Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2024 – 11:34 pm BST

PDB ID	:	2VVL
Title	:	The structure of MAO-N-D3, a variant of monoamine oxidase from Aspergillus niger.
Authors	:	Atkin, K.E.; Hart, S.; Turkenburg, J.P.; Brzozowski, A.M.; Grogan, G.J.
Deposited on	:	2008-06-10
Resolution	:	2.45 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:

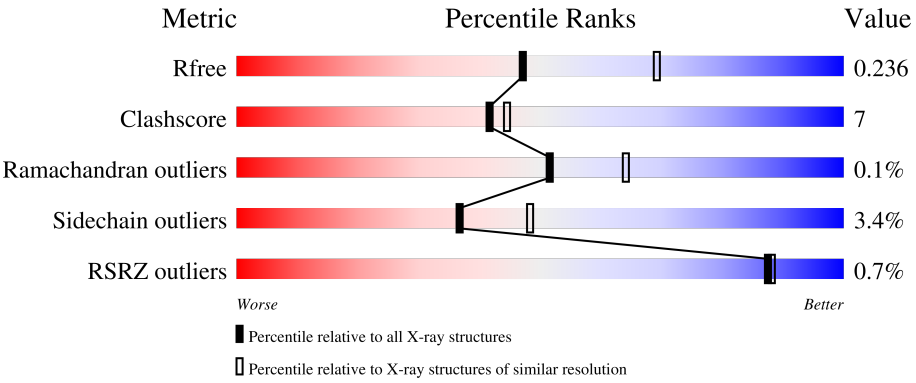
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	495	83% 12%
1	B	495	82% 12%
1	C	495	79% 15%
1	D	495	80% 14%
1	E	495	80% 15%

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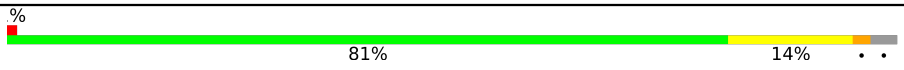
Mol	Chain	Length	Quality of chain
1	F	495	
1	H	495	
2	G	495	

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	FAD	A	600	X	-	-	-
3	FAD	B	600	X	-	-	-
3	FAD	C	600	X	-	-	-
3	FAD	D	600	X	-	-	-
3	FAD	E	600	X	-	-	-
3	FAD	F	600	X	-	-	-
3	FAD	G	600	X	-	-	-
3	FAD	H	600	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 31496 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 MONOAMINE OXIDASE N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	29	1	0
			3782	2390	669	700	23			
1	B	476	Total	C	N	O	S	40	1	0
			3770	2382	667	698	23			
1	C	477	Total	C	N	O	S	43	1	0
			3778	2387	668	701	22			
1	D	478	Total	C	N	O	S	55	0	0
			3778	2387	666	702	23			
1	E	477	Total	C	N	O	S	50	1	0
			3777	2387	668	699	23			
1	F	478	Total	C	N	O	S	53	1	0
			3782	2389	669	702	22			
1	H	478	Total	C	N	O	S	60	1	0
			3785	2393	669	700	23			

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	246	MET	ILE	engineered mutation	UNP P46882
A	336	SER	ASN	engineered mutation	UNP P46882
B	246	MET	ILE	engineered mutation	UNP P46882
B	336	SER	ASN	engineered mutation	UNP P46882
C	246	MET	ILE	engineered mutation	UNP P46882
C	336	SER	ASN	engineered mutation	UNP P46882
D	246	MET	ILE	engineered mutation	UNP P46882
D	336	SER	ASN	engineered mutation	UNP P46882
E	246	MET	ILE	engineered mutation	UNP P46882
E	336	SER	ASN	engineered mutation	UNP P46882
F	246	MET	ILE	engineered mutation	UNP P46882
F	336	SER	ASN	engineered mutation	UNP P46882
H	246	MET	ILE	engineered mutation	UNP P46882
H	336	SER	ASN	engineered mutation	UNP P46882
A	300	VAL	ALA	conflict	UNP P46882

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Chain	Residue	Modelled	Actual	Comment	Reference
A	304	VAL	LEU	conflict	UNP P46882
A	450	GLY	ARG	conflict	UNP P46882
B	300	VAL	ALA	conflict	UNP P46882
B	304	VAL	LEU	conflict	UNP P46882
B	450	GLY	ARG	conflict	UNP P46882
C	300	VAL	ALA	conflict	UNP P46882
C	304	VAL	LEU	conflict	UNP P46882
C	450	GLY	ARG	conflict	UNP P46882
D	300	VAL	ALA	conflict	UNP P46882
D	304	VAL	LEU	conflict	UNP P46882
D	450	GLY	ARG	conflict	UNP P46882
E	300	VAL	ALA	conflict	UNP P46882
E	304	VAL	LEU	conflict	UNP P46882
E	450	GLY	ARG	conflict	UNP P46882
F	300	VAL	ALA	conflict	UNP P46882
F	304	VAL	LEU	conflict	UNP P46882
F	450	GLY	ARG	conflict	UNP P46882
H	300	VAL	ALA	conflict	UNP P46882
H	304	VAL	LEU	conflict	UNP P46882
H	450	GLY	ARG	conflict	UNP P46882

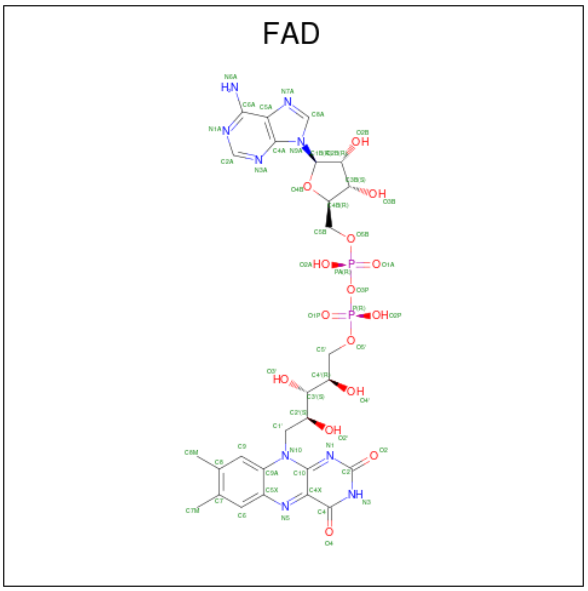
- Molecule 2 is a protein called MONOAMINE OXIDASE N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	478	3785	2392	669	701	23	46	1	0

There are 6 discrepancies between the modelled and reference sequences:

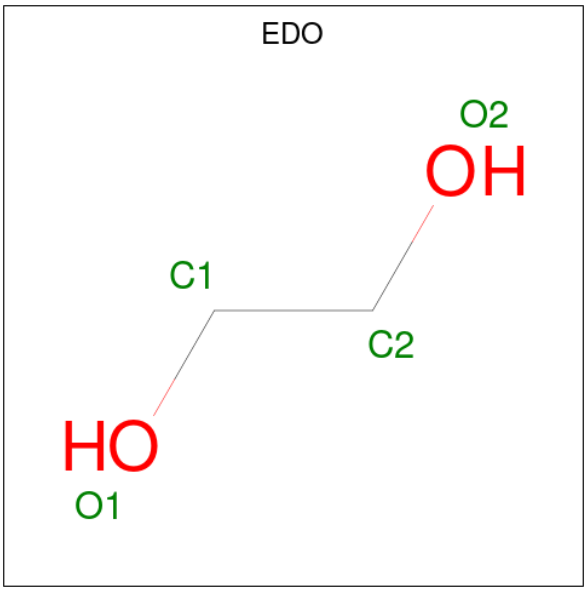
Chain	Residue	Modelled	Actual	Comment	Reference
G	246	MET	ILE	engineered mutation	UNP P46882
G	336	SER	ASN	engineered mutation	UNP P46882
G	20	THR	PRO	conflict	UNP P46882
G	300	VAL	ALA	conflict	UNP P46882
G	304	VAL	LEU	conflict	UNP P46882
G	450	GLY	ARG	conflict	UNP P46882

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



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	118	Total O 118 118	0	0
5	B	134	Total O 134 134	0	0
5	C	95	Total O 95 95	0	0
5	D	102	Total O 102 102	0	0
5	E	122	Total O 122 122	0	0

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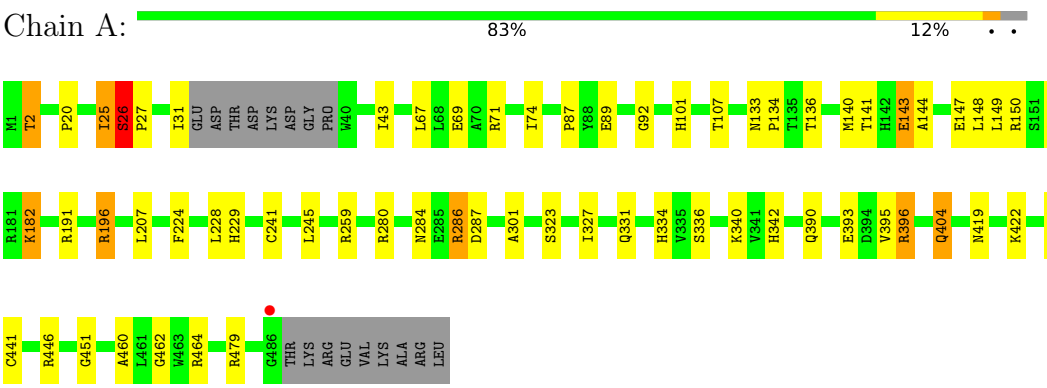
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	103	Total O 103 103	0	0
5	G	53	Total O 53 53	0	0
5	H	80	Total O 80 80	0	0

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.

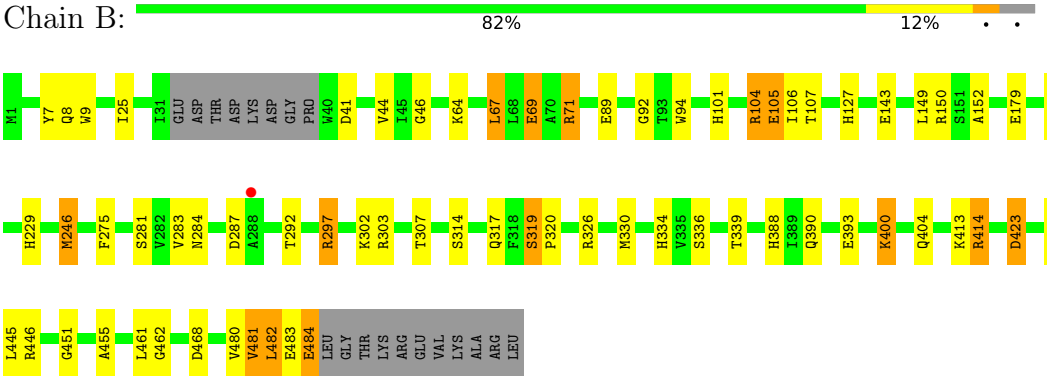
• Molecule 1: MONOAMINE OXIDASE N

Chain A:



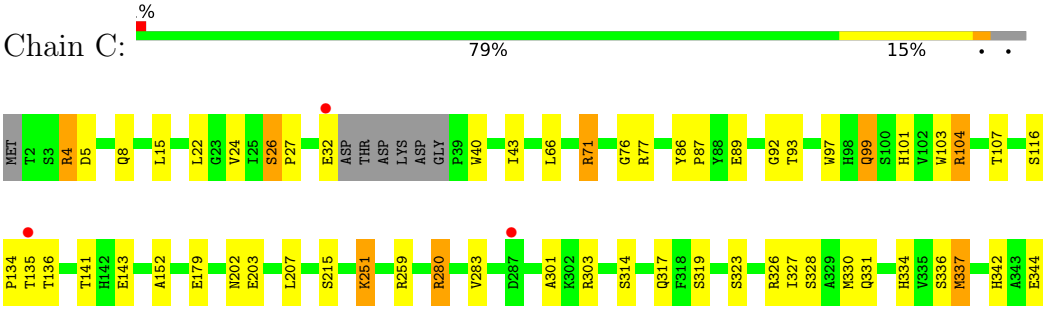
• Molecule 1: MONOAMINE OXIDASE N

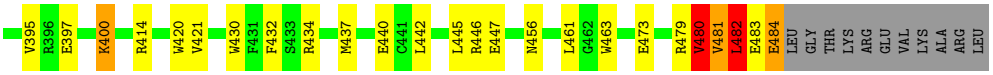
Chain B:



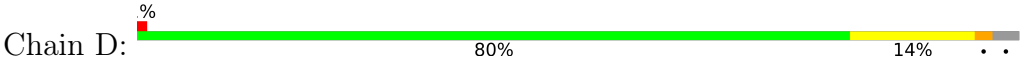
• Molecule 1: MONOAMINE OXIDASE N

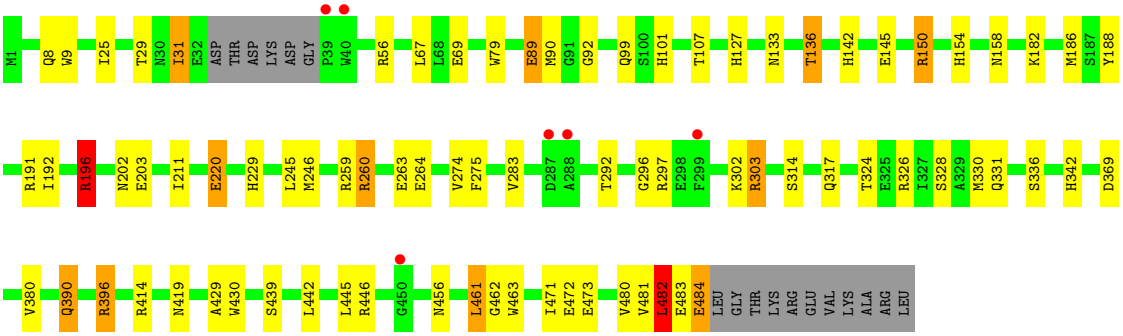
Chain C:



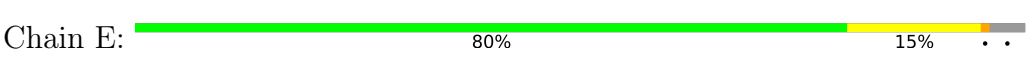


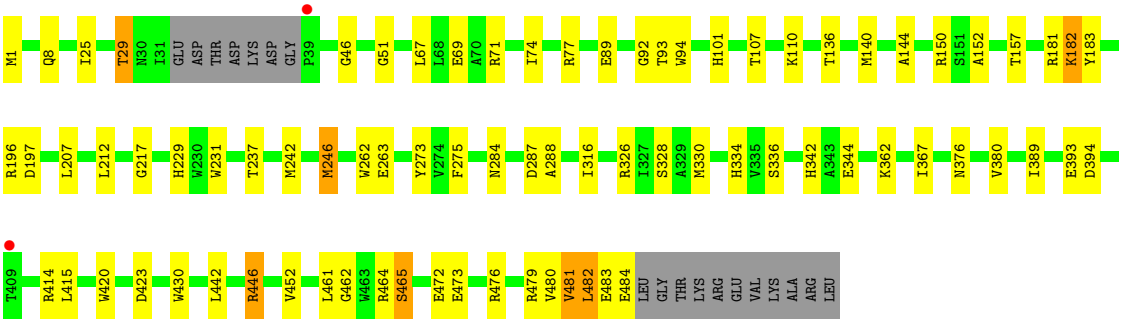
• Molecule 1: MONOAMINE OXIDASE N



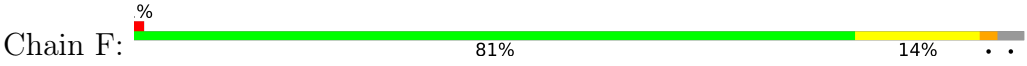


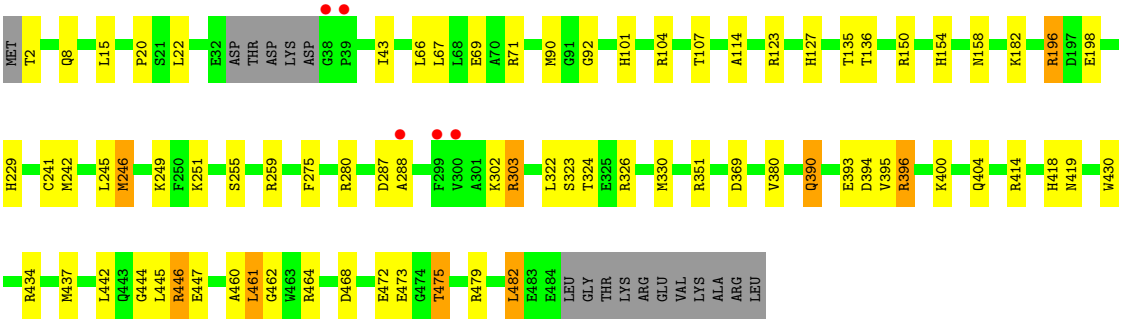
• Molecule 1: MONOAMINE OXIDASE N



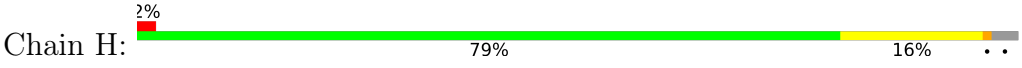


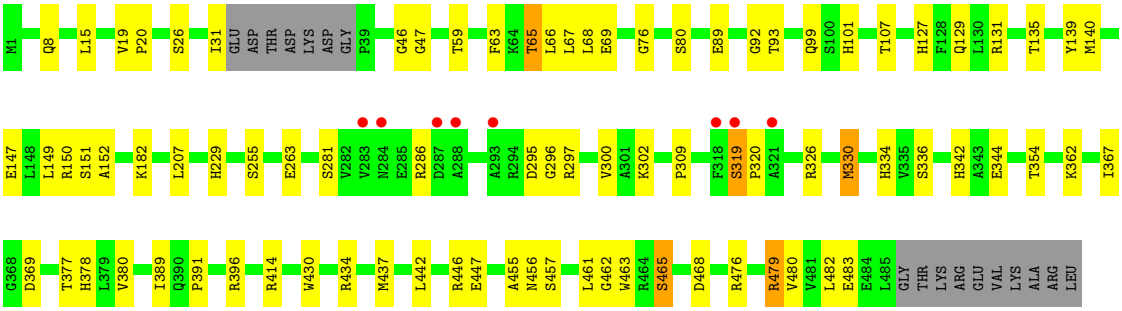
• Molecule 1: MONOAMINE OXIDASE N





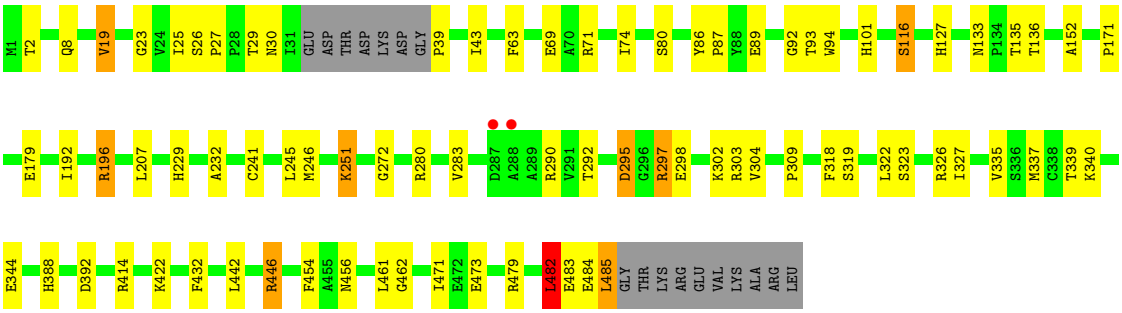
• Molecule 1: MONOAMINE OXIDASE N





• Molecule 2: MONOAMINE OXIDASE N

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	103.29Å 187.25Å 132.43Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	132.45 – 2.45 49.53 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.1 (132.45-2.45) 97.2 (49.53-2.45)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.85 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.4.0065	Depositor
R, R_{free}	0.182 , 0.236 0.190 , 0.236	Depositor DCC
R_{free} test set	9016 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	24.2	Xtriage
Anisotropy	0.636	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 33.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.148 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	31496	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 3.22% 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: EDO, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.95	6/3885 (0.2%)	0.82	4/5266 (0.1%)
1	B	0.97	8/3873 (0.2%)	0.92	17/5250 (0.3%)
1	C	0.89	7/3882 (0.2%)	0.87	10/5263 (0.2%)
1	D	0.92	6/3879 (0.2%)	0.84	9/5259 (0.2%)
1	E	0.84	6/3881 (0.2%)	0.80	11/5261 (0.2%)
1	F	0.87	5/3886 (0.1%)	0.89	15/5269 (0.3%)
1	H	0.91	9/3889 (0.2%)	0.79	9/5272 (0.2%)
2	G	0.91	6/3888 (0.2%)	0.80	8/5270 (0.2%)
All	All	0.91	53/31063 (0.2%)	0.84	83/42110 (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	A	0	4
1	B	0	2
1	C	0	2
1	D	0	2
1	F	0	1
1	H	0	1
All	All	0	12

