	0.20	38,42,43,45	0
5	GOL	A	810	6/6	0.67	0.20	37,46,48,49	0
5	GOL	A	809	6/6	0.70	0.18	67,68,68,68	0
5	GOL	A	813	6/6	0.70	0.19	55,57,58,58	0
5	GOL	B	802	6/6	0.73	0.20	67,67,67,68	0
5	GOL	A	817	6/6	0.73	0.19	57,60,60,60	0
3	ELI	A	958	21/21	0.77	0.17	31,38,46,49	0
5	GOL	B	812	6/6	0.77	0.23	55,58,58,58	0
3	ELI	B	958	21/21	0.78	0.17	33,40,43,45	0
5	GOL	A	808	6/6	0.78	0.14	40,42,44,48	0
5	GOL	B	811	6/6	0.81	0.15	62,63,63,63	0
5	GOL	B	806	6/6	0.87	0.12	27,39,41,43	0
5	GOL	B	803	6/6	0.88	0.12	28,38,40,44	0
2	PO4	B	5705	5/5	0.91	0.12	33,33,36,37	0
4	FAD	A	479	53/53	0.94	0.09	13,18,32,34	0
4	FAD	B	479	53/53	0.94	0.09	15,20,38,39	0
2	PO4	A	5703	5/5	0.95	0.08	34,36,36,37	0
2	PO4	B	5704	5/5	0.96	0.07	27,27,28,28	0
2	PO4	A	5706	5/5	0.96	0.09	29,33,34,34	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.

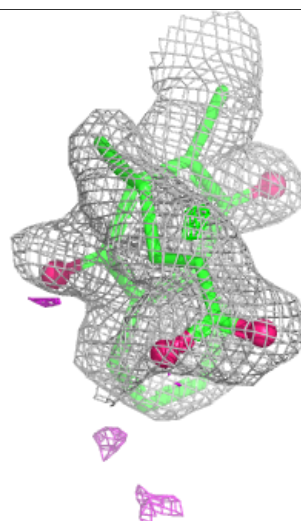
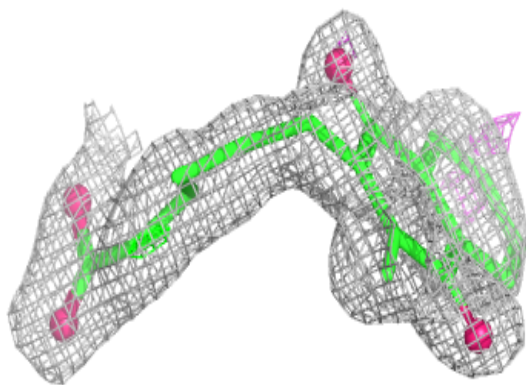
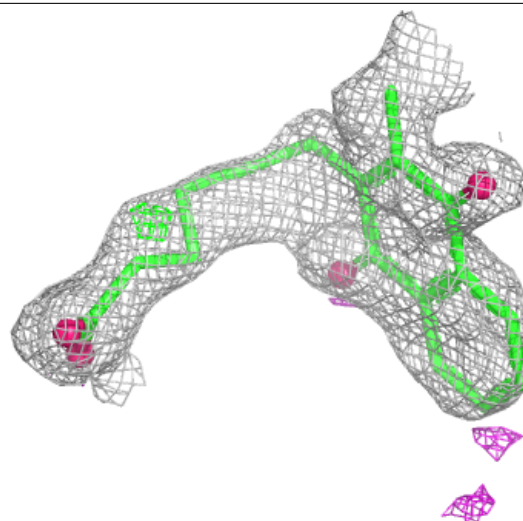
Electron density around ELI A 958:

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



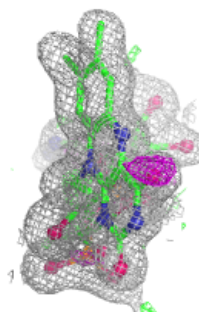
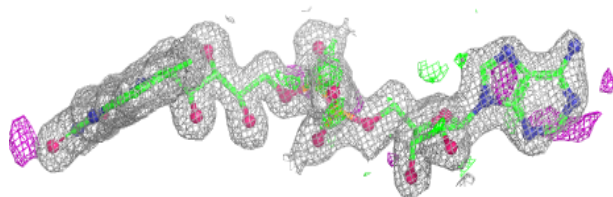
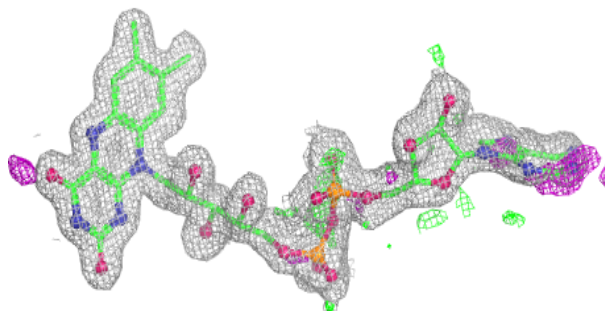
Electron density around ELI B 958:

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

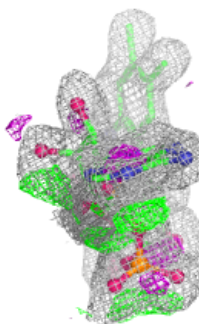
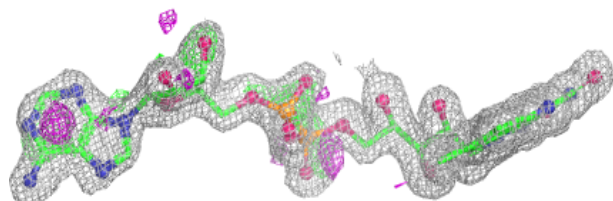
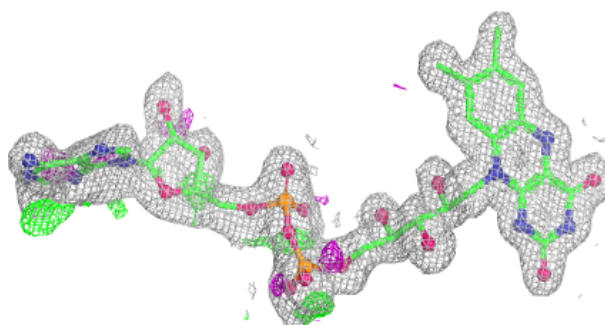


Electron density around FAD A 479:

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

**Electron density around FAD B 479:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.