Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2022 – 03:44 pm GMT

PDB ID	:	7YWV
Title	:	Eugenol oxidase from rhodococcus jostii: mutant S81H, D151E, A423M, H434Y, S394V, Q425S, I445D, S518P
Authors	:	Alvigini, L.; Mattevi, A.
Deposited on	:	2022-02-14
Resolution	:	2.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

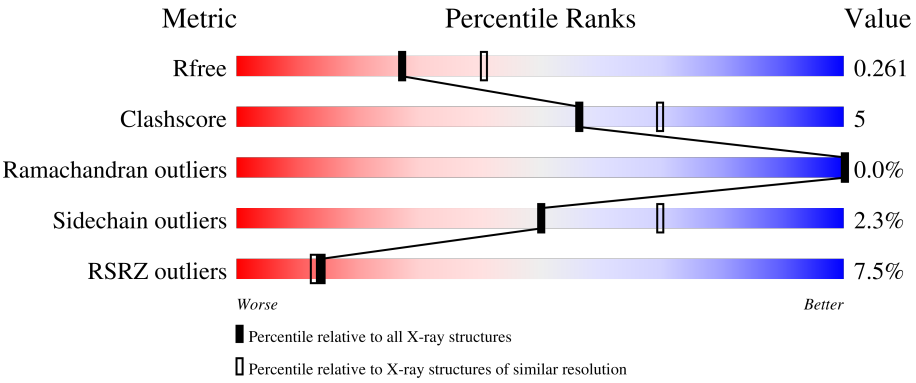
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	526	4% 87% 12%
1	B	526	3% 89% 10%
1	C	526	3% 88% 11%
1	D	526	8% 87% 12%
1	E	526	6% 87% 12%

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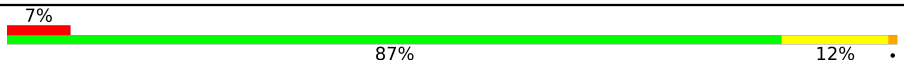
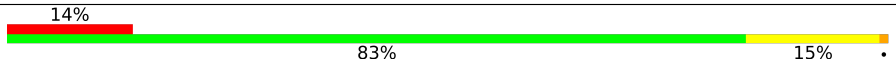
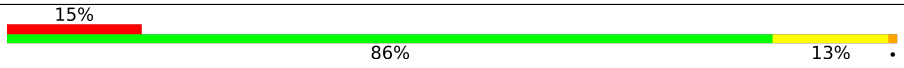
Mol	Chain	Length	Quality of chain
1	F	526	
1	G	526	
1	H	526	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 33775 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 Probable vanillyl-alcohol oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			4130	2635	699	772	24			
1	B	525	Total	C	N	O	S	0	0	0
			4123	2630	699	770	24			
1	C	524	Total	C	N	O	S	0	0	0
			4116	2628	698	766	24			
1	D	524	Total	C	N	O	S	0	0	0
			4110	2623	696	767	24			
1	E	524	Total	C	N	O	S	0	0	0
			4126	2632	699	771	24			
1	F	524	Total	C	N	O	S	0	0	0
			4118	2627	698	769	24			
1	G	525	Total	C	N	O	S	0	0	0
			4127	2633	697	773	24			
1	H	525	Total	C	N	O	S	0	0	0
			4123	2630	696	773	24			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	HIS	SER	engineered mutation	UNP Q0SBK1
A	151	GLU	ASP	engineered mutation	UNP Q0SBK1
A	394	VAL	SER	engineered mutation	UNP Q0SBK1
A	423	MET	ALA	engineered mutation	UNP Q0SBK1
A	425	SER	GLN	engineered mutation	UNP Q0SBK1
A	434	TYR	HIS	engineered mutation	UNP Q0SBK1
A	445	ASP	ILE	engineered mutation	UNP Q0SBK1
A	518	PRO	SER	engineered mutation	UNP Q0SBK1
B	81	HIS	SER	engineered mutation	UNP Q0SBK1
B	151	GLU	ASP	engineered mutation	UNP Q0SBK1
B	394	VAL	SER	engineered mutation	UNP Q0SBK1
B	423	MET	ALA	engineered mutation	UNP Q0SBK1
B	425	SER	GLN	engineered mutation	UNP Q0SBK1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	434	TYR	HIS	engineered mutation	UNP Q0SBK1
B	445	ASP	ILE	engineered mutation	UNP Q0SBK1
B	518	PRO	SER	engineered mutation	UNP Q0SBK1
C	81	HIS	SER	engineered mutation	UNP Q0SBK1
C	151	GLU	ASP	engineered mutation	UNP Q0SBK1
C	394	VAL	SER	engineered mutation	UNP Q0SBK1
C	423	MET	ALA	engineered mutation	UNP Q0SBK1
C	425	SER	GLN	engineered mutation	UNP Q0SBK1
C	434	TYR	HIS	engineered mutation	UNP Q0SBK1
C	445	ASP	ILE	engineered mutation	UNP Q0SBK1
C	518	PRO	SER	engineered mutation	UNP Q0SBK1
D	81	HIS	SER	engineered mutation	UNP Q0SBK1
D	151	GLU	ASP	engineered mutation	UNP Q0SBK1
D	394	VAL	SER	engineered mutation	UNP Q0SBK1
D	423	MET	ALA	engineered mutation	UNP Q0SBK1
D	425	SER	GLN	engineered mutation	UNP Q0SBK1
D	434	TYR	HIS	engineered mutation	UNP Q0SBK1
D	445	ASP	ILE	engineered mutation	UNP Q0SBK1
D	518	PRO	SER	engineered mutation	UNP Q0SBK1
E	81	HIS	SER	engineered mutation	UNP Q0SBK1
E	151	GLU	ASP	engineered mutation	UNP Q0SBK1
E	394	VAL	SER	engineered mutation	UNP Q0SBK1
E	423	MET	ALA	engineered mutation	UNP Q0SBK1
E	425	SER	GLN	engineered mutation	UNP Q0SBK1
E	434	TYR	HIS	engineered mutation	UNP Q0SBK1
E	445	ASP	ILE	engineered mutation	UNP Q0SBK1
E	518	PRO	SER	engineered mutation	UNP Q0SBK1
F	81	HIS	SER	engineered mutation	UNP Q0SBK1
F	151	GLU	ASP	engineered mutation	UNP Q0SBK1
F	394	VAL	SER	engineered mutation	UNP Q0SBK1
F	423	MET	ALA	engineered mutation	UNP Q0SBK1
F	425	SER	GLN	engineered mutation	UNP Q0SBK1
F	434	TYR	HIS	engineered mutation	UNP Q0SBK1
F	445	ASP	ILE	engineered mutation	UNP Q0SBK1
F	518	PRO	SER	engineered mutation	UNP Q0SBK1
G	81	HIS	SER	engineered mutation	UNP Q0SBK1
G	151	GLU	ASP	engineered mutation	UNP Q0SBK1
G	394	VAL	SER	engineered mutation	UNP Q0SBK1
G	423	MET	ALA	engineered mutation	UNP Q0SBK1
G	425	SER	GLN	engineered mutation	UNP Q0SBK1
G	434	TYR	HIS	engineered mutation	UNP Q0SBK1
G	445	ASP	ILE	engineered mutation	UNP Q0SBK1

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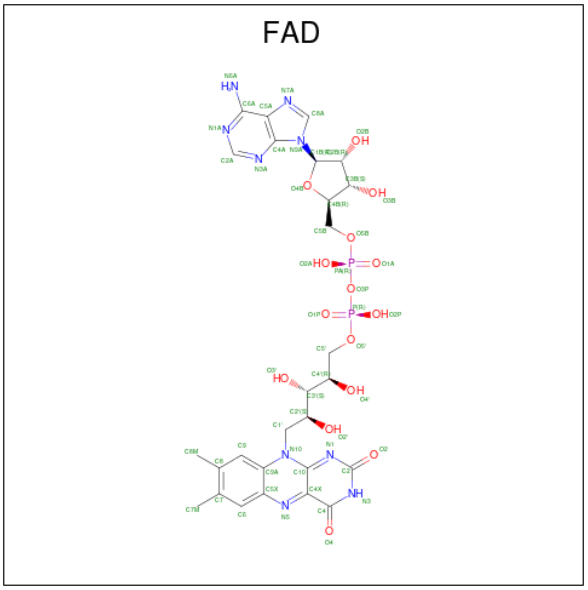
Chain	Residue	Modelled	Actual	Comment	Reference
G	518	PRO	SER	engineered mutation	UNP Q0SBK1
H	81	HIS	SER	engineered mutation	UNP Q0SBK1
H	151	GLU	ASP	engineered mutation	UNP Q0SBK1
H	394	VAL	SER	engineered mutation	UNP Q0SBK1
H	423	MET	ALA	engineered mutation	UNP Q0SBK1
H	425	SER	GLN	engineered mutation	UNP Q0SBK1
H	434	TYR	HIS	engineered mutation	UNP Q0SBK1
H	445	ASP	ILE	engineered mutation	UNP Q0SBK1
H	518	PRO	SER	engineered mutation	UNP Q0SBK1

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



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		

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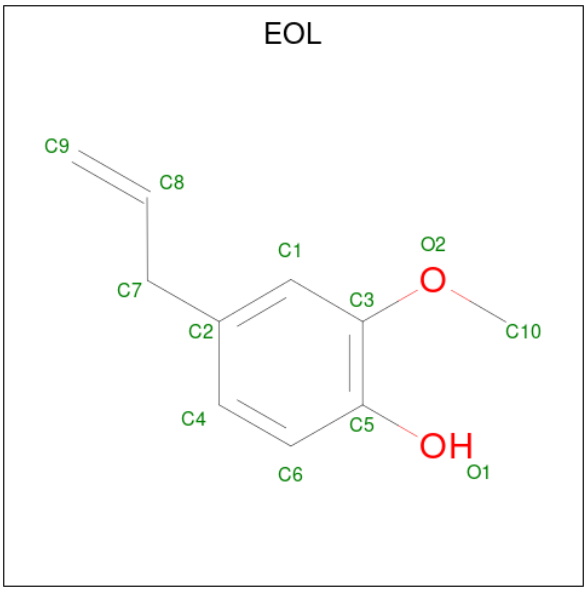
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total C N O P 53 27 9 15 2	0	0
2	H	1	Total C N O P 53 27 9 15 2	0	0

- Molecule 3 is 2-methoxy-4-(prop-2-en-1-yl)phenol (three-letter code: EOL) (formula: $C_{10}H_{12}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 10 2	0	0
3	B	1	Total C O 12 10 2	0	0
3	C	1	Total C O 12 10 2	0	0
3	D	1	Total C O 12 10 2	0	0
3	E	1	Total C O 12 10 2	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	B	2	Total Ca 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Ca 1 1	0	0
4	E	1	Total Ca 1 1	0	0

- Molecule 5 is water.

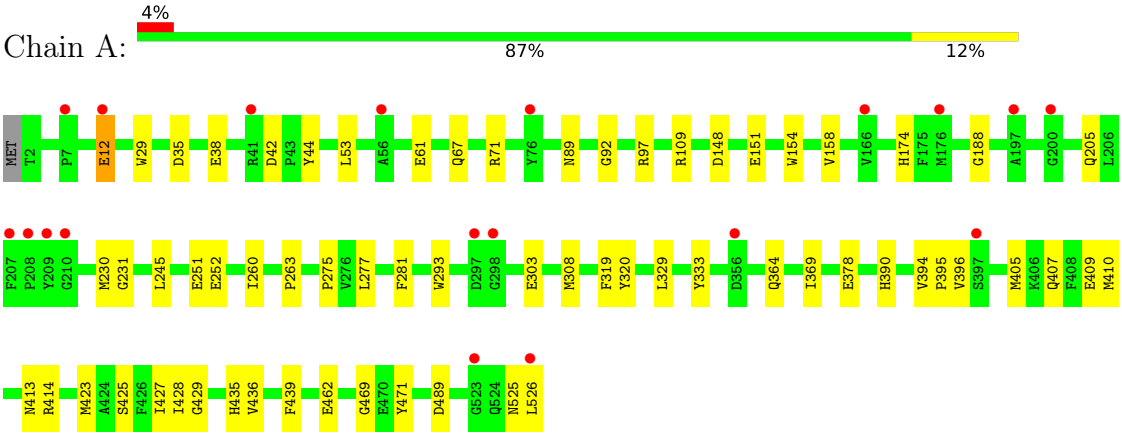
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	49	Total O 49 49	0	0
5	B	51	Total O 51 51	0	0
5	C	34	Total O 34 34	0	0
5	D	42	Total O 42 42	0	0
5	E	48	Total O 48 48	0	0
5	F	31	Total O 31 31	0	0
5	G	24	Total O 24 24	0	0
5	H	34	Total O 34 34	0	0

3 Residue-property plots (i)

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

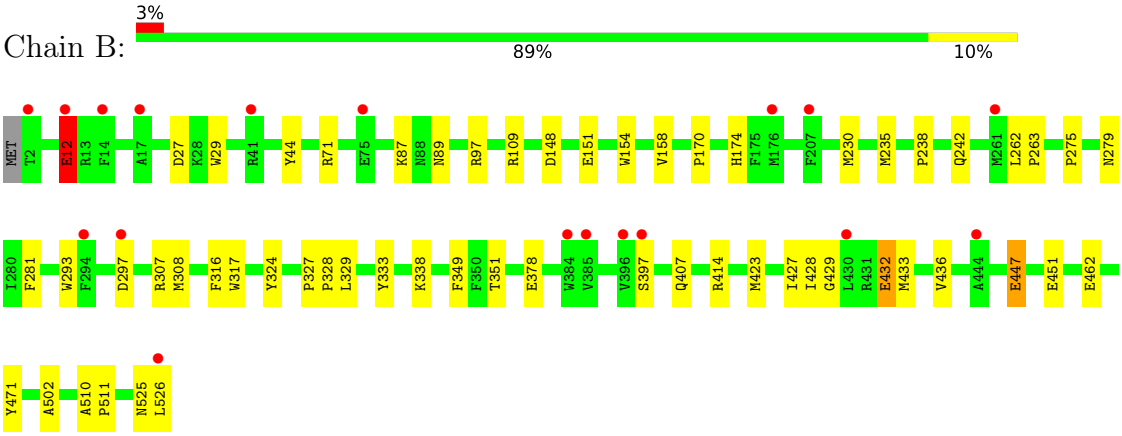
• Molecule 1: Probable vanillyl-alcohol oxidase

Chain A:



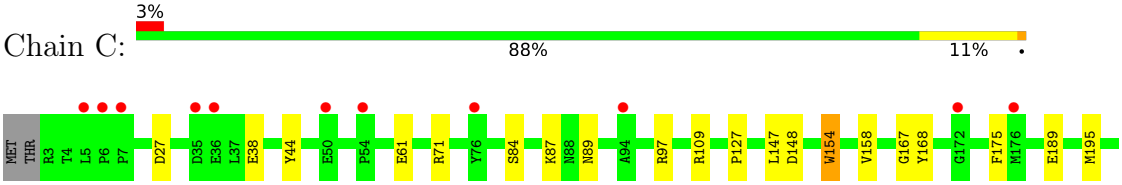
• Molecule 1: Probable vanillyl-alcohol oxidase

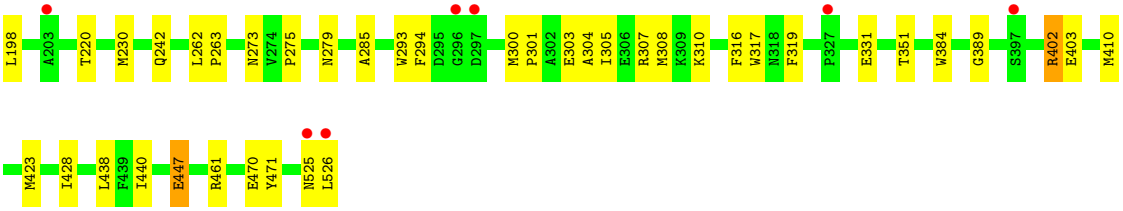
Chain B:



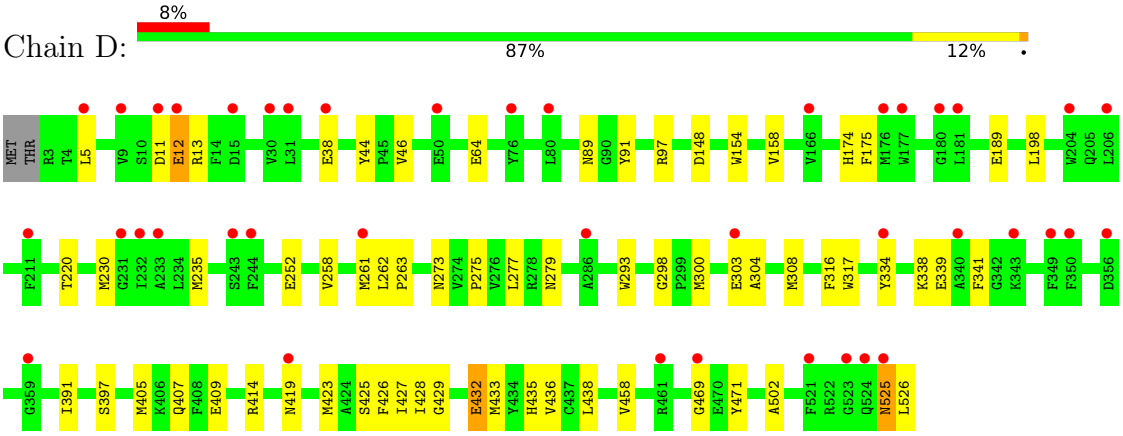
• Molecule 1: Probable vanillyl-alcohol oxidase

