Full wwPDB X-ray Structure Validation Report (i)

Sep 28, 2023 – 11:12 AM EDT

PDB ID	:	2IGK
Title	:	Crystal structure of recombinant pyranose 2-oxidase
Authors	:	Divne, C.
Deposited on	:	2006-09-22
Resolution	:	1.80 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 (i) 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 (i)) were used in the production of this report:

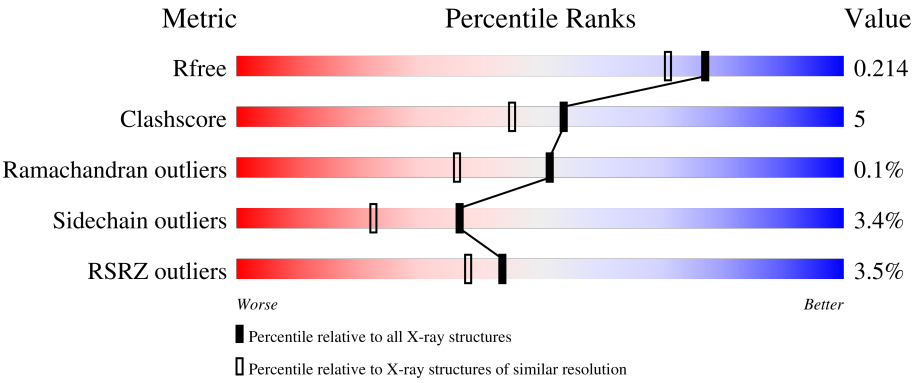
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	623	3% 85% 8% 7%
1	B	623	3% 81% 11% 7%
1	C	623	4% 83% 9% 7%
1	D	623	3% 84% 8% 7%
1	E	623	3% 81% 11% 7%

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Mol	Chain	Length	Quality of chain
1	F	623	3% 82% 9% • 7%
1	G	623	4% 82% 10% • 7%
1	H	623	2% 83% 8% • 7%

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
3	MES	A	902	-	-	X	-
3	MES	B	901	-	-	X	-
3	MES	C	904	-	-	X	-
3	MES	D	903	-	-	X	-
3	MES	E	906	-	-	X	-
3	MES	G	908	-	-	X	-
3	MES	H	907	-	-	X	-

2 Entry composition (i)

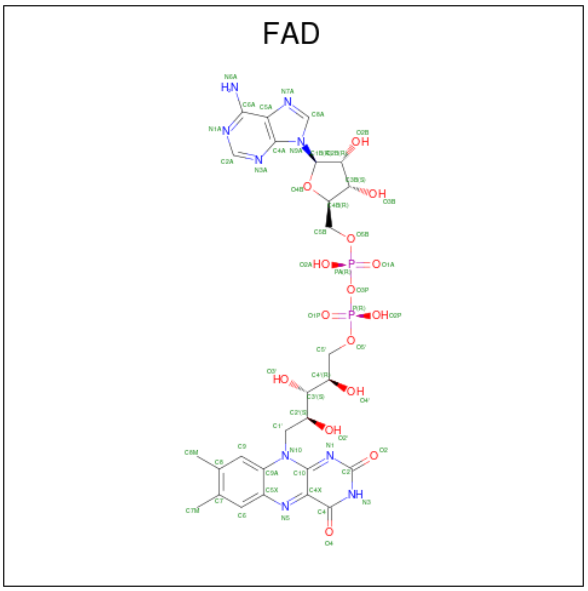
There are 4 unique types of molecules in this entry. The entry contains 39837 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pyranose oxidase.

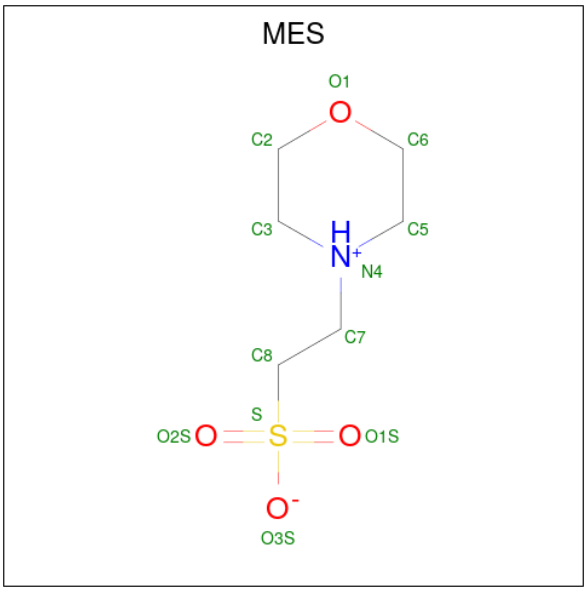
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	577	Total	C	N	O	S	0	0	0
			4549	2872	778	874	25			
1	B	577	Total	C	N	O	S	0	0	0
			4549	2872	778	874	25			
1	C	577	Total	C	N	O	S	0	0	0
			4549	2872	778	874	25			
1	D	577	Total	C	N	O	S	0	0	0
			4549	2872	778	874	25			
1	E	577	Total	C	N	O	S	0	0	0
			4549	2872	778	874	25			
1	F	577	Total	C	N	O	S	0	0	0
			4549	2872	778	874	25			
1	G	577	Total	C	N	O	S	0	0	0
			4549	2872	778	874	25			
1	H	577	Total	C	N	O	S	0	0	0
			4549	2872	778	874	25			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
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 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	417	Total	O	0	0
			417	417		
4	B	418	Total	O	0	0
			418	418		
4	C	307	Total	O	0	0
			307	307		
4	D	354	Total	O	0	0
			354	354		

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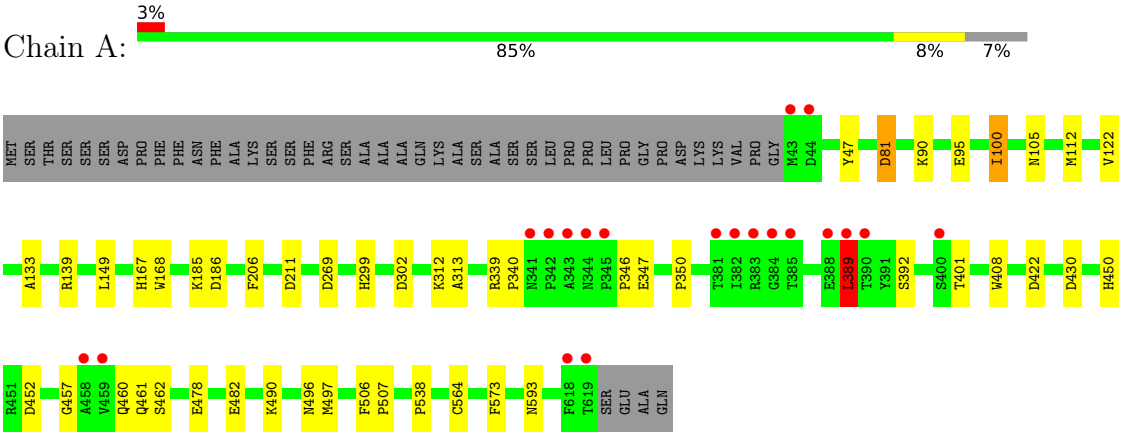
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	336	Total O 336 336	0	0
4	F	318	Total O 318 318	0	0
4	G	379	Total O 379 379	0	0
4	H	396	Total O 396 396	0	0

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.

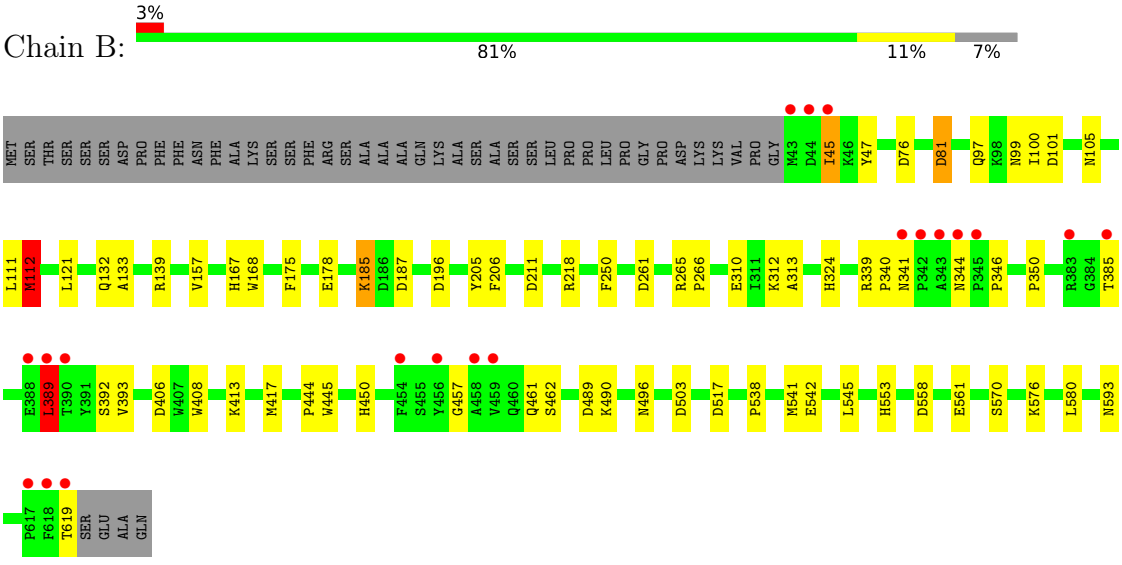
• Molecule 1: Pyranose oxidase

Chain A:



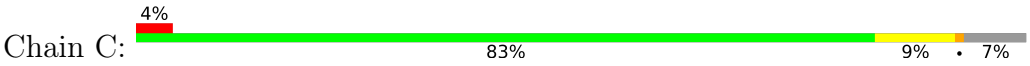
• Molecule 1: Pyranose oxidase

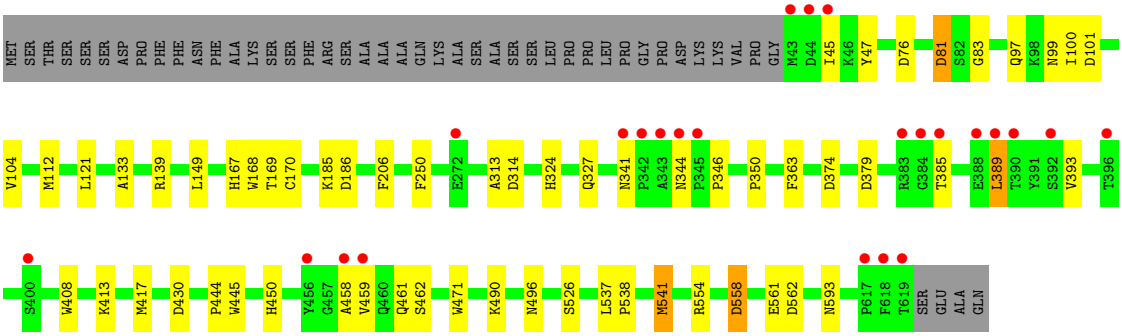
Chain B:



• Molecule 1: Pyranose oxidase

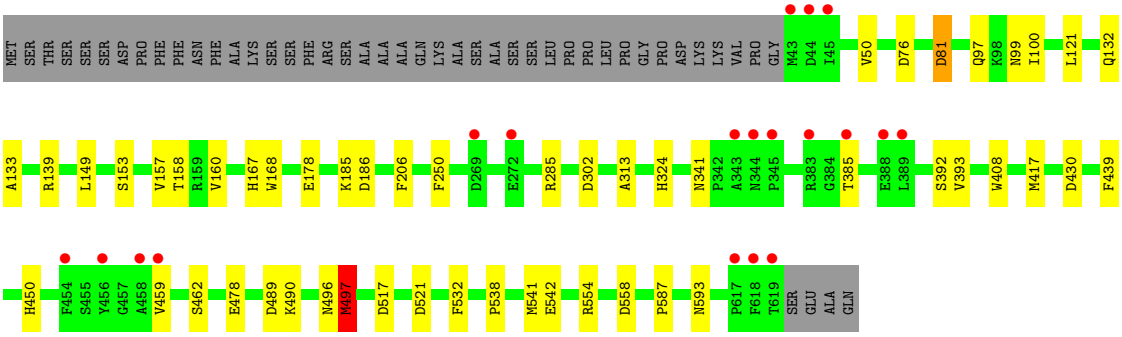
Chain C:





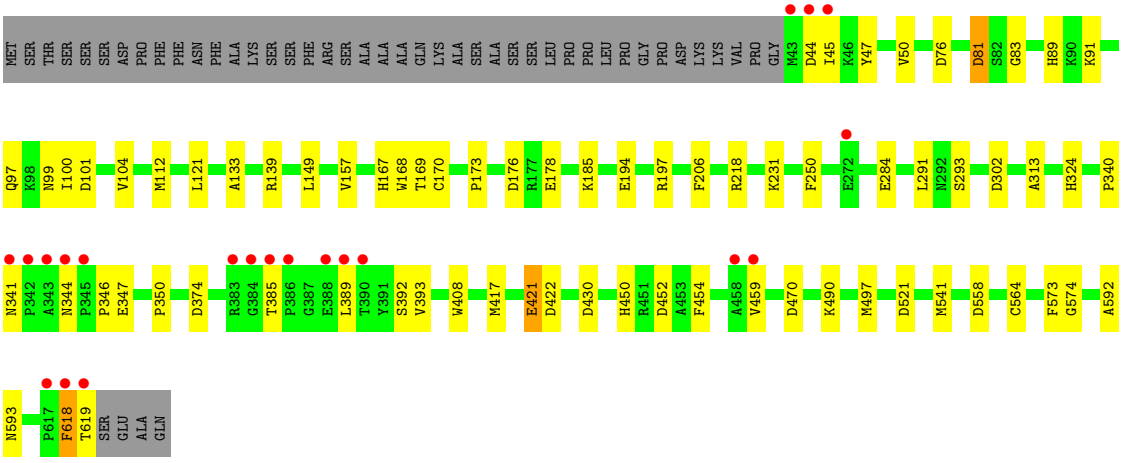
• Molecule 1: Pyranose oxidase

Chain D:



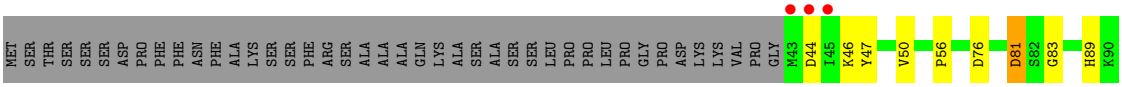
• Molecule 1: Pyranose oxidase

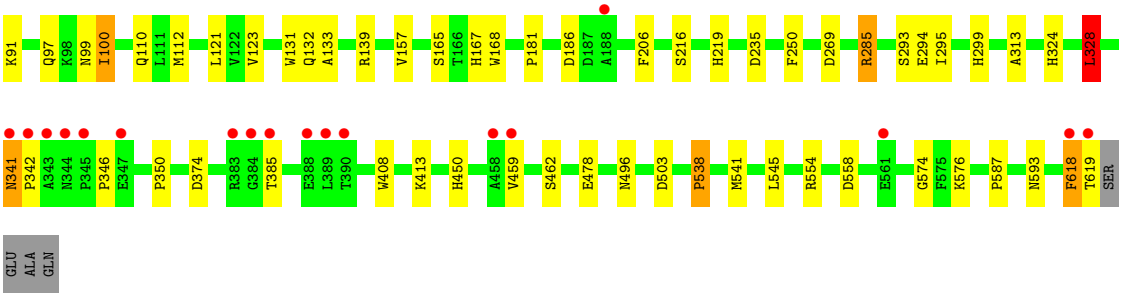
Chain E:



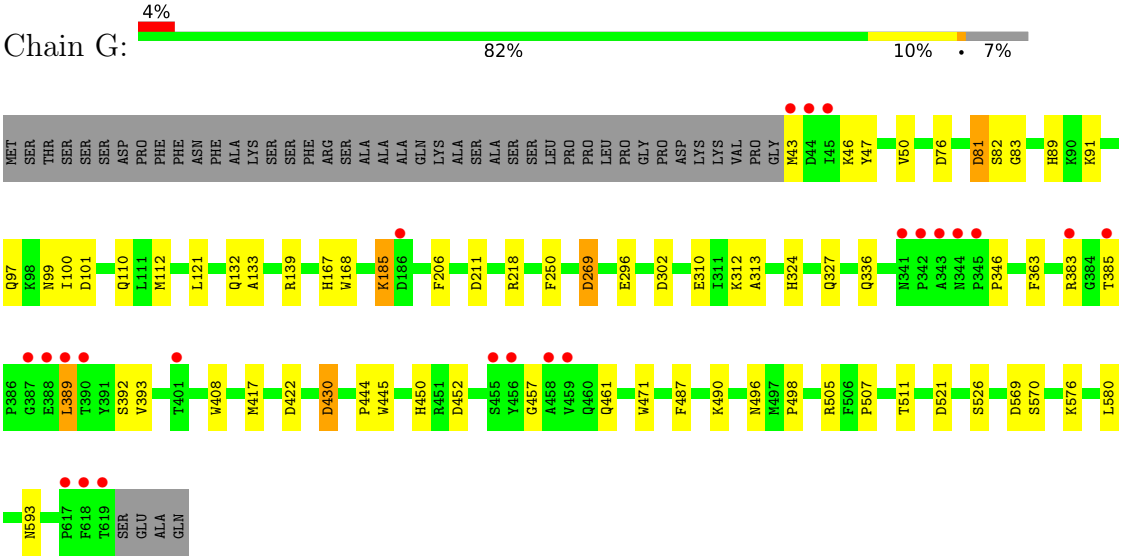
• Molecule 1: Pyranose oxidase

Chain F:

