Full wwPDB X-ray Structure Validation Report (i)

Mar 16, 2026 – 04:38 PM UTC

PDB ID	:	9H8P / pdb_00009h8p
Title	:	Eugenol Oxidase (EUGO) from Rhodococcus jostii RHA1, mutant DTT
Authors	:	Rozeboom, H.J.; Fraaije, M.W.
Deposited on	:	2024-10-29
Resolution	:	1.47 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:

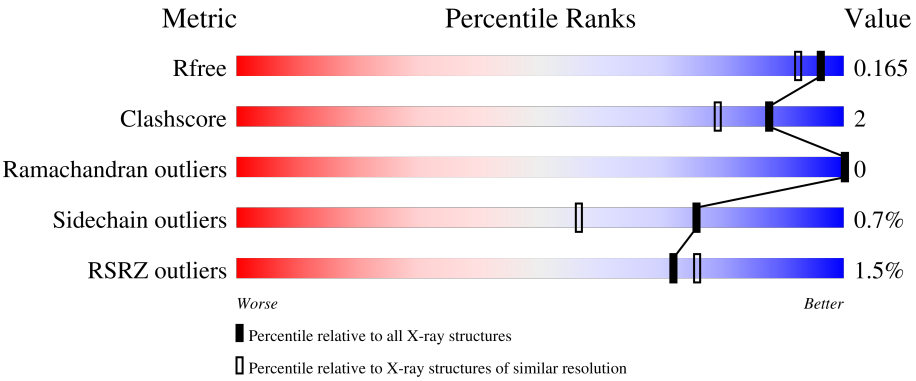
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.47 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6779 (1.50-1.46)
Clashscore	190562	7025 (1.50-1.46)
Ramachandran outliers	187476	6917 (1.50-1.46)
Sidechain outliers	187428	6914 (1.50-1.46)
RSRZ outliers	180081	6781 (1.50-1.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	526	94% 5%
1	B	526	95%
1	C	526	95%
1	D	526	96%
1	E	526	93% 6%

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Mol	Chain	Length	Quality of chain
1	F	526	2% 96%
1	G	526	% 95%
1	H	526	2% 95%

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
6	CL	E	604	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 36894 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Probable vanillyl-alcohol oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			4133	2634	700	775	24			
1	B	525	Total	C	N	O	S	0	1	0
			4141	2639	701	776	25			
1	C	525	Total	C	N	O	S	0	1	0
			4141	2638	701	778	24			
1	D	525	Total	C	N	O	S	0	1	0
			4141	2639	701	776	25			
1	E	525	Total	C	N	O	S	0	1	0
			4141	2639	701	776	25			
1	F	525	Total	C	N	O	S	0	1	0
			4141	2639	701	776	25			
1	G	525	Total	C	N	O	S	0	1	0
			4141	2640	701	776	24			
1	H	525	Total	C	N	O	S	0	1	0
			4141	2638	701	778	24			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	HIS	SER	engineered mutation	UNP Q0SBK1
A	394	VAL	SER	engineered mutation	UNP Q0SBK1
A	423	MET	ALA	engineered mutation	UNP Q0SBK1
A	425	THR	GLN	engineered mutation	UNP Q0SBK1
A	427	THR	ILE	engineered mutation	UNP Q0SBK1
A	434	TYR	HIS	engineered mutation	UNP Q0SBK1
A	445	ASP	ILE	engineered mutation	UNP Q0SBK1
A	518	PRO	SER	engineered mutation	UNP Q0SBK1
B	81	HIS	SER	engineered mutation	UNP Q0SBK1
B	394	VAL	SER	engineered mutation	UNP Q0SBK1
B	423	MET	ALA	engineered mutation	UNP Q0SBK1
B	425	THR	GLN	engineered mutation	UNP Q0SBK1
B	427	THR	ILE	engineered mutation	UNP Q0SBK1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	434	TYR	HIS	engineered mutation	UNP Q0SBK1
B	445	ASP	ILE	engineered mutation	UNP Q0SBK1
B	518	PRO	SER	engineered mutation	UNP Q0SBK1
C	81	HIS	SER	engineered mutation	UNP Q0SBK1
C	394	VAL	SER	engineered mutation	UNP Q0SBK1
C	423	MET	ALA	engineered mutation	UNP Q0SBK1
C	425	THR	GLN	engineered mutation	UNP Q0SBK1
C	427	THR	ILE	engineered mutation	UNP Q0SBK1
C	434	TYR	HIS	engineered mutation	UNP Q0SBK1
C	445	ASP	ILE	engineered mutation	UNP Q0SBK1
C	518	PRO	SER	engineered mutation	UNP Q0SBK1
D	81	HIS	SER	engineered mutation	UNP Q0SBK1
D	394	VAL	SER	engineered mutation	UNP Q0SBK1
D	423	MET	ALA	engineered mutation	UNP Q0SBK1
D	425	THR	GLN	engineered mutation	UNP Q0SBK1
D	427	THR	ILE	engineered mutation	UNP Q0SBK1
D	434	TYR	HIS	engineered mutation	UNP Q0SBK1
D	445	ASP	ILE	engineered mutation	UNP Q0SBK1
D	518	PRO	SER	engineered mutation	UNP Q0SBK1
E	81	HIS	SER	engineered mutation	UNP Q0SBK1
E	394	VAL	SER	engineered mutation	UNP Q0SBK1
E	423	MET	ALA	engineered mutation	UNP Q0SBK1
E	425	THR	GLN	engineered mutation	UNP Q0SBK1
E	427	THR	ILE	engineered mutation	UNP Q0SBK1
E	434	TYR	HIS	engineered mutation	UNP Q0SBK1
E	445	ASP	ILE	engineered mutation	UNP Q0SBK1
E	518	PRO	SER	engineered mutation	UNP Q0SBK1
F	81	HIS	SER	engineered mutation	UNP Q0SBK1
F	394	VAL	SER	engineered mutation	UNP Q0SBK1
F	423	MET	ALA	engineered mutation	UNP Q0SBK1
F	425	THR	GLN	engineered mutation	UNP Q0SBK1
F	427	THR	ILE	engineered mutation	UNP Q0SBK1
F	434	TYR	HIS	engineered mutation	UNP Q0SBK1
F	445	ASP	ILE	engineered mutation	UNP Q0SBK1
F	518	PRO	SER	engineered mutation	UNP Q0SBK1
G	81	HIS	SER	engineered mutation	UNP Q0SBK1
G	394	VAL	SER	engineered mutation	UNP Q0SBK1
G	423	MET	ALA	engineered mutation	UNP Q0SBK1
G	425	THR	GLN	engineered mutation	UNP Q0SBK1
G	427	THR	ILE	engineered mutation	UNP Q0SBK1
G	434	TYR	HIS	engineered mutation	UNP Q0SBK1
G	445	ASP	ILE	engineered mutation	UNP Q0SBK1

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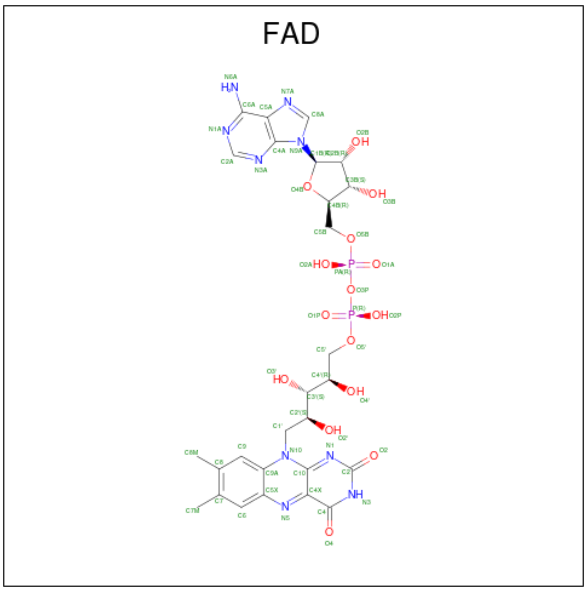
Chain	Residue	Modelled	Actual	Comment	Reference
G	518	PRO	SER	engineered mutation	UNP Q0SBK1
H	81	HIS	SER	engineered mutation	UNP Q0SBK1
H	394	VAL	SER	engineered mutation	UNP Q0SBK1
H	423	MET	ALA	engineered mutation	UNP Q0SBK1
H	425	THR	GLN	engineered mutation	UNP Q0SBK1
H	427	THR	ILE	engineered mutation	UNP Q0SBK1
H	434	TYR	HIS	engineered mutation	UNP Q0SBK1
H	445	ASP	ILE	engineered mutation	UNP Q0SBK1
H	518	PRO	SER	engineered mutation	UNP Q0SBK1

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: 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		

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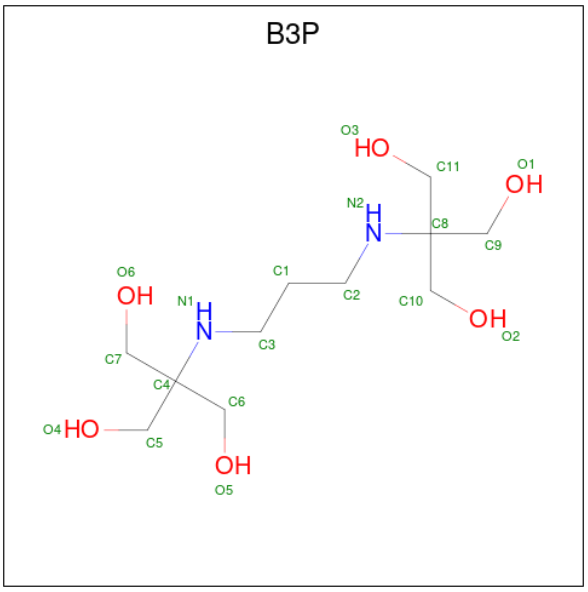
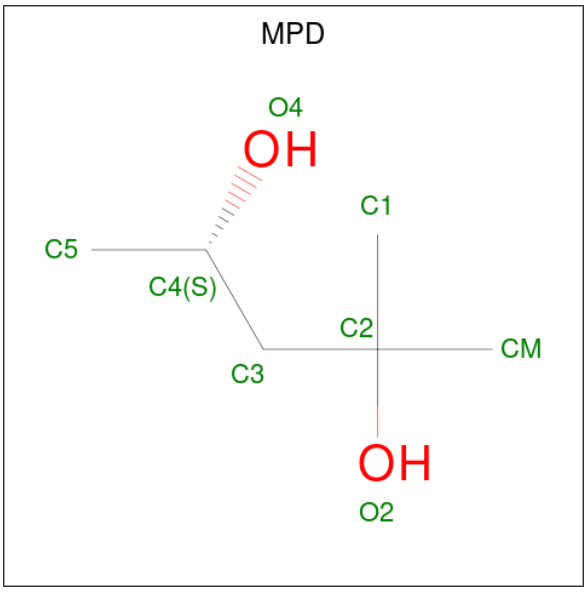
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYLAMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: B3P) (formula: $C_{11}H_{26}N_2O_6$).



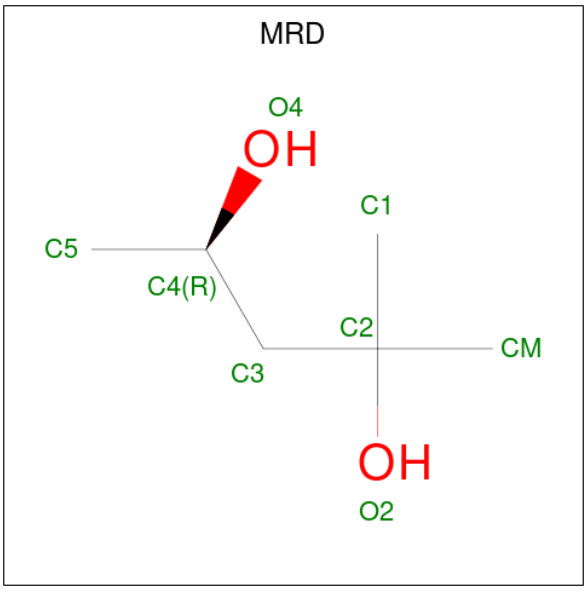
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	11	2	6		
3	A	1	Total	C	N	O	0	0
			19	11	2	6		
3	B	1	Total	C	N	O	0	0
			19	11	2	6		
3	C	1	Total	C	N	O	0	0
			19	11	2	6		
3	D	1	Total	C	N	O	0	0
			19	11	2	6		
3	E	1	Total	C	N	O	0	0
			19	11	2	6		
3	F	1	Total	C	N	O	0	0
			19	11	2	6		
3	H	1	Total	C	N	O	0	0
			19	11	2	6		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	E	1	Total C O 8 6 2	0	0
4	F	1	Total C O 8 6 2	0	0

- Molecule 5 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 8 6 2	0	0

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0
6	B	1	Total Cl 1 1	0	0
6	C	1	Total Cl 1 1	0	0
6	D	2	Total Cl 2 2	0	0
6	E	1	Total Cl 1 1	0	0
6	F	1	Total Cl 1 1	0	0
6	G	1	Total Cl 1 1	0	0
6	H	1	Total Cl 1 1	0	0

- Molecule 7 is water.