Chain C:

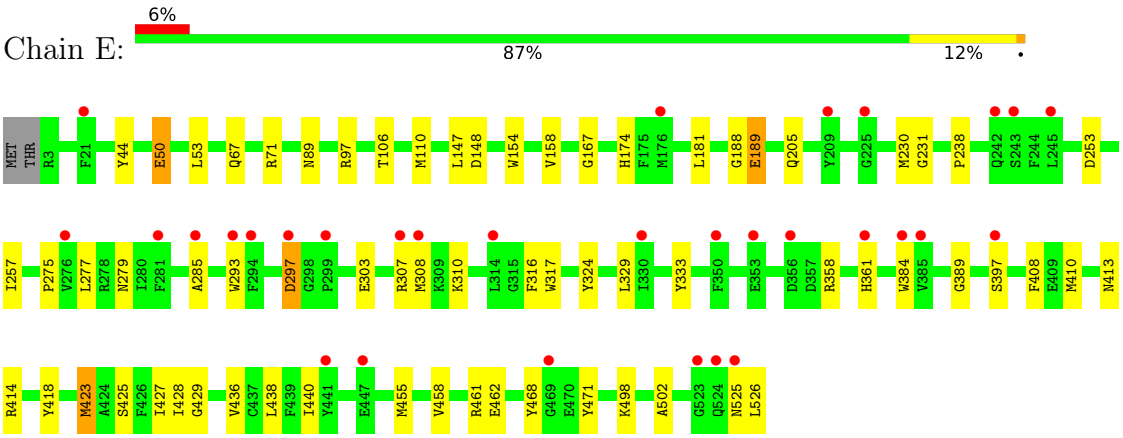




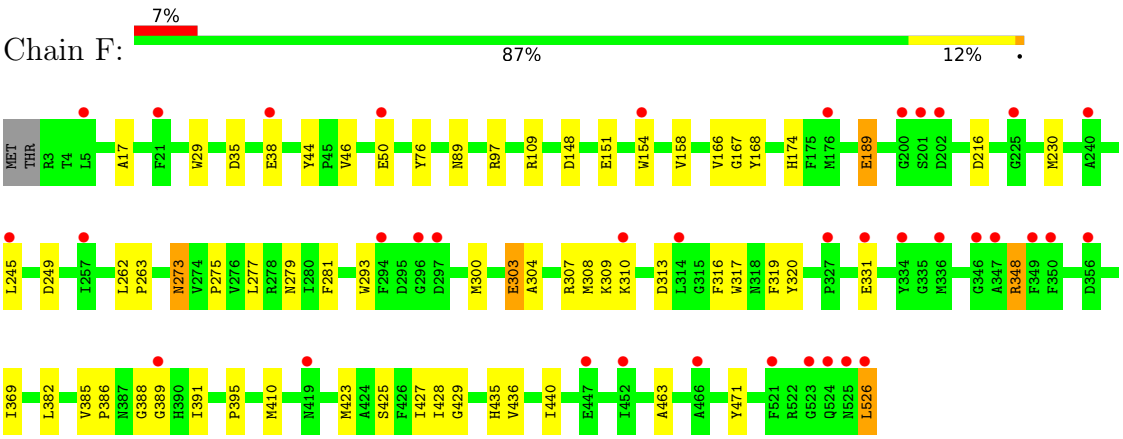
• Molecule 1: Probable vanillyl-alcohol oxidase



• Molecule 1: Probable vanillyl-alcohol oxidase

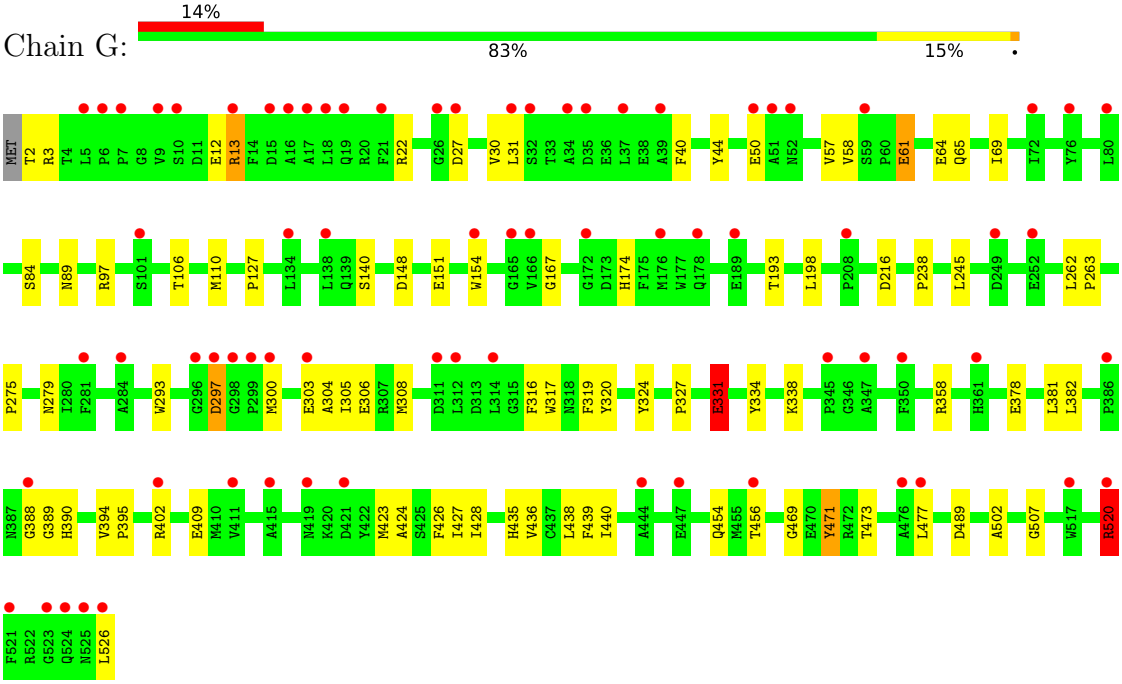


• Molecule 1: Probable vanillyl-alcohol oxidase



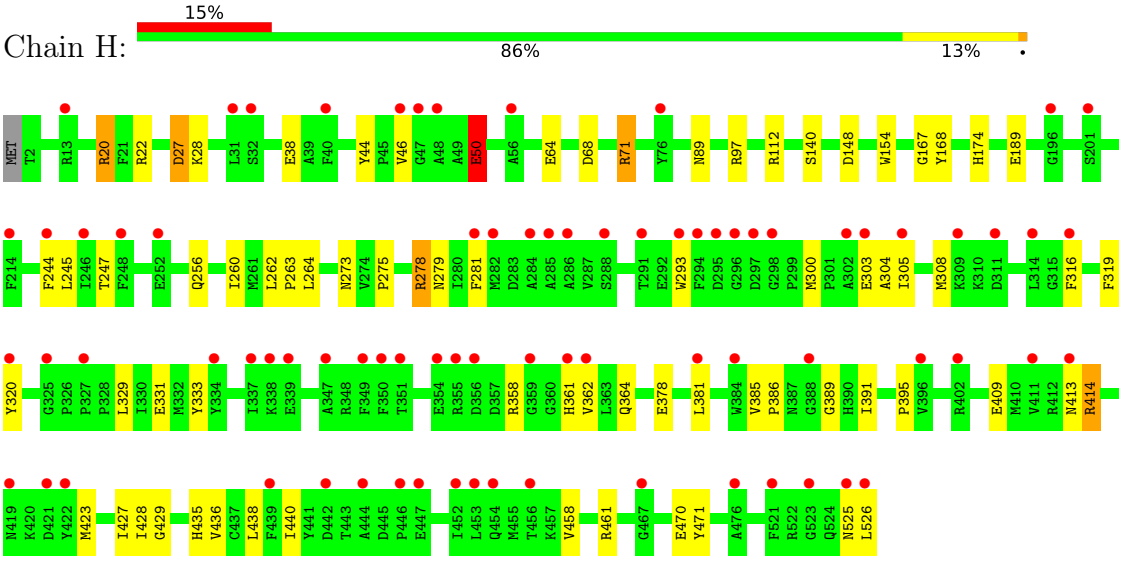
• Molecule 1: Probable vanillyl-alcohol oxidase

Chain G:



• Molecule 1: Probable vanillyl-alcohol oxidase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	114.19Å 142.40Å 288.52Å 90.00° 100.41° 90.00°	Depositor
Resolution (Å)	49.30 – 2.40 49.38 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.30-2.40) 99.2 (49.38-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.222 , 0.262 0.223 , 0.261	Depositor DCC
R_{free} test set	8823 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	40.7	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	33775	wwPDB-VP
Average B, all atoms (Å^2)	58.0	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.*

[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, EOL, CA

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	0.68	2/4239 (0.0%)	0.79	1/5753 (0.0%)
1	B	0.66	0/4232	0.78	1/5745 (0.0%)
1	C	0.70	2/4225 (0.0%)	0.79	3/5734 (0.1%)
1	D	0.69	3/4219 (0.1%)	0.80	3/5727 (0.1%)
1	E	0.68	1/4235 (0.0%)	0.79	3/5747 (0.1%)
1	F	0.66	1/4227 (0.0%)	0.79	2/5738 (0.0%)
1	G	0.71	3/4236 (0.1%)	0.84	6/5750 (0.1%)
1	H	0.98	3/4232 (0.1%)	0.83	6/5746 (0.1%)
All	All	0.73	15/33845 (0.0%)	0.80	25/45940 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	H	0	1
All	All	0	2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	50	GLU	CD-OE2	43.88	1.74	1.25
1	C	447	GLU	CD-OE1	12.29	1.39	1.25
1	G	331	GLU	CD-OE2	8.95	1.35	1.25
1	C	470	GLU	CD-OE1	-8.50	1.16	1.25
1	H	50	GLU	CD-OE1	-8.33	1.16	1.25
1	D	12	GLU	CD-OE1	-7.61	1.17	1.25
1	G	12	GLU	CD-OE2	6.62	1.32	1.25
1	A	12	GLU	CD-OE2	-6.52	1.18	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	189	GLU	CD-OE2	-6.08	1.19	1.25
1	E	189	GLU	CD-OE2	-6.01	1.19	1.25
1	A	251	GLU	CD-OE2	-5.97	1.19	1.25
1	H	64	GLU	CD-OE1	-5.47	1.19	1.25
1	G	61	GLU	CD-OE1	5.16	1.31	1.25
1	D	64	GLU	CD-OE1	-5.14	1.20	1.25
1	D	38	GLU	CD-OE1	-5.08	1.20	1.25

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	520	ARG	NE-CZ-NH1	-10.11	115.25	120.30
1	D	12	GLU	CB-CA-C	9.73	129.86	110.40
1	G	12	GLU	CB-CA-C	-7.50	95.39	110.40
1	A	12	GLU	CB-CA-C	-7.40	95.60	110.40
1	H	28	LYS	CB-CA-C	-7.35	95.70	110.40
1	G	520	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	C	461	ARG	CG-CD-NE	-7.21	96.67	111.80
1	F	348	ARG	NE-CZ-NH2	6.69	123.64	120.30
1	E	71	ARG	NE-CZ-NH1	-6.58	117.01	120.30
1	G	13	ARG	CG-CD-NE	-6.53	98.10	111.80
1	H	50	GLU	CB-CA-C	-6.52	97.36	110.40
1	H	461	ARG	CG-CD-NE	-6.38	98.40	111.80
1	C	402	ARG	CG-CD-NE	-6.35	98.46	111.80
1	H	20	ARG	CG-CD-NE	-6.24	98.69	111.80
1	D	13	ARG	CG-CD-NE	-5.81	99.60	111.80
1	H	50	GLU	OE1-CD-OE2	-5.77	116.37	123.30
1	B	12	GLU	CB-CA-C	5.76	121.92	110.40
1	E	71	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	D	339	GLU	CB-CA-C	-5.59	99.21	110.40
1	G	358	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	G	12	GLU	N-CA-CB	5.29	120.13	110.60
1	H	278	ARG	NE-CZ-NH2	5.19	122.89	120.30
1	F	348	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	C	310	LYS	CB-CA-C	-5.06	100.28	110.40
1	E	50	GLU	N-CA-CB	-5.04	101.53	110.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	447	GLU	Sidechain

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Mol	Chain	Res	Type	Group
1	H	50	GLU	Sidechain

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	4130	0	4000	37	0
1	B	4123	0	3984	36	0
1	C	4116	0	3987	36	0
1	D	4110	0	3971	38	1
1	E	4126	0	3997	39	0
1	F	4118	0	3982	41	0
1	G	4127	0	3993	61	0
1	H	4123	0	3982	42	0
2	A	53	0	29	1	0
2	B	53	0	30	2	0
2	C	53	0	29	1	0
2	D	53	0	30	2	0
2	E	53	0	29	1	0
2	F	53	0	29	1	0
2	G	53	0	30	1	0
2	H	53	0	29	1	0
3	A	12	0	11	0	0
3	B	12	0	11	0	0
3	C	12	0	12	0	0
3	D	12	0	11	1	0
3	E	12	0	11	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	A	49	0	0	0	0
5	B	51	0	0	2	0
5	C	34	0	0	0	0
5	D	42	0	0	0	0
5	E	48	0	0	1	0
5	F	31	0	0	3	0
5	G	24	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	34	0	0	4	0
All	All	33775	0	32187	329	1

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 5.