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	483	GLU	C-N	-13.38	1.03	1.34
1	C	4	ARG	C-N	-9.81	1.11	1.34
1	H	455	ALA	C-N	-9.05	1.13	1.34
1	H	67	LEU	C-N	-9.02	1.13	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	ARG	C-N	-8.99	1.13	1.34
1	B	481	VAL	CB-CG1	-8.79	1.34	1.52
1	C	104	ARG	C-N	-8.68	1.14	1.34
1	B	393	GLU	C-N	-8.57	1.14	1.34
1	C	303	ARG	C-N	-8.47	1.14	1.34
1	H	391	PRO	C-N	-8.13	1.15	1.34
1	D	196	ARG	C-N	-7.94	1.15	1.34
1	A	143	GLU	C-N	-7.90	1.15	1.34
1	F	393	GLU	C-N	-7.75	1.16	1.34
1	H	66	LEU	C-N	-7.36	1.17	1.34
1	B	303	ARG	C-N	-7.20	1.17	1.34
1	A	441	CYS	CB-SG	-7.18	1.70	1.82
1	E	183	TYR	CD1-CE1	-6.90	1.28	1.39
1	H	263	GLU	CB-CG	-6.87	1.39	1.52
2	G	471	ILE	C-N	-6.39	1.19	1.34
2	G	303	ARG	C-N	-6.33	1.19	1.34
1	F	395	VAL	CB-CG2	-6.30	1.39	1.52
1	E	394	ASP	C-N	-6.29	1.19	1.34
1	C	99	GLN	C-N	-6.05	1.20	1.34
1	E	393	GLU	C-N	-5.94	1.20	1.34
1	B	7	TYR	C-N	-5.92	1.20	1.34
1	D	89	GLU	CD-OE1	-5.86	1.19	1.25
1	F	67	LEU	C-N	-5.81	1.20	1.34
1	H	68	LEU	C-N	-5.79	1.20	1.34
2	G	340	LYS	C-N	-5.77	1.20	1.34
1	D	471	ILE	C-N	-5.73	1.20	1.34
1	F	475	THR	C-N	-5.64	1.21	1.34
1	C	447	GLU	CB-CG	-5.63	1.41	1.52
1	E	472	GLU	CD-OE2	-5.62	1.19	1.25
1	A	393	GLU	C-N	-5.54	1.21	1.34
1	H	447	GLU	CB-CG	-5.52	1.41	1.52
1	A	340	LYS	C-N	-5.44	1.21	1.34
1	F	198	GLU	C-N	-5.43	1.21	1.34
1	H	300	VAL	CB-CG1	-5.42	1.41	1.52
1	B	189	SER	CB-OG	-5.40	1.35	1.42
1	B	190	GLU	CD-OE1	-5.36	1.19	1.25
1	H	286	ARG	CB-CG	-5.34	1.38	1.52
1	D	472	GLU	C-N	-5.33	1.21	1.34
2	G	29	THR	N-CA	-5.33	1.35	1.46
1	B	105	GLU	CD-OE2	-5.31	1.19	1.25
1	D	331	GLN	CB-CG	-5.24	1.38	1.52
1	B	339	THR	C-N	-5.20	1.22	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	404	GLN	CB-CG	-5.14	1.38	1.52
1	D	69	GLU	CD-OE1	-5.13	1.20	1.25
1	E	472	GLU	CD-OE1	-5.09	1.20	1.25
2	G	339	THR	C-N	-5.05	1.22	1.34
1	C	480	VAL	CB-CG2	-5.04	1.42	1.52
1	C	202	ASN	C-N	-5.00	1.22	1.34
1	E	183	TYR	CD2-CE2	-5.00	1.31	1.39

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	136	THR	O-C-N	-16.38	96.49	122.70
1	B	297	ARG	O-C-N	16.17	148.58	122.70
1	F	150[A]	ARG	NE-CZ-NH1	-13.08	113.76	120.30
1	F	150[B]	ARG	NE-CZ-NH1	-13.08	113.76	120.30
1	F	150[A]	ARG	NE-CZ-NH2	12.14	126.37	120.30
1	F	150[B]	ARG	NE-CZ-NH2	12.14	126.37	120.30
1	B	297	ARG	CA-C-N	-11.92	90.97	117.20
1	C	136	THR	CA-C-N	11.76	143.08	117.20
1	B	287	ASP	CB-CG-OD1	-11.39	108.05	118.30
2	G	302	LYS	O-C-N	-8.63	108.89	122.70
1	D	196	ARG	O-C-N	-8.30	109.42	122.70
1	H	139	TYR	O-C-N	-8.25	109.49	122.70
1	B	297	ARG	C-N-CA	-8.25	101.07	121.70
1	B	303	ARG	O-C-N	8.25	135.90	122.70
1	E	446	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	B	143	GLU	CG-CD-OE2	-7.96	102.37	118.30
1	B	143	GLU	CG-CD-OE1	7.79	133.87	118.30
1	E	446	ARG	C-N-CA	7.66	140.84	121.70
1	B	413	LYS	CD-CE-NZ	7.66	129.31	111.70
1	H	300	VAL	CG1-CB-CG2	7.58	123.03	110.90
1	A	26	SER	N-CA-C	-7.49	90.79	111.00
1	B	71	ARG	NE-CZ-NH2	-7.27	116.67	120.30
2	G	302	LYS	C-N-CA	7.19	139.68	121.70
1	C	4	ARG	O-C-N	-6.62	112.11	122.70
1	C	203	GLU	O-C-N	-6.59	112.15	122.70
1	B	446	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	D	203	GLU	O-C-N	-6.56	112.20	122.70
2	G	482	LEU	CA-CB-CG	6.49	130.23	115.30
1	C	99	GLN	O-C-N	-6.48	112.33	122.70
1	E	446	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	E	376	ASN	C-N-CA	6.31	137.48	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	139	TYR	C-N-CA	6.28	137.41	121.70
1	B	303	ARG	CA-C-N	-6.27	103.40	117.20
2	G	446	ARG	NE-CZ-NH2	-6.21	117.19	120.30
2	G	485	LEU	CA-CB-CG	-6.19	101.07	115.30
1	C	135	THR	C-N-CA	6.17	137.12	121.70
1	F	104	ARG	O-C-N	6.16	132.55	122.70
2	G	446	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	C	280	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	C	71	ARG	NE-CZ-NH1	-6.09	117.25	120.30
1	B	423	ASP	CB-CG-OD1	6.08	123.77	118.30
1	D	246	MET	N-CA-C	6.08	127.41	111.00
1	E	287	ASP	CB-CA-C	-6.05	98.29	110.40
1	E	288	ALA	N-CA-CB	6.05	118.57	110.10
1	E	394	ASP	O-C-N	-6.04	113.04	122.70
1	E	197	ASP	CB-CG-OD1	6.03	123.73	118.30
1	F	15	LEU	O-C-N	-5.97	113.15	122.70
1	B	104	ARG	C-N-CA	-5.91	106.93	121.70
2	G	29	THR	CA-C-N	-5.88	104.25	117.20
1	A	446	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	E	483	GLU	N-CA-C	5.83	126.74	111.00
1	H	302	LYS	O-C-N	-5.82	113.39	122.70
1	D	283	VAL	CG1-CB-CG2	-5.80	101.61	110.90
2	G	302	LYS	CA-C-N	5.80	129.95	117.20
1	F	461	LEU	CA-CB-CG	5.76	128.56	115.30
1	F	288	ALA	N-CA-CB	5.75	118.15	110.10
1	E	110	LYS	CD-CE-NZ	-5.75	98.47	111.70
1	F	482	LEU	CB-CG-CD1	-5.67	101.37	111.00
1	F	15	LEU	C-N-CA	5.64	135.80	121.70
1	B	67	LEU	CA-CB-CG	5.63	128.25	115.30
1	D	31	ILE	CB-CG1-CD1	5.62	129.65	113.90
1	H	135	THR	N-CA-C	5.55	125.98	111.00
1	D	296	GLY	N-CA-C	5.50	126.85	113.10
1	C	136	THR	C-N-CA	5.47	135.38	121.70
1	A	228	LEU	CD1-CG-CD2	5.47	126.90	110.50
1	F	287	ASP	CB-CA-C	-5.45	99.50	110.40
1	A	286	ARG	N-CA-C	-5.41	96.39	111.00
1	H	377	THR	O-C-N	5.34	131.25	122.70
1	F	396	ARG	O-C-N	-5.31	114.20	122.70
1	D	296	GLY	C-N-CA	5.31	134.97	121.70
1	H	302	LYS	C-N-CA	5.29	134.92	121.70
1	H	139	TYR	CA-C-N	5.27	128.79	117.20
1	D	260	ARG	NE-CZ-NH2	-5.22	117.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	316	ILE	CA-C-N	-5.18	105.81	117.20
1	B	7	TYR	C-N-CA	5.17	134.64	121.70
1	F	482	LEU	C-N-CA	5.17	134.62	121.70
1	H	377	THR	CA-C-N	-5.14	105.89	117.20
1	F	446	ARG	O-C-N	-5.10	114.53	122.70
1	C	303	ARG	O-C-N	5.10	130.86	122.70
1	B	69	GLU	O-C-N	5.08	130.83	122.70
1	F	482	LEU	CB-CG-CD2	-5.02	102.46	111.00
1	B	414	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	D	202	ASN	CA-C-N	-5.02	106.16	117.20

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	ARG	Mainchain
1	A	25	ILE	Peptide
1	A	26	SER	Peptide
1	A	440	GLU	Mainchain
1	B	150[A]	ARG	Sidechain
1	B	150[B]	ARG	Sidechain
1	C	4	ARG	Mainchain
1	C	482	LEU	Peptide
1	D	196	ARG	Mainchain
1	D	482	LEU	Peptide
1	F	475	THR	Mainchain
1	H	140	MET	Mainchain