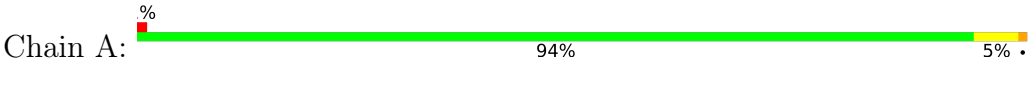
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	443	Total O 443 443	0	0
7	B	392	Total O 392 392	0	0
7	C	373	Total O 373 373	0	0
7	D	410	Total O 410 410	0	0
7	E	441	Total O 441 441	0	0
7	F	407	Total O 407 407	0	0
7	G	320	Total O 320 320	0	0
7	H	363	Total O 363 363	0	0

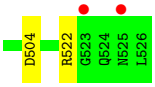
3 Residue-property plots (i)

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

• Molecule 1: Probable vanillyl-alcohol oxidase

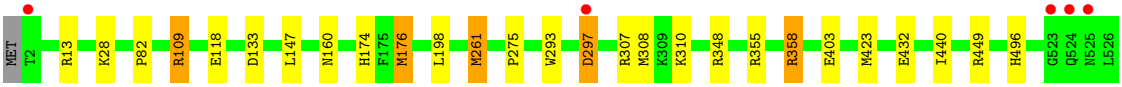
Chain A:





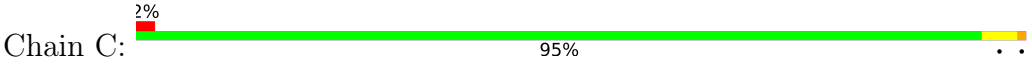
• Molecule 1: Probable vanillyl-alcohol oxidase

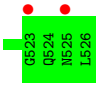
Chain B:



• Molecule 1: Probable vanillyl-alcohol oxidase

Chain C:



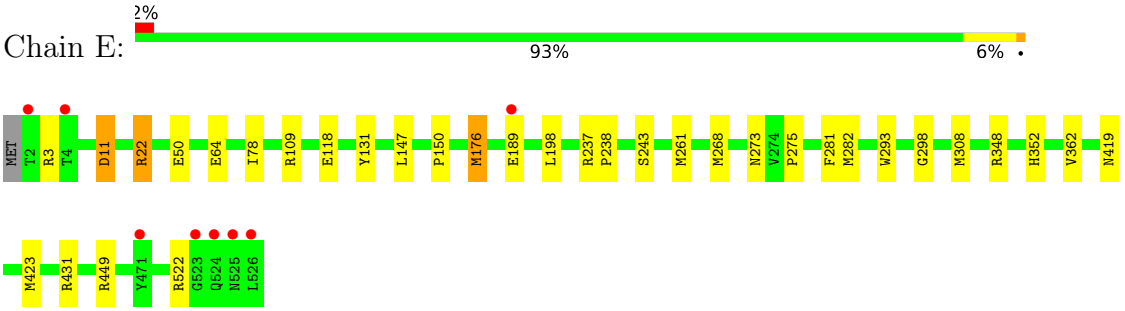


• Molecule 1: Probable vanillyl-alcohol oxidase

Chain D:

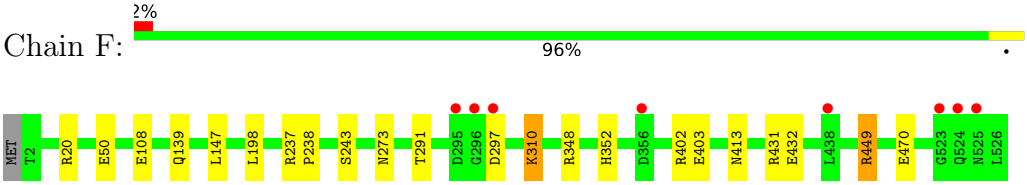
• Molecule 1: Probable vanillyl-alcohol oxidase

Chain E:



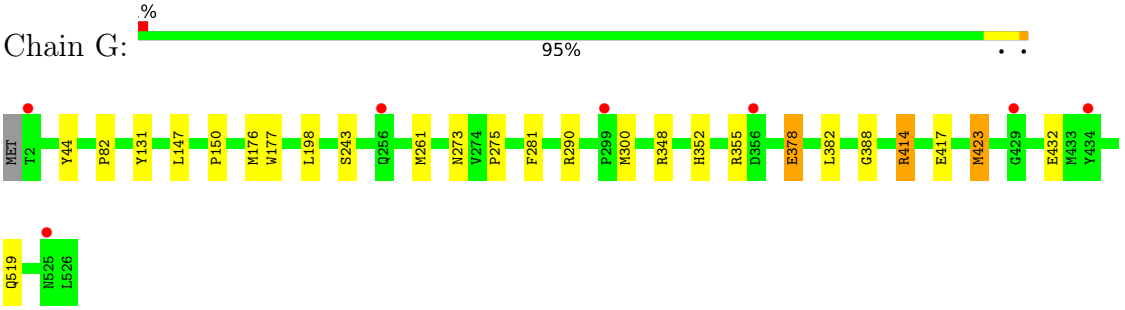
• Molecule 1: Probable vanillyl-alcohol oxidase

Chain F:



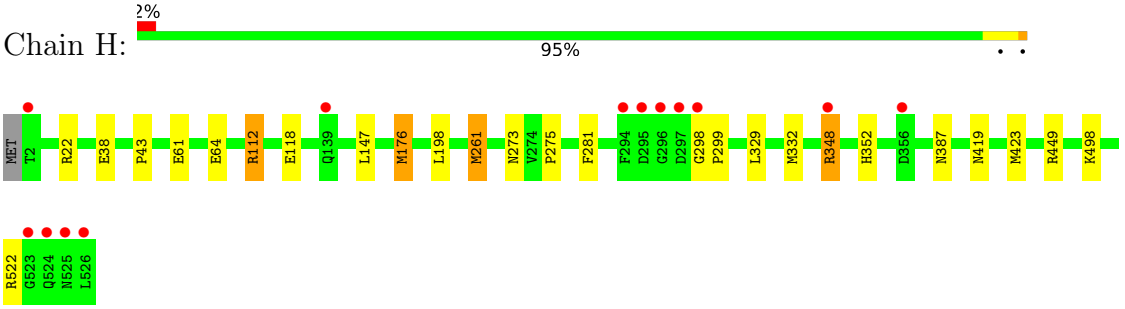
• Molecule 1: Probable vanillyl-alcohol oxidase

Chain G:



• Molecule 1: Probable vanillyl-alcohol oxidase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	90.35Å 110.23Å 117.26Å 89.75° 89.50° 68.43°	Depositor
Resolution (Å)	102.72 – 1.47 102.72 – 1.47	Depositor EDS
% Data completeness (in resolution range)	92.2 (102.72-1.47) 92.5 (102.72-1.47)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 1.46Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.149 , 0.165 0.149 , 0.165	Depositor DCC
R_{free} test set	32662 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å^2)	14.7	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 31.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.013 for h,h-k,-l 0.056 for -h,-k,l 0.011 for -h,-h+k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	36894	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MRD, FAD, B3P, CL, MPD

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	0.76	0/4242	1.06	15/5757 (0.3%)
1	B	0.72	0/4250	1.05	16/5767 (0.3%)
1	C	0.72	0/4250	1.00	5/5768 (0.1%)
1	D	0.74	0/4250	1.04	8/5767 (0.1%)
1	E	0.78	0/4250	1.04	11/5767 (0.2%)
1	F	0.74	0/4250	1.02	6/5767 (0.1%)
1	G	0.66	0/4250	0.96	4/5768 (0.1%)
1	H	0.69	0/4250	1.01	12/5768 (0.2%)
All	All	0.73	0/33992	1.02	77/46129 (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	2
1	B	0	2
1	C	0	1
1	D	0	1
1	E	0	2
1	F	0	3
1	G	0	4
1	H	0	3
All	All	0	18

There are no bond length outliers.

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	176	MET	CG-SD-CE	-11.45	75.70	100.90
1	C	176	MET	CG-SD-CE	-10.42	77.97	100.90
1	B	176	MET	CG-SD-CE	-9.81	79.31	100.90
1	E	176	MET	CG-SD-CE	-9.01	81.08	100.90
1	H	118	GLU	CG-CD-OE2	-8.58	98.67	118.40
1	D	118	GLU	CG-CD-OE2	-8.57	98.68	118.40
1	E	118	GLU	CG-CD-OE2	-8.56	98.72	118.40
1	A	118	GLU	CG-CD-OE2	-8.55	98.73	118.40
1	A	176	MET	CG-SD-CE	-8.28	82.69	100.90
1	G	378	GLU	CG-CD-OE2	-7.93	100.15	118.40
1	B	358	ARG	CB-CG-CD	7.24	127.96	111.30
1	B	403	GLU	CG-CD-OE1	7.06	134.64	118.40
1	H	261	MET	CG-SD-CE	-7.02	85.45	100.90
1	C	432	GLU	CB-CG-CD	6.98	124.47	112.60
1	A	11	ASP	CA-CB-CG	6.78	119.38	112.60
1	B	297	ASP	CA-CB-CG	6.55	119.15	112.60
1	A	431	ARG	CB-CA-C	-6.53	98.52	109.75
1	A	261	MET	CG-SD-CE	-6.45	86.72	100.90
1	B	261	MET	CG-SD-CE	-6.43	86.75	100.90
1	E	22	ARG	NE-CZ-NH2	-6.31	113.52	119.20
1	G	423	MET	CB-CG-SD	-6.18	94.16	112.70
1	F	402	ARG	CG-CD-NE	6.12	125.47	112.00
1	D	355	ARG	NE-CZ-NH1	-6.09	115.41	121.50
1	D	71	ARG	NE-CZ-NH2	-6.00	113.80	119.20
1	C	410	MET	CG-SD-CE	-6.00	87.71	100.90
1	B	403	GLU	CG-CD-OE2	-6.00	104.61	118.40
1	B	28	LYS	CG-CD-CE	5.97	125.03	111.30
1	D	64	GLU	CG-CD-OE1	5.93	132.04	118.40
1	E	11	ASP	CA-CB-CG	5.89	118.49	112.60
1	D	61	GLU	N-CA-CB	-5.86	101.80	110.53
1	H	64	GLU	CG-CD-OE1	5.79	131.72	118.40
1	B	310	LYS	CB-CG-CD	5.77	124.58	111.30
1	E	64	GLU	CG-CD-OE1	5.76	131.65	118.40
1	H	64	GLU	CB-CG-CD	5.73	122.34	112.60
1	F	310	LYS	CB-CG-CD	5.71	124.43	111.30
1	H	118	GLU	CG-CD-OE1	5.69	131.50	118.40
1	B	355	ARG	CA-CB-CG	-5.65	102.80	114.10
1	A	22	ARG	NH1-CZ-NH2	-5.63	111.98	119.30
1	G	432	GLU	CB-CG-CD	5.61	122.13	112.60
1	D	109	ARG	CD-NE-CZ	5.59	132.23	124.40
1	F	403	GLU	CG-CD-OE1	5.52	131.10	118.40
1	A	22	ARG	NE-CZ-NH1	5.47	126.97	121.50
1	E	118	GLU	CG-CD-OE1	5.46	130.97	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	300	MET	CG-SD-CE	-5.46	88.90	100.90
1	A	408	PHE	CA-CB-CG	5.45	119.25	113.80
1	A	423	MET	CB-CG-SD	-5.45	96.36	112.70
1	C	297	ASP	CB-CA-C	5.42	118.65	109.50
1	A	112	ARG	CG-CD-NE	-5.37	100.18	112.00
1	A	118	GLU	CG-CD-OE1	5.37	130.74	118.40
1	D	355	ARG	CA-CB-CG	-5.36	103.38	114.10
1	F	431	ARG	CB-CA-C	-5.34	100.56	109.75
1	B	355	ARG	CG-CD-NE	-5.34	100.26	112.00
1	H	112	ARG	CG-CD-NE	-5.33	100.28	112.00
1	B	133	ASP	CA-CB-CG	5.29	117.89	112.60
1	C	378	GLU	CG-CD-OE2	-5.29	106.24	118.40
1	A	64	GLU	CB-CG-CD	5.26	121.55	112.60
1	F	432	GLU	CB-CG-CD	5.26	121.54	112.60
1	E	78	ILE	CA-C-O	5.25	122.25	119.15
1	H	522	ARG	CA-CB-CG	-5.22	103.66	114.10
1	E	109	ARG	CD-NE-CZ	5.21	131.70	124.40
1	H	387	ASN	CA-CB-CG	-5.14	107.46	112.60
1	F	449	ARG	CG-CD-NE	5.14	123.30	112.00
1	A	64	GLU	CG-CD-OE2	-5.13	106.59	118.40
1	D	355	ARG	CD-NE-CZ	5.13	131.58	124.40
1	A	504	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	522	ARG	CA-CB-CG	-5.09	103.92	114.10
1	B	310	LYS	CD-CE-NZ	5.09	128.19	111.90
1	B	432	GLU	CB-CG-CD	5.09	121.25	112.60
1	H	352	HIS	CB-CG-CD2	-5.09	124.58	131.20
1	E	522	ARG	CA-CB-CG	-5.09	103.93	114.10
1	H	61	GLU	N-CA-CB	-5.08	102.96	110.53
1	H	64	GLU	CG-CD-OE2	-5.06	106.77	118.40
1	B	355	ARG	N-CA-CB	-5.04	103.03	110.90
1	E	64	GLU	CG-CD-OE2	-5.02	106.85	118.40
1	B	109	ARG	CD-NE-CZ	5.02	131.42	124.40
1	B	118	GLU	CG-CD-OE2	-5.01	106.87	118.40
1	E	431	ARG	CB-CA-C	-5.00	101.14	109.75