All (329) 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:H:50:GLU:CD	1:H:50:GLU:OE2	1.73	1.25
1:B:397:SER:OG	1:B:407:GLN:OE1	1.59	1.18
1:G:40:PHE:CD2	1:G:57:VAL:HG21	1.85	1.12
1:H:22:ARG:HD3	1:H:27:ASP:HB3	1.44	0.99
1:E:189:GLU:HG2	5:E:743:HOH:O	1.61	0.98
1:F:97:ARG:HH22	1:F:526:LEU:HD21	1.29	0.96
1:G:97:ARG:HH12	1:G:526:LEU:HD11	1.34	0.92
1:B:71:ARG:NH1	5:B:702:HOH:O	2.04	0.90
1:E:293:TRP:O	1:E:307:ARG:NH2	2.04	0.90
1:B:12:GLU:OE2	5:B:701:HOH:O	1.89	0.90
1:G:44:TYR:CD1	1:G:389:GLY:HA2	2.10	0.86
1:G:97:ARG:NH1	1:G:526:LEU:HD11	1.93	0.84
1:F:97:ARG:NH2	1:F:526:LEU:HD21	1.94	0.82
1:H:189:GLU:HG2	5:H:725:HOH:O	1.79	0.82
1:F:97:ARG:HH22	1:F:526:LEU:CD2	1.94	0.80
1:F:189:GLU:HG2	5:F:724:HOH:O	1.82	0.78
1:G:44:TYR:HD1	1:G:389:GLY:CA	1.99	0.75
2:A:601:FAD:H8A	2:A:601:FAD:O5B	1.87	0.74
1:B:97:ARG:HH12	1:B:526:LEU:HD11	1.52	0.73
1:F:245:LEU:HD13	1:F:320:TYR:CE2	2.24	0.73
1:B:151:GLU:OE2	1:B:378:GLU:HG2	1.90	0.71
1:A:151:GLU:OE2	1:A:378:GLU:HG2	1.90	0.71
1:E:358:ARG:HA	1:E:361:HIS:ND1	2.04	0.71
1:G:44:TYR:HD1	1:G:389:GLY:HA2	1.56	0.71
1:H:358:ARG:HA	1:H:361:HIS:ND1	2.05	0.70
1:G:44:TYR:CE1	1:G:389:GLY:HA2	2.27	0.70
2:F:600:FAD:O5B	2:F:600:FAD:H8A	1.96	0.66
1:G:40:PHE:CE2	1:G:57:VAL:HG21	2.30	0.66
1:G:151:GLU:OE2	1:G:378:GLU:HG2	1.95	0.66
1:G:44:TYR:CE2	1:G:89:ASN:HB3	2.30	0.66
1:A:44:TYR:CE2	1:A:89:ASN:HB3	2.32	0.65
1:F:423:MET:HE1	5:F:710:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:397:SER:CB	1:D:407:GLN:HE22	2.10	0.65
1:H:97:ARG:HH12	1:H:526:LEU:HD11	1.61	0.65
1:E:414:ARG:NH1	1:E:462:GLU:OE2	2.30	0.64
1:G:245:LEU:HD13	1:G:320:TYR:CE2	2.31	0.64
1:C:158:VAL:HA	1:C:230:MET:HE3	1.80	0.63
1:H:245:LEU:HD12	1:H:320:TYR:CE2	2.33	0.63
1:G:2:THR:HG22	1:G:3:ARG:H	1.64	0.62
1:B:429:GLY:HA3	1:B:432:GLU:OE1	2.00	0.62
1:F:148:ASP:OD1	1:F:174:HIS:NE2	2.33	0.61
1:H:148:ASP:OD1	1:H:167:GLY:HA3	2.01	0.61
2:D:601:FAD:H8A	2:D:601:FAD:O5B	2.01	0.60
1:D:97:ARG:HH12	1:D:526:LEU:HD11	1.66	0.60
1:G:58:VAL:HG11	1:G:69:ILE:HD12	1.83	0.60
2:H:600:FAD:H8A	2:H:600:FAD:O5B	2.02	0.60
1:F:97:ARG:HH12	1:F:526:LEU:HD21	1.66	0.59
1:H:293:TRP:HB2	1:H:300:MET:HE1	1.84	0.59
2:C:601:FAD:H8A	2:C:601:FAD:O5B	2.02	0.59
1:F:382:LEU:HD12	1:F:388:GLY:O	2.03	0.59
1:F:423:MET:CE	5:F:710:HOH:O	2.50	0.59
2:B:601:FAD:H8A	2:B:601:FAD:O5B	2.03	0.59
1:F:427:ILE:HD12	1:F:436:VAL:HG21	1.85	0.58
1:C:97:ARG:HH12	1:C:526:LEU:HD11	1.67	0.58
1:G:44:TYR:CD1	1:G:389:GLY:CA	2.77	0.58
1:B:242:GLN:NE2	1:B:351:THR:HG21	2.19	0.58
1:B:428:ILE:HG22	1:B:429:GLY:O	2.04	0.58
1:H:293:TRP:HB2	1:H:300:MET:CE	2.33	0.58
1:G:40:PHE:HD2	1:G:57:VAL:HG21	1.62	0.57
1:G:334:TYR:CE2	1:G:338:LYS:HE3	2.40	0.57
1:H:245:LEU:HD12	1:H:320:TYR:HE2	1.70	0.57
1:C:242:GLN:NE2	1:C:351:THR:HG21	2.20	0.56
1:H:358:ARG:HA	1:H:361:HIS:CE1	2.39	0.56
1:B:293:TRP:O	1:B:307:ARG:NH2	2.34	0.56
1:B:97:ARG:NH1	1:B:526:LEU:HD11	2.20	0.56
1:B:414:ARG:NH2	1:B:462:GLU:OE2	2.38	0.56
1:F:97:ARG:CZ	1:F:526:LEU:HD21	2.36	0.56
1:C:148:ASP:OD2	1:C:167:GLY:HA3	2.06	0.56
1:B:158:VAL:HG22	1:B:230:MET:HB3	1.87	0.55
1:D:275:PRO:HD2	1:D:428:ILE:O	2.06	0.55
1:A:525:ASN:O	1:A:526:LEU:HB2	2.06	0.55
1:A:61:GLU:HB2	1:A:109:ARG:NH2	2.22	0.55
1:B:447:GLU:O	1:B:451:GLU:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:97:ARG:NH1	1:F:526:LEU:HD21	2.20	0.55
1:G:389:GLY:O	1:G:440:ILE:HA	2.07	0.55
1:G:507:GLY:O	1:G:520:ARG:NH2	2.39	0.55
1:B:525:ASN:O	1:B:526:LEU:HB2	2.07	0.55
1:A:97:ARG:HH12	1:A:526:LEU:HD11	1.71	0.54
1:G:334:TYR:CE2	1:G:338:LYS:CE	2.90	0.54
1:H:525:ASN:O	1:H:526:LEU:HB2	2.07	0.54
1:F:44:TYR:CE2	1:F:89:ASN:HB3	2.43	0.54
1:H:423:MET:HB2	1:H:438:LEU:O	2.08	0.54
1:A:281:PHE:HB3	1:A:423:MET:SD	2.48	0.54
1:G:300:MET:HE3	1:G:304:ALA:HB1	1.90	0.53
1:E:106:THR:O	1:E:110:MET:HB2	2.08	0.53
1:G:297:ASP:OD1	1:G:297:ASP:N	2.42	0.53
1:F:148:ASP:OD1	1:F:167:GLY:HA3	2.08	0.53
1:H:329:LEU:HD11	1:H:333:TYR:CZ	2.44	0.53
1:D:502:ALA:HB2	1:G:502:ALA:HB2	1.91	0.53
1:A:407:GLN:HA	1:A:410:MET:HE3	1.91	0.53
1:D:427:ILE:HD12	1:D:436:VAL:HG21	1.90	0.53
1:F:249:ASP:O	1:F:309:LYS:NZ	2.41	0.53
1:F:275:PRO:HB3	1:F:319:PHE:CZ	2.43	0.53
1:H:275:PRO:HB3	1:H:319:PHE:CZ	2.44	0.53
1:A:158:VAL:HG22	1:A:230:MET:HB3	1.91	0.52
1:H:364:GLN:OE1	1:H:364:GLN:HA	2.09	0.52
1:H:44:TYR:CE2	1:H:89:ASN:HB3	2.45	0.52
1:A:97:ARG:HH22	1:A:526:LEU:HD21	1.75	0.52
1:D:414:ARG:HE	1:D:458:VAL:HG11	1.74	0.52
2:E:601:FAD:H8A	2:E:601:FAD:O5B	2.10	0.52
1:H:279:ASN:HA	1:H:316:PHE:O	2.10	0.51
1:E:277:LEU:HD11	1:E:317:TRP:HB3	1.92	0.51
1:B:293:TRP:CD2	1:B:308:MET:HG2	2.45	0.51
1:G:423:MET:HB2	1:G:438:LEU:O	2.10	0.51
1:G:454:GLN:HA	1:G:454:GLN:NE2	2.26	0.51
1:B:262:LEU:HB3	1:B:263:PRO:HD3	1.92	0.51
1:F:382:LEU:HD12	1:F:388:GLY:C	2.31	0.51
1:D:46:VAL:HG21	1:D:391:ILE:HD12	1.92	0.51
1:G:148:ASP:OD1	1:G:167:GLY:HA3	2.11	0.51
1:A:414:ARG:NH2	1:A:462:GLU:OE2	2.44	0.51
1:F:279:ASN:HB3	1:F:317:TRP:CZ3	2.46	0.51
1:G:306:GLU:OE2	1:G:306:GLU:HA	2.11	0.51
1:H:148:ASP:OD1	1:H:174:HIS:NE2	2.44	0.51
1:F:410:MET:CE	1:F:463:ALA:HA	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:395:PRO:HD2	1:H:435:HIS:O	2.10	0.50
1:C:294:PHE:CE1	1:C:301:PRO:HD3	2.46	0.50
1:A:61:GLU:HB2	1:A:109:ARG:CZ	2.41	0.50
1:H:278:ARG:HH11	1:H:362:VAL:HG11	1.77	0.50
1:H:414:ARG:HD2	1:H:458:VAL:HG11	1.92	0.50
1:F:279:ASN:HA	1:F:316:PHE:O	2.11	0.50
1:B:87:LYS:HB2	2:B:601:FAD:O1P	2.12	0.50
1:G:245:LEU:HD13	1:G:320:TYR:CZ	2.47	0.50
1:C:44:TYR:CE2	1:C:89:ASN:HB3	2.47	0.50
1:A:396:VAL:HB	1:C:195:MET:CE	2.41	0.49
1:B:275:PRO:HD2	1:B:428:ILE:O	2.12	0.49
1:H:427:ILE:HD12	1:H:436:VAL:HG21	1.94	0.49
1:A:409:GLU:O	1:A:413:ASN:HB2	2.13	0.49
1:F:275:PRO:HD2	1:F:428:ILE:O	2.12	0.49
1:C:61:GLU:HB2	1:C:109:ARG:CZ	2.42	0.49
1:C:305:ILE:HA	1:C:308:MET:HE2	1.94	0.49
1:E:358:ARG:HA	1:E:361:HIS:CE1	2.47	0.49
1:F:158:VAL:HG22	1:F:230:MET:HB3	1.95	0.49
1:B:502:ALA:HB2	1:E:502:ALA:HB2	1.93	0.49
1:G:427:ILE:HD12	1:G:436:VAL:HG21	1.95	0.49
1:H:245:LEU:CD2	1:H:247:THR:HG23	2.43	0.49
1:C:525:ASN:O	1:C:526:LEU:HB2	2.13	0.49
1:C:71:ARG:NH2	1:G:402:ARG:CZ	2.75	0.49
1:A:29:TRP:CE2	1:A:109:ARG:HD3	2.47	0.49
1:H:68:ASP:OD1	5:H:701:HOH:O	2.20	0.49
1:B:148:ASP:OD1	1:B:174:HIS:NE2	2.45	0.48
1:H:428:ILE:HG22	1:H:429:GLY:O	2.12	0.48
1:C:158:VAL:HG22	1:C:230:MET:HB3	1.93	0.48
1:D:525:ASN:O	1:D:526:LEU:HB2	2.12	0.48
1:A:303:GLU:OE1	1:A:303:GLU:N	2.46	0.48
1:C:262:LEU:HB3	1:C:263:PRO:HD3	1.94	0.48
1:D:397:SER:HB2	1:D:407:GLN:HE22	1.77	0.48
1:C:87:LYS:HE3	1:C:154:TRP:CD2	2.48	0.48
1:C:293:TRP:O	1:C:307:ARG:NH2	2.41	0.48
1:D:469:GLY:CA	1:G:198:LEU:HD13	2.43	0.48
1:H:378:GLU:O	1:H:381:LEU:HB2	2.13	0.48
1:F:262:LEU:HB3	1:F:263:PRO:HD3	1.96	0.48
1:C:97:ARG:HH22	1:C:526:LEU:HD21	1.79	0.48
1:D:423:MET:HB2	1:D:438:LEU:O	2.14	0.48
1:G:262:LEU:HB3	1:G:263:PRO:HD3	1.96	0.48
1:H:71:ARG:NH1	5:H:701:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:GLU:OE1	1:C:303:GLU:N	2.47	0.47
1:D:89:ASN:O	2:D:601:FAD:H9	2.14	0.47
1:C:147:LEU:C	1:C:147:LEU:HD12	2.35	0.47
1:D:252:GLU:HA	1:D:405:MET:CE	2.44	0.47
1:H:97:ARG:NH1	1:H:526:LEU:HD11	2.29	0.47
1:G:394:VAL:HA	1:G:435:HIS:O	2.14	0.47
1:B:329:LEU:HD11	1:B:333:TYR:CZ	2.49	0.47
1:E:410:MET:HE1	1:E:468:TYR:HE2	1.80	0.47
1:A:275:PRO:HB3	1:A:319:PHE:CZ	2.49	0.47
1:C:279:ASN:HA	1:C:316:PHE:O	2.14	0.47
1:D:397:SER:OG	1:D:407:GLN:NE2	2.43	0.47
1:E:148:ASP:OD1	1:E:174:HIS:NE2	2.47	0.47
1:D:252:GLU:HA	1:D:405:MET:HE3	1.96	0.47
1:B:44:TYR:CE2	1:B:89:ASN:HB3	2.50	0.47
1:D:44:TYR:CE2	1:D:89:ASN:HB3	2.50	0.47
1:G:31:LEU:HD12	1:G:40:PHE:HE2	1.80	0.47
2:G:600:FAD:O5B	2:G:600:FAD:H8A	2.15	0.47
1:A:394:VAL:HA	1:A:435:HIS:O	2.15	0.46
1:C:84:SER:OG	1:C:127:PRO:HB3	2.15	0.46
1:F:46:VAL:HG21	1:F:391:ILE:HD12	1.98	0.46
1:G:394:VAL:HG13	1:G:394:VAL:O	2.15	0.46
1:A:252:GLU:HA	1:A:405:MET:CE	2.46	0.46
1:D:148:ASP:OD1	1:D:174:HIS:NE2	2.48	0.46
1:H:304:ALA:O	1:H:308:MET:HG3	2.15	0.46
1:F:281:PHE:HB3	1:F:423:MET:SD	2.56	0.46
1:G:279:ASN:HA	1:G:316:PHE:O	2.15	0.46
1:G:305:ILE:HA	1:G:308:MET:HE2	1.97	0.46
1:B:170:PRO:HB2	1:B:235:MET:HE3	1.96	0.46
1:C:410:MET:HB2	1:C:410:MET:HE2	1.82	0.46
1:G:378:GLU:O	1:G:381:LEU:HB2	2.16	0.46
1:E:44:TYR:CE2	1:E:89:ASN:HB3	2.51	0.46
1:E:428:ILE:HG22	1:E:429:GLY:O	2.16	0.46
1:G:148:ASP:OD1	1:G:174:HIS:NE2	2.49	0.46
1:G:394:VAL:HG11	1:G:471:TYR:CE1	2.51	0.46
1:A:67:GLN:HG2	1:A:188:GLY:O	2.16	0.46
1:A:364:GLN:OE1	1:A:364:GLN:HA	2.15	0.46
1:D:198:LEU:HD13	1:G:469:GLY:CA	2.46	0.46
1:A:469:GLY:CA	1:C:198:LEU:HD13	2.46	0.45
1:E:158:VAL:HG22	1:E:230:MET:HB3	1.98	0.45
1:A:148:ASP:OD1	1:A:174:HIS:NE2	2.41	0.45
1:F:395:PRO:HG2	1:F:435:HIS:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:281:PHE:CZ	1:H:305:ILE:CD1	2.99	0.45
1:D:277:LEU:O	1:D:425:SER:HA	2.15	0.45
1:E:303:GLU:N	1:E:303:GLU:OE1	2.49	0.45
1:G:279:ASN:HB3	1:G:317:TRP:CZ3	2.52	0.45
1:H:395:PRO:HG2	1:H:435:HIS:HB3	1.98	0.45
1:A:42:ASP:OD2	1:A:92:GLY:HA2	2.17	0.45
1:C:275:PRO:HD2	1:C:428:ILE:O	2.17	0.45
1:D:293:TRP:CD2	1:D:308:MET:HG2	2.51	0.45
1:E:97:ARG:HH12	1:E:526:LEU:HD11	1.81	0.45
1:A:427:ILE:HD12	1:A:436:VAL:HG21	1.99	0.45
1:G:97:ARG:HH22	1:G:526:LEU:HD21	1.82	0.45
1:B:238:PRO:HG3	1:B:324:TYR:HB3	1.97	0.45
1:G:395:PRO:HD2	1:G:435:HIS:O	2.17	0.45
1:C:423:MET:HB2	1:C:438:LEU:O	2.17	0.45
1:E:418:TYR:CD1	1:E:455:MET:HG3	2.52	0.45
1:H:256:GLN:O	1:H:260:ILE:HG13	2.16	0.45
1:D:262:LEU:HB3	1:D:263:PRO:HD3	1.99	0.45
1:E:279:ASN:HA	1:E:316:PHE:O	2.17	0.45
1:D:426:PHE:CZ	1:D:435:HIS:CD2	3.05	0.44
1:G:275:PRO:HB3	1:G:319:PHE:CZ	2.51	0.44
1:G:382:LEU:O	1:G:388:GLY:HA3	2.17	0.44
1:A:275:PRO:HD2	1:A:428:ILE:O	2.16	0.44
1:H:409:GLU:O	1:H:413:ASN:HB2	2.16	0.44
1:E:329:LEU:HD11	1:E:333:TYR:CZ	2.53	0.44
1:F:29:TRP:CD2	1:F:109:ARG:HD2	2.52	0.44
1:G:275:PRO:HD2	1:G:428:ILE:O	2.17	0.44
1:B:279:ASN:HA	1:B:316:PHE:O	2.18	0.44
1:D:97:ARG:HH22	1:D:526:LEU:HD21	1.82	0.44
1:F:300:MET:HG2	1:F:304:ALA:HB3	1.99	0.44
1:F:389:GLY:O	1:F:440:ILE:HA	2.16	0.44
1:G:327:PRO:O	1:G:331:GLU:HB2	2.18	0.44
1:C:279:ASN:HB3	1:C:317:TRP:CZ3	2.53	0.44
1:G:65:GLN:O	1:G:69:ILE:HG12	2.17	0.44
1:G:390:HIS:HA	1:G:439:PHE:O	2.17	0.44
1:E:285:ALA:HA	1:E:384:TRP:CE3	2.53	0.44
1:A:245:LEU:HD13	1:A:320:TYR:CE2	2.53	0.43
1:B:338:LYS:HG2	1:B:349:PHE:CD2	2.53	0.43
1:D:97:ARG:NH1	1:D:526:LEU:HD11	2.33	0.43
1:D:300:MET:HG2	1:D:304:ALA:HB3	2.00	0.43
1:E:297:ASP:OD1	1:E:297:ASP:N	2.51	0.43
1:D:279:ASN:HA	1:D:316:PHE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:410:MET:HE1	1:E:468:TYR:CE2	2.53	0.43
1:H:385:VAL:HB	1:H:386:PRO:HD2	2.01	0.43
1:B:281:PHE:HB3	1:B:423:MET:SD	2.58	0.43
1:F:313:ASP:OD1	1:F:348:ARG:NH2	2.52	0.43
1:F:428:ILE:HG22	1:F:429:GLY:O	2.19	0.43
1:C:175:PHE:CD1	1:C:220:THR:HG21	2.54	0.43
1:F:385:VAL:HB	1:F:386:PRO:HD2	2.00	0.43
1:H:389:GLY:O	1:H:440:ILE:HA	2.19	0.43
1:D:298:GLY:HA2	1:D:419:ASN:OD1	2.19	0.43
1:E:67:GLN:HG2	1:E:188:GLY:O	2.19	0.43
1:A:252:GLU:HA	1:A:405:MET:HE2	2.01	0.43
1:B:97:ARG:HH22	1:B:526:LEU:HD21	1.84	0.43
1:C:285:ALA:HA	1:C:384:TRP:CE3	2.53	0.43
1:C:389:GLY:O	1:C:440:ILE:HA	2.18	0.43
1:D:397:SER:HB3	1:D:433:MET:HB3	2.00	0.43
1:C:305:ILE:HA	1:C:308:MET:CE	2.47	0.43
1:C:403:GLU:OE1	1:C:403:GLU:HA	2.19	0.43
1:D:175:PHE:CD1	1:D:220:THR:HG21	2.54	0.42
1:F:151:GLU:HA	1:F:369:ILE:HD13	2.00	0.42
1:F:303:GLU:N	1:F:303:GLU:OE1	2.52	0.42
1:B:397:SER:HB2	1:B:433:MET:HB3	2.00	0.42
1:D:5:LEU:HD11	1:D:11:ASP:OD2	2.19	0.42
1:E:275:PRO:HD2	1:E:428:ILE:O	2.19	0.42
1:G:106:THR:O	1:G:110:MET:HB2	2.20	0.42
1:A:260:ILE:O	1:A:263:PRO:HD2	2.19	0.42
1:E:148:ASP:OD1	1:E:167:GLY:HA3	2.19	0.42
1:E:427:ILE:HD12	1:E:436:VAL:HG21	2.01	0.42
1:A:293:TRP:CD2	1:A:308:MET:HG2	2.54	0.42
1:E:389:GLY:O	1:E:440:ILE:HA	2.19	0.42
1:F:395:PRO:HD2	1:F:435:HIS:O	2.20	0.42
1:H:97:ARG:HH22	1:H:526:LEU:HD21	1.85	0.42
1:D:91:TYR:OH	3:D:602:EOL:O2	2.33	0.42
1:C:87:LYS:HE3	1:C:154:TRP:CE2	2.55	0.42
1:G:293:TRP:CD2	1:G:308:MET:HG2	2.55	0.42
1:E:414:ARG:HD2	1:E:458:VAL:CG1	2.50	0.42
1:F:277:LEU:O	1:F:425:SER:HA	2.20	0.42
1:F:293:TRP:O	1:F:307:ARG:NH2	2.44	0.42
1:B:279:ASN:HB3	1:B:317:TRP:CZ3	2.55	0.42
1:C:61:GLU:HB2	1:C:109:ARG:NH2	2.34	0.42
1:D:429:GLY:HA3	1:D:432:GLU:OE1	2.20	0.42
1:E:97:ARG:HH12	1:E:526:LEU:HD21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:GLN:NE2	1:B:351:THR:CG2	2.83	0.42
1:A:395:PRO:HD2	1:A:435:HIS:O	2.19	0.41
1:E:205:GLN:HG3	1:E:231:GLY:HA3	2.02	0.41
1:G:22:ARG:HD3	1:G:27:ASP:HA	2.03	0.41
1:H:262:LEU:HB3	1:H:263:PRO:HD3	2.02	0.41
1:B:327:PRO:N	1:B:328:PRO:HD2	2.35	0.41
1:C:300:MET:HG2	1:C:304:ALA:HB3	2.02	0.41
1:E:423:MET:HB2	1:E:438:LEU:O	2.20	0.41
1:E:525:ASN:O	1:E:526:LEU:HB2	2.20	0.41
1:F:293:TRP:CD2	1:F:308:MET:HG2	2.55	0.41
1:G:2:THR:HG22	1:G:3:ARG:N	2.32	0.41
1:G:22:ARG:HG2	1:G:30:VAL:HG21	2.01	0.41
1:A:205:GLN:HG3	1:A:231:GLY:HA3	2.02	0.41
1:B:502:ALA:HB2	1:E:502:ALA:CB	2.51	0.41
1:A:277:LEU:O	1:A:425:SER:HA	2.20	0.41
1:D:158:VAL:HG22	1:D:230:MET:HB3	2.02	0.41
1:D:261:MET:HB3	1:D:341:PHE:HZ	1.85	0.41
1:G:84:SER:OG	1:G:127:PRO:HB3	2.20	0.41
1:H:46:VAL:HG21	1:H:391:ILE:HD12	2.02	0.41
1:D:334:TYR:CE2	1:D:338:LYS:HE2	2.55	0.41
1:E:253:ASP:O	1:E:257:ILE:HG13	2.21	0.41
1:G:424:ALA:HA	1:G:436:VAL:O	2.20	0.41
1:G:426:PHE:CZ	1:G:435:HIS:CD2	3.08	0.41
1:H:168:TYR:O	1:H:273:ASN:HB2	2.21	0.41
1:E:277:LEU:O	1:E:425:SER:HA	2.21	0.41
1:E:293:TRP:CD2	1:E:308:MET:HG2	2.56	0.41
1:A:97:ARG:NH1	1:A:526:LEU:HD11	2.35	0.41
1:B:29:TRP:CE2	1:B:109:ARG:HD3	2.56	0.41
1:C:71:ARG:NH2	1:G:402:ARG:NH1	2.68	0.41
1:C:275:PRO:HB3	1:C:319:PHE:CZ	2.55	0.41
1:F:17:ALA:HB2	1:F:76:TYR:CD2	2.56	0.41
1:A:428:ILE:HG22	1:A:429:GLY:O	2.21	0.40
1:G:238:PRO:HG3	1:G:324:TYR:HB3	2.02	0.40
1:G:456:THR:OG1	1:G:477:LEU:HD21	2.21	0.40
1:H:71:ARG:HD3	5:H:717:HOH:O	2.21	0.40
1:A:329:LEU:HD11	1:A:333:TYR:CZ	2.56	0.40
1:D:258:VAL:HA	1:D:261:MET:HG2	2.04	0.40
1:E:238:PRO:CG	1:E:324:TYR:HB3	2.50	0.40
1:A:151:GLU:HA	1:A:369:ILE:HD13	2.03	0.40
1:B:427:ILE:HD12	1:B:436:VAL:HG21	2.03	0.40
1:B:510:ALA:N	1:B:511:PRO:HD3	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:168:TYR:O	1:F:273:ASN:HB2	2.21	0.40
1:C:168:TYR:O	1:C:273:ASN:HB2	2.21	0.40
1:E:50:GLU:HG3	1:E:53:LEU:HD11	2.04	0.40
1:E:181:LEU:C	1:E:181:LEU:HD12	2.42	0.40
1:G:193:THR:HB	1:G:216:ASP:OD1	2.20	0.40
1:A:390:HIS:HA	1:A:439:PHE:O	2.21	0.40
1:D:235:MET:HE2	1:D:235:MET:HB3	1.78	0.40
1:D:279:ASN:HB3	1:D:317:TRP:CZ3	2.56	0.40
1:E:147:LEU:HD12	1:E:147:LEU:C	2.41	0.40
1:H:245:LEU:CD1	1:H:320:TYR:CE2	3.01	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:409:GLU:OE1	1:D:414:ARG:NH2[2_655]	2.04	0.16