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	3782	0	3629	42	0
1	B	3770	0	3615	57	0
1	C	3778	0	3613	65	0
1	D	3778	0	3616	50	0
1	E	3777	0	3623	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3782	0	3617	49	0
1	H	3785	0	3630	52	0
2	G	3785	0	3633	47	0
3	A	53	0	30	5	0
3	B	53	0	30	4	0
3	C	53	0	30	5	0
3	D	53	0	30	5	0
3	E	53	0	31	4	0
3	F	53	0	30	4	0
3	G	53	0	31	5	0
3	H	53	0	30	4	0
4	A	4	0	6	0	0
4	C	8	0	12	1	0
4	D	4	0	6	0	0
4	F	4	0	6	0	0
4	G	8	0	12	3	0
5	A	118	0	0	1	0
5	B	134	0	0	1	0
5	C	95	0	0	0	0
5	D	102	0	0	2	0
5	E	122	0	0	1	0
5	F	103	0	0	1	0
5	G	53	0	0	0	0
5	H	80	0	0	1	0
All	All	31496	0	29260	414	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (414) 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:C:481:VAL:C	1:C:482:LEU:HD12	1.44	1.36
1:B:483:GLU:O	1:B:484:GLU:HG2	1.40	1.20
1:B:482:LEU:HD12	1:B:482:LEU:N	1.69	1.06
1:D:483:GLU:O	1:D:484:GLU:HB3	1.49	1.05
1:C:481:VAL:O	1:C:482:LEU:HD12	1.55	1.04
1:E:481:VAL:C	1:E:482:LEU:HD12	1.78	1.03
1:E:482:LEU:N	1:E:482:LEU:CD1	2.18	1.01
1:C:434:ARG:H	1:C:437:MET:HE2	1.27	0.97
1:C:482:LEU:N	1:C:482:LEU:CD1	2.25	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:LEU:N	1:B:482:LEU:CD1	2.29	0.94
1:C:481:VAL:C	1:C:482:LEU:CD1	2.35	0.94
1:B:104:ARG:HD3	1:C:104:ARG:HD2	1.48	0.94
1:D:482:LEU:N	1:D:482:LEU:CD1	2.29	0.94
1:C:482:LEU:HD12	1:C:482:LEU:N	1.75	0.94
1:C:351:ARG:HE	4:C:601:EDO:H22	1.35	0.90
1:B:481:VAL:C	1:B:482:LEU:HD12	1.92	0.90
3:G:600:FAD:H2'	3:G:600:FAD:H9	1.54	0.89
1:D:482:LEU:N	1:D:482:LEU:HD12	1.87	0.88
1:B:104:ARG:CD	1:C:104:ARG:CD	2.52	0.88
1:B:104:ARG:HD3	1:C:104:ARG:CD	2.03	0.87
1:F:196:ARG:HG2	5:F:2056:HOH:O	1.75	0.87
1:E:482:LEU:N	1:E:482:LEU:HD13	1.87	0.86
1:H:342:HIS:HD2	1:H:378:HIS:NE2	1.75	0.85
1:B:284:ASN:HD21	1:B:451:GLY:H	1.23	0.84
1:H:309:PRO:HA	1:H:456:ASN:ND2	1.93	0.84
1:E:481:VAL:C	1:E:482:LEU:CD1	2.44	0.84
3:B:600:FAD:H2'	3:B:600:FAD:H9	1.59	0.84
1:E:482:LEU:HD12	1:E:482:LEU:N	1.88	0.83
1:H:89:GLU:HG3	1:H:93:THR:HG23	1.61	0.82
1:B:483:GLU:C	1:B:484:GLU:HG2	1.95	0.81
1:D:481:VAL:C	1:D:482:LEU:HD12	2.00	0.81
3:C:600:FAD:H2'	3:C:600:FAD:H9	1.61	0.80
1:H:8:GLN:HE21	1:H:414:ARG:HE	1.29	0.80
3:F:600:FAD:H2'	3:F:600:FAD:H9	1.64	0.80
1:F:434:ARG:H	1:F:437:MET:HE2	1.46	0.79
2:G:309:PRO:HA	2:G:456:ASN:ND2	1.98	0.79
3:E:600:FAD:H2'	3:E:600:FAD:H9	1.64	0.78
1:B:104:ARG:CD	1:C:104:ARG:HD2	2.11	0.78
1:C:337:MET:CE	1:C:421:VAL:HG13	2.14	0.78
3:D:600:FAD:H2'	3:D:600:FAD:H9	1.66	0.77
1:C:337:MET:HE2	1:C:421:VAL:HG13	1.66	0.77
1:H:434:ARG:HG3	1:H:437:MET:CE	2.16	0.75
3:H:600:FAD:H2'	3:H:600:FAD:H9	1.69	0.74
1:C:442:LEU:O	1:C:446:ARG:HG3	1.87	0.74
1:F:8:GLN:HE21	1:F:414:ARG:HE	1.33	0.74
1:A:147:GLU:OE1	1:A:150[A]:ARG:NH1	2.21	0.74
1:D:483:GLU:O	1:D:484:GLU:CB	2.30	0.73
1:B:483:GLU:O	1:B:484:GLU:CG	2.30	0.73
1:B:8:GLN:NE2	1:B:414:ARG:HH21	1.87	0.73
1:C:481:VAL:O	1:C:481:VAL:HG12	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:150:ARG:HG3	1:H:151:SER:N	2.03	0.72
1:B:104:ARG:O	1:B:105:GLU:C	2.20	0.72
2:G:485:LEU:N	2:G:485:LEU:HD12	2.04	0.72
1:B:104:ARG:CD	1:C:104:ARG:HD3	2.20	0.72
1:E:67:LEU:HD23	1:E:262:TRP:HZ3	1.53	0.71
1:A:334:HIS:HD2	1:A:336:SER:H	1.40	0.70
1:C:323:SER:O	1:C:327:ILE:HG12	1.91	0.70
1:H:434:ARG:HG3	1:H:437:MET:HE3	1.74	0.70
1:A:69:GLU:OE2	1:A:71:ARG:HG3	1.92	0.70
1:A:390:GLN:HG3	1:A:419:ASN:HD21	1.57	0.69
1:E:25:ILE:HD13	1:E:275:PHE:CZ	2.26	0.69
2:G:344:GLU:OE1	2:G:414:ARG:NH1	2.24	0.69
1:F:8:GLN:NE2	1:F:414:ARG:HE	1.90	0.69
1:A:26:SER:HB3	1:A:27:PRO:HD2	1.75	0.69
1:B:483:GLU:C	1:B:484:GLU:CG	2.62	0.69
1:E:71:ARG:NH2	1:E:423:ASP:OD2	2.26	0.69
1:E:140:MET:HG2	1:E:144:ALA:HB3	1.75	0.69
1:F:69:GLU:OE2	1:F:71:ARG:HG3	1.93	0.69
1:D:302:LYS:O	1:D:303:ARG:HD3	1.93	0.68
1:B:104:ARG:HD2	1:C:104:ARG:HD3	1.76	0.68
1:A:323:SER:O	1:A:327:ILE:HG12	1.94	0.68
1:H:59:THR:CG2	1:H:65:THR:HG23	2.24	0.68
1:C:434:ARG:H	1:C:437:MET:CE	2.05	0.68
1:F:444:GLY:O	1:F:447:GLU:HG2	1.92	0.68
1:H:229:HIS:HE1	1:H:462:GLY:O	1.77	0.68
1:E:229:HIS:HE1	1:E:462:GLY:O	1.77	0.67
1:B:334:HIS:HD2	1:B:336:SER:H	1.41	0.67
1:F:229:HIS:HE1	1:F:462:GLY:O	1.77	0.67
2:G:482:LEU:HD12	2:G:482:LEU:O	1.95	0.67
1:C:331:GLN:HA	1:C:331:GLN:NE2	2.10	0.66
1:A:284:ASN:HD21	1:A:451:GLY:H	1.44	0.66
3:A:600:FAD:H2'	3:A:600:FAD:H9	1.78	0.65
2:G:30:ASN:HD22	2:G:272:GLY:HA2	1.60	0.65
2:G:442:LEU:O	2:G:446:ARG:HG3	1.97	0.65
1:D:482:LEU:N	1:D:482:LEU:HD13	2.10	0.65
1:A:179:GLU:HG3	1:A:182:LYS:NZ	2.11	0.64
1:F:242:MET:HE3	1:F:246:MET:HE3	1.79	0.64
1:A:327:ILE:O	1:A:331:GLN:HG2	1.98	0.64
2:G:482:LEU:HD12	2:G:482:LEU:C	2.18	0.64
1:E:69:GLU:OE1	3:E:600:FAD:H3B	1.98	0.63
1:E:334:HIS:HD2	1:E:336:SER:H	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:123:ARG:HH21	4:G:601:EDO:HO2	1.47	0.63
1:A:25:ILE:HA	1:A:26:SER:HB2	1.81	0.63
1:C:215:SER:O	1:C:336:SER:HB2	1.98	0.63
1:F:351:ARG:HE	4:G:601:EDO:H11	1.62	0.62
2:G:323:SER:O	2:G:327:ILE:HG12	1.99	0.62
1:B:229:HIS:HE1	1:B:462:GLY:O	1.82	0.62
1:A:140:MET:HG2	1:A:144:ALA:HB3	1.82	0.62
2:G:485:LEU:N	2:G:485:LEU:CD1	2.62	0.62
1:H:147:GLU:HA	1:H:150:ARG:HG2	1.81	0.62
1:H:59:THR:HG23	1:H:65:THR:CG2	2.30	0.61
1:A:25:ILE:HA	1:A:26:SER:CB	2.29	0.61
1:B:104:ARG:HD2	1:C:104:ARG:CD	2.27	0.61
1:C:434:ARG:N	1:C:437:MET:HE2	2.09	0.61
1:H:46:GLY:HA2	1:H:69:GLU:OE1	2.01	0.61
1:C:482:LEU:N	1:C:482:LEU:HD13	2.14	0.61
1:D:482:LEU:HD13	1:D:482:LEU:H	1.65	0.61
1:F:390:GLN:HE21	1:F:419:ASN:HD21	1.49	0.60
1:F:22:LEU:O	1:F:259:ARG:HD3	2.01	0.60
2:G:2:THR:HG23	2:G:19:VAL:C	2.21	0.60
1:E:482:LEU:HA	1:E:484:GLU:H	1.67	0.60
1:A:25:ILE:HG23	1:A:26:SER:HB2	1.83	0.60
1:E:442:LEU:O	1:E:446:ARG:HG3	2.02	0.60
1:H:59:THR:HG23	1:H:65:THR:HG23	1.83	0.59
1:B:8:GLN:HE22	1:B:414:ARG:HH21	1.50	0.59
1:E:481:VAL:O	1:E:482:LEU:HD12	2.00	0.59
1:B:314:SER:HB3	1:B:330:MET:HG2	1.83	0.59
2:G:30:ASN:ND2	2:G:272:GLY:HA2	2.16	0.59
1:E:326:ARG:O	1:E:330:MET:HG2	2.03	0.59
1:E:284:ASN:HD21	1:E:452:VAL:HG23	1.67	0.59
1:B:46:GLY:HA2	1:B:69:GLU:OE1	2.03	0.58
1:B:92:GLY:HA2	3:B:600:FAD:C4X	2.33	0.58
1:H:8:GLN:NE2	1:H:414:ARG:HE	1.98	0.58
1:B:388:HIS:NE2	1:B:390:GLN:NE2	2.52	0.58
2:G:25:ILE:HD13	2:G:74:ILE:HG23	1.84	0.58
1:B:41:ASP:HB2	1:B:64:LYS:O	2.02	0.58
2:G:229:HIS:HE1	2:G:462:GLY:O	1.86	0.58
1:C:481:VAL:O	1:C:481:VAL:CG1	2.52	0.58
1:F:242:MET:CE	1:F:246:MET:HE3	2.34	0.58
1:E:67:LEU:CD2	1:E:262:TRP:HZ3	2.15	0.58
1:C:480:VAL:O	1:C:483:GLU:HB2	2.03	0.58
1:H:59:THR:CG2	1:H:65:THR:CG2	2.82	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:SER:HB3	1:A:27:PRO:CD	2.33	0.57
2:G:89:GLU:HG3	2:G:93:THR:HG23	1.87	0.57
1:H:334:HIS:HD2	1:H:336:SER:H	1.53	0.57
2:G:26:SER:HA	2:G:27:PRO:C	2.23	0.57
1:B:179:GLU:O	1:B:179:GLU:HG2	2.04	0.56
1:E:67:LEU:HD23	1:E:262:TRP:CZ3	2.37	0.56
1:E:430:TRP:HB3	3:E:600:FAD:H1'1	1.86	0.56
2:G:192:ILE:O	2:G:196:ARG:HB3	2.06	0.56
1:A:101:HIS:HE1	1:E:107:THR:OG1	1.88	0.56
1:A:229:HIS:HE1	1:A:462:GLY:O	1.89	0.56
1:E:92:GLY:HA2	3:E:600:FAD:C4X	2.35	0.56
1:D:442:LEU:O	1:D:446:ARG:HG3	2.05	0.56
1:E:29:THR:HG22	1:E:273:TYR:O	2.04	0.56
1:E:482:LEU:HA	1:E:484:GLU:N	2.19	0.56
1:H:309:PRO:HA	1:H:456:ASN:HD21	1.71	0.56
1:F:2:THR:HA	1:F:20:PRO:HA	1.88	0.56
1:E:8:GLN:HE21	1:E:414:ARG:HE	1.54	0.55
2:G:309:PRO:HA	2:G:456:ASN:HD21	1.70	0.55
2:G:456:ASN:O	2:G:473:GLU:HG3	2.06	0.55
1:F:242:MET:CE	1:F:246:MET:CE	2.84	0.55
1:H:309:PRO:HA	1:H:456:ASN:HD22	1.69	0.55
1:D:142:HIS:O	1:D:145:GLU:HB3	2.06	0.55
1:E:150[B]:ARG:HH21	1:E:237:THR:HB	1.72	0.55
1:C:397:GLU:OE1	1:C:400:LYS:HE2	2.07	0.55
1:A:179:GLU:HG3	1:A:182:LYS:CE	2.37	0.54
1:D:79:TRP:CZ2	1:D:90:MET:HG3	2.42	0.54
1:H:47:GLY:N	1:H:69:GLU:OE1	2.40	0.54
1:H:319:SER:HA	1:H:320:PRO:C	2.27	0.54
1:F:242:MET:HE3	1:F:246:MET:CE	2.37	0.54
1:E:242:MET:CE	1:E:246:MET:CE	2.86	0.54
2:G:133:ASN:OD1	2:G:135:THR:HG22	2.08	0.54
1:H:354:THR:HG22	1:H:367:ILE:HG22	1.89	0.54
1:F:302:LYS:O	1:F:303:ARG:HD3	2.07	0.54
2:G:69:GLU:OE1	3:G:600:FAD:H3B	2.07	0.54
1:H:369:ASP:HB2	1:H:380:VAL:HG12	1.89	0.54
1:D:101:HIS:HE1	1:H:107:THR:OG1	1.90	0.54
1:F:390:GLN:NE2	1:F:419:ASN:HD21	2.05	0.54
1:H:434:ARG:HG3	1:H:437:MET:HE1	1.90	0.54
1:E:242:MET:CE	1:E:246:MET:HE3	2.38	0.54
1:B:44:VAL:O	1:B:67:LEU:HA	2.08	0.53
1:C:92:GLY:HA2	3:C:600:FAD:C4X	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:242:MET:HE1	1:E:246:MET:CE	2.38	0.53
1:C:97:TRP:HB3	1:C:103:TRP:CE2	2.44	0.53
1:E:242:MET:HE3	1:E:246:MET:HE3	1.90	0.53
1:D:8:GLN:NE2	1:D:414:ARG:HH21	2.06	0.53
1:F:400:LYS:O	1:F:404:GLN:HG3	2.08	0.53
1:C:8:GLN:HE21	1:C:414:ARG:HE	1.57	0.53
2:G:241:CYS:O	2:G:245:LEU:HG	2.09	0.53
1:D:229:HIS:HE1	1:D:462:GLY:O	1.92	0.53
2:G:482:LEU:O	2:G:482:LEU:CD1	2.56	0.53
1:F:123:ARG:NH2	4:G:601:EDO:O2	2.32	0.53
1:C:152:ALA:HB1	1:C:207:LEU:HB2	1.91	0.52
1:F:442:LEU:O	1:F:446:ARG:HG3	2.10	0.52
2:G:94:TRP:CG	2:G:246:MET:HA	2.45	0.52
1:A:390:GLN:HG3	1:A:419:ASN:ND2	2.24	0.52
1:B:283:VAL:HG22	1:B:319:SER:HB2	1.91	0.52
1:D:107:THR:OG1	1:H:101:HIS:HE1	1.92	0.52
2:G:92:GLY:HA2	3:G:600:FAD:C4X	2.39	0.52
1:A:191:ARG:HG2	1:A:224:PHE:CE1	2.44	0.52
1:F:90:MET:CE	1:F:418:HIS:HB2	2.38	0.52
1:A:2:THR:HA	1:A:20:PRO:HA	1.91	0.52
1:F:43:ILE:HA	1:F:66:LEU:O	2.10	0.52
1:H:89:GLU:O	1:H:342:HIS:HE1	1.92	0.52
1:A:92:GLY:HA2	3:A:600:FAD:C4X	2.39	0.52
1:B:107:THR:OG1	1:C:101:HIS:HE1	1.93	0.52
3:G:600:FAD:H9	3:G:600:FAD:C2'	2.35	0.52
1:E:89:GLU:HG3	1:E:93:THR:HG23	1.91	0.52
1:D:56:ARG:HD3	1:D:264:GLU:OE1	2.10	0.52
1:H:342:HIS:CD2	1:H:378:HIS:NE2	2.67	0.52
1:C:8:GLN:NE2	1:C:414:ARG:HE	2.08	0.51
1:E:362:LYS:HB3	1:E:389:ILE:HB	1.92	0.51
1:C:5:ASP:OD2	1:C:71:ARG:HD3	2.11	0.51
3:B:600:FAD:H9	3:B:600:FAD:C2'	2.36	0.51
1:C:334:HIS:HD2	1:C:336:SER:H	1.58	0.51
1:C:326:ARG:HG2	1:C:445:LEU:HD23	1.93	0.51
1:E:330:MET:HE3	5:E:2089:HOH:O	2.10	0.51
1:F:430:TRP:HB3	3:F:600:FAD:H1'1	1.93	0.51
1:E:482:LEU:HD13	1:E:482:LEU:H	1.73	0.51
1:A:460:ALA:HB3	1:A:464:ARG:HA	1.93	0.51
1:D:92:GLY:HA2	3:D:600:FAD:C4X	2.41	0.50
1:F:369:ASP:HB2	1:F:380:VAL:HG12	1.93	0.50
1:F:69:GLU:OE1	3:F:600:FAD:H3B	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:19:VAL:HB	1:H:20:PRO:HD2	1.92	0.50
1:A:89:GLU:O	1:A:342:HIS:NE2	2.38	0.50
1:B:71:ARG:NH2	1:B:423:ASP:OD2	2.34	0.50
1:H:326:ARG:O	1:H:330:MET:HG2	2.12	0.50
1:D:314:SER:HB3	1:D:330:MET:HG2	1.93	0.50
1:D:326:ARG:O	1:D:330:MET:HB2	2.12	0.50
1:H:442:LEU:O	1:H:446:ARG:HG3	2.12	0.50
1:A:69:GLU:OE1	3:A:600:FAD:H3B	2.11	0.50
1:D:92:GLY:HA2	3:D:600:FAD:C5X	2.42	0.50
1:A:133:ASN:HB2	1:A:134:PRO:HD2	1.92	0.49
1:A:179:GLU:O	1:A:180:PHE:C	2.50	0.49
2:G:309:PRO:HA	2:G:456:ASN:HD22	1.74	0.49
1:D:79:TRP:CE2	1:D:90:MET:HG3	2.48	0.49
1:E:480:VAL:HG12	1:E:481:VAL:N	2.27	0.49
1:D:429:ALA:HB1	3:D:600:FAD:HM83	1.95	0.49
1:B:101:HIS:HE1	1:C:107:THR:OG1	1.95	0.49
1:A:287:ASP:OD1	1:A:287:ASP:O	2.30	0.49
1:E:89:GLU:O	1:E:342:HIS:NE2	2.41	0.49
1:F:101:HIS:HD2	1:F:468:ASP:OD2	1.95	0.49
3:C:600:FAD:H2'	3:C:600:FAD:C9	2.37	0.49
1:H:92:GLY:HA2	3:H:600:FAD:C4X	2.43	0.49
1:B:307:THR:HA	1:B:455:ALA:O	2.13	0.49
1:H:19:VAL:HB	1:H:20:PRO:CD	2.43	0.49
1:H:80:SER:HB3	1:H:255:SER:H	1.78	0.48
1:H:430:TRP:HB3	3:H:600:FAD:H1'1	1.95	0.48
1:B:481:VAL:O	1:B:484:GLU:HG3	2.13	0.48
1:F:154:HIS:O	1:F:158:ASN:HB2	2.13	0.48
1:D:396:ARG:HA	1:D:396:ARG:HD3	1.70	0.48
1:E:25:ILE:HD11	1:E:74:ILE:HG23	1.96	0.48
2:G:392:ASP:OD1	2:G:422:LYS:NZ	2.39	0.48
1:H:63:PHE:O	1:H:65:THR:HG22	2.14	0.48
1:H:129:GLN:HE21	1:H:131:ARG:HD3	1.79	0.48
1:H:362:LYS:HB3	1:H:389:ILE:HB	1.95	0.48
1:C:89:GLU:O	1:C:342:HIS:NE2	2.43	0.48
2:G:152:ALA:HB1	2:G:207:LEU:HB2	1.95	0.48
2:G:326:ARG:CZ	2:G:454:PHE:CD2	2.96	0.48
1:B:94:TRP:CD2	1:B:246:MET:HA	2.49	0.48
1:C:133:ASN:HB2	1:C:134:PRO:CD	2.44	0.48
2:G:116:SER:OG	2:G:251:LYS:HB2	2.14	0.48
1:H:295:ASP:OD1	1:H:296:GLY:N	2.46	0.48
2:G:337:MET:O	2:G:388:HIS:HE1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:ASN:HB2	1:B:320:PRO:HD3	1.96	0.47
1:F:107:THR:OG1	2:G:101:HIS:HE1	1.97	0.47
1:A:430:TRP:HB3	3:A:600:FAD:H1'1	1.95	0.47
1:C:89:GLU:HG3	1:C:93:THR:HG23	1.95	0.47
1:A:241:CYS:O	1:A:245:LEU:HG	2.14	0.47
1:F:434:ARG:N	1:F:437:MET:HE2	2.24	0.47
1:H:76:GLY:HA2	3:H:600:FAD:O3B	2.15	0.47
1:E:473:GLU:OE1	1:E:476:ARG:NH2	2.36	0.47
1:C:116:SER:OG	1:C:251:LYS:HG3	2.15	0.46
1:H:479[A]:ARG:HE	1:H:479[A]:ARG:HB2	1.51	0.46
1:B:430:TRP:HB3	3:B:600:FAD:H1'1	1.98	0.46
1:D:390:GLN:HG3	1:D:419:ASN:HD21	1.80	0.46
5:B:2122:HOH:O	1:F:396:ARG:HD2	2.16	0.46
1:F:394:ASP:OD1	1:F:396:ARG:HB3	2.15	0.46
1:D:336:SER:HB3	1:D:430:TRP:O	2.16	0.46
1:A:152:ALA:HB1	1:A:207:LEU:HB2	1.97	0.46
1:B:334:HIS:HB2	1:B:432:PHE:O	2.15	0.46
1:D:326:ARG:HG2	1:D:445:LEU:HD23	1.98	0.46
1:E:344:GLU:HB3	1:E:414:ARG:HB3	1.97	0.46
1:F:460:ALA:HB3	1:F:464:ARG:HA	1.97	0.46
2:G:482:LEU:C	2:G:482:LEU:CD1	2.84	0.46
1:F:323:SER:HB3	1:F:447:GLU:OE2	2.16	0.46
1:C:327:ILE:O	1:C:331:GLN:HG2	2.15	0.45
1:A:390:GLN:HG2	1:A:422:LYS:HD2	1.98	0.45
1:A:396:ARG:HA	1:A:396:ARG:HD3	1.54	0.45
1:B:94:TRP:CG	1:B:246:MET:HA	2.52	0.45
1:B:9:TRP:O	1:B:414:ARG:HA	2.17	0.45
1:C:482:LEU:HA	1:C:484:GLU:N	2.31	0.45
1:B:292:THR:HA	1:B:297:ARG:O	2.17	0.45
1:F:69:GLU:HB3	1:F:275:PHE:CD1	2.51	0.45
2:G:179:GLU:O	2:G:179:GLU:CG	2.64	0.45
1:H:456:ASN:OD1	1:H:457:SER:N	2.50	0.45
1:E:336:SER:HB3	1:E:430:TRP:O	2.17	0.45
1:A:92:GLY:HA2	3:A:600:FAD:C5X	2.47	0.45
1:C:8:GLN:O	1:C:15:LEU:HA	2.17	0.45
1:B:482:LEU:CD1	1:B:482:LEU:H	2.22	0.45
1:D:259:ARG:HA	1:D:259:ARG:HD3	1.66	0.45
1:D:259:ARG:O	1:D:263:GLU:HG2	2.16	0.45
1:D:480:VAL:O	1:D:483:GLU:HB3	2.17	0.45
1:D:483:GLU:O	1:D:483:GLU:CG	2.66	0.44
1:F:242:MET:HE1	1:F:246:MET:CE	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:89:GLU:O	1:H:342:HIS:CE1	2.69	0.44
1:B:480:VAL:O	1:B:483:GLU:HB2	2.17	0.44
1:C:337:MET:HE2	1:C:421:VAL:CG1	2.42	0.44
1:C:456:ASN:O	1:C:473:GLU:HG3	2.17	0.44
1:B:400:LYS:O	1:B:404:GLN:HG3	2.17	0.44
1:D:260:ARG:NH2	5:D:2070:HOH:O	2.50	0.44
1:B:326:ARG:HG2	1:B:445:LEU:HD23	2.00	0.44
1:C:283:VAL:HG13	1:C:319:SER:HB2	2.00	0.44
2:G:484:GLU:O	2:G:485:LEU:HB2	2.18	0.44
1:F:446:ARG:NH2	1:F:473:GLU:OE2	2.50	0.43
2:G:335:VAL:HG22	2:G:432:PHE:O	2.18	0.43
1:F:8:GLN:NE2	1:F:414:ARG:HH21	2.16	0.43
1:H:479[B]:ARG:CZ	1:H:479[B]:ARG:HB3	2.48	0.43
1:C:99:GLN:HG2	1:C:463:TRP:CE2	2.53	0.43
1:H:465:SER:HA	5:H:2075:HOH:O	2.19	0.43
1:B:330:MET:HE2	1:B:330:MET:HB2	1.81	0.43
1:C:86:TYR:HA	1:C:87:PRO:HD3	1.87	0.43
1:D:29:THR:HG22	1:D:274:VAL:HG22	2.00	0.43
1:F:90:MET:HE2	1:F:418:HIS:HB2	1.99	0.43
1:A:107:THR:OG1	1:E:101:HIS:HE1	2.00	0.43
2:G:295:ASP:HB3	2:G:297:ARG:H	1.83	0.43
1:H:99:GLN:HG2	1:H:463:TRP:CE2	2.54	0.43
1:C:43:ILE:HG12	1:C:66:LEU:HD23	2.00	0.43
1:C:440:GLU:O	1:C:440:GLU:HG2	2.19	0.43
1:D:188:TYR:CD2	1:D:211:ILE:HD12	2.54	0.43
1:D:369:ASP:HB2	1:D:380:VAL:HG12	2.01	0.43
1:E:212:LEU:HD22	1:E:217:GLY:O	2.18	0.43
1:F:92:GLY:HA2	3:F:600:FAD:C4X	2.49	0.43
1:F:101:HIS:N	1:F:468:ASP:OD1	2.50	0.43
2:G:290:ARG:HD3	2:G:298:GLU:OE1	2.19	0.43
1:D:99:GLN:HG2	1:D:463:TRP:CE2	2.54	0.43
3:G:600:FAD:H2'	3:G:600:FAD:C9	2.37	0.43
1:H:344:GLU:OE1	1:H:414:ARG:NH1	2.50	0.43
1:A:25:ILE:CD1	1:A:74:ILE:HG23	2.49	0.42
1:D:220:GLU:CD	1:D:220:GLU:H	2.21	0.42
1:A:259:ARG:HD2	1:A:259:ARG:HA	1.83	0.42
1:C:482:LEU:HA	1:C:484:GLU:H	1.83	0.42
1:C:26:SER:HA	1:C:27:PRO:C	2.39	0.42
2:G:8:GLN:NE2	2:G:414:ARG:HE	2.17	0.42
1:C:344:GLU:HB3	1:C:414:ARG:HB3	2.01	0.42
1:B:482:LEU:N	1:B:482:LEU:HD13	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:MET:HE3	1:C:421:VAL:HG22	2.01	0.42
1:B:69:GLU:HG3	1:B:71:ARG:H	1.85	0.42
1:C:314:SER:HA	1:C:330:MET:HE3	2.02	0.42
1:D:456:ASN:O	1:D:473:GLU:HG3	2.20	0.42
1:H:101:HIS:HD2	1:H:468:ASP:OD2	2.03	0.42
1:D:133:ASN:ND2	1:D:136:THR:HG22	2.35	0.42
1:E:77:ARG:HA	1:E:420:TRP:CH2	2.55	0.42
1:F:255:SER:O	1:F:259:ARG:HG2	2.19	0.42
1:B:281:SER:HA	1:B:317:GLN:O	2.19	0.42
1:D:245:LEU:HA	1:D:245:LEU:HD23	1.78	0.42
1:E:46:GLY:O	1:E:51:GLY:HA3	2.19	0.42
1:E:181:ARG:O	1:E:182:LYS:C	2.55	0.42
1:F:241:CYS:O	1:F:245:LEU:HG	2.19	0.42
1:F:434:ARG:H	1:F:437:MET:CE	2.23	0.42
1:C:133:ASN:HB2	1:C:134:PRO:HD2	2.01	0.42
1:D:430:TRP:HB3	3:D:600:FAD:H1'1	2.01	0.42
2:G:171:PRO:HG3	2:G:232:ALA:HB1	2.02	0.42
1:H:31:ILE:HG21	1:H:31:ILE:HD13	1.64	0.42
1:B:69:GLU:OE2	1:B:71:ARG:HG3	2.19	0.42
1:E:25:ILE:CD1	1:E:74:ILE:HG23	2.49	0.42
1:F:101:HIS:CD2	1:F:472:GLU:HB2	2.55	0.42
1:A:43:ILE:HG13	1:A:301:ALA:HB2	2.01	0.41
1:B:25:ILE:HG13	1:B:275:PHE:CZ	2.54	0.41
1:B:482:LEU:HA	1:B:484:GLU:N	2.35	0.41
1:E:94:TRP:CD2	1:E:246:MET:HA	2.55	0.41
1:E:157:THR:HG21	1:E:231:TRP:CE2	2.55	0.41
1:C:430:TRP:HB3	3:C:600:FAD:H1'1	2.02	0.41
1:D:186:MET:HE3	1:D:191:ARG:HD3	2.00	0.41
1:D:192:ILE:O	1:D:196:ARG:HB2	2.20	0.41
1:C:141:THR:HB	1:C:143:GLU:OE1	2.19	0.41
1:D:29:THR:HB	1:D:31:ILE:H	1.86	0.41
1:F:114:ALA:O	1:F:251:LYS:HG2	2.20	0.41
2:G:283:VAL:HG13	2:G:319:SER:HB2	2.03	0.41
2:G:318:PHE:CD2	2:G:322:LEU:HD11	2.55	0.41
1:B:179:GLU:O	1:B:179:GLU:CG	2.67	0.41
1:D:292:THR:HA	1:D:297:ARG:O	2.20	0.41
1:E:8:GLN:NE2	1:E:414:ARG:HE	2.16	0.41
1:E:464:ARG:O	1:E:465:SER:CB	2.66	0.41
1:A:395:VAL:HG23	5:A:2102:HOH:O	2.21	0.41
1:C:215:SER:HB2	1:C:432:PHE:CD1	2.55	0.41
1:D:150:ARG:NH2	5:D:2039:HOH:O	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ILE:CA	1:A:26:SER:HB2	2.49	0.41
1:A:147:GLU:O	1:A:148:LEU:C	2.58	0.41
1:B:152:ALA:HB1	1:B:207:LEU:HB2	2.03	0.41
1:D:154:HIS:O	1:D:158:ASN:HB2	2.20	0.41
2:G:43:ILE:HB	2:G:304:VAL:HG22	2.02	0.41
2:G:63:PHE:HE2	2:G:482:LEU:HD22	1.85	0.41
1:H:152:ALA:HB1	1:H:207:LEU:HB2	2.01	0.41
1:A:141:THR:HB	1:A:143:GLU:OE1	2.21	0.41
1:E:342:HIS:O	1:E:415:LEU:HA	2.20	0.41
1:E:367:ILE:HG13	1:E:380:VAL:HG12	2.03	0.41
2:G:23:GLY:O	2:G:25:ILE:HD12	2.20	0.41
2:G:86:TYR:HA	2:G:87:PRO:HD3	1.99	0.41
2:G:292:THR:HG23	2:G:298:GLU:HG2	2.03	0.41
1:H:476:ARG:O	1:H:480:VAL:HG23	2.21	0.41
1:C:40:TRP:O	1:C:301:ALA:HA	2.21	0.41
1:C:76:GLY:HA2	3:C:600:FAD:O3B	2.21	0.41
1:C:331:GLN:NE2	1:C:331:GLN:CA	2.76	0.41
1:D:9:TRP:O	1:D:414:ARG:HA	2.20	0.41
1:D:89:GLU:O	1:D:342:HIS:NE2	2.50	0.41
1:A:179:GLU:HG3	1:A:182:LYS:HZ1	1.84	0.40
1:B:104:ARG:C	1:B:106:ILE:N	2.70	0.40
1:B:482:LEU:H	1:B:482:LEU:HD13	1.86	0.40
1:E:152:ALA:HB1	1:E:207:LEU:HB2	2.03	0.40
1:F:326:ARG:HG2	1:F:445:LEU:HD23	2.02	0.40
2:G:69:GLU:OE2	2:G:71:ARG:HG3	2.21	0.40
1:H:59:THR:HG22	1:H:65:THR:CG2	2.51	0.40
1:B:89:GLU:HA	1:B:89:GLU:OE1	2.22	0.40
1:B:101:HIS:HD2	1:B:468:ASP:OD2	2.05	0.40
1:C:77:ARG:HA	1:C:420:TRP:CH2	2.56	0.40
1:F:249:LYS:NZ	1:F:369:ASP:OD2	2.45	0.40
1:D:25:ILE:HG13	1:D:275:PHE:CZ	2.57	0.40
1:D:446:ARG:CZ	1:D:461:LEU:HD13	2.51	0.40
1:C:22:LEU:O	1:C:259:ARG:HD3	2.22	0.40
1:E:481:VAL:HG12	1:E:482:LEU:CD1	2.52	0.40
1:F:322:LEU:HD13	1:F:330:MET:HE1	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	475/495 (96%)	454 (96%)	20 (4%)	1 (0%)	47 57
1	B	473/495 (96%)	457 (97%)	16 (3%)	0	100 100
1	C	474/495 (96%)	453 (96%)	19 (4%)	2 (0%)	34 41
1	D	474/495 (96%)	458 (97%)	16 (3%)	0	100 100
1	E	474/495 (96%)	451 (95%)	22 (5%)	1 (0%)	47 57
1	F	475/495 (96%)	456 (96%)	19 (4%)	0	100 100
1	H	475/495 (96%)	460 (97%)	15 (3%)	0	100 100
2	G	475/495 (96%)	449 (94%)	26 (6%)	0	100 100
All	All	3795/3960 (96%)	3638 (96%)	153 (4%)	4 (0%)	51 64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	SER
1	E	481	VAL
1	C	481	VAL
1	C	179	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	400/414 (97%)	386 (96%)	14 (4%)	36 47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	399/414 (96%)	390 (98%)	9 (2%)	50 63
1	C	400/414 (97%)	383 (96%)	17 (4%)	29 38
1	D	400/414 (97%)	384 (96%)	16 (4%)	31 41
1	E	400/414 (97%)	388 (97%)	12 (3%)	41 52
1	F	400/414 (97%)	387 (97%)	13 (3%)	38 49
1	H	401/414 (97%)	385 (96%)	16 (4%)	31 41
2	G	401/414 (97%)	387 (96%)	14 (4%)	36 47
All	All	3201/3312 (97%)	3090 (96%)	111 (4%)	37 47