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	ARG	Sidechain
1	A	348	ARG	Sidechain
1	B	109	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	348	ARG	Sidechain
1	C	348	ARG	Sidechain
1	D	348	ARG	Sidechain
1	E	22	ARG	Sidechain
1	E	348	ARG	Sidechain
1	F	20	ARG	Sidechain
1	F	348	ARG	Sidechain
1	F	449	ARG	Sidechain
1	G	290	ARG	Sidechain
1	G	348	ARG	Sidechain
1	G	355	ARG	Sidechain
1	G	414	ARG	Sidechain
1	H	112	ARG	Sidechain
1	H	22	ARG	Sidechain
1	H	348	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4133	0	4000	24	0
1	B	4141	0	4008	15	0
1	C	4141	0	4003	17	0
1	D	4141	0	4008	13	0
1	E	4141	0	4008	18	0
1	F	4141	0	4008	10	0
1	G	4141	0	4010	19	0
1	H	4141	0	4003	15	0
2	A	53	0	30	1	0
2	B	53	0	30	1	0
2	C	53	0	30	1	0
2	D	53	0	30	1	0
2	E	53	0	30	1	0
2	F	53	0	30	1	0
2	G	53	0	30	1	0
2	H	53	0	30	1	0
3	A	38	0	52	0	0
3	B	19	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	19	0	26	0	0
3	D	19	0	26	3	0
3	E	19	0	26	0	0
3	F	19	0	26	0	0
3	H	19	0	26	4	0
4	A	8	0	14	1	0
4	B	8	0	14	1	0
4	E	8	0	14	1	0
4	F	8	0	14	0	0
5	A	8	0	14	0	0
6	A	1	0	0	1	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
6	E	1	0	0	2	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	A	443	0	0	10	0
7	B	392	0	0	5	0
7	C	373	0	0	4	0
7	D	410	0	0	4	0
7	E	441	0	0	3	0
7	F	407	0	0	4	0
7	G	320	0	0	2	0
7	H	363	0	0	8	0
All	All	36894	0	32566	134	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 2.

All (134) 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:G:44:TYR:CZ	1:G:382[A]:LEU:HD11	2.00	0.96
3:H:602:B3P:H92	7:H:816:HOH:O	1.72	0.89
1:A:343:LYS:CE	7:A:3409:HOH:O	2.24	0.83
1:A:176:MET:HE2	1:B:176:MET:HE2	1.61	0.82
1:C:343:LYS:CE	7:C:800:HOH:O	2.27	0.82
1:G:44:TYR:OH	1:G:382[A]:LEU:HD11	1.81	0.81
1:A:343:LYS:HE3	7:A:3409:HOH:O	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLU:HG2	7:A:3389:HOH:O	1.84	0.77
1:F:108:GLU:HG2	7:F:784:HOH:O	1.85	0.75
1:E:189:GLU:HG2	6:E:604:CL:CL	2.26	0.73
1:B:358:ARG:HD2	7:B:1030:HOH:O	1.91	0.71
1:D:356:ASP:OD1	3:D:604:B3P:H91	1.92	0.69
1:B:82:PRO:HD2	7:B:731:HOH:O	1.92	0.69
1:A:108:GLU:OE2	7:A:3201:HOH:O	2.12	0.68
1:D:75:GLU:HG3	7:D:1068:HOH:O	1.92	0.68
1:D:36:GLU:OE1	7:D:701:HOH:O	2.12	0.68
1:C:343:LYS:HE2	7:C:800:HOH:O	1.92	0.67
1:A:176:MET:HE2	1:B:176:MET:CE	2.24	0.67
1:G:82:PRO:HD2	7:G:758:HOH:O	1.95	0.66
1:A:176:MET:HE1	4:A:604:MPD:H52	1.77	0.66
1:G:44:TYR:OH	1:G:382[A]:LEU:CD1	2.43	0.65
1:C:343:LYS:HE3	7:C:800:HOH:O	1.94	0.65
1:C:295[B]:ASP:CG	1:C:295[B]:ASP:O	2.40	0.63
1:G:382[A]:LEU:HD12	7:G:771:HOH:O	1.98	0.63
1:H:348:ARG:HD2	7:H:1031:HOH:O	1.98	0.63
1:D:361:HIS:ND1	3:D:604:B3P:H112	2.14	0.62
1:F:139:GLN:HG3	7:F:769:HOH:O	1.99	0.62
1:A:82:PRO:HD2	7:A:3229:HOH:O	1.99	0.62
7:D:1025:HOH:O	1:F:413:ASN:HB2	2.00	0.62
1:E:176:MET:HE1	4:E:603:MPD:H52	1.83	0.61
1:A:176:MET:CE	1:B:176:MET:HE2	2.30	0.61
1:H:449:ARG:CZ	7:H:733:HOH:O	2.48	0.61
1:E:282:MET:SD	1:E:423[B]:MET:HG2	2.42	0.59
1:E:268:MET:HE3	7:E:967:HOH:O	2.03	0.58
1:C:295[B]:ASP:O	1:C:295[B]:ASP:OD1	2.22	0.57
2:B:601:FAD:O5B	2:B:601:FAD:H8A	2.06	0.56
1:A:268:MET:HE3	7:A:3485:HOH:O	2.05	0.56
1:A:412:ARG:NH1	7:A:3202:HOH:O	2.20	0.56
1:A:343:LYS:HE2	7:A:3409:HOH:O	1.99	0.55
1:G:44:TYR:CZ	1:G:382[A]:LEU:CD1	2.82	0.55
1:A:3:ARG:HH11	1:A:11:ASP:CG	2.15	0.55
2:E:601:FAD:O5B	2:E:601:FAD:H8A	2.07	0.55
1:G:243:SER:H	1:G:352:HIS:CD2	2.25	0.55
1:C:243:SER:H	1:C:352:HIS:CD2	2.24	0.55
1:E:243:SER:H	1:E:352:HIS:CD2	2.25	0.54
1:D:112:ARG:NH2	7:D:704:HOH:O	2.38	0.54
1:B:449:ARG:CZ	7:B:733:HOH:O	2.55	0.54
1:F:243:SER:H	1:F:352:HIS:CD2	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:ASP:OD1	3:D:604:B3P:C9	2.56	0.53
1:F:470:GLU:HG2	7:F:885:HOH:O	2.08	0.53
1:A:298:GLY:HA2	1:A:419:ASN:ND2	2.24	0.52
1:B:176:MET:HE1	4:B:603:MPD:H52	1.91	0.52
1:G:414:ARG:NH1	1:G:417:GLU:OE1	2.44	0.51
1:G:176:MET:HE3	1:H:176:MET:HE1	1.92	0.50
1:H:43:PRO:O	3:H:602:B3P:H101	2.10	0.50
1:E:243:SER:H	1:E:352:HIS:HD2	1.60	0.50
1:E:261:MET:HE3	1:E:275:PRO:HB2	1.93	0.50
1:C:243:SER:H	1:C:352:HIS:HD2	1.58	0.50
1:G:44:TYR:HH	1:G:382[A]:LEU:HD11	1.76	0.49
2:G:601:FAD:H8A	2:G:601:FAD:O5B	2.12	0.49
1:F:243:SER:H	1:F:352:HIS:HD2	1.59	0.49
2:H:601:FAD:O5B	2:H:601:FAD:H8A	2.11	0.49
1:C:261:MET:HE3	1:C:275:PRO:HB2	1.95	0.49
2:C:601:FAD:H8A	2:C:601:FAD:O5B	2.12	0.48
1:G:261:MET:HE3	1:G:275:PRO:HB2	1.94	0.48
1:G:243:SER:H	1:G:352:HIS:HD2	1.59	0.48
2:F:601:FAD:O5B	2:F:601:FAD:H8A	2.13	0.47
1:G:382[A]:LEU:HD13	1:G:388:GLY:O	2.14	0.47
1:E:189:GLU:CG	6:E:604:CL:CL	2.99	0.47
1:E:449:ARG:CZ	7:E:781:HOH:O	2.62	0.47
1:A:108:GLU:CG	7:A:3389:HOH:O	2.50	0.47
1:H:299:PRO:HD3	1:H:419:ASN:HD22	1.80	0.47
1:A:50:GLU:HA	1:A:50:GLU:OE1	2.14	0.47
1:H:329:LEU:HD12	1:H:332:MET:HE2	1.96	0.47
1:E:50:GLU:HA	1:E:50:GLU:OE1	2.14	0.46
1:E:298:GLY:HA2	1:E:419:ASN:ND2	2.30	0.46
1:H:348:ARG:CG	7:H:1031:HOH:O	2.64	0.46
1:B:13:ARG:NE	1:B:13:ARG:HA	2.32	0.45
1:H:281:PHE:HB3	1:H:423:MET:HG2	1.98	0.45
1:F:50:GLU:HA	1:F:50:GLU:OE1	2.16	0.45
1:G:281:PHE:HB3	1:G:423:MET:HG2	1.98	0.45
1:C:410:MET:HE2	7:C:1059:HOH:O	2.17	0.45
1:F:147:LEU:C	1:F:147:LEU:HD12	2.42	0.44
2:A:601:FAD:O5B	2:A:601:FAD:H8A	2.17	0.44
1:H:261:MET:HE3	1:H:275:PRO:HB2	2.00	0.44
1:C:176:MET:CE	1:D:176:MET:HE3	2.47	0.44
1:H:498:LYS:HE2	7:H:898:HOH:O	2.18	0.44
1:C:298:GLY:HA2	1:C:419:ASN:ND2	2.32	0.44
2:D:601:FAD:H8A	2:D:601:FAD:O5B	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:ARG:HD3	1:E:11:ASP:OD1	2.18	0.44
1:G:131:TYR:CZ	1:G:150:PRO:HD3	2.53	0.44
3:H:602:B3P:C9	7:H:816:HOH:O	2.46	0.44
1:B:261:MET:HE3	1:B:275:PRO:HB2	2.00	0.43
1:C:50:GLU:HA	1:C:50:GLU:OE1	2.17	0.43
1:E:362:VAL:HG23	7:E:748:HOH:O	2.17	0.43
1:H:348:ARG:CD	7:H:1031:HOH:O	2.64	0.43
1:B:423[A]:MET:SD	1:B:440:ILE:HD12	2.58	0.43
1:C:176:MET:HE1	1:D:176:MET:HE3	2.00	0.43
1:H:348:ARG:HG2	7:H:1031:HOH:O	2.18	0.43
1:E:147:LEU:C	1:E:147:LEU:HD12	2.43	0.43
1:B:147:LEU:C	1:B:147:LEU:HD12	2.43	0.43
1:E:293:TRP:CD2	1:E:308:MET:HG2	2.54	0.43
1:H:147:LEU:C	1:H:147:LEU:HD12	2.44	0.43
1:H:298:GLY:HA2	1:H:419:ASN:ND2	2.34	0.42
1:B:160:ASN:ND2	1:B:174:HIS:ND1	2.67	0.42
1:B:293:TRP:CD2	1:B:308:MET:HG2	2.55	0.42
1:C:147:LEU:HD12	1:C:147:LEU:C	2.45	0.42
1:D:261:MET:HE3	1:D:261:MET:HB2	1.84	0.42
1:A:3:ARG:NH1	1:A:11:ASP:CG	2.76	0.42
1:A:281:PHE:HB3	1:A:423:MET:HG2	2.01	0.42
1:G:147:LEU:HD12	1:G:147:LEU:C	2.45	0.42
1:D:356:ASP:HB3	1:G:519:GLN:NE2	2.35	0.41
1:A:3:ARG:NH1	1:A:11:ASP:OD2	2.39	0.41
1:D:147:LEU:C	1:D:147:LEU:HD12	2.45	0.41
1:H:38:GLU:OE2	3:H:602:B3P:O5	2.33	0.41
1:E:281:PHE:HB3	1:E:423[A]:MET:HG2	2.01	0.41
1:A:147:LEU:C	1:A:147:LEU:HD12	2.46	0.41
1:A:261:MET:HE3	1:A:275:PRO:HB2	2.02	0.41
1:E:131:TYR:CZ	1:E:150:PRO:HD3	2.56	0.41
7:A:3347:HOH:O	1:B:496:HIS:HE1	2.04	0.41
1:B:307:ARG:HD2	7:B:1033:HOH:O	2.21	0.41
1:C:176:MET:HB2	1:C:176:MET:HE3	1.91	0.41
1:G:176:MET:HE2	1:G:177:TRP:CZ2	2.55	0.41
1:A:261:MET:HE2	1:A:261:MET:HB3	1.71	0.41
1:F:237:ARG:HA	1:F:238:PRO:HD3	1.95	0.41
1:E:237:ARG:HA	1:E:238:PRO:HD3	1.96	0.40
1:C:148:ASP:OD1	1:C:167:GLY:HA3	2.22	0.40
1:F:291:THR:HG23	7:F:1085:HOH:O	2.19	0.40
1:A:189:GLU:HB2	6:A:606:CL:CL	2.59	0.40
1:A:496:HIS:HE1	7:B:780:HOH:O	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:GLY:O	1:D:440:ILE:HA	2.22	0.40
1:G:44:TYR:CE1	1:G:382[A]:LEU:CD1	3.04	0.40
1:C:131:TYR:CZ	1:C:150:PRO:HD3	2.56	0.40
1:D:131:TYR:CZ	1:D:150:PRO:HD3	2.55	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	523/526 (99%)	512 (98%)	11 (2%)	0	100	100
1	B	524/526 (100%)	513 (98%)	11 (2%)	0	100	100
1	C	524/526 (100%)	512 (98%)	12 (2%)	0	100	100
1	D	524/526 (100%)	512 (98%)	12 (2%)	0	100	100
1	E	524/526 (100%)	511 (98%)	13 (2%)	0	100	100
1	F	524/526 (100%)	513 (98%)	11 (2%)	0	100	100
1	G	524/526 (100%)	512 (98%)	12 (2%)	0	100	100
1	H	524/526 (100%)	512 (98%)	12 (2%)	0	100	100
All	All	4191/4208 (100%)	4097 (98%)	94 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	434/435 (100%)	432 (100%)	2 (0%)	81	65
1	B	435/435 (100%)	433 (100%)	2 (0%)	81	65
1	C	435/435 (100%)	429 (99%)	6 (1%)	59	31
1	D	435/435 (100%)	432 (99%)	3 (1%)	76	56
1	E	435/435 (100%)	433 (100%)	2 (0%)	81	65
1	F	435/435 (100%)	431 (99%)	4 (1%)	70	48
1	G	435/435 (100%)	432 (99%)	3 (1%)	76	56
1	H	435/435 (100%)	433 (100%)	2 (0%)	81	65
All	All	3479/3480 (100%)	3455 (99%)	24 (1%)	76	56