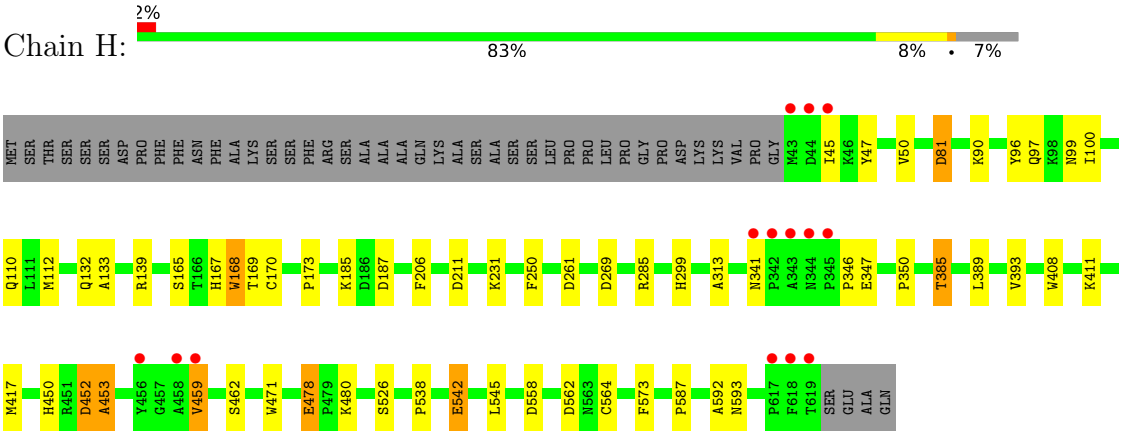




• Molecule 1: Pyranose oxidase



• Molecule 1: Pyranose oxidase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	168.78Å 103.86Å 169.26Å 90.00° 106.36° 90.00°	Depositor
Resolution (Å)	39.20 – 1.80 39.17 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.20-1.80) 99.9 (39.17-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.177 , 0.214 0.177 , 0.214	Depositor DCC
R_{free} test set	5182 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	19.1	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	39837	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.94% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, MES

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	1.01	3/4665 (0.1%)	0.95	13/6343 (0.2%)
1	B	0.97	3/4665 (0.1%)	0.98	15/6343 (0.2%)
1	C	0.87	0/4665	0.91	13/6343 (0.2%)
1	D	0.90	2/4665 (0.0%)	0.91	12/6343 (0.2%)
1	E	0.89	0/4665	0.90	14/6343 (0.2%)
1	F	0.88	1/4665 (0.0%)	0.92	14/6343 (0.2%)
1	G	0.95	1/4665 (0.0%)	0.96	14/6343 (0.2%)
1	H	0.96	2/4665 (0.0%)	0.97	13/6343 (0.2%)
All	All	0.93	12/37320 (0.0%)	0.94	108/50744 (0.2%)

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	B	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	112	MET	CB-CG	6.50	1.72	1.51
1	D	478	GLU	CD-OE1	5.70	1.31	1.25
1	B	205	TYR	CD1-CE1	5.67	1.47	1.39
1	H	96	TYR	CD2-CE2	-5.54	1.31	1.39
1	B	175	PHE	CE2-CZ	5.48	1.47	1.37
1	G	81	ASP	CA-C	5.42	1.67	1.52
1	A	482	GLU	CD-OE1	5.29	1.31	1.25
1	D	497	MET	SD-CE	-5.08	1.49	1.77
1	F	478	GLU	CD-OE1	5.08	1.31	1.25
1	A	122	VAL	CB-CG1	5.04	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	478	GLU	CD-OE1	5.01	1.31	1.25
1	A	478	GLU	CD-OE1	5.00	1.31	1.25

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	139	ARG	NE-CZ-NH2	-19.04	110.78	120.30
1	B	139	ARG	NE-CZ-NH2	-15.60	112.50	120.30
1	G	139	ARG	NE-CZ-NH2	-14.95	112.83	120.30
1	H	389	LEU	CA-CB-CG	14.62	148.93	115.30
1	B	139	ARG	NE-CZ-NH1	13.94	127.27	120.30
1	F	139	ARG	NE-CZ-NH1	13.24	126.92	120.30
1	D	139	ARG	NE-CZ-NH2	-12.78	113.91	120.30
1	C	139	ARG	NE-CZ-NH2	-12.73	113.93	120.30
1	E	139	ARG	NE-CZ-NH2	-12.48	114.06	120.30
1	G	81	ASP	CB-CG-OD2	12.41	129.47	118.30
1	G	139	ARG	NE-CZ-NH1	12.41	126.50	120.30
1	A	139	ARG	NE-CZ-NH2	-11.97	114.31	120.30
1	E	81	ASP	CB-CG-OD2	11.83	128.95	118.30
1	B	81	ASP	CB-CG-OD2	11.81	128.93	118.30
1	C	81	ASP	CB-CG-OD2	11.55	128.70	118.30
1	H	139	ARG	NE-CZ-NH2	-11.17	114.72	120.30
1	A	81	ASP	CB-CG-OD2	11.03	128.23	118.30
1	C	139	ARG	NE-CZ-NH1	10.69	125.64	120.30
1	H	81	ASP	CB-CG-OD2	10.63	127.87	118.30
1	H	81	ASP	CB-CG-OD1	-10.23	109.09	118.30
1	D	81	ASP	CB-CG-OD2	10.16	127.44	118.30
1	D	139	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	G	81	ASP	CB-CG-OD1	-9.15	110.06	118.30
1	F	76	ASP	CB-CG-OD2	9.08	126.47	118.30
1	F	81	ASP	CB-CG-OD2	9.00	126.40	118.30
1	A	81	ASP	CB-CG-OD1	-8.92	110.27	118.30
1	B	81	ASP	CB-CG-OD1	-8.70	110.47	118.30
1	G	76	ASP	CB-CG-OD2	8.29	125.76	118.30
1	E	81	ASP	CB-CG-OD1	-8.18	110.94	118.30
1	H	389	LEU	CB-CG-CD2	-7.85	97.66	111.00
1	D	302	ASP	CB-CG-OD2	7.67	125.20	118.30
1	E	139	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	H	139	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	A	139	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	C	81	ASP	CB-CG-OD1	-7.08	111.93	118.30
1	H	211	ASP	CB-CG-OD1	7.07	124.66	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	389	LEU	CB-CG-CD1	6.99	122.89	111.00
1	A	186	ASP	CB-CG-OD2	6.96	124.56	118.30
1	G	211	ASP	CB-CG-OD1	6.84	124.46	118.30
1	B	406	ASP	CB-CG-OD1	6.75	124.37	118.30
1	E	521	ASP	CB-CG-OD2	6.73	124.35	118.30
1	E	374	ASP	CB-CG-OD2	6.72	124.35	118.30
1	F	44	ASP	CB-CG-OD2	6.67	124.30	118.30
1	A	269	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	422	ASP	CB-CG-OD2	6.50	124.15	118.30
1	B	76	ASP	CB-CG-OD2	6.45	124.10	118.30
1	F	328	LEU	CA-CB-CG	6.34	129.89	115.30
1	B	489	ASP	CB-CG-OD1	6.31	123.98	118.30
1	G	101	ASP	CB-CG-OD2	6.24	123.92	118.30
1	C	558	ASP	CB-CG-OD2	6.17	123.85	118.30
1	B	503	ASP	CB-CG-OD2	6.12	123.80	118.30
1	A	389	LEU	CA-CB-CG	6.06	129.25	115.30
1	C	562	ASP	CB-CG-OD2	6.01	123.71	118.30
1	D	517	ASP	CB-CG-OD2	6.00	123.70	118.30
1	D	76	ASP	CB-CG-OD2	5.99	123.69	118.30
1	D	81	ASP	CB-CG-OD1	-5.94	112.95	118.30
1	H	562	ASP	CB-CG-OD2	5.94	123.64	118.30
1	C	541	MET	CG-SD-CE	5.93	109.69	100.20
1	F	81	ASP	CB-CG-OD1	-5.92	112.97	118.30
1	G	269	ASP	CB-CG-OD2	5.92	123.62	118.30
1	B	517	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	211	ASP	CB-CG-OD1	5.87	123.58	118.30
1	G	521	ASP	CB-CG-OD2	5.80	123.52	118.30
1	E	76	ASP	CB-CG-OD2	5.79	123.51	118.30
1	H	261	ASP	CB-CG-OD2	5.77	123.50	118.30
1	D	489	ASP	CB-CG-OD2	5.75	123.48	118.30
1	F	558	ASP	CB-CG-OD2	5.75	123.48	118.30
1	B	139	ARG	CD-NE-CZ	5.72	131.60	123.60
1	G	569	ASP	CB-CG-OD2	5.65	123.39	118.30
1	E	452	ASP	CB-CG-OD2	5.56	123.31	118.30
1	D	521	ASP	CB-CG-OD2	5.52	123.27	118.30
1	E	558	ASP	CB-CG-OD2	5.50	123.25	118.30
1	H	385	THR	OG1-CB-CG2	-5.48	97.41	110.00
1	G	452	ASP	CB-CG-OD2	5.43	123.18	118.30
1	C	314	ASP	CB-CG-OD1	5.41	123.17	118.30
1	H	558	ASP	CB-CG-OD2	5.41	123.17	118.30
1	C	374	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	261	ASP	CB-CG-OD1	5.40	123.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	187	ASP	CB-CG-OD2	5.37	123.13	118.30
1	E	302	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	101	ASP	CB-CG-OD2	5.34	123.11	118.30
1	F	374	ASP	CB-CG-OD2	5.33	123.10	118.30
1	E	422	ASP	CB-CG-OD2	5.32	123.08	118.30
1	A	302	ASP	CB-CG-OD2	5.31	123.08	118.30
1	D	558	ASP	CB-CG-OD2	5.31	123.08	118.30
1	F	186	ASP	CB-CG-OD2	5.29	123.06	118.30
1	G	430	ASP	CB-CG-OD2	5.27	123.04	118.30
1	F	269	ASP	CB-CG-OD2	5.21	122.99	118.30
1	G	302	ASP	CB-CG-OD2	5.21	122.99	118.30
1	G	422	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	139	ARG	CG-CD-NE	-5.18	100.92	111.80
1	A	430	ASP	CB-CG-OD2	5.17	122.96	118.30
1	C	379	ASP	CB-CG-OD2	5.17	122.95	118.30
1	E	44	ASP	CB-CG-OD2	5.16	122.94	118.30
1	F	139	ARG	CD-NE-CZ	5.14	130.80	123.60
1	F	503	ASP	CB-CG-OD2	5.14	122.92	118.30
1	E	470	ASP	CB-CG-OD1	5.12	122.91	118.30
1	B	211	ASP	CB-CG-OD1	5.08	122.88	118.30
1	B	196	ASP	CB-CG-OD1	5.08	122.87	118.30
1	C	186	ASP	CB-CG-OD2	5.08	122.87	118.30
1	F	235	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	452	ASP	CB-CG-OD2	5.08	122.87	118.30
1	D	430	ASP	CB-CG-OD2	5.06	122.86	118.30
1	D	541	MET	CG-SD-CE	5.04	108.27	100.20
1	C	430	ASP	CB-CG-OD2	5.04	122.83	118.30
1	C	76	ASP	CB-CG-OD2	5.03	122.83	118.30
1	H	269	ASP	CB-CG-OD2	5.02	122.82	118.30
1	E	430	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	553	HIS	Peptide