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	26	SER
1	A	31	ILE
1	A	67	LEU
1	A	87	PRO
1	A	136	THR
1	A	149	LEU
1	A	182	LYS
1	A	280	ARG
1	A	286	ARG
1	A	396	ARG
1	A	404	GLN
1	A	439	SER
1	A	479	ARG
1	B	127	HIS
1	B	149	LEU
1	B	246	MET
1	B	302	LYS
1	B	319	SER
1	B	400	LYS
1	B	461	LEU
1	B	482	LEU
1	B	484	GLU
1	C	24	VAL
1	C	26	SER
1	C	32	GLU
1	C	127	HIS
1	C	251	LYS

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Mol	Chain	Res	Type
1	C	280	ARG
1	C	317	GLN
1	C	328	SER
1	C	337	MET
1	C	380	VAL
1	C	395	VAL
1	C	400	LYS
1	C	461	LEU
1	C	479	ARG
1	C	480	VAL
1	C	482	LEU
1	C	484	GLU
1	D	67	LEU
1	D	127	HIS
1	D	136	THR
1	D	150	ARG
1	D	182	LYS
1	D	220	GLU
1	D	303	ARG
1	D	317	GLN
1	D	324	THR
1	D	328	SER
1	D	390	GLN
1	D	396	ARG
1	D	439	SER
1	D	461	LEU
1	D	482	LEU
1	D	484	GLU
1	E	1	MET
1	E	29	THR
1	E	136	THR
1	E	182	LYS
1	E	196	ARG
1	E	246	MET
1	E	263	GLU
1	E	328	SER
1	E	461	LEU
1	E	465	SER
1	E	479	ARG
1	E	482	LEU
1	F	127	HIS
1	F	135	THR

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Mol	Chain	Res	Type
1	F	136	THR
1	F	182	LYS
1	F	196	ARG
1	F	246	MET
1	F	280	ARG
1	F	303	ARG
1	F	324	THR
1	F	390	GLN
1	F	461	LEU
1	F	479	ARG
1	F	482	LEU
2	G	19	VAL
2	G	39	PRO
2	G	80	SER
2	G	116	SER
2	G	127	HIS
2	G	136	THR
2	G	196	ARG
2	G	251	LYS
2	G	280	ARG
2	G	295	ASP
2	G	297	ARG
2	G	461	LEU
2	G	479	ARG
2	G	482	LEU
1	H	15	LEU
1	H	26	SER
1	H	65	THR
1	H	127	HIS
1	H	149	LEU
1	H	182	LYS
1	H	281	SER
1	H	297	ARG
1	H	319	SER
1	H	330	MET
1	H	396	ARG
1	H	461	LEU
1	H	465	SER
1	H	479[A]	ARG
1	H	479[B]	ARG
1	H	482	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	101	HIS
1	A	127	HIS
1	A	154	HIS
1	A	163	ASN
1	A	229	HIS
1	A	284	ASN
1	A	334	HIS
1	A	388	HIS
1	A	390	GLN
1	B	8	GLN
1	B	101	HIS
1	B	163	ASN
1	B	229	HIS
1	B	284	ASN
1	B	331	GLN
1	B	334	HIS
1	B	404	GLN
1	B	449	HIS
1	C	8	GLN
1	C	82	ASN
1	C	101	HIS
1	C	331	GLN
1	C	334	HIS
1	D	8	GLN
1	D	101	HIS
1	D	163	ASN
1	D	284	ASN
1	E	8	GLN
1	E	101	HIS
1	E	163	ASN
1	E	229	HIS
1	E	284	ASN
1	E	334	HIS
1	E	404	GLN
1	F	8	GLN
1	F	101	HIS
1	F	229	HIS
1	F	284	ASN
1	F	390	GLN
1	F	404	GLN
2	G	8	GLN

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Mol	Chain	Res	Type
2	G	30	ASN
2	G	101	HIS
2	G	163	ASN
2	G	229	HIS
2	G	284	ASN
2	G	388	HIS
1	H	8	GLN
1	H	101	HIS
1	H	163	ASN
1	H	229	HIS
1	H	284	ASN
1	H	334	HIS
1	H	342	HIS
1	H	404	GLN
1	H	449	HIS

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)

15 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	$\#\|Z\|>2$
3	FAD	F	600	-	53,58,58	1.63	6 (11%)	68,89,89	2.21	19 (27%)
3	FAD	B	600	-	53,58,58	1.65	5 (9%)	68,89,89	2.64	20 (29%)
3	FAD	E	600	-	53,58,58	1.72	6 (11%)	68,89,89	2.35	21 (30%)
3	FAD	H	600	-	53,58,58	1.60	4 (7%)	68,89,89	2.26	22 (32%)
4	EDO	F	601	-	3,3,3	0.41	0	2,2,2	0.65	0
3	FAD	D	600	-	53,58,58	1.51	5 (9%)	68,89,89	2.30	17 (25%)
3	FAD	C	600	-	53,58,58	1.48	3 (5%)	68,89,89	2.27	18 (26%)
3	FAD	A	600	-	53,58,58	1.44	6 (11%)	68,89,89	2.42	19 (27%)
3	FAD	G	600	-	53,58,58	1.51	5 (9%)	68,89,89	2.36	19 (27%)
4	EDO	G	602	-	3,3,3	0.49	0	2,2,2	0.38	0
4	EDO	G	601	-	3,3,3	0.44	0	2,2,2	0.79	0
4	EDO	C	601	-	3,3,3	0.41	0	2,2,2	0.65	0
4	EDO	D	601	-	3,3,3	0.43	0	2,2,2	0.22	0
4	EDO	C	602	-	3,3,3	0.48	0	2,2,2	0.39	0
4	EDO	A	601	-	3,3,3	0.45	0	2,2,2	0.71	0

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
3	FAD	F	600	-	3/3/9/9	11/30/50/50	0/6/6/6
3	FAD	B	600	-	3/3/9/9	9/30/50/50	0/6/6/6
3	FAD	E	600	-	3/3/9/9	13/30/50/50	0/6/6/6
3	FAD	H	600	-	3/3/9/9	10/30/50/50	0/6/6/6
4	EDO	F	601	-	-	1/1/1/1	-
3	FAD	D	600	-	3/3/9/9	10/30/50/50	0/6/6/6
3	FAD	C	600	-	3/3/9/9	9/30/50/50	0/6/6/6
3	FAD	A	600	-	3/3/9/9	11/30/50/50	0/6/6/6
3	FAD	G	600	-	3/3/9/9	18/30/50/50	0/6/6/6
4	EDO	G	602	-	-	1/1/1/1	-
4	EDO	G	601	-	-	1/1/1/1	-
4	EDO	C	601	-	-	1/1/1/1	-
4	EDO	D	601	-	-	1/1/1/1	-
4	EDO	C	602	-	-	1/1/1/1	-
4	EDO	A	601	-	-	1/1/1/1	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	600	FAD	O4B-C1B	7.27	1.51	1.41
3	H	600	FAD	O4B-C1B	6.93	1.50	1.41
3	B	600	FAD	C4X-N5	6.87	1.44	1.30
3	F	600	FAD	C4X-N5	6.74	1.43	1.30
3	E	600	FAD	C4X-N5	6.52	1.43	1.30
3	C	600	FAD	C4X-N5	6.42	1.43	1.30
3	D	600	FAD	C4X-N5	6.16	1.42	1.30
3	F	600	FAD	O4B-C1B	5.99	1.49	1.41
3	G	600	FAD	C4X-N5	5.92	1.42	1.30
3	H	600	FAD	C4X-N5	5.59	1.41	1.30
3	G	600	FAD	O4B-C1B	5.47	1.48	1.41
3	B	600	FAD	O4B-C1B	5.46	1.48	1.41
3	C	600	FAD	O4B-C1B	5.18	1.48	1.41
3	A	600	FAD	C4X-N5	5.11	1.40	1.30
3	A	600	FAD	O4B-C1B	4.41	1.47	1.41
3	D	600	FAD	O4B-C1B	4.35	1.47	1.41
3	B	600	FAD	O4B-C4B	3.38	1.52	1.45
3	D	600	FAD	C10-N1	3.24	1.39	1.33
3	H	600	FAD	C10-N1	3.20	1.39	1.33
3	A	600	FAD	C10-N1	3.18	1.39	1.33
3	B	600	FAD	C10-N1	3.03	1.39	1.33
3	F	600	FAD	C10-N1	2.90	1.39	1.33
3	E	600	FAD	P-O1P	2.83	1.60	1.50
3	G	600	FAD	C10-N1	2.77	1.38	1.33
3	C	600	FAD	C10-N1	2.64	1.38	1.33
3	D	600	FAD	O4B-C4B	2.62	1.50	1.45
3	D	600	FAD	P-O1P	2.62	1.60	1.50
3	B	600	FAD	P-O1P	2.56	1.60	1.50
3	F	600	FAD	P-O1P	2.52	1.59	1.50
3	A	600	FAD	P-O1P	2.45	1.59	1.50
3	H	600	FAD	P-O1P	2.34	1.59	1.50
3	F	600	FAD	O4B-C4B	2.30	1.50	1.45
3	F	600	FAD	C8M-C8	2.29	1.55	1.51
3	E	600	FAD	O5B-C5B	-2.24	1.36	1.44
3	E	600	FAD	C10-N1	2.24	1.37	1.33
3	G	600	FAD	O5B-C5B	-2.18	1.36	1.44
3	A	600	FAD	C7M-C7	2.17	1.55	1.51
3	A	600	FAD	O4B-C4B	2.07	1.49	1.45
3	E	600	FAD	C2'-C3'	2.05	1.57	1.53
3	G	600	FAD	O4B-C4B	2.02	1.49	1.45

