Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2022 – 04:54 pm GMT

PDB ID	:	7YWU
Title	:	Eugenol oxidase from rhodococcus jostii: mutant S81H, A423M, H434Y, S394V, I445D, S518P
Authors	:	Alvigini, L.; Mattevi, A.
Deposited on	:	2022-02-14
Resolution	:	2.80 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:

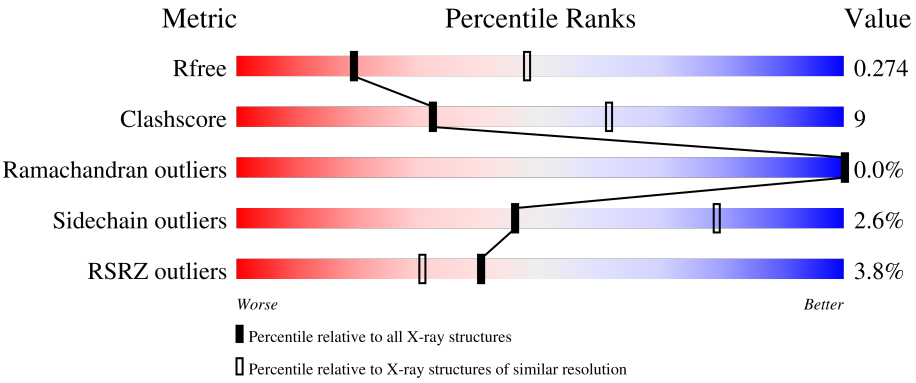
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	87% 12%
1	B	526	2% 85% 14%
1	C	526	85% 13%
1	D	526	86% 13%
1	E	526	4% 78% 20%

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Mol	Chain	Length	Quality of chain
1	F	526	6% 79% 19%
1	G	526	10% 71% 26%
1	H	526	7% 78% 20%

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
4	GOL	C	602	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 33232 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
			4125	2633	700	768	24			
1	B	525	Total	C	N	O	S	0	0	0
			4120	2629	699	768	24			
1	C	522	Total	C	N	O	S	0	0	0
			4097	2616	693	764	24			
1	D	525	Total	C	N	O	S	0	0	0
			4131	2635	701	771	24			
1	E	521	Total	C	N	O	S	0	0	0
			4075	2604	688	759	24			
1	F	524	Total	C	N	O	S	0	0	0
			4058	2593	685	756	24			
1	G	522	Total	C	N	O	S	0	0	0
			4031	2578	666	763	24			
1	H	522	Total	C	N	O	S	0	0	0
			4010	2566	664	755	25			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	HIS	SER	engineered mutation	UNP Q0SBK1
A	394	VAL	SER	engineered mutation	UNP Q0SBK1
A	423	MET	ALA	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	394	VAL	SER	engineered mutation	UNP Q0SBK1
B	423	MET	ALA	engineered mutation	UNP Q0SBK1
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

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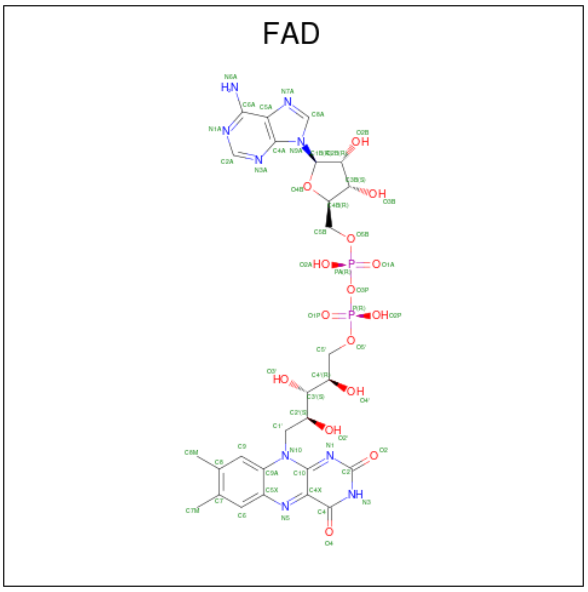
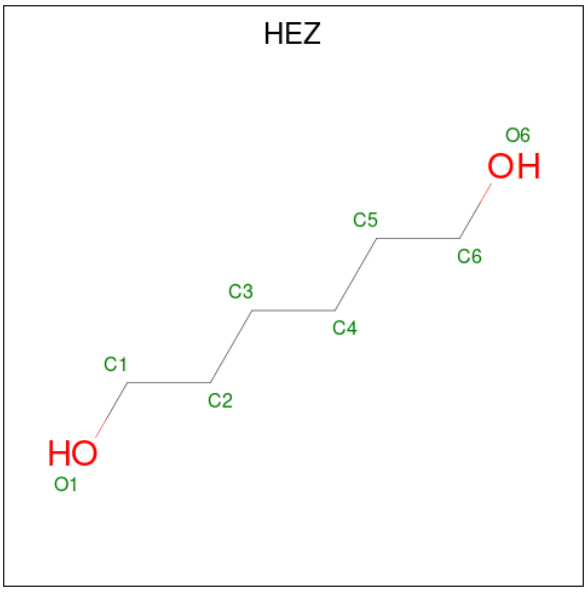
Chain	Residue	Modelled	Actual	Comment	Reference
C	394	VAL	SER	engineered mutation	UNP Q0SBK1
C	423	MET	ALA	engineered mutation	UNP Q0SBK1
C	434	TYR	HIS	engineered mutation	UNP Q0SBK1
C	445	ASP	ILE	engineered mutation	UNP Q0SBK1
C	518	PRO	SER	engineered mutation	UNP Q0SBK1
D	81	HIS	SER	engineered mutation	UNP Q0SBK1
D	394	VAL	SER	engineered mutation	UNP Q0SBK1
D	423	MET	ALA	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	394	VAL	SER	engineered mutation	UNP Q0SBK1
E	423	MET	ALA	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	394	VAL	SER	engineered mutation	UNP Q0SBK1
F	423	MET	ALA	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	394	VAL	SER	engineered mutation	UNP Q0SBK1
G	423	MET	ALA	engineered mutation	UNP Q0SBK1
G	434	TYR	HIS	engineered mutation	UNP Q0SBK1
G	445	ASP	ILE	engineered mutation	UNP Q0SBK1
G	518	PRO	SER	engineered mutation	UNP Q0SBK1
H	81	HIS	SER	engineered mutation	UNP Q0SBK1
H	394	VAL	SER	engineered mutation	UNP Q0SBK1
H	423	MET	ALA	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).



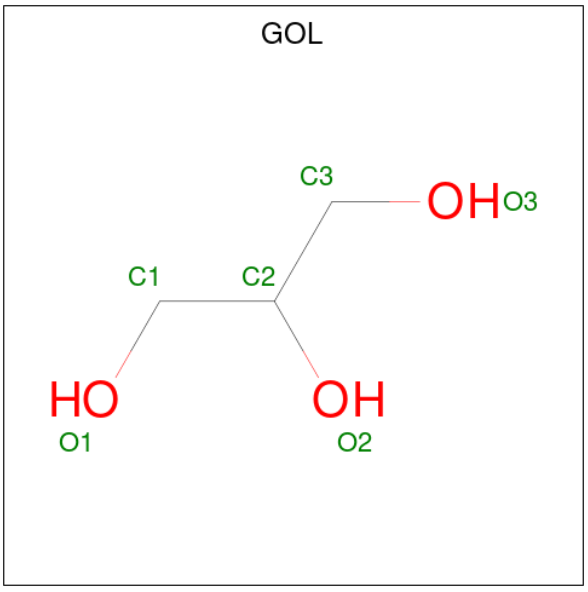
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: $C_6H_{14}O_2$).



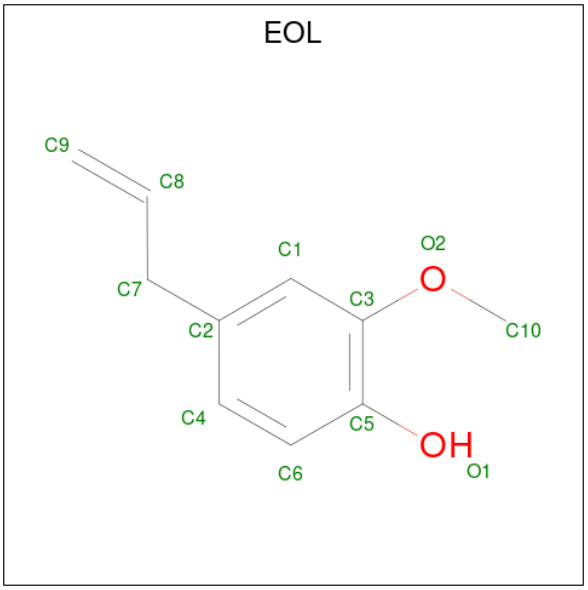
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 8 6 2	0	0
3	A	1	Total C O 8 6 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	D	1	Total C O 8 6 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



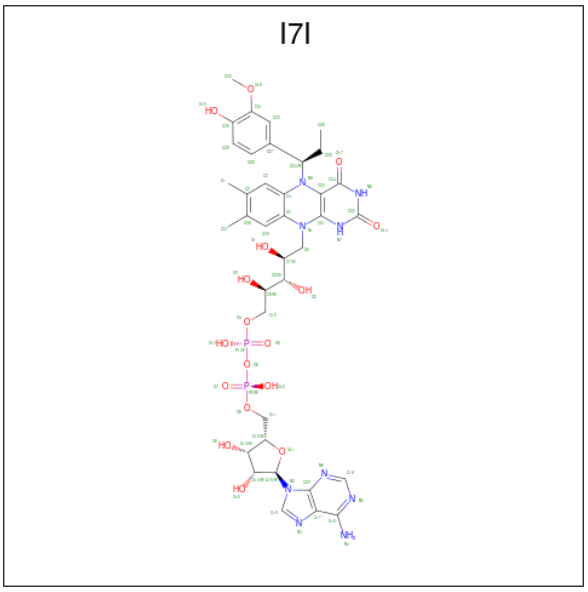
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0

- Molecule 5 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
5	A	1	Total C O 12 10 2	0	0
5	C	1	Total C O 12 10 2	0	0
5	D	1	Total C O 12 10 2	0	0
5	E	1	Total C O 12 10 2	0	0
5	G	1	Total C O 12 10 2	0	0

- Molecule 6 is [[(2 {S},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(2 {R},3 {S},4 {S})-5-[5-[(1 {R})-1-(3-methoxy-4-oxidanyl-phenyl)propyl]-7,8-dimethyl-2,4-bis(oxidanylidene)-1 {H}-benzo[g]pteridin-10-yl]-2,3,4-tris(oxidanyl)pentyl] hydrogen phosphate (three-letter code: I7I) (formula: $C_{37}H_{47}N_9O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O P 65 37 9 17 2	0	0
6	F	1	Total C N O P 65 37 9 17 2	0	0

- Molecule 7 is water.

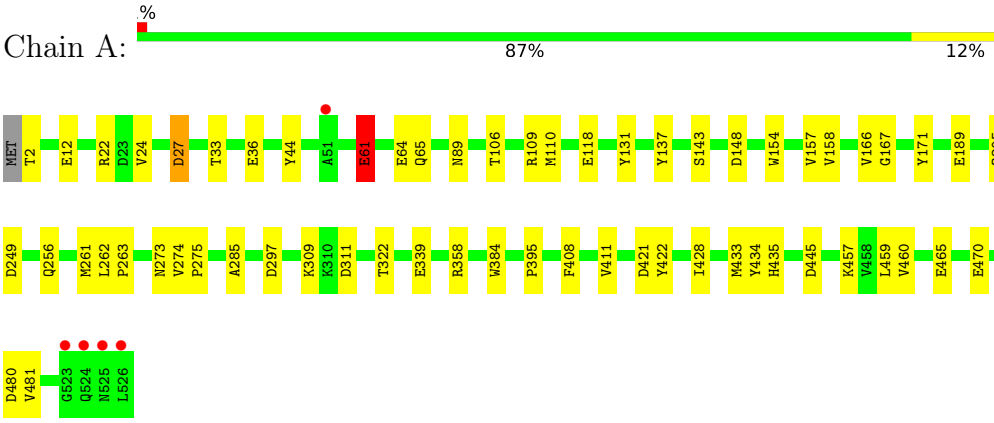
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	8	Total O 8 8	0	0
7	B	5	Total O 5 5	0	0
7	C	5	Total O 5 5	0	0
7	D	8	Total O 8 8	0	0
7	E	2	Total O 2 2	0	0
7	G	4	Total O 4 4	0	0
7	H	1	Total O 1 1	0	0

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.

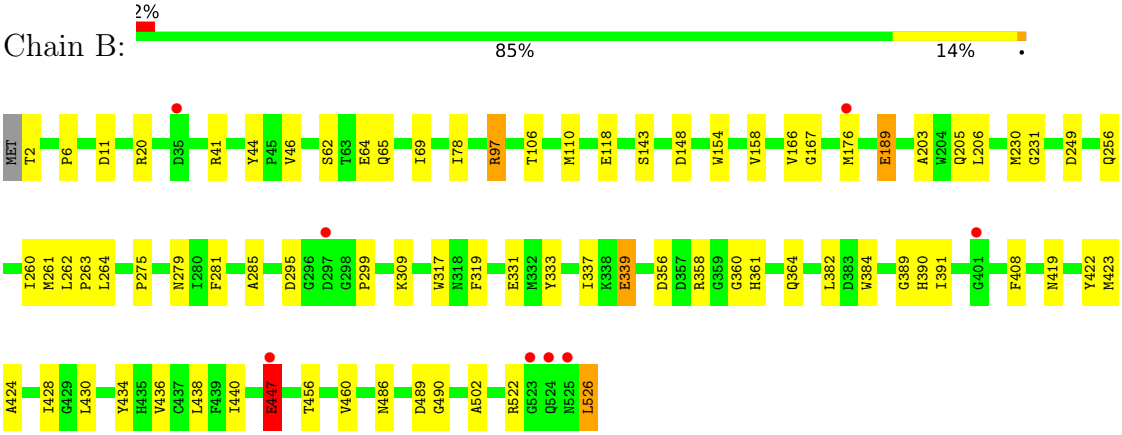
• Molecule 1: Probable vanillyl-alcohol oxidase

Chain A:



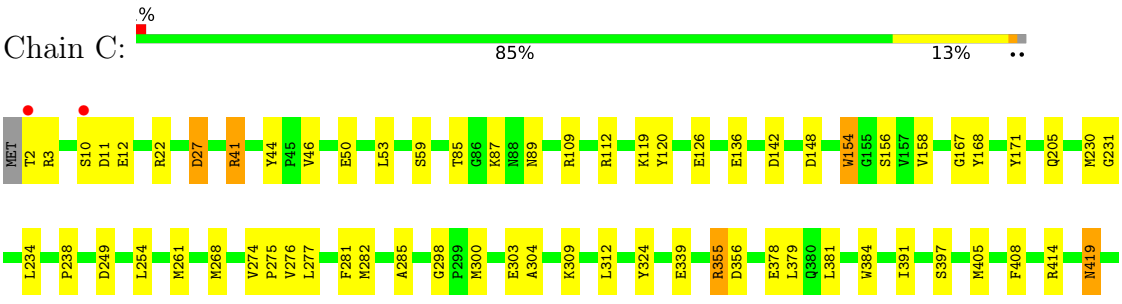
• Molecule 1: Probable vanillyl-alcohol oxidase

Chain B:

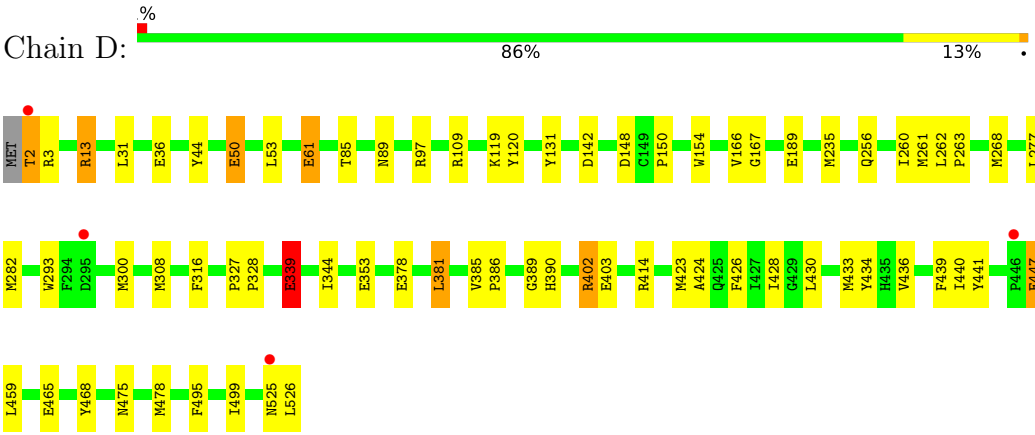


• Molecule 1: Probable vanillyl-alcohol oxidase

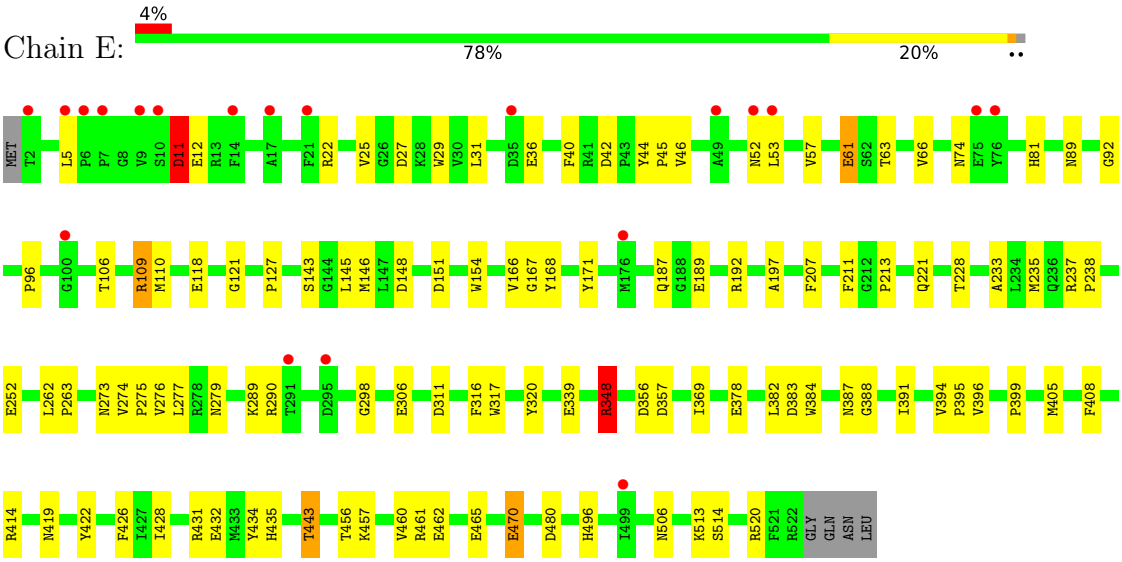
Chain C:



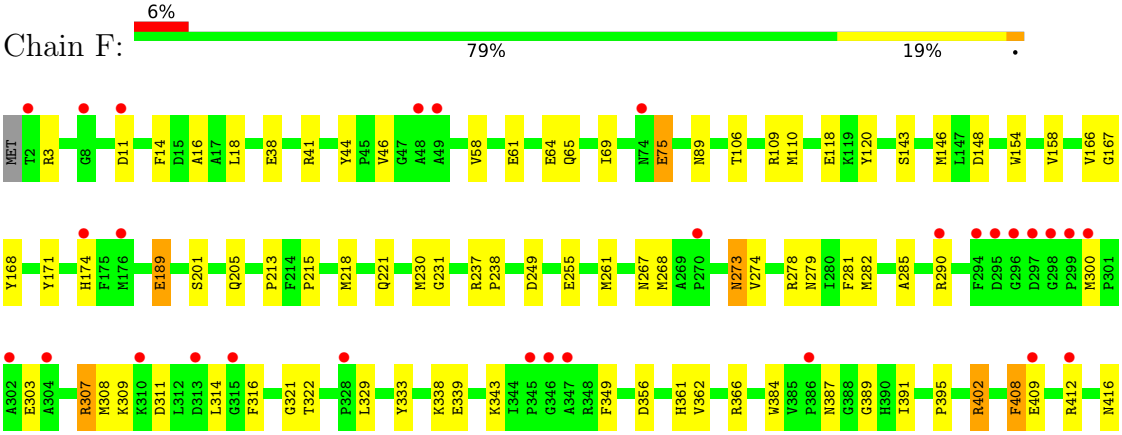
• Molecule 1: Probable vanillyl-alcohol oxidase