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	LEU
1	A	273	ASN
1	B	198	LEU
1	B	297	ASP
1	C	28	LYS
1	C	198	LEU
1	C	273	ASN
1	C	378	GLU
1	C	406	LYS
1	C	471	TYR
1	D	41	ARG
1	D	198	LEU
1	D	273	ASN
1	E	198	LEU
1	E	273	ASN
1	F	198	LEU
1	F	273	ASN
1	F	297	ASP
1	F	310	LYS
1	G	198	LEU
1	G	273	ASN
1	G	378	GLU
1	H	198	LEU
1	H	273	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	419	ASN
1	A	496	HIS
1	B	139	GLN
1	B	160	ASN
1	B	496	HIS
1	C	139	GLN
1	C	205	GLN
1	C	256	GLN
1	C	352	HIS
1	C	454	GLN
1	D	205	GLN
1	D	267	ASN
1	D	371	ASN
1	E	139	GLN
1	E	205	GLN
1	E	267	ASN
1	E	352	HIS
1	E	419	ASN
1	F	205	GLN
1	F	279	ASN
1	F	352	HIS
1	F	506	ASN
1	G	139	GLN
1	G	205	GLN
1	G	352	HIS
1	H	139	GLN
1	H	205	GLN
1	H	387	ASN
1	H	419	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 9 are monoatomic - leaving 21 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	MPD	A	604	-	7,7,7	0.43	0	9,10,10	1.10	1 (11%)
3	B3P	C	602	-	18,18,18	0.40	0	23,23,23	1.14	2 (8%)
2	FAD	H	601	1	58,58,58	0.77	1 (1%)	85,89,89	0.82	1 (1%)
2	FAD	F	601	1	58,58,58	0.88	2 (3%)	85,89,89	0.84	3 (3%)
3	B3P	B	602	-	18,18,18	0.27	0	23,23,23	1.04	2 (8%)
5	MRD	A	605	-	7,7,7	0.21	0	9,10,10	0.83	0
2	FAD	D	601	1	58,58,58	1.02	2 (3%)	85,89,89	0.89	2 (2%)
3	B3P	F	602	-	18,18,18	0.30	0	23,23,23	0.92	1 (4%)
3	B3P	D	604	-	18,18,18	0.34	0	23,23,23	1.03	1 (4%)
3	B3P	A	602	-	18,18,18	0.57	0	23,23,23	0.81	1 (4%)
4	MPD	E	603	-	7,7,7	0.57	0	9,10,10	1.31	2 (22%)
4	MPD	B	603	-	7,7,7	0.85	0	9,10,10	1.05	1 (11%)
3	B3P	A	603	-	18,18,18	0.38	0	23,23,23	1.23	3 (13%)
3	B3P	E	602	-	18,18,18	0.46	0	23,23,23	0.93	1 (4%)
3	B3P	H	602	-	18,18,18	0.30	0	23,23,23	1.64	6 (26%)
4	MPD	F	603	-	7,7,7	0.64	0	9,10,10	1.04	1 (11%)
2	FAD	B	601	1	58,58,58	1.00	5 (8%)	85,89,89	0.89	4 (4%)
2	FAD	A	601	1	58,58,58	1.03	2 (3%)	85,89,89	1.03	4 (4%)
2	FAD	C	601	-	58,58,58	0.85	1 (1%)	85,89,89	0.83	4 (4%)
2	FAD	G	601	-	58,58,58	1.10	2 (3%)	85,89,89	0.85	2 (2%)
2	FAD	E	601	1	58,58,58	1.18	3 (5%)	85,89,89	0.82	2 (2%)

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
4	MPD	A	604	-	-	3/5/5/5	-
3	B3P	C	602	-	-	7/28/28/28	-
2	FAD	H	601	1	-	4/34/50/50	0/6/6/6
2	FAD	F	601	1	-	5/34/50/50	0/6/6/6
3	B3P	B	602	-	-	8/28/28/28	-
5	MRD	A	605	-	-	0/5/5/5	-
2	FAD	D	601	1	-	7/34/50/50	0/6/6/6
3	B3P	F	602	-	-	1/28/28/28	-
3	B3P	D	604	-	-	5/28/28/28	-
3	B3P	A	602	-	-	0/28/28/28	-
4	MPD	E	603	-	-	2/5/5/5	-
4	MPD	B	603	-	-	3/5/5/5	-
3	B3P	A	603	-	-	2/28/28/28	-
3	B3P	E	602	-	-	3/28/28/28	-
3	B3P	H	602	-	-	8/28/28/28	-
4	MPD	F	603	-	-	2/5/5/5	-
2	FAD	B	601	1	-	6/34/50/50	0/6/6/6
2	FAD	A	601	1	-	4/34/50/50	0/6/6/6
2	FAD	C	601	-	-	5/34/50/50	0/6/6/6
2	FAD	G	601	-	-	4/34/50/50	0/6/6/6
2	FAD	E	601	1	-	6/34/50/50	0/6/6/6

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	601	FAD	PA-O3P	-5.85	1.53	1.59
2	E	601	FAD	P-O3P	5.05	1.65	1.59
2	D	601	FAD	P-O3P	4.61	1.64	1.59
2	E	601	FAD	PA-O3P	-4.37	1.54	1.59
2	A	601	FAD	P-O3P	4.25	1.64	1.59
2	B	601	FAD	C1'-C2'	-3.19	1.48	1.52
2	B	601	FAD	C4X-N5	2.62	1.36	1.30
2	E	601	FAD	C6-C7	-2.51	1.36	1.39
2	F	601	FAD	C4X-N5	2.51	1.36	1.30
2	B	601	FAD	PA-O2A	-2.35	1.44	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	601	FAD	P-O3P	2.32	1.62	1.59
2	C	601	FAD	PA-O3P	2.32	1.62	1.59
2	A	601	FAD	C5'-C4'	2.32	1.55	1.51
2	F	601	FAD	PA-O3P	2.32	1.62	1.59
2	B	601	FAD	C5'-C4'	2.19	1.54	1.51
2	B	601	FAD	P-O3P	2.13	1.61	1.59
2	D	601	FAD	O2'-C2'	2.03	1.47	1.43
2	H	601	FAD	C4X-N5	2.00	1.35	1.30

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	602	B3P	C9-C8-N2	3.82	120.43	109.02
3	D	604	B3P	C3-N1-C4	3.48	121.25	116.17
2	A	601	FAD	O2'-C2'-C3'	-3.44	101.19	109.25
2	D	601	FAD	O2'-C2'-C3'	-3.37	101.36	109.25
2	A	601	FAD	N3A-C2A-N1A	3.23	133.47	128.58
3	C	602	B3P	C3-N1-C4	3.16	120.79	116.17
3	H	602	B3P	C2-N2-C8	3.04	120.61	116.17
2	B	601	FAD	C1'-C2'-C3'	3.00	117.79	109.66
2	G	601	FAD	C1'-C2'-C3'	2.90	117.53	109.66
2	D	601	FAD	C1'-C2'-C3'	2.83	117.32	109.66
2	B	601	FAD	O2'-C2'-C3'	-2.82	102.64	109.25
2	E	601	FAD	C1'-C2'-C3'	2.76	117.15	109.66
3	B	602	B3P	C6-C4-N1	2.67	116.99	109.02
3	A	603	B3P	C5-C4-N1	-2.67	101.04	109.02
4	B	603	MPD	O4-C4-C3	2.62	121.76	111.35
2	B	601	FAD	N3A-C2A-N1A	2.59	132.50	128.58
2	H	601	FAD	O2'-C2'-C3'	-2.57	103.24	109.25
3	A	603	B3P	C3-N1-C4	2.54	119.88	116.17
3	A	602	B3P	C7-C4-C5	-2.49	104.57	110.02
2	F	601	FAD	O2'-C2'-C3'	-2.45	103.52	109.25
3	E	602	B3P	C3-N1-C4	2.44	119.73	116.17
2	C	601	FAD	O2'-C2'-C3'	-2.39	103.65	109.25
3	H	602	B3P	O1-C9-C8	-2.38	106.85	111.68
3	H	602	B3P	C6-C4-N1	2.35	116.02	109.02
2	C	601	FAD	C6A-C5A-C4A	2.34	120.37	117.18
3	H	602	B3P	C10-C8-C9	-2.29	104.99	110.02
3	B	602	B3P	C2-N2-C8	2.28	119.50	116.17
2	A	601	FAD	C6A-C5A-C4A	2.27	120.28	117.18
2	F	601	FAD	C5X-C9A-N10	2.26	120.01	117.97
2	G	601	FAD	O3P-P-O1P	-2.22	104.02	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	603	MPD	O2-C2-C3	-2.21	100.99	109.27
3	C	602	B3P	C6-C4-N1	2.20	115.59	109.02
2	A	601	FAD	C2A-N3A-C4A	-2.20	106.46	111.83
4	A	604	MPD	O4-C4-C3	2.19	120.08	111.35
3	H	602	B3P	C11-C8-C9	-2.17	105.25	110.02
3	A	603	B3P	C11-C8-C9	-2.17	105.26	110.02
2	C	601	FAD	C1'-C2'-C3'	2.16	115.50	109.66
4	E	603	MPD	O4-C4-C3	2.15	119.92	111.35
2	B	601	FAD	O5'-C5'-C4'	2.14	115.07	109.36
4	F	603	MPD	O4-C4-C3	2.12	119.80	111.35
3	F	602	B3P	O3-C11-C8	-2.09	107.43	111.68
2	F	601	FAD	C1'-C2'-C3'	2.09	115.32	109.66
2	C	601	FAD	N3A-C2A-N1A	2.08	131.74	128.58
2	E	601	FAD	O2'-C2'-C3'	-2.08	104.37	109.25

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	B3P	N1-C4-C6-O5
3	B	602	B3P	C5-C4-C6-O5
3	B	602	B3P	C7-C4-C6-O5
3	B	602	B3P	C10-C8-C9-O1
3	B	602	B3P	C11-C8-C9-O1
3	C	602	B3P	C5-C4-C6-O5
3	D	604	B3P	C1-C3-N1-C4
3	H	602	B3P	C5-C4-N1-C3
3	H	602	B3P	C6-C4-N1-C3
3	H	602	B3P	C7-C4-N1-C3
3	H	602	B3P	C10-C8-N2-C2
3	H	602	B3P	C11-C8-N2-C2
3	C	602	B3P	C2-C1-C3-N1
3	H	602	B3P	C2-C1-C3-N1
3	B	602	B3P	N2-C8-C9-O1
3	C	602	B3P	N1-C4-C6-O5
3	D	604	B3P	O3-C11-C8-N2
3	B	602	B3P	C6-C4-C7-O6
2	A	601	FAD	C3'-C4'-C5'-O5'
2	E	601	FAD	C3'-C4'-C5'-O5'
3	C	602	B3P	C6-C4-N1-C3
3	C	602	B3P	C1-C2-N2-C8
3	C	602	B3P	C1-C3-N1-C4