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	523/526 (99%)	510 (98%)	13 (2%)	0	100	100
1	B	523/526 (99%)	507 (97%)	16 (3%)	0	100	100
1	C	522/526 (99%)	508 (97%)	14 (3%)	0	100	100
1	D	522/526 (99%)	506 (97%)	16 (3%)	0	100	100
1	E	522/526 (99%)	503 (96%)	19 (4%)	0	100	100
1	F	522/526 (99%)	506 (97%)	15 (3%)	1 (0%)	47	62
1	G	523/526 (99%)	504 (96%)	19 (4%)	0	100	100
1	H	523/526 (99%)	502 (96%)	21 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4180/4208 (99%)	4046 (97%)	133 (3%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	50	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	433/435 (100%)	425 (98%)	8 (2%)	59 76
1	B	431/435 (99%)	424 (98%)	7 (2%)	62 79
1	C	430/435 (99%)	423 (98%)	7 (2%)	62 79
1	D	429/435 (99%)	421 (98%)	8 (2%)	57 75
1	E	433/435 (100%)	423 (98%)	10 (2%)	50 70
1	F	431/435 (99%)	420 (97%)	11 (3%)	46 66
1	G	433/435 (100%)	419 (97%)	14 (3%)	39 59
1	H	432/435 (99%)	417 (96%)	15 (4%)	36 55
All	All	3452/3480 (99%)	3372 (98%)	80 (2%)	50 70

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLU
1	A	35	ASP
1	A	38	GLU
1	A	53	LEU
1	A	71	ARG
1	A	154	TRP
1	A	471	TYR
1	A	489	ASP
1	B	12	GLU

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Mol	Chain	Res	Type
1	B	27	ASP
1	B	154	TRP
1	B	297	ASP
1	B	432	GLU
1	B	447	GLU
1	B	471	TYR
1	C	27	ASP
1	C	38	GLU
1	C	154	TRP
1	C	189	GLU
1	C	331	GLU
1	C	402	ARG
1	C	471	TYR
1	D	12	GLU
1	D	154	TRP
1	D	189	GLU
1	D	273	ASN
1	D	303	GLU
1	D	432	GLU
1	D	471	TYR
1	D	525	ASN
1	E	154	TRP
1	E	297	ASP
1	E	310	LYS
1	E	397	SER
1	E	408	PHE
1	E	413	ASN
1	E	423	MET
1	E	461	ARG
1	E	471	TYR
1	E	498	LYS
1	F	35	ASP
1	F	38	GLU
1	F	154	TRP
1	F	166	VAL
1	F	216	ASP
1	F	273	ASN
1	F	303	GLU
1	F	310	LYS
1	F	331	GLU
1	F	471	TYR
1	F	526	LEU

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Mol	Chain	Res	Type
1	G	13	ARG
1	G	50	GLU
1	G	61	GLU
1	G	64	GLU
1	G	140	SER
1	G	154	TRP
1	G	297	ASP
1	G	303	GLU
1	G	331	GLU
1	G	409	GLU
1	G	471	TYR
1	G	473	THR
1	G	489	ASP
1	G	520	ARG
1	H	20	ARG
1	H	27	ASP
1	H	38	GLU
1	H	50	GLU
1	H	71	ARG
1	H	112	ARG
1	H	140	SER
1	H	154	TRP
1	H	244	PHE
1	H	264	LEU
1	H	303	GLU
1	H	331	GLU
1	H	414	ARG
1	H	470	GLU
1	H	471	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	GLN
1	B	67	GLN
1	B	81	HIS
1	C	242	GLN
1	D	187	GLN
1	D	242	GLN
1	D	407	GLN
1	E	242	GLN
1	E	419	ASN

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Mol	Chain	Res	Type
1	F	242	GLN
1	F	267	ASN
1	G	242	GLN
1	G	419	ASN
1	G	454	GLN
1	H	242	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 5 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FAD	D	601	1	53,58,58	0.67	0	68,89,89	0.83	3 (4%)
3	EOL	B	602	-	12,12,12	1.41	1 (8%)	15,15,15	1.65	3 (20%)
2	FAD	A	601	1	53,58,58	0.69	0	68,89,89	0.93	2 (2%)
2	FAD	G	600	1	53,58,58	0.66	0	68,89,89	0.80	0
2	FAD	F	600	1	53,58,58	0.68	0	68,89,89	0.80	2 (2%)
2	FAD	B	601	1	53,58,58	0.63	0	68,89,89	0.82	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EOL	C	602	-	12,12,12	1.28	1 (8%)	15,15,15	1.57	4 (26%)
2	FAD	E	601	1	53,58,58	0.63	0	68,89,89	0.79	1 (1%)
3	EOL	A	602	-	12,12,12	1.44	1 (8%)	15,15,15	1.62	1 (6%)
2	FAD	H	600	1	53,58,58	0.65	0	68,89,89	0.70	1 (1%)
3	EOL	E	602	-	12,12,12	1.32	1 (8%)	15,15,15	1.74	4 (26%)
2	FAD	C	601	1	53,58,58	0.67	1 (1%)	68,89,89	0.80	1 (1%)
3	EOL	D	602	-	12,12,12	1.33	1 (8%)	15,15,15	1.51	4 (26%)

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	D	601	1	-	6/30/50/50	0/6/6/6
3	EOL	B	602	-	-	1/5/5/5	0/1/1/1
2	FAD	A	601	1	-	8/30/50/50	0/6/6/6
2	FAD	G	600	1	-	13/30/50/50	0/6/6/6
2	FAD	F	600	1	-	9/30/50/50	0/6/6/6
2	FAD	B	601	1	-	6/30/50/50	0/6/6/6
3	EOL	C	602	-	-	1/5/5/5	0/1/1/1
2	FAD	E	601	1	-	10/30/50/50	0/6/6/6
3	EOL	A	602	-	-	1/5/5/5	0/1/1/1
2	FAD	H	600	1	-	8/30/50/50	0/6/6/6
3	EOL	E	602	-	-	1/5/5/5	0/1/1/1
2	FAD	C	601	1	-	3/30/50/50	0/6/6/6
3	EOL	D	602	-	-	1/5/5/5	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	EOL	C9-C8	3.93	1.55	1.28
3	D	602	EOL	C9-C8	3.92	1.55	1.28
3	B	602	EOL	C9-C8	3.87	1.54	1.28
3	C	602	EOL	C9-C8	3.76	1.54	1.28
3	E	602	EOL	C9-C8	3.63	1.53	1.28
2	C	601	FAD	C1'-C2'	2.20	1.55	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	EOL	C4-C6-C5	-3.83	116.57	120.50
3	B	602	EOL	C4-C6-C5	-3.72	116.68	120.50
2	A	601	FAD	P-O3P-PA	-3.48	120.87	132.83
3	E	602	EOL	C10-O2-C3	3.39	122.64	117.53
3	E	602	EOL	C4-C6-C5	-3.27	117.14	120.50
3	C	602	EOL	C7-C2-C1	-2.85	115.30	120.56
3	C	602	EOL	C4-C6-C5	-2.84	117.59	120.50
2	D	601	FAD	P-O3P-PA	-2.80	123.23	132.83
3	D	602	EOL	C4-C6-C5	-2.78	117.64	120.50
2	B	601	FAD	C5A-C6A-N6A	2.67	124.42	120.35
2	C	601	FAD	C5A-C6A-N6A	2.56	124.24	120.35
3	E	602	EOL	C7-C2-C1	-2.50	115.95	120.56
2	E	601	FAD	C5A-C6A-N6A	2.41	124.02	120.35
3	E	602	EOL	C6-C5-C3	2.41	122.32	119.53
3	D	602	EOL	C10-O2-C3	2.38	121.13	117.53
3	B	602	EOL	C10-O2-C3	2.37	121.10	117.53
2	D	601	FAD	C1'-C2'-C3'	2.33	116.29	109.79
3	D	602	EOL	O1-C5-C3	-2.20	114.96	120.09
2	F	600	FAD	C1'-C2'-C3'	2.19	115.92	109.79
2	A	601	FAD	C1'-C2'-C3'	2.16	115.83	109.79
2	F	600	FAD	C5A-C6A-N6A	2.15	123.61	120.35
3	C	602	EOL	C10-O2-C3	2.13	120.75	117.53
2	H	600	FAD	C5A-C6A-N6A	2.10	123.55	120.35
2	D	601	FAD	C5A-C6A-N6A	2.10	123.54	120.35
3	B	602	EOL	C7-C2-C1	-2.08	116.72	120.56
3	C	602	EOL	C7-C8-C9	-2.07	110.28	127.58
3	D	602	EOL	C7-C2-C1	-2.02	116.83	120.56

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	601	FAD	C5'-O5'-P-O2P
2	F	600	FAD	C5'-O5'-P-O2P
2	G	600	FAD	N10-C1'-C2'-C3'
2	G	600	FAD	C1'-C2'-C3'-O3'
2	G	600	FAD	C1'-C2'-C3'-C4'
2	G	600	FAD	C5'-O5'-P-O2P
2	G	600	FAD	O3'-C3'-C4'-O4'
2	H	600	FAD	O3'-C3'-C4'-O4'
2	A	601	FAD	C2'-C3'-C4'-O4'
2	D	601	FAD	C2'-C3'-C4'-O4'
2	G	600	FAD	C2'-C3'-C4'-O4'

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Mol	Chain	Res	Type	Atoms
2	H	600	FAD	C2'-C3'-C4'-O4'
2	B	601	FAD	O4'-C4'-C5'-O5'
2	C	601	FAD	O4'-C4'-C5'-O5'
2	E	601	FAD	O4'-C4'-C5'-O5'
2	H	600	FAD	O4'-C4'-C5'-O5'
2	A	601	FAD	C2'-C3'-C4'-C5'
2	D	601	FAD	C2'-C3'-C4'-C5'
2	G	600	FAD	C2'-C3'-C4'-C5'
2	H	600	FAD	C2'-C3'-C4'-C5'
2	A	601	FAD	O3'-C3'-C4'-O4'
2	D	601	FAD	O3'-C3'-C4'-O4'
2	B	601	FAD	C2'-C3'-C4'-O4'
2	A	601	FAD	C3'-C4'-C5'-O5'
2	B	601	FAD	C3'-C4'-C5'-O5'
2	C	601	FAD	C3'-C4'-C5'-O5'
2	E	601	FAD	C3'-C4'-C5'-O5'
2	H	600	FAD	C3'-C4'-C5'-O5'
2	G	600	FAD	O2'-C2'-C3'-O3'
2	E	601	FAD	C2'-C3'-C4'-O4'
2	F	600	FAD	C4'-C5'-O5'-P
2	G	600	FAD	C4'-C5'-O5'-P
2	G	600	FAD	O3'-C3'-C4'-C5'
2	H	600	FAD	O3'-C3'-C4'-C5'
2	B	601	FAD	C2'-C3'-C4'-C5'
2	D	601	FAD	C4'-C5'-O5'-P
2	E	601	FAD	C4'-C5'-O5'-P
2	C	601	FAD	C4'-C5'-O5'-P
2	E	601	FAD	C5'-O5'-P-O3P
2	F	600	FAD	C5'-O5'-P-O3P
2	G	600	FAD	C5'-O5'-P-O3P
3	E	602	EOL	C2-C7-C8-C9
2	G	600	FAD	O2'-C2'-C3'-C4'
2	A	601	FAD	C4'-C5'-O5'-P
2	B	601	FAD	C4'-C5'-O5'-P
3	B	602	EOL	C2-C7-C8-C9
2	H	600	FAD	N10-C1'-C2'-C3'
2	A	601	FAD	O4'-C4'-C5'-O5'
2	E	601	FAD	C2'-C3'-C4'-C5'
3	A	602	EOL	C2-C7-C8-C9
3	C	602	EOL	C2-C7-C8-C9
2	D	601	FAD	O3'-C3'-C4'-C5'
2	F	600	FAD	O2'-C2'-C3'-O3'

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Mol	Chain	Res	Type	Atoms
2	F	600	FAD	C2'-C3'-C4'-O4'
2	H	600	FAD	C4'-C5'-O5'-P
2	B	601	FAD	O3'-C3'-C4'-O4'
2	D	601	FAD	C3'-C4'-C5'-O5'
3	D	602	EOL	C2-C7-C8-C9
2	A	601	FAD	O3'-C3'-C4'-C5'
2	E	601	FAD	O2'-C2'-C3'-O3'
2	E	601	FAD	O3'-C3'-C4'-O4'
2	F	600	FAD	C3'-C4'-C5'-O5'
2	F	600	FAD	C5'-O5'-P-O1P
2	G	600	FAD	C5'-O5'-P-O1P
2	A	601	FAD	C1'-C2'-C3'-O3'
2	E	601	FAD	C1'-C2'-C3'-O3'
2	F	600	FAD	C1'-C2'-C3'-O3'
2	F	600	FAD	O4'-C4'-C5'-O5'

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	FAD	2	0
2	A	601	FAD	1	0
2	G	600	FAD	1	0
2	F	600	FAD	1	0
2	B	601	FAD	2	0
2	E	601	FAD	1	0
2	H	600	FAD	1	0
2	C	601	FAD	1	0
3	D	602	EOL	1	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.