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	4549	0	4395	37	0
1	B	4549	0	4395	53	0
1	C	4549	0	4395	44	0
1	D	4549	0	4395	37	0
1	E	4549	0	4395	68	1
1	F	4549	0	4395	52	0
1	G	4549	0	4395	57	0
1	H	4549	0	4395	48	0
2	A	53	0	31	8	0
2	B	53	0	31	8	0
2	C	53	0	31	4	0
2	D	53	0	31	6	0
2	E	53	0	31	7	0
2	F	53	0	30	3	0
2	G	53	0	30	0	0
2	H	53	0	30	3	0
3	A	12	0	13	9	0
3	B	12	0	13	15	0
3	C	12	0	13	12	0
3	D	12	0	13	14	0
3	E	24	0	26	13	0
3	G	12	0	13	13	0
3	H	12	0	13	13	0
4	A	417	0	0	4	0
4	B	418	0	0	6	0
4	C	307	0	0	3	0
4	D	354	0	0	2	1
4	E	336	0	0	14	0
4	F	318	0	0	9	0
4	G	379	0	0	21	0
4	H	396	0	0	5	0
All	All	39837	0	35509	379	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 (379) 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:D:167:HIS:HE2	2:D:801:FAD:C8M	0.98	1.61
1:A:167:HIS:HE2	2:A:801:FAD:C8M	0.98	1.58
1:C:167:HIS:HE2	2:C:801:FAD:C8M	0.91	1.56
1:E:167:HIS:HE2	2:E:801:FAD:C8M	0.92	1.56
1:B:167:HIS:HE2	2:B:801:FAD:C8M	0.92	1.55
1:D:133:ALA:HB3	3:D:903:MES:C7	1.51	1.39
1:H:133:ALA:HB3	3:H:907:MES:C7	1.58	1.31
1:A:167:HIS:NE2	2:A:801:FAD:HM82	0.97	1.28
1:B:167:HIS:NE2	2:B:801:FAD:HM82	0.94	1.27
1:D:167:HIS:NE2	2:D:801:FAD:HM82	0.93	1.24
1:H:133:ALA:CB	3:H:907:MES:C7	2.15	1.24
1:E:167:HIS:NE2	2:E:801:FAD:HM82	0.88	1.21
1:C:167:HIS:CD2	2:C:801:FAD:HM82	1.76	1.20
1:C:133:ALA:HB3	3:C:904:MES:C7	1.72	1.20
1:G:133:ALA:HB3	3:G:908:MES:C7	1.72	1.19
1:B:133:ALA:HB3	3:B:901:MES:C7	1.73	1.19
1:A:133:ALA:HB3	3:A:902:MES:C7	1.73	1.18
1:C:167:HIS:NE2	2:C:801:FAD:HM82	0.86	1.18
1:D:133:ALA:CB	3:D:903:MES:C7	2.20	1.18
1:E:133:ALA:HB3	3:E:906:MES:C7	1.72	1.17
1:H:133:ALA:CB	3:H:907:MES:H72	1.72	1.17
1:C:133:ALA:HB3	3:C:904:MES:H72	1.17	1.15
1:D:133:ALA:CB	3:D:903:MES:H72	1.77	1.14
1:E:121:LEU:CD2	1:F:459:VAL:HA	1.76	1.14
1:D:133:ALA:HB3	3:D:903:MES:H71	1.32	1.11
1:E:167:HIS:CD2	2:E:801:FAD:HM82	1.87	1.09
1:B:133:ALA:HB3	3:B:901:MES:H72	1.29	1.09
1:A:133:ALA:HB3	3:A:902:MES:H72	1.28	1.08
1:H:133:ALA:HB3	3:H:907:MES:H72	1.13	1.08
1:B:167:HIS:CD2	2:B:801:FAD:HM82	1.88	1.07
1:G:133:ALA:HB3	3:G:908:MES:H72	1.31	1.07
1:G:133:ALA:CB	3:G:908:MES:C7	2.32	1.07
1:E:133:ALA:HB3	3:E:906:MES:H72	1.37	1.06
1:G:81:ASP:CA	4:G:3105:HOH:O	2.03	1.06
1:D:133:ALA:HB3	3:D:903:MES:H72	1.11	1.04
1:B:133:ALA:CB	3:B:901:MES:C7	2.34	1.03
1:E:121:LEU:HD23	1:F:459:VAL:HA	1.37	1.03
1:H:133:ALA:CB	3:H:907:MES:H71	1.88	1.03
1:D:167:HIS:CD2	2:D:801:FAD:HM82	1.94	1.02
1:H:133:ALA:HB3	3:H:907:MES:H71	1.42	1.02
1:F:81:ASP:HB2	4:F:3658:HOH:O	1.60	1.01
1:E:133:ALA:CB	3:E:906:MES:C7	2.37	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:ALA:HB3	3:E:906:MES:H71	1.39	1.00
1:G:133:ALA:CB	3:G:908:MES:H72	1.90	0.99
1:A:167:HIS:CD2	2:A:801:FAD:HM82	1.98	0.98
1:C:133:ALA:CB	3:C:904:MES:C7	2.44	0.96
1:B:167:HIS:HE2	2:B:801:FAD:HM81	1.25	0.96
1:G:81:ASP:CA	4:G:3782:HOH:O	2.14	0.95
1:G:110:GLN:HE21	1:G:167:HIS:HD1	1.15	0.95
1:C:133:ALA:CB	3:C:904:MES:H72	1.97	0.95
1:G:133:ALA:CB	3:G:908:MES:H71	1.97	0.94
1:H:393:VAL:H	1:H:417:MET:HE1	1.33	0.94
1:B:133:ALA:CB	3:B:901:MES:H72	1.95	0.93
1:D:133:ALA:CB	3:D:903:MES:H71	1.90	0.93
1:G:133:ALA:HB3	3:G:908:MES:H71	1.46	0.93
1:E:133:ALA:CB	3:E:906:MES:H72	1.98	0.93
1:E:133:ALA:CB	3:E:906:MES:H71	1.99	0.92
1:E:167:HIS:HE2	2:E:801:FAD:HM81	1.30	0.92
1:B:393:VAL:H	1:B:417:MET:CE	1.83	0.92
1:E:121:LEU:HD21	1:F:459:VAL:HG22	1.50	0.92
1:F:110:GLN:HE21	1:F:167:HIS:HD1	1.11	0.92
1:G:81:ASP:C	4:G:3782:HOH:O	2.07	0.91
1:B:133:ALA:HB3	3:B:901:MES:H71	1.49	0.91
4:E:2488:HOH:O	1:F:132:GLN:HG2	1.69	0.91
1:B:133:ALA:CB	3:B:901:MES:H71	2.01	0.90
1:G:81:ASP:C	4:G:3105:HOH:O	2.07	0.90
1:B:393:VAL:H	1:B:417:MET:HE2	1.35	0.90
1:A:133:ALA:HB3	3:A:902:MES:H71	1.53	0.89
1:D:133:ALA:HB2	3:D:903:MES:O1S	1.71	0.89
1:H:133:ALA:HB2	3:H:907:MES:C7	2.01	0.88
1:E:167:HIS:CE1	2:E:801:FAD:HM82	2.03	0.88
1:C:167:HIS:HE2	2:C:801:FAD:HM81	1.33	0.88
1:H:110:GLN:HE21	1:H:167:HIS:HD1	1.20	0.87
1:A:167:HIS:CE1	2:A:801:FAD:HM82	2.09	0.86
1:G:81:ASP:HA	4:G:3782:HOH:O	1.70	0.86
1:A:133:ALA:CB	3:A:902:MES:C7	2.52	0.85
1:B:133:ALA:HB2	3:B:901:MES:O1S	1.77	0.84
1:B:178:GLU:HG3	4:B:3228:HOH:O	1.77	0.83
1:D:393:VAL:H	1:D:417:MET:HE2	1.42	0.83
1:G:82:SER:N	4:G:3782:HOH:O	2.10	0.83
1:A:167:HIS:HE2	2:A:801:FAD:HM81	1.39	0.83
1:C:133:ALA:HB3	3:C:904:MES:H71	1.60	0.82
1:E:81:ASP:HA	4:F:3642:HOH:O	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:83:GLY:N	4:F:3642:HOH:O	2.13	0.82
1:F:83:GLY:HA2	4:F:3642:HOH:O	1.79	0.81
1:D:167:HIS:CE1	2:D:801:FAD:HM82	2.08	0.81
1:E:393:VAL:H	1:E:417:MET:HE1	1.45	0.81
1:G:133:ALA:HB2	3:G:908:MES:O1S	1.81	0.80
1:G:505:ARG:NH2	4:G:3175:HOH:O	2.14	0.80
1:E:393:VAL:H	1:E:417:MET:CE	1.95	0.80
1:G:83:GLY:N	4:G:2294:HOH:O	1.97	0.79
1:B:167:HIS:CE1	2:B:801:FAD:HM82	2.10	0.79
4:C:3530:HOH:O	1:D:81:ASP:HA	1.83	0.78
4:E:3661:HOH:O	1:F:81:ASP:HA	1.85	0.77
1:G:393:VAL:H	1:G:417:MET:CE	1.98	0.77
1:E:133:ALA:HB2	3:E:906:MES:O1S	1.85	0.76
1:F:97:GLN:HG3	1:F:250:PHE:CD2	2.20	0.76
1:F:538:PRO:HG2	1:H:538:PRO:HG2	1.67	0.76
1:A:133:ALA:CB	3:A:902:MES:H72	2.12	0.76
1:C:393:VAL:H	1:C:417:MET:HE1	1.52	0.74
1:F:167:HIS:CD2	2:F:801:FAD:C8M	2.67	0.74
3:E:906:MES:H52	4:E:2112:HOH:O	1.87	0.74
1:E:121:LEU:HD21	1:F:459:VAL:CG2	2.17	0.73
1:G:393:VAL:H	1:G:417:MET:HE2	1.53	0.73
1:B:576:LYS:HG3	4:B:3770:HOH:O	1.89	0.73
1:E:121:LEU:CD2	1:F:459:VAL:CA	2.63	0.72
1:D:133:ALA:HB2	3:D:903:MES:C7	2.19	0.72
1:H:167:HIS:CD2	2:H:801:FAD:C8M	2.71	0.72
1:G:97:GLN:HG3	1:G:250:PHE:CD2	2.24	0.72
1:F:83:GLY:CA	4:F:3642:HOH:O	2.33	0.71
1:A:133:ALA:HB2	3:A:902:MES:O1S	1.89	0.71
1:H:133:ALA:HB2	3:H:907:MES:O1S	1.91	0.71
1:A:100:ILE:HD13	1:A:100:ILE:O	1.92	0.70
1:E:541:MET:HA	1:E:541:MET:HE2	1.74	0.70
1:G:133:ALA:HB2	3:G:908:MES:C7	2.21	0.70
3:C:904:MES:H52	4:C:1926:HOH:O	1.91	0.69
1:B:133:ALA:HB2	3:B:901:MES:C7	2.23	0.69
3:G:908:MES:H52	4:G:1962:HOH:O	1.93	0.68
1:G:97:GLN:HG3	1:G:250:PHE:CE2	2.28	0.68
1:F:97:GLN:HG3	1:F:250:PHE:CE2	2.29	0.68
1:G:132:GLN:HG2	4:G:3160:HOH:O	1.93	0.68
1:D:393:VAL:H	1:D:417:MET:CE	2.06	0.68
1:G:81:ASP:O	4:G:3105:HOH:O	2.10	0.67
1:G:83:GLY:CA	4:G:2294:HOH:O	2.39	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:HIS:HE2	2:D:801:FAD:HM81	1.43	0.67
1:G:99:ASN:CB	1:H:112:MET:HE1	2.25	0.67
1:A:167:HIS:HE2	2:A:801:FAD:C8	2.00	0.67
1:C:133:ALA:CB	3:C:904:MES:H71	2.18	0.67
1:A:133:ALA:CB	3:A:902:MES:H71	2.21	0.66
1:G:81:ASP:C	1:G:81:ASP:OD1	2.32	0.65
4:G:2294:HOH:O	1:H:81:ASP:HA	1.96	0.65
1:H:167:HIS:CE1	2:H:801:FAD:C8M	2.75	0.65
1:H:393:VAL:H	1:H:417:MET:CE	2.08	0.65
1:G:81:ASP:HA	4:G:3105:HOH:O	1.79	0.65
1:C:393:VAL:H	1:C:417:MET:CE	2.09	0.64
1:E:121:LEU:HD21	1:F:459:VAL:CB	2.28	0.64
1:G:81:ASP:CB	4:G:3105:HOH:O	2.39	0.64
1:E:497:MET:CE	4:E:3557:HOH:O	2.47	0.63
1:E:497:MET:HE3	4:E:3557:HOH:O	1.98	0.63
1:B:81:ASP:OD1	1:B:81:ASP:C	2.35	0.63
1:E:121:LEU:CD2	1:F:459:VAL:HG22	2.27	0.63
1:F:133:ALA:O	4:G:3175:HOH:O	2.16	0.63
1:F:299:HIS:HB3	4:F:3325:HOH:O	1.98	0.63
1:H:167:HIS:NE2	2:H:801:FAD:HM81	2.00	0.63
1:E:83:GLY:N	4:E:3661:HOH:O	2.23	0.63
3:E:905:MES:H52	4:E:2488:HOH:O	1.97	0.63
1:F:541:MET:CE	1:F:545:LEU:HD23	2.29	0.62
1:B:457:GLY:O	1:B:461:GLN:HG3	2.00	0.61
1:G:336:GLN:HB2	1:G:346:PRO:HG3	1.83	0.61
1:C:112:MET:HE1	1:D:99:ASN:CB	2.31	0.61
1:H:50:VAL:HG13	1:H:313:ALA:HB2	1.83	0.61
1:G:392:SER:HA	1:G:417:MET:HE1	1.83	0.60
3:C:904:MES:H21	1:D:462:SER:OG	2.01	0.60
1:G:133:ALA:HB2	3:G:908:MES:H71	1.79	0.60
1:F:81:ASP:CA	4:F:3658:HOH:O	2.50	0.60
1:E:89:HIS:CE1	1:E:91:LYS:HG2	2.36	0.60
1:C:133:ALA:HB2	3:C:904:MES:O1S	2.01	0.59
1:C:462:SER:OG	3:D:903:MES:H21	2.03	0.58
1:A:462:SER:OG	3:B:901:MES:H21	2.04	0.58
1:F:167:HIS:CE1	2:F:801:FAD:C8M	2.76	0.58
1:G:83:GLY:HA2	4:G:2294:HOH:O	2.02	0.58
1:H:393:VAL:N	1:H:417:MET:HE1	2.10	0.58
1:C:97:GLN:HG3	1:C:250:PHE:CD2	2.38	0.58
1:B:393:VAL:H	1:B:417:MET:HE1	1.64	0.57
3:D:903:MES:H52	4:D:1743:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:ALA:HB2	3:E:906:MES:C7	2.30	0.57
1:E:121:LEU:HD21	1:F:459:VAL:HG13	1.87	0.57
3:E:905:MES:H32	3:E:905:MES:O3S	2.05	0.57
1:B:393:VAL:N	1:B:417:MET:HE2	2.12	0.56
1:E:167:HIS:CE1	2:E:801:FAD:C8M	2.77	0.56
1:B:167:HIS:HE2	2:B:801:FAD:C8	1.99	0.56
1:B:45:ILE:HD12	1:B:45:ILE:H	1.71	0.56
1:H:133:ALA:HB2	3:H:907:MES:C8	2.36	0.55
1:H:417:MET:CE	4:H:3504:HOH:O	2.54	0.55
1:E:421:GLU:CD	1:E:421:GLU:H	2.08	0.55
1:D:133:ALA:HB2	3:D:903:MES:H71	1.84	0.55
1:E:393:VAL:N	1:E:417:MET:HE1	2.20	0.55
1:A:457:GLY:H	1:A:460:GLN:HE21	1.52	0.55
1:H:346:PRO:HG2	1:H:350:PRO:HA	1.89	0.55
1:F:541:MET:HE3	1:F:545:LEU:HD23	1.88	0.55
1:G:296:GLU:O	1:G:312:LYS:HE3	2.08	0.54
1:G:81:ASP:HB2	4:G:3105:HOH:O	2.02	0.54
1:D:50:VAL:HG13	1:D:313:ALA:HB2	1.90	0.54
1:H:81:ASP:O	1:H:90:LYS:HE2	2.08	0.54
1:C:393:VAL:N	1:C:417:MET:HE1	2.21	0.53
1:D:97:GLN:HG3	1:D:250:PHE:CD2	2.42	0.53
1:B:97:GLN:HG3	1:B:250:PHE:CD2	2.43	0.53
1:E:97:GLN:HG3	1:E:250:PHE:CE2	2.43	0.53
1:H:133:ALA:HB2	3:H:907:MES:H71	1.71	0.53
1:H:564:CYS:HG	1:H:573:PHE:HE2	1.57	0.53
1:D:393:VAL:N	1:D:417:MET:HE2	2.19	0.53
1:B:389:LEU:H	1:B:389:LEU:HD13	1.74	0.52
1:B:538:PRO:HG2	1:D:538:PRO:HG2	1.90	0.52
1:E:459:VAL:HG12	1:F:123:VAL:HG22	1.92	0.52
1:G:112:MET:HE1	1:H:99:ASN:CB	2.38	0.52
1:F:346:PRO:HG2	1:F:350:PRO:HA	1.91	0.52
1:A:149:LEU:HD22	3:D:903:MES:H51	1.92	0.52
1:A:81:ASP:O	1:A:90:LYS:HE2	2.09	0.51
3:C:904:MES:H32	3:C:904:MES:O3S	2.10	0.51
1:E:618:PHE:CD1	1:E:618:PHE:C	2.84	0.51
1:E:97:GLN:HG3	1:E:250:PHE:CD2	2.45	0.51
1:E:169:THR:O	1:E:170:CYS:HB2	2.11	0.51
1:D:167:HIS:CE1	2:D:801:FAD:C8M	2.83	0.51
1:G:487:PHE:HB3	1:G:498:PRO:HB2	1.93	0.51
3:B:901:MES:H52	4:B:2032:HOH:O	2.10	0.51
1:B:167:HIS:CE1	2:B:801:FAD:C8M	2.81	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:618:PHE:C	1:E:618:PHE:HD1	2.15	0.50
1:H:417:MET:HE2	4:H:3504:HOH:O	2.10	0.50
1:B:133:ALA:HB2	3:B:901:MES:H71	1.84	0.50
1:G:393:VAL:H	1:G:417:MET:HE1	1.72	0.50
1:B:218:ARG:HD2	4:B:1194:HOH:O	2.12	0.50
1:C:324:HIS:HD2	1:C:327:GLN:OE1	1.94	0.50
1:B:167:HIS:NE2	2:B:801:FAD:C8	2.66	0.50
1:G:112:MET:HE1	1:H:99:ASN:HB3	1.94	0.50
3:G:908:MES:H21	1:H:462:SER:OG	2.10	0.50
1:A:81:ASP:C	1:A:81:ASP:OD1	2.50	0.49
1:D:158:THR:HG22	1:D:160:VAL:HG22	1.94	0.49
1:C:389:LEU:HD13	1:C:389:LEU:N	2.28	0.49
1:D:497:MET:HE3	1:D:497:MET:HA	1.94	0.49
1:C:133:ALA:HB2	3:C:904:MES:C7	2.39	0.49
1:E:121:LEU:HD21	1:F:459:VAL:CG1	2.43	0.49
1:F:285:ARG:HA	1:F:328:LEU:HD13	1.95	0.49
1:H:459:VAL:O	1:H:462:SER:HB3	2.13	0.49
1:D:178:GLU:CD	1:D:439:PHE:HE1	2.16	0.49
1:E:121:LEU:HD23	1:F:459:VAL:CA	2.27	0.49
1:G:324:HIS:HD2	1:G:327:GLN:OE1	1.96	0.49
1:G:324:HIS:CE1	4:G:2467:HOH:O	2.66	0.48
1:A:497:MET:CE	4:A:3235:HOH:O	2.60	0.48
1:E:392:SER:HA	1:E:417:MET:HE3	1.95	0.48
1:E:176:ASP:OD2	1:E:178:GLU:OE2	2.31	0.48
3:B:901:MES:H51	1:C:149:LEU:HD22	1.96	0.48
1:B:97:GLN:HG3	1:B:250:PHE:CE2	2.49	0.48
1:F:89:HIS:CE1	1:F:91:LYS:HB2	2.49	0.48
1:A:538:PRO:HG2	1:C:538:PRO:HG2	1.95	0.48
1:B:157:VAL:HG21	1:B:324:HIS:HE1	1.79	0.48
1:E:619:THR:HG22	4:E:2505:HOH:O	2.12	0.48
1:F:100:ILE:HG22	4:F:3798:HOH:O	2.14	0.47
1:H:165:SER:HA	1:H:168:TRP:CD1	2.49	0.47
1:G:457:GLY:O	1:G:461:GLN:HG3	2.14	0.47
3:C:904:MES:H31	3:C:904:MES:H82	1.56	0.47
1:G:444:PRO:HD2	1:G:445:TRP:CZ3	2.49	0.47
3:G:908:MES:H32	3:G:908:MES:O3S	2.15	0.47
1:F:81:ASP:CB	4:F:3658:HOH:O	2.32	0.47
1:G:471:TRP:CH2	1:G:526:SER:HA	2.49	0.47
1:A:389:LEU:HD13	1:A:389:LEU:H	1.80	0.47
1:C:459:VAL:O	1:C:462:SER:CB	2.63	0.47
1:H:478:GLU:OE2	1:H:480:LYS:HE2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:HIS:CE1	2:A:801:FAD:C8M	2.81	0.47
1:G:50:VAL:HG13	1:G:313:ALA:HB2	1.97	0.47
1:B:346:PRO:HG2	1:B:350:PRO:HA	1.97	0.47
1:F:50:VAL:HG13	1:F:313:ALA:HB2	1.96	0.47
1:G:576:LYS:HG2	4:G:2971:HOH:O	2.15	0.47
1:A:538:PRO:HG2	1:C:538:PRO:CG	2.44	0.47
1:E:284:GLU:HA	1:E:497:MET:CE	2.45	0.46
1:F:56:PRO:HD3	1:F:165:SER:HB3	1.96	0.46
1:G:507:PRO:HD2	1:G:511:THR:HG21	1.95	0.46
1:C:459:VAL:O	1:C:462:SER:HB3	2.15	0.46
1:E:99:ASN:CB	1:F:112:MET:HE1	2.45	0.46
1:H:47:TYR:O	1:H:313:ALA:HA	2.16	0.46
1:C:47:TYR:O	1:C:313:ALA:HA	2.15	0.46
1:E:133:ALA:HB2	3:E:906:MES:H71	1.92	0.46
1:E:157:VAL:HG21	1:E:324:HIS:HE1	1.81	0.46
1:E:618:PHE:HD1	1:E:619:THR:N	2.12	0.46
1:C:541:MET:CE	1:C:541:MET:HA	2.46	0.46
1:D:97:GLN:HG3	1:D:250:PHE:CE2	2.50	0.46
1:B:558:ASP:HB3	1:B:561:GLU:HB2	1.98	0.46
1:F:538:PRO:HG2	1:H:538:PRO:CG	2.43	0.46
1:H:285:ARG:HH22	1:H:299:HIS:CE1	2.34	0.46
1:H:478:GLU:CD	1:H:480:LYS:HE2	2.35	0.46
1:C:458:ALA:O	1:D:121:LEU:HD12	2.15	0.46
1:G:89:HIS:CE1	1:G:91:LYS:HB2	2.51	0.46
1:C:97:GLN:HG3	1:C:250:PHE:CE2	2.52	0.45
1:E:83:GLY:CA	4:E:3661:HOH:O	2.64	0.45
1:H:542:GLU:OE1	1:H:545:LEU:HD13	2.17	0.45
1:F:47:TYR:O	1:F:313:ALA:HA	2.17	0.45
1:H:97:GLN:HG3	1:H:250:PHE:CD2	2.52	0.45
3:E:906:MES:H21	1:F:462:SER:OG	2.16	0.45
1:F:541:MET:HE2	1:F:545:LEU:HD23	1.97	0.45
1:A:112:MET:HE1	1:B:99:ASN:CB	2.46	0.45
1:B:132:GLN:NE2	4:B:2718:HOH:O	2.41	0.45
1:B:541:MET:CE	1:B:545:LEU:HD23	2.47	0.45
1:F:167:HIS:NE2	2:F:801:FAD:HM81	2.07	0.45
3:D:903:MES:H71	4:D:1743:HOH:O	2.17	0.44
1:E:50:VAL:HG13	1:E:313:ALA:HB2	1.99	0.44
1:E:194:GLU:CD	1:E:197:ARG:HH21	2.20	0.44
1:E:497:MET:HE1	4:E:3557:HOH:O	2.15	0.44
1:E:149:LEU:HD22	3:H:907:MES:H51	1.99	0.44
1:E:393:VAL:H	1:E:417:MET:HE3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:169:THR:O	1:H:170:CYS:HB2	2.17	0.44
1:C:83:GLY:N	4:C:3530:HOH:O	2.27	0.44
1:C:81:ASP:OD1	1:C:81:ASP:C	2.54	0.44
1:F:294:GLU:HG2	1:F:295:ILE:N	2.32	0.44
1:H:97:GLN:HG3	1:H:250:PHE:CE2	2.52	0.44
1:C:101:ASP:O	1:C:104:VAL:HG12	2.18	0.43
1:E:173:PRO:HG2	1:E:592:ALA:HB1	2.00	0.43
1:B:47:TYR:O	1:B:313:ALA:HA	2.18	0.43
1:D:392:SER:HA	1:D:417:MET:HE1	2.00	0.43
1:E:47:TYR:O	1:E:313:ALA:HA	2.18	0.43
1:H:173:PRO:HG2	1:H:592:ALA:HB1	2.00	0.43
1:C:324:HIS:CD2	1:C:327:GLN:OE1	2.71	0.43
1:F:293:SER:HA	1:F:574:GLY:O	2.18	0.43
1:G:47:TYR:O	1:G:313:ALA:HA	2.18	0.43
3:H:907:MES:H82	3:H:907:MES:H31	1.36	0.43
1:A:105:ASN:O	1:B:105:ASN:HB3	2.19	0.43
1:B:392:SER:HA	1:B:417:MET:HE1	2.00	0.43
1:F:181:PRO:HG3	1:F:587:PRO:HD2	2.00	0.43
3:G:908:MES:H31	3:G:908:MES:H82	1.64	0.43
1:C:363:PHE:HA	1:C:471:TRP:O	2.19	0.43
1:D:153:SER:OG	1:D:542:GLU:HG3	2.18	0.43
1:E:346:PRO:HG2	1:E:350:PRO:HA	1.99	0.43
1:C:537:LEU:HB3	1:C:538:PRO:HD2	2.01	0.43
1:G:389:LEU:N	1:G:389:LEU:CD1	2.82	0.43
1:C:346:PRO:HG2	1:C:350:PRO:HA	2.00	0.43
1:E:112:MET:HE1	1:F:99:ASN:CB	2.49	0.43
1:H:411:LYS:HD3	4:H:2747:HOH:O	2.18	0.43
1:B:121:LEU:CD2	1:C:121:LEU:CD2	2.97	0.42
1:G:218:ARG:HD2	4:G:1363:HOH:O	2.19	0.42
1:A:95:GLU:HG3	1:B:112:MET:CE	2.49	0.42
1:E:101:ASP:O	1:E:104:VAL:HG12	2.19	0.42
1:E:218:ARG:HD2	4:E:1455:HOH:O	2.19	0.42
3:H:907:MES:H52	4:H:2336:HOH:O	2.18	0.42
1:A:564:CYS:HG	1:A:573:PHE:HE2	1.63	0.42
1:D:157:VAL:HG21	1:D:324:HIS:HE1	1.84	0.42
1:F:341:ASN:HD22	1:F:342:PRO:HD2	1.83	0.42
1:C:112:MET:CE	1:D:99:ASN:CG	2.87	0.42
1:C:558:ASP:HB3	1:C:561:GLU:HB2	2.01	0.42
1:B:81:ASP:OD1	1:B:81:ASP:O	2.38	0.42
1:A:497:MET:HE1	4:A:3235:HOH:O	2.19	0.42
1:G:570:SER:HB3	1:G:580:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:452:ASP:O	1:H:453:ALA:C	2.57	0.42
1:E:121:LEU:HD12	4:E:2793:HOH:O	2.20	0.42
1:A:167:HIS:NE2	2:A:801:FAD:C8	2.72	0.42
1:A:339:ARG:HA	1:A:340:PRO:HD3	1.93	0.42
1:E:167:HIS:NE2	2:E:801:FAD:C8	2.71	0.42
1:A:299:HIS:HB3	4:A:2839:HOH:O	2.20	0.42
1:D:532:PHE:CZ	1:D:538:PRO:HG3	2.55	0.42
1:F:131:TRP:CH2	1:F:133:ALA:HB2	2.55	0.42
1:A:497:MET:HE2	4:A:3235:HOH:O	2.19	0.41
1:B:185:LYS:HB2	1:B:185:LYS:HE3	1.89	0.41
1:C:471:TRP:CH2	1:C:526:SER:HA	2.55	0.41
3:A:902:MES:H51	1:D:149:LEU:HD22	2.01	0.41
1:B:339:ARG:HA	1:B:340:PRO:HD3	1.89	0.41
1:E:564:CYS:HG	1:E:573:PHE:HE2	1.66	0.41
1:G:218:ARG:HG3	1:G:430:ASP:OD2	2.21	0.41
1:A:47:TYR:O	1:A:313:ALA:HA	2.21	0.41
1:A:95:GLU:HG3	1:B:112:MET:HE2	2.01	0.41
1:B:542:GLU:OE1	1:B:545:LEU:HD13	2.20	0.41
3:B:901:MES:H71	4:B:2032:HOH:O	2.20	0.41
1:F:216:SER:HB3	1:F:219:HIS:HB3	2.03	0.41
1:C:444:PRO:HD2	1:C:445:TRP:CZ3	2.56	0.41
1:F:618:PHE:C	1:F:618:PHE:CD1	2.94	0.41
1:H:471:TRP:CH2	1:H:526:SER:HA	2.56	0.41
1:B:444:PRO:HD2	1:B:445:TRP:CZ3	2.56	0.41
1:F:157:VAL:HG21	1:F:324:HIS:HE1	1.86	0.41
1:G:112:MET:CE	1:H:99:ASN:CG	2.89	0.41
1:G:363:PHE:HA	1:G:471:TRP:O	2.20	0.41
1:C:112:MET:HE1	1:D:99:ASN:CG	2.40	0.41
1:C:169:THR:O	1:C:170:CYS:HB2	2.21	0.41
1:D:459:VAL:O	1:D:462:SER:HB3	2.20	0.41
1:E:83:GLY:HA2	4:E:3661:HOH:O	2.20	0.41
1:E:121:LEU:CD2	1:F:459:VAL:HG13	2.51	0.41
1:E:454:PHE:HA	4:E:3652:HOH:O	2.21	0.41
1:G:185:LYS:H	1:G:185:LYS:HG2	1.69	0.41
1:F:121:LEU:HD21	1:G:121:LEU:CD2	2.51	0.41
1:H:285:ARG:NH2	1:H:299:HIS:CE1	2.89	0.41
1:B:265:ARG:HA	1:B:266:PRO:C	2.42	0.40
1:E:293:SER:HA	1:E:574:GLY:O	2.21	0.40
3:A:902:MES:H21	1:B:462:SER:OG	2.22	0.40
1:B:111:LEU:HD23	1:B:111:LEU:HA	1.97	0.40
1:E:81:ASP:OD1	1:E:81:ASP:C	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:99:ASN:CG	1:H:112:MET:CE	2.90	0.40
1:A:346:PRO:HG2	1:A:350:PRO:HA	2.03	0.40
3:D:903:MES:H32	3:D:903:MES:O3S	2.21	0.40
1:B:133:ALA:HB2	3:B:901:MES:C8	2.51	0.40
1:H:299:HIS:HB3	4:H:3326:HOH:O	2.20	0.40
1:A:506:PHE:HA	1:A:507:PRO:HD3	1.94	0.40
1:B:570:SER:HB3	1:B:580:LEU:O	2.21	0.40
3:B:901:MES:H31	3:B:901:MES:H82	1.63	0.40
1:C:541:MET:HA	1:C:541:MET:HE3	2.04	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:E:291:LEU:CD2	4:D:3818:HOH:O[2_665]	1.77	0.43