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Mol	Chain	Res	Type	Atoms
2	D	601	FAD	C2'-C3'-C4'-C5'
2	B	601	FAD	C4'-C5'-O5'-P
2	D	601	FAD	O4'-C4'-C5'-O5'
2	C	601	FAD	C2'-C3'-C4'-O4'
2	H	601	FAD	C2'-C3'-C4'-O4'
3	H	602	B3P	N2-C8-C9-O1
2	A	601	FAD	C4'-C5'-O5'-P
2	F	601	FAD	C4'-C5'-O5'-P
2	G	601	FAD	C4'-C5'-O5'-P
2	H	601	FAD	C4'-C5'-O5'-P
2	E	601	FAD	C2'-C3'-C4'-C5'
2	E	601	FAD	C2'-C3'-C4'-O4'
3	B	602	B3P	C3-C1-C2-N2
3	E	602	B3P	C6-C4-C7-O6
2	A	601	FAD	C2'-C3'-C4'-O4'
2	B	601	FAD	C2'-C3'-C4'-O4'
2	D	601	FAD	C2'-C3'-C4'-O4'
2	G	601	FAD	C2'-C3'-C4'-O4'
2	C	601	FAD	C3'-C4'-C5'-O5'
2	H	601	FAD	C3'-C4'-C5'-O5'
4	E	603	MPD	O2-C2-C3-C4
2	E	601	FAD	O4'-C4'-C5'-O5'
2	F	601	FAD	O4'-C4'-C5'-O5'
2	C	601	FAD	C4'-C5'-O5'-P
2	D	601	FAD	C4'-C5'-O5'-P
3	H	602	B3P	C9-C8-N2-C2
3	D	604	B3P	C10-C8-C9-O1
2	F	601	FAD	C2'-C3'-C4'-C5'
2	E	601	FAD	C4'-C5'-O5'-P
2	B	601	FAD	C2'-C3'-C4'-C5'
3	F	602	B3P	C6-C4-C7-O6
2	F	601	FAD	C2'-C3'-C4'-O4'
2	B	601	FAD	C3'-C4'-C5'-O5'
2	F	601	FAD	C3'-C4'-C5'-O5'
3	E	602	B3P	C2-C1-C3-N1
3	D	604	B3P	C3-C1-C2-N2
2	E	601	FAD	O3'-C3'-C4'-O4'
3	C	602	B3P	C7-C4-C6-O5
2	B	601	FAD	O4'-C4'-C5'-O5'
2	D	601	FAD	C1'-C2'-C3'-O3'
2	D	601	FAD	O2'-C2'-C3'-O3'
3	A	603	B3P	O2-C10-C8-N2

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Mol	Chain	Res	Type	Atoms
2	G	601	FAD	O3'-C3'-C4'-O4'
2	H	601	FAD	O3'-C3'-C4'-O4'
2	B	601	FAD	O3'-C3'-C4'-O4'
2	C	601	FAD	O3'-C3'-C4'-O4'
2	D	601	FAD	C3'-C4'-C5'-O5'
2	G	601	FAD	C3'-C4'-C5'-O5'
4	A	604	MPD	O2-C2-C3-C4
4	B	603	MPD	O2-C2-C3-C4
4	F	603	MPD	O2-C2-C3-C4
2	A	601	FAD	O3'-C3'-C4'-O4'
3	D	604	B3P	O3-C11-C8-C10
4	A	604	MPD	C2-C3-C4-O4
4	B	603	MPD	C2-C3-C4-O4
4	E	603	MPD	C2-C3-C4-O4
4	A	604	MPD	CM-C2-C3-C4
4	B	603	MPD	CM-C2-C3-C4
4	F	603	MPD	CM-C2-C3-C4
2	C	601	FAD	C2'-C3'-C4'-C5'
3	A	603	B3P	C9-C8-N2-C2
3	E	602	B3P	N1-C4-C7-O6

There are no ring outliers.

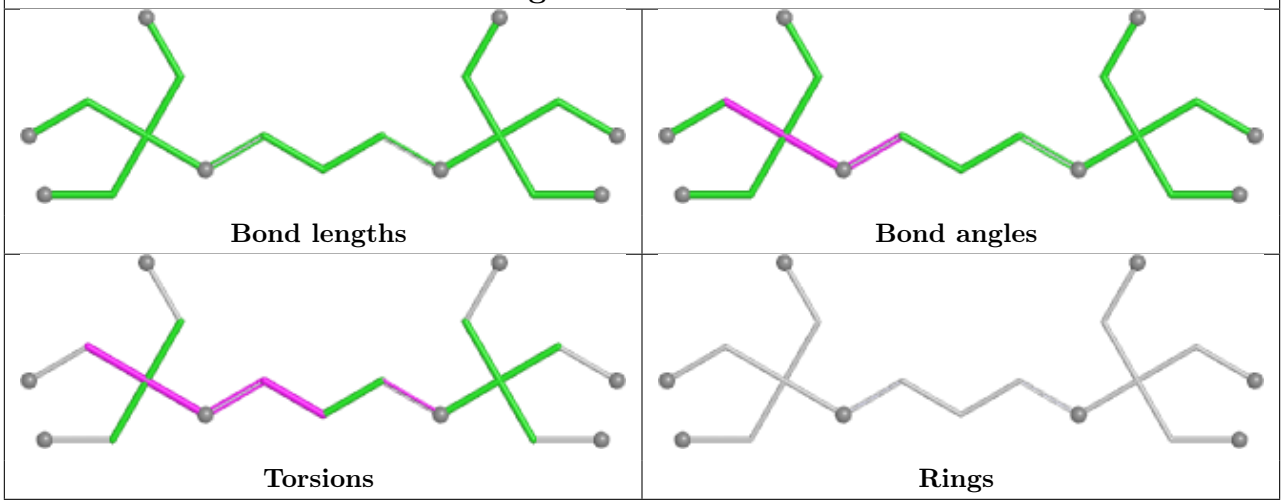
13 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	604	MPD	1	0
2	H	601	FAD	1	0
2	F	601	FAD	1	0
2	D	601	FAD	1	0
3	D	604	B3P	3	0
4	E	603	MPD	1	0
4	B	603	MPD	1	0
3	H	602	B3P	4	0
2	B	601	FAD	1	0
2	A	601	FAD	1	0
2	C	601	FAD	1	0
2	G	601	FAD	1	0
2	E	601	FAD	1	0

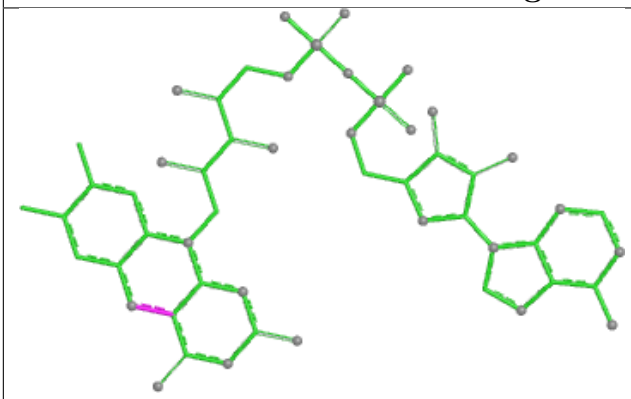
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

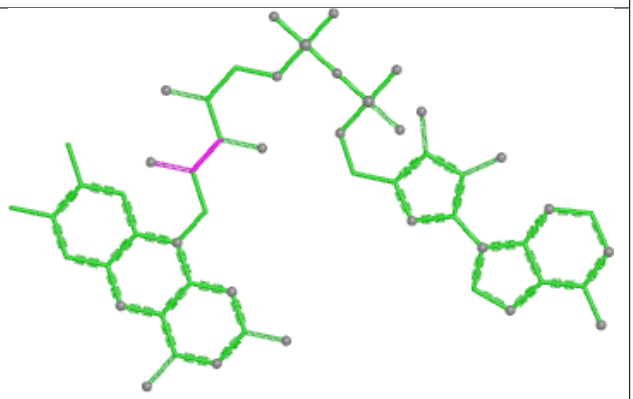
Ligand B3P C 602



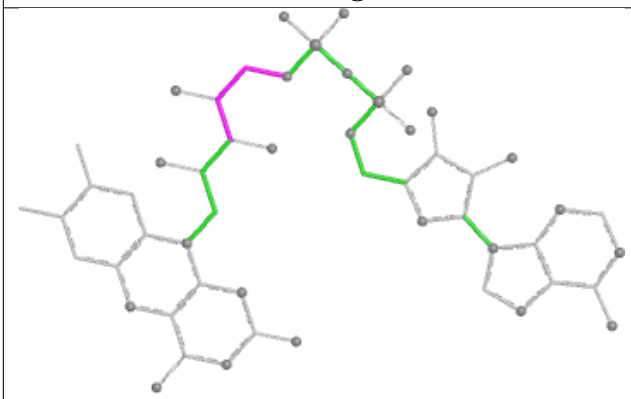
Ligand FAD H 601



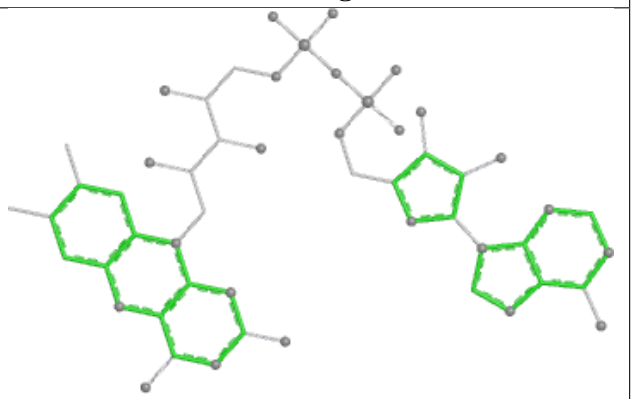
Bond lengths



Bond angles

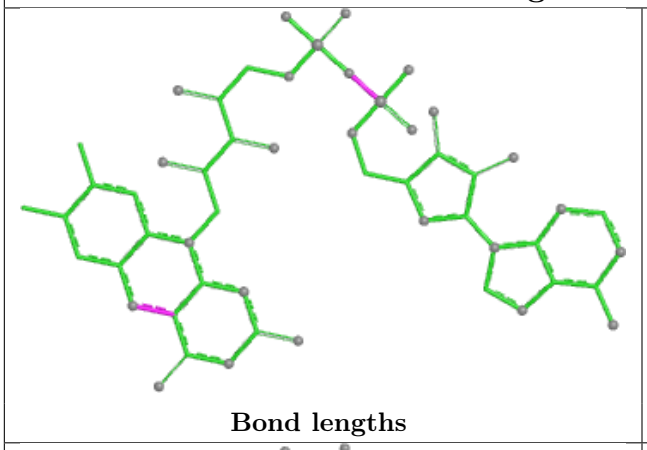


Torsions

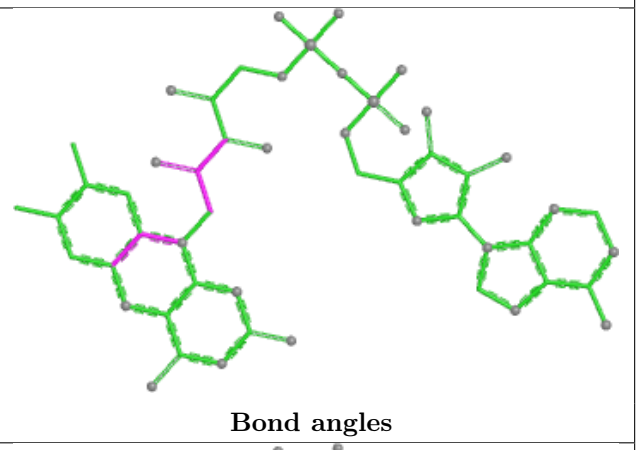


Rings

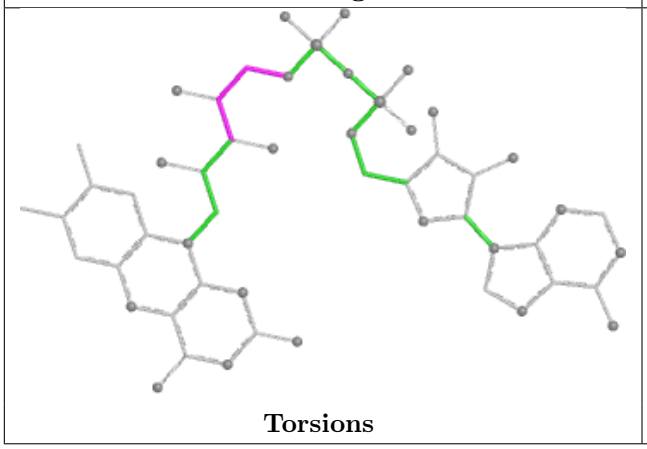
Ligand FAD F 601



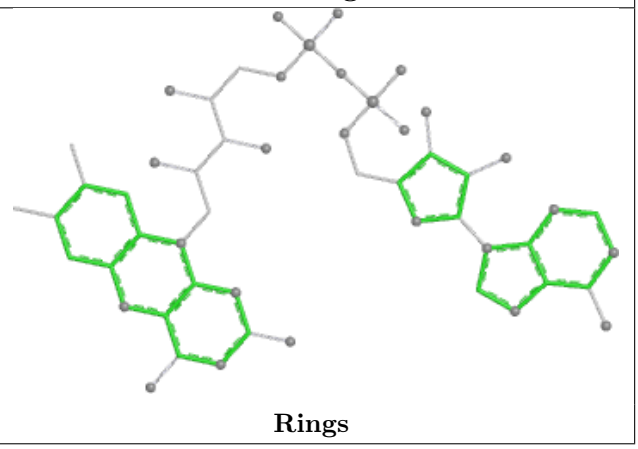
Bond lengths



Bond angles

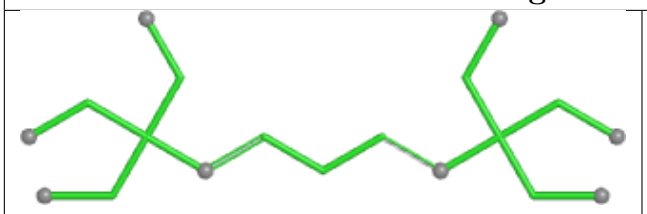


Torsions

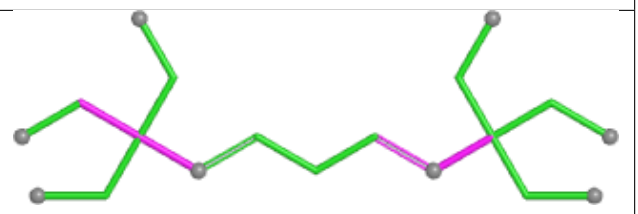


Rings

Ligand B3P B 602



Bond lengths



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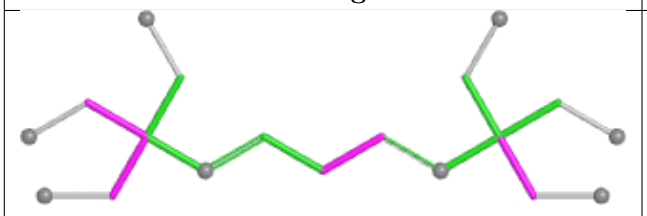