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	600	FAD	C3B-C2B-C1B	-9.80	86.22	100.98
3	B	600	FAD	C3B-C2B-C1B	-9.41	86.82	100.98
3	A	600	FAD	C3B-C2B-C1B	-8.99	87.44	100.98
3	E	600	FAD	C3B-C2B-C1B	-8.97	87.47	100.98
3	A	600	FAD	C2B-C3B-C4B	-8.66	85.82	102.64
3	B	600	FAD	C2B-C3B-C4B	-8.40	86.32	102.64
3	C	600	FAD	C3B-C2B-C1B	-8.28	88.51	100.98
3	H	600	FAD	C3B-C2B-C1B	-8.10	88.78	100.98
3	D	600	FAD	C2B-C3B-C4B	-8.00	87.10	102.64
3	D	600	FAD	C3B-C2B-C1B	-7.65	89.46	100.98
3	C	600	FAD	C2B-C3B-C4B	-7.61	87.86	102.64
3	F	600	FAD	C3B-C2B-C1B	-7.58	89.57	100.98
3	F	600	FAD	C2B-C3B-C4B	-7.46	88.15	102.64
3	H	600	FAD	C2B-C3B-C4B	-7.24	88.58	102.64
3	G	600	FAD	C2B-C3B-C4B	-7.11	88.83	102.64
3	E	600	FAD	C2B-C3B-C4B	-6.98	89.09	102.64
3	A	600	FAD	O4B-C4B-C3B	-6.41	92.44	105.11
3	B	600	FAD	O4B-C4B-C3B	-6.31	92.62	105.11
3	C	600	FAD	O4B-C4B-C3B	-6.10	93.04	105.11
3	D	600	FAD	O4B-C4B-C3B	-5.58	94.07	105.11
3	B	600	FAD	O2A-PA-O5B	-5.43	82.52	107.75
3	G	600	FAD	O4B-C4B-C5B	5.43	127.24	109.37
3	F	600	FAD	N3A-C2A-N1A	-5.06	120.77	128.68
3	G	600	FAD	N3A-C2A-N1A	-5.00	120.87	128.68
3	D	600	FAD	N3A-C2A-N1A	-4.98	120.90	128.68
3	F	600	FAD	O4B-C4B-C3B	-4.91	95.40	105.11
3	G	600	FAD	O4B-C4B-C3B	-4.83	95.56	105.11
3	H	600	FAD	N3A-C2A-N1A	-4.79	121.20	128.68
3	A	600	FAD	O4B-C1B-C2B	-4.69	100.07	106.93
3	B	600	FAD	N3A-C2A-N1A	-4.68	121.36	128.68
3	H	600	FAD	O4B-C4B-C3B	-4.65	95.90	105.11
3	B	600	FAD	C5B-C4B-C3B	4.65	132.59	115.18
3	E	600	FAD	C4-C4X-N5	4.44	124.55	118.23
3	C	600	FAD	N3A-C2A-N1A	-4.42	121.78	128.68
3	E	600	FAD	N3A-C2A-N1A	-4.39	121.81	128.68
3	E	600	FAD	O4B-C4B-C3B	-4.29	96.62	105.11
3	A	600	FAD	C5B-C4B-C3B	4.22	131.00	115.18
3	B	600	FAD	C9A-C5X-N5	-4.07	118.01	122.43
3	B	600	FAD	O3B-C3B-C4B	4.04	122.72	111.05
3	B	600	FAD	O4B-C1B-C2B	-3.98	101.11	106.93
3	D	600	FAD	O4B-C1B-C2B	-3.97	101.12	106.93
3	A	600	FAD	N3A-C2A-N1A	-3.97	122.47	128.68
3	B	600	FAD	O5B-PA-O1A	-3.92	93.76	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	600	FAD	O4B-C1B-C2B	-3.92	101.20	106.93
3	B	600	FAD	C5'-C4'-C3'	-3.88	104.71	112.20
3	G	600	FAD	C4-C4X-N5	3.84	123.70	118.23
3	H	600	FAD	C5B-C4B-C3B	3.79	129.39	115.18
3	F	600	FAD	C4-C4X-N5	3.79	123.62	118.23
3	E	600	FAD	O4B-C4B-C5B	3.78	121.80	109.37
3	C	600	FAD	O4B-C1B-C2B	-3.75	101.44	106.93
3	H	600	FAD	C4-N3-C2	-3.67	118.85	125.64
3	G	600	FAD	O4B-C1B-C2B	-3.60	101.66	106.93
3	D	600	FAD	C5B-C4B-C3B	3.60	128.68	115.18
3	B	600	FAD	C4-N3-C2	-3.55	119.08	125.64
3	C	600	FAD	C9A-C5X-N5	-3.54	118.58	122.43
3	D	600	FAD	C5'-C4'-C3'	-3.54	105.37	112.20
3	A	600	FAD	C5'-C4'-C3'	-3.52	105.40	112.20
3	E	600	FAD	C4X-C10-N10	3.50	121.60	116.48
3	D	600	FAD	C9A-C5X-N5	-3.44	118.70	122.43
3	C	600	FAD	C4-C4X-N5	3.40	123.07	118.23
3	E	600	FAD	O2'-C2'-C3'	3.39	117.34	109.10
3	H	600	FAD	O4B-C1B-C2B	-3.38	101.98	106.93
3	H	600	FAD	P-O3P-PA	-3.37	121.25	132.83
3	F	600	FAD	O4B-C1B-C2B	-3.32	102.08	106.93
3	D	600	FAD	C4-C4X-N5	3.31	122.95	118.23
3	F	600	FAD	C5B-C4B-C3B	3.30	127.54	115.18
3	E	600	FAD	C1'-N10-C9A	3.29	126.00	120.51
3	A	600	FAD	C4-C4X-N5	3.29	122.92	118.23
3	E	600	FAD	C10-C4X-N5	-3.29	117.88	124.86
3	E	600	FAD	C4'-C3'-C2'	3.23	120.08	113.36
3	B	600	FAD	C4'-C3'-C2'	3.22	120.06	113.36
3	A	600	FAD	O3B-C3B-C4B	3.18	120.23	111.05
3	B	600	FAD	P-O3P-PA	-3.17	121.96	132.83
3	F	600	FAD	C10-C4X-N5	-3.14	118.19	124.86
3	H	600	FAD	C4'-C3'-C2'	3.14	119.89	113.36
3	D	600	FAD	C4-N3-C2	-3.13	119.86	125.64
3	H	600	FAD	C5'-C4'-C3'	-3.10	106.22	112.20
3	F	600	FAD	C5'-C4'-C3'	-3.09	106.23	112.20
3	C	600	FAD	C5'-C4'-C3'	-3.09	106.24	112.20
3	G	600	FAD	C10-C4X-N5	-3.08	118.31	124.86
3	B	600	FAD	C4X-C4-N3	3.08	121.02	113.19
3	D	600	FAD	C4X-C4-N3	3.07	120.98	113.19
3	G	600	FAD	C5'-C4'-C3'	-3.04	106.33	112.20
3	H	600	FAD	C4X-C4-N3	3.03	120.88	113.19
3	E	600	FAD	C9A-C5X-N5	-3.03	119.14	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	600	FAD	C9A-C5X-N5	-3.00	119.17	122.43
3	C	600	FAD	C5B-C4B-C3B	2.97	126.29	115.18
3	C	600	FAD	C10-C4X-N5	-2.95	118.59	124.86
3	H	600	FAD	C10-C4X-N5	-2.90	118.70	124.86
3	A	600	FAD	C10-C4X-N5	-2.89	118.72	124.86
3	A	600	FAD	C4X-C10-N10	2.89	120.70	116.48
3	E	600	FAD	C4-N3-C2	-2.88	120.31	125.64
3	B	600	FAD	C4-C4X-N5	2.87	122.32	118.23
3	C	600	FAD	C4-N3-C2	-2.85	120.37	125.64
3	C	600	FAD	C1B-N9A-C4A	-2.82	121.68	126.64
3	D	600	FAD	C10-C4X-N5	-2.81	118.89	124.86
3	F	600	FAD	C1B-N9A-C4A	-2.80	121.73	126.64
3	C	600	FAD	C4X-C4-N3	2.79	120.28	113.19
3	H	600	FAD	O3B-C3B-C4B	2.79	119.11	111.05
3	G	600	FAD	C4X-C10-N10	2.77	120.52	116.48
3	E	600	FAD	C5'-C4'-C3'	-2.74	106.90	112.20
3	C	600	FAD	O3B-C3B-C4B	2.73	118.95	111.05
3	G	600	FAD	C5B-C4B-C3B	-2.70	105.06	115.18
3	H	600	FAD	O2'-C2'-C3'	2.67	115.60	109.10
3	G	600	FAD	C9A-C5X-N5	-2.67	119.53	122.43
3	F	600	FAD	C4X-C10-N10	2.67	120.38	116.48
3	A	600	FAD	C1'-N10-C9A	2.66	124.95	120.51
3	D	600	FAD	O3B-C3B-C4B	2.65	118.72	111.05
3	F	600	FAD	P-O3P-PA	-2.65	123.75	132.83
3	G	600	FAD	C4'-C3'-C2'	2.62	118.81	113.36
3	F	600	FAD	C9A-C5X-N5	-2.62	119.59	122.43
3	E	600	FAD	O2-C2-N1	-2.60	117.52	121.83
3	A	600	FAD	C4A-C5A-N7A	-2.55	106.74	109.40
3	H	600	FAD	C9A-C5X-N5	-2.55	119.66	122.43
3	E	600	FAD	C4X-C4-N3	2.55	119.67	113.19
3	A	600	FAD	C4X-C4-N3	2.53	119.61	113.19
3	G	600	FAD	C4X-C4-N3	2.52	119.59	113.19
3	D	600	FAD	C4'-C3'-C2'	2.52	118.60	113.36
3	G	600	FAD	C4-N3-C2	-2.51	121.00	125.64
3	B	600	FAD	O4-C4-C4X	-2.51	119.94	126.60
3	H	600	FAD	C4-C4X-N5	2.51	121.80	118.23
3	G	600	FAD	P-O3P-PA	-2.48	124.31	132.83
3	B	600	FAD	C10-C4X-N5	-2.48	119.59	124.86
3	F	600	FAD	C4-N3-C2	-2.47	121.08	125.64
3	H	600	FAD	O4-C4-C4X	-2.45	120.10	126.60
3	C	600	FAD	C4X-C10-N10	2.45	120.06	116.48
3	H	600	FAD	C1B-N9A-C4A	-2.44	122.35	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	600	FAD	C1'-N10-C9A	2.44	124.58	120.51
3	F	600	FAD	C1'-N10-C9A	2.44	124.58	120.51
3	F	600	FAD	C4'-C3'-C2'	2.41	118.38	113.36
3	C	600	FAD	P-O3P-PA	-2.41	124.55	132.83
3	D	600	FAD	C1B-N9A-C4A	-2.41	122.41	126.64
3	F	600	FAD	C4X-C4-N3	2.35	119.15	113.19
3	H	600	FAD	O5'-P-O1P	-2.31	100.05	109.07
3	D	600	FAD	C4X-C10-N10	2.30	119.84	116.48
3	C	600	FAD	C1'-N10-C9A	2.28	124.32	120.51
3	E	600	FAD	O2-C2-N3	2.26	123.04	118.65
3	A	600	FAD	C4'-C3'-C2'	2.25	118.05	113.36
3	A	600	FAD	C4-N3-C2	-2.25	121.49	125.64
3	E	600	FAD	O5B-PA-O1A	2.24	117.82	109.07
3	C	600	FAD	C6-C5X-C9A	2.24	122.10	118.94
3	H	600	FAD	C4X-C10-N10	2.24	119.75	116.48
3	G	600	FAD	C4A-C5A-N7A	-2.22	107.08	109.40
3	G	600	FAD	O2'-C2'-C3'	2.20	114.45	109.10
3	E	600	FAD	C4A-C5A-N7A	-2.19	107.12	109.40
3	B	600	FAD	O2'-C2'-C3'	2.18	114.40	109.10
3	E	600	FAD	P-O3P-PA	-2.17	125.39	132.83
3	D	600	FAD	O4-C4-C4X	-2.15	120.89	126.60
3	A	600	FAD	C1B-N9A-C4A	-2.15	122.87	126.64
3	B	600	FAD	C5X-C9A-N10	2.14	120.17	117.95
3	F	600	FAD	O3B-C3B-C4B	2.09	117.10	111.05
3	F	600	FAD	O2-C2-N1	-2.08	118.39	121.83
3	H	600	FAD	O2-C2-N1	-2.05	118.43	121.83
3	A	600	FAD	P-O3P-PA	-2.03	125.84	132.83
3	H	600	FAD	O4'-C4'-C3'	2.03	114.05	109.10

All (24) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	600	FAD	C3B
3	A	600	FAD	C4B
3	A	600	FAD	C2'
3	B	600	FAD	C3B
3	B	600	FAD	C4B
3	B	600	FAD	C2'
3	C	600	FAD	C3B
3	C	600	FAD	C4B
3	C	600	FAD	C2'
3	D	600	FAD	C3B

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Mol	Chain	Res	Type	Atom
3	D	600	FAD	C4B
3	D	600	FAD	C2'
3	E	600	FAD	C3B
3	E	600	FAD	C4B
3	E	600	FAD	C2'
3	F	600	FAD	C3B
3	F	600	FAD	C4B
3	F	600	FAD	C2'
3	G	600	FAD	C3B
3	G	600	FAD	C4B
3	G	600	FAD	C2'
3	H	600	FAD	C3B
3	H	600	FAD	C4B
3	H	600	FAD	C2'

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	600	FAD	C1'-C2'-C3'-O3'
3	A	600	FAD	C1'-C2'-C3'-C4'
3	A	600	FAD	O2'-C2'-C3'-O3'
3	A	600	FAD	O2'-C2'-C3'-C4'
3	A	600	FAD	PA-O3P-P-O5'
3	B	600	FAD	C1'-C2'-C3'-O3'
3	B	600	FAD	C1'-C2'-C3'-C4'
3	B	600	FAD	O2'-C2'-C3'-O3'
3	B	600	FAD	O2'-C2'-C3'-C4'
3	C	600	FAD	C1'-C2'-C3'-O3'
3	C	600	FAD	C1'-C2'-C3'-C4'
3	C	600	FAD	O2'-C2'-C3'-O3'
3	C	600	FAD	O2'-C2'-C3'-C4'
3	C	600	FAD	PA-O3P-P-O5'
3	D	600	FAD	C1'-C2'-C3'-O3'
3	D	600	FAD	C1'-C2'-C3'-C4'
3	D	600	FAD	O2'-C2'-C3'-O3'
3	D	600	FAD	O2'-C2'-C3'-C4'
3	E	600	FAD	C5B-O5B-PA-O1A
3	E	600	FAD	C5B-O5B-PA-O2A
3	E	600	FAD	C5B-O5B-PA-O3P
3	E	600	FAD	C3B-C4B-C5B-O5B
3	E	600	FAD	C1'-C2'-C3'-O3'
3	E	600	FAD	C1'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
3	E	600	FAD	O2'-C2'-C3'-O3'
3	E	600	FAD	O2'-C2'-C3'-C4'
3	F	600	FAD	C1'-C2'-C3'-O3'
3	F	600	FAD	C1'-C2'-C3'-C4'
3	F	600	FAD	O2'-C2'-C3'-O3'
3	F	600	FAD	O2'-C2'-C3'-C4'
3	G	600	FAD	C5B-O5B-PA-O2A
3	G	600	FAD	C5B-O5B-PA-O3P
3	G	600	FAD	C2'-C1'-N10-C10
3	G	600	FAD	C1'-C2'-C3'-O3'
3	G	600	FAD	C1'-C2'-C3'-C4'
3	G	600	FAD	O2'-C2'-C3'-O3'
3	G	600	FAD	O2'-C2'-C3'-C4'
3	G	600	FAD	C5'-O5'-P-O3P
3	H	600	FAD	C1'-C2'-C3'-O3'
3	H	600	FAD	C1'-C2'-C3'-C4'
3	H	600	FAD	O2'-C2'-C3'-O3'
3	H	600	FAD	O2'-C2'-C3'-C4'
3	H	600	FAD	PA-O3P-P-O5'
3	G	600	FAD	C3B-C4B-C5B-O5B
3	A	600	FAD	C2'-C3'-C4'-C5'
3	E	600	FAD	C2'-C3'-C4'-O4'
3	B	600	FAD	C2'-C3'-C4'-C5'
3	D	600	FAD	C2'-C3'-C4'-C5'
3	E	600	FAD	C2'-C3'-C4'-C5'
3	F	600	FAD	C2'-C3'-C4'-C5'
3	G	600	FAD	C2'-C3'-C4'-C5'
3	H	600	FAD	C2'-C3'-C4'-C5'
3	A	600	FAD	C2'-C3'-C4'-O4'
3	F	600	FAD	C2'-C3'-C4'-O4'
3	H	600	FAD	C2'-C3'-C4'-O4'
3	G	600	FAD	O4B-C4B-C5B-O5B
3	B	600	FAD	C2'-C3'-C4'-O4'
3	E	600	FAD	O4B-C4B-C5B-O5B
3	D	600	FAD	C2'-C3'-C4'-O4'
3	G	600	FAD	C2'-C3'-C4'-O4'
3	G	600	FAD	C2'-C1'-N10-C9A
3	G	600	FAD	O3'-C3'-C4'-C5'
3	C	600	FAD	O4B-C4B-C5B-O5B
3	A	600	FAD	O3'-C3'-C4'-C5'
3	C	600	FAD	C2'-C3'-C4'-C5'
4	F	601	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	D	600	FAD	PA-O3P-P-O5'
3	F	600	FAD	PA-O3P-P-O5'
3	D	600	FAD	C4B-C5B-O5B-PA
3	G	600	FAD	C4B-C5B-O5B-PA
3	H	600	FAD	C4B-C5B-O5B-PA
3	G	600	FAD	C5'-O5'-P-O2P
4	C	601	EDO	O1-C1-C2-O2
3	A	600	FAD	C4B-C5B-O5B-PA
3	E	600	FAD	C4B-C5B-O5B-PA
4	G	602	EDO	O1-C1-C2-O2
3	C	600	FAD	C4B-C5B-O5B-PA
3	F	600	FAD	C4B-C5B-O5B-PA
3	D	600	FAD	O4B-C4B-C5B-O5B
3	C	600	FAD	C2'-C3'-C4'-O4'
3	B	600	FAD	C4B-C5B-O5B-PA
4	C	602	EDO	O1-C1-C2-O2
3	B	600	FAD	PA-O3P-P-O5'
3	G	600	FAD	O3'-C3'-C4'-O4'
3	F	600	FAD	O3'-C3'-C4'-C5'
3	A	600	FAD	O4B-C4B-C5B-O5B
4	A	601	EDO	O1-C1-C2-O2
4	G	601	EDO	O1-C1-C2-O2
3	E	600	FAD	O3'-C3'-C4'-C5'
3	F	600	FAD	O4B-C4B-C5B-O5B
3	H	600	FAD	O4B-C4B-C5B-O5B
3	G	600	FAD	C5'-O5'-P-O1P
3	B	600	FAD	O4B-C4B-C5B-O5B
4	D	601	EDO	O1-C1-C2-O2
3	A	600	FAD	O3'-C3'-C4'-O4'
3	F	600	FAD	C2'-C1'-N10-C10
3	D	600	FAD	O3'-C3'-C4'-C5'
3	H	600	FAD	O3'-C3'-C4'-C5'

There are no ring outliers.