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	575/623 (92%)	556 (97%)	19 (3%)	0	100	100
1	B	575/623 (92%)	562 (98%)	12 (2%)	1 (0%)	47	33
1	C	575/623 (92%)	559 (97%)	16 (3%)	0	100	100
1	D	575/623 (92%)	561 (98%)	14 (2%)	0	100	100
1	E	575/623 (92%)	555 (96%)	20 (4%)	0	100	100
1	F	575/623 (92%)	559 (97%)	16 (3%)	0	100	100
1	G	575/623 (92%)	557 (97%)	17 (3%)	1 (0%)	47	33
1	H	575/623 (92%)	561 (98%)	12 (2%)	2 (0%)	41	27
All	All	4600/4984 (92%)	4470 (97%)	126 (3%)	4 (0%)	51	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	46	LYS
1	H	187	ASP
1	H	453	ALA
1	B	389	LEU

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	505/542 (93%)	490 (97%)	15 (3%)	41	27
1	B	505/542 (93%)	486 (96%)	19 (4%)	33	18
1	C	505/542 (93%)	487 (96%)	18 (4%)	35	20
1	D	505/542 (93%)	488 (97%)	17 (3%)	37	22
1	E	505/542 (93%)	487 (96%)	18 (4%)	35	20
1	F	505/542 (93%)	487 (96%)	18 (4%)	35	20
1	G	505/542 (93%)	490 (97%)	15 (3%)	41	27
1	H	505/542 (93%)	488 (97%)	17 (3%)	37	22
All	All	4040/4336 (93%)	3903 (97%)	137 (3%)	37	22

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ILE
1	A	168	TRP
1	A	185	LYS
1	A	206	PHE
1	A	312	LYS
1	A	347	GLU
1	A	389	LEU
1	A	392	SER
1	A	401	THR
1	A	408	TRP

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Mol	Chain	Res	Type
1	A	450	HIS
1	A	461	GLN
1	A	490	LYS
1	A	496	ASN
1	A	593	ASN
1	B	45	ILE
1	B	100	ILE
1	B	112	MET
1	B	168	TRP
1	B	185	LYS
1	B	206	PHE
1	B	310	GLU
1	B	312	LYS
1	B	341	ASN
1	B	344	ASN
1	B	385	THR
1	B	389	LEU
1	B	408	TRP
1	B	413	LYS
1	B	450	HIS
1	B	490	LYS
1	B	496	ASN
1	B	593	ASN
1	B	619	THR
1	C	45	ILE
1	C	99	ASN
1	C	100	ILE
1	C	168	TRP
1	C	185	LYS
1	C	206	PHE
1	C	341	ASN
1	C	344	ASN
1	C	385	THR
1	C	389	LEU
1	C	408	TRP
1	C	413	LYS
1	C	450	HIS
1	C	461	GLN
1	C	490	LYS
1	C	496	ASN
1	C	554	ARG
1	C	593	ASN

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Mol	Chain	Res	Type
1	D	100	ILE
1	D	132	GLN
1	D	168	TRP
1	D	185	LYS
1	D	186	ASP
1	D	206	PHE
1	D	285	ARG
1	D	341	ASN
1	D	385	THR
1	D	408	TRP
1	D	450	HIS
1	D	490	LYS
1	D	496	ASN
1	D	497	MET
1	D	554	ARG
1	D	587	PRO
1	D	593	ASN
1	E	45	ILE
1	E	100	ILE
1	E	168	TRP
1	E	185	LYS
1	E	206	PHE
1	E	231	LYS
1	E	340	PRO
1	E	341	ASN
1	E	344	ASN
1	E	347	GLU
1	E	385	THR
1	E	389	LEU
1	E	408	TRP
1	E	421	GLU
1	E	450	HIS
1	E	490	LYS
1	E	593	ASN
1	E	618	PHE
1	F	46	LYS
1	F	100	ILE
1	F	168	TRP
1	F	206	PHE
1	F	285	ARG
1	F	328	LEU
1	F	341	ASN

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Mol	Chain	Res	Type
1	F	385	THR
1	F	408	TRP
1	F	413	LYS
1	F	450	HIS
1	F	496	ASN
1	F	538	PRO
1	F	554	ARG
1	F	576	LYS
1	F	593	ASN
1	F	618	PHE
1	F	619	THR
1	G	43	MET
1	G	100	ILE
1	G	168	TRP
1	G	185	LYS
1	G	206	PHE
1	G	269	ASP
1	G	310	GLU
1	G	383	ARG
1	G	385	THR
1	G	389	LEU
1	G	408	TRP
1	G	450	HIS
1	G	490	LYS
1	G	496	ASN
1	G	593	ASN
1	H	45	ILE
1	H	100	ILE
1	H	132	GLN
1	H	168	TRP
1	H	185	LYS
1	H	206	PHE
1	H	231	LYS
1	H	341	ASN
1	H	347	GLU
1	H	385	THR
1	H	408	TRP
1	H	450	HIS
1	H	452	ASP
1	H	459	VAL
1	H	542	GLU
1	H	587	PRO

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Mol	Chain	Res	Type
1	H	593	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	A	324	HIS
1	A	341	ASN
1	A	460	GLN
1	B	263	GLN
1	B	324	HIS
1	B	341	ASN
1	B	460	GLN
1	C	99	ASN
1	C	263	GLN
1	C	324	HIS
1	C	341	ASN
1	D	263	GLN
1	D	324	HIS
1	D	331	ASN
1	D	341	ASN
1	D	460	GLN
1	D	461	GLN
1	E	99	ASN
1	E	263	GLN
1	E	324	HIS
1	E	341	ASN
1	E	460	GLN
1	E	461	GLN
1	F	324	HIS
1	F	341	ASN
1	F	460	GLN
1	G	263	GLN
1	G	324	HIS
1	G	341	ASN
1	G	460	GLN
1	G	611	GLN
1	H	324	HIS
1	H	341	ASN
1	H	460	GLN
1	H	611	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)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FAD	C	801	1	53,58,58	1.39	7 (13%)	68,89,89	1.44	9 (13%)
3	MES	A	902	-	12,12,12	1.24	2 (16%)	14,16,16	11.33	9 (64%)
2	FAD	H	801	1	53,58,58	1.30	6 (11%)	68,89,89	1.57	10 (14%)
3	MES	D	903	-	12,12,12	1.17	1 (8%)	14,16,16	14.50	9 (64%)
3	MES	E	905	-	12,12,12	1.14	1 (8%)	14,16,16	12.15	8 (57%)
2	FAD	D	801	1	53,58,58	1.24	4 (7%)	68,89,89	1.50	12 (17%)
2	FAD	A	801	1	53,58,58	1.47	5 (9%)	68,89,89	1.60	7 (10%)
3	MES	B	901	-	12,12,12	1.29	2 (16%)	14,16,16	12.78	8 (57%)
3	MES	E	906	-	12,12,12	0.89	1 (8%)	14,16,16	12.81	9 (64%)
3	MES	H	907	-	12,12,12	0.97	1 (8%)	14,16,16	11.77	8 (57%)
3	MES	G	908	-	12,12,12	1.11	2 (16%)	14,16,16	12.97	10 (71%)
2	FAD	G	801	1	53,58,58	1.36	5 (9%)	68,89,89	1.52	9 (13%)
3	MES	C	904	-	12,12,12	1.38	1 (8%)	14,16,16	13.27	9 (64%)
2	FAD	E	801	1	53,58,58	1.25	5 (9%)	68,89,89	1.50	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FAD	F	801	1	53,58,58	1.24	5 (9%)	68,89,89	1.41	12 (17%)
2	FAD	B	801	1	53,58,58	1.21	6 (11%)	68,89,89	1.64	13 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	C	801	1	-	2/30/50/50	0/6/6/6
3	MES	A	902	-	-	2/6/14/14	0/1/1/1
2	FAD	H	801	1	-	1/30/50/50	0/6/6/6
3	MES	D	903	-	-	4/6/14/14	0/1/1/1
3	MES	E	905	-	-	2/6/14/14	0/1/1/1
2	FAD	D	801	1	-	4/30/50/50	0/6/6/6
2	FAD	A	801	1	-	2/30/50/50	0/6/6/6
3	MES	B	901	-	-	2/6/14/14	0/1/1/1
3	MES	E	906	-	-	4/6/14/14	0/1/1/1
3	MES	H	907	-	-	3/6/14/14	0/1/1/1
3	MES	G	908	-	-	4/6/14/14	0/1/1/1
2	FAD	G	801	1	-	1/30/50/50	0/6/6/6
3	MES	C	904	-	-	2/6/14/14	0/1/1/1
2	FAD	E	801	1	-	1/30/50/50	0/6/6/6
2	FAD	F	801	1	-	2/30/50/50	0/6/6/6
2	FAD	B	801	1	-	2/30/50/50	0/6/6/6

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	FAD	C4X-N5	5.42	1.41	1.30
2	H	801	FAD	C2A-N3A	5.16	1.40	1.32
2	A	801	FAD	C2A-N3A	5.10	1.40	1.32
2	F	801	FAD	C4X-N5	5.04	1.40	1.30
2	B	801	FAD	C4X-N5	5.02	1.40	1.30
2	G	801	FAD	C2A-N3A	4.99	1.40	1.32
2	A	801	FAD	C4X-N5	4.96	1.40	1.30
2	C	801	FAD	C4X-N5	4.80	1.40	1.30
2	G	801	FAD	C4X-N5	4.20	1.38	1.30
3	C	904	MES	C8-S	4.08	1.83	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	801	FAD	C2A-N3A	4.03	1.38	1.32
2	E	801	FAD	C4X-N5	3.94	1.38	1.30
2	C	801	FAD	C10-N1	3.65	1.40	1.33
2	H	801	FAD	C4X-N5	3.48	1.37	1.30
3	B	901	MES	C8-S	3.45	1.82	1.77
2	D	801	FAD	O4B-C1B	3.44	1.45	1.41
2	C	801	FAD	C2A-N3A	3.32	1.37	1.32
3	A	902	MES	C8-S	3.25	1.82	1.77
2	E	801	FAD	C2A-N1A	3.23	1.39	1.33
2	F	801	FAD	C2A-N3A	3.22	1.37	1.32
2	F	801	FAD	C2A-N1A	3.21	1.39	1.33
2	D	801	FAD	C2A-N3A	3.08	1.37	1.32
2	H	801	FAD	C2A-N1A	3.06	1.39	1.33
2	B	801	FAD	C2A-N3A	3.04	1.37	1.32
3	E	905	MES	C8-S	3.00	1.81	1.77
2	C	801	FAD	C2A-N1A	2.93	1.39	1.33
3	D	903	MES	C8-S	2.91	1.81	1.77
2	G	801	FAD	C10-N1	2.87	1.39	1.33
2	H	801	FAD	C10-N1	2.75	1.38	1.33
2	B	801	FAD	C5'-C4'	2.68	1.55	1.51
2	G	801	FAD	C5'-C4'	2.68	1.55	1.51
2	D	801	FAD	C10-N1	2.66	1.38	1.33
2	B	801	FAD	C10-N1	2.62	1.38	1.33
2	A	801	FAD	C5'-C4'	2.61	1.55	1.51
3	H	907	MES	C8-S	2.48	1.81	1.77
2	F	801	FAD	C10-N1	2.47	1.38	1.33
2	B	801	FAD	C2A-N1A	2.47	1.38	1.33
2	A	801	FAD	O4B-C1B	2.44	1.44	1.41
3	G	908	MES	C8-S	2.43	1.81	1.77
2	H	801	FAD	C5'-C4'	2.40	1.55	1.51
2	E	801	FAD	O4B-C1B	2.31	1.44	1.41
2	A	801	FAD	C10-N1	2.31	1.37	1.33
2	E	801	FAD	C10-N1	2.25	1.37	1.33
2	C	801	FAD	C9-C8	2.22	1.42	1.39
2	C	801	FAD	PA-O1A	-2.15	1.43	1.50
3	E	906	MES	C8-S	2.14	1.80	1.77
3	G	908	MES	O1S-S	2.11	1.51	1.45
2	C	801	FAD	C5X-N5	-2.11	1.35	1.39
3	A	902	MES	O1S-S	2.06	1.51	1.45
2	B	801	FAD	C4X-C10	-2.06	1.38	1.44
2	G	801	FAD	C2A-N1A	2.05	1.37	1.33
2	H	801	FAD	O4-C4	2.04	1.27	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	901	MES	O1S-S	2.04	1.51	1.45
2	F	801	FAD	C4A-N3A	2.02	1.38	1.35