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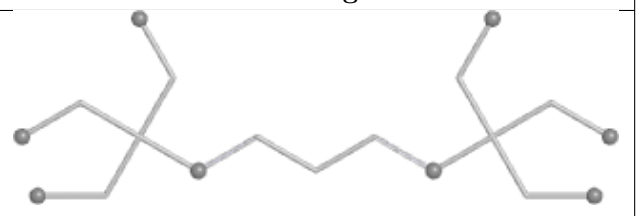
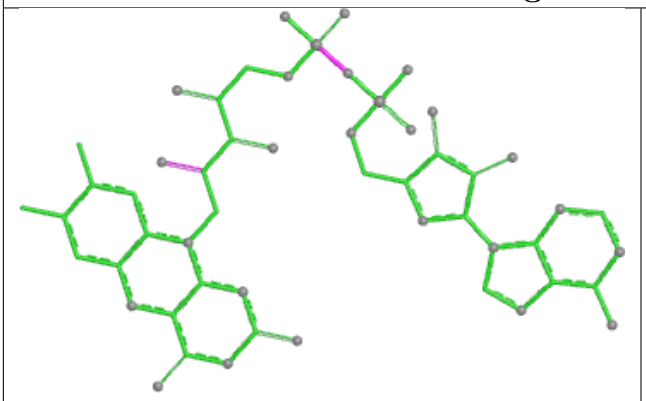


Rings

Ligand FAD D 601



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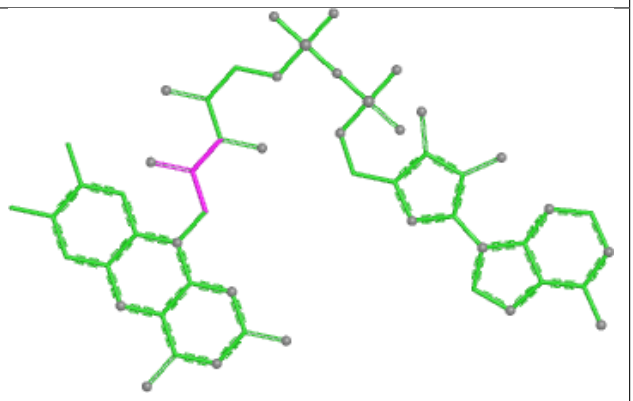
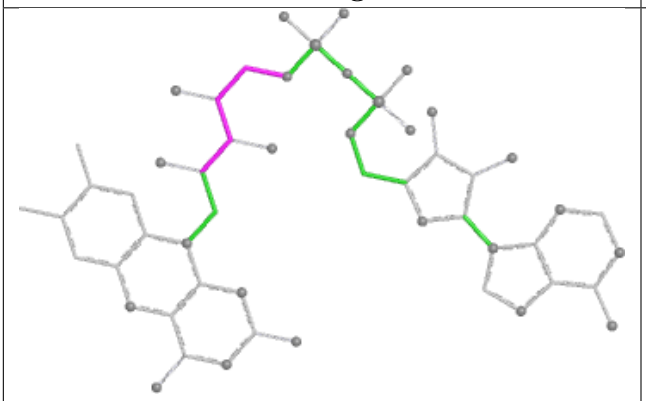


Bond angles



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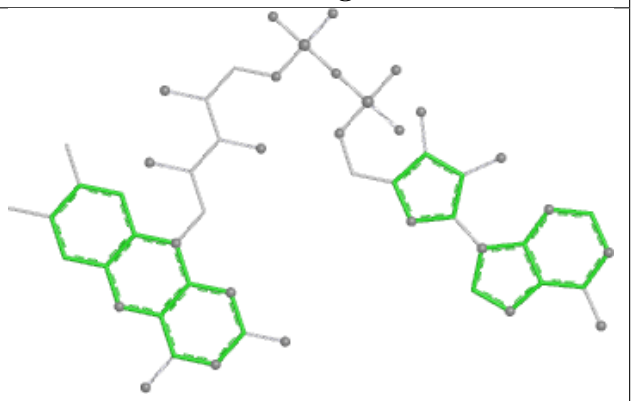
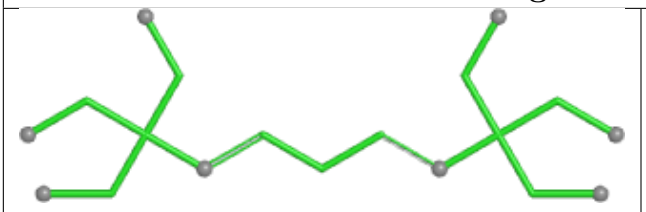
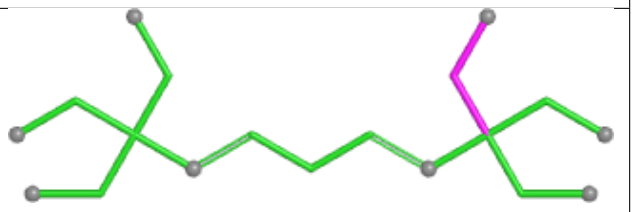