10 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	600	FAD	4	0
3	B	600	FAD	4	0
3	E	600	FAD	4	0
3	H	600	FAD	4	0
3	D	600	FAD	5	0

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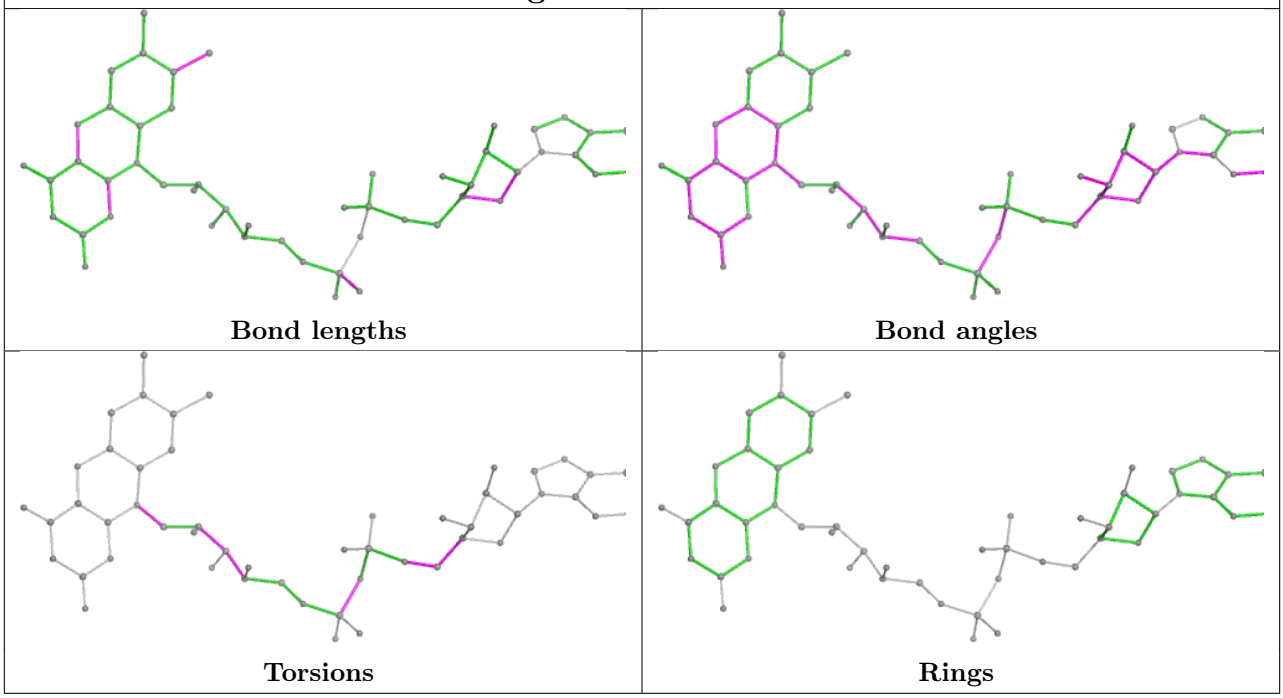
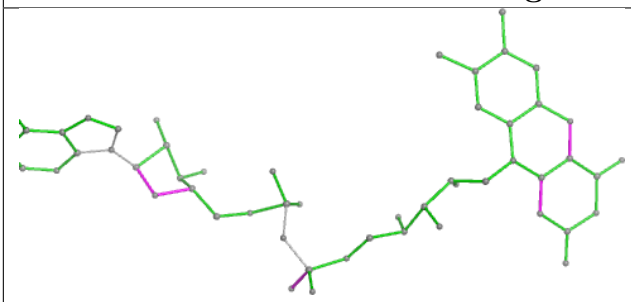
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	600	FAD	5	0
3	A	600	FAD	5	0
3	G	600	FAD	5	0
4	G	601	EDO	3	0
4	C	601	EDO	1	0