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	903	MES	O2S-S-C8	51.56	169.00	106.92
3	C	904	MES	O2S-S-C8	47.21	163.77	106.92
3	G	908	MES	O2S-S-C8	45.73	161.99	106.92
3	E	906	MES	O2S-S-C8	45.58	161.79	106.92
3	B	901	MES	O2S-S-C8	45.38	161.56	106.92
3	E	905	MES	O2S-S-C8	43.13	158.85	106.92
3	H	907	MES	O2S-S-C8	41.93	157.41	106.92
3	A	902	MES	O2S-S-C8	40.26	155.39	106.92
3	G	908	MES	O3S-S-C8	-9.52	90.37	105.77
3	D	903	MES	O3S-S-C8	-8.99	91.23	105.77
3	B	901	MES	O3S-S-O2S	-8.69	90.03	111.27
3	C	904	MES	O3S-S-C8	-8.11	92.65	105.77
2	A	801	FAD	N3A-C2A-N1A	-8.06	116.08	128.68
3	D	903	MES	O3S-S-O2S	-8.02	91.67	111.27
3	H	907	MES	O3S-S-O2S	-7.70	92.47	111.27
3	E	906	MES	O3S-S-O2S	-7.47	93.01	111.27
3	C	904	MES	O3S-S-O2S	-7.36	93.29	111.27
3	D	903	MES	O1S-S-C8	-7.05	98.42	106.92
3	G	908	MES	O1S-S-C8	-6.86	98.65	106.92
3	E	906	MES	O3S-S-C8	-6.79	94.79	105.77
3	D	903	MES	O2S-S-O1S	-6.65	90.94	113.95
3	E	905	MES	O1S-S-C8	-6.65	98.91	106.92
2	H	801	FAD	N3A-C2A-N1A	-6.50	118.52	128.68
3	E	905	MES	O3S-S-C8	-6.49	95.27	105.77
3	E	905	MES	O3S-S-O2S	-6.21	96.11	111.27
3	A	902	MES	O3S-S-O2S	-6.16	96.23	111.27
3	C	904	MES	O2S-S-O1S	-5.97	93.28	113.95
3	G	908	MES	O3S-S-O2S	-5.95	96.74	111.27
3	B	901	MES	O1S-S-C8	-5.89	99.82	106.92
2	B	801	FAD	N3A-C2A-N1A	-5.87	119.51	128.68
3	A	902	MES	O3S-S-C8	-5.84	96.33	105.77
3	C	904	MES	O1S-S-C8	-5.71	100.04	106.92
3	E	906	MES	O2S-S-O1S	-5.70	94.23	113.95
3	A	902	MES	O3S-S-O1S	-5.63	97.53	111.27
2	G	801	FAD	N3A-C2A-N1A	-5.61	119.90	128.68
2	E	801	FAD	N3A-C2A-N1A	-5.40	120.24	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	907	MES	O2S-S-O1S	-5.39	95.28	113.95
3	B	901	MES	O3S-S-O1S	-5.34	98.22	111.27
3	B	901	MES	O2S-S-O1S	-5.29	95.65	113.95
3	E	906	MES	O3S-S-O1S	-5.26	98.42	111.27
2	F	801	FAD	N3A-C2A-N1A	-5.22	120.51	128.68
3	G	908	MES	O3S-S-O1S	-5.16	98.68	111.27
3	B	901	MES	O3S-S-C8	-5.06	97.58	105.77
2	C	801	FAD	N3A-C2A-N1A	-5.04	120.81	128.68
3	E	905	MES	O2S-S-O1S	-5.04	96.52	113.95
3	E	906	MES	O1S-S-C8	-5.04	100.85	106.92
3	G	908	MES	O2S-S-O1S	-5.01	96.62	113.95
3	A	902	MES	O2S-S-O1S	-5.00	96.66	113.95
3	E	905	MES	C5-N4-C3	4.60	119.19	108.83
3	A	902	MES	C5-N4-C3	4.52	119.00	108.83
3	G	908	MES	C5-N4-C3	4.51	118.98	108.83
3	H	907	MES	O3S-S-O1S	-4.51	100.26	111.27
3	E	905	MES	O3S-S-O1S	-4.50	100.29	111.27
3	H	907	MES	O3S-S-C8	-4.49	98.50	105.77
3	D	903	MES	C5-N4-C3	4.27	118.44	108.83
3	C	904	MES	C5-N4-C3	4.20	118.28	108.83
3	H	907	MES	C5-N4-C3	4.12	118.09	108.83
3	H	907	MES	O1S-S-C8	-4.03	102.06	106.92
2	D	801	FAD	C5A-C6A-N6A	3.94	126.33	120.35
3	B	901	MES	O1-C6-C5	-3.92	103.17	111.80
3	B	901	MES	C5-N4-C3	3.84	117.48	108.83
3	H	907	MES	O1-C6-C5	-3.72	103.61	111.80
2	B	801	FAD	C4-N3-C2	-3.65	118.90	125.64
3	A	902	MES	O1S-S-C8	-3.61	102.56	106.92
2	D	801	FAD	N3A-C2A-N1A	-3.43	123.32	128.68
3	C	904	MES	O1-C6-C5	-3.42	104.26	111.80
2	D	801	FAD	C4X-C10-N10	3.41	121.46	116.48
2	E	801	FAD	C4X-C10-N10	3.35	121.38	116.48
2	D	801	FAD	C4A-C5A-N7A	-3.35	105.91	109.40
2	B	801	FAD	C4X-C10-N10	3.33	121.34	116.48
2	H	801	FAD	C5'-C4'-C3'	-3.32	105.78	112.20
2	A	801	FAD	C1B-N9A-C4A	-3.31	120.82	126.64
2	A	801	FAD	C2A-N1A-C6A	3.30	124.41	118.75
3	C	904	MES	O3S-S-O1S	-3.29	103.22	111.27
2	E	801	FAD	C5X-C9A-N10	3.27	121.33	117.95
2	E	801	FAD	C4-N3-C2	-3.15	119.83	125.64
2	G	801	FAD	C4X-C10-N10	3.14	121.08	116.48
3	E	906	MES	C5-N4-C3	3.13	115.87	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	801	FAD	O4B-C1B-C2B	-3.11	102.38	106.93
2	H	801	FAD	C10-C4X-N5	-3.08	118.32	124.86
2	B	801	FAD	C6-C5X-C9A	3.07	123.29	118.94
2	H	801	FAD	C4X-C10-N10	2.93	120.77	116.48
2	C	801	FAD	C4X-C10-N10	2.93	120.76	116.48
2	E	801	FAD	O4-C4-C4X	-2.87	119.00	126.60
2	G	801	FAD	C10-C4X-N5	-2.82	118.88	124.86
2	C	801	FAD	C6-C5X-C9A	2.79	122.89	118.94
2	E	801	FAD	C5'-C4'-C3'	-2.79	106.81	112.20
2	B	801	FAD	C2A-N1A-C6A	2.79	123.52	118.75
2	H	801	FAD	C2A-N1A-C6A	2.75	123.46	118.75
2	C	801	FAD	C2B-C3B-C4B	2.75	107.99	102.64
2	F	801	FAD	C4X-C10-N10	2.75	120.50	116.48
2	A	801	FAD	O4-C4-C4X	-2.74	119.33	126.60
3	E	906	MES	O1-C6-C5	-2.74	105.77	111.80
3	D	903	MES	O1-C6-C5	-2.66	105.93	111.80
2	F	801	FAD	C5X-C9A-N10	2.64	120.68	117.95
2	F	801	FAD	C9A-C5X-N5	-2.62	119.58	122.43
2	B	801	FAD	C10-C4X-N5	-2.61	119.32	124.86
2	F	801	FAD	C4-C4X-N5	2.60	121.93	118.23
2	A	801	FAD	C5'-C4'-C3'	-2.58	107.22	112.20
2	E	801	FAD	C4X-C4-N3	2.57	119.71	113.19
2	A	801	FAD	C4X-C10-N10	2.56	120.22	116.48
2	C	801	FAD	C9A-C5X-N5	-2.56	119.66	122.43
2	C	801	FAD	C5X-C9A-N10	2.54	120.58	117.95
2	D	801	FAD	C4-C4X-N5	2.51	121.81	118.23
2	B	801	FAD	C4X-C4-N3	2.51	119.56	113.19
3	E	906	MES	O1-C2-C3	-2.50	106.30	111.80
2	D	801	FAD	C5X-C9A-N10	2.49	120.53	117.95
2	G	801	FAD	C4A-C5A-N7A	-2.49	106.80	109.40
2	D	801	FAD	O4'-C4'-C3'	2.48	115.12	109.10
3	G	908	MES	O1-C2-C3	-2.47	106.35	111.80
2	H	801	FAD	O2B-C2B-C3B	2.47	119.82	111.82
2	F	801	FAD	C4X-C4-N3	2.47	119.46	113.19
2	G	801	FAD	O2-C2-N1	-2.46	117.76	121.83
2	H	801	FAD	C4-C4X-C10	2.45	120.91	116.79
2	D	801	FAD	C10-C4X-N5	-2.41	119.73	124.86
2	C	801	FAD	C1B-N9A-C4A	-2.39	122.45	126.64
3	D	903	MES	C2-C3-N4	2.39	113.72	110.10
2	G	801	FAD	C9A-C5X-N5	-2.37	119.86	122.43
3	A	902	MES	C2-C3-N4	2.34	113.66	110.10
2	B	801	FAD	C1B-N9A-C4A	-2.34	122.53	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	801	FAD	C9A-C5X-N5	-2.32	119.91	122.43
2	C	801	FAD	C10-C4X-N5	-2.30	119.97	124.86
3	E	905	MES	C2-C3-N4	2.30	113.59	110.10
2	F	801	FAD	C1B-N9A-C4A	-2.29	122.62	126.64
2	H	801	FAD	C5A-C6A-N6A	2.27	123.81	120.35
2	A	801	FAD	C10-N1-C2	2.27	121.45	116.90
2	H	801	FAD	O2-C2-N1	-2.27	118.06	121.83
2	B	801	FAD	C4X-C10-N1	-2.25	119.51	124.73
2	H	801	FAD	C9A-C5X-N5	-2.25	119.99	122.43
2	B	801	FAD	C9-C8-C7	2.24	122.88	119.67
2	D	801	FAD	C9A-C5X-N5	-2.24	120.00	122.43
2	G	801	FAD	C1B-N9A-C4A	-2.22	122.74	126.64
2	D	801	FAD	O4-C4-C4X	-2.21	120.74	126.60
2	F	801	FAD	O4-C4-N3	-2.20	115.90	120.12
3	G	908	MES	C2-C3-N4	2.16	113.39	110.10
2	F	801	FAD	C6-C5X-C9A	2.16	122.00	118.94
3	A	902	MES	O1-C6-C5	-2.15	107.05	111.80
2	B	801	FAD	O4B-C1B-C2B	-2.12	103.83	106.93
2	F	801	FAD	C2A-N1A-C6A	2.10	122.34	118.75
2	D	801	FAD	C9-C8-C7	2.10	122.67	119.67
2	B	801	FAD	C4-C4X-C10	2.08	120.29	116.79
3	D	903	MES	O3S-S-O1S	-2.07	106.22	111.27
3	C	904	MES	O1-C2-C3	-2.05	107.28	111.80
3	G	908	MES	O1-C6-C5	-2.05	107.29	111.80
2	F	801	FAD	C10-C4X-N5	-2.04	120.53	124.86
2	F	801	FAD	C5'-C4'-C3'	-2.04	108.26	112.20
2	C	801	FAD	O2A-PA-O1A	2.04	122.32	112.24
2	E	801	FAD	O2-C2-N1	-2.03	118.47	121.83
2	B	801	FAD	O4-C4-C4X	-2.01	121.26	126.60
2	G	801	FAD	C5'-C4'-C3'	-2.01	108.32	112.20
2	E	801	FAD	C10-N1-C2	2.01	120.92	116.90
2	D	801	FAD	C9-C9A-N10	-2.00	119.13	121.84

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	MES	C8-C7-N4-C3
3	A	902	MES	N4-C7-C8-S
3	B	901	MES	C8-C7-N4-C3
3	B	901	MES	N4-C7-C8-S
3	C	904	MES	C8-C7-N4-C3

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Mol	Chain	Res	Type	Atoms
3	C	904	MES	N4-C7-C8-S
3	D	903	MES	C8-C7-N4-C3
3	D	903	MES	N4-C7-C8-S
3	E	905	MES	C8-C7-N4-C3
3	E	905	MES	N4-C7-C8-S
3	E	906	MES	C8-C7-N4-C3
3	E	906	MES	N4-C7-C8-S
3	G	908	MES	C8-C7-N4-C3
3	G	908	MES	N4-C7-C8-S
3	H	907	MES	C8-C7-N4-C3
3	H	907	MES	N4-C7-C8-S
2	A	801	FAD	PA-O3P-P-O5'
2	B	801	FAD	PA-O3P-P-O5'
2	C	801	FAD	PA-O3P-P-O5'
2	D	801	FAD	PA-O3P-P-O5'
2	F	801	FAD	PA-O3P-P-O5'
3	D	903	MES	C7-C8-S-O1S
3	E	906	MES	C7-C8-S-O1S
3	G	908	MES	C7-C8-S-O1S
3	H	907	MES	C7-C8-S-O1S
3	E	906	MES	C8-C7-N4-C5
2	D	801	FAD	P-O3P-PA-O1A
2	F	801	FAD	O4B-C4B-C5B-O5B
2	G	801	FAD	O4B-C4B-C5B-O5B
2	A	801	FAD	O4B-C4B-C5B-O5B
2	B	801	FAD	O4B-C4B-C5B-O5B
2	D	801	FAD	O4B-C4B-C5B-O5B
2	H	801	FAD	O4B-C4B-C5B-O5B
2	D	801	FAD	P-O3P-PA-O2A
2	C	801	FAD	O4B-C4B-C5B-O5B
2	E	801	FAD	O4B-C4B-C5B-O5B
3	D	903	MES	C8-C7-N4-C5
3	G	908	MES	C8-C7-N4-C5

There are no ring outliers.

15 monomers are involved in 128 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	801	FAD	4	0
3	A	902	MES	9	0
2	H	801	FAD	3	0
3	D	903	MES	14	0

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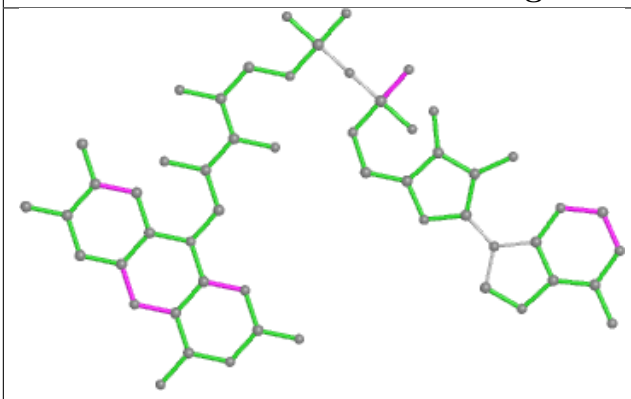
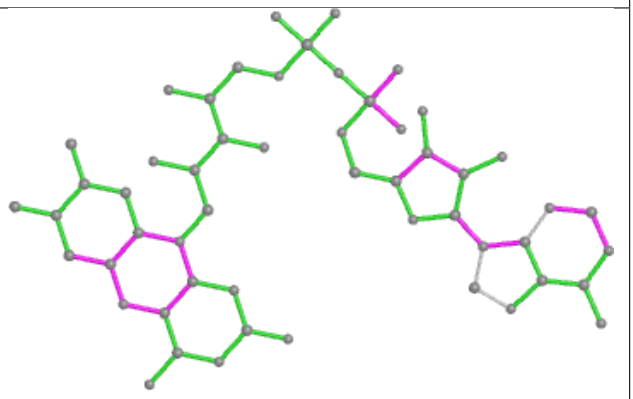
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	905	MES	2	0
2	D	801	FAD	6	0
2	A	801	FAD	8	0
3	B	901	MES	15	0
3	E	906	MES	11	0
3	H	907	MES	13	0
3	G	908	MES	13	0
3	C	904	MES	12	0
2	E	801	FAD	7	0
2	F	801	FAD	3	0
2	B	801	FAD	8	0

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.