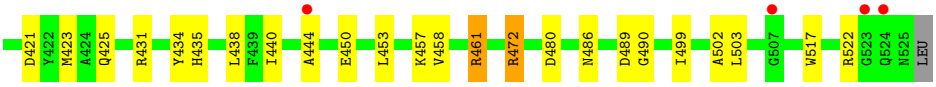


• Molecule 1: Probable vanillyl-alcohol oxidase



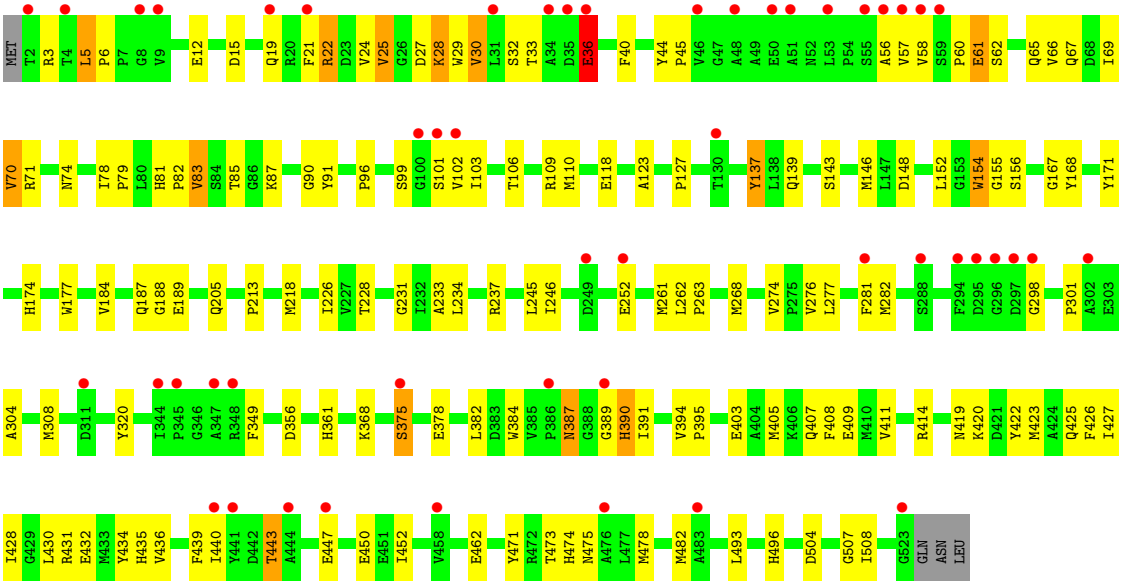
• Molecule 1: Probable vanillyl-alcohol oxidase





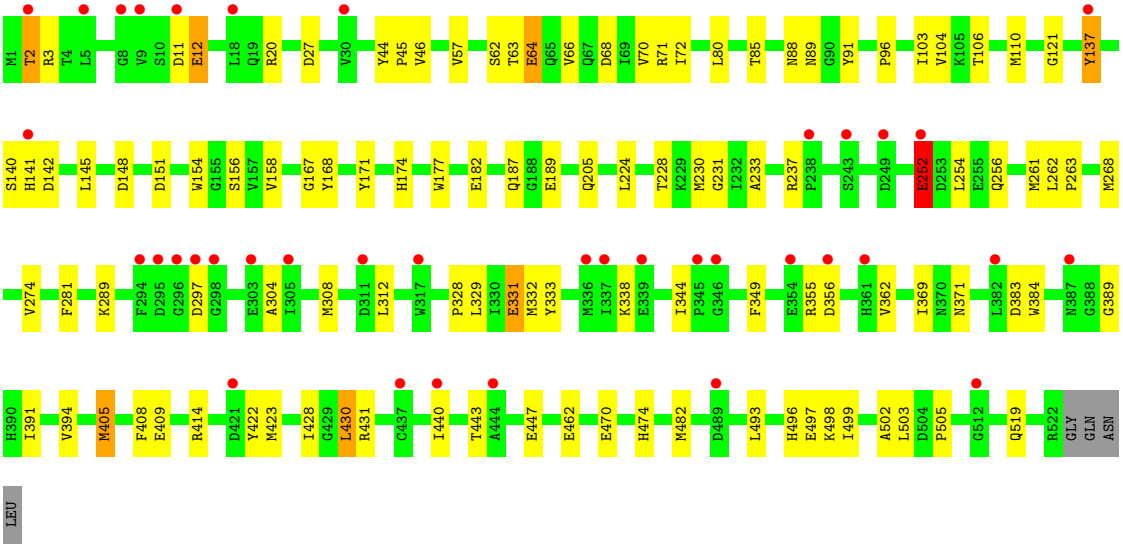
• Molecule 1: Probable vanillyl-alcohol oxidase

Chain G:



• Molecule 1: Probable vanillyl-alcohol oxidase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	149.64Å 79.43Å 189.18Å 90.00° 96.25° 90.00°	Depositor
Resolution (Å)	49.34 – 2.80 49.29 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (49.34-2.80) 97.5 (49.29-2.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.227 , 0.274 0.227 , 0.274	Depositor DCC
R_{free} test set	5453 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	50.6	Xtriage
Anisotropy	0.102	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	0.91	EDS
Total number of atoms	33232	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.39% 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: GOL, HEZ, FAD, I7I, EOL

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	0.74	3/4234 (0.1%)	0.80	4/5747 (0.1%)
1	B	0.69	1/4229 (0.0%)	0.81	5/5742 (0.1%)
1	C	0.68	1/4206 (0.0%)	0.80	3/5710 (0.1%)
1	D	0.75	7/4240 (0.2%)	0.83	6/5755 (0.1%)
1	E	0.74	4/4184 (0.1%)	0.87	9/5684 (0.2%)
1	F	0.86	4/4167 (0.1%)	0.84	6/5668 (0.1%)
1	G	0.88	5/4140 (0.1%)	0.89	6/5636 (0.1%)
1	H	0.86	7/4119 (0.2%)	0.92	9/5612 (0.2%)
All	All	0.78	32/33519 (0.1%)	0.85	48/45554 (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	D	0	1
1	F	0	2
All	All	0	3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	447	GLU	CD-OE2	28.59	1.57	1.25
1	F	409	GLU	CD-OE2	22.32	1.50	1.25
1	H	2	THR	CB-OG1	22.06	1.87	1.43
1	F	409	GLU	CD-OE1	-18.49	1.05	1.25
1	A	61	GLU	CD-OE1	-18.33	1.05	1.25
1	H	189	GLU	CD-OE2	-15.26	1.08	1.25
1	D	339	GLU	CD-OE1	13.61	1.40	1.25
1	G	36	GLU	CD-OE1	-12.79	1.11	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	306	GLU	CD-OE2	8.87	1.35	1.25
1	E	61	GLU	CD-OE1	-8.85	1.16	1.25
1	H	12	GLU	CD-OE2	8.33	1.34	1.25
1	H	331	GLU	CD-OE1	7.26	1.33	1.25
1	D	339	GLU	CG-CD	7.03	1.62	1.51
1	H	462	GLU	CD-OE2	6.68	1.32	1.25
1	F	450	GLU	CD-OE1	-6.66	1.18	1.25
1	D	189	GLU	CD-OE1	-6.61	1.18	1.25
1	H	447	GLU	CD-OE1	-6.47	1.18	1.25
1	A	465	GLU	CD-OE1	-5.80	1.19	1.25
1	D	353	GLU	CD-OE2	-5.78	1.19	1.25
1	D	353	GLU	CD-OE1	-5.76	1.19	1.25
1	G	450	GLU	CD-OE2	-5.63	1.19	1.25
1	F	189	GLU	CD-OE1	-5.62	1.19	1.25
1	A	64	GLU	CD-OE2	-5.58	1.19	1.25
1	G	409	GLU	CD-OE1	-5.58	1.19	1.25
1	E	470	GLU	CD-OE1	-5.36	1.19	1.25
1	G	450	GLU	CD-OE1	-5.29	1.19	1.25
1	H	409	GLU	CD-OE1	-5.23	1.19	1.25
1	D	447	GLU	CD-OE1	-5.18	1.20	1.25
1	E	470	GLU	CD-OE2	-5.12	1.20	1.25
1	C	470	GLU	CD-OE2	-5.10	1.20	1.25
1	D	189	GLU	CD-OE2	-5.07	1.20	1.25
1	B	189	GLU	CD-OE1	-5.05	1.20	1.25

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	339	GLU	OE1-CD-OE2	-14.00	106.50	123.30
1	G	36	GLU	OE1-CD-OE2	-12.87	107.86	123.30
1	H	189	GLU	OE1-CD-OE2	-11.96	108.95	123.30
1	D	339	GLU	OE1-CD-OE2	-11.68	109.29	123.30
1	G	447	GLU	OE1-CD-OE2	-11.12	109.96	123.30
1	F	461	ARG	CG-CD-NE	-10.08	90.64	111.80
1	H	519	GLN	OE1-CD-NE2	-9.76	99.45	121.90
1	H	519	GLN	CG-CD-NE2	8.91	138.09	116.70
1	G	22	ARG	NE-CZ-NH1	-8.88	115.86	120.30
1	H	189	GLU	CB-CG-CD	-8.78	90.50	114.20
1	E	11	ASP	CB-CA-C	7.63	125.67	110.40
1	C	41	ARG	CG-CD-NE	-7.56	95.93	111.80
1	G	36	GLU	CG-CD-OE1	7.42	133.13	118.30
1	E	348	ARG	NE-CZ-NH1	7.38	123.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	339	GLU	CG-CD-OE2	7.32	132.93	118.30
1	F	461	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	A	61	GLU	OE1-CD-OE2	-6.85	115.08	123.30
1	D	61	GLU	CB-CA-C	-6.77	96.85	110.40
1	A	64	GLU	N-CA-CB	-6.75	98.46	110.60
1	A	64	GLU	CB-CA-C	6.74	123.87	110.40
1	H	519	GLN	CB-CG-CD	-6.66	94.28	111.60
1	G	447	GLU	CB-CA-C	6.58	123.56	110.40
1	B	20	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	E	22	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	G	28	LYS	CB-CG-CD	-6.29	95.23	111.60
1	D	50	GLU	CB-CA-C	-6.12	98.17	110.40
1	H	2	THR	OG1-CB-CG2	-6.09	95.99	110.00
1	D	447	GLU	CG-CD-OE2	-6.06	106.18	118.30
1	E	348	ARG	CG-CD-NE	-6.03	99.15	111.80
1	B	97	ARG	NE-CZ-NH1	-5.89	117.36	120.30
1	H	189	GLU	CG-CD-OE2	5.82	129.94	118.30
1	H	12	GLU	OE1-CD-OE2	-5.72	116.44	123.30
1	D	13	ARG	CB-CG-CD	5.71	126.44	111.60
1	H	64	GLU	N-CA-CB	-5.67	100.40	110.60
1	D	13	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	A	339	GLU	CB-CG-CD	-5.58	99.14	114.20
1	F	461	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	C	339	GLU	CB-CA-C	-5.46	99.47	110.40
1	E	306	GLU	OE1-CD-OE2	5.40	129.78	123.30
1	B	522	ARG	NE-CZ-NH1	-5.39	117.60	120.30
1	E	189	GLU	N-CA-CB	5.29	120.13	110.60
1	F	472	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	B	447	GLU	OE1-CD-OE2	5.23	129.58	123.30
1	F	75	GLU	CG-CD-OE2	-5.20	107.91	118.30
1	F	409	GLU	CG-CD-OE2	-5.19	107.92	118.30
1	C	355	ARG	CG-CD-NE	-5.16	100.96	111.80
1	E	109	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	B	331	GLU	CB-CA-C	-5.03	100.34	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	447	GLU	Sidechain
1	F	361	HIS	Sidechain
1	F	75	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	4125	0	3995	46	1
1	B	4120	0	3982	57	1
1	C	4097	0	3963	49	4
1	D	4131	0	4001	51	0
1	E	4075	0	3930	86	3
1	F	4058	0	3875	92	0
1	G	4031	0	3825	131	1
1	H	4010	0	3792	78	0
2	A	53	0	29	2	0
2	C	53	0	30	1	0
2	D	53	0	30	3	0
2	E	53	0	29	2	0
2	G	53	0	29	1	0
2	H	53	0	29	3	0
3	A	16	0	28	3	0
3	B	8	0	14	1	0
3	D	8	0	14	0	0
4	A	6	0	8	0	0
4	C	6	0	8	5	0
5	A	12	0	11	1	0
5	C	12	0	12	0	0
5	D	12	0	11	2	0
5	E	12	0	12	1	0
5	G	12	0	12	3	0
6	B	65	0	0	3	0
6	F	65	0	0	3	0
7	A	8	0	0	1	0
7	B	5	0	0	0	0
7	C	5	0	0	0	0
7	D	8	0	0	0	0
7	E	2	0	0	0	0
7	G	4	0	0	0	0
7	H	1	0	0	1	0
All	All	33232	0	31669	573	5

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.