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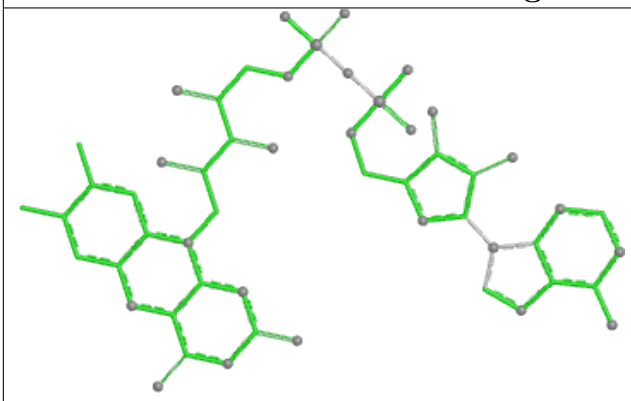
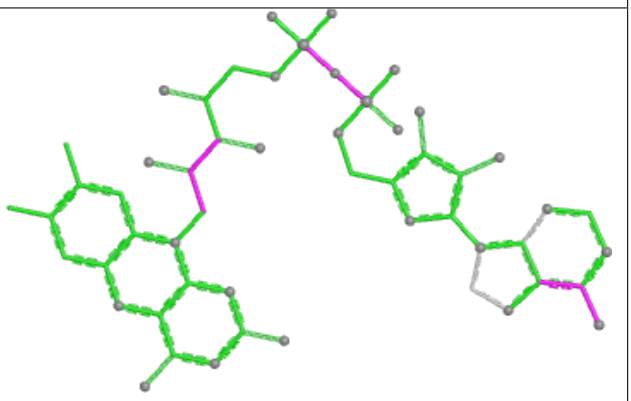
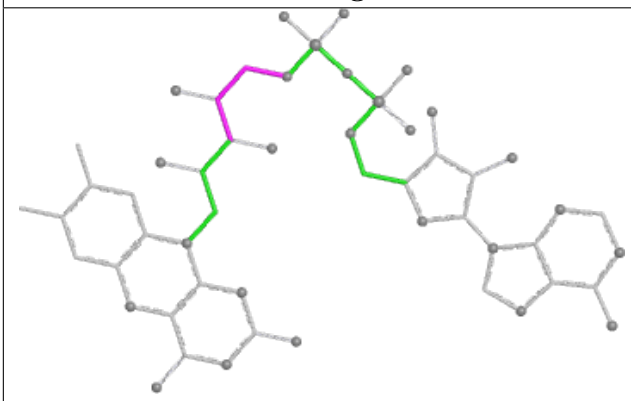
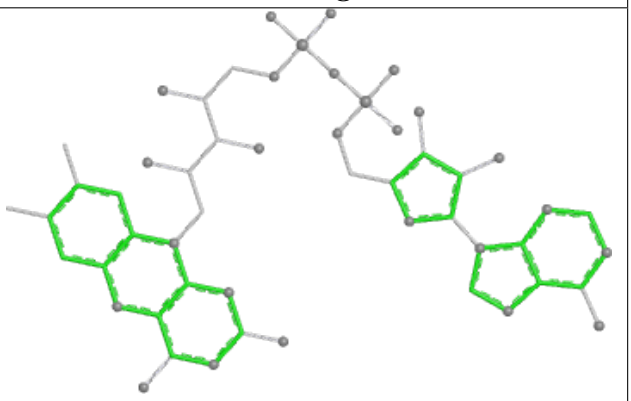
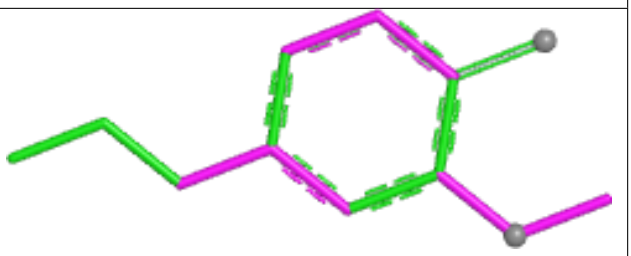
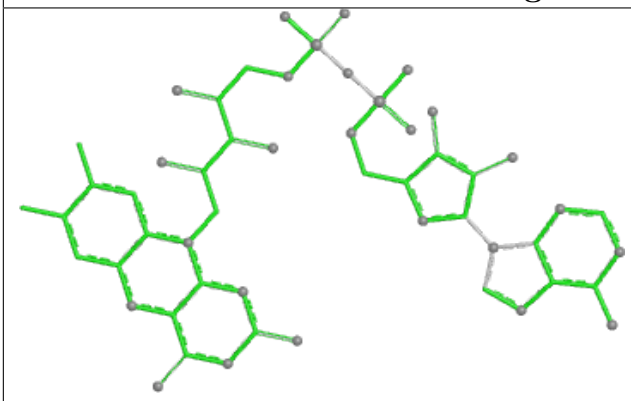
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand EOL B 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FAD A 601



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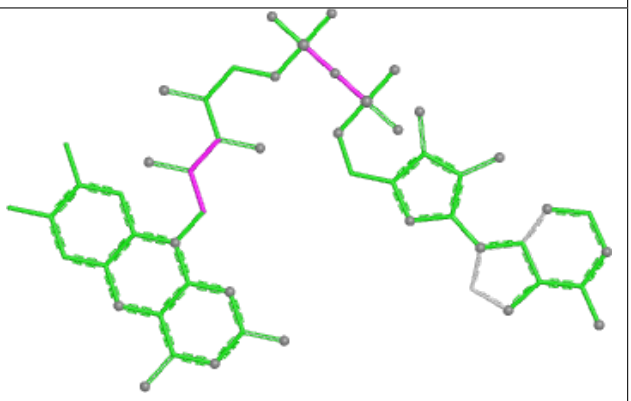

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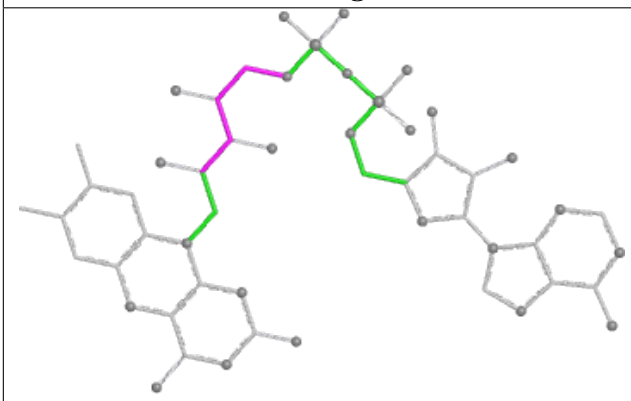

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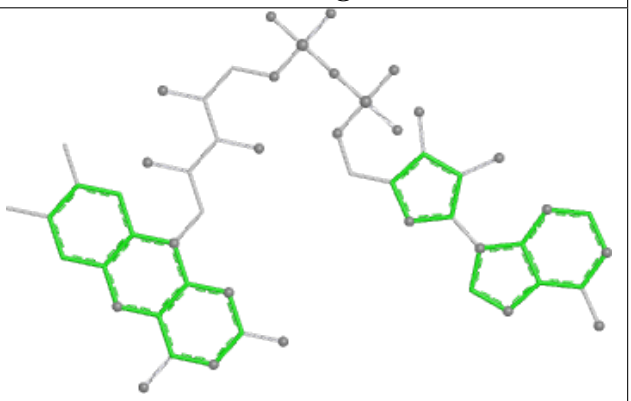

Rings

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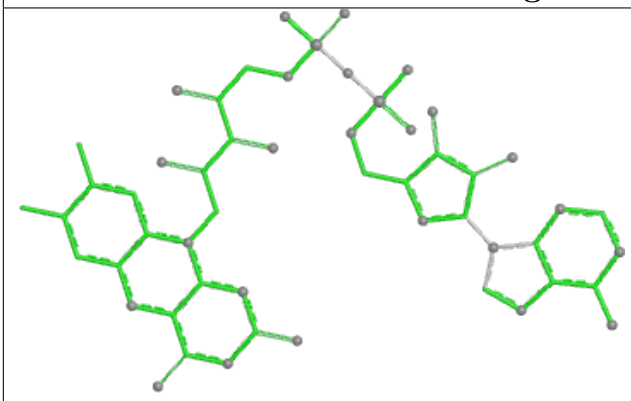

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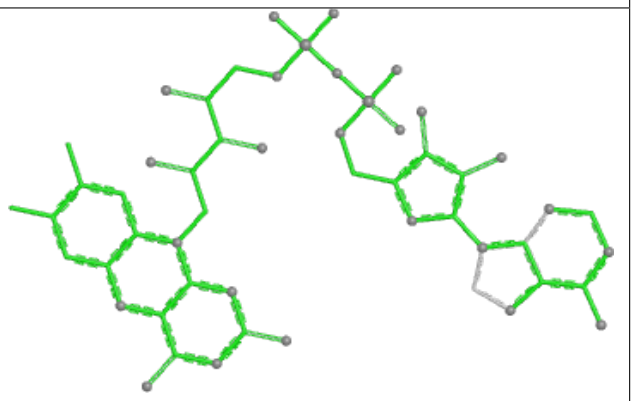

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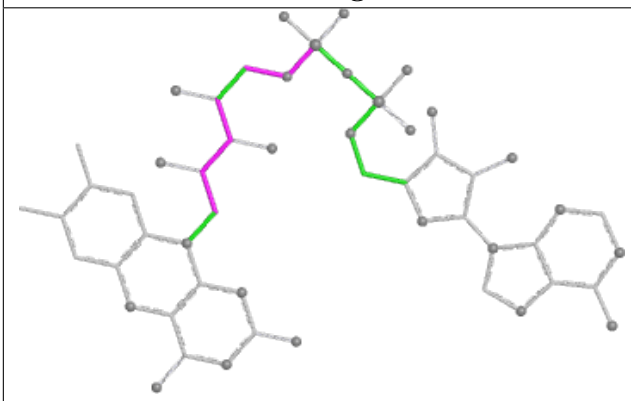

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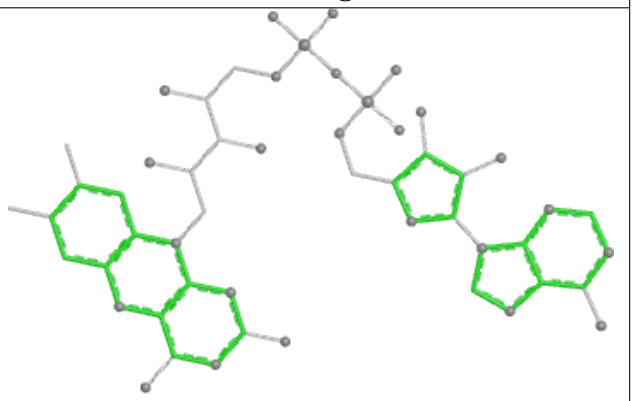

Rings

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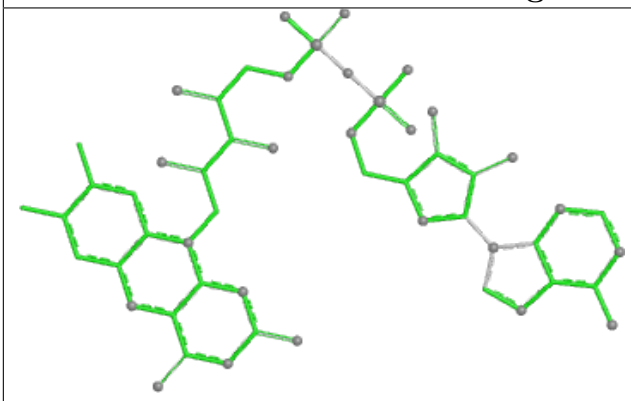

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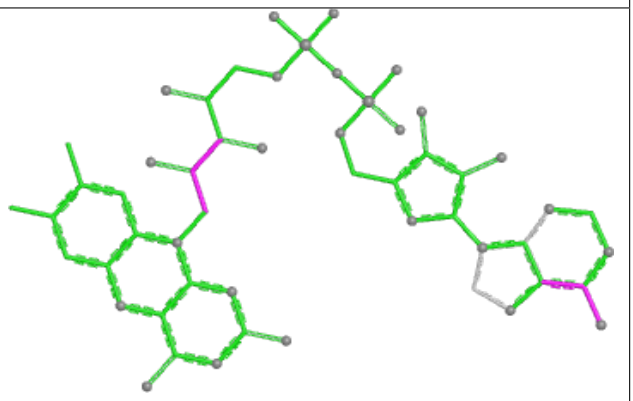
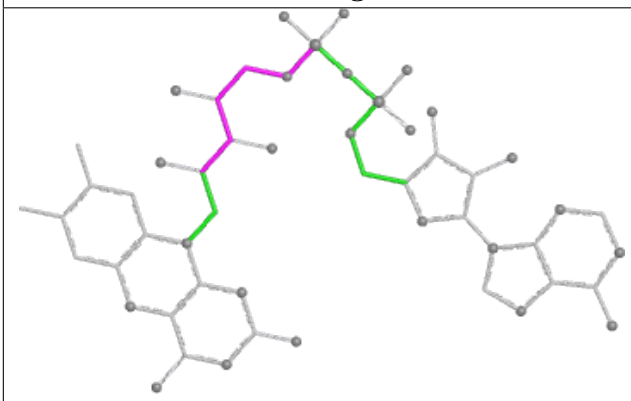


Bond angles



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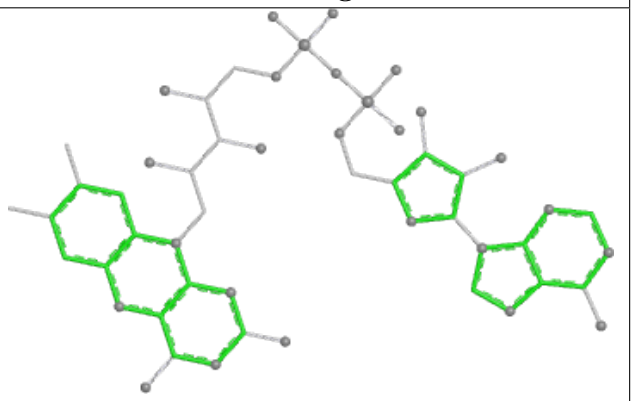

Rings

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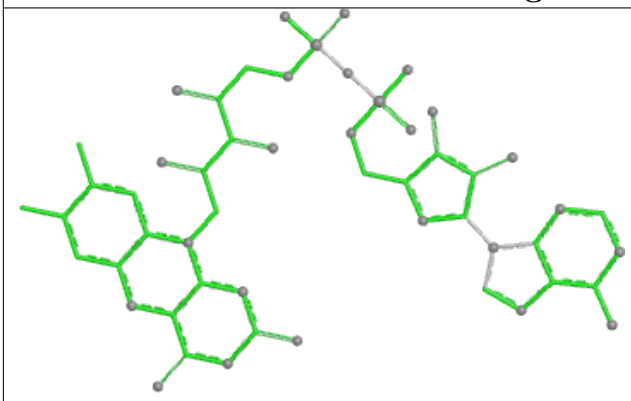

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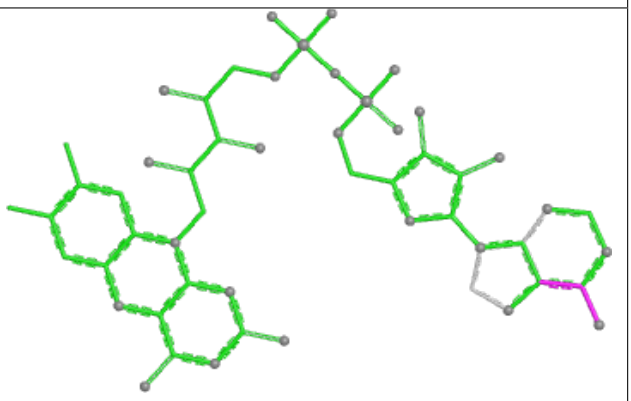
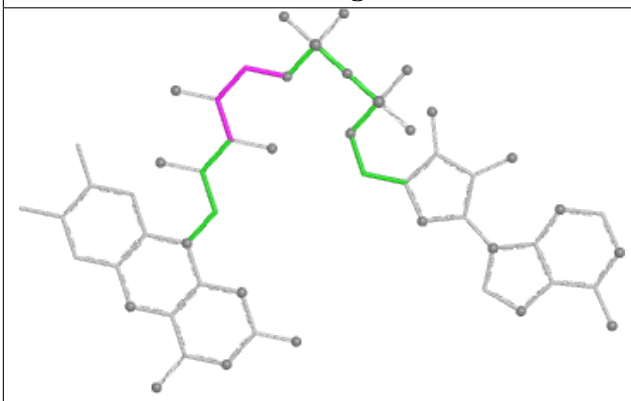