Rings

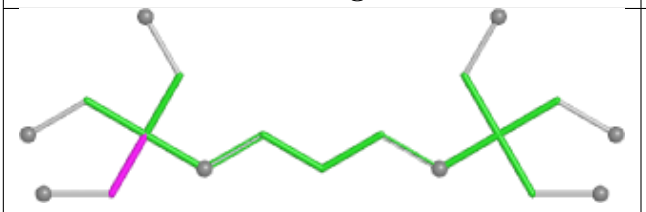
Ligand B3P F 602



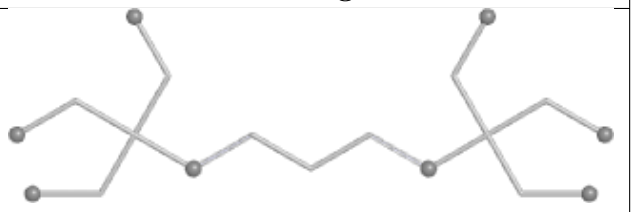
Bond lengths



Bond angles

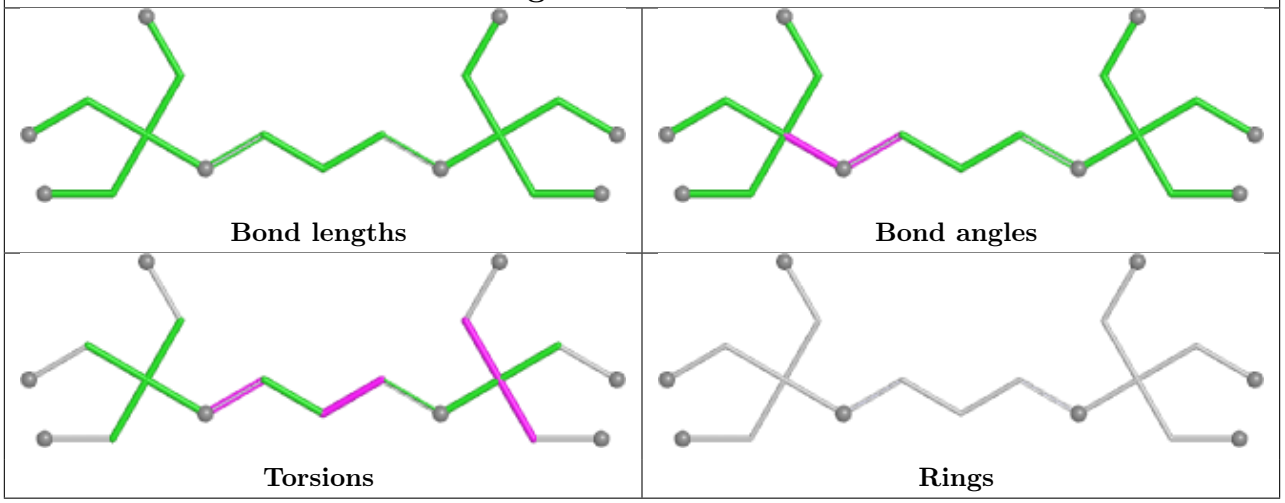


Torsions

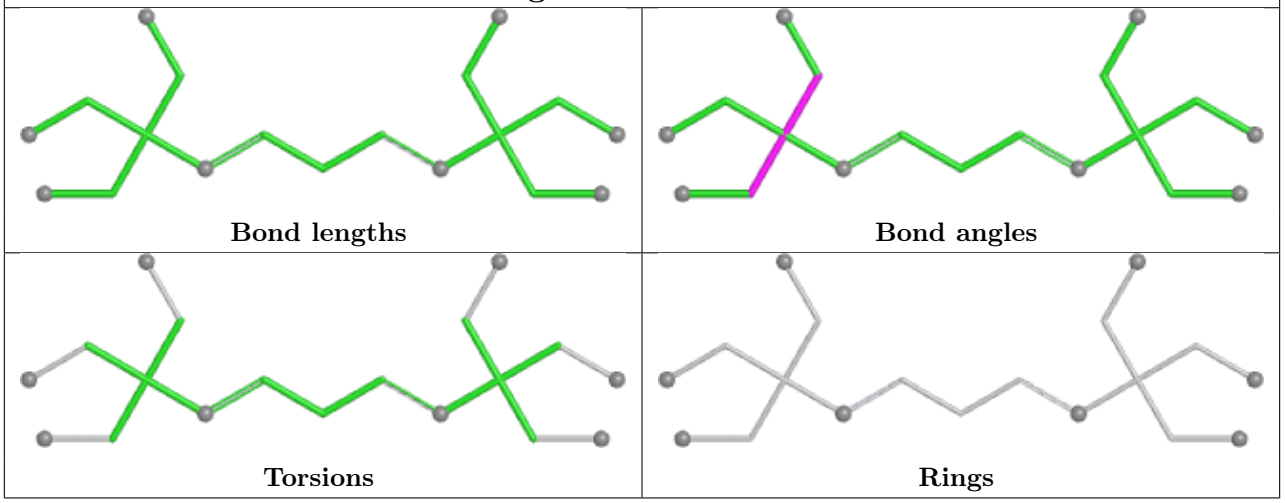


Rings

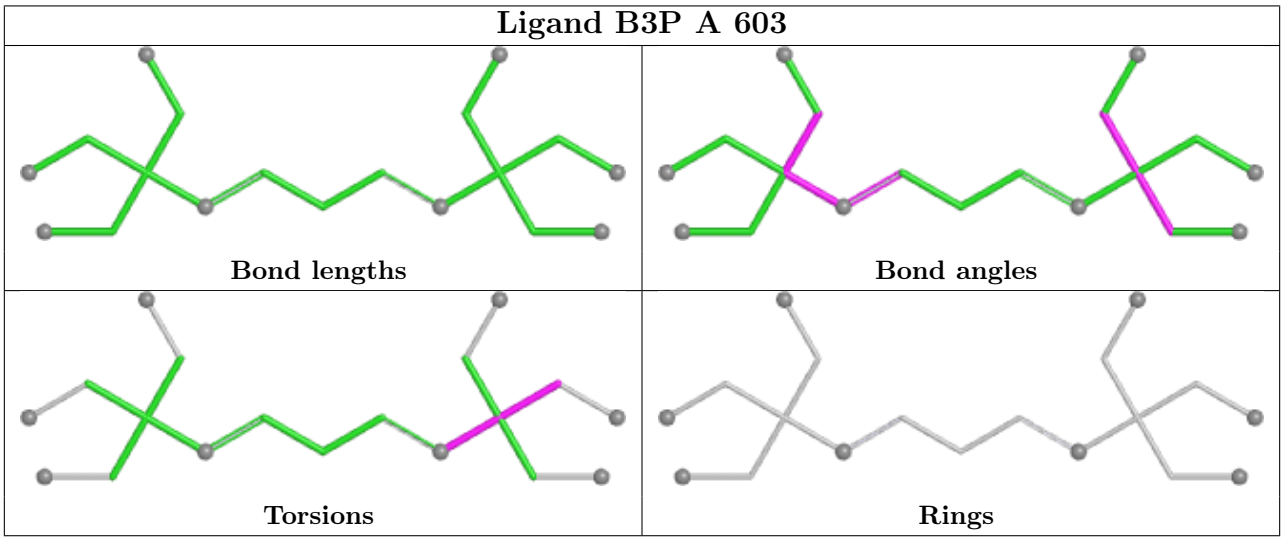
Ligand B3P D 604



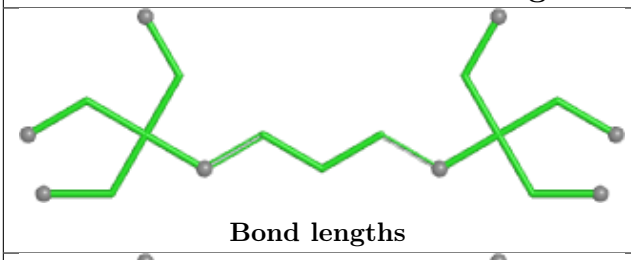
Ligand B3P A 602



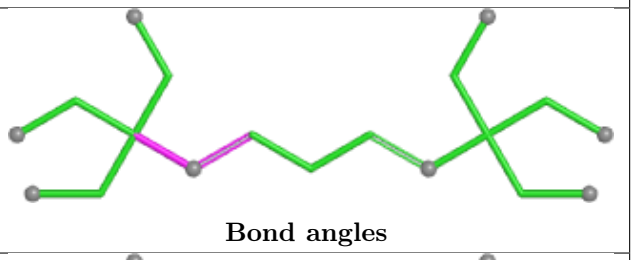
Ligand B3P A 603



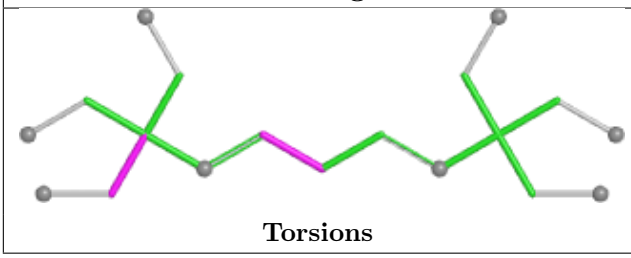
Ligand B3P E 602



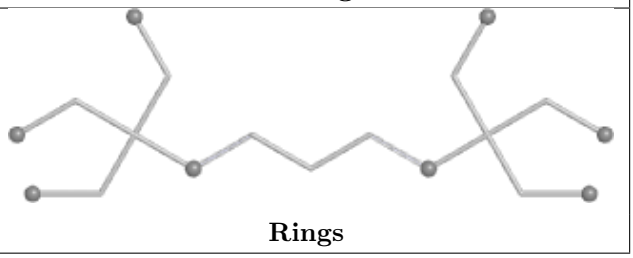
Bond lengths



Bond angles

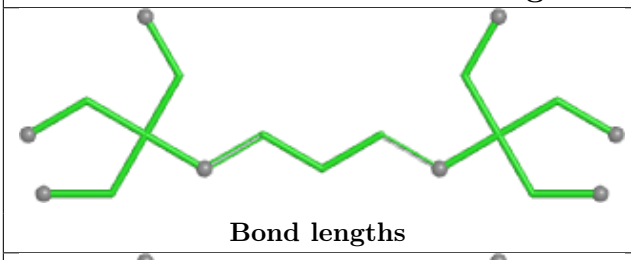


Torsions



Rings

Ligand B3P H 602



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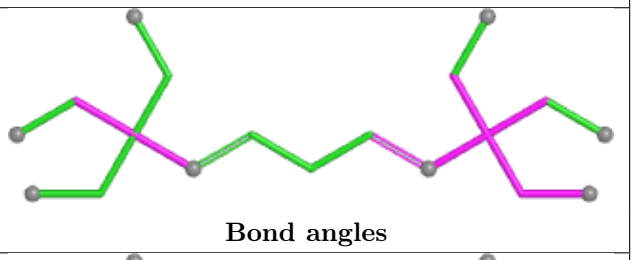
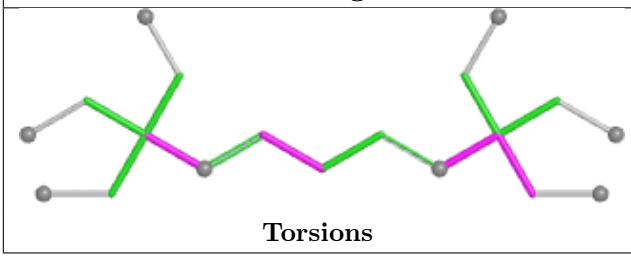


Bond angles



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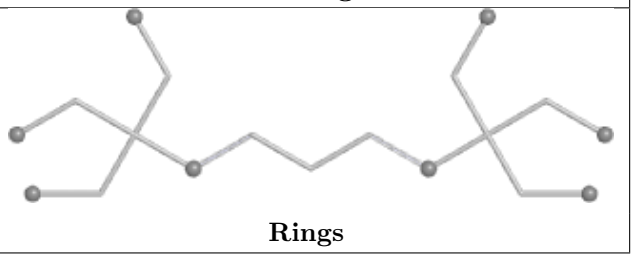
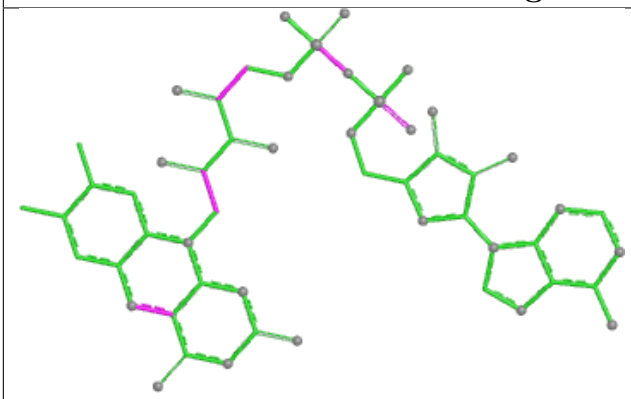


Rings

Ligand FAD B 601



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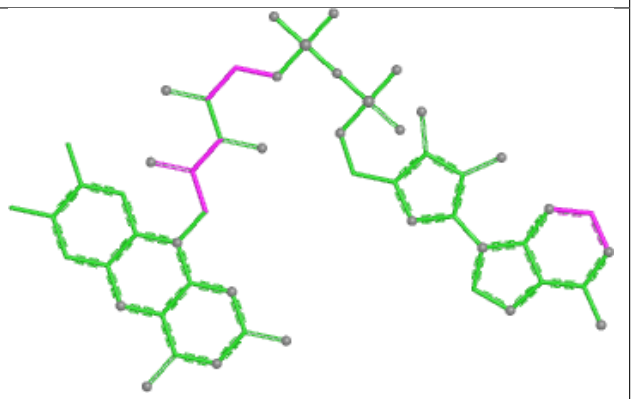
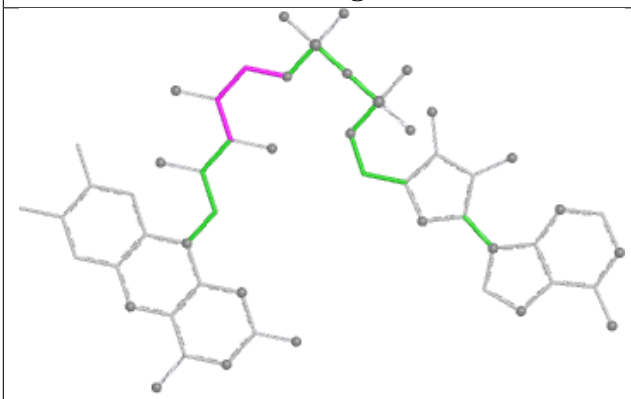
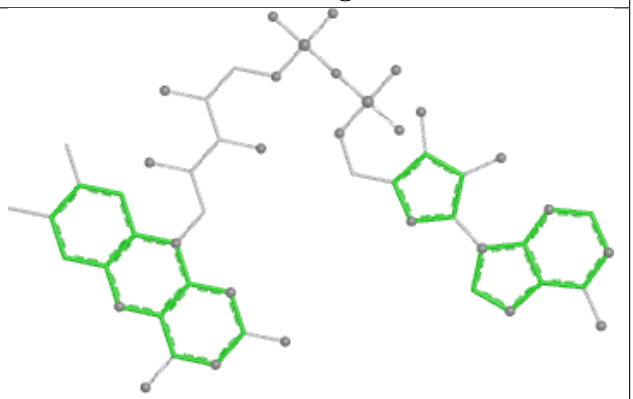


Bond angles

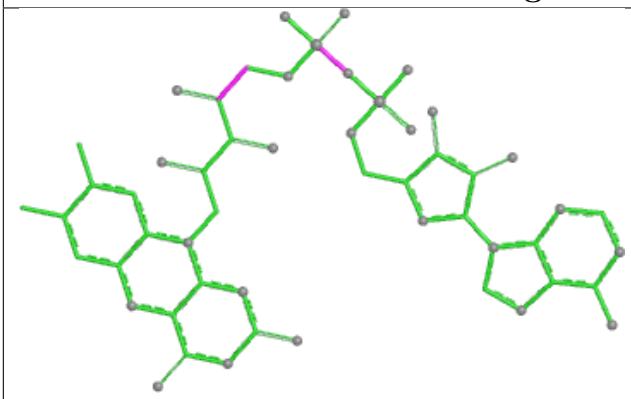


Torsions



Rings

Ligand FAD A 601



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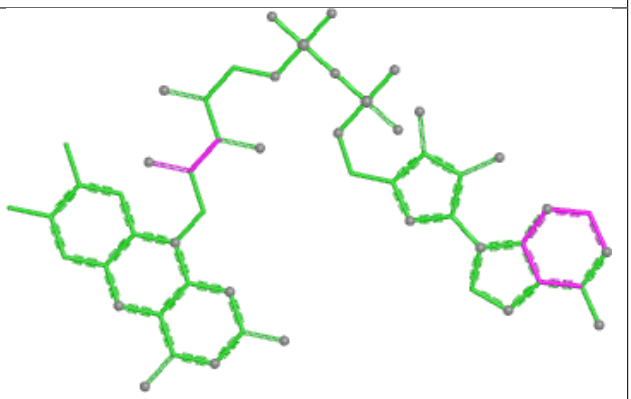
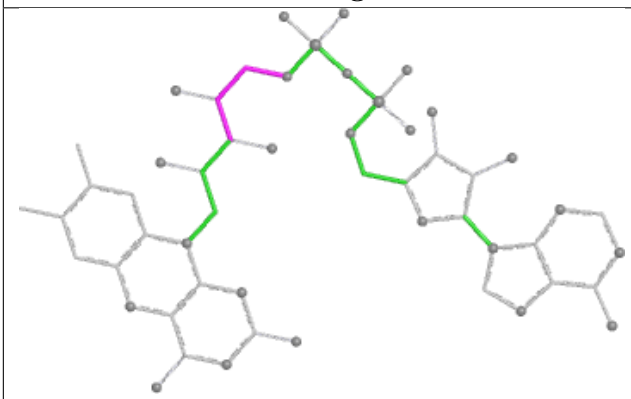


Bond angles



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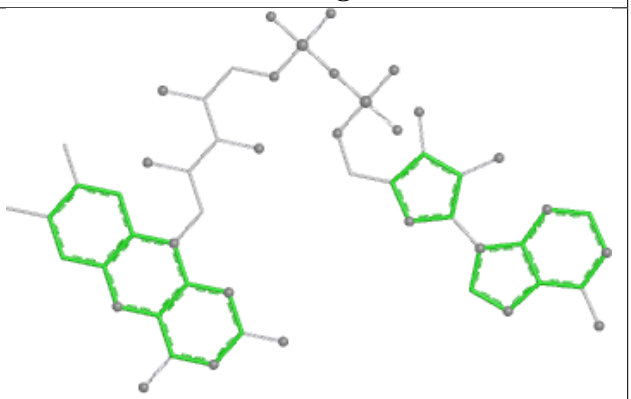
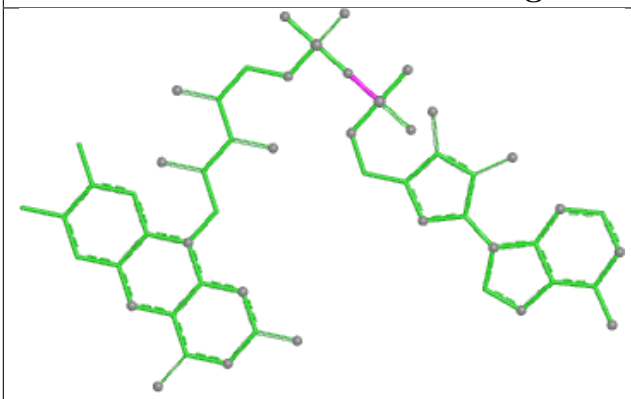