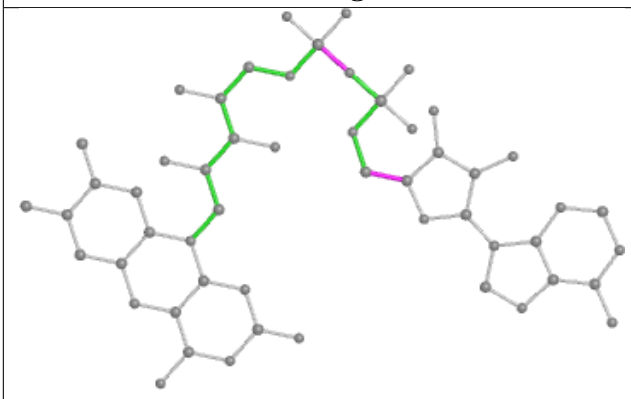
Ligand FAD C 801



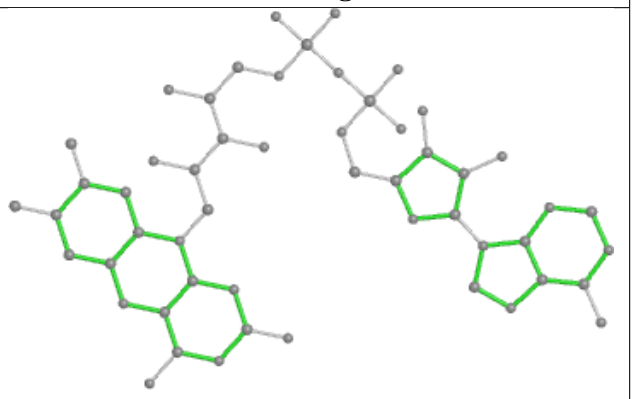
Bond lengths



Bond angles

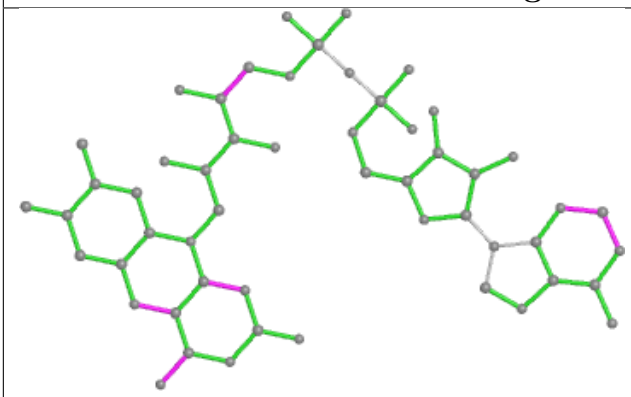


Torsions

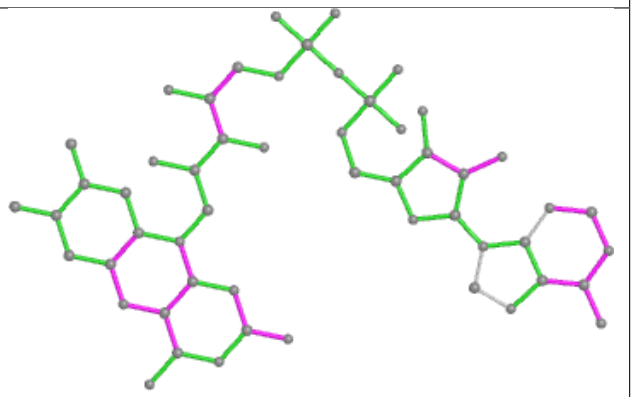


Rings

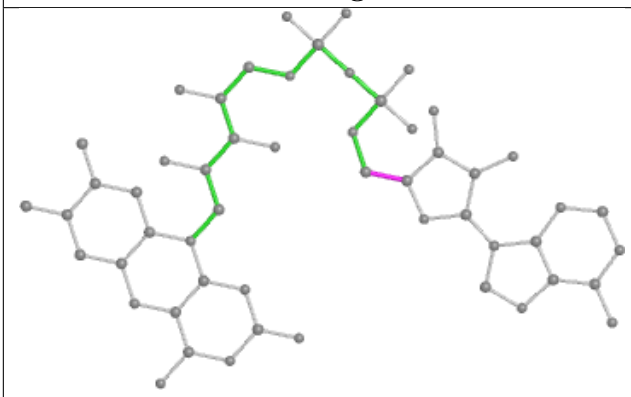
Ligand FAD H 801



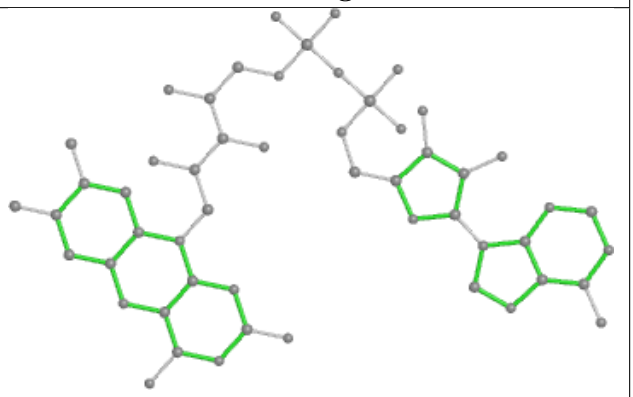
Bond lengths



Bond angles

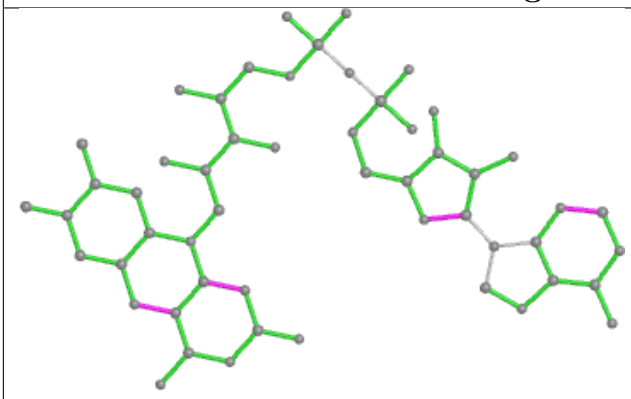


Torsions

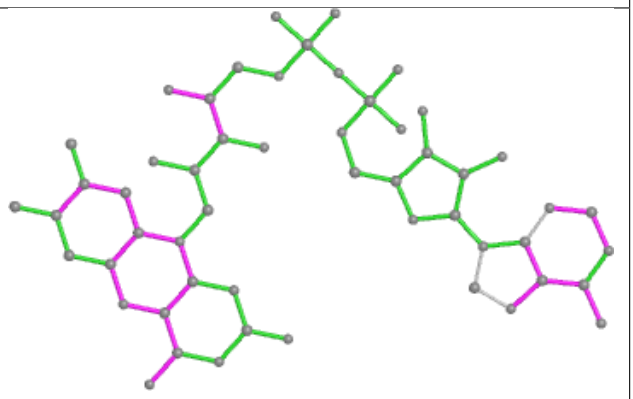


Rings

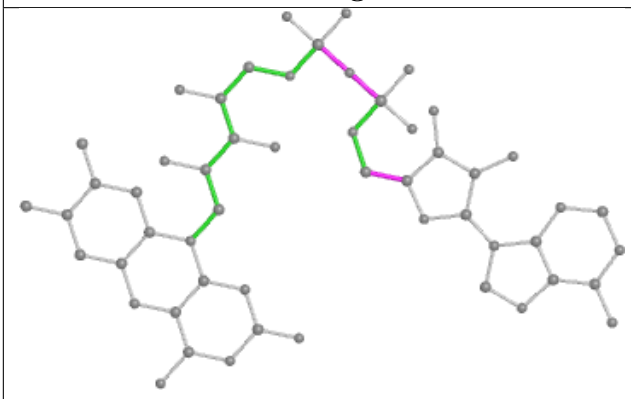
Ligand FAD D 801



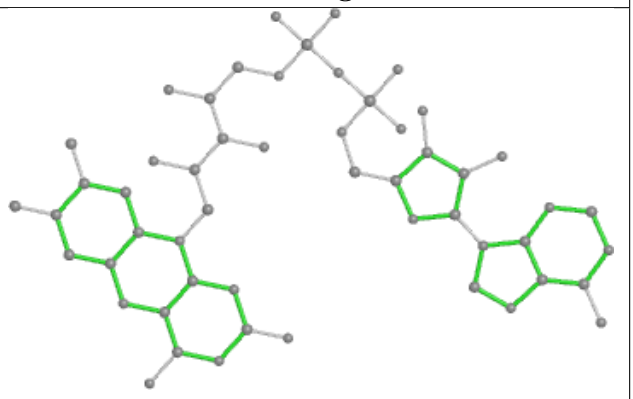
Bond lengths



Bond angles

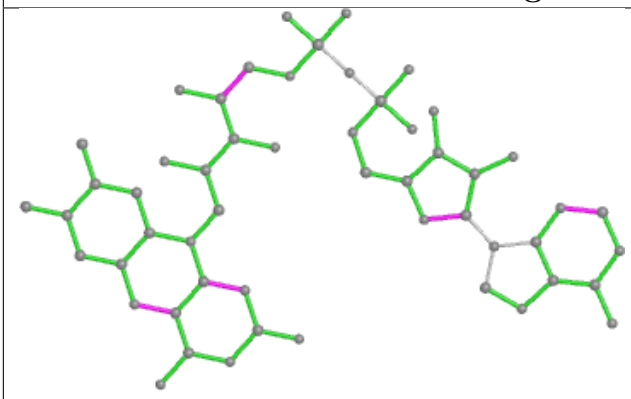


Torsions

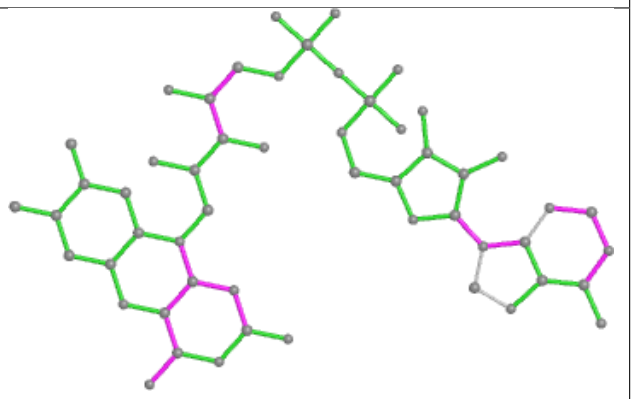


Rings

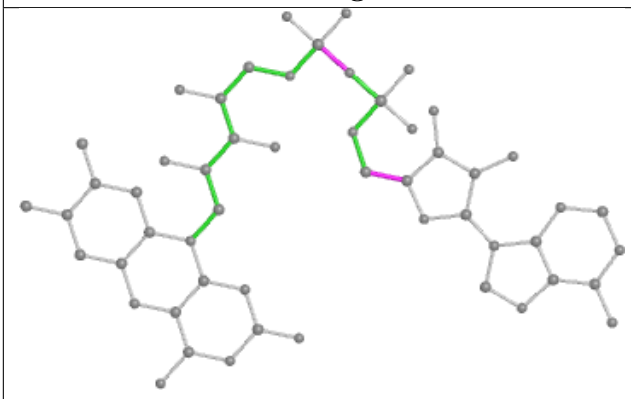
Ligand FAD A 801



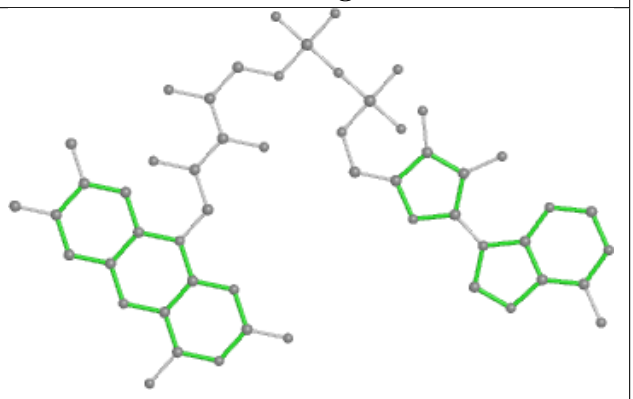
Bond lengths



Bond angles

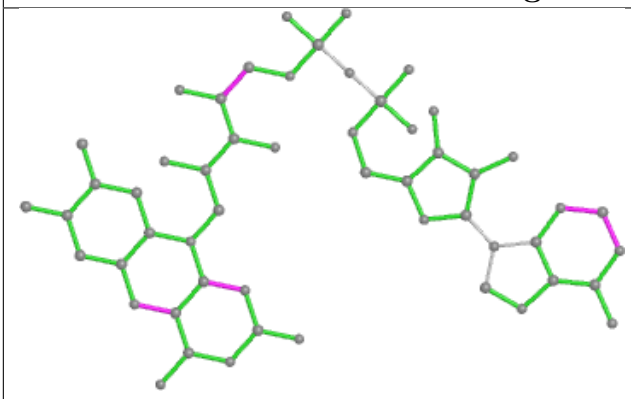


Torsions



Rings

Ligand FAD G 801



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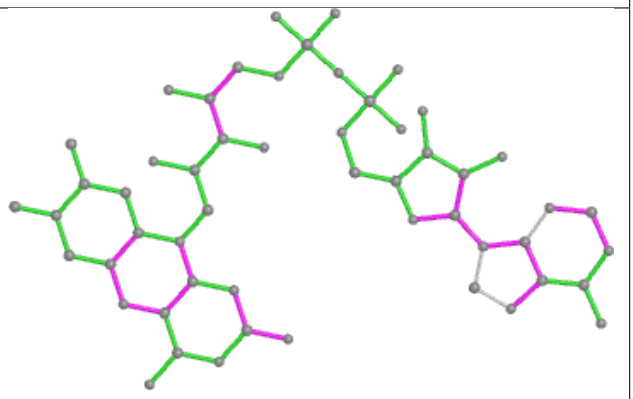
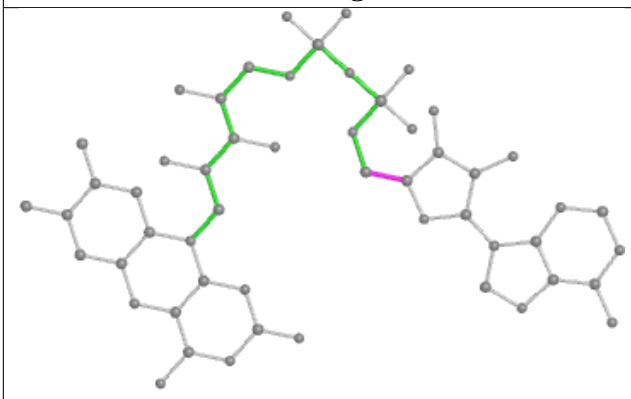


Bond angles



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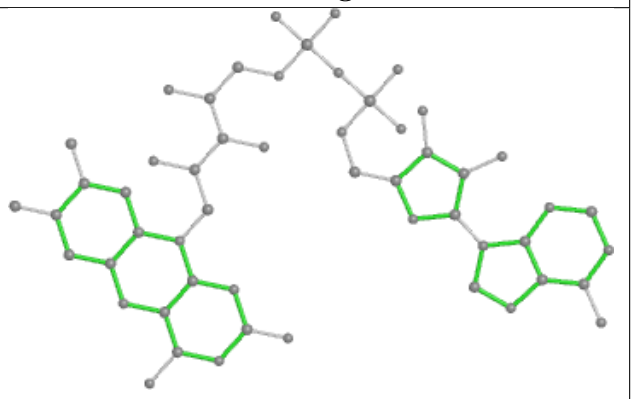
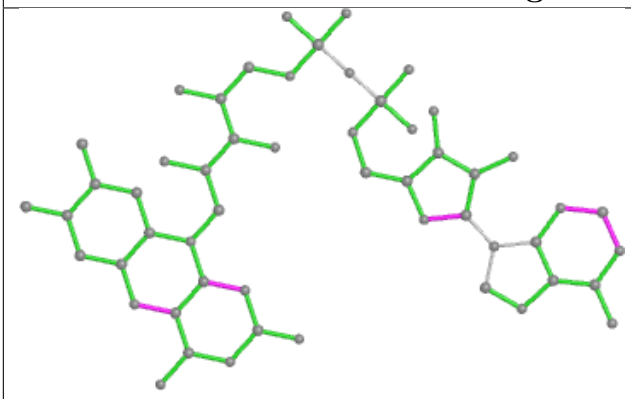


Rings

Ligand FAD E 801



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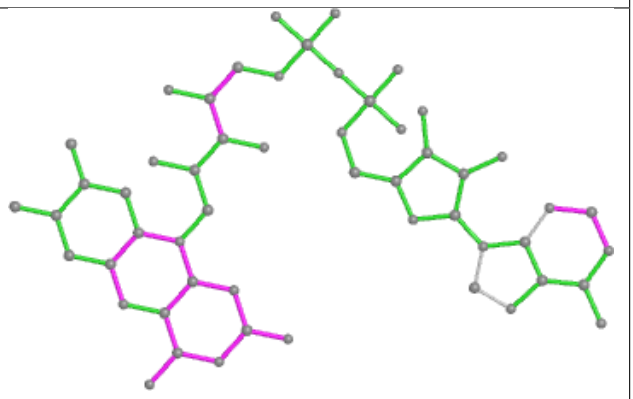
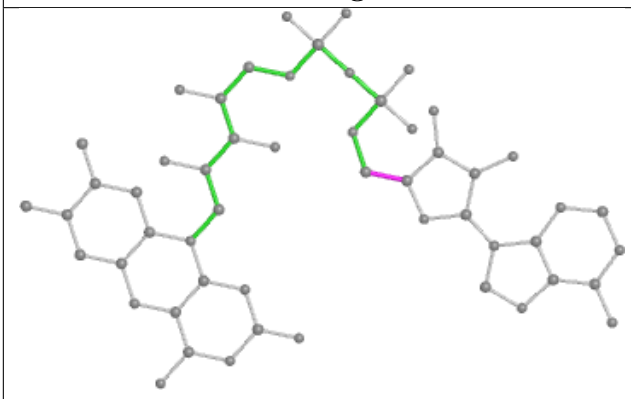


Bond angles



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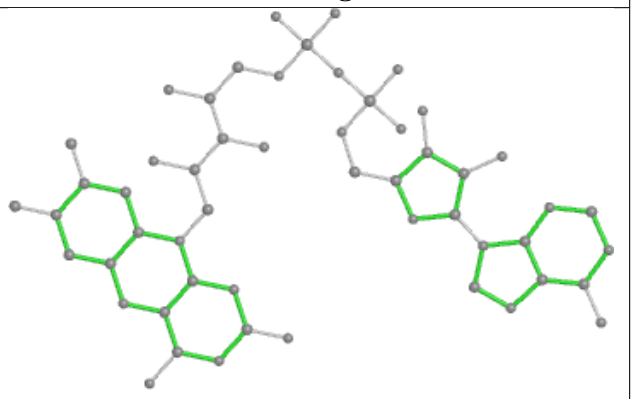
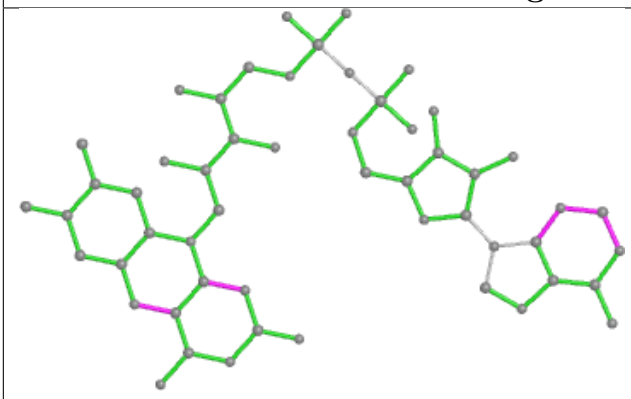