Bond angles



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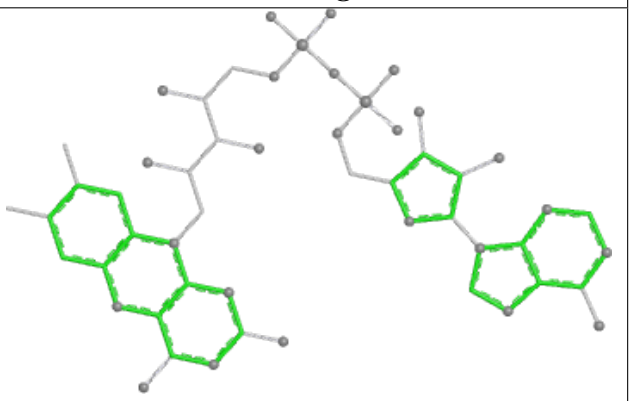
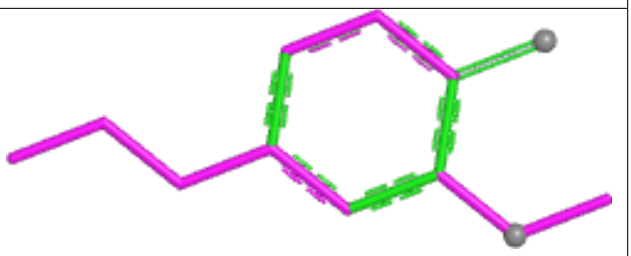


Rings

Ligand EOL C 602

Bond lengths

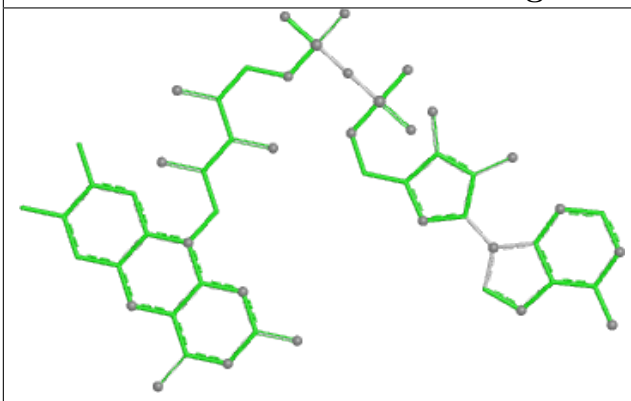


Bond angles

Torsions

Rings

Ligand FAD E 601



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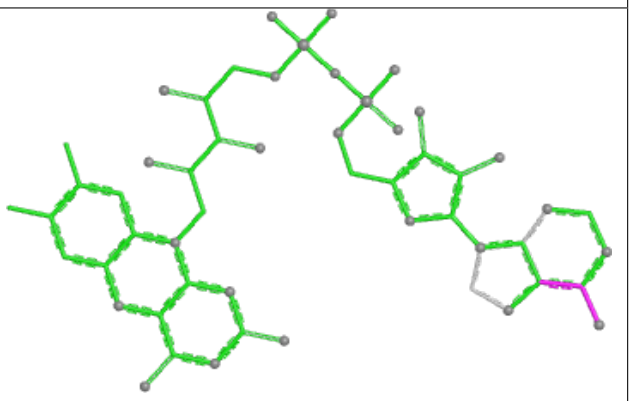

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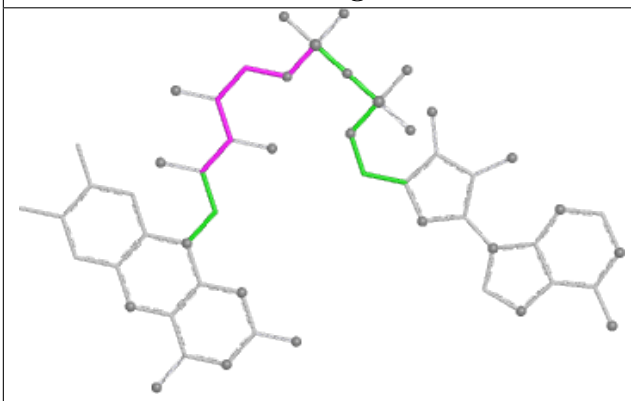

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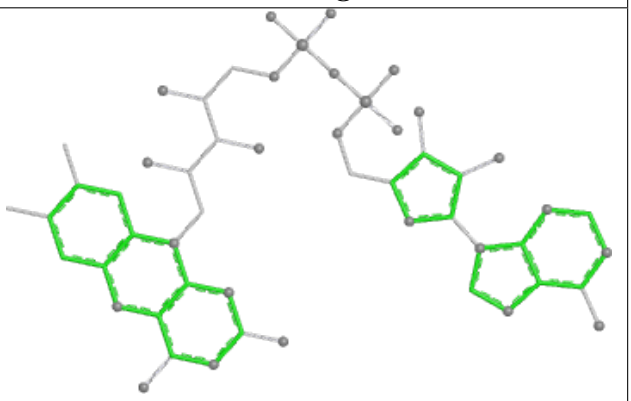
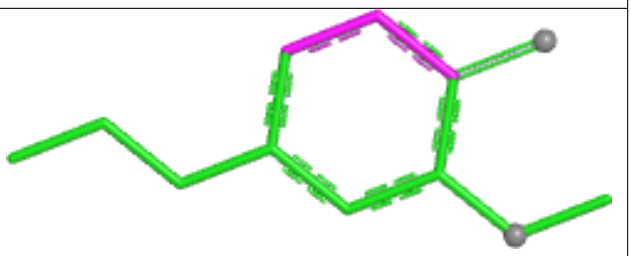


Rings

Ligand EOL A 602

Bond lengths

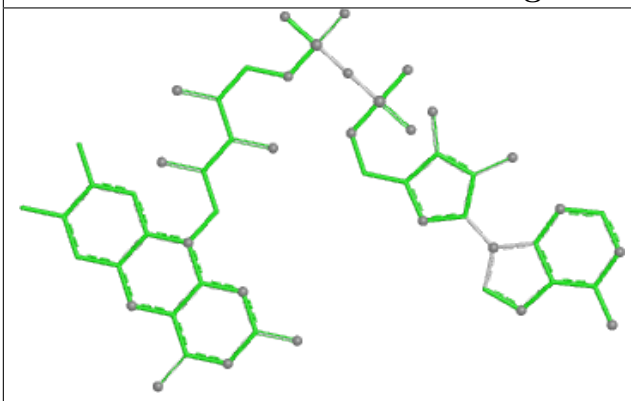


Bond angles

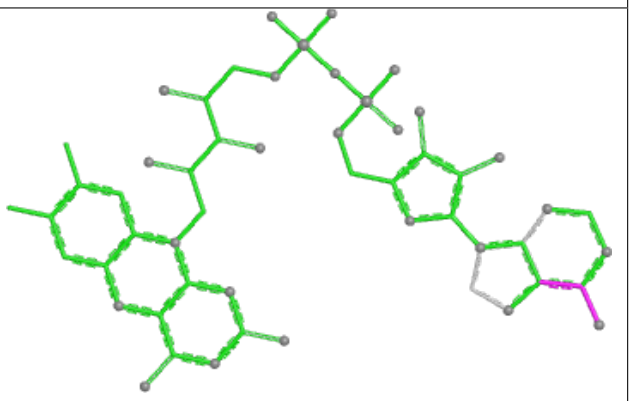
Torsions

Rings

Ligand FAD H 600



Bond lengths



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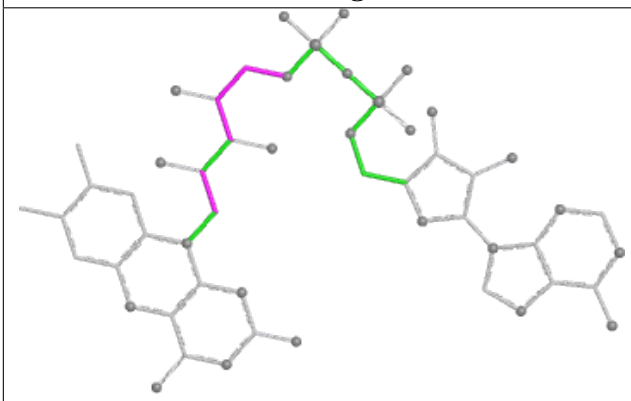

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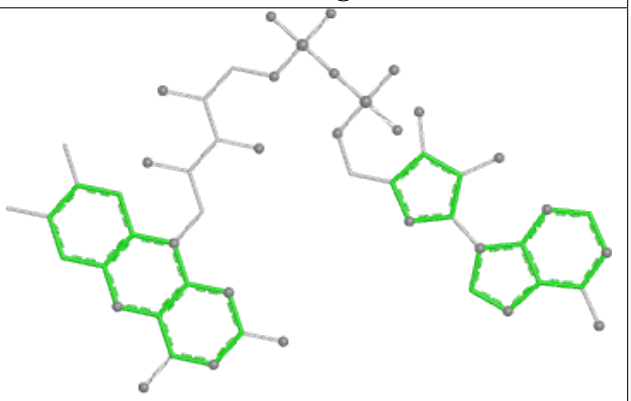
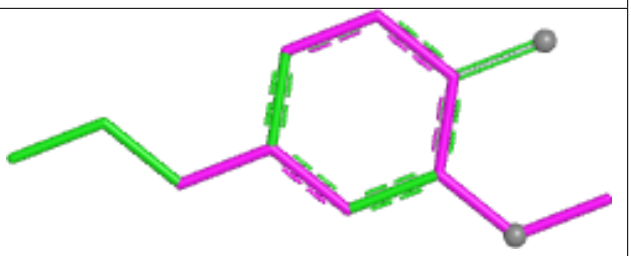


Rings

Ligand EOL E 602

Bond lengths

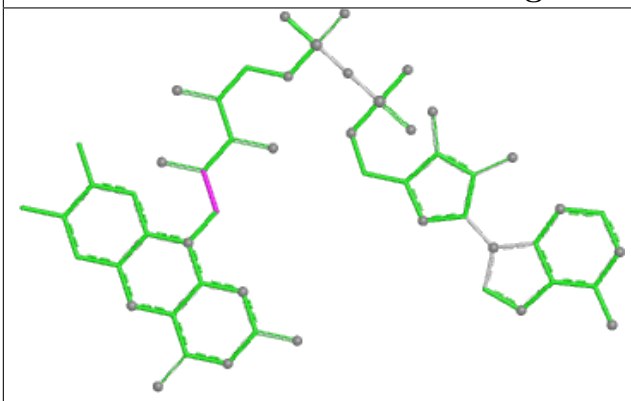


Bond angles

Torsions

Rings

Ligand FAD C 601



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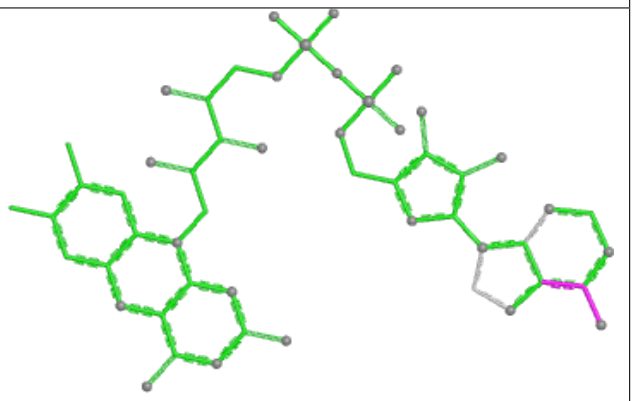

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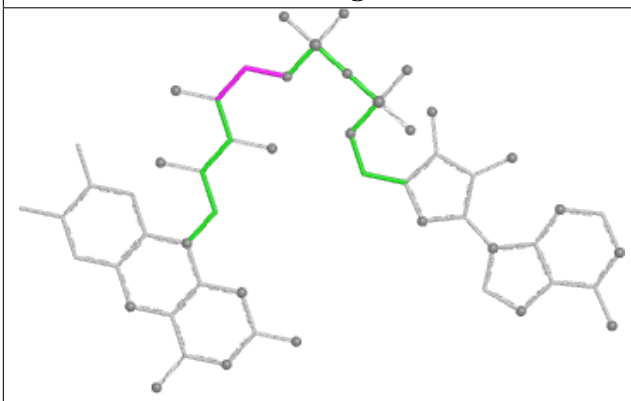

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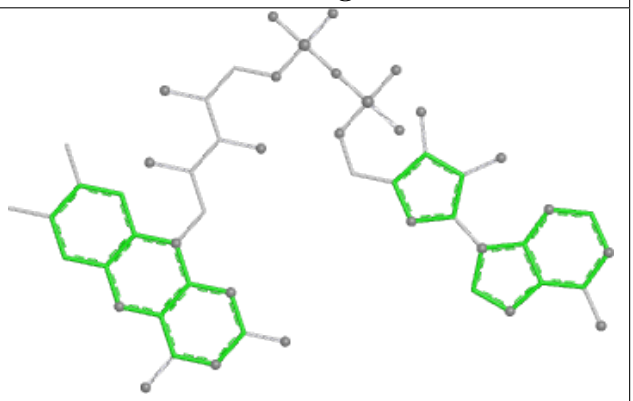
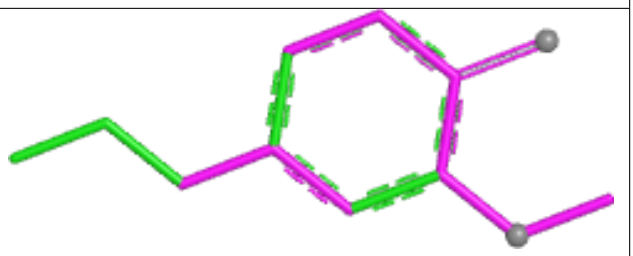


Rings

Ligand EOL D 602

Bond lengths



Bond angles

Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	525/526 (99%)	0.66	19 (3%)	42	42	32, 45, 67, 94	0
1	B	525/526 (99%)	0.66	18 (3%)	45	44	35, 48, 70, 112	0
1	C	524/526 (99%)	0.66	18 (3%)	45	44	35, 50, 75, 108	0
1	D	524/526 (99%)	0.81	41 (7%)	13	11	36, 54, 76, 112	0
1	E	524/526 (99%)	0.73	31 (5%)	22	21	37, 56, 84, 111	0
1	F	524/526 (99%)	0.73	37 (7%)	16	14	43, 62, 85, 125	0
1	G	525/526 (99%)	1.23	74 (14%)	2	2	44, 70, 95, 133	0
1	H	525/526 (99%)	1.03	78 (14%)	2	2	42, 68, 98, 130	0
All	All	4196/4208 (99%)	0.81	316 (7%)	14	13	32, 56, 87, 133	0