All (573) 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:97:ARG:HH12	1:B:526:LEU:CD1	1.25	1.48
1:H:2:THR:OG1	1:H:2:THR:CB	1.87	1.22
1:B:97:ARG:NH1	1:B:526:LEU:CD1	2.04	1.18
1:B:97:ARG:HH12	1:B:526:LEU:HD11	1.06	1.15
1:B:339:GLU:HA	1:B:339:GLU:OE1	1.58	1.04
1:B:97:ARG:HH12	1:B:526:LEU:HD13	1.19	1.02
1:E:118:GLU:OE2	1:E:143:SER:OG	1.77	1.02
1:F:402:ARG:HG2	1:F:402:ARG:HH11	1.21	1.02
1:E:61:GLU:HG2	1:E:109:ARG:HH21	1.22	1.01
1:G:44:TYR:CD1	1:G:389:GLY:HA2	1.94	1.01
1:E:61:GLU:CG	1:E:109:ARG:HH21	1.73	1.00
1:F:249:ASP:O	1:F:309:LYS:NZ	1.94	1.00
1:E:42:ASP:OD1	1:E:92:GLY:HA2	1.63	0.98
1:G:85:THR:HG23	1:G:156:SER:HB2	1.45	0.95
1:G:30:VAL:HG12	1:G:58:VAL:HG22	1.48	0.93
1:B:44:TYR:HD1	1:B:390:HIS:H	1.15	0.92
1:B:447:GLU:OE1	1:D:465:GLU:OE2	1.88	0.90
1:E:61:GLU:HG2	1:E:109:ARG:NH2	1.86	0.90
1:E:61:GLU:CG	1:E:109:ARG:NH2	2.35	0.89
1:B:97:ARG:NH1	1:B:526:LEU:HD13	1.79	0.89
1:F:3:ARG:NH1	1:F:11:ASP:OD1	2.06	0.88
1:G:44:TYR:CE1	1:G:389:GLY:HA2	2.08	0.88
1:G:74:ASN:HD21	1:G:187:GLN:HA	1.40	0.85
1:F:402:ARG:HG2	1:F:402:ARG:NH1	1.90	0.85
1:F:402:ARG:N	1:F:402:ARG:HD3	1.92	0.84
1:G:25:VAL:HG23	1:G:29:TRP:HB2	1.58	0.83
1:G:40:PHE:CD1	1:G:57:VAL:HG21	2.14	0.82
1:G:414:ARG:NH2	1:G:462:GLU:OE2	2.13	0.82
1:H:252:GLU:HA	1:H:405:MET:HE3	1.62	0.81
1:G:82:PRO:HB3	1:G:226:ILE:HD13	1.64	0.79
1:D:378:GLU:O	1:D:381:LEU:HD12	1.82	0.79
1:G:40:PHE:HE1	1:G:57:VAL:HG11	1.47	0.79
1:A:33:THR:HG22	1:A:36:GLU:OE2	1.83	0.79
1:G:40:PHE:CE1	1:G:57:VAL:HG11	2.17	0.78
1:G:44:TYR:HD1	1:G:389:GLY:HA2	1.41	0.78
1:C:234:LEU:HD23	4:C:602:GOL:H12	1.66	0.78
1:B:97:ARG:CZ	1:B:526:LEU:HD13	2.13	0.78
1:B:339:GLU:OE1	1:B:339:GLU:CA	2.32	0.78
1:G:85:THR:CG2	1:G:156:SER:HB2	2.14	0.77
1:C:298:GLY:HA2	1:C:419:ASN:OD1	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:482:MET:HG3	1:G:493:LEU:HD12	1.67	0.77
1:B:97:ARG:NH2	1:B:526:LEU:HD13	2.00	0.76
1:D:31:LEU:CD2	1:D:36:GLU:HB3	2.16	0.76
1:B:97:ARG:NH1	1:B:526:LEU:HD11	1.86	0.76
1:F:273:ASN:ND2	1:F:322:THR:H	1.84	0.76
1:A:189:GLU:HG3	7:A:706:HOH:O	1.86	0.75
1:B:97:ARG:HH22	1:B:526:LEU:HD13	1.50	0.75
1:G:22:ARG:NH1	1:G:27:ASP:O	2.20	0.74
1:E:61:GLU:HG3	1:E:109:ARG:NH2	2.02	0.74
2:G:601:FAD:H8A	2:G:601:FAD:O5B	1.87	0.74
1:A:273:ASN:OD1	1:A:274:VAL:N	2.20	0.74
1:C:22:ARG:HD3	1:C:27:ASP:CB	2.17	0.74
1:F:273:ASN:ND2	1:F:322:THR:N	2.36	0.74
1:H:3:ARG:NH2	1:H:11:ASP:OD1	2.21	0.73
1:E:457:LYS:HE3	1:E:480:ASP:OD2	1.89	0.73
1:A:22:ARG:HD3	1:A:27:ASP:HB3	1.68	0.73
1:E:106:THR:O	1:E:110:MET:HB2	1.88	0.73
1:F:402:ARG:HH11	1:F:402:ARG:CG	1.99	0.73
1:G:91:TYR:CE1	5:G:602:EOL:H10	2.24	0.73
1:G:184:VAL:HG22	1:G:226:ILE:HB	1.70	0.73
1:G:189:GLU:N	1:G:189:GLU:OE2	2.21	0.72
1:B:447:GLU:OE2	1:D:465:GLU:HG2	1.90	0.72
1:H:137:TYR:O	1:H:137:TYR:HD1	1.73	0.71
1:E:146:MET:HE3	1:E:237:ARG:HA	1.72	0.71
1:F:273:ASN:HD22	1:F:322:THR:N	1.88	0.71
1:H:3:ARG:CZ	1:H:11:ASP:OD1	2.39	0.70
1:H:121:GLY:HA2	1:H:145:LEU:HD21	1.74	0.70
1:A:118:GLU:OE2	1:A:143:SER:OG	2.08	0.69
1:E:45:PRO:HD2	1:E:443:THR:CG2	2.22	0.69
1:F:146:MET:HE3	1:F:238:PRO:HD2	1.74	0.69
1:D:2:THR:OG1	1:D:3:ARG:N	2.20	0.69
1:G:44:TYR:HD1	1:G:389:GLY:CA	2.05	0.69
1:H:338:LYS:HA	1:H:349:PHE:CE1	2.28	0.69
1:E:29:TRP:CD1	1:E:109:ARG:NH1	2.61	0.69
1:B:447:GLU:CD	1:D:465:GLU:OE2	2.30	0.69
1:G:281:PHE:HB3	1:G:423:MET:SD	2.33	0.69
1:D:31:LEU:HD23	1:D:36:GLU:OE1	1.93	0.68
1:F:273:ASN:HD22	1:F:322:THR:H	1.41	0.68
1:E:45:PRO:HD2	1:E:443:THR:HG21	1.74	0.68
1:H:96:PRO:HD3	1:H:103:ILE:HD11	1.75	0.68
1:H:328:PRO:O	1:H:331:GLU:HB3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:408:PHE:CE2	1:H:422:TYR:HE2	2.12	0.67
1:F:282:MET:HE1	1:F:438:LEU:HD12	1.75	0.67
1:E:414:ARG:NH2	1:E:462:GLU:OE2	2.28	0.66
1:G:74:ASN:ND2	1:G:187:GLN:HA	2.10	0.66
1:G:66:VAL:HG12	1:G:184:VAL:HG21	1.77	0.66
1:H:3:ARG:NH1	1:H:11:ASP:OD2	2.27	0.66
1:E:29:TRP:CB	1:E:109:ARG:HH11	2.09	0.66
1:G:45:PRO:HD2	1:G:443:THR:CG2	2.26	0.66
1:C:87:LYS:HD2	1:C:154:TRP:CE2	2.31	0.65
1:F:61:GLU:HG2	1:F:109:ARG:CZ	2.26	0.65
1:F:338:LYS:HA	1:F:349:PHE:CE1	2.31	0.65
1:H:148:ASP:OD1	1:H:167:GLY:HA3	1.97	0.65
1:C:22:ARG:HD3	1:C:27:ASP:HB3	1.80	0.64
1:H:338:LYS:HA	1:H:349:PHE:HE1	1.61	0.64
1:E:387:ASN:O	1:E:443:THR:OG1	2.17	0.63
1:B:249:ASP:O	1:B:309:LYS:NZ	2.22	0.63
1:G:245:LEU:HD13	1:G:320:TYR:CE1	2.34	0.63
1:A:470:GLU:N	1:A:470:GLU:OE2	2.32	0.62
1:D:31:LEU:HD22	1:D:36:GLU:HB3	1.79	0.62
1:G:389:GLY:O	1:G:440:ILE:HA	1.99	0.62
1:F:273:ASN:OD1	1:F:274:VAL:N	2.33	0.62
1:F:307:ARG:O	1:F:311:ASP:HB2	1.98	0.62
1:F:329:LEU:HD11	1:F:333:TYR:CZ	2.33	0.62
2:H:600:FAD:H8A	2:H:600:FAD:O5B	1.98	0.62
1:H:44:TYR:CD1	1:H:389:GLY:HA2	2.34	0.62
1:H:224:LEU:HD23	1:H:503:LEU:HD12	1.81	0.62
1:B:118:GLU:OE2	1:B:143:SER:OG	2.11	0.62
1:A:273:ASN:HD22	1:A:322:THR:N	1.98	0.62
1:E:252:GLU:HA	1:E:405:MET:HE3	1.82	0.62
1:E:25:VAL:O	1:E:109:ARG:NH1	2.24	0.61
1:G:301:PRO:HD2	1:G:304:ALA:HB3	1.82	0.61
1:H:408:PHE:CD2	1:H:422:TYR:HE2	2.19	0.61
1:F:499:ILE:HD12	1:H:499:ILE:HG23	1.81	0.61
1:E:40:PHE:CE1	1:E:57:VAL:HG11	2.36	0.61
1:A:61:GLU:O	1:A:61:GLU:HG2	1.98	0.61
1:H:66:VAL:O	1:H:70:VAL:HG23	2.01	0.61
2:A:601:FAD:H8A	2:A:601:FAD:O5B	2.01	0.60
1:H:46:VAL:HG21	1:H:391:ILE:HD12	1.82	0.60
1:F:423:MET:SD	1:F:440:ILE:HD13	2.40	0.60
1:E:31:LEU:HD23	1:E:36:GLU:HB3	1.82	0.60
1:F:46:VAL:HG21	1:F:391:ILE:HD12	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:300:MET:CE	1:F:308:MET:CE	2.79	0.60
1:G:30:VAL:CG1	1:G:58:VAL:HG22	2.29	0.60
1:D:403:GLU:OE1	1:D:468:TYR:HE1	1.84	0.60
1:G:61:GLU:HG3	1:G:109:ARG:CZ	2.32	0.60
1:C:282:MET:CE	1:C:381:LEU:HD21	2.32	0.60
1:G:407:GLN:O	1:G:411:VAL:HG22	2.02	0.60
1:E:166:VAL:HG11	1:E:434:TYR:HE2	1.65	0.59
1:H:252:GLU:HA	1:H:405:MET:CE	2.31	0.59
1:F:300:MET:HE3	1:F:308:MET:HE3	1.84	0.59
1:F:499:ILE:HD11	1:H:503:LEU:HD11	1.84	0.59
1:G:82:PRO:HB3	1:G:226:ILE:CD1	2.31	0.59
1:A:22:ARG:HD3	1:A:27:ASP:CB	2.32	0.59
1:A:249:ASP:O	1:A:309:LYS:NZ	2.23	0.58
1:A:460:VAL:HG22	1:A:470:GLU:OE1	2.02	0.58
1:E:146:MET:HE1	1:E:238:PRO:HD2	1.85	0.58
1:G:67:GLN:HB3	1:G:71:ARG:NH2	2.18	0.58
1:B:447:GLU:CD	1:D:465:GLU:CD	2.62	0.58
1:H:68:ASP:O	1:H:72:ILE:HG12	2.03	0.58
1:E:29:TRP:CG	1:E:109:ARG:NH1	2.72	0.58
1:A:33:THR:HG22	1:A:36:GLU:CD	2.23	0.58
1:E:213:PRO:CB	1:G:218:MET:HE2	2.33	0.58
1:E:213:PRO:HB3	1:G:218:MET:HE2	1.85	0.58
1:B:148:ASP:OD1	1:B:167:GLY:HA3	2.03	0.58
1:G:282:MET:HA	1:G:423:MET:HG3	1.86	0.58
1:F:166:VAL:HG11	1:F:434:TYR:CE2	2.38	0.58
1:G:33:THR:OG1	1:G:36:GLU:HG2	2.03	0.58
1:H:329:LEU:HD21	1:H:333:TYR:CE1	2.38	0.57
1:B:356:ASP:O	1:E:357:ASP:HA	2.05	0.57
1:H:137:TYR:CD1	1:H:137:TYR:C	2.77	0.57
1:C:148:ASP:OD1	1:C:167:GLY:HA3	2.04	0.57
1:H:137:TYR:HD1	1:H:137:TYR:C	2.07	0.57
1:G:3:ARG:NH2	1:G:15:ASP:OD1	2.37	0.57
1:H:137:TYR:CE1	1:H:141:HIS:ND1	2.73	0.57
1:F:189:GLU:HA	1:F:189:GLU:OE1	2.04	0.57
1:G:139:GLN:OE1	1:G:139:GLN:HA	2.05	0.57
1:B:333:TYR:O	1:B:337:ILE:HG13	2.05	0.57
1:E:348:ARG:HG2	1:E:348:ARG:HH21	1.70	0.57
1:B:261:MET:SD	1:B:428:ILE:HG21	2.44	0.56
1:D:261:MET:C	1:D:261:MET:SD	2.84	0.56
1:F:281:PHE:HB3	1:F:423:MET:HG2	1.87	0.56
1:F:148:ASP:OD1	1:F:167:GLY:HA3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:MET:HG2	1:C:430:LEU:HD21	1.85	0.56
1:D:389:GLY:O	1:D:440:ILE:HA	2.05	0.56
1:D:403:GLU:OE1	1:D:468:TYR:CE1	2.58	0.56
1:E:298:GLY:HA2	1:E:419:ASN:OD1	2.03	0.56
1:F:387:ASN:HD22	1:F:444:ALA:CB	2.18	0.56
1:G:83:VAL:HG21	1:G:103:ILE:HG23	1.88	0.56
1:H:80:LEU:HD22	1:H:104:VAL:CG2	2.36	0.56
1:H:237:ARG:NH1	1:H:371:ASN:O	2.37	0.56
1:E:348:ARG:NH2	1:E:348:ARG:CG	2.65	0.56
1:E:252:GLU:HA	1:E:405:MET:CE	2.36	0.56
1:H:2:THR:OG1	1:H:2:THR:CG2	2.52	0.56
1:F:387:ASN:HD22	1:F:444:ALA:HB2	1.71	0.56
1:G:184:VAL:CG2	1:G:226:ILE:HB	2.36	0.56
1:H:44:TYR:CE1	1:H:389:GLY:HA2	2.41	0.56
1:E:146:MET:CE	1:E:238:PRO:HD2	2.36	0.55
1:H:44:TYR:CE2	1:H:89:ASN:HB3	2.41	0.55
1:F:300:MET:HE3	1:F:308:MET:CE	2.36	0.55
1:F:408:PHE:C	1:F:408:PHE:CD2	2.79	0.55
1:A:33:THR:HG22	1:A:36:GLU:HG2	1.89	0.55
1:F:120:TYR:O	1:H:431:ARG:HD3	2.06	0.55
1:G:83:VAL:CG2	1:G:103:ILE:HG23	2.36	0.55
1:G:391:ILE:HD11	1:G:474:HIS:HB2	1.88	0.55
1:E:44:TYR:CE2	1:E:89:ASN:HB3	2.42	0.55
1:B:65:GLN:O	1:B:69:ILE:HG12	2.06	0.54
1:F:255:GLU:CD	1:F:402:ARG:HD2	2.27	0.54
1:H:20:ARG:HG3	1:H:72:ILE:HD12	1.87	0.54
1:G:277:LEU:HB3	1:G:426:PHE:HB2	1.90	0.54
1:H:312:LEU:O	1:H:355:ARG:NH2	2.41	0.54
1:F:408:PHE:HD2	1:F:408:PHE:O	1.90	0.54
1:B:489:ASP:OD2	1:F:16:ALA:CB	2.55	0.54
1:F:171:TYR:OH	1:H:431:ARG:NH2	2.40	0.54
1:F:408:PHE:C	1:F:408:PHE:HD2	2.11	0.54
1:E:211:PHE:HD2	1:G:482:MET:HE2	1.73	0.54
1:B:260:ILE:O	1:B:264:LEU:HD23	2.08	0.54
1:C:148:ASP:HB3	4:C:602:GOL:H2	1.90	0.54
1:H:384:TRP:HB3	1:H:440:ILE:HG21	1.89	0.54
1:A:61:GLU:O	1:A:61:GLU:CG	2.56	0.53
1:D:50:GLU:HB3	1:D:53:LEU:HD21	1.90	0.53
1:D:378:GLU:HG2	1:D:381:LEU:CD1	2.38	0.53
1:G:62:SER:C	1:G:110:MET:HE3	2.28	0.53
1:G:65:GLN:O	1:G:69:ILE:HG13	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:85:THR:HG23	1:G:156:SER:CB	2.29	0.53
1:C:50:GLU:HG2	1:C:53:LEU:HD21	1.89	0.53
1:G:384:TRP:HB3	1:G:440:ILE:HG21	1.90	0.53
1:B:358:ARG:HB2	1:E:356:ASP:OD2	2.08	0.53
1:E:42:ASP:OD2	1:E:44:TYR:C	2.47	0.53
1:E:46:VAL:HG21	1:E:391:ILE:HD12	1.90	0.53
1:F:309:LYS:HB3	1:F:314:LEU:O	2.08	0.53
1:D:166:VAL:HG11	1:D:434:TYR:HE2	1.73	0.53
1:G:56:ALA:HB3	1:G:102:VAL:HG22	1.90	0.53
1:E:5:LEU:HD11	1:E:11:ASP:HB2	1.89	0.53
1:F:329:LEU:HD11	1:F:333:TYR:CE2	2.44	0.53
1:H:106:THR:O	1:H:110:MET:HB2	2.08	0.53
1:F:261:MET:SD	1:F:261:MET:C	2.87	0.53
1:G:3:ARG:HG2	1:G:5:LEU:CD2	2.38	0.53
1:G:33:THR:OG1	1:G:36:GLU:CG	2.57	0.53
1:F:146:MET:HE2	1:F:237:ARG:HA	1.91	0.53
1:G:168:TYR:HA	1:G:274:VAL:HB	1.91	0.53
1:C:85:THR:HG23	1:C:156:SER:HB2	1.91	0.53
1:E:213:PRO:HD2	1:G:496:HIS:CE1	2.43	0.52
1:B:275:PRO:HB2	1:B:428:ILE:HD12	1.91	0.52
1:D:300:MET:SD	1:D:308:MET:CE	2.98	0.52
1:D:378:GLU:HG2	1:D:381:LEU:HD11	1.91	0.52
1:E:207:PHE:HE1	1:G:434:TYR:OH	1.92	0.52
1:H:158:VAL:HG22	1:H:230:MET:HB3	1.92	0.52
1:F:329:LEU:HD12	1:F:329:LEU:O	2.10	0.52
1:G:276:VAL:HA	1:G:426:PHE:O	2.10	0.52
1:H:268:MET:HG3	1:H:430:LEU:HD11	1.92	0.52
1:F:146:MET:CE	1:F:238:PRO:HD2	2.40	0.52
6:B:802:I7I:C3	6:B:802:I7I:C25	2.87	0.52
1:C:234:LEU:CD2	4:C:602:GOL:H12	2.39	0.51
1:E:262:LEU:HD13	1:E:399:PRO:HB2	1.92	0.51
1:G:70:VAL:CG1	1:G:188:GLY:HA2	2.40	0.51
1:C:171:TYR:HB3	4:C:602:GOL:H32	1.92	0.51
1:A:44:TYR:CE2	1:A:89:ASN:HB3	2.45	0.51
1:B:299:PRO:HD3	1:B:419:ASN:OD1	2.11	0.51
1:D:327:PRO:N	1:D:328:PRO:HD2	2.26	0.51
1:E:277:LEU:HB3	1:E:426:PHE:HB2	1.93	0.51
1:G:25:VAL:CG2	1:G:29:TRP:HB2	2.35	0.51
1:H:187:GLN:OE1	1:H:505:PRO:CG	2.59	0.51
1:H:63:THR:HG22	1:H:228:THR:HB	1.93	0.51
1:D:339:GLU:O	1:D:339:GLU:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:486:ASN:HA	1:F:490:GLY:HA2	1.92	0.51
1:G:44:TYR:CD1	1:G:389:GLY:CA	2.77	0.51
1:G:391:ILE:HD11	1:G:474:HIS:CB	2.41	0.51
1:H:187:GLN:OE1	1:H:505:PRO:HG2	2.11	0.51
6:F:901:I7I:C3	6:F:901:I7I:C25	2.89	0.51
1:A:148:ASP:OD1	1:A:167:GLY:HA3	2.11	0.51
1:D:148:ASP:OD2	1:D:167:GLY:HA3	2.11	0.51
1:D:495:PHE:O	1:D:499:ILE:HD12	2.11	0.51
1:E:61:GLU:HG2	1:E:109:ARG:HD2	1.93	0.51
1:F:412:ARG:HG2	1:F:416:ASN:ND2	2.26	0.51
1:H:85:THR:OG1	2:H:600:FAD:O1P	2.29	0.51
1:H:256:GLN:HB2	1:H:344:ILE:HD12	1.92	0.51
1:E:42:ASP:OD1	1:E:92:GLY:CA	2.49	0.51
1:F:44:TYR:CE2	1:F:89:ASN:HB3	2.45	0.51
1:F:38:GLU:O	1:F:41:ARG:HG2	2.11	0.50
1:A:61:GLU:HB2	1:A:109:ARG:HB3	1.93	0.50
1:C:500:LYS:HE3	1:C:518:PRO:HG3	1.92	0.50
1:G:282:MET:CA	1:G:423:MET:HG3	2.40	0.50
1:E:289:LYS:HG2	1:E:383:ASP:O	2.11	0.50
1:F:65:GLN:O	1:F:69:ILE:HG12	2.11	0.50
1:F:267:ASN:O	1:F:268:MET:HB2	2.12	0.50
1:C:281:PHE:HB3	1:C:423:MET:HG2	1.93	0.50
1:E:348:ARG:HH21	1:E:348:ARG:CG	2.24	0.50
1:H:329:LEU:HD23	1:H:329:LEU:C	2.32	0.50
1:G:218:MET:HE2	1:G:218:MET:HA	1.92	0.50
1:D:281:PHE:HB3	1:D:423:MET:HG2	1.94	0.50
1:F:517:TRP:O	1:F:522:ARG:NH1	2.44	0.50
1:G:91:TYR:CE1	5:G:602:EOL:C10	2.95	0.50
1:G:154:TRP:HD1	1:G:155:GLY:N	2.10	0.50
1:G:427:ILE:HB	1:G:434:TYR:HB2	1.93	0.50
1:A:358:ARG:HD3	1:F:356:ASP:CB	2.42	0.49
1:D:31:LEU:CD2	1:D:36:GLU:CB	2.88	0.49
1:D:414:ARG:HE	1:D:458:VAL:HG11	1.77	0.49
1:B:166:VAL:HG11	1:B:434:TYR:HE2	1.76	0.49
1:D:277:LEU:HB3	1:D:426:PHE:HB2	1.94	0.49
1:D:300:MET:SD	1:D:308:MET:HE2	2.52	0.49
1:F:290:ARG:NH1	1:F:421:ASP:OD2	2.45	0.49
1:A:61:GLU:HB2	1:A:109:ARG:CB	2.43	0.49
1:C:22:ARG:HD3	1:C:27:ASP:HB2	1.91	0.49
1:G:246:ILE:HG12	1:G:349:PHE:CD2	2.47	0.49
1:B:275:PRO:HB3	1:B:319:PHE:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:81:HIS:HB2	1:G:96:PRO:HB3	1.95	0.49
1:H:71:ARG:CB	7:H:701:HOH:O	2.60	0.49
1:H:482:MET:HG3	1:H:493:LEU:HD12	1.94	0.49
1:B:489:ASP:OD2	1:F:16:ALA:HB1	2.12	0.49
1:E:348:ARG:HG2	1:E:348:ARG:NH2	2.27	0.49
1:G:44:TYR:OH	1:G:382:LEU:HG	2.13	0.49
1:H:62:SER:O	1:H:66:VAL:HG23	2.12	0.49
1:E:168:TYR:HA	1:E:274:VAL:HB	1.94	0.49
1:E:207:PHE:CE1	1:G:434:TYR:OH	2.66	0.49
6:F:901:I7I:C28	6:F:901:I7I:C34	2.91	0.49
1:C:3:ARG:NH1	1:C:11:ASP:OD1	2.35	0.48
1:D:402:ARG:HD3	1:D:402:ARG:N	2.28	0.48
1:E:121:GLY:HA2	1:E:145:LEU:HD11	1.95	0.48
1:E:279:ASN:HB3	1:E:317:TRP:CZ3	2.48	0.48
1:F:300:MET:CE	1:F:308:MET:HE1	2.42	0.48
1:G:137:TYR:CD1	1:G:137:TYR:C	2.86	0.48
1:G:420:LYS:HE2	1:G:452:ILE:HG12	1.95	0.48
1:H:151:ASP:HA	1:H:369:ILE:HD12	1.94	0.48
1:D:44:TYR:CE2	1:D:89:ASN:HB3	2.48	0.48
1:E:148:ASP:OD1	1:E:167:GLY:HA3	2.14	0.48
1:F:14:PHE:CZ	1:F:18:LEU:HD21	2.48	0.48
1:B:189:GLU:OE1	1:B:189:GLU:HA	2.12	0.48
1:D:61:GLU:HG2	1:D:109:ARG:CZ	2.44	0.48
1:F:64:GLU:OE1	1:F:64:GLU:HA	2.12	0.48
1:G:60:PRO:HB3	1:G:69:ILE:HD12	1.95	0.48
1:G:87:LYS:HG2	1:G:154:TRP:CD1	2.48	0.48
1:H:261:MET:SD	1:H:428:ILE:HG21	2.53	0.48
1:C:168:TYR:HA	1:C:274:VAL:HB	1.96	0.48
1:G:148:ASP:OD1	1:G:174:HIS:NE2	2.39	0.48
1:D:424:ALA:HA	1:D:436:VAL:O	2.14	0.48
1:E:408:PHE:CD1	1:E:422:TYR:HE2	2.32	0.48
1:F:58:VAL:HG11	1:F:69:ILE:HD12	1.95	0.48
1:G:390:HIS:HA	1:G:439:PHE:O	2.14	0.48
1:E:290:ARG:HG3	1:E:384:TRP:CZ2	2.49	0.48
1:G:123:ALA:HB2	1:G:234:LEU:HD11	1.96	0.48
1:F:273:ASN:OD1	1:F:273:ASN:C	2.51	0.47
1:A:33:THR:HG22	1:A:36:GLU:CG	2.43	0.47
1:B:502:ALA:HB2	1:C:502:ALA:HB2	1.96	0.47
1:A:285:ALA:HA	1:A:384:TRP:CE3	2.49	0.47
1:F:221:GLN:NE2	1:F:472:ARG:HB3	2.29	0.47
1:H:289:LYS:HG2	1:H:383:ASP:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:ASN:HA	1:B:490:GLY:HA2	1.95	0.47
1:D:31:LEU:HD21	1:D:36:GLU:HB3	1.93	0.47
1:E:207:PHE:HD1	1:G:432:GLU:OE1	1.96	0.47
1:G:62:SER:O	1:G:110:MET:HE3	2.15	0.47
1:G:78:ILE:O	1:G:508:ILE:HD12	2.14	0.47
1:B:358:ARG:HD3	1:E:356:ASP:OD2	2.14	0.47
1:C:300:MET:HG2	1:C:304:ALA:HB3	1.97	0.47
1:E:262:LEU:HB3	1:E:263:PRO:HD3	1.97	0.47
1:B:97:ARG:CZ	1:B:526:LEU:CD1	2.80	0.47
1:B:176:MET:O	3:B:801:HEZ:H51	2.15	0.47
1:E:221:GLN:HA	1:E:513:LYS:HE2	1.97	0.47
1:G:45:PRO:HD2	1:G:443:THR:HG23	1.95	0.47
1:G:382:LEU:N	1:G:382:LEU:HD22	2.30	0.47
1:H:63:THR:HG21	1:H:182:GLU:OE1	2.14	0.47
1:H:261:MET:SD	1:H:261:MET:C	2.93	0.47
1:D:261:MET:SD	1:D:428:ILE:HG21	2.55	0.47
1:E:396:VAL:HG12	1:E:434:TYR:CD1	2.50	0.47
1:A:158:VAL:HG22	1:A:230:MET:HB3	1.96	0.47
1:C:112:ARG:HG2	1:C:126:GLU:OE1	2.15	0.47
1:G:24:VAL:HG12	1:G:25:VAL:HG12	1.96	0.47
1:G:58:VAL:HG11	1:G:69:ILE:HD13	1.96	0.47
6:B:802:I7I:C16	6:B:802:I7I:C12	2.93	0.46
1:F:213:PRO:HB2	1:H:496:HIS:CE1	2.49	0.46
1:A:273:ASN:HD22	1:A:322:THR:H	1.60	0.46
1:E:45:PRO:HD2	1:E:443:THR:HG22	1.96	0.46
1:B:203:ALA:HA	1:B:206:LEU:HD12	1.96	0.46
1:G:148:ASP:OD1	1:G:167:GLY:HA3	2.15	0.46
1:G:432:GLU:O	1:G:432:GLU:HG3	2.16	0.46
1:D:390:HIS:HA	1:D:439:PHE:O	2.15	0.46
1:F:118:GLU:OE2	1:F:143:SER:OG	2.27	0.46
1:G:67:GLN:HB3	1:G:71:ARG:HH21	1.80	0.46
1:G:252:GLU:HA	1:G:405:MET:CE	2.45	0.46
1:G:368:LYS:NZ	1:G:375:SER:HB2	2.30	0.46
1:B:408:PHE:CE1	1:B:422:TYR:HE2	2.34	0.46
1:G:127:PRO:HD3	1:G:228:THR:O	2.15	0.46
1:C:261:MET:SD	1:C:261:MET:C	2.95	0.46
2:D:601:FAD:H8A	2:D:601:FAD:O5B	2.16	0.46
1:E:171:TYR:CE1	1:E:235:MET:HB2	2.51	0.46
1:D:97:ARG:HH12	1:D:526:LEU:HD11	1.80	0.46
1:D:414:ARG:HB2	1:D:459:LEU:HD21	1.98	0.46
6:F:901:I7I:C16	6:F:901:I7I:C12	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:21:PHE:HB3	1:G:30:VAL:HG11	1.97	0.46
1:G:29:TRP:CD1	1:G:109:ARG:CZ	2.99	0.46
1:G:282:MET:N	1:G:423:MET:HG3	2.31	0.46
1:A:22:ARG:CD	1:A:27:ASP:HB3	2.41	0.45
1:E:127:PRO:HD3	1:E:228:THR:O	2.16	0.45
1:A:261:MET:SD	1:A:261:MET:C	2.94	0.45
3:A:602:HEZ:H11	1:D:235:MET:HG3	1.98	0.45
1:C:275:PRO:HB2	1:C:428:ILE:HD12	1.97	0.45
1:G:395:PRO:HD2	1:G:435:HIS:O	2.16	0.45
1:A:408:PHE:CD1	1:A:422:TYR:HE2	2.34	0.45
1:C:158:VAL:HG22	1:C:230:MET:HB3	1.99	0.45
1:E:395:PRO:HD2	1:E:435:HIS:O	2.16	0.45
2:D:601:FAD:C6	5:D:603:EOL:H7	2.47	0.45
1:F:453:LEU:O	1:F:457:LYS:HB2	2.15	0.45
1:G:408:PHE:CD1	1:G:422:TYR:HE2	2.35	0.45
1:B:360:GLY:O	1:B:364:GLN:HG2	2.16	0.45
1:F:300:MET:CE	1:F:308:MET:HE3	2.43	0.45
1:G:504:ASP:OD2	1:G:507:GLY:N	2.49	0.45
1:G:6:PRO:HG2	1:G:78:ILE:CD1	2.47	0.45
1:H:205:GLN:HG3	1:H:231:GLY:HA3	1.98	0.45
1:E:461:ARG:NH1	1:E:465:GLU:OE2	2.48	0.45
1:G:70:VAL:HG11	1:G:188:GLY:HA2	1.99	0.45
1:F:300:MET:HB3	1:F:300:MET:HE2	1.49	0.45
1:G:261:MET:SD	1:G:261:MET:C	2.95	0.45
1:G:408:PHE:CE1	1:G:422:TYR:HE2	2.35	0.45
1:H:44:TYR:HE2	1:H:89:ASN:HB3	1.81	0.45
1:B:106:THR:O	1:B:110:MET:HB2	2.17	0.44
1:E:52:ASN:HB3	1:E:96:PRO:O	2.16	0.44
1:B:279:ASN:HB3	1:B:317:TRP:CZ3	2.51	0.44
1:C:378:GLU:O	1:C:381:LEU:HB2	2.17	0.44
1:D:475:ASN:HA	1:D:478:MET:HE3	2.00	0.44
1:F:303:GLU:O	1:F:307:ARG:HG2	2.17	0.44
1:A:473:THR:HG21	1:A:481:VAL:HG21	1.99	0.44
1:E:277:LEU:HD11	1:E:317:TRP:HB3	1.99	0.44
1:F:166:VAL:HG11	1:F:434:TYR:HE2	1.79	0.44
1:G:58:VAL:CG1	1:G:69:ILE:HD13	2.48	0.44
1:A:61:GLU:CB	1:A:109:ARG:HB3	2.47	0.44
1:B:46:VAL:HG21	1:B:391:ILE:HD12	1.98	0.44
1:E:81:HIS:ND1	1:E:96:PRO:HA	2.32	0.44
1:E:431:ARG:CZ	1:G:233:ALA:HB1	2.47	0.44
1:F:273:ASN:OD1	1:F:274:VAL:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:154:TRP:CD1	1:G:154:TRP:C	2.91	0.44
2:A:601:FAD:C6	5:A:605:EOL:H7	2.47	0.44
1:E:432:GLU:O	1:E:432:GLU:HG2	2.16	0.44
2:E:601:FAD:H8A	2:E:601:FAD:O5B	2.18	0.44
1:A:131:TYR:CE1	1:A:157:VAL:HG22	2.53	0.44
1:A:166:VAL:HG11	1:A:434:TYR:HE2	1.83	0.44
1:B:424:ALA:HA	1:B:436:VAL:O	2.17	0.44
1:C:46:VAL:HG21	1:C:391:ILE:HD12	1.99	0.44
1:C:85:THR:OG1	2:C:601:FAD:O1P	2.35	0.44
1:C:414:ARG:HD3	1:C:414:ARG:HA	1.87	0.44
1:F:168:TYR:HA	1:F:274:VAL:HB	1.99	0.44
1:G:394:VAL:HG22	1:G:436:VAL:HA	2.00	0.44
1:H:281:PHE:HB3	1:H:423:MET:HG3	2.00	0.44
1:A:273:ASN:OD1	1:A:273:ASN:C	2.56	0.44
1:C:205:GLN:HG3	1:C:231:GLY:HA3	1.99	0.44
1:C:470:GLU:OE1	1:C:470:GLU:N	2.51	0.44
1:F:285:ALA:HA	1:F:384:TRP:CE3	2.53	0.44
1:C:119:LYS:HD3	1:C:120:TYR:CZ	2.52	0.43
1:C:254:LEU:HB3	1:C:405:MET:HE1	2.00	0.43
1:C:312:LEU:O	1:C:355:ARG:NH2	2.52	0.43
1:E:279:ASN:HA	1:E:316:PHE:O	2.18	0.43
1:H:88:ASN:HA	2:H:600:FAD:H5'2	1.99	0.43
1:D:268:MET:CG	1:D:430:LEU:HD21	2.48	0.43
1:E:456:THR:O	1:E:460:VAL:HG23	2.18	0.43
1:F:273:ASN:HD21	1:F:321:GLY:HA2	1.83	0.43
1:F:362:VAL:O	1:F:366:ARG:HG2	2.19	0.43
1:A:106:THR:O	1:A:110:MET:HB2	2.18	0.43
1:G:61:GLU:HG3	1:G:109:ARG:NH2	2.34	0.43
1:G:425:GLN:O	1:G:436:VAL:HB	2.19	0.43
6:B:802:I7I:C28	6:B:802:I7I:C34	2.96	0.43
1:C:44:TYR:CE2	1:C:89:ASN:HB3	2.53	0.43
1:C:238:PRO:HG3	1:C:324:TYR:HB3	2.00	0.43
1:E:276:VAL:HG23	1:E:320:TYR:HB2	2.00	0.43
1:E:408:PHE:CE1	1:E:422:TYR:HE2	2.36	0.43
1:G:40:PHE:CD1	1:G:57:VAL:CG2	2.94	0.43
1:G:152:LEU:CD1	1:G:378:GLU:HB3	2.48	0.43
1:H:45:PRO:HD2	1:H:443:THR:HG22	2.00	0.43
1:H:148:ASP:OD1	1:H:174:HIS:NE2	2.51	0.43
1:A:475:ASN:HA	1:A:478:MET:HE3	2.00	0.43
1:B:6:PRO:HG2	1:B:78:ILE:HD12	1.99	0.43
1:E:273:ASN:O	1:E:275:PRO:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:457:LYS:HG2	1:E:480:ASP:OD2	2.18	0.43
1:A:411:VAL:HA	1:A:459:LEU:HD21	2.01	0.43
1:B:64:GLU:OE1	1:B:64:GLU:N	2.48	0.43
1:D:85:THR:OG1	2:D:601:FAD:O1P	2.33	0.43
1:E:166:VAL:HG11	1:E:434:TYR:CE2	2.50	0.43
1:E:506:ASN:O	1:E:520:ARG:NE	2.51	0.43
1:F:158:VAL:HG22	1:F:230:MET:HB3	1.99	0.43
1:F:395:PRO:HD2	1:F:435:HIS:O	2.18	0.43
1:A:421:ASP:H	3:A:603:HEZ:C6	2.32	0.43
1:B:456:THR:O	1:B:460:VAL:HG23	2.18	0.43
1:C:285:ALA:HA	1:C:384:TRP:CE3	2.54	0.43
1:E:275:PRO:HB2	1:E:428:ILE:HD12	2.00	0.43
1:F:300:MET:SD	1:F:308:MET:HE1	2.59	0.43
1:H:262:LEU:HB3	1:H:263:PRO:HD3	2.00	0.43
1:E:276:VAL:HA	1:E:426:PHE:O	2.19	0.43
1:F:278:ARG:HH11	1:F:425:GLN:HE22	1.65	0.43
1:A:262:LEU:HB3	1:A:263:PRO:HD3	2.00	0.43
2:E:601:FAD:C6	5:E:602:EOL:H7	2.49	0.43
1:F:278:ARG:HH11	1:F:425:GLN:NE2	2.17	0.43
1:H:329:LEU:HD21	1:H:333:TYR:CD1	2.54	0.43
1:D:260:ILE:HD12	1:D:344:ILE:HD11	1.99	0.42
1:G:171:TYR:HA	1:G:177:TRP:NE1	2.34	0.42
1:H:254:LEU:HB3	1:H:405:MET:HE2	2.02	0.42
1:G:90:GLY:HA3	1:G:390:HIS:CE1	2.54	0.42
1:G:262:LEU:HB3	1:G:263:PRO:HD3	2.01	0.42
1:H:304:ALA:O	1:H:308:MET:HG3	2.19	0.42
1:H:408:PHE:CD2	1:H:422:TYR:CE2	3.05	0.42
1:A:408:PHE:CE1	1:A:422:TYR:HE2	2.36	0.42
1:F:431:ARG:NH2	1:H:171:TYR:OH	2.51	0.42
1:H:85:THR:HG23	1:H:156:SER:HB2	2.02	0.42
1:B:262:LEU:HB3	1:B:263:PRO:HD3	2.01	0.42
1:D:279:ASN:HA	1:D:316:PHE:O	2.19	0.42
1:E:192:ARG:O	1:E:197:ALA:HB2	2.19	0.42
1:E:382:LEU:O	1:E:388:GLY:HA3	2.18	0.42
1:F:215:PRO:O	1:F:218:MET:HB2	2.19	0.42
1:G:60:PRO:HB3	1:G:69:ILE:CD1	2.49	0.42
1:G:387:ASN:O	1:G:443:THR:OG1	2.26	0.42
1:A:171:TYR:CE1	1:A:235:MET:HB2	2.54	0.42
1:A:457:LYS:HE3	1:A:480:ASP:OD2	2.19	0.42
1:B:158:VAL:HG22	1:B:230:MET:HB3	2.00	0.42
1:F:281:PHE:HB3	1:F:423:MET:CG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:3:ARG:NH1	1:H:11:ASP:CG	2.73	0.42
1:H:168:TYR:HA	1:H:274:VAL:HB	2.01	0.42
1:F:148:ASP:OD1	1:F:174:HIS:NE2	2.50	0.42
1:F:431:ARG:CZ	1:H:233:ALA:HB1	2.49	0.42
1:H:91:TYR:HA	1:H:474:HIS:HA	2.02	0.42
1:A:428:ILE:HA	1:A:433:MET:HG2	2.02	0.42
1:D:441:TYR:CD1	1:D:452:ILE:HG13	2.55	0.42
1:G:106:THR:O	1:G:110:MET:HB2	2.19	0.42
1:A:24:VAL:HG12	1:A:65:GLN:HG2	2.02	0.42
1:A:273:ASN:O	1:A:275:PRO:HD3	2.19	0.42
1:B:389:GLY:O	1:B:440:ILE:HA	2.20	0.42
1:D:131:TYR:CZ	1:D:150:PRO:HD3	2.55	0.42
1:E:74:ASN:HD21	1:E:187:GLN:HA	1.84	0.42
1:F:503:LEU:HD23	1:H:498:LYS:HD2	2.02	0.42
1:G:276:VAL:HG23	1:G:320:TYR:HB2	2.02	0.42
1:C:148:ASP:CB	4:C:602:GOL:H2	2.50	0.42
1:F:205:GLN:HG3	1:F:231:GLY:HA3	2.02	0.42
1:C:59:SER:O	1:C:109:ARG:NH1	2.53	0.41
1:C:282:MET:HE3	1:C:381:LEU:HD21	1.99	0.41
1:D:293:TRP:CD2	1:D:308:MET:HG2	2.55	0.41
1:G:281:PHE:HD2	1:G:308:MET:HE1	1.83	0.41
1:D:268:MET:HG2	1:D:430:LEU:HD21	2.02	0.41
1:D:525:ASN:O	1:D:526:LEU:HB3	2.20	0.41
1:A:137:TYR:CD1	1:A:137:TYR:C	2.93	0.41
1:B:44:TYR:HE1	1:B:382:LEU:HD11	1.85	0.41
1:F:14:PHE:O	1:F:18:LEU:HG	2.20	0.41
1:F:106:THR:O	1:F:110:MET:HB2	2.21	0.41
1:G:79:PRO:HG2	1:G:101:SER:HA	2.01	0.41
1:D:119:LYS:HD3	1:D:120:TYR:CZ	2.55	0.41
1:E:151:ASP:HA	1:E:369:ILE:HD13	2.02	0.41
1:E:394:VAL:O	1:E:470:GLU:HA	2.20	0.41
1:F:502:ALA:HB2	1:H:502:ALA:HB2	2.02	0.41
1:H:44:TYR:CD2	1:H:89:ASN:HB3	2.55	0.41
1:A:205:GLN:HG3	1:A:231:GLY:HA3	2.03	0.41
1:B:205:GLN:HG3	1:B:231:GLY:HA3	2.03	0.41
1:B:438:LEU:HD23	1:B:438:LEU:HA	1.87	0.41
1:C:254:LEU:HB3	1:C:405:MET:CE	2.50	0.41
1:G:3:ARG:HG2	1:G:5:LEU:HD21	2.02	0.41
1:G:81:HIS:CB	1:G:96:PRO:HB3	2.50	0.41
1:D:262:LEU:HB3	1:D:263:PRO:HD3	2.03	0.41
1:D:282:MET:HE2	5:D:603:EOL:C9	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:457:LYS:HE3	1:F:480:ASP:OD2	2.20	0.41
1:G:40:PHE:CE1	1:G:57:VAL:HG21	2.55	0.41
1:G:205:GLN:HG3	1:G:231:GLY:HA3	2.03	0.41
1:C:2:THR:HG22	1:C:3:ARG:N	2.36	0.41
1:G:471:TYR:HH	5:G:602:EOL:HO1	1.66	0.41
1:B:423:MET:SD	1:B:440:ILE:HD12	2.60	0.41
1:C:154:TRP:CH2	1:C:379:LEU:HD11	2.56	0.41
1:C:249:ASP:O	1:C:309:LYS:NZ	2.45	0.41
1:C:276:VAL:HA	1:C:426:PHE:O	2.21	0.41
1:C:408:PHE:CD1	1:C:422:TYR:HE2	2.39	0.41
1:E:233:ALA:HB1	1:G:431:ARG:CZ	2.50	0.41
1:F:279:ASN:HA	1:F:316:PHE:O	2.20	0.41
1:F:389:GLY:O	1:F:440:ILE:HA	2.21	0.41
1:G:61:GLU:CG	1:G:109:ARG:CZ	2.98	0.41
1:G:118:GLU:OE2	1:G:143:SER:OG	2.24	0.41
1:H:394:VAL:O	1:H:470:GLU:HA	2.20	0.41
1:C:10:SER:OG	1:C:12:GLU:HB2	2.21	0.41
1:D:385:VAL:HB	1:D:386:PRO:HD2	2.03	0.41
1:E:496:HIS:CE1	1:G:213:PRO:HD2	2.56	0.41
1:H:171:TYR:HA	1:H:177:TRP:NE1	2.35	0.41
1:H:493:LEU:HD23	1:H:497:GLU:HG3	2.02	0.41
1:B:285:ALA:HA	1:B:384:TRP:CE3	2.56	0.40
1:G:473:THR:HG23	1:G:478:MET:HG2	2.02	0.40
1:A:297:ASP:OD1	3:A:603:HEZ:C1	2.69	0.40
1:A:395:PRO:HD2	1:A:435:HIS:O	2.21	0.40
1:E:63:THR:O	1:E:66:VAL:HG22	2.21	0.40
1:F:221:GLN:HE22	1:F:472:ARG:HB3	1.85	0.40
1:F:278:ARG:NH1	1:F:425:GLN:HE22	2.20	0.40
1:G:252:GLU:HA	1:G:405:MET:HE1	2.03	0.40
1:G:261:MET:SD	1:G:428:ILE:HG21	2.61	0.40
1:G:268:MET:HG2	1:G:430:LEU:HD21	2.02	0.40
1:G:298:GLY:HA2	1:G:419:ASN:OD1	2.21	0.40
1:B:206:LEU:HD22	1:C:431:ARG:O	2.22	0.40
1:B:281:PHE:HB3	1:B:423:MET:CG	2.52	0.40
1:C:277:LEU:HB3	1:C:426:PHE:HB2	2.03	0.40
1:H:57:VAL:HG22	1:H:103:ILE:HB	2.04	0.40
1:C:408:PHE:CE1	1:C:422:TYR:HE2	2.39	0.40
1:F:458:VAL:O	1:F:461:ARG:HB3	2.21	0.40
1:G:146:MET:SD	1:G:237:ARG:HA	2.62	0.40
1:G:246:ILE:HG12	1:G:349:PHE:CE2	2.57	0.40
1:G:474:HIS:ND1	1:G:475:ASN:N	2.69	0.40