Rings

Ligand FAD F 801



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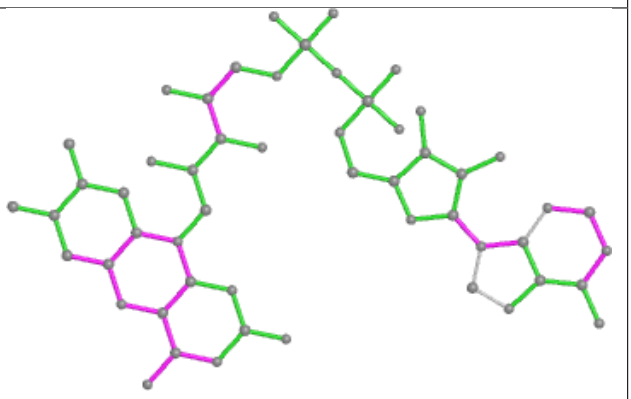
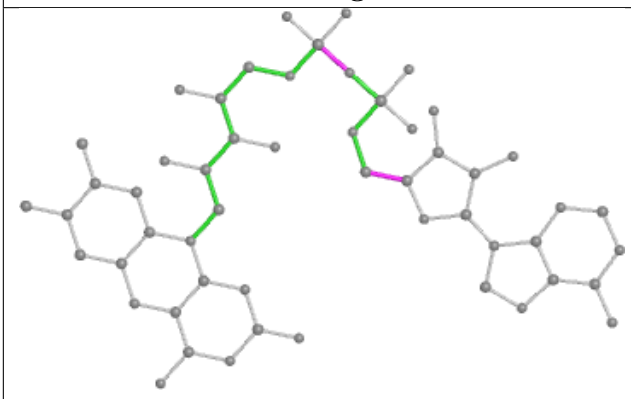


Bond angles



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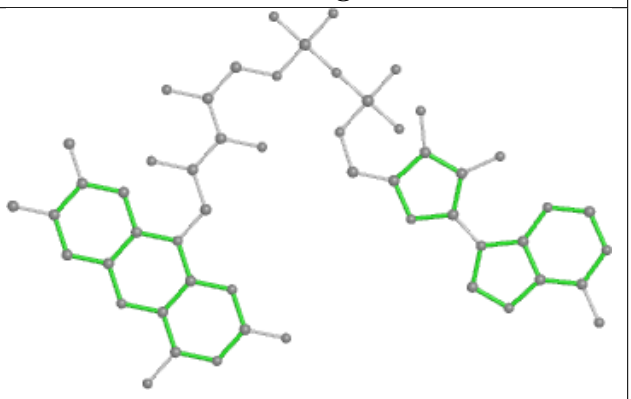
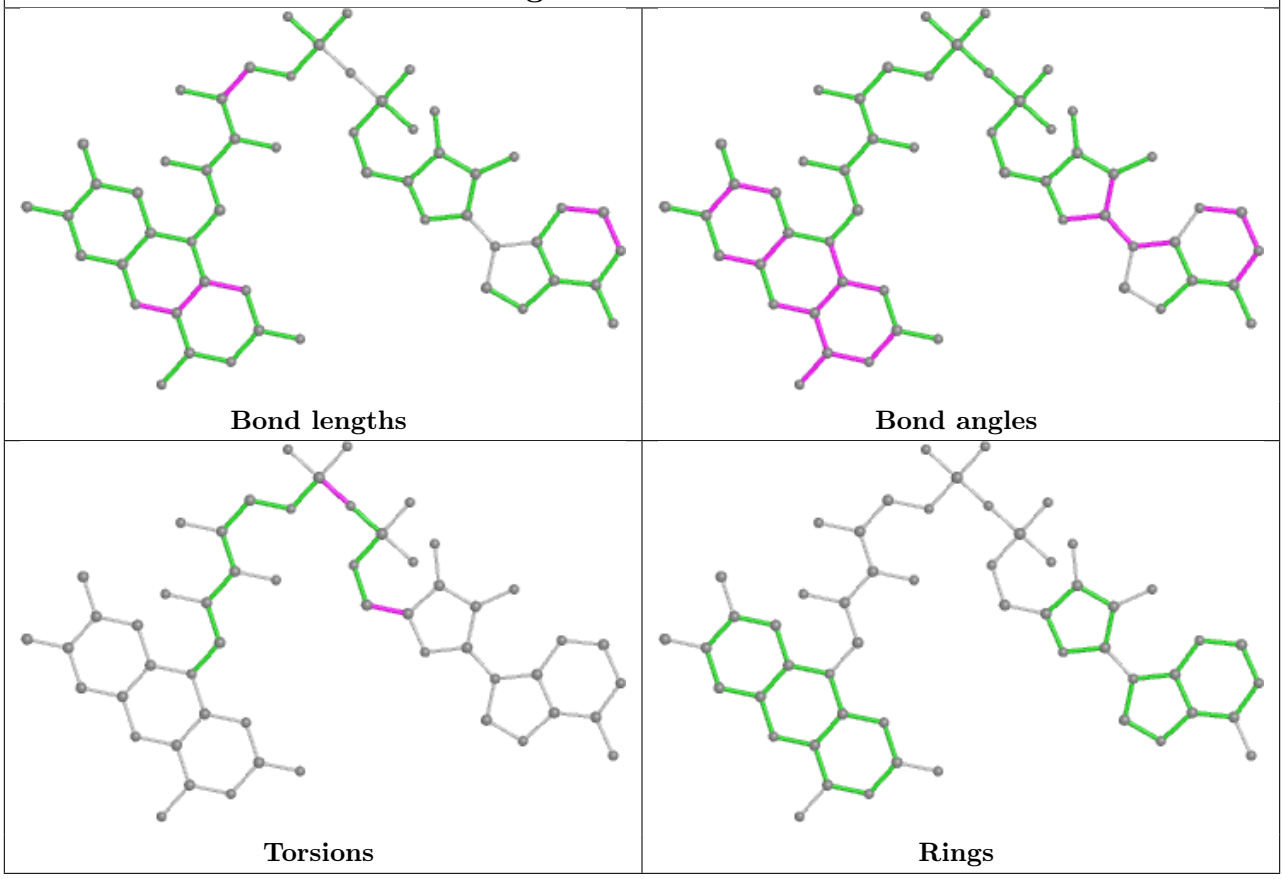


Rings

Ligand FAD B 801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	577/623 (92%)	-0.43	20 (3%)	44	38	10, 16, 42, 61	0
1	B	577/623 (92%)	-0.46	20 (3%)	44	38	10, 17, 39, 61	0
1	C	577/623 (92%)	-0.23	24 (4%)	36	30	13, 23, 47, 67	0
1	D	577/623 (92%)	-0.36	19 (3%)	46	40	12, 21, 42, 63	0
1	E	577/623 (92%)	-0.33	21 (3%)	42	37	13, 21, 43, 64	0
1	F	577/623 (92%)	-0.32	21 (3%)	42	37	11, 22, 43, 65	0
1	G	577/623 (92%)	-0.38	23 (3%)	38	32	12, 19, 43, 66	0
1	H	577/623 (92%)	-0.49	14 (2%)	59	54	11, 18, 39, 62	0
All	All	4616/4984 (92%)	-0.38	162 (3%)	44	38	10, 20, 43, 67	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	619	THR	11.3
1	H	619	THR	10.3
1	A	619	THR	9.8
1	B	619	THR	8.7
1	G	619	THR	8.6
1	D	619	THR	8.4
1	A	459	VAL	8.1
1	G	44	ASP	7.5
1	C	45	ILE	7.1
1	F	459	VAL	7.1
1	E	619	THR	7.0
1	E	43	MET	7.0
1	F	343	ALA	6.7
1	C	459	VAL	6.6
1	C	389	LEU	6.6
1	F	619	THR	6.5

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Mol	Chain	Res	Type	RSRZ
1	E	45	ILE	6.3
1	C	618	PHE	6.2
1	D	459	VAL	6.2
1	H	343	ALA	6.0
1	C	343	ALA	5.9
1	H	459	VAL	5.8
1	A	343	ALA	5.7
1	B	43	MET	5.6
1	G	458	ALA	5.6
1	G	343	ALA	5.5
1	G	459	VAL	5.4
1	D	458	ALA	5.4
1	E	389	LEU	5.4
1	D	343	ALA	5.4
1	C	44	ASP	5.4
1	B	343	ALA	5.2
1	F	342	PRO	5.2
1	H	44	ASP	5.1
1	E	385	THR	5.1
1	F	389	LEU	4.9
1	H	344	ASN	4.9
1	F	43	MET	4.9
1	B	458	ALA	4.9
1	A	43	MET	4.9
1	B	459	VAL	4.9
1	E	459	VAL	4.8
1	F	44	ASP	4.8
1	A	389	LEU	4.8
1	G	43	MET	4.8
1	C	345	PRO	4.7
1	D	618	PHE	4.7
1	E	343	ALA	4.6
1	D	45	ILE	4.6
1	B	44	ASP	4.6
1	B	618	PHE	4.6
1	D	345	PRO	4.5
1	D	44	ASP	4.5
1	G	389	LEU	4.5
1	C	43	MET	4.4
1	F	45	ILE	4.4
1	F	385	THR	4.3
1	B	45	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	H	45	ILE	4.2
1	H	43	MET	4.1
1	B	344	ASN	4.1
1	G	618	PHE	4.1
1	H	458	ALA	4.1
1	A	385	THR	4.1
1	C	383	ARG	4.0
1	F	458	ALA	4.0
1	A	345	PRO	4.0
1	F	344	ASN	4.0
1	E	458	ALA	4.0
1	C	617	PRO	4.0
1	D	389	LEU	4.0
1	G	344	ASN	3.9
1	A	458	ALA	3.8
1	C	390	THR	3.8
1	H	618	PHE	3.8
1	D	43	MET	3.8
1	G	342	PRO	3.8
1	E	384	GLY	3.7
1	E	388	GLU	3.7
1	F	345	PRO	3.7
1	A	388	GLU	3.7
1	E	618	PHE	3.7
1	G	388	GLU	3.7
1	E	345	PRO	3.7
1	E	342	PRO	3.6
1	H	345	PRO	3.6
1	E	44	ASP	3.6
1	B	389	LEU	3.6
1	D	388	GLU	3.6
1	A	344	ASN	3.5
1	G	345	PRO	3.5
1	D	385	THR	3.5
1	H	456	TYR	3.4
1	F	618	PHE	3.4
1	H	342	PRO	3.4
1	C	384	GLY	3.4
1	A	44	ASP	3.4
1	A	390	THR	3.4
1	B	456	TYR	3.4
1	F	390	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	385	THR	3.2
1	C	458	ALA	3.2
1	C	385	THR	3.1
1	F	384	GLY	3.1
1	E	386	PRO	3.0
1	E	383	ARG	3.0
1	F	341	ASN	3.0
1	C	388	GLU	3.0
1	A	618	PHE	3.0
1	C	456	TYR	3.0
1	E	344	ASN	3.0
1	D	344	ASN	3.0
1	G	341	ASN	3.0
1	G	45	ILE	2.9
1	C	344	ASN	2.8
1	B	388	GLU	2.8
1	F	383	ARG	2.7
1	G	186	ASP	2.7
1	G	387	GLY	2.7
1	D	617	PRO	2.7
1	G	617	PRO	2.7
1	C	392	SER	2.7
1	D	272	GLU	2.7
1	E	617	PRO	2.6
1	H	617	PRO	2.6
1	B	342	PRO	2.6
1	C	400	SER	2.6
1	B	341	ASN	2.6
1	C	272	GLU	2.6
1	F	388	GLU	2.6
1	D	383	ARG	2.5
1	E	390	THR	2.5
1	B	345	PRO	2.4
1	D	454	PHE	2.4
1	C	342	PRO	2.4
1	G	383	ARG	2.4
1	G	390	THR	2.4
1	A	382	ILE	2.3
1	A	341	ASN	2.3
1	F	188	ALA	2.3
1	F	347	GLU	2.3
1	A	383	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	269	ASP	2.3
1	A	384	GLY	2.3
1	A	381	THR	2.3
1	G	456	TYR	2.2
1	G	401	THR	2.2
1	B	390	THR	2.2
1	A	342	PRO	2.2
1	A	400	SER	2.2
1	C	396	THR	2.2
1	E	341	ASN	2.2
1	B	617	PRO	2.2
1	B	385	THR	2.1
1	E	272	GLU	2.1
1	F	561	GLU	2.1
1	C	341	ASN	2.1
1	H	341	ASN	2.1
1	G	455	SER	2.0
1	D	456	TYR	2.0
1	B	383	ARG	2.0
1	B	454	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
3	MES	C	904	12/12	0.85	0.31	27,37,45,46	0
3	MES	E	906	12/12	0.85	0.28	31,38,41,42	0
3	MES	G	908	12/12	0.85	0.28	28,37,41,41	0

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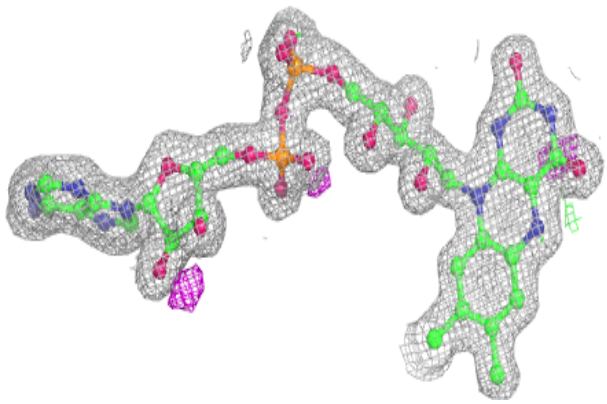
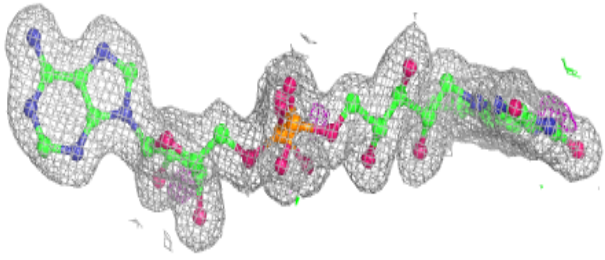
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MES	B	901	12/12	0.88	0.27	28,35,38,39	0
3	MES	D	903	12/12	0.88	0.29	32,37,41,44	0
3	MES	A	902	12/12	0.92	0.20	24,29,34,34	0
3	MES	H	907	12/12	0.93	0.19	29,33,37,37	0
3	MES	E	905	12/12	0.94	0.18	21,29,32,32	0
2	FAD	E	801	53/53	0.97	0.09	15,18,21,22	0
2	FAD	A	801	53/53	0.98	0.09	9,13,17,18	0
2	FAD	F	801	53/53	0.98	0.09	15,18,21,21	0
2	FAD	G	801	53/53	0.98	0.08	12,14,18,19	0
2	FAD	H	801	53/53	0.98	0.09	11,14,17,19	0
2	FAD	C	801	53/53	0.98	0.09	16,20,22,24	0
2	FAD	D	801	53/53	0.98	0.10	14,17,20,22	0
2	FAD	B	801	53/53	0.99	0.09	9,14,16,17	0

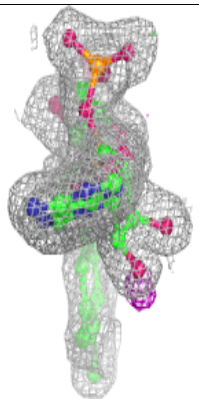
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD E 801:

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

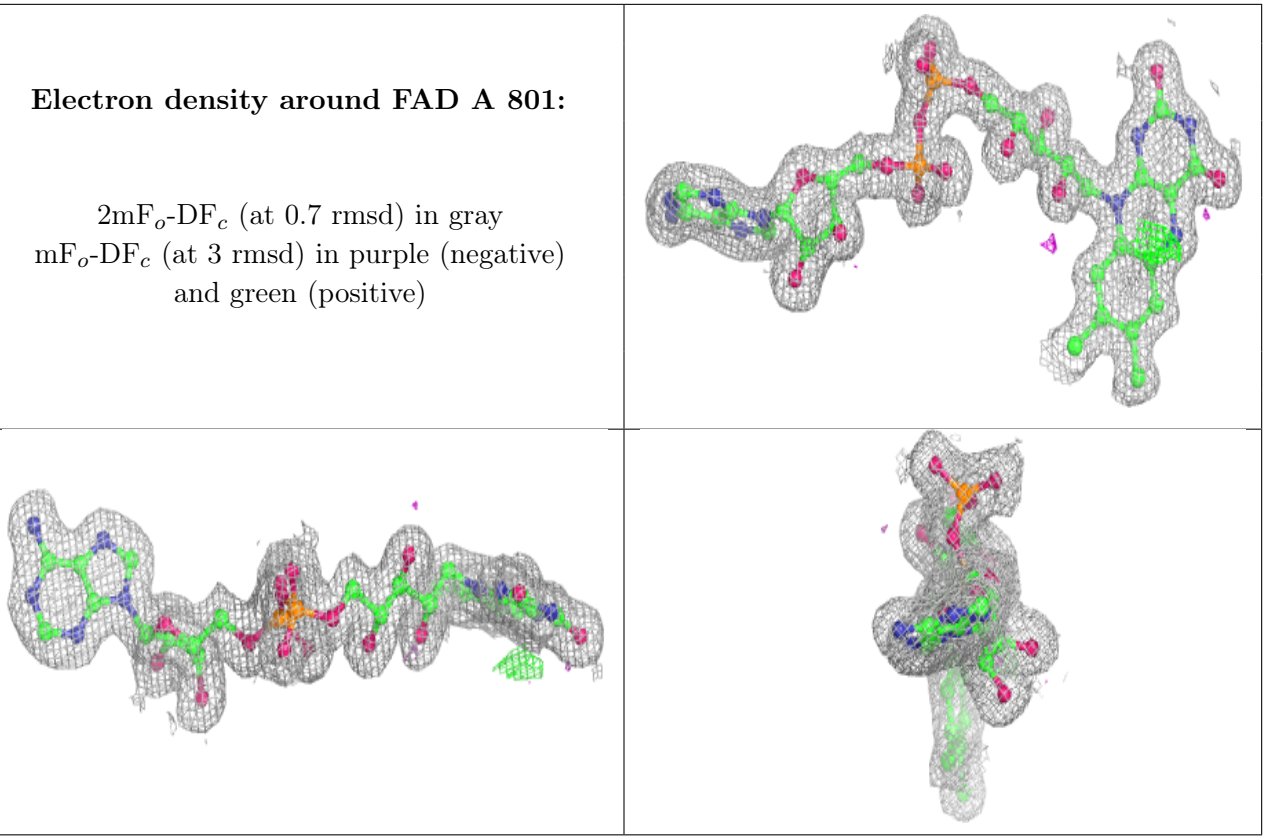






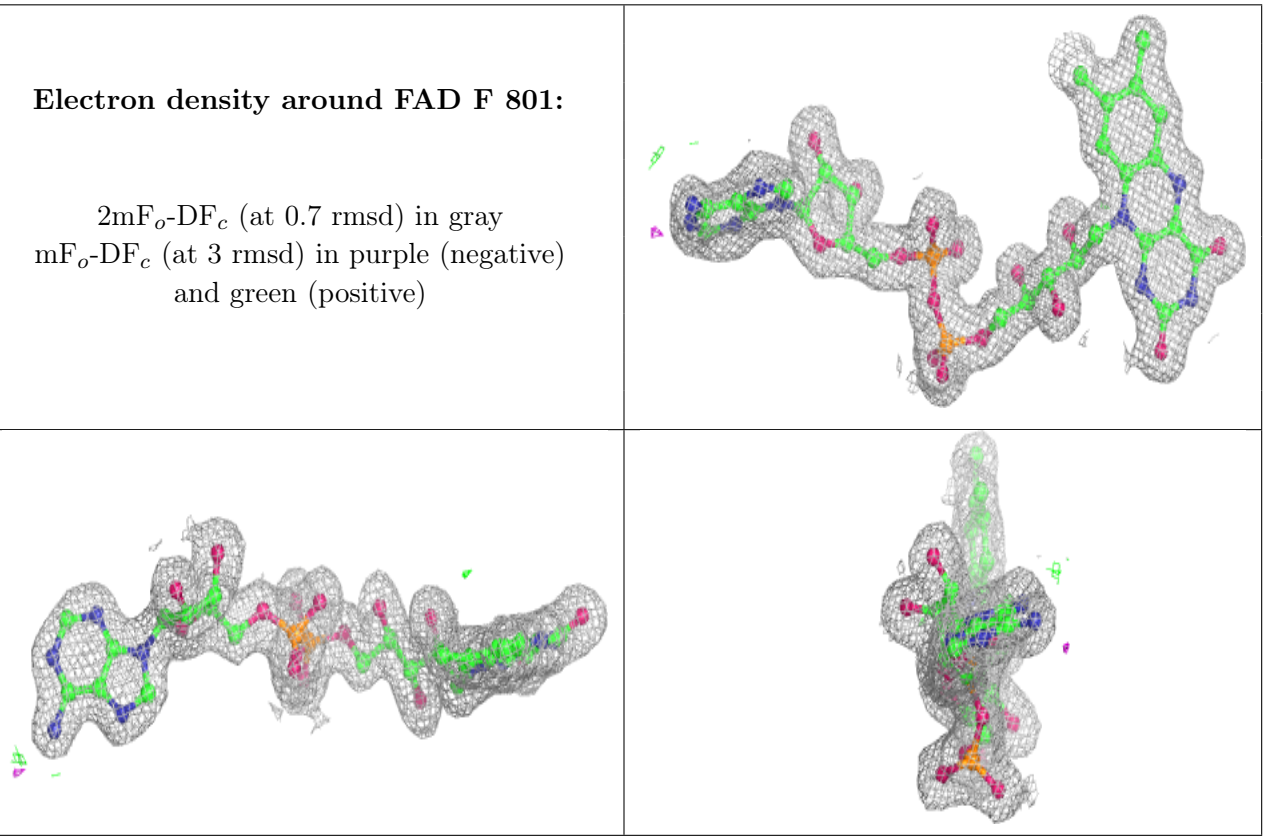
Electron density around FAD A 801:

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



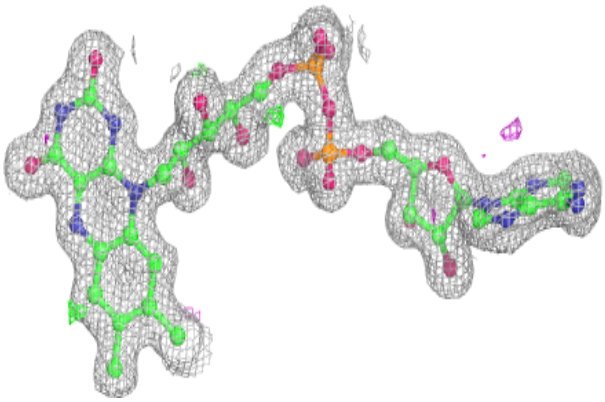
Electron density around FAD F 801:

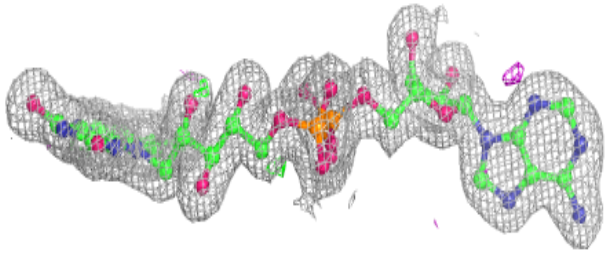
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

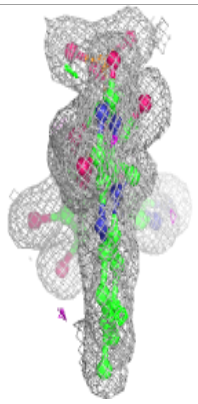


Electron density around FAD G 801:

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

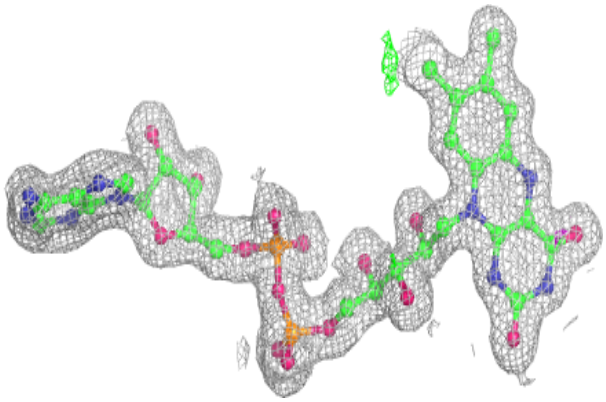


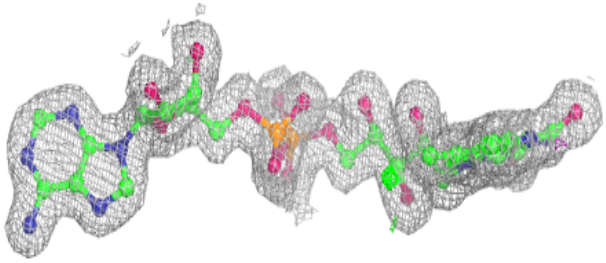


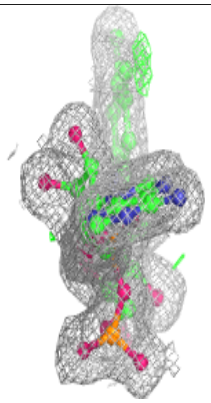


Electron density around FAD H 801:

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

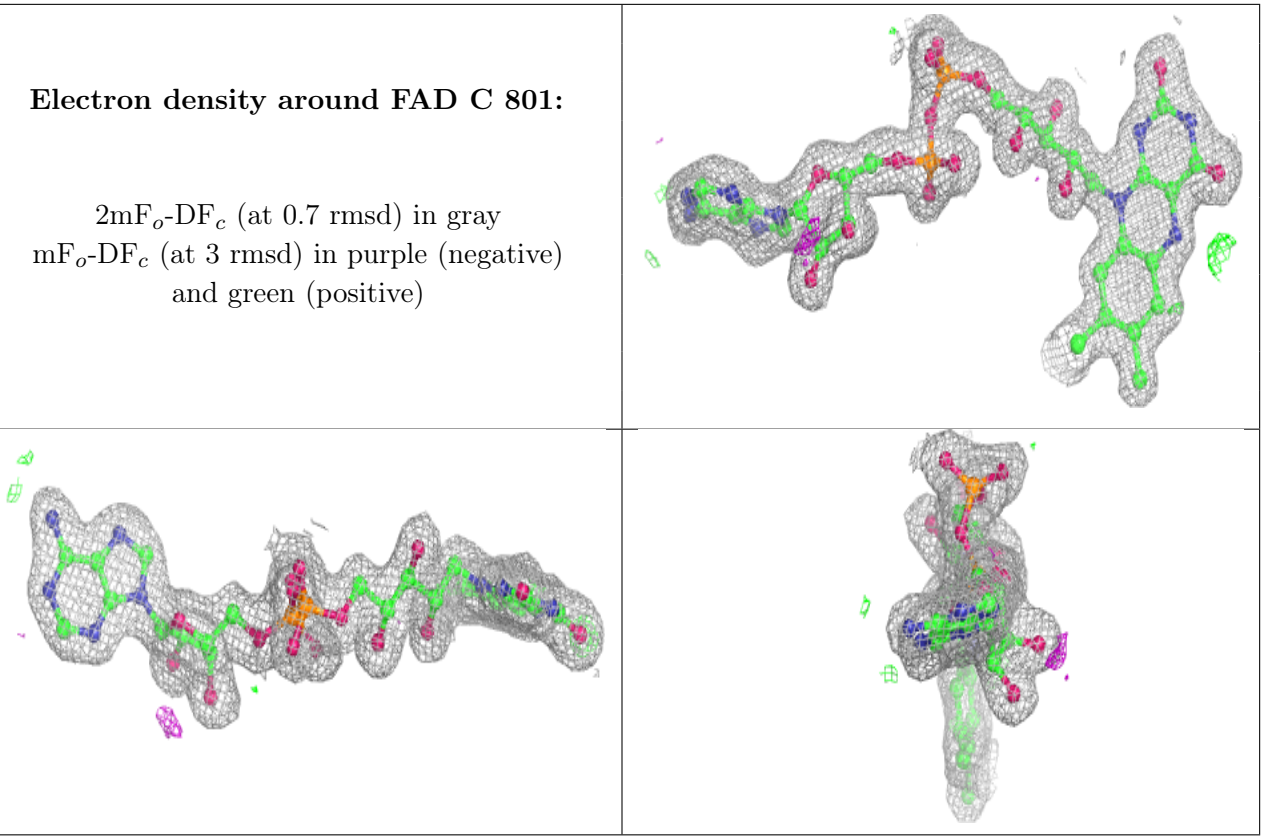






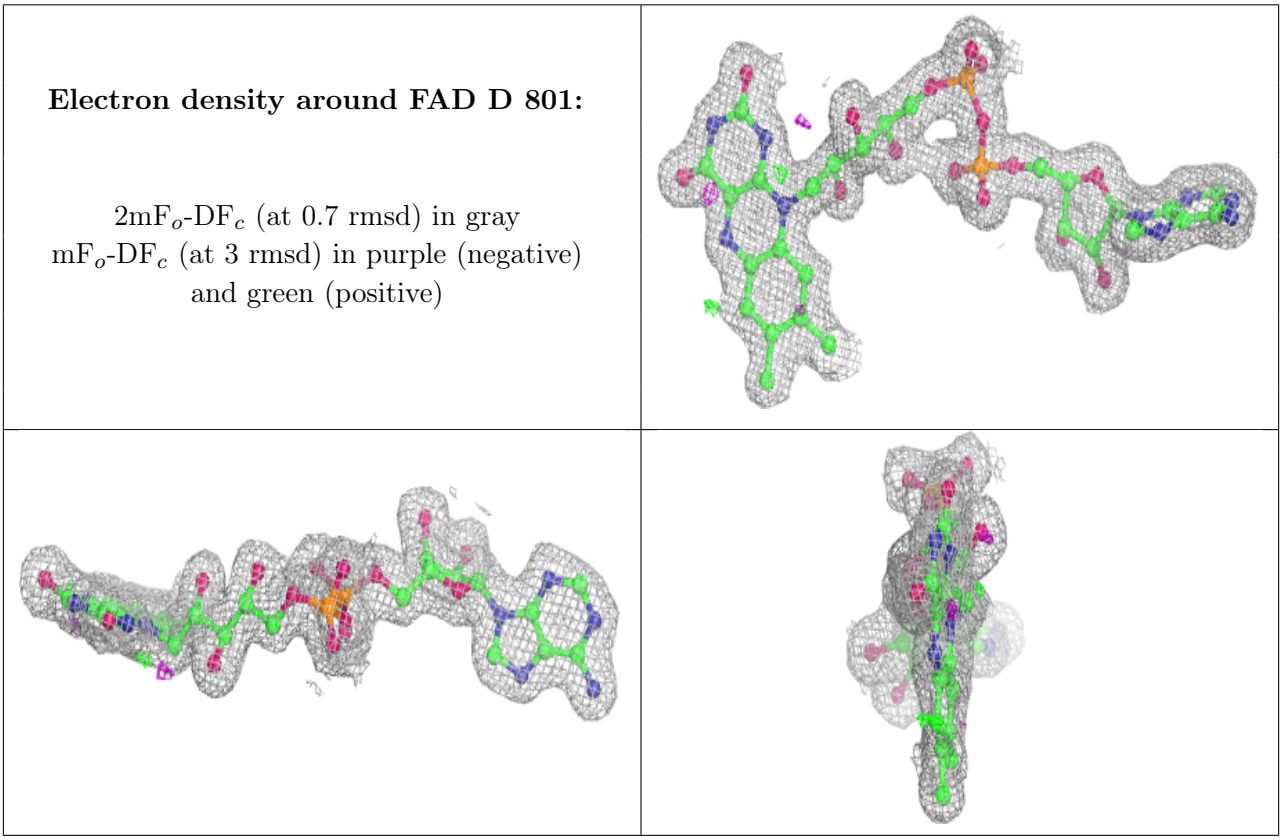
Electron density around FAD C 801:

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



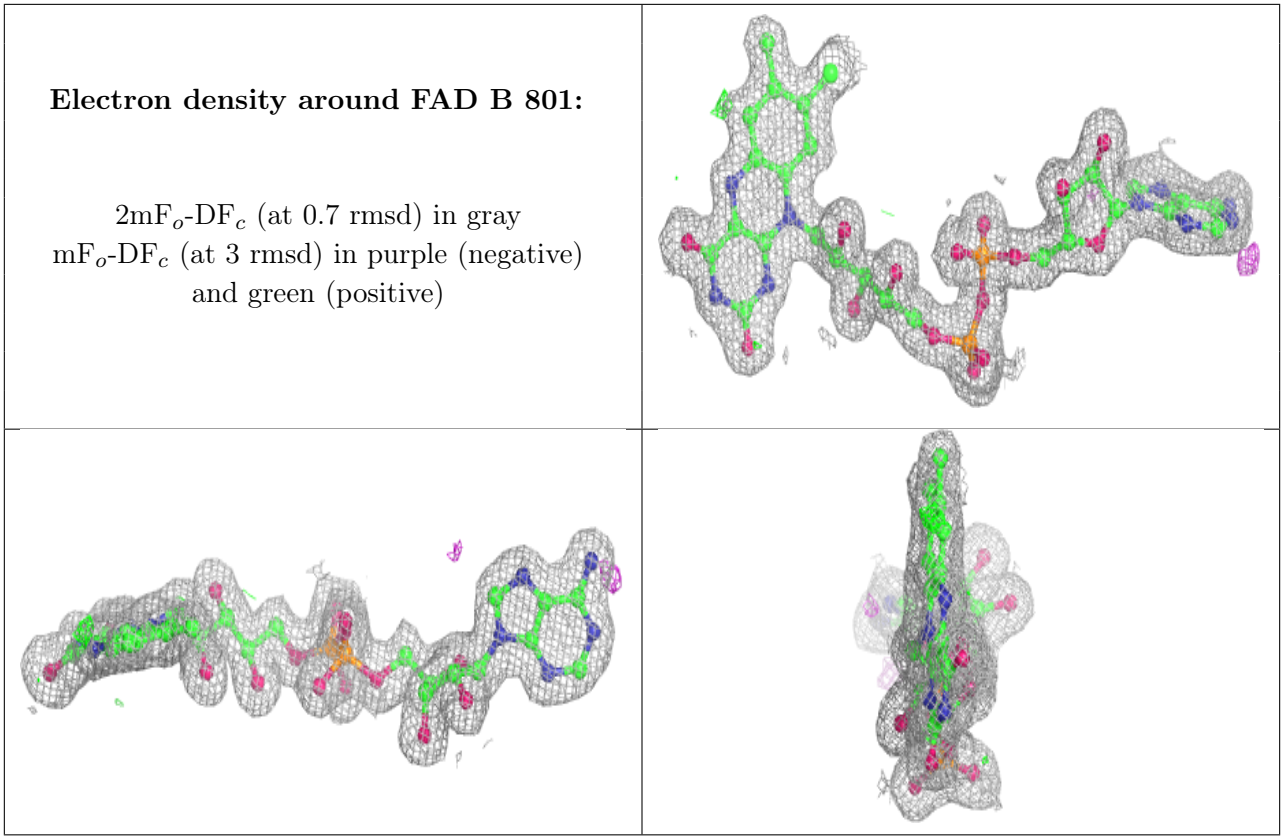
Electron density around FAD D 801:

$2mF_o$-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 801:

$2mF_o$-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.