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

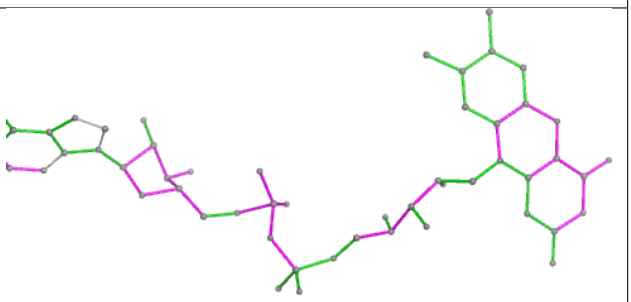
Ligand FAD F 600



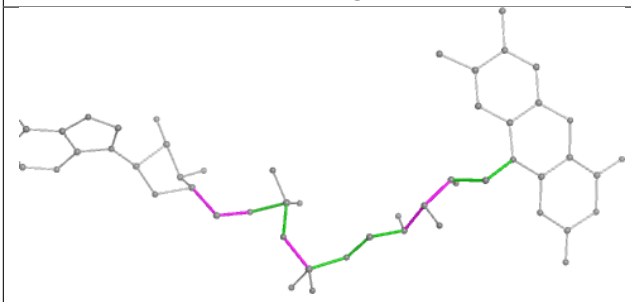
Ligand FAD B 600



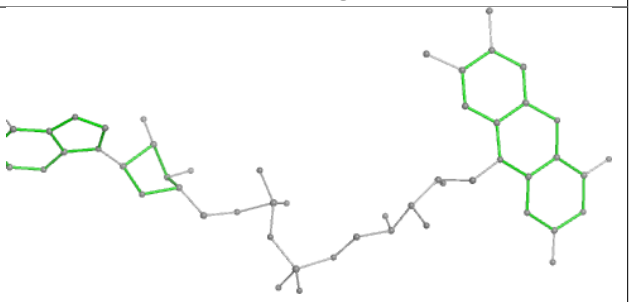
Bond lengths



Bond angles

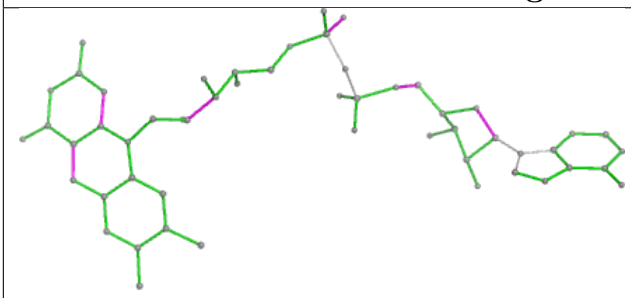


Torsions

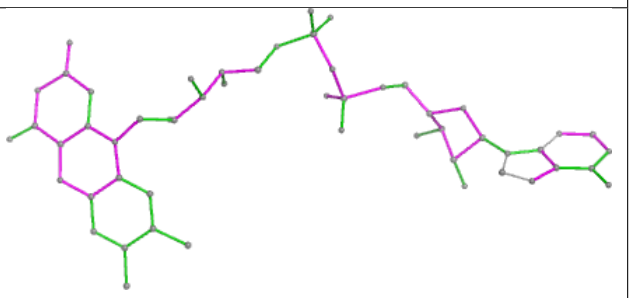


Rings

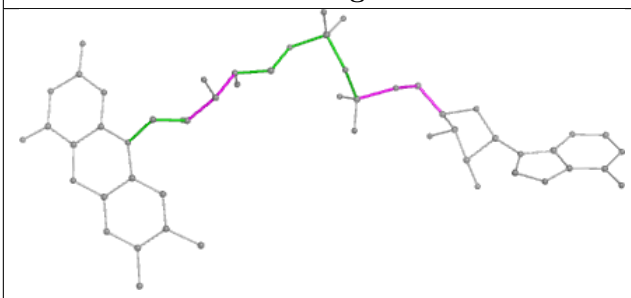
Ligand FAD E 600



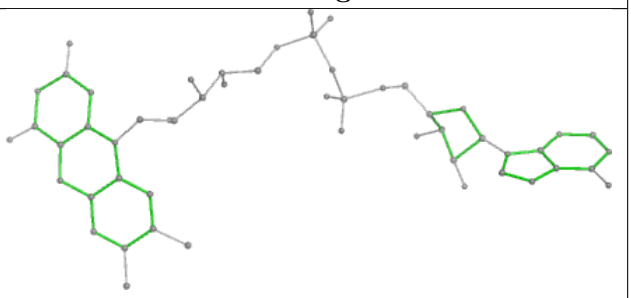
Bond lengths



Bond angles

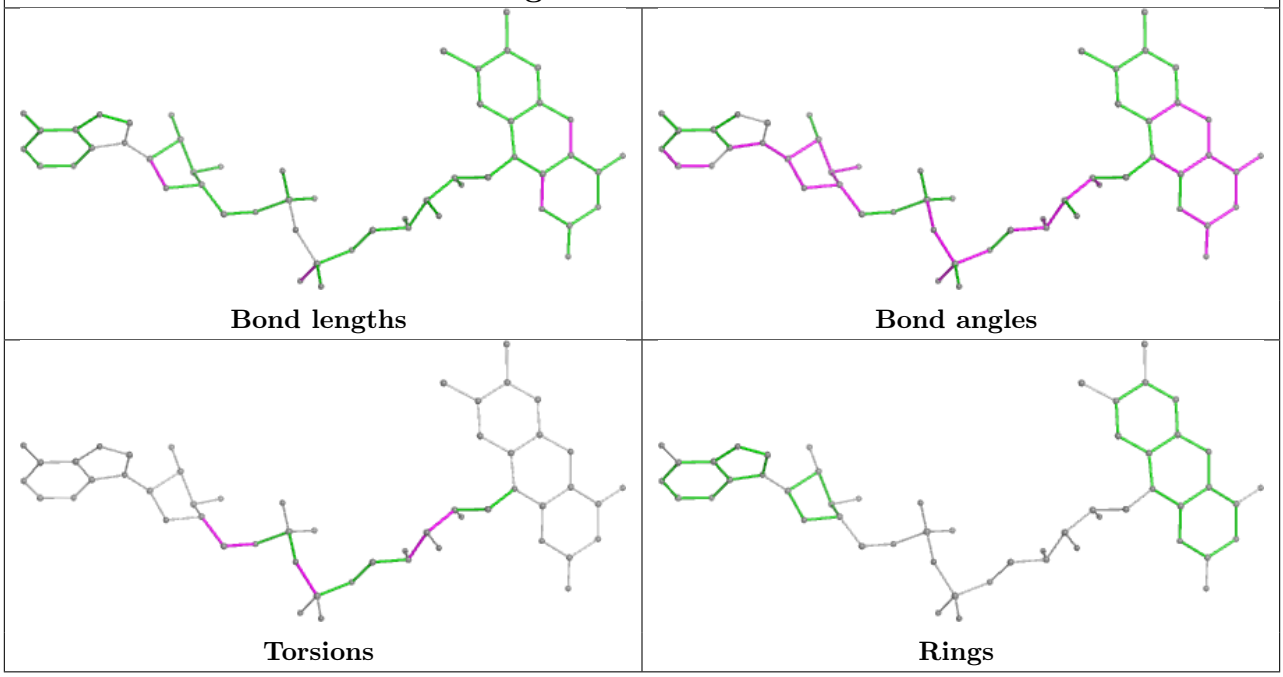


Torsions

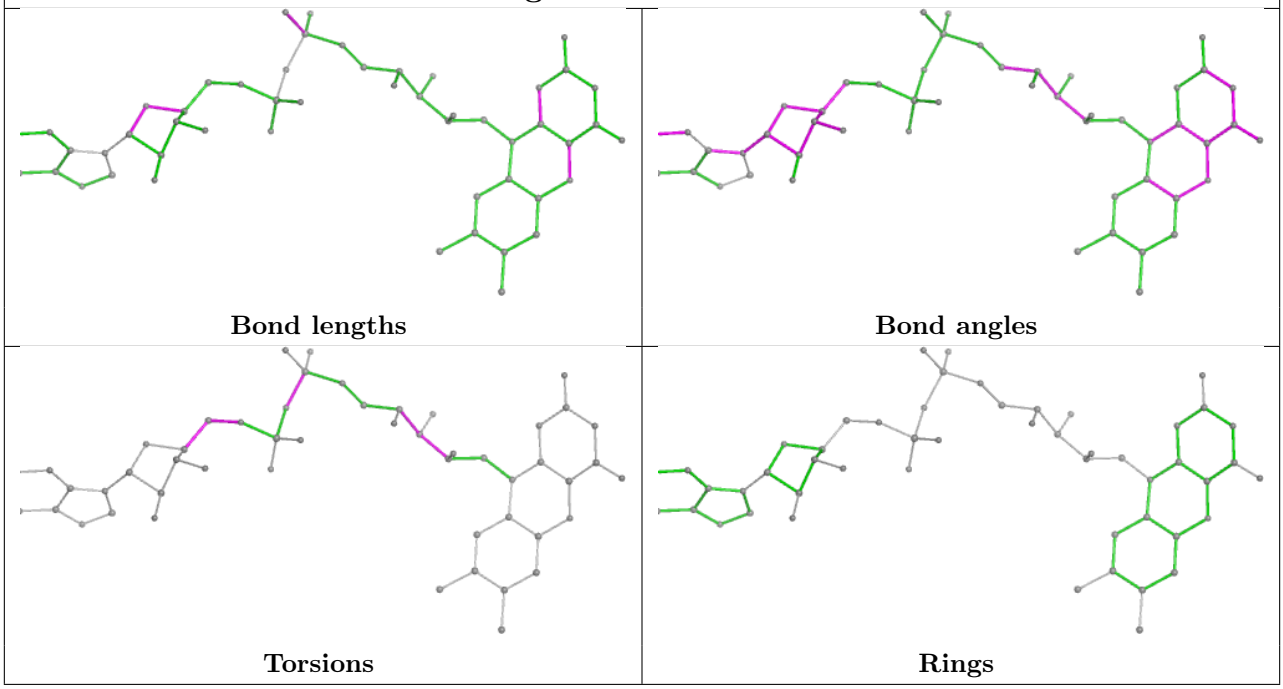


Rings

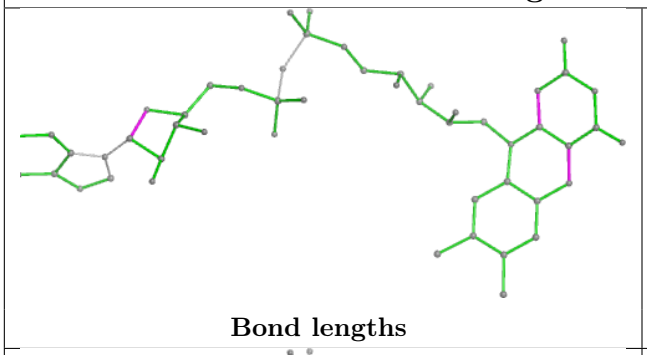
Ligand FAD H 600



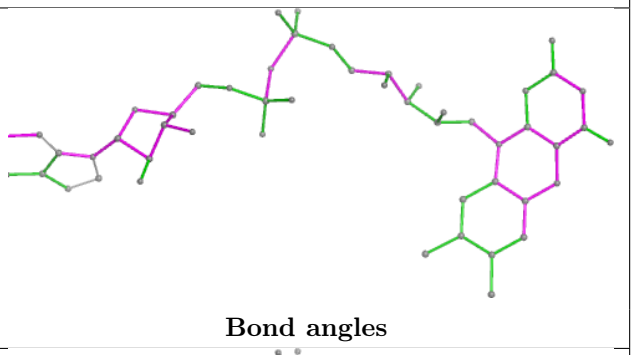
Ligand FAD D 600



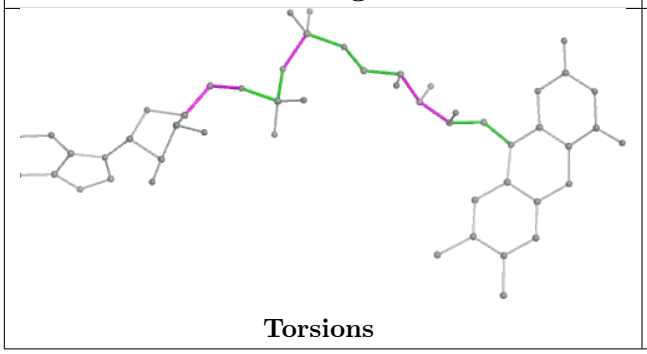
Ligand FAD C 600



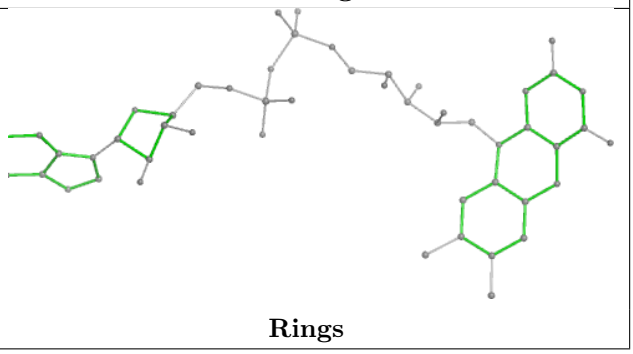
Bond lengths



Bond angles

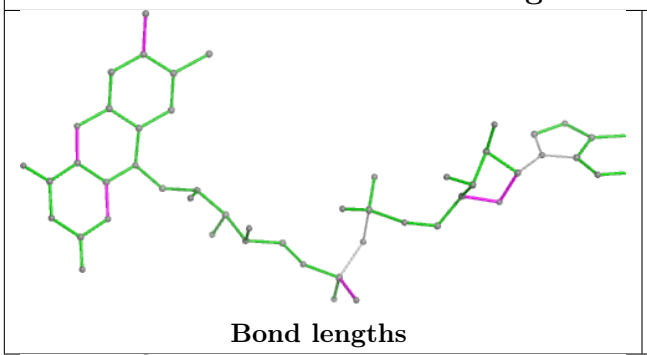


Torsions

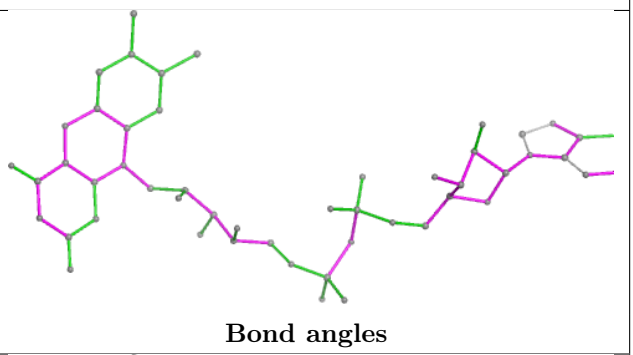


Rings

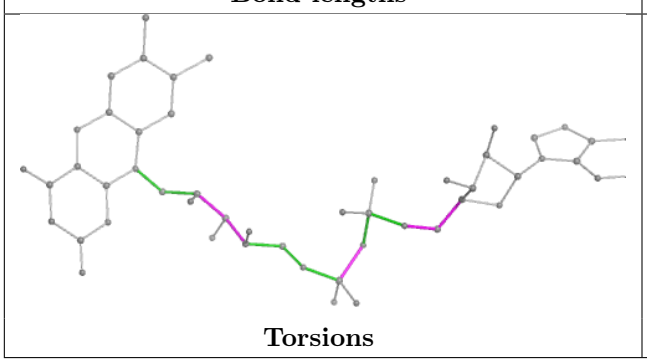
Ligand FAD A 600



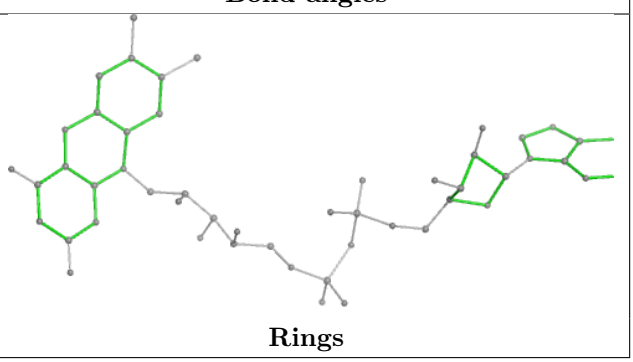
Bond lengths



Bond angles

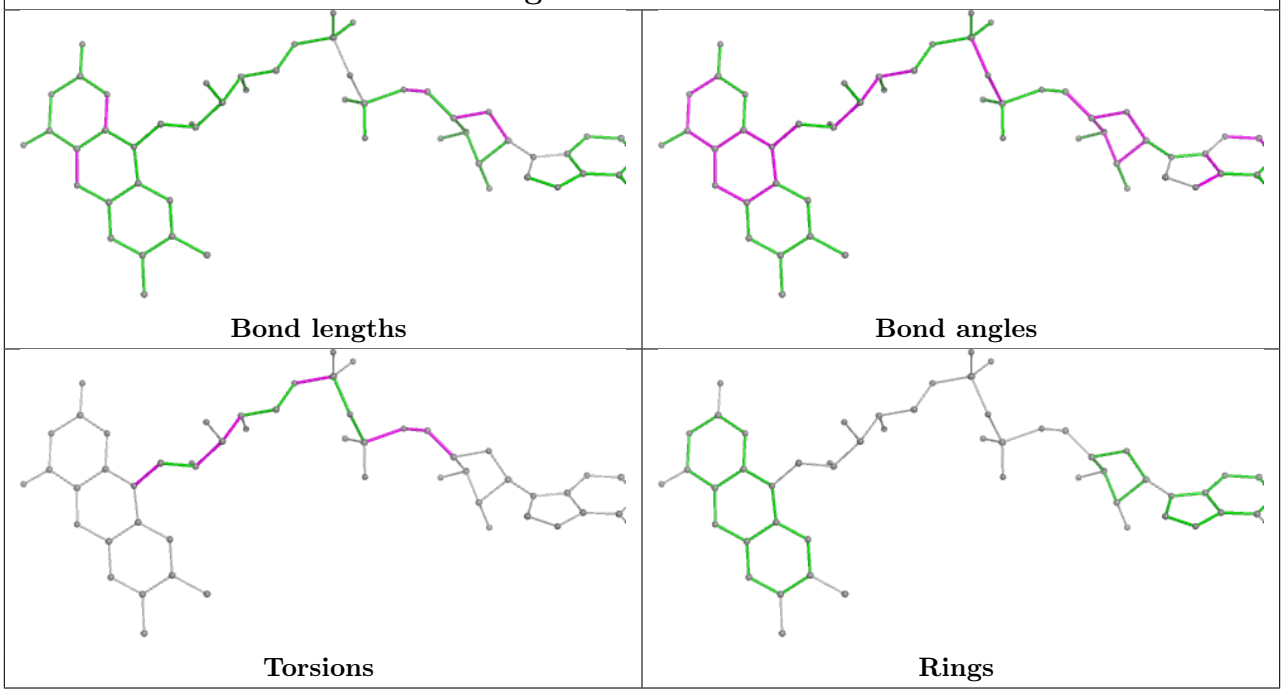


Torsions



Rings

Ligand FAD G 600



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	4
1	H	4
1	B	3
2	G	3
1	E	2
1	A	2
1	F	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	7:TYR	C	8:GLN	N	1.20
1	C	99:GLN	C	100:SER	N	1.20
1	E	393:GLU	C	394:ASP	N	1.20

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	394:ASP	C	395:VAL	N	1.19
1	G	303:ARG	C	304:VAL	N	1.19
1	G	471:ILE	C	472:GLU	N	1.19
1	B	303:ARG	C	304:VAL	N	1.17
1	H	66:LEU	C	67:LEU	N	1.17
1	F	393:GLU	C	394:ASP	N	1.16
1	A	143:GLU	C	144:ALA	N	1.15
1	D	196:ARG	C	197:ASP	N	1.15
1	H	391:PRO	C	392:ASP	N	1.15
1	B	393:GLU	C	394:ASP	N	1.14
1	C	104:ARG	C	105:GLU	N	1.14
1	C	303:ARG	C	304:VAL	N	1.14
1	A	196:ARG	C	197:ASP	N	1.13
1	H	67:LEU	C	68:LEU	N	1.13
1	H	455:ALA	C	456:ASN	N	1.13
1	C	4:ARG	C	5:ASP	N	1.11
1	G	483:GLU	C	484:GLU	N	1.03

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	478/495 (96%)	-0.60	1 (0%)	95	95	9, 19, 30, 47	10 (2%)
1	B	476/495 (96%)	-0.54	1 (0%)	95	95	9, 19, 35, 48	14 (2%)
1	C	477/495 (96%)	-0.44	3 (0%)	89	89	10, 23, 38, 50	16 (3%)
1	D	478/495 (96%)	-0.38	6 (1%)	77	76	11, 22, 41, 56	18 (3%)
1	E	477/495 (96%)	-0.41	2 (0%)	92	93	9, 23, 41, 50	16 (3%)
1	F	478/495 (96%)	-0.37	5 (1%)	82	83	10, 23, 38, 46	16 (3%)
1	H	478/495 (96%)	-0.23	8 (1%)	70	67	12, 26, 44, 52	18 (3%)
2	G	478/495 (96%)	-0.38	2 (0%)	92	93	11, 23, 39, 51	14 (2%)
All	All	3820/3960 (96%)	-0.42	28 (0%)	87	88	9, 22, 39, 56	122 (3%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	39	PRO	4.0
1	D	288	ALA	3.7
1	F	288	ALA	3.5
1	H	321	ALA	3.2
1	F	38	GLY	3.1
1	E	39	PRO	3.0
1	D	450	GLY	3.0
1	F	300	VAL	3.0
2	G	287	ASP	2.7
1	H	284	ASN	2.5
1	H	283	VAL	2.5
1	H	319	SER	2.5
1	B	288	ALA	2.5
1	E	409	THR	2.5
1	D	287	ASP	2.4
1	C	287	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	293	ALA	2.4
1	C	32	GLU	2.3
2	G	288	ALA	2.3
1	C	135	THR	2.3
1	H	288	ALA	2.3
1	F	299	PHE	2.3
1	H	287	ASP	2.3
1	H	318	PHE	2.2
1	D	299	PHE	2.2
1	A	486	GLY	2.2
1	D	40	TRP	2.2
1	D	39	PRO	2.1

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	EDO	C	601	4/4	0.82	0.18	24,27,31,32	0
4	EDO	G	601	4/4	0.85	0.21	26,28,31,34	0
4	EDO	F	601	4/4	0.95	0.17	21,24,27,31	0
3	FAD	H	600	53/53	0.96	0.13	19,24,29,30	0
3	FAD	D	600	53/53	0.96	0.13	10,19,26,27	0
3	FAD	F	600	53/53	0.96	0.12	15,20,25,25	0
3	FAD	G	600	53/53	0.96	0.13	17,22,32,32	0
4	EDO	D	601	4/4	0.97	0.14	20,23,25,27	0
3	FAD	C	600	53/53	0.97	0.13	13,19,27,28	0
3	FAD	E	600	53/53	0.97	0.12	14,19,29,30	0
4	EDO	G	602	4/4	0.97	0.12	29,31,31,31	0

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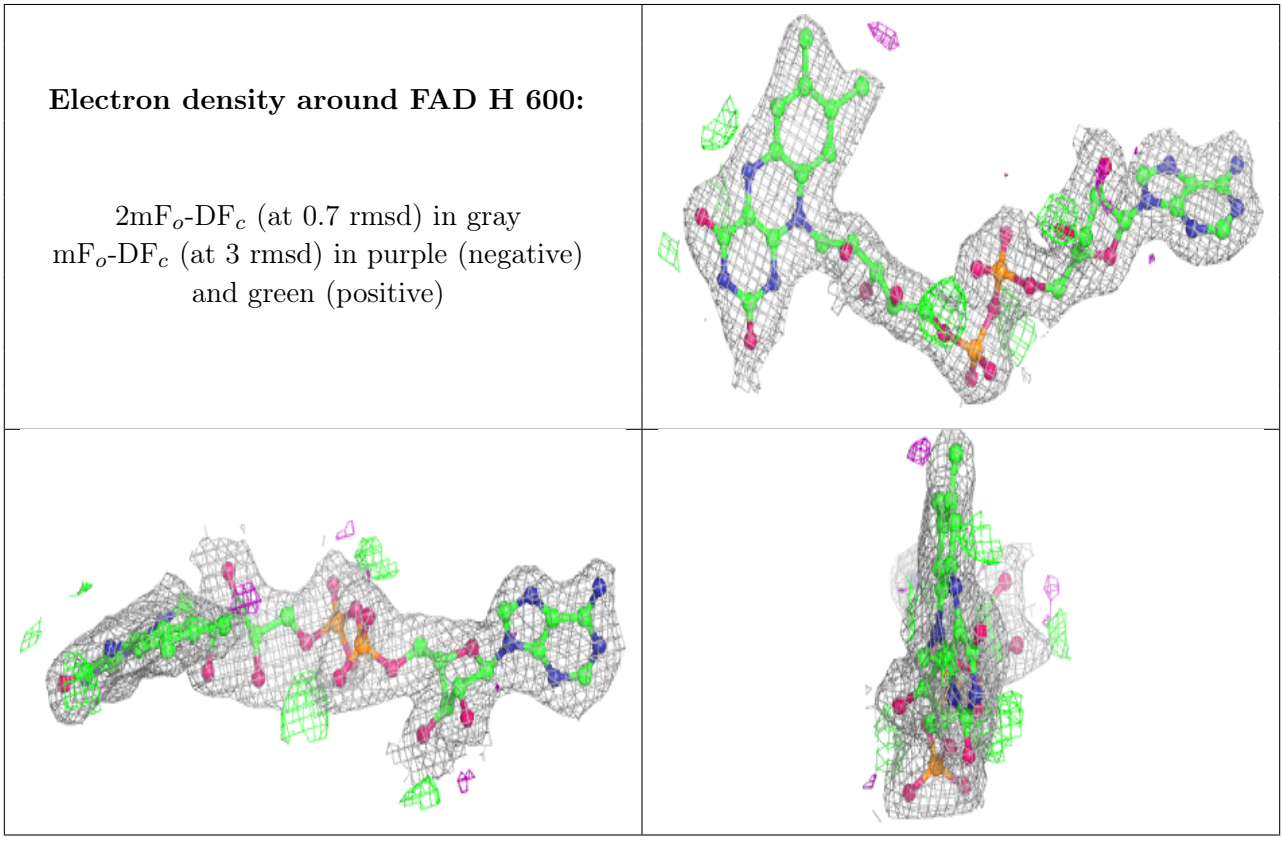
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FAD	B	600	53/53	0.98	0.12	10,18,22,23	0
4	EDO	A	601	4/4	0.98	0.13	23,25,26,26	0
3	FAD	A	600	53/53	0.98	0.12	13,18,20,22	0
4	EDO	C	602	4/4	0.98	0.09	29,32,33,33	0

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.

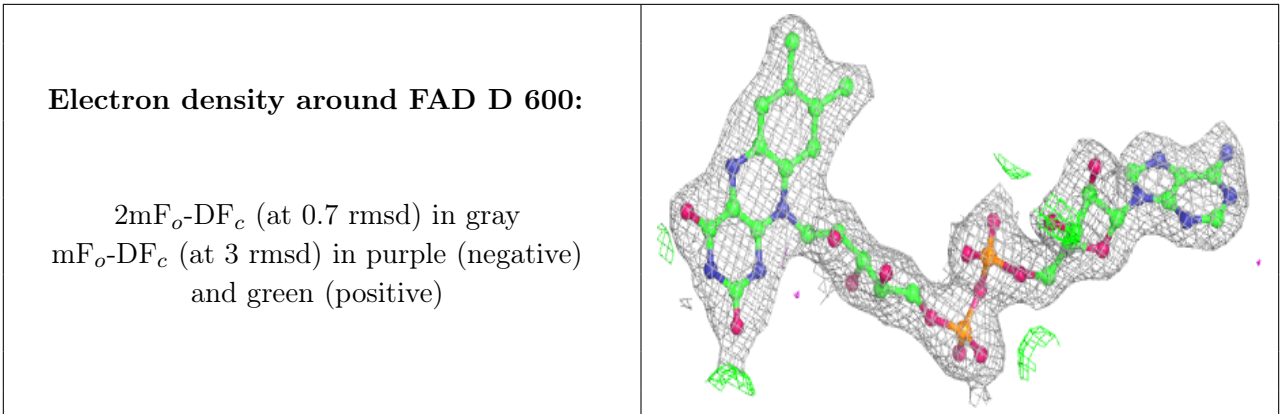
Electron density around FAD H 600:

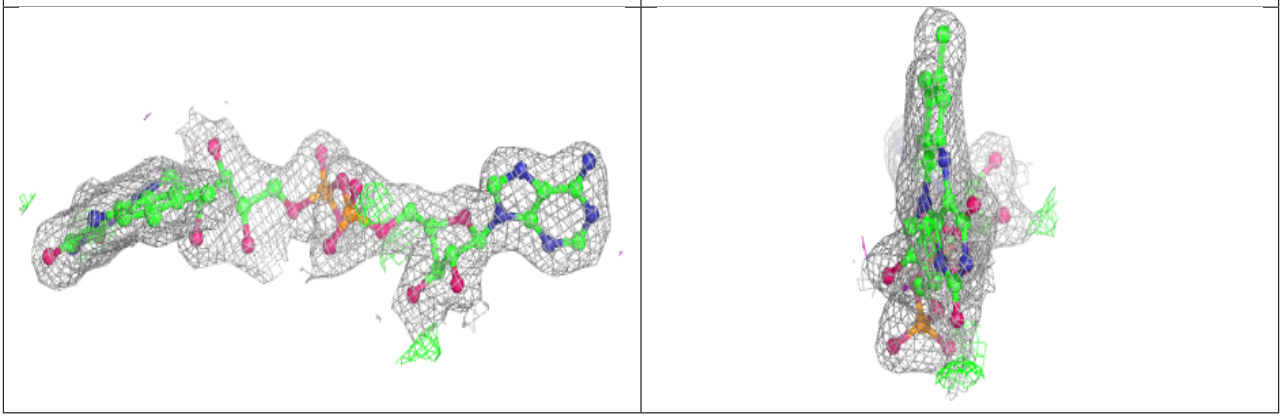
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around FAD D 600:

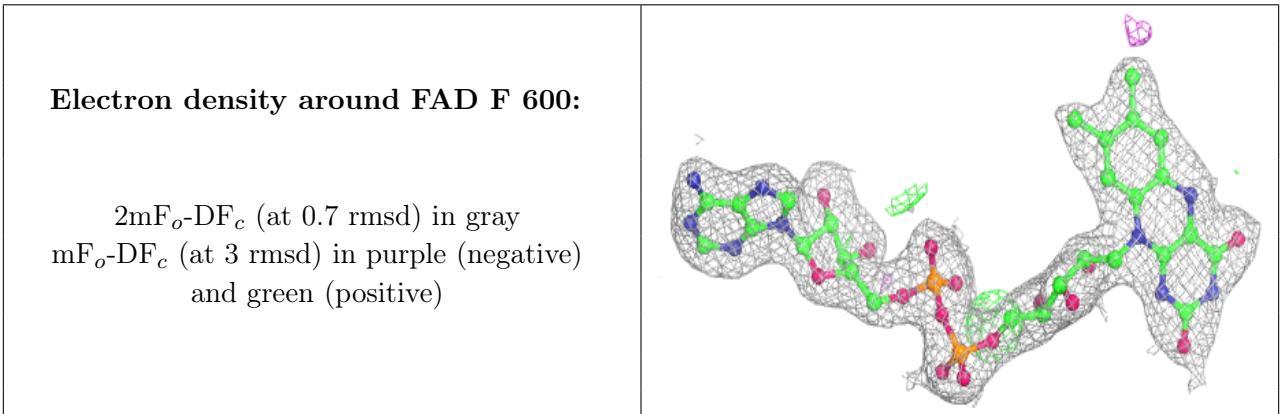
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