All (5) 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:C:12:GLU:OE1	1:E:12:GLU:OE1[2_656]	1.76	0.44
1:C:12:GLU:OE2	1:E:12:GLU:OE1[2_656]	1.89	0.31
1:C:12:GLU:CD	1:E:12:GLU:OE1[2_656]	1.98	0.22
1:A:12:GLU:N	1:G:12:GLU:OE2[1_455]	2.02	0.18
1:B:62:SER:OG	1:C:303:GLU:OE2[2_656]	2.16	0.04

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%)	505 (97%)	18 (3%)	0	100	100
1	B	523/526 (99%)	513 (98%)	10 (2%)	0	100	100
1	C	520/526 (99%)	500 (96%)	20 (4%)	0	100	100
1	D	523/526 (99%)	510 (98%)	13 (2%)	0	100	100
1	E	519/526 (99%)	506 (98%)	13 (2%)	0	100	100
1	F	522/526 (99%)	507 (97%)	15 (3%)	0	100	100
1	G	520/526 (99%)	506 (97%)	14 (3%)	0	100	100
1	H	520/526 (99%)	500 (96%)	19 (4%)	1 (0%)	47	78
All	All	4170/4208 (99%)	4047 (97%)	122 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	252	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	431/435 (99%)	424 (98%)	7 (2%)	62	88
1	B	430/435 (99%)	419 (97%)	11 (3%)	46	79
1	C	428/435 (98%)	419 (98%)	9 (2%)	53	84
1	D	433/435 (100%)	424 (98%)	9 (2%)	53	84
1	E	424/435 (98%)	415 (98%)	9 (2%)	53	84
1	F	416/435 (96%)	407 (98%)	9 (2%)	52	83
1	G	415/435 (95%)	395 (95%)	20 (5%)	25	58
1	H	410/435 (94%)	395 (96%)	15 (4%)	34	68
All	All	3387/3480 (97%)	3298 (97%)	89 (3%)	46	79

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	27	ASP
1	A	61	GLU
1	A	154	TRP
1	A	256	GLN
1	A	311	ASP
1	A	445	ASP
1	B	2	THR
1	B	11	ASP
1	B	41	ARG
1	B	154	TRP
1	B	256	GLN
1	B	295	ASP
1	B	339	GLU
1	B	361	HIS
1	B	430	LEU
1	B	447	GLU
1	B	526	LEU
1	C	27	ASP

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Mol	Chain	Res	Type
1	C	41	ARG
1	C	136	GLU
1	C	142	ASP
1	C	154	TRP
1	C	356	ASP
1	C	397	SER
1	C	419	ASN
1	C	461	ARG
1	D	2	THR
1	D	13	ARG
1	D	142	ASP
1	D	154	TRP
1	D	256	GLN
1	D	339	GLU
1	D	381	LEU
1	D	402	ARG
1	D	433	MET
1	E	11	ASP
1	E	27	ASP
1	E	53	LEU
1	E	154	TRP
1	E	311	ASP
1	E	348	ARG
1	E	378	GLU
1	E	443	THR
1	E	514	SER
1	F	154	TRP
1	F	201	SER
1	F	273	ASN
1	F	307	ARG
1	F	339	GLU
1	F	343	LYS
1	F	402	ARG
1	F	408	PHE
1	F	489	ASP
1	G	5	LEU
1	G	19	GLN
1	G	25	VAL
1	G	28	LYS
1	G	30	VAL
1	G	32	SER
1	G	36	GLU

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Mol	Chain	Res	Type
1	G	61	GLU
1	G	70	VAL
1	G	83	VAL
1	G	99	SER
1	G	137	TYR
1	G	154	TRP
1	G	356	ASP
1	G	361	HIS
1	G	375	SER
1	G	387	ASN
1	G	390	HIS
1	G	403	GLU
1	G	443	THR
1	H	12	GLU
1	H	27	ASP
1	H	64	GLU
1	H	137	TYR
1	H	140	SER
1	H	142	ASP
1	H	154	TRP
1	H	252	GLU
1	H	297	ASP
1	H	332	MET
1	H	356	ASP
1	H	362	VAL
1	H	405	MET
1	H	414	ARG
1	H	430	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	370	ASN
1	B	256	GLN
1	B	416	ASN
1	C	387	ASN
1	E	496	HIS
1	F	387	ASN
1	F	425	GLN
1	G	74	ASN
1	H	273	ASN
1	H	496	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