All (316) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	297	ASP	8.5
1	G	525	ASN	7.9
1	G	76	TYR	6.7
1	H	523	GLY	6.3
1	G	9	VAL	5.7
1	F	297	ASP	5.7
1	G	296	GLY	5.7
1	G	444	ALA	5.6
1	G	51	ALA	5.5
1	H	297	ASP	5.4
1	H	284	ALA	5.3
1	H	525	ASN	5.3
1	G	6	PRO	5.3
1	G	298	GLY	5.0
1	F	524	GLN	4.8
1	H	476	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	F	525	ASN	4.7
1	E	245	LEU	4.6
1	G	526	LEU	4.5
1	H	349	PHE	4.5
1	F	521	PHE	4.5
1	H	526	LEU	4.4
1	H	291	THR	4.4
1	F	346	GLY	4.4
1	H	421	ASP	4.3
1	G	419	ASN	4.3
1	E	21	PHE	4.3
1	D	343	LYS	4.1
1	C	297	ASP	4.1
1	G	415	ALA	4.0
1	H	302	ALA	4.0
1	G	523	GLY	4.0
1	D	523	GLY	3.9
1	C	526	LEU	3.8
1	F	523	GLY	3.8
1	F	347	ALA	3.8
1	E	384	TRP	3.8
1	B	297	ASP	3.8
1	H	303	GLU	3.7
1	G	21	PHE	3.7
1	H	314	LEU	3.7
1	H	422	TYR	3.7
1	A	12	GLU	3.7
1	H	381	LEU	3.7
1	H	47	GLY	3.7
1	G	299	PRO	3.7
1	E	294	PHE	3.6
1	H	355	ARG	3.6
1	G	311	ASP	3.6
1	G	303	GLU	3.6
1	G	347	ALA	3.6
1	G	72	ILE	3.6
1	E	361	HIS	3.6
1	F	314	LEU	3.6
1	H	316	PHE	3.6
1	H	444	ALA	3.6
1	G	345	PRO	3.5
1	G	350	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	5	LEU	3.5
1	G	101	SER	3.5
1	E	297	ASP	3.5
1	H	447	GLU	3.5
1	H	337	ILE	3.4
1	D	349	PHE	3.4
1	H	419	ASN	3.4
1	F	200	GLY	3.3
1	E	356	ASP	3.3
1	G	411	VAL	3.3
1	D	5	LEU	3.3
1	A	56	ALA	3.3
1	G	138	LEU	3.2
1	G	50	GLU	3.2
1	F	21	PHE	3.2
1	A	76	TYR	3.2
1	H	320	TYR	3.2
1	B	526	LEU	3.2
1	B	294	PHE	3.2
1	H	31	LEU	3.2
1	H	281	PHE	3.2
1	G	281	PHE	3.1
1	D	303	GLU	3.1
1	C	327	PRO	3.1
1	H	286	ALA	3.1
1	D	334	TYR	3.1
1	H	288	SER	3.1
1	C	525	ASN	3.0
1	G	31	LEU	3.0
1	F	154	TRP	3.0
1	G	18	LEU	3.0
1	G	312	LEU	3.0
1	G	15	ASP	3.0
1	D	419	ASN	3.0
1	F	349	PHE	3.0
1	F	356	ASP	3.0
1	F	419	ASN	3.0
1	G	26	GLY	3.0
1	E	353	GLU	3.0
1	D	261	MET	2.9
1	F	294	PHE	2.9
1	G	402	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	361	HIS	2.9
1	E	350	PHE	2.9
1	H	402	ARG	2.9
1	H	439	PHE	2.9
1	A	397	SER	2.8
1	F	389	GLY	2.8
1	G	39	ALA	2.8
1	G	80	LEU	2.8
1	H	252	GLU	2.8
1	H	295	ASP	2.8
1	H	350	PHE	2.8
1	G	249	ASP	2.8
1	H	296	GLY	2.8
1	H	334	TYR	2.8
1	H	298	GLY	2.8
1	H	327	PRO	2.7
1	A	208	PRO	2.7
1	A	210	GLY	2.7
1	G	13	ARG	2.7
1	D	286	ALA	2.7
1	G	59	SER	2.7
1	H	244	PHE	2.7
1	G	386	PRO	2.7
1	D	356	ASP	2.7
1	F	350	PHE	2.7
1	H	338	LYS	2.7
1	F	176	MET	2.7
1	H	339	GLU	2.6
1	H	32	SER	2.6
1	G	447	GLU	2.6
1	B	385	VAL	2.6
1	A	197	ALA	2.6
1	D	521	PHE	2.6
1	A	297	ASP	2.6
1	B	12	GLU	2.6
1	D	176	MET	2.6
1	H	201	SER	2.6
1	G	154	TRP	2.6
1	H	294	PHE	2.6
1	D	204	TRP	2.6
1	D	524	GLN	2.6
1	H	309	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	17	ALA	2.6
1	H	48	ALA	2.6
1	D	244	PHE	2.6
1	H	356	ASP	2.6
1	H	351	THR	2.6
1	G	314	LEU	2.6
1	H	384	TRP	2.6
1	D	180	GLY	2.6
1	F	526	LEU	2.5
1	G	7	PRO	2.5
1	A	298	GLY	2.5
1	F	225	GLY	2.5
1	G	35	ASP	2.5
1	G	208	PRO	2.5
1	A	523	GLY	2.5
1	G	284	ALA	2.5
1	B	384	TRP	2.5
1	E	447	GLU	2.5
1	F	331	GLU	2.5
1	D	525	ASN	2.5
1	E	293	TRP	2.5
1	G	166	VAL	2.5
1	H	325	GLY	2.5
1	H	362	VAL	2.5
1	B	14	PHE	2.5
1	H	446	PRO	2.5
1	D	11	ASP	2.5
1	A	209	TYR	2.4
1	H	46	VAL	2.4
1	C	176	MET	2.4
1	F	50	GLU	2.4
1	A	41	ARG	2.4
1	B	2	THR	2.4
1	B	261	MET	2.4
1	F	310	LYS	2.4
1	A	526	LEU	2.4
1	D	9	VAL	2.4
1	F	334	TYR	2.4
1	C	35	ASP	2.4
1	G	520	ARG	2.4
1	F	296	GLY	2.4
1	H	214	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	172	GLY	2.4
1	H	413	ASN	2.4
1	H	467	GLY	2.4
1	D	38	GLU	2.4
1	E	176	MET	2.4
1	G	189	GLU	2.4
1	H	293	TRP	2.4
1	G	476	ALA	2.4
1	H	285	ALA	2.4
1	C	5	LEU	2.4
1	C	50	GLU	2.4
1	G	517	TRP	2.4
1	F	5	LEU	2.4
1	B	396	VAL	2.3
1	B	176	MET	2.3
1	D	76	TYR	2.3
1	G	524	GLN	2.3
1	H	76	TYR	2.3
1	E	243	SER	2.3
1	F	447	GLU	2.3
1	E	225	GLY	2.3
1	D	12	GLU	2.3
1	D	231	GLY	2.3
1	A	7	PRO	2.3
1	B	207	PHE	2.3
1	A	200	GLY	2.3
1	B	75	GLU	2.3
1	C	296	GLY	2.3
1	D	340	ALA	2.3
1	F	466	ALA	2.3
1	G	16	ALA	2.3
1	G	172	GLY	2.3
1	G	134	LEU	2.3
1	H	311	ASP	2.3
1	D	350	PHE	2.3
1	E	523	GLY	2.3
1	G	10	SER	2.3
1	G	165	GLY	2.3
1	G	34	ALA	2.3
1	H	56	ALA	2.3
1	D	461	ARG	2.3
1	E	307	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	282	MET	2.3
1	D	469	GLY	2.3
1	C	94	ALA	2.3
1	E	281	PHE	2.3
1	G	178	GLN	2.3
1	G	37	LEU	2.3
1	D	166	VAL	2.2
1	E	524	GLN	2.2
1	D	177	TRP	2.2
1	H	453	LEU	2.2
1	C	6	PRO	2.2
1	F	327	PRO	2.2
1	E	242	GLN	2.2
1	A	176	MET	2.2
1	G	421	ASP	2.2
1	H	456	THR	2.2
1	E	314	LEU	2.2
1	C	7	PRO	2.2
1	E	469	GLY	2.2
1	E	385	VAL	2.2
1	F	201	SER	2.2
1	G	176	MET	2.2
1	D	232	ILE	2.2
1	A	207	PHE	2.2
1	D	80	LEU	2.2
1	D	50	GLU	2.2
1	E	525	ASN	2.2
1	E	209	TYR	2.2
1	D	233	ALA	2.2
1	D	211	PHE	2.2
1	E	299	PRO	2.2
1	C	76	TYR	2.2
1	H	361	HIS	2.2
1	H	442	ASP	2.2
1	F	245	LEU	2.2
1	G	300	MET	2.2
1	H	411	VAL	2.2
1	F	240	ALA	2.2
1	H	347	ALA	2.2
1	H	305	ILE	2.2
1	B	397	SER	2.2
1	G	32	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	15	ASP	2.1
1	E	285	ALA	2.1
1	G	17	ALA	2.1
1	G	521	PHE	2.1
1	H	40	PHE	2.1
1	H	454	GLN	2.1
1	F	336	MET	2.1
1	H	13	ARG	2.1
1	G	456	THR	2.1
1	H	248	PHE	2.1
1	F	202	ASP	2.1
1	B	444	ALA	2.1
1	E	276	VAL	2.1
1	F	257	ILE	2.1
1	G	477	LEU	2.1
1	C	36	GLU	2.1
1	H	359	GLY	2.1
1	C	203	ALA	2.1
1	G	252	GLU	2.1
1	E	397	SER	2.1
1	G	388	GLY	2.1
1	E	308	MET	2.1
1	B	41	ARG	2.1
1	D	181	LEU	2.1
1	G	52	ASN	2.1
1	A	166	VAL	2.1
1	D	30	VAL	2.1
1	G	27	ASP	2.1
1	F	452	ILE	2.1
1	H	196	GLY	2.1
1	H	396	VAL	2.0
1	D	243	SER	2.0
1	E	441	TYR	2.0
1	D	206	LEU	2.0
1	D	359	GLY	2.0
1	A	356	ASP	2.0
1	C	54	PRO	2.0
1	C	397	SER	2.0
1	G	19	GLN	2.0
1	D	31	LEU	2.0
1	E	330	ILE	2.0
1	F	38	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	354	GLU	2.0
1	H	388	GLY	2.0
1	B	430	LEU	2.0
1	H	246	ILE	2.0
1	H	452	ILE	2.0
1	H	521	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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
4	CA	B	604	1/1	0.78	0.19	52,52,52,52	0
4	CA	B	603	1/1	0.82	0.18	47,47,47,47	0
3	EOL	B	602	12/12	0.82	0.36	67,72,98,105	0
3	EOL	E	602	12/12	0.85	0.31	67,70,99,103	0
4	CA	C	603	1/1	0.86	0.24	55,55,55,55	0
3	EOL	C	602	12/12	0.87	0.34	66,71,97,103	0
2	FAD	G	600	53/53	0.89	0.19	47,59,67,70	0
2	FAD	C	601	53/53	0.90	0.19	41,48,54,58	0
3	EOL	A	602	12/12	0.90	0.30	53,56,82,93	0
2	FAD	H	600	53/53	0.91	0.17	50,61,68,75	0
2	FAD	E	601	53/53	0.91	0.17	43,48,59,62	0
2	FAD	F	600	53/53	0.92	0.17	47,55,61,66	0
2	FAD	D	601	53/53	0.92	0.18	37,49,52,56	0
4	CA	A	603	1/1	0.93	0.06	79,79,79,79	0
2	FAD	A	601	53/53	0.93	0.18	31,37,41,47	0
3	EOL	D	602	12/12	0.93	0.31	56,59,89,98	0
2	FAD	B	601	53/53	0.93	0.19	33,39,47,52	0

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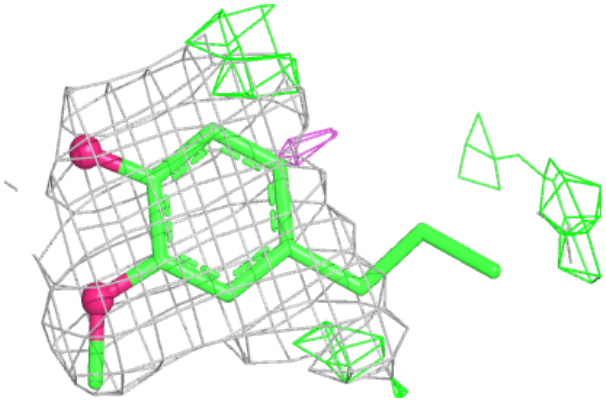
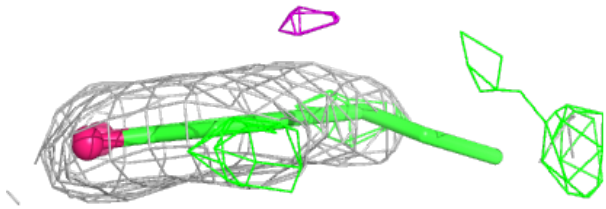
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	E	603	1/1	0.95	0.26	57,57,57,57	0

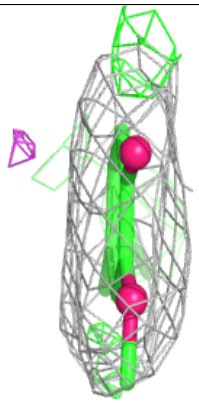
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EOL B 602:

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

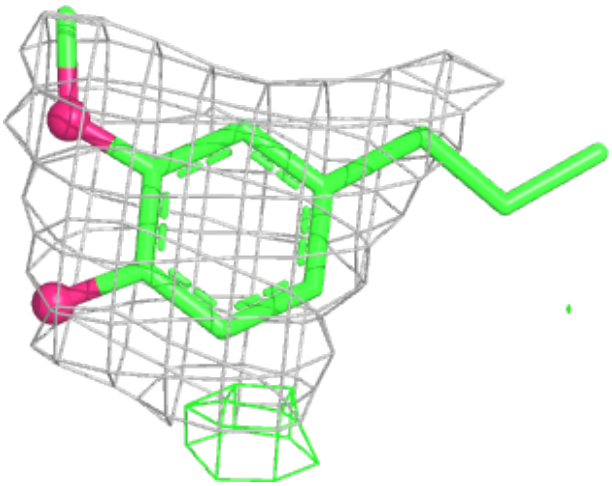


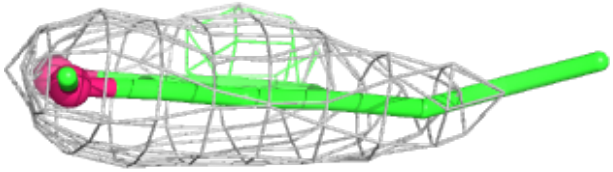


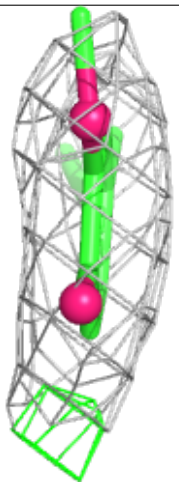


Electron density around EOL E 602:

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

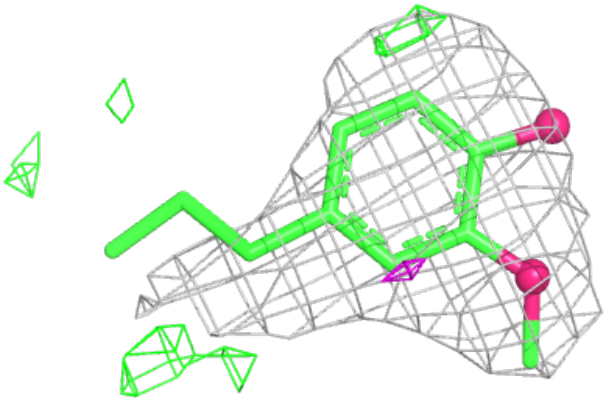


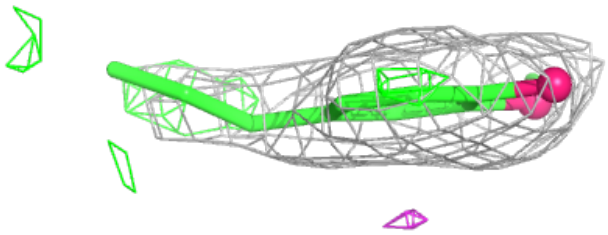


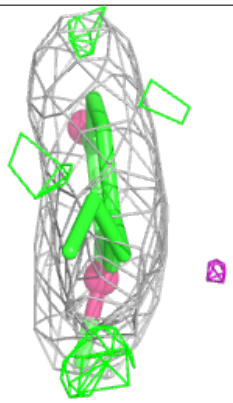


Electron density around EOL C 602:

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

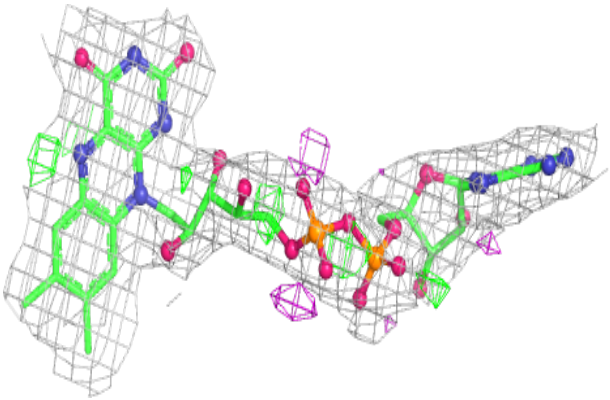


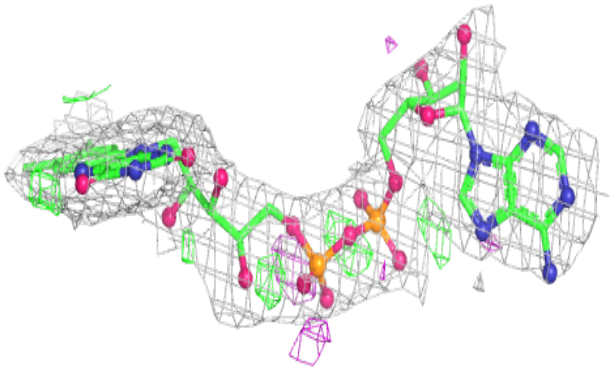


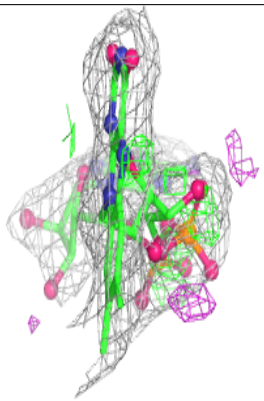


Electron density around FAD G 600:

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

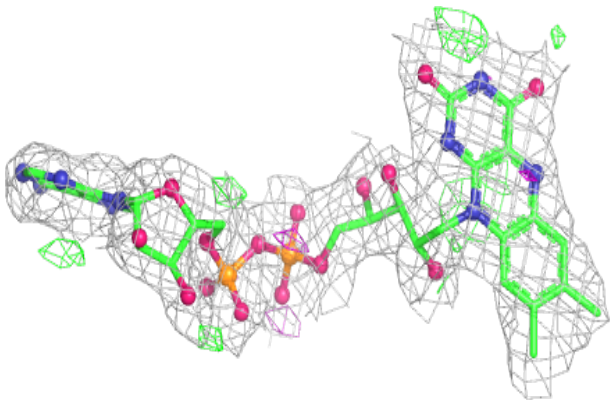


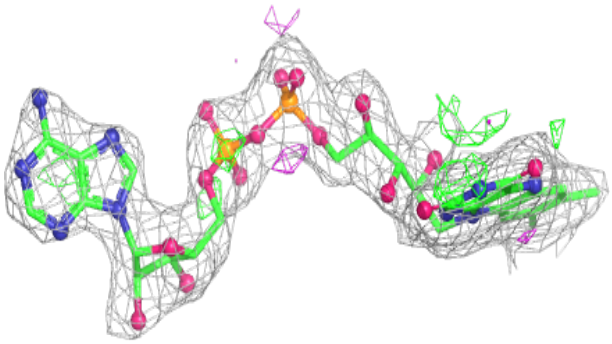


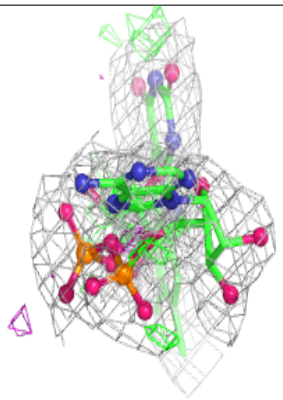


Electron density around FAD C 601:

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

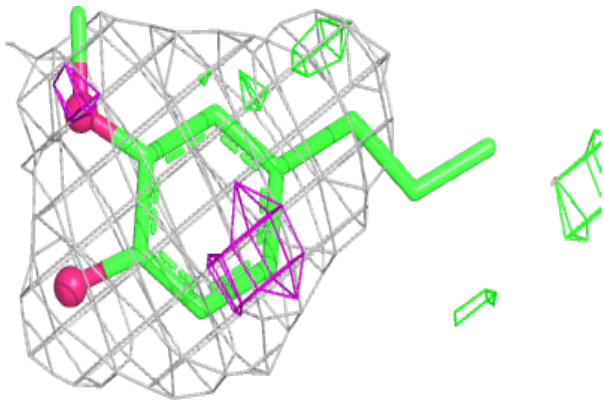


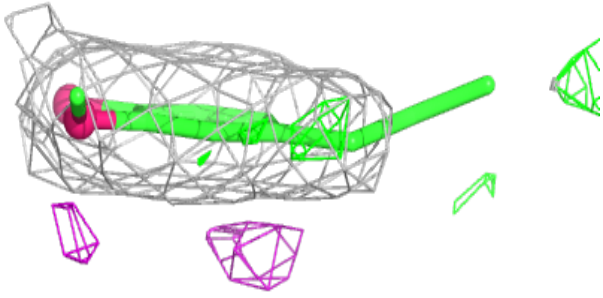


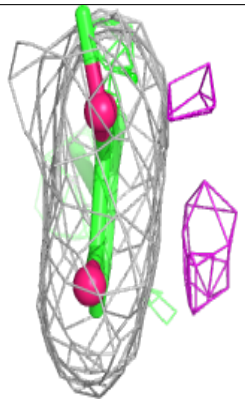


Electron density around EOL A 602:

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

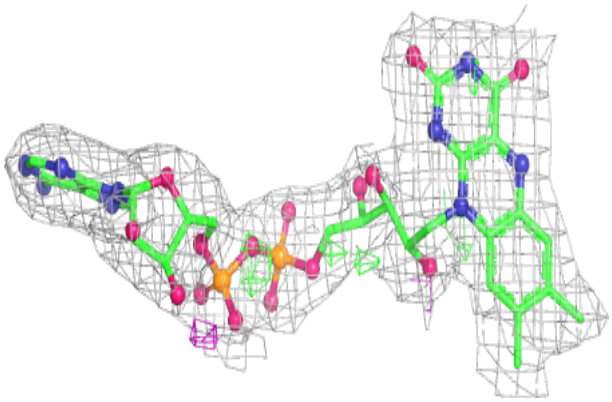


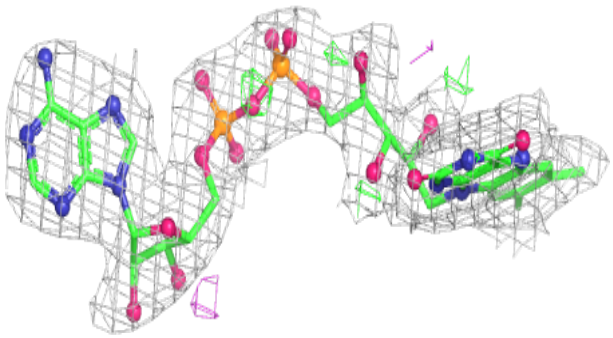


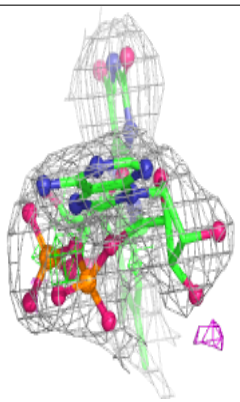


Electron density around FAD H 600:

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

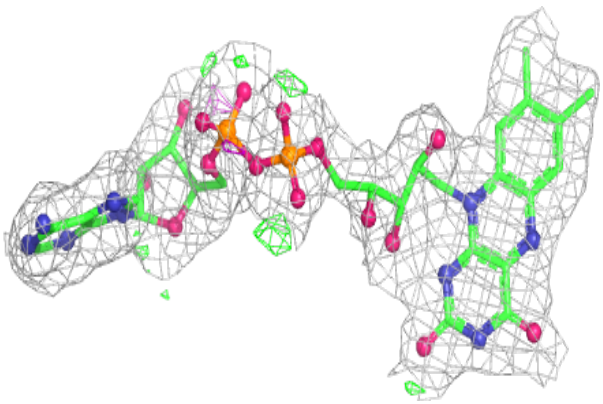


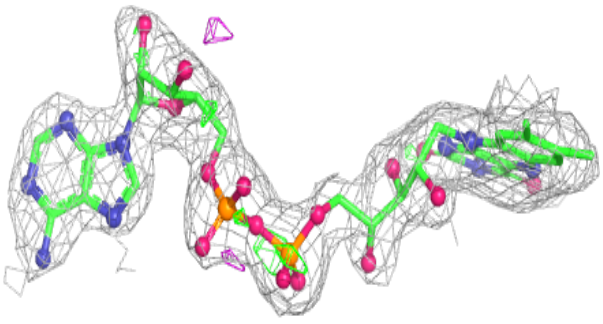


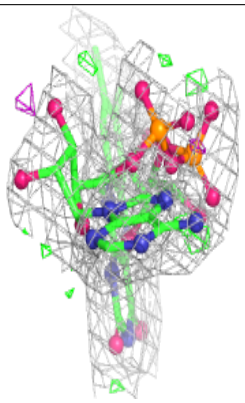


Electron density around FAD E 601:

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

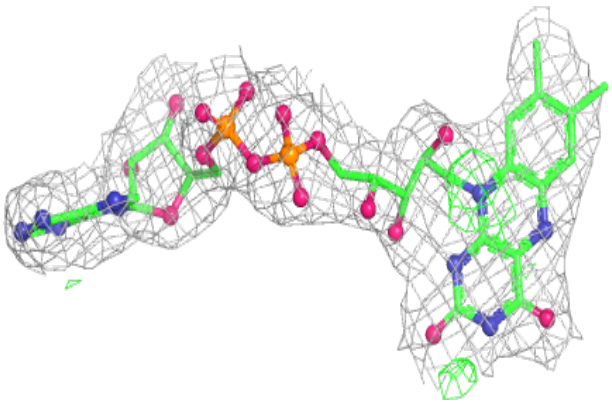


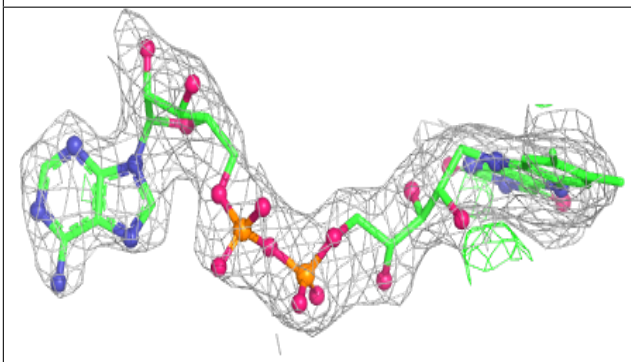


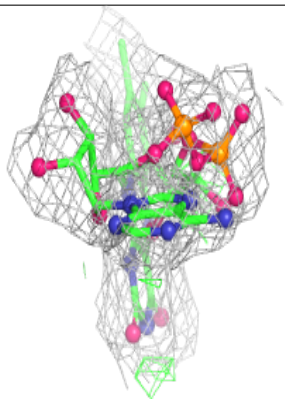


Electron density around FAD F 600:

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

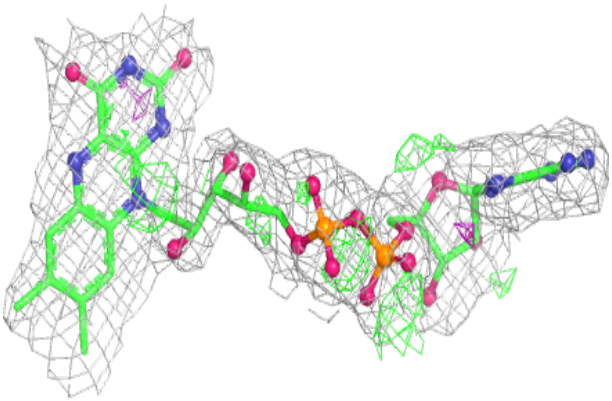


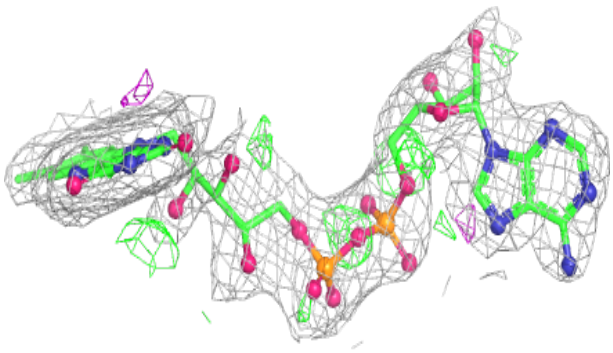


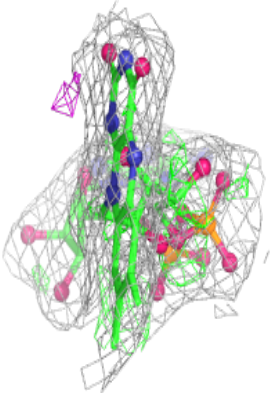


Electron density around FAD D 601:

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

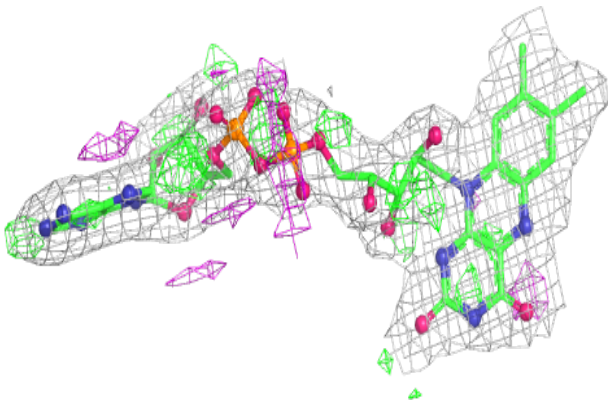


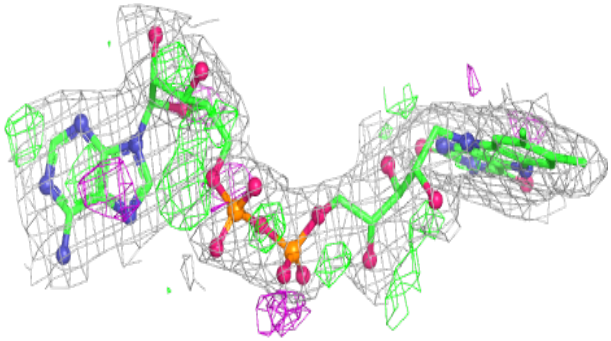


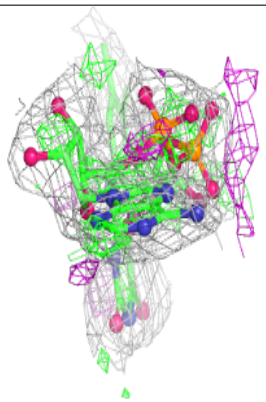


Electron density around FAD A 601:

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

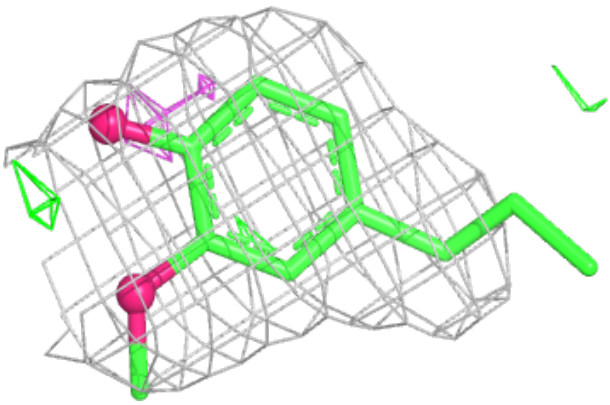


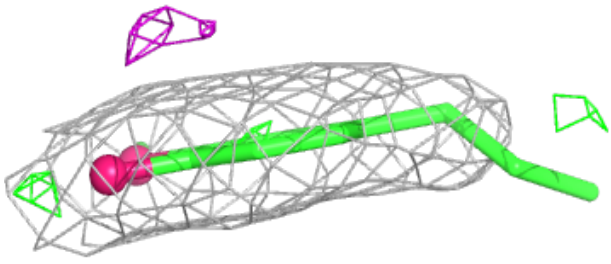


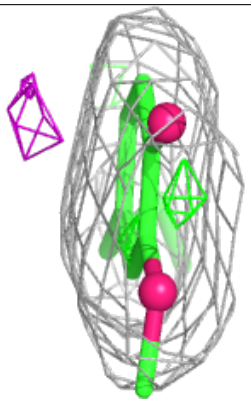


Electron density around EOL D 602:

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

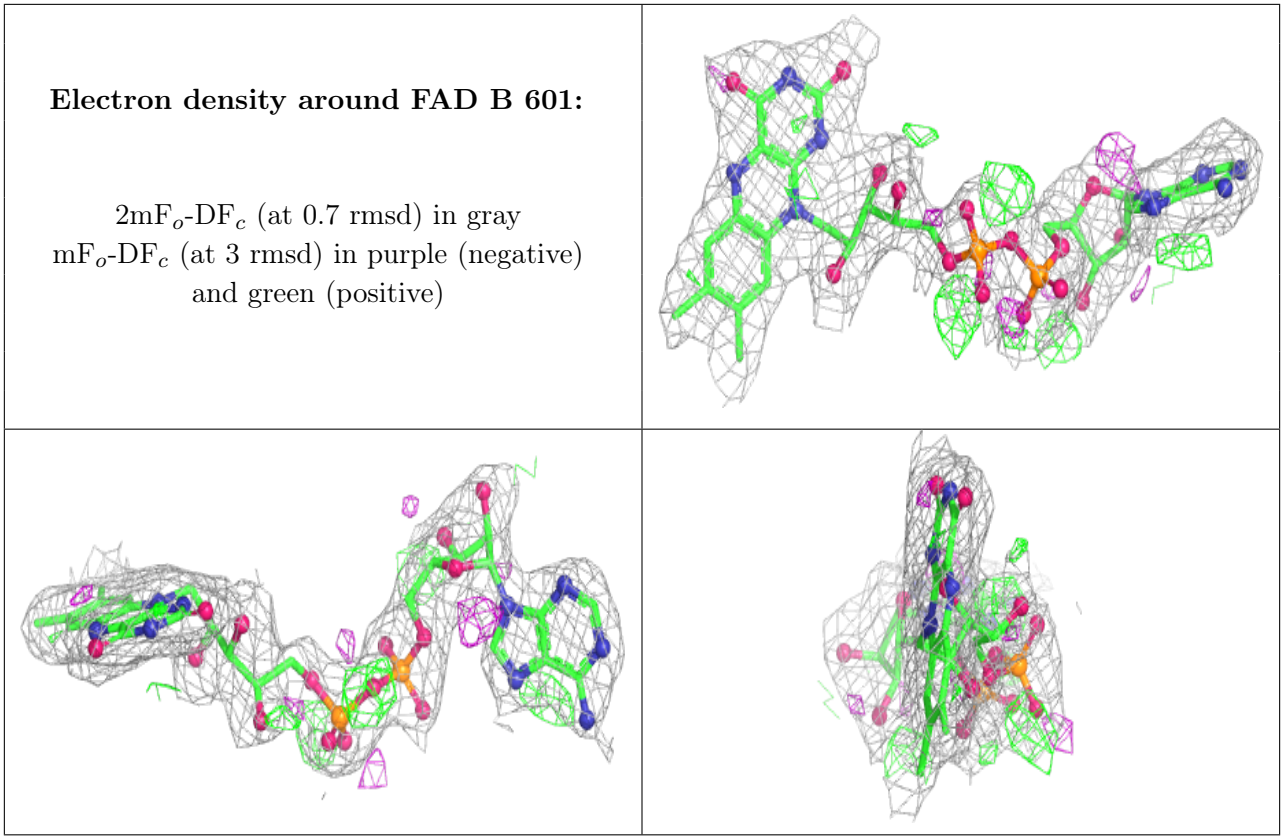






Electron density around FAD B 601:

$2mF_o$-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.