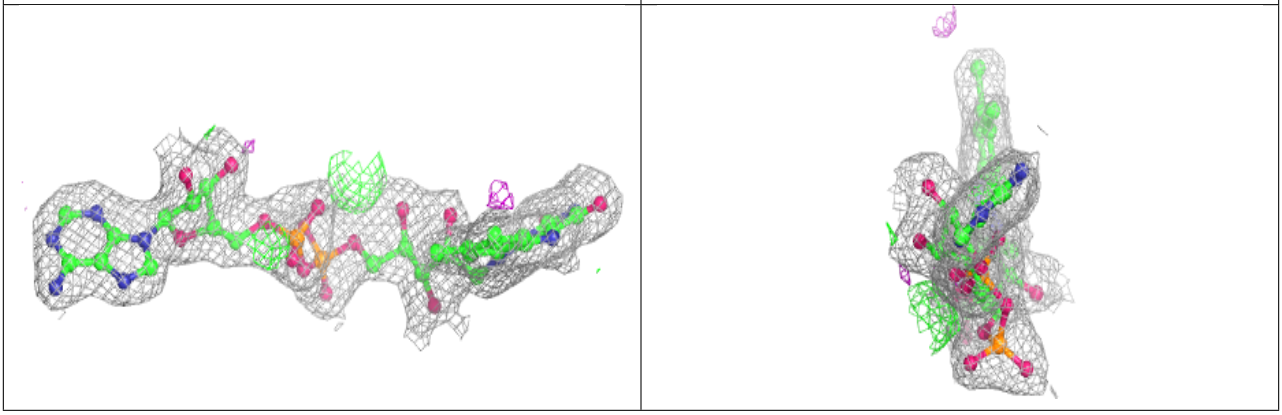




Electron density around FAD F 600:

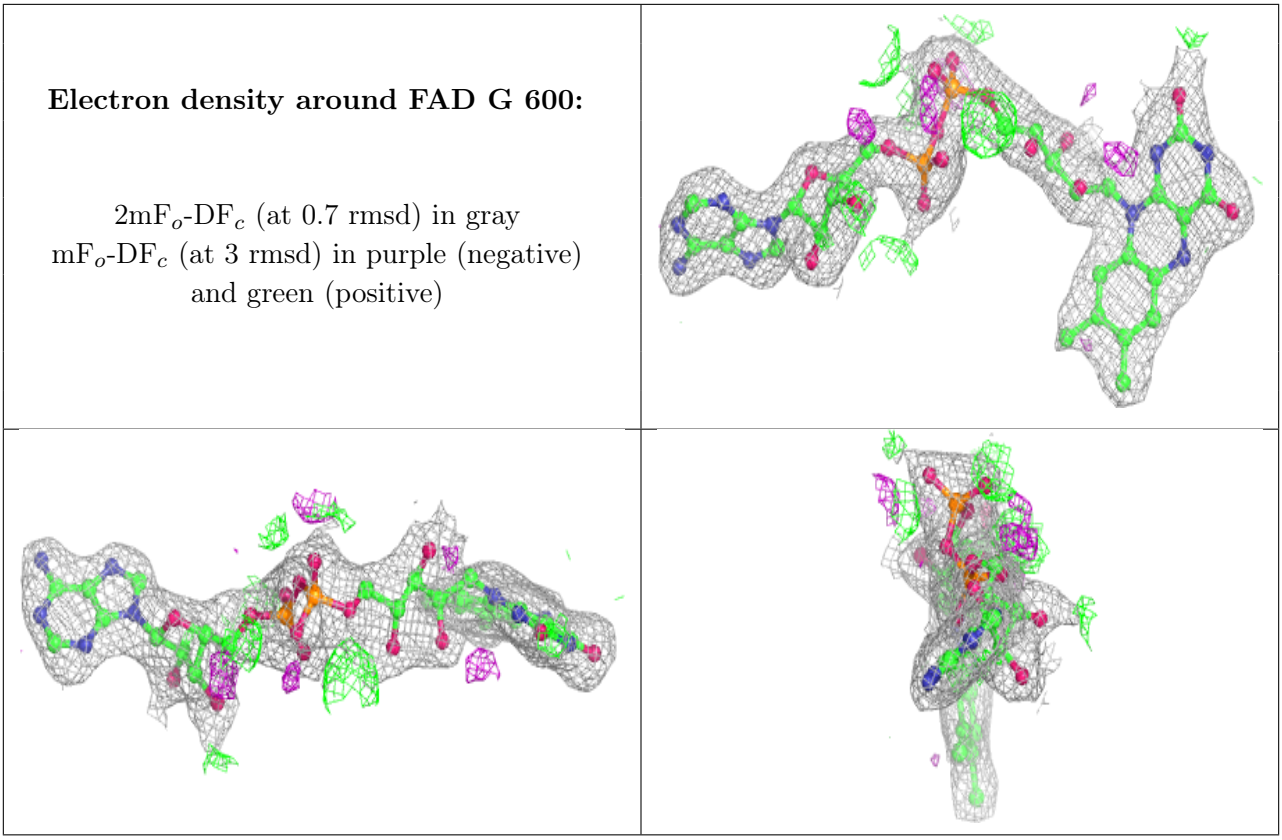
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





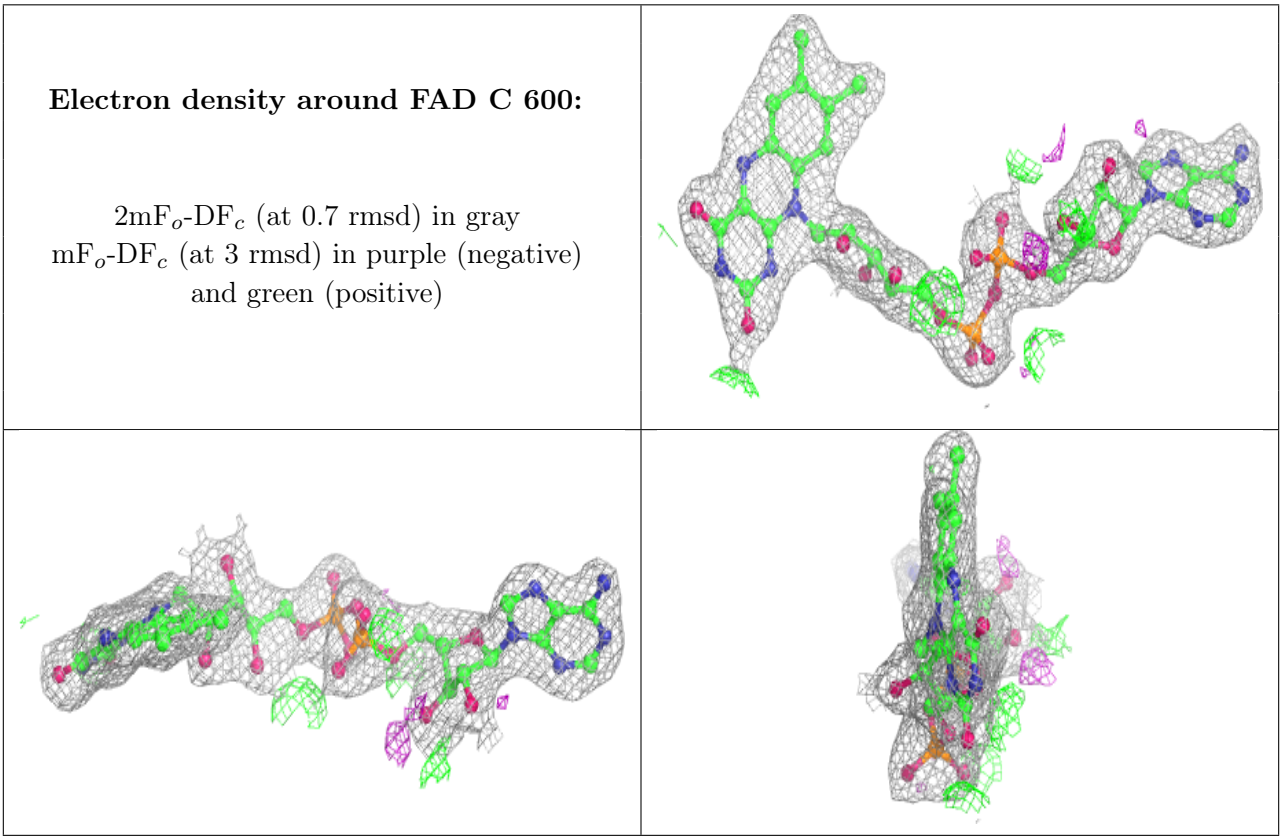
Electron density around FAD G 600:

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



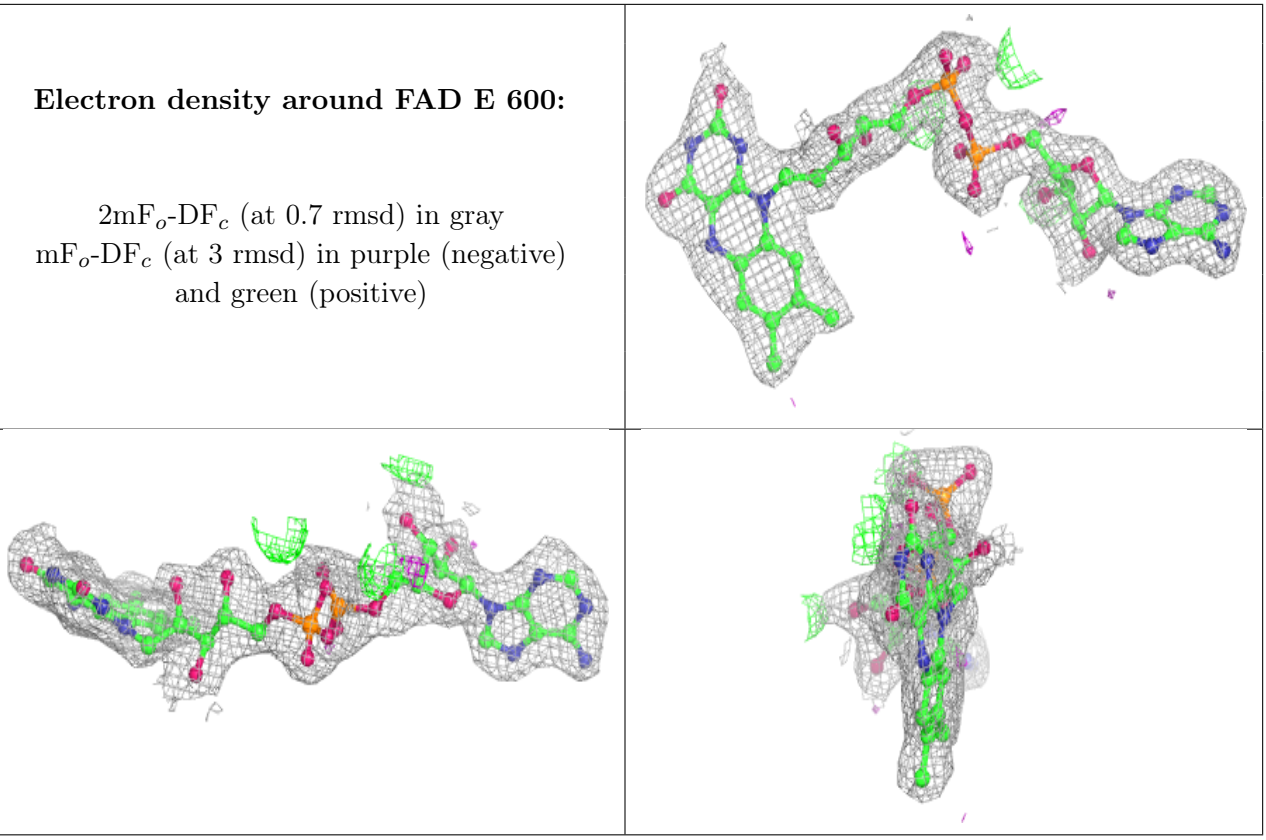
Electron density around FAD C 600:

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



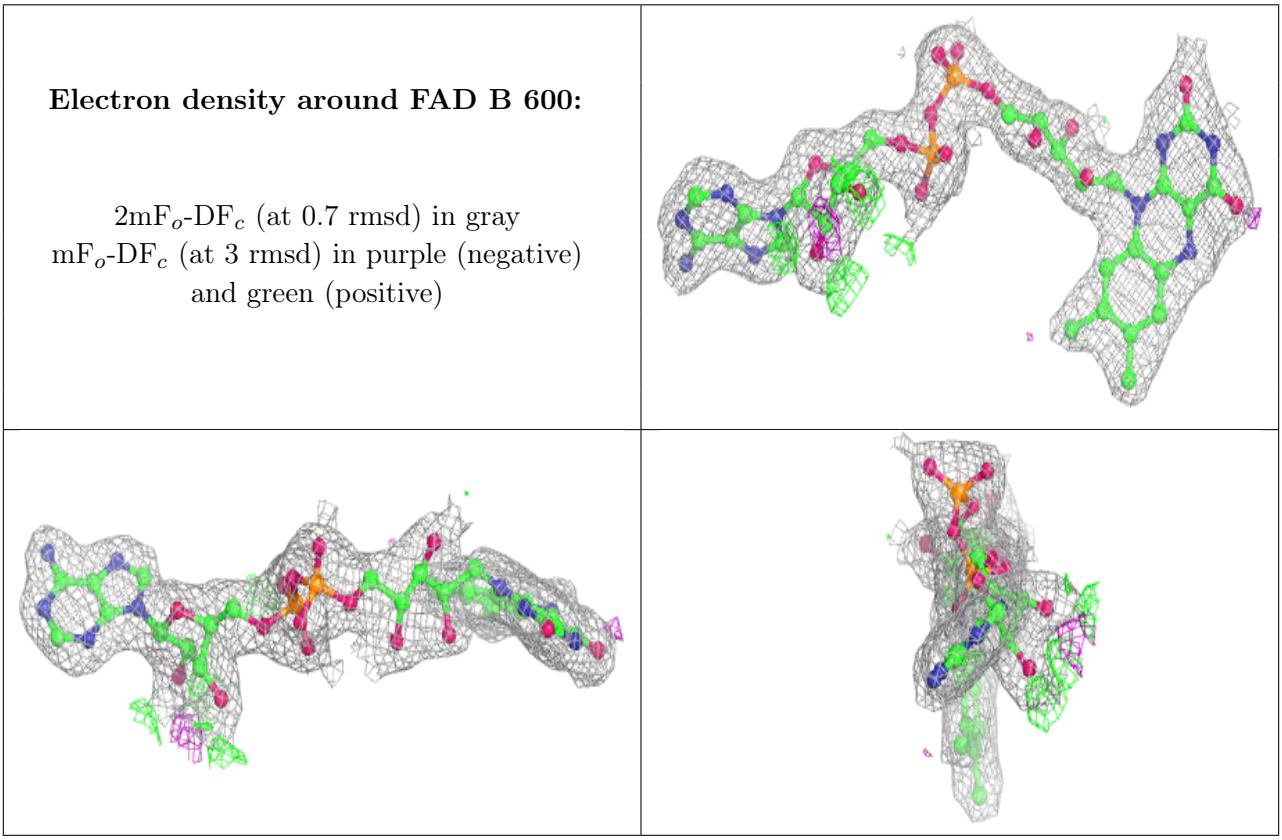
Electron density around FAD E 600:

$2mF_o$-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 B 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 A 600:

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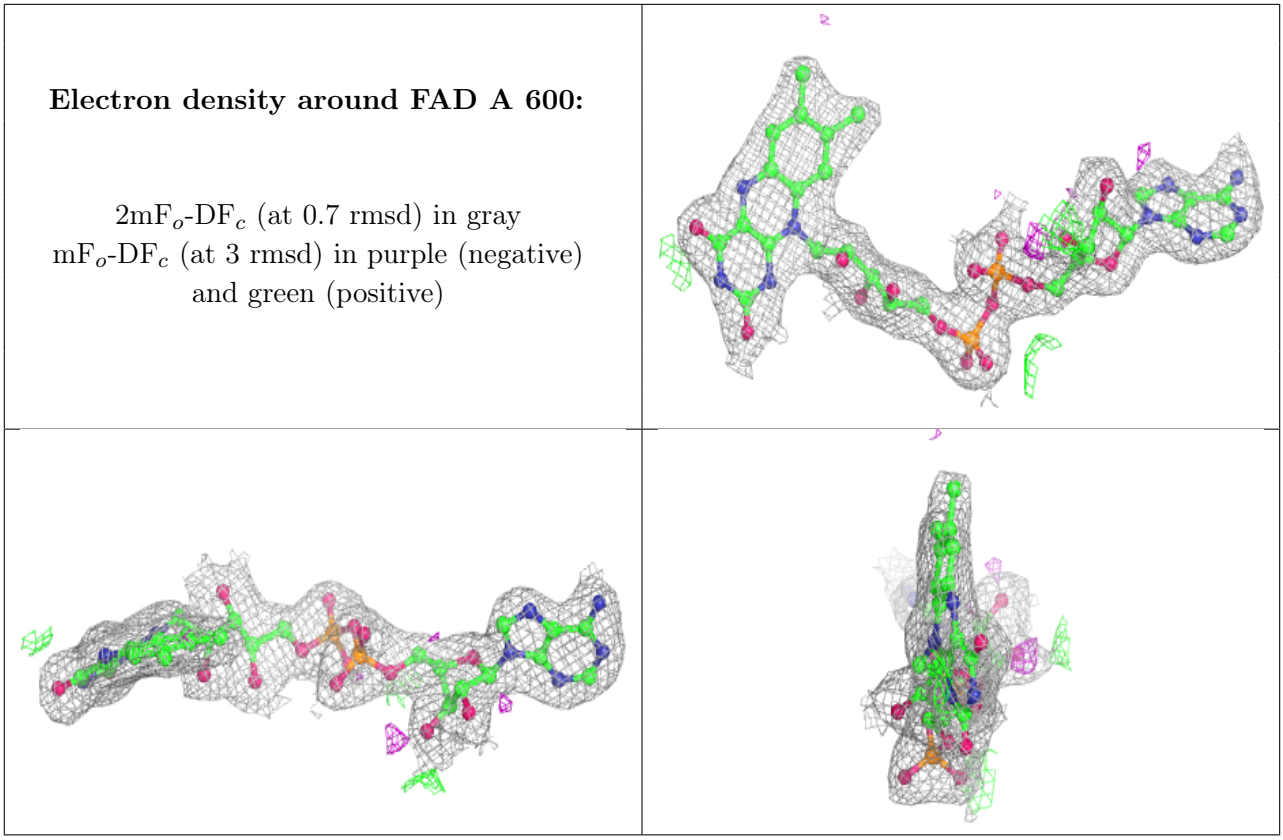
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.