19 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FAD	D	601	1	53,58,58	0.65	0	68,89,89	0.81	1 (1%)
3	HEZ	A	603	-	7,7,7	0.25	0	6,6,6	0.28	0
5	EOL	E	602	-	12,12,12	2.49	2 (16%)	15,15,15	1.65	3 (20%)
2	FAD	H	600	1	53,58,58	0.62	0	68,89,89	0.73	1 (1%)
3	HEZ	A	602	-	7,7,7	0.15	0	6,6,6	0.26	0
4	GOL	A	604	-	5,5,5	0.18	0	5,5,5	0.39	0
3	HEZ	B	801	-	7,7,7	0.22	0	6,6,6	0.31	0
6	I7I	F	901	1	65,71,71	0.97	2 (3%)	75,108,108	1.13	6 (8%)
2	FAD	G	601	1	53,58,58	0.66	0	68,89,89	0.80	2 (2%)
4	GOL	C	602	-	5,5,5	0.23	0	5,5,5	0.46	0
6	I7I	B	802	1	65,71,71	1.01	2 (3%)	75,108,108	1.12	7 (9%)
2	FAD	C	601	1	53,58,58	0.60	0	68,89,89	0.80	1 (1%)
5	EOL	C	603	-	12,12,12	2.27	2 (16%)	15,15,15	1.77	4 (26%)
5	EOL	D	603	-	12,12,12	2.41	2 (16%)	15,15,15	1.51	2 (13%)
5	EOL	A	605	-	12,12,12	2.30	2 (16%)	15,15,15	2.06	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EOL	G	602	-	12,12,12	2.26	2 (16%)	15,15,15	1.69	3 (20%)
2	FAD	A	601	1	53,58,58	0.63	0	68,89,89	0.80	2 (2%)
3	HEZ	D	602	-	7,7,7	0.13	0	6,6,6	0.20	0
2	FAD	E	601	1	53,58,58	0.61	0	68,89,89	0.77	1 (1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	D	601	1	-	3/30/50/50	0/6/6/6
3	HEZ	A	603	-	-	1/5/5/5	-
5	EOL	E	602	-	-	3/5/5/5	0/1/1/1
2	FAD	H	600	1	-	6/30/50/50	0/6/6/6
3	HEZ	A	602	-	-	2/5/5/5	-
4	GOL	A	604	-	-	2/4/4/4	-
3	HEZ	B	801	-	-	2/5/5/5	-
6	I7I	F	901	1	-	15/42/62/62	0/6/7/7
2	FAD	G	601	1	-	12/30/50/50	0/6/6/6
4	GOL	C	602	-	-	4/4/4/4	-
6	I7I	B	802	1	-	16/42/62/62	0/6/7/7
2	FAD	C	601	1	-	11/30/50/50	0/6/6/6
5	EOL	C	603	-	-	1/5/5/5	0/1/1/1
5	EOL	D	603	-	-	3/5/5/5	0/1/1/1
5	EOL	A	605	-	-	3/5/5/5	0/1/1/1
5	EOL	G	602	-	-	2/5/5/5	0/1/1/1
2	FAD	A	601	1	-	14/30/50/50	0/6/6/6
3	HEZ	D	602	-	-	4/5/5/5	-
2	FAD	E	601	1	-	8/30/50/50	0/6/6/6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	603	EOL	C7-C2	-7.33	1.38	1.52
5	E	602	EOL	C7-C2	-7.29	1.38	1.52
5	C	603	EOL	C7-C2	-6.65	1.39	1.52
5	A	605	EOL	C7-C2	-6.36	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	602	EOL	C7-C2	-6.31	1.40	1.52
6	B	802	I7I	C24-N9	5.32	1.53	1.47
6	F	901	I7I	C24-N9	4.82	1.53	1.47
5	A	605	EOL	C9-C8	3.81	1.54	1.28
6	F	901	I7I	C23-N9	3.80	1.43	1.37
5	G	602	EOL	C9-C8	3.76	1.54	1.28
5	E	602	EOL	C9-C8	3.76	1.53	1.28
5	C	603	EOL	C9-C8	3.74	1.53	1.28
5	D	603	EOL	C9-C8	3.62	1.53	1.28
6	B	802	I7I	C23-N9	3.41	1.43	1.37

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	605	EOL	C7-C2-C1	-4.95	111.42	120.56
6	F	901	I7I	C27-C24-N9	-4.15	107.02	111.67
5	C	603	EOL	C7-C2-C1	-4.11	112.98	120.56
5	E	602	EOL	C7-C2-C1	-3.95	113.28	120.56
5	G	602	EOL	C7-C2-C1	-3.93	113.31	120.56
6	F	901	I7I	C23-C34-N8	3.59	117.31	110.99
6	B	802	I7I	C23-C34-N8	3.55	117.25	110.99
5	D	603	EOL	C7-C2-C1	-3.35	114.38	120.56
6	B	802	I7I	C27-C24-N9	-3.25	108.03	111.67
5	A	605	EOL	C7-C2-C4	3.13	129.63	120.96
5	A	605	EOL	C7-C8-C9	-2.82	103.98	127.58
2	E	601	FAD	C5A-C6A-N6A	2.71	124.47	120.35
5	D	603	EOL	C7-C8-C9	-2.68	105.16	127.58
5	C	603	EOL	C7-C8-C9	-2.63	105.62	127.58
6	B	802	I7I	C6-C7-C8	2.60	117.05	109.79
2	G	601	FAD	P-O3P-PA	-2.59	123.95	132.83
6	B	802	I7I	C28-C27-C24	2.59	125.65	120.76
5	G	602	EOL	C7-C2-C4	2.51	127.90	120.96
5	G	602	EOL	C7-C8-C9	-2.50	106.66	127.58
2	C	601	FAD	C5A-C6A-N6A	2.49	124.14	120.35
6	B	802	I7I	C33-C27-C24	-2.49	115.65	120.42
6	F	901	I7I	O11-C15-C14	-2.49	103.29	106.93
5	C	603	EOL	C7-C2-C4	2.46	127.75	120.96
5	C	603	EOL	O2-C3-C5	2.45	118.12	114.57
5	E	602	EOL	C7-C8-C9	-2.45	107.10	127.58
2	A	601	FAD	P-O3P-PA	-2.30	124.92	132.83
6	F	901	I7I	C33-C27-C24	-2.27	116.06	120.42
6	B	802	I7I	C17-C18-N4	2.16	123.63	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	901	I7I	C6-C7-C8	2.14	115.77	109.79
2	D	601	FAD	C5A-C6A-N6A	2.13	123.59	120.35
6	B	802	I7I	C26-C25-C24	2.10	115.82	113.33
6	F	901	I7I	C17-C18-N4	2.08	123.51	120.35
5	E	602	EOL	O1-C5-C6	2.07	124.96	119.33
5	A	605	EOL	O1-C5-C3	-2.05	115.31	120.09
2	H	600	FAD	C5A-C6A-N6A	2.04	123.46	120.35
2	A	601	FAD	C5A-C6A-N6A	2.04	123.46	120.35
5	A	605	EOL	O1-C5-C6	2.02	124.82	119.33
2	G	601	FAD	C5A-C6A-N6A	2.01	123.41	120.35

There are no chirality outliers.

All (112) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	N10-C1'-C2'-C3'
2	C	601	FAD	N10-C1'-C2'-C3'
2	G	601	FAD	N10-C1'-C2'-C3'
2	G	601	FAD	C2'-C3'-C4'-O4'
2	G	601	FAD	C2'-C3'-C4'-C5'
2	G	601	FAD	O3'-C3'-C4'-O4'
2	G	601	FAD	O3'-C3'-C4'-C5'
2	G	601	FAD	C5'-O5'-P-O2P
4	A	604	GOL	C1-C2-C3-O3
6	B	802	I7I	C11-O8-P2-O6
6	B	802	I7I	C27-C24-C25-C26
6	F	901	I7I	N1-C6-C7-C8
6	F	901	I7I	O2-C8-C9-C10
6	F	901	I7I	O4-C10-C9-C8
6	F	901	I7I	O4-C10-C9-O3
6	F	901	I7I	C25-C24-N9-C23
6	F	901	I7I	N9-C24-C25-C26
6	F	901	I7I	C7-C8-C9-C10
6	F	901	I7I	C7-C8-C9-O3
5	D	603	EOL	C2-C7-C8-C9
5	E	602	EOL	C2-C7-C8-C9
2	A	601	FAD	C2'-C3'-C4'-C5'
6	F	901	I7I	O2-C8-C9-O3
2	A	601	FAD	C2'-C3'-C4'-O4'
2	C	601	FAD	C2'-C3'-C4'-O4'
6	B	802	I7I	C7-C8-C9-O3
6	B	802	I7I	C25-C24-N9-C23

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Mol	Chain	Res	Type	Atoms
4	C	602	GOL	O1-C1-C2-C3
4	C	602	GOL	C1-C2-C3-O3
3	A	602	HEZ	C1-C2-C3-C4
2	A	601	FAD	O4'-C4'-C5'-O5'
2	C	601	FAD	O4'-C4'-C5'-O5'
2	C	601	FAD	C2'-C3'-C4'-C5'
2	E	601	FAD	C2'-C3'-C4'-C5'
6	B	802	I7I	C7-C8-C9-C10
4	C	602	GOL	O1-C1-C2-O2
2	A	601	FAD	O3'-C3'-C4'-O4'
2	C	601	FAD	O3'-C3'-C4'-O4'
2	E	601	FAD	O3'-C3'-C4'-O4'
6	B	802	I7I	O2-C8-C9-O3
2	E	601	FAD	C2'-C3'-C4'-O4'
5	A	605	EOL	C2-C7-C8-C9
3	B	801	HEZ	C3-C4-C5-C6
2	H	600	FAD	C2'-C3'-C4'-O4'
2	A	601	FAD	C3'-C4'-C5'-O5'
2	C	601	FAD	C3'-C4'-C5'-O5'
2	E	601	FAD	C3'-C4'-C5'-O5'
6	B	802	I7I	O4-C10-C9-C8
3	D	602	HEZ	O1-C1-C2-C3
5	C	603	EOL	C2-C7-C8-C9
4	C	602	GOL	O2-C2-C3-O3
6	B	802	I7I	C25-C24-N9-C4
6	F	901	I7I	C25-C24-N9-C4
3	D	602	HEZ	C4-C5-C6-O6
6	B	802	I7I	N9-C24-C25-C26
5	G	602	EOL	C2-C7-C8-C9
2	C	601	FAD	C4'-C5'-O5'-P
2	E	601	FAD	O4'-C4'-C5'-O5'
2	E	601	FAD	O3'-C3'-C4'-C5'
2	H	600	FAD	C2'-C3'-C4'-C5'
2	D	601	FAD	C4'-C5'-O5'-P
2	G	601	FAD	C4'-C5'-O5'-P
6	B	802	I7I	C9-C10-O4-P1
6	F	901	I7I	C9-C10-O4-P1
2	A	601	FAD	O3'-C3'-C4'-C5'
2	C	601	FAD	O3'-C3'-C4'-C5'
6	B	802	I7I	O2-C8-C9-C10
6	B	802	I7I	C12-C11-O8-P2
2	G	601	FAD	C5'-O5'-P-O3P

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Mol	Chain	Res	Type	Atoms
4	A	604	GOL	O2-C2-C3-O3
6	B	802	I7I	C10-O4-P1-O6
6	B	802	I7I	C27-C24-N9-C23
2	A	601	FAD	C4'-C5'-O5'-P
2	H	600	FAD	C4'-C5'-O5'-P
6	F	901	I7I	C12-C11-O8-P2
2	D	601	FAD	C3'-C4'-C5'-O5'
6	B	802	I7I	C11-O8-P2-O12
2	G	601	FAD	N10-C1'-C2'-O2'
2	H	600	FAD	N10-C1'-C2'-C3'
6	B	802	I7I	O4-C10-C9-O3
3	D	602	HEZ	C2-C3-C4-C5
3	B	801	HEZ	C4-C5-C6-O6
5	D	603	EOL	C4-C2-C7-C8
3	A	602	HEZ	C4-C5-C6-O6
3	A	603	HEZ	O1-C1-C2-C3
5	D	603	EOL	C1-C2-C7-C8
3	D	602	HEZ	C3-C4-C5-C6
2	A	601	FAD	PA-O3P-P-O1P
2	E	601	FAD	PA-O3P-P-O1P
2	A	601	FAD	O2'-C2'-C3'-O3'
2	E	601	FAD	C4'-C5'-O5'-P
5	E	602	EOL	C1-C2-C7-C8
5	A	605	EOL	C4-C2-C7-C8
2	D	601	FAD	O4'-C4'-C5'-O5'
2	H	600	FAD	O3'-C3'-C4'-O4'
6	F	901	I7I	C11-O8-P2-O6
2	A	601	FAD	PA-O3P-P-O2P
2	C	601	FAD	O2'-C2'-C3'-O3'
6	F	901	I7I	C27-C24-N9-C23
5	E	602	EOL	C4-C2-C7-C8
5	G	602	EOL	C4-C2-C7-C8
2	A	601	FAD	C5B-O5B-PA-O1A
2	G	601	FAD	C5'-O5'-P-O1P
2	H	600	FAD	C3'-C4'-C5'-O5'
2	A	601	FAD	C1'-C2'-C3'-O3'
2	C	601	FAD	C1'-C2'-C3'-O3'
2	G	601	FAD	C1'-C2'-C3'-O3'
2	G	601	FAD	O2'-C2'-C3'-O3'
2	A	601	FAD	N10-C1'-C2'-O2'
2	C	601	FAD	N10-C1'-C2'-O2'
6	F	901	I7I	C27-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
5	A	605	EOL	C1-C2-C7-C8

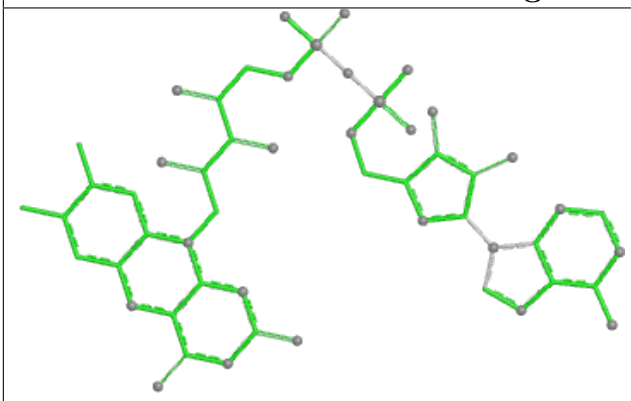
There are no ring outliers.

16 monomers are involved in 31 short contacts:

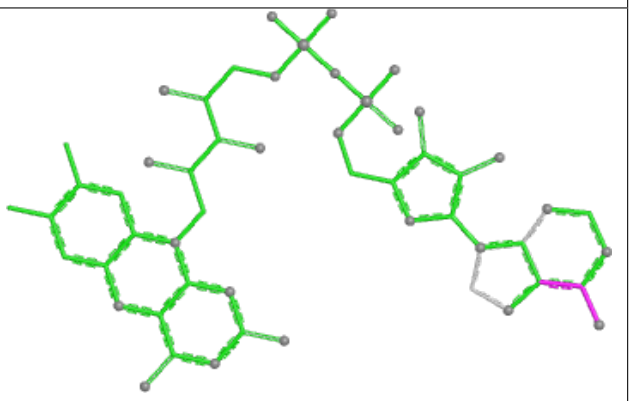
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	FAD	3	0
3	A	603	HEZ	2	0
5	E	602	EOL	1	0
2	H	600	FAD	3	0
3	A	602	HEZ	1	0
3	B	801	HEZ	1	0
6	F	901	I7I	3	0
2	G	601	FAD	1	0
4	C	602	GOL	5	0
6	B	802	I7I	3	0
2	C	601	FAD	1	0
5	D	603	EOL	2	0
5	A	605	EOL	1	0
5	G	602	EOL	3	0
2	A	601	FAD	2	0
2	E	601	FAD	2	0

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

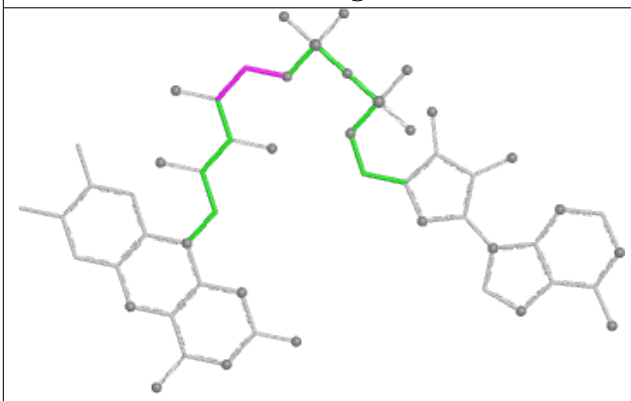
Ligand FAD D 601



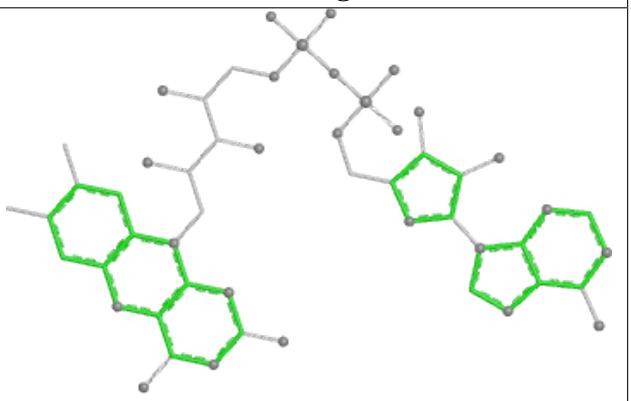
Bond lengths



Bond angles



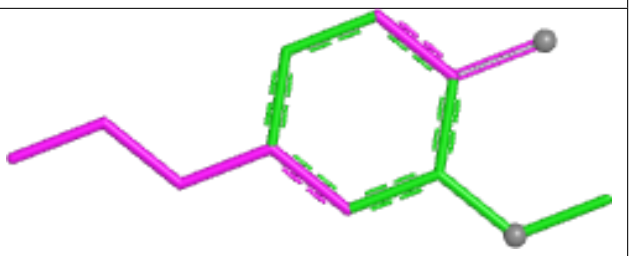
Torsions



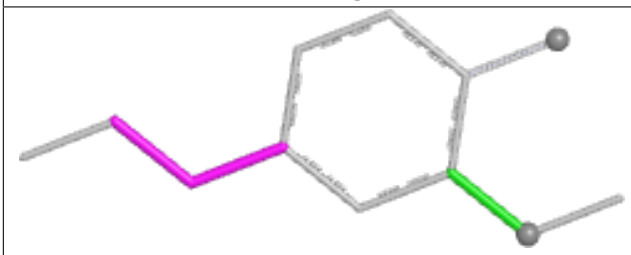
Rings

Ligand EOL E 602

Bond lengths



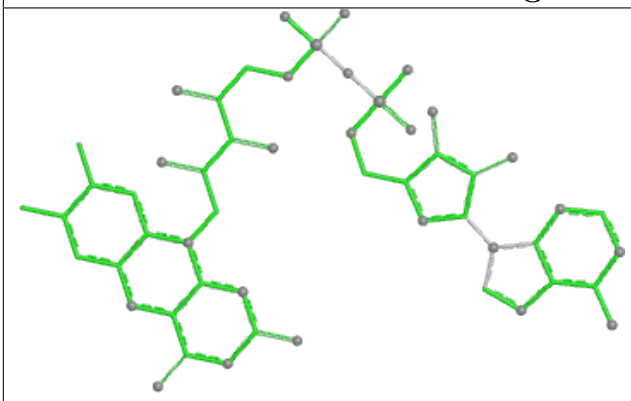
Bond angles



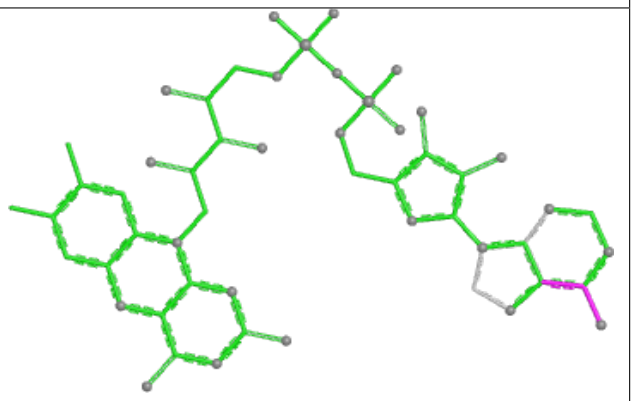
Torsions

Rings

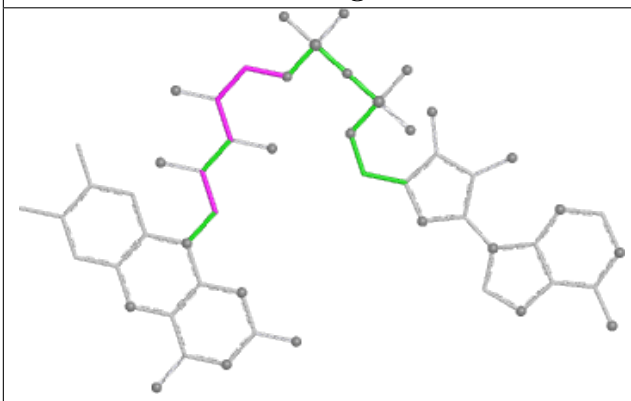
Ligand FAD H 600



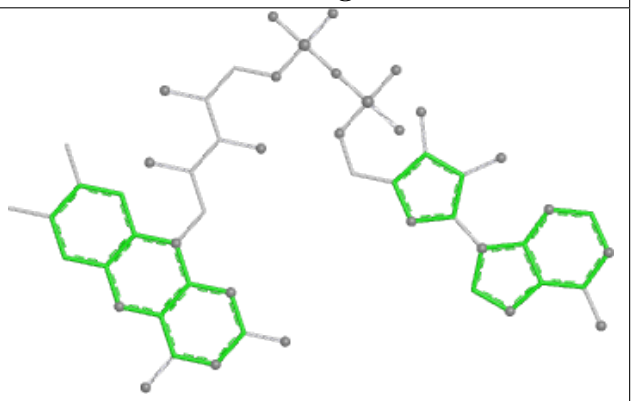
Bond lengths



Bond angles

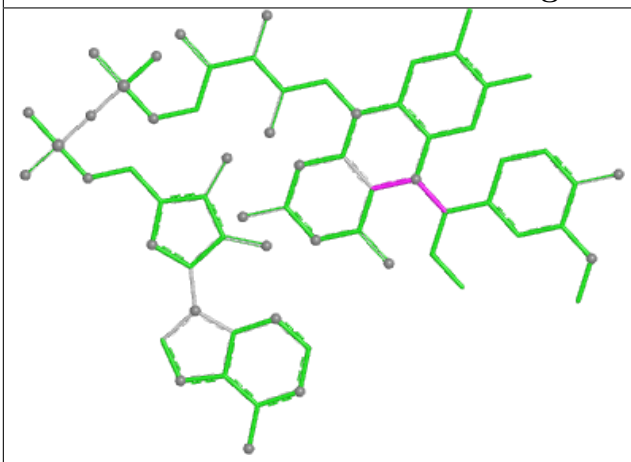


Torsions

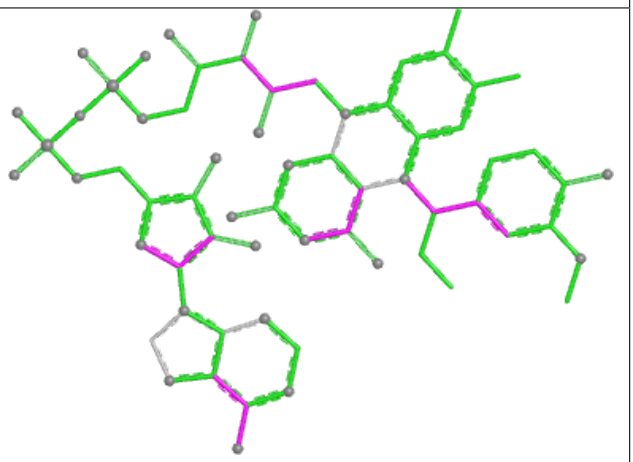


Rings

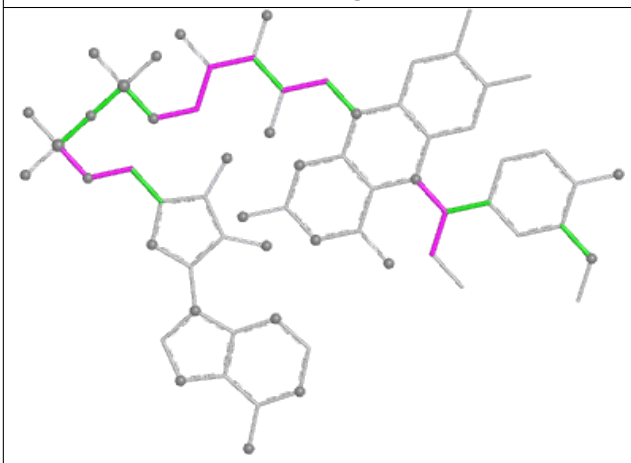
Ligand I7I F 901



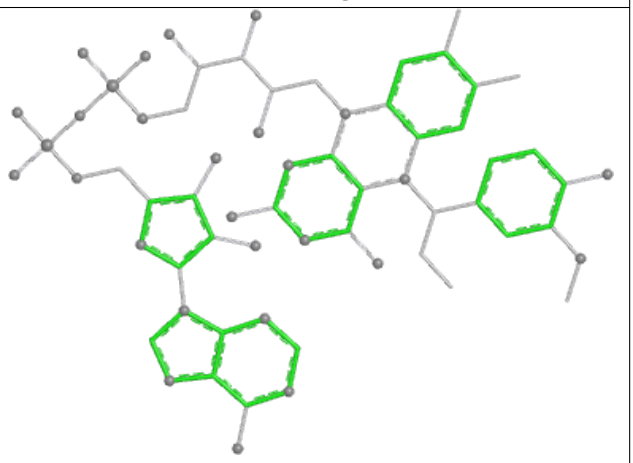
Bond lengths



Bond angles

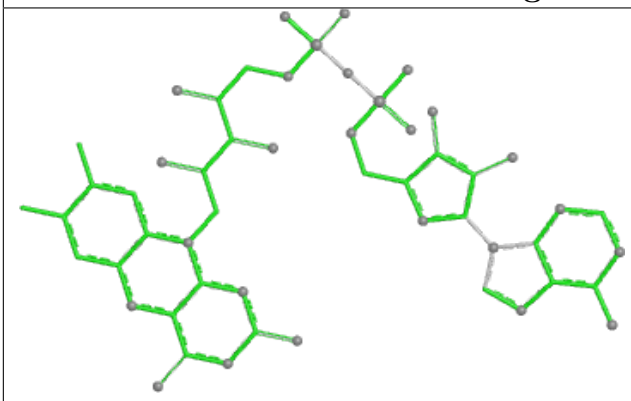


Torsions

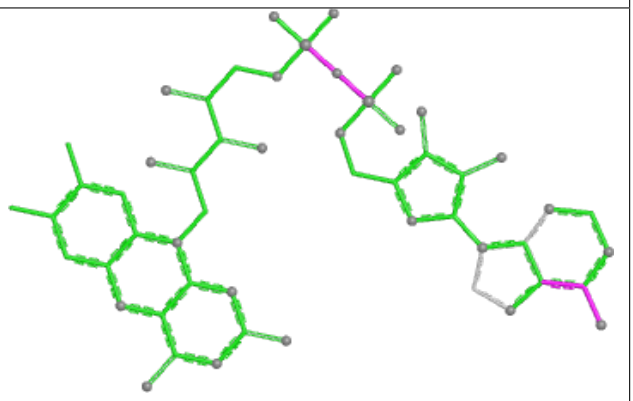


Rings

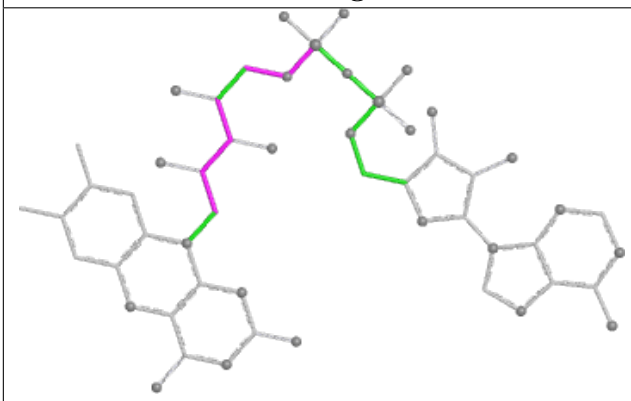
Ligand FAD G 601



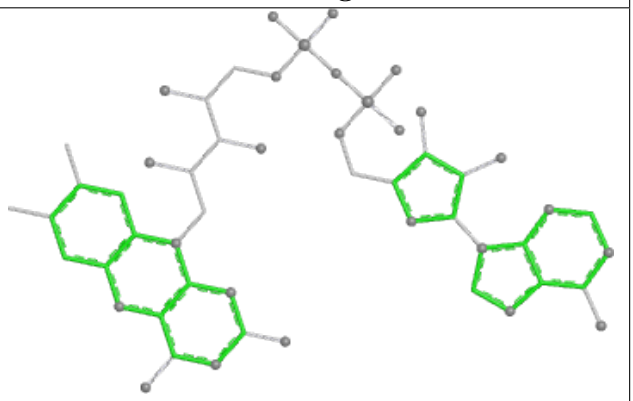
Bond lengths



Bond angles

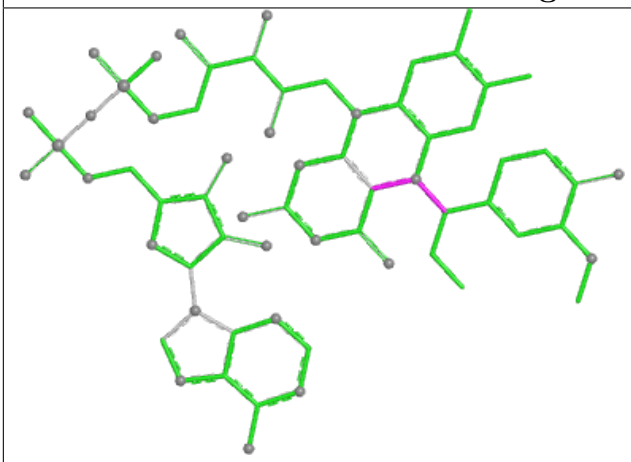


Torsions

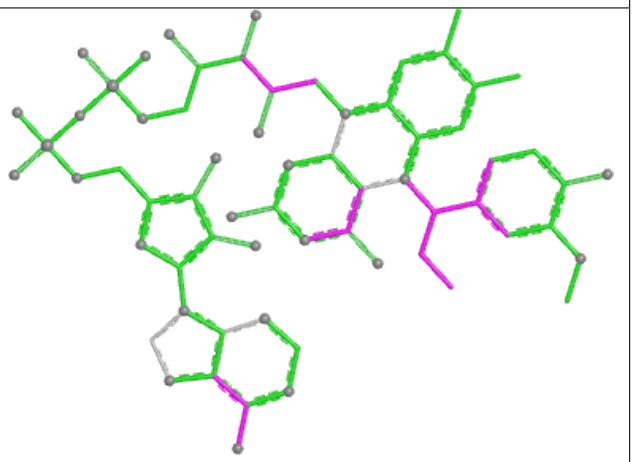


Rings

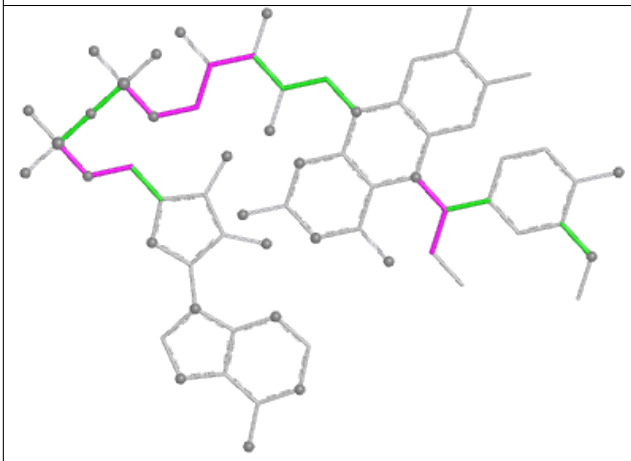
Ligand I7I B 802



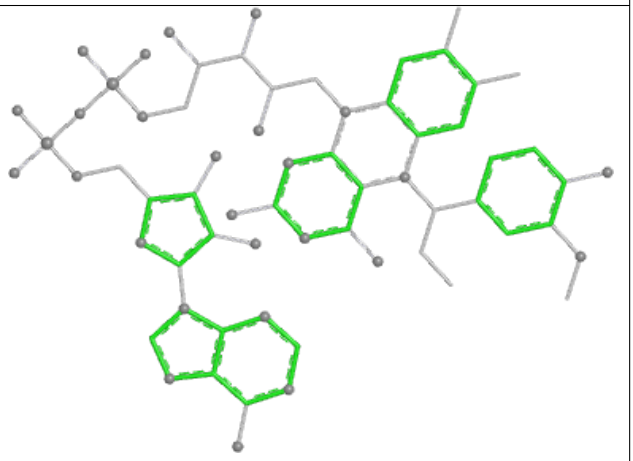
Bond lengths



Bond angles

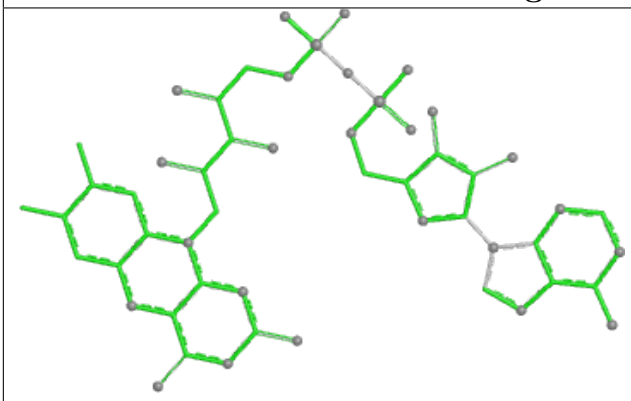


Torsions

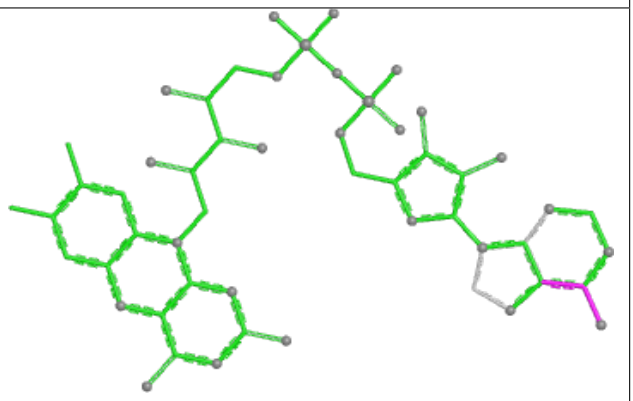


Rings

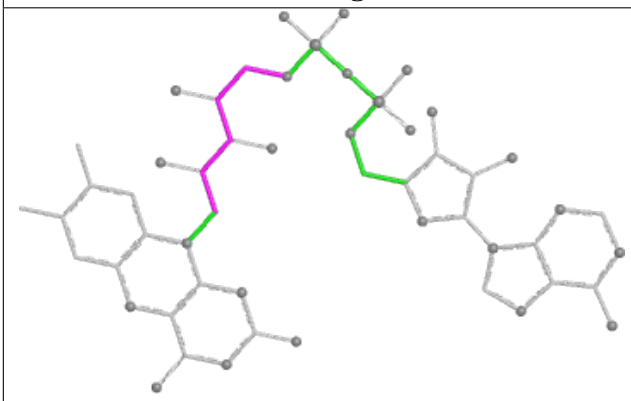
Ligand FAD C 601



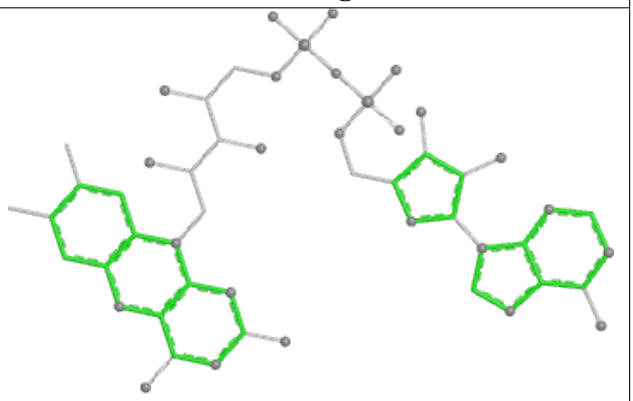
Bond lengths



Bond angles



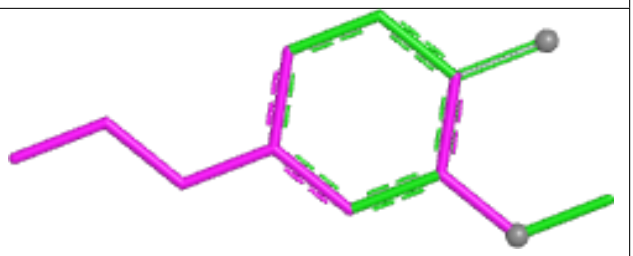
Torsions



Rings

Ligand EOL C 603

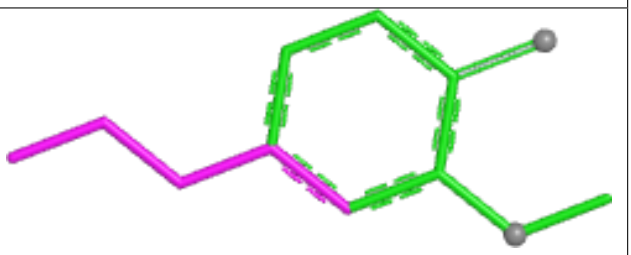
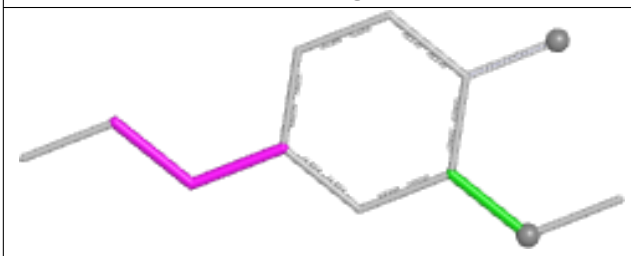
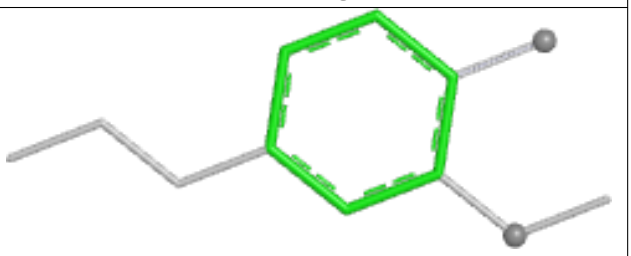
Bond lengths

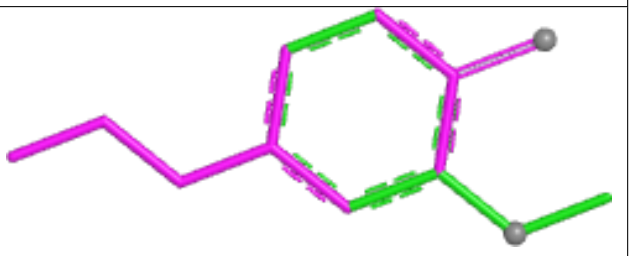
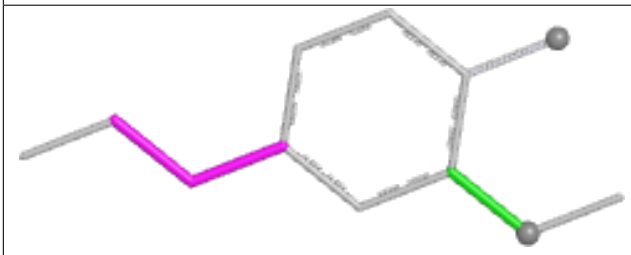
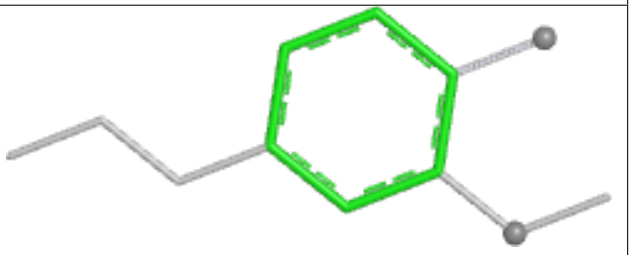


Bond angles

Torsions

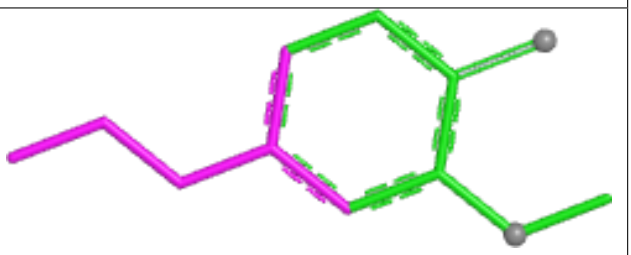
Rings

Ligand EOL D 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

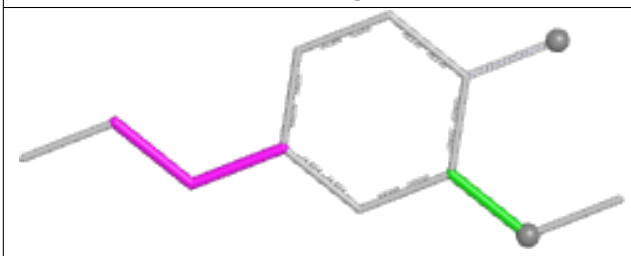
Ligand EOL A 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand EOL G 602

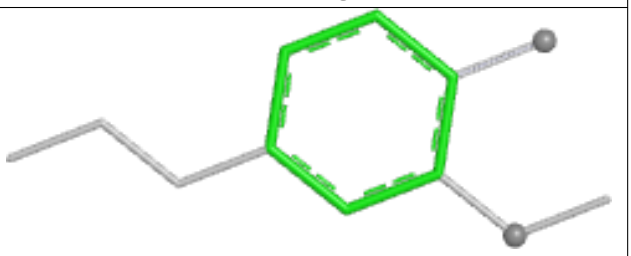
Bond lengths



Bond angles

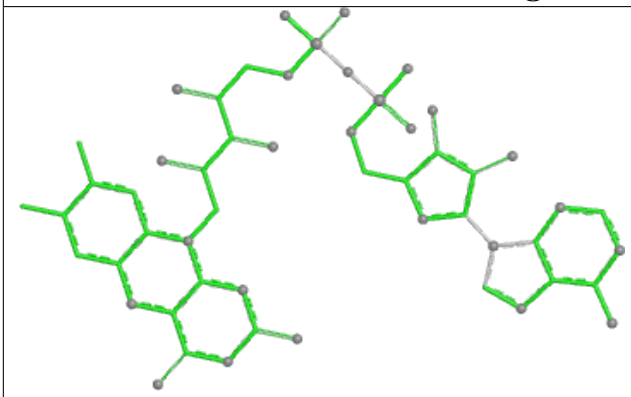


Torsions

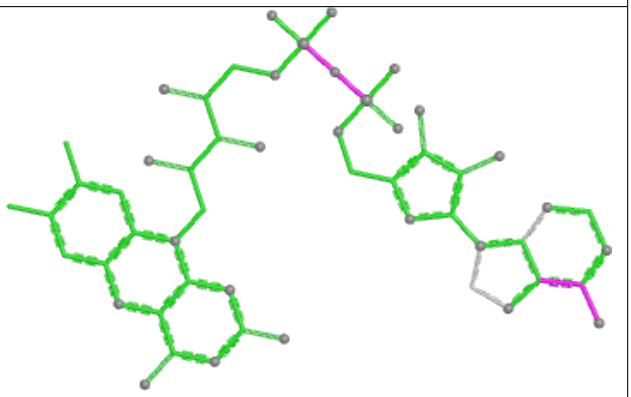


Rings

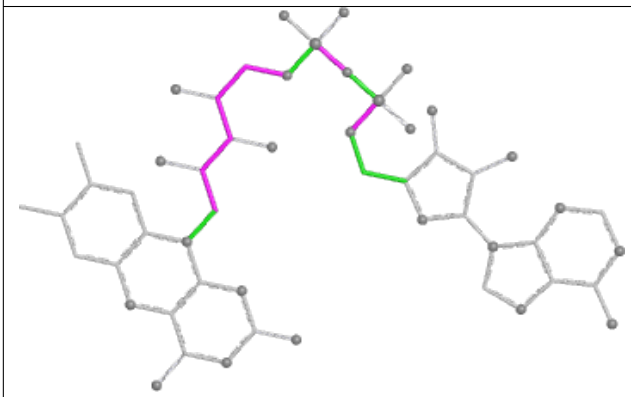
Ligand FAD A 601



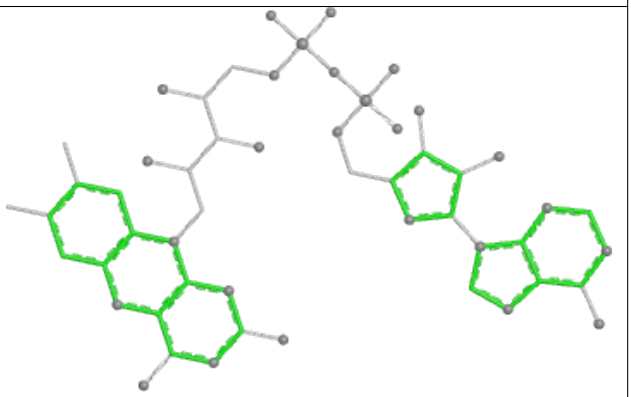
Bond lengths



Bond angles

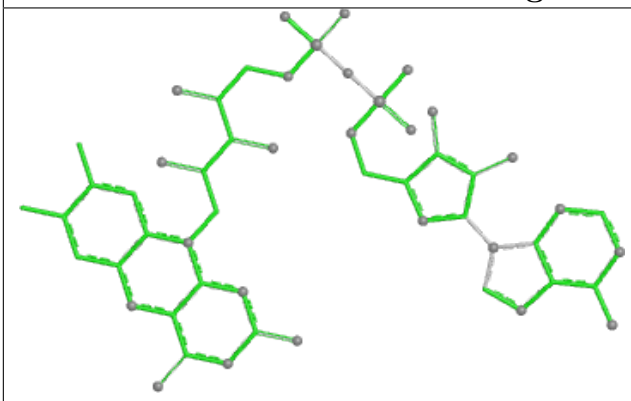


Torsions

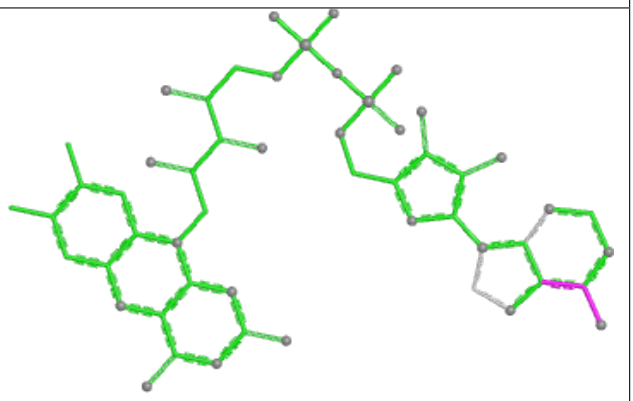


Rings

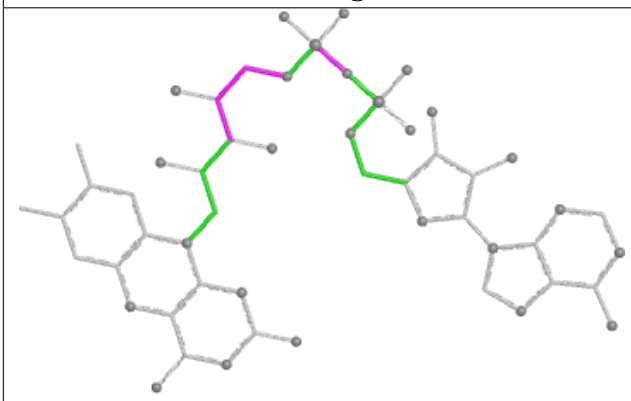
Ligand FAD E 601



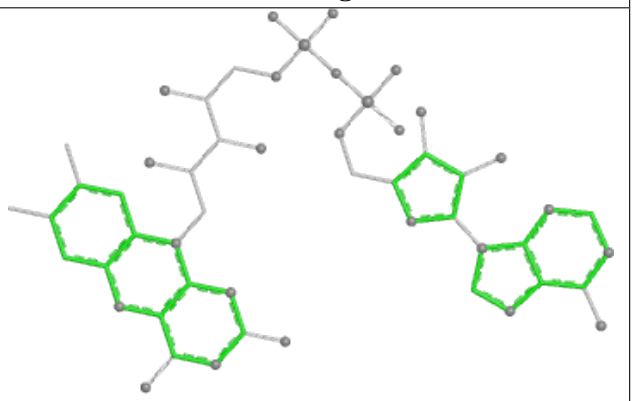
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.07	5 (0%)	82	77	27, 38, 56, 110	0
1	B	525/526 (99%)	0.06	8 (1%)	73	68	27, 46, 70, 113	0
1	C	522/526 (99%)	0.05	3 (0%)	89	86	30, 42, 62, 91	0
1	D	525/526 (99%)	-0.01	4 (0%)	86	81	25, 40, 63, 95	0
1	E	521/526 (99%)	0.34	20 (3%)	40	30	30, 59, 89, 132	0
1	F	524/526 (99%)	0.57	33 (6%)	20	12	43, 66, 90, 111	0
1	G	522/526 (99%)	0.78	50 (9%)	8	4	38, 69, 96, 130	0
1	H	522/526 (99%)	0.64	38 (7%)	15	8	47, 75, 99, 123	0
All	All	4186/4208 (99%)	0.29	161 (3%)	40	30	25, 53, 89, 132	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	525	ASN	10.1
1	A	526	LEU	6.6
1	H	8	GLY	6.1
1	F	523	GLY	5.8
1	H	2	THR	4.6
1	B	525	ASN	4.4
1	G	56	ALA	4.3
1	E	6	PRO	4.2
1	B	523	GLY	4.2
1	E	9	VAL	4.1
1	H	9	VAL	4.1
1	G	294	PHE	4.0
1	E	100	GLY	3.9
1	G	444	ALA	3.9
1	H	346	GLY	3.9
1	G	389	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	H	303	GLU	3.7
1	G	476	ALA	3.7
1	A	524	GLN	3.7
1	G	55	SER	3.7
1	H	345	PRO	3.7
1	G	295	ASP	3.7
1	F	297	ASP	3.7
1	H	294	PHE	3.6
1	G	101	SER	3.6
1	A	523	GLY	3.5
1	H	30	VAL	3.5
1	F	524	GLN	3.5
1	B	524	GLN	3.4
1	H	387	ASN	3.4
1	G	523	GLY	3.4
1	H	444	ALA	3.3
1	G	21	PHE	3.3
1	E	21	PHE	3.3
1	E	49	ALA	3.3
1	H	437	CYS	3.2
1	H	382	LEU	3.2
1	D	525	ASN	3.2
1	G	483	ALA	3.1
1	G	9	VAL	3.1
1	H	252	GLU	3.1
1	C	2	THR	3.1
1	E	52	ASN	3.1
1	E	76	TYR	3.1
1	H	311	ASP	3.1
1	H	421	ASP	3.1
1	G	59	SER	3.1
1	F	270	PRO	3.1
1	F	347	ALA	3.0
1	G	46	VAL	3.0
1	G	57	VAL	3.0
1	G	440	ILE	3.0
1	F	345	PRO	3.0
1	G	311	ASP	3.0
1	G	302	ALA	2.9
1	G	53	LEU	2.9
1	E	35	ASP	2.9
1	C	523	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	53	LEU	2.9
1	G	19	GLN	2.8
1	G	50	GLU	2.8
1	E	291	THR	2.8
1	B	401	GLY	2.8
1	E	2	THR	2.8
1	F	295	ASP	2.8
1	H	356	ASP	2.8
1	D	2	THR	2.8
1	F	313	ASP	2.8
1	G	48	ALA	2.8
1	F	2	THR	2.7
1	H	440	ILE	2.7
1	G	51	ALA	2.7
1	H	361	HIS	2.7
1	E	17	ALA	2.6
1	G	102	VAL	2.6
1	E	7	PRO	2.6
1	G	35	ASP	2.6
1	H	336	MET	2.6
1	G	8	GLY	2.6
1	F	8	GLY	2.6
1	H	297	ASP	2.6
1	H	18	LEU	2.5
1	H	295	ASP	2.5
1	F	444	ALA	2.5
1	H	5	LEU	2.5
1	H	11	ASP	2.5
1	F	296	GLY	2.5
1	G	386	PRO	2.5
1	F	290	ARG	2.5
1	G	31	LEU	2.5
1	E	295	ASP	2.5
1	G	4	THR	2.5
1	F	294	PHE	2.5
1	F	412	ARG	2.4
1	E	5	LEU	2.4
1	F	304	ALA	2.4
1	F	386	PRO	2.4
1	H	238	PRO	2.4
1	G	298	GLY	2.4
1	H	249	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	252	GLU	2.4
1	G	58	VAL	2.4
1	C	10	SER	2.4
1	F	300	MET	2.4
1	G	347	ALA	2.4
1	F	176	MET	2.4
1	H	512	GLY	2.4
1	G	297	ASP	2.3
1	H	337	ILE	2.3
1	G	100	GLY	2.3
1	G	447	GLU	2.3
1	F	310	LYS	2.3
1	B	297	ASP	2.3
1	E	14	PHE	2.3
1	F	11	ASP	2.3
1	F	346	GLY	2.3
1	G	288	SER	2.3
1	F	298	GLY	2.3
1	G	458	VAL	2.3
1	G	130	THR	2.2
1	B	176	MET	2.2
1	G	296	GLY	2.2
1	H	489	ASP	2.2
1	G	34	ALA	2.2
1	G	344	ILE	2.2
1	G	36	GLU	2.2
1	G	281	PHE	2.2
1	H	339	GLU	2.2
1	E	499	ILE	2.2
1	F	299	PRO	2.2
1	E	75	GLU	2.2
1	G	375	SER	2.2
1	H	243	SER	2.2
1	H	137	TYR	2.2
1	H	298	GLY	2.2
1	D	295	ASP	2.2
1	F	49	ALA	2.2
1	F	507	GLY	2.1
1	G	348	ARG	2.1
1	B	35	ASP	2.1
1	E	176	MET	2.1
1	A	51	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	446	PRO	2.1
1	G	345	PRO	2.1
1	F	315	GLY	2.1
1	F	328	PRO	2.1
1	G	441	TYR	2.1
1	G	249	ASP	2.1
1	F	409	GLU	2.1
1	F	174	HIS	2.0
1	E	10	SER	2.0
1	G	2	THR	2.0
1	F	74	ASN	2.0
1	F	48	ALA	2.0
1	B	447	GLU	2.0
1	H	141	HIS	2.0
1	H	296	GLY	2.0
1	H	354	GLU	2.0
1	H	305	ILE	2.0
1	F	302	ALA	2.0
1	H	317	TRP	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	GOL	C	602	6/6	0.76	0.35	36,39,40,41	0
4	GOL	A	604	6/6	0.79	0.29	52,55,56,56	0
3	HEZ	A	603	8/8	0.88	0.31	55,58,68,72	0
5	EOL	D	603	12/12	0.91	0.22	55,57,61,62	0

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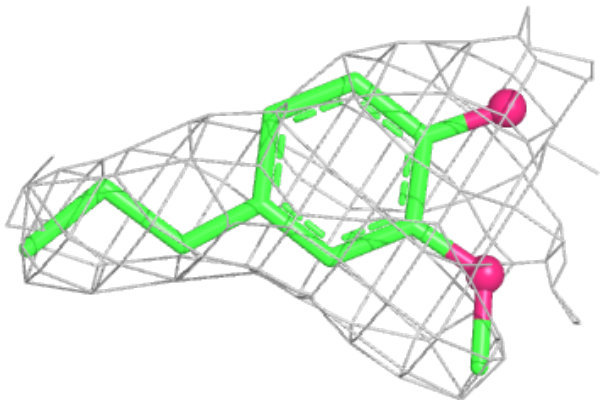
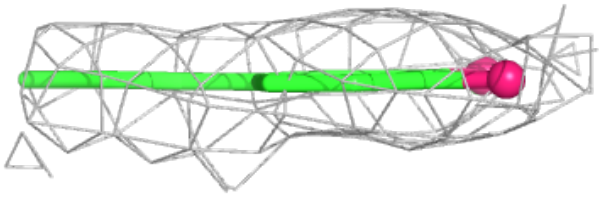
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	I7I	F	901	65/65	0.91	0.24	44,55,62,71	0
5	EOL	G	602	12/12	0.92	0.27	49,51,60,60	0
5	EOL	A	605	12/12	0.93	0.19	36,38,40,42	0
5	EOL	C	603	12/12	0.93	0.23	42,46,47,49	0
2	FAD	G	601	53/53	0.93	0.21	46,56,62,63	0
2	FAD	H	600	53/53	0.93	0.17	51,64,82,87	0
3	HEZ	A	602	8/8	0.93	0.22	42,43,45,46	0
3	HEZ	B	801	8/8	0.94	0.59	38,40,43,44	0
2	FAD	E	601	53/53	0.94	0.19	39,54,63,68	0
3	HEZ	D	602	8/8	0.95	0.27	33,33,34,34	0
6	I7I	B	802	65/65	0.95	0.21	32,42,56,62	0
5	EOL	E	602	12/12	0.95	0.20	46,49,58,59	0
2	FAD	C	601	53/53	0.96	0.19	31,38,42,43	0
2	FAD	D	601	53/53	0.96	0.20	28,34,41,43	0
2	FAD	A	601	53/53	0.96	0.19	26,32,36,40	0

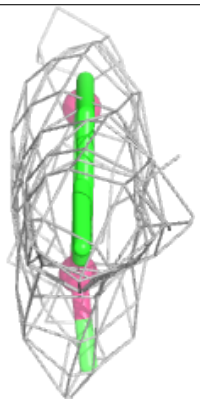
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EOL D 603:

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

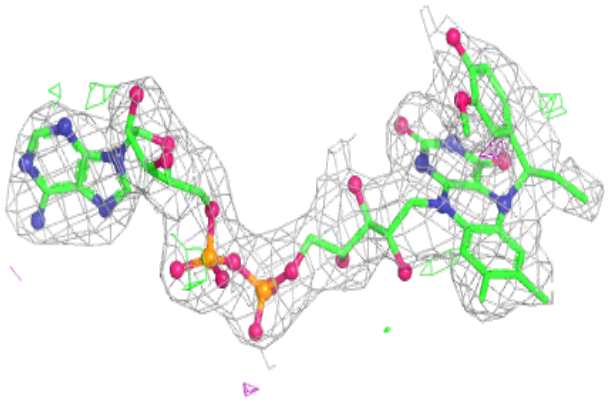


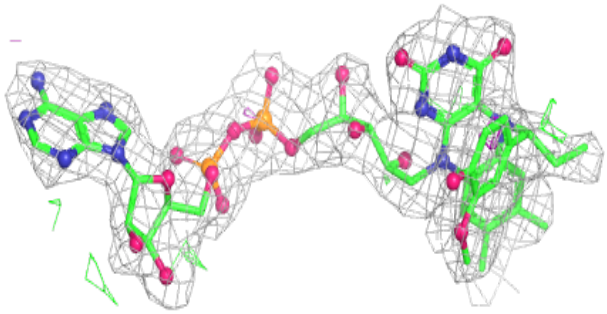




Electron density around I7I F 901:

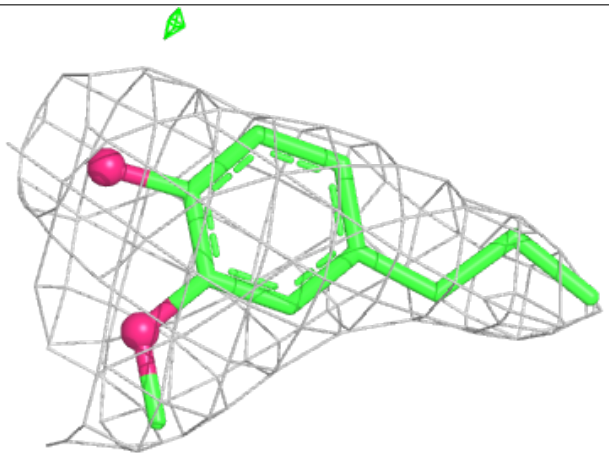
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

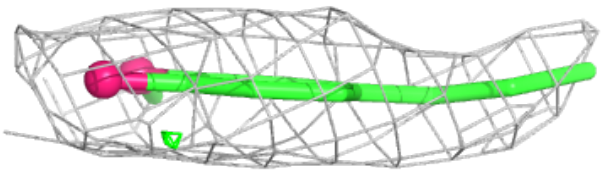


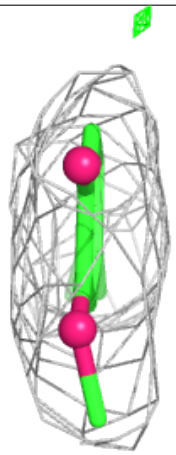


Electron density around EOL G 602:

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

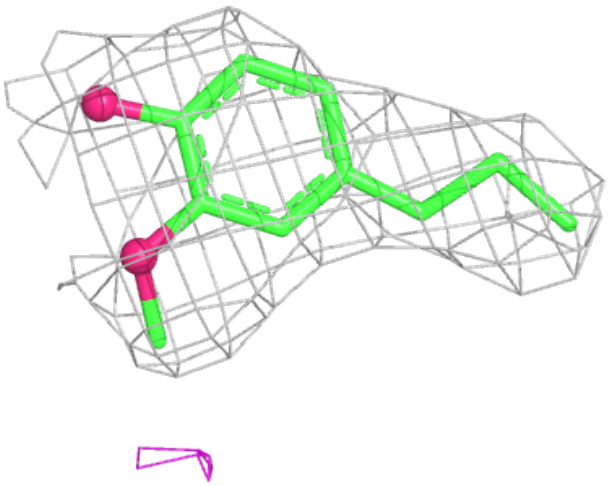


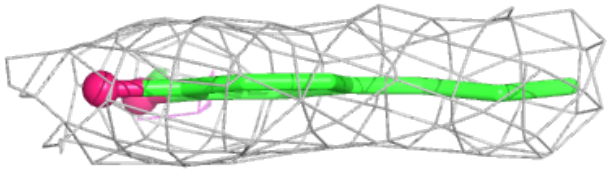


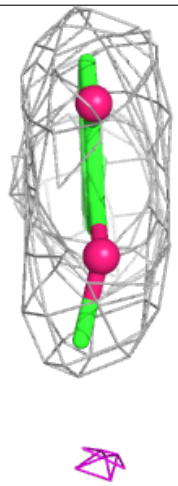


Electron density around EOL A 605:

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

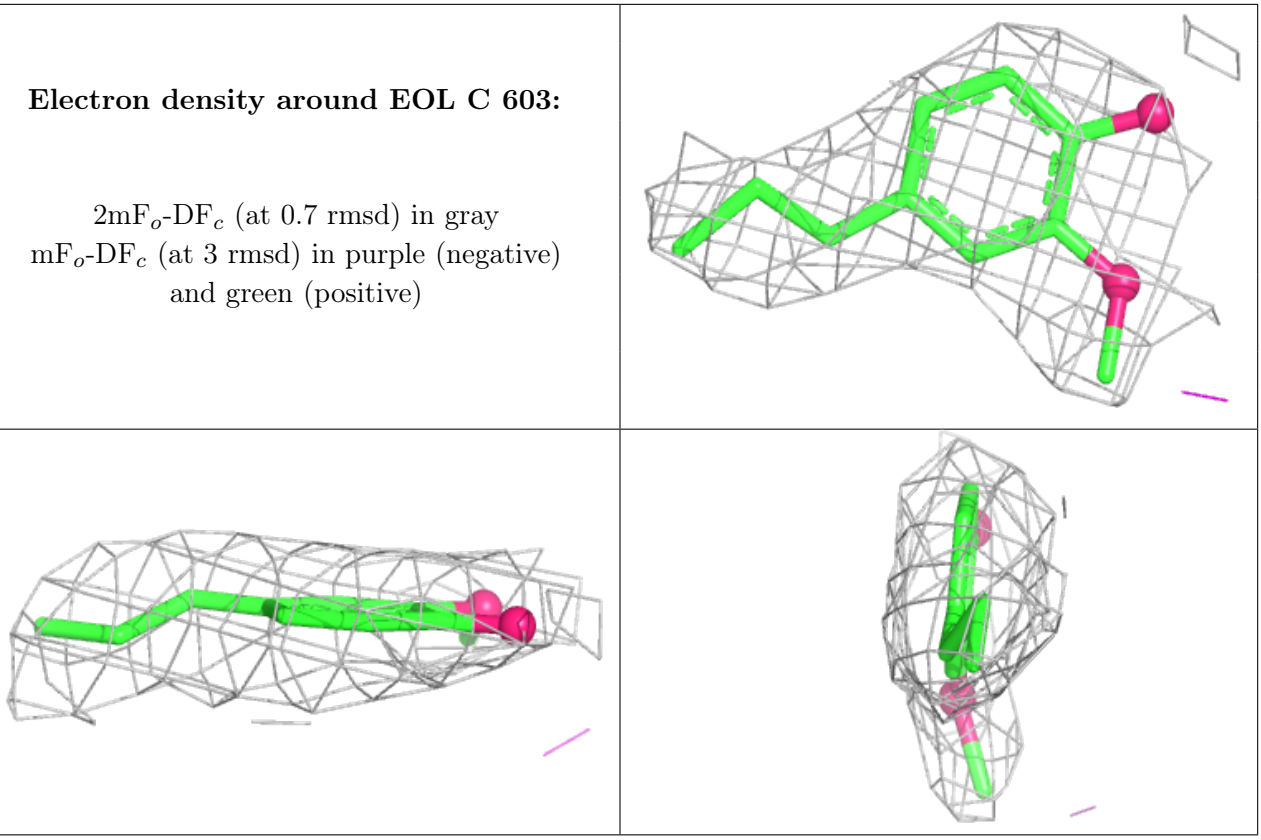






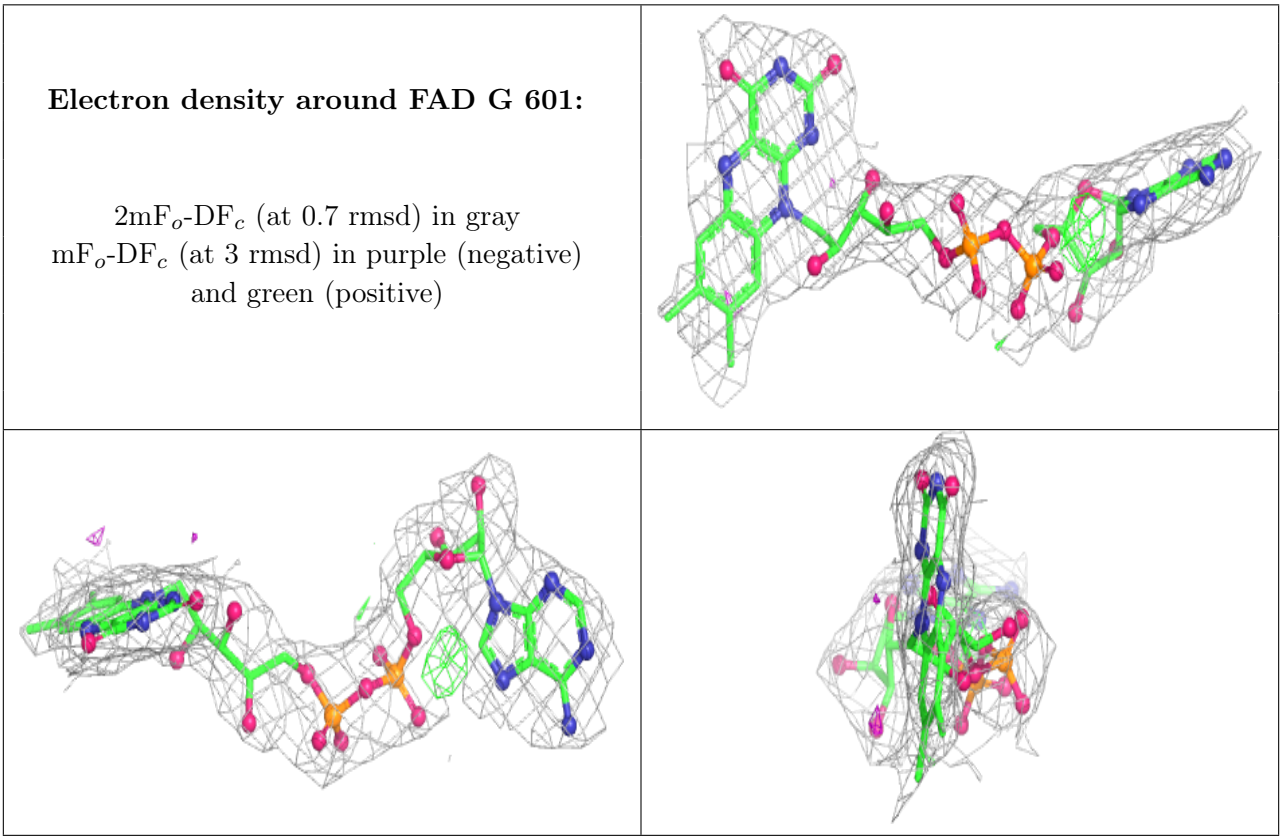
Electron density around EOL C 603:

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



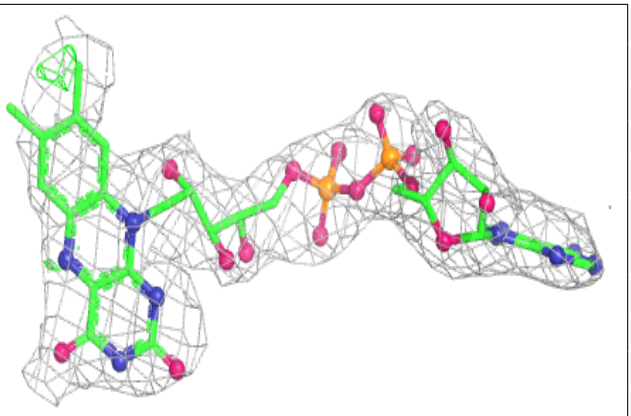
Electron density around FAD G 601:

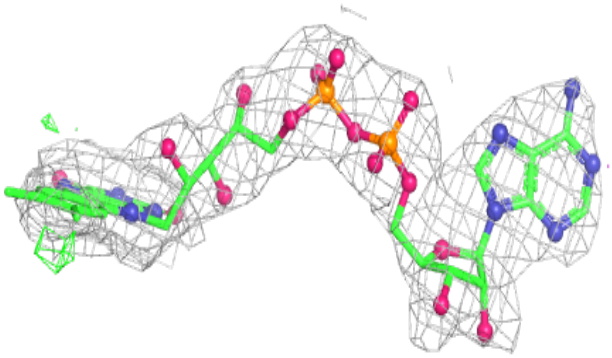
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

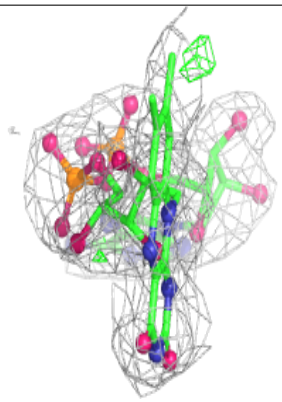


Electron density around FAD H 600:

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

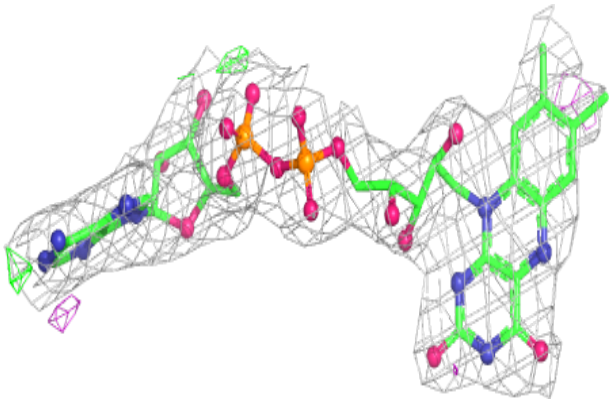


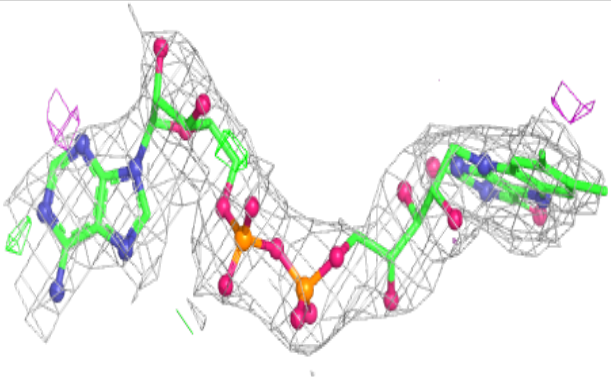


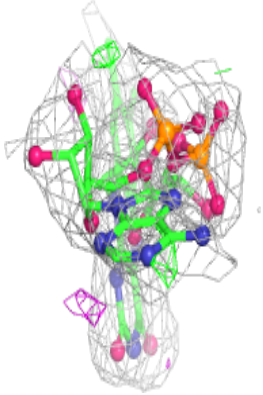


Electron density around FAD E 601:

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

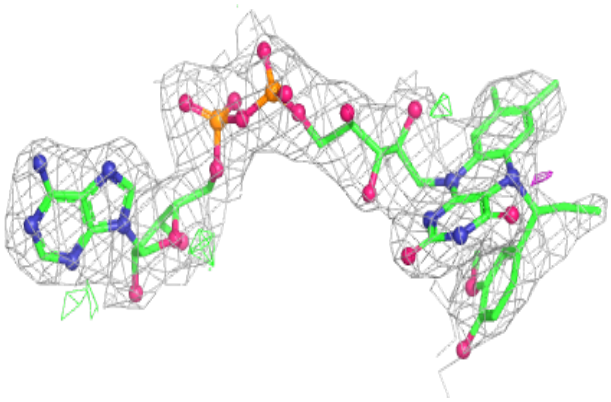


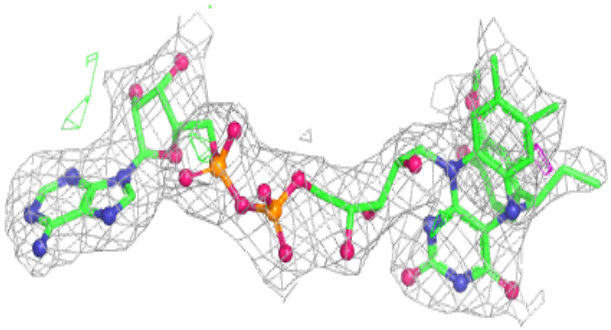


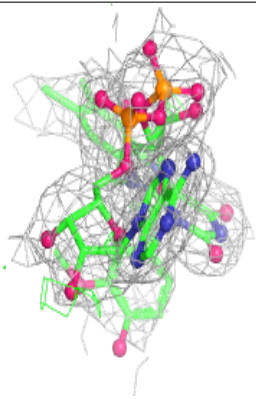


Electron density around I7I B 802:

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

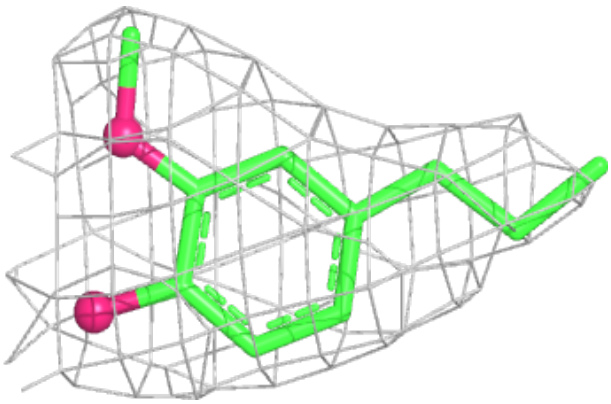


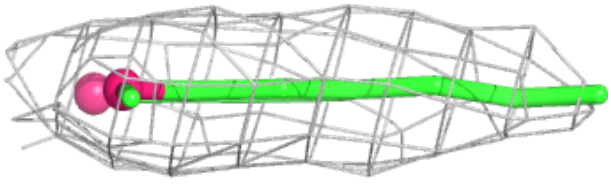


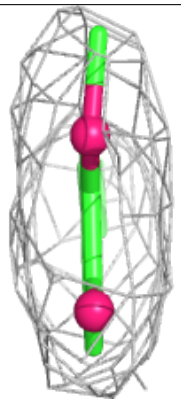


Electron density around EOL E 602:

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

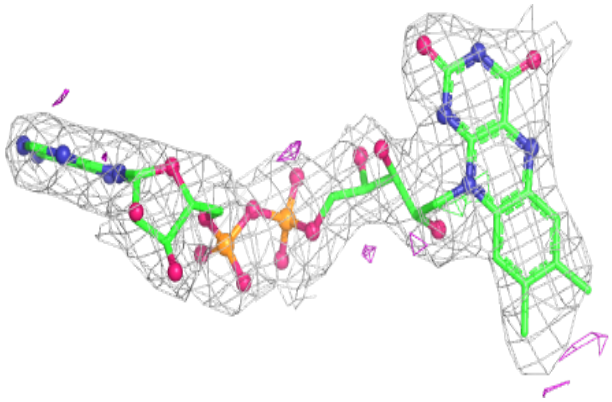


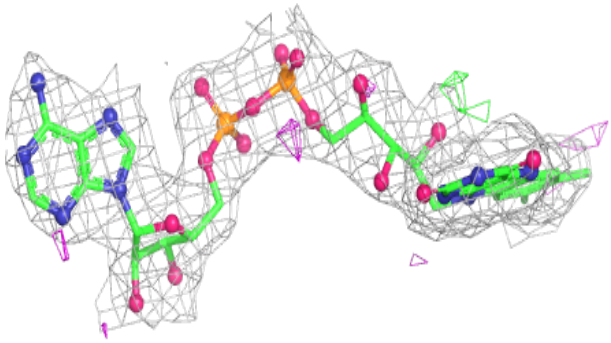


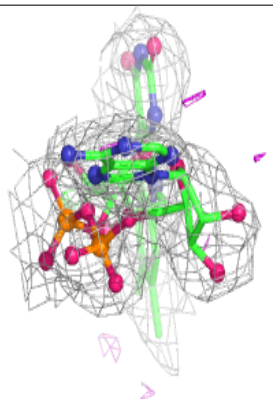


Electron density around FAD C 601:

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

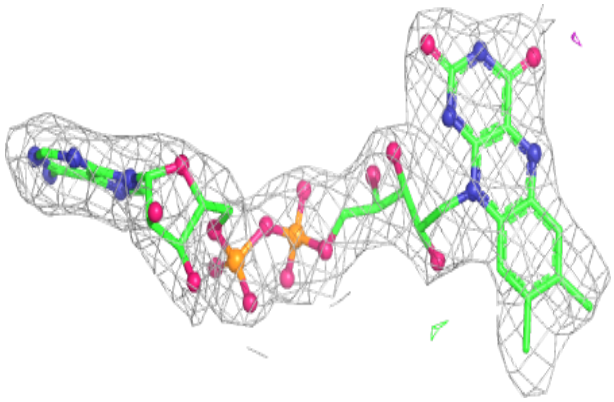


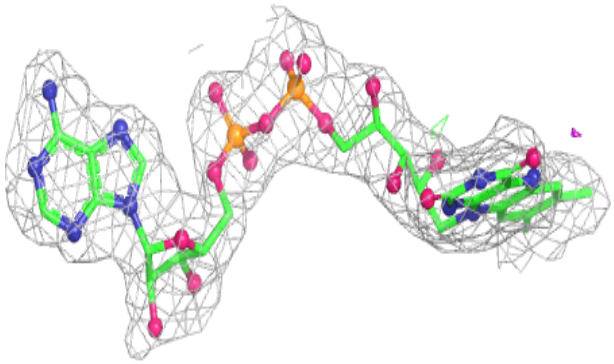


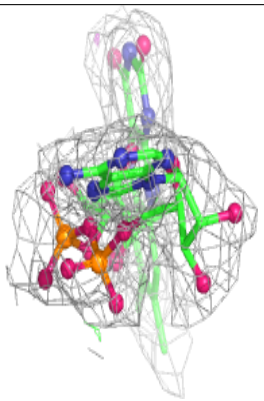


Electron density around FAD D 601:

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

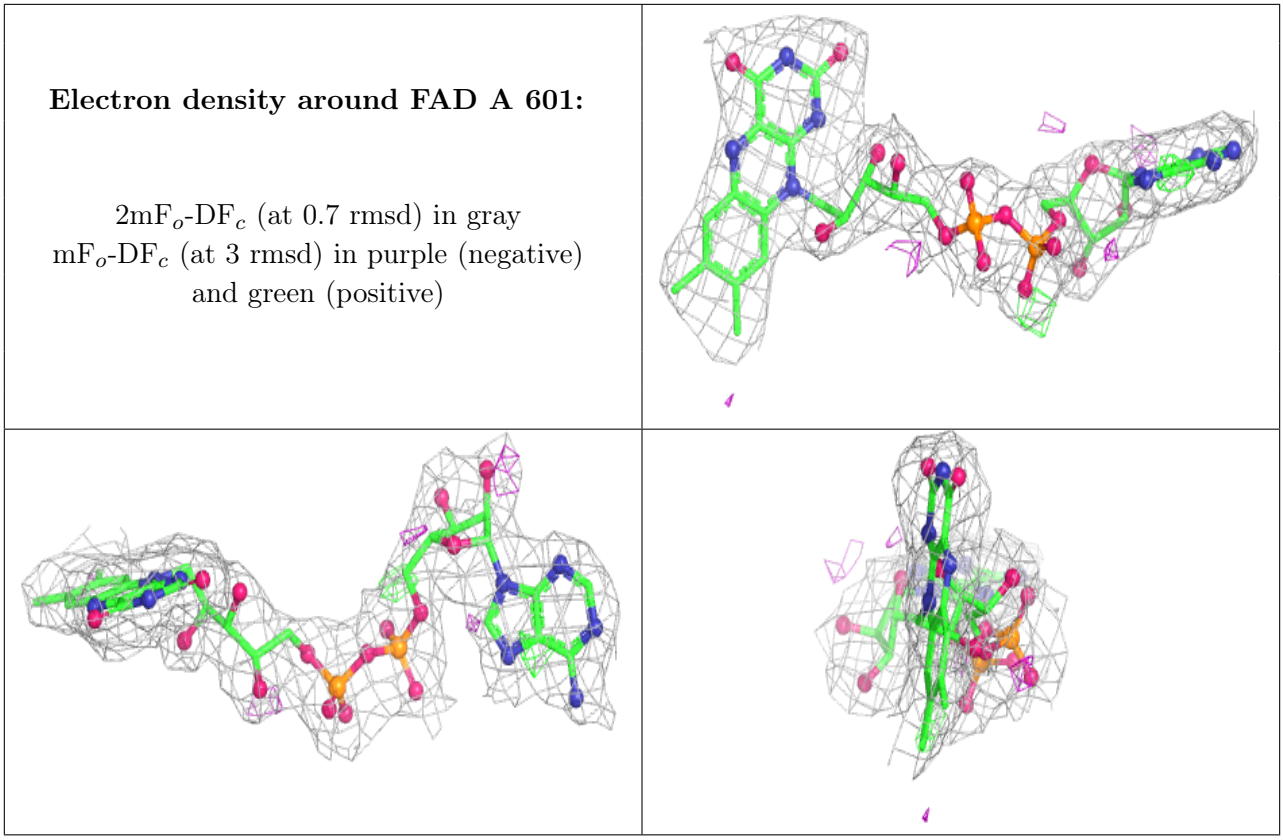






Electron density around FAD A 601:

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



6.5 Other polymers (i)

There are no such residues in this entry.