Rings

Ligand FAD C 601



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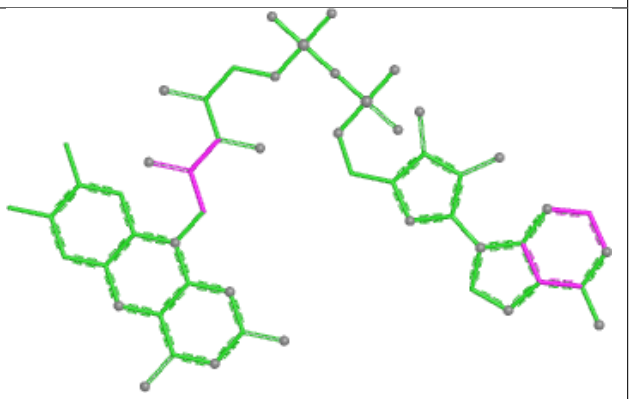

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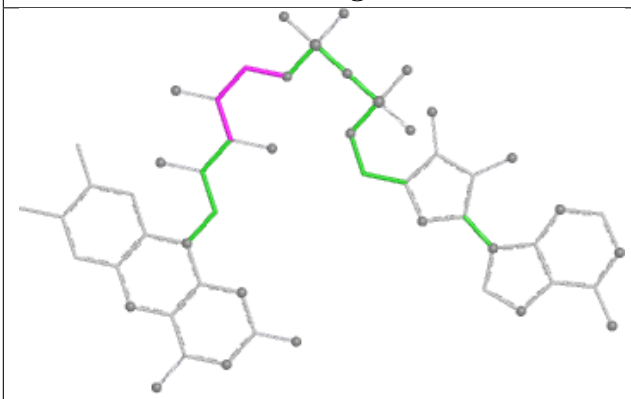

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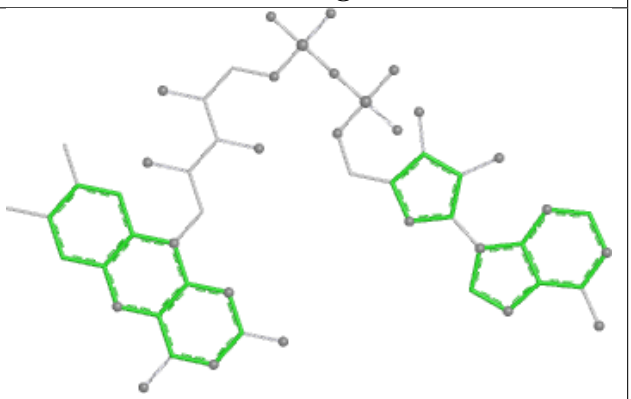
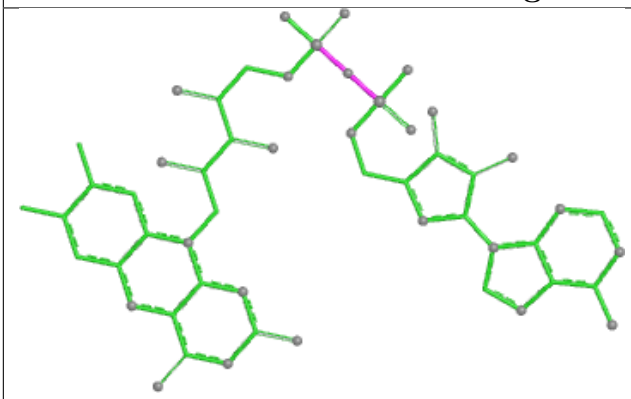


Rings

Ligand FAD G 601



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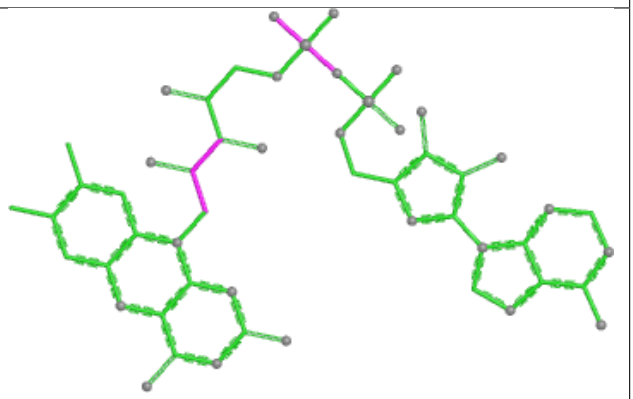
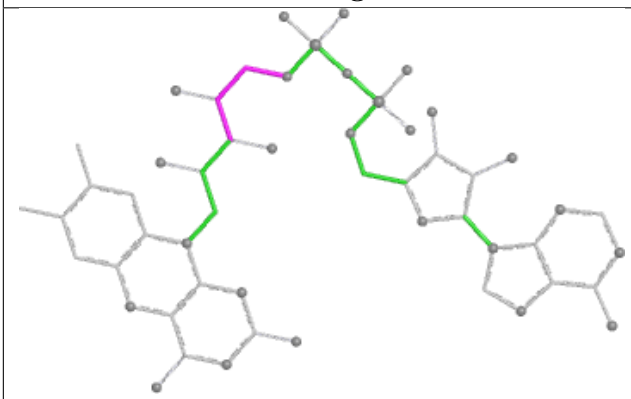


Bond angles



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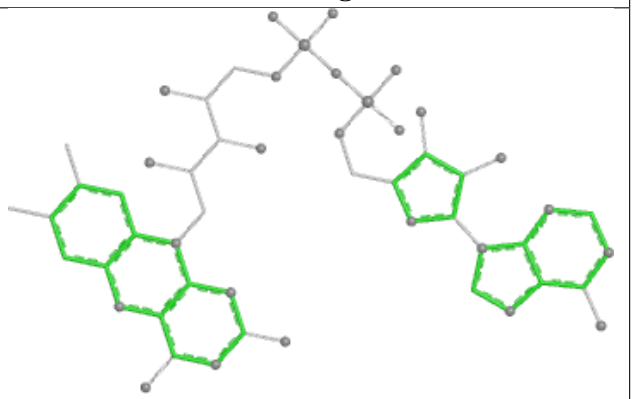
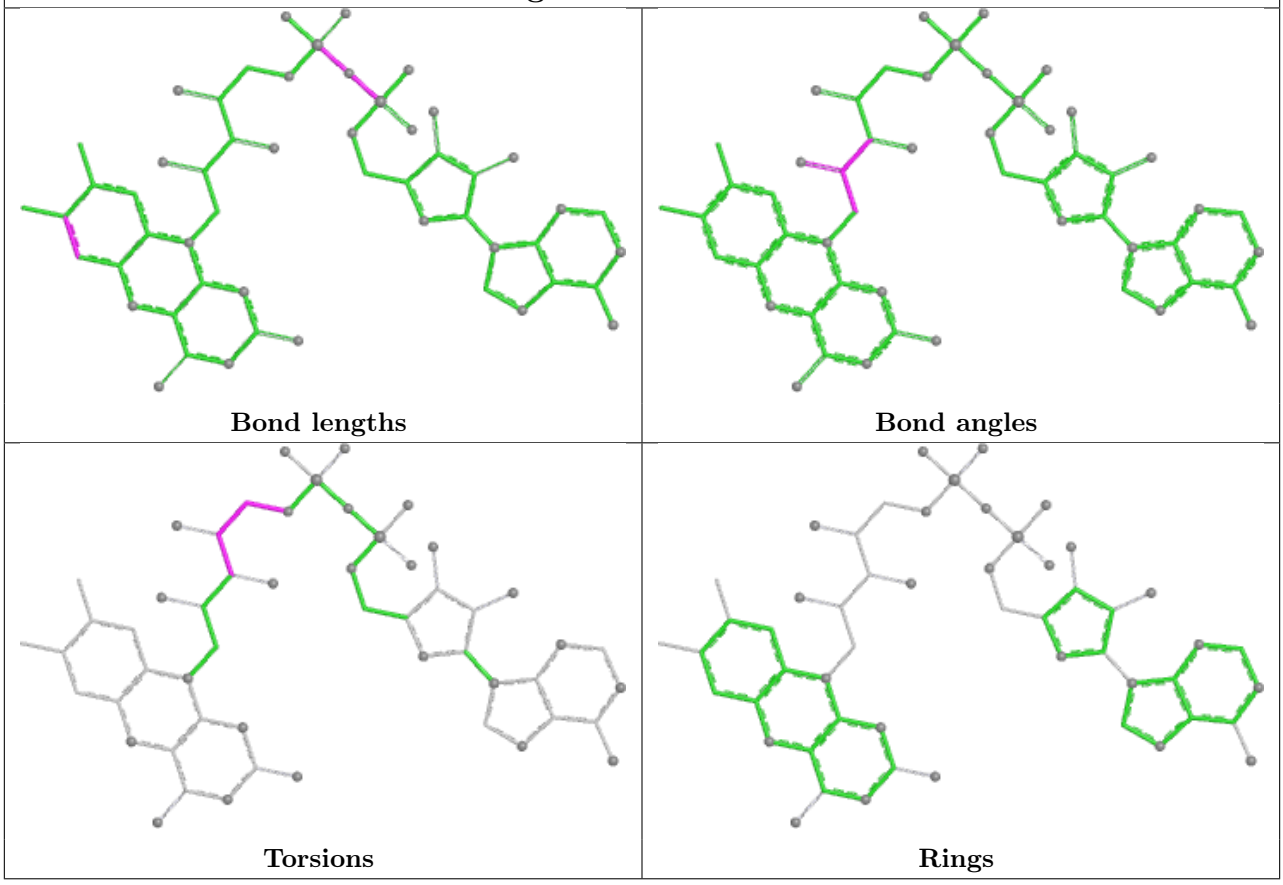


Rings

Ligand FAD E 601



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	525/526 (99%)	-0.34	6 (1%)	78	81	9, 13, 25, 61	0
1	B	525/526 (99%)	-0.20	5 (0%)	79	83	9, 15, 29, 56	1 (0%)
1	C	525/526 (99%)	-0.09	10 (1%)	66	70	9, 16, 31, 58	1 (0%)
1	D	525/526 (99%)	-0.25	5 (0%)	79	83	9, 14, 29, 53	1 (0%)
1	E	525/526 (99%)	-0.34	8 (1%)	72	76	8, 13, 25, 66	1 (0%)
1	F	525/526 (99%)	-0.24	8 (1%)	72	76	8, 14, 28, 66	1 (0%)
1	G	525/526 (99%)	0.06	7 (1%)	75	79	10, 20, 40, 60	1 (0%)
1	H	525/526 (99%)	-0.04	13 (2%)	58	62	11, 17, 34, 72	1 (0%)
All	All	4200/4208 (99%)	-0.18	62 (1%)	72	76	8, 15, 31, 72	7 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	THR	6.2
1	E	2	THR	5.6
1	B	297	ASP	4.6
1	H	297	ASP	3.9
1	A	525	ASN	3.9
1	C	297	ASP	3.9
1	F	297	ASP	3.8
1	C	523	GLY	3.6
1	C	434	TYR	3.5
1	B	525	ASN	3.4
1	H	525	ASN	3.3
1	A	2	THR	3.3
1	A	523	GLY	3.2
1	G	2	THR	3.2
1	C	428	ILE	3.1
1	B	523	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	524	GLN	2.9
1	G	525	ASN	2.9
1	E	525	ASN	2.8
1	F	523	GLY	2.8
1	H	2	THR	2.7
1	F	356	ASP	2.7
1	F	296	GLY	2.7
1	H	526	LEU	2.7
1	C	429	GLY	2.6
1	D	2	THR	2.6
1	H	523	GLY	2.6
1	H	296	GLY	2.6
1	E	4	THR	2.5
1	E	523	GLY	2.5
1	E	524	GLN	2.4
1	H	524	GLN	2.4
1	C	525	ASN	2.4
1	B	2	THR	2.3
1	E	189	GLU	2.3
1	C	12	GLU	2.3
1	D	297	ASP	2.3
1	G	356	ASP	2.3
1	H	356	ASP	2.3
1	E	526	LEU	2.3
1	H	294	PHE	2.2
1	C	9	VAL	2.2
1	H	348	ARG	2.2
1	B	524	GLN	2.2
1	H	139	GLN	2.2
1	F	295	ASP	2.2
1	A	297	ASP	2.1
1	F	524	GLN	2.1
1	G	429	GLY	2.1
1	D	525	ASN	2.1
1	F	525	ASN	2.1
1	G	256	GLN	2.1
1	F	438	LEU	2.1
1	H	295	ASP	2.1
1	H	298	GLY	2.1
1	C	427	THR	2.0
1	A	438	LEU	2.0
1	E	471	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	434	TYR	2.0
1	G	299	PRO	2.0
1	A	303	GLU	2.0
1	D	142	ASP	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 oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B3P	H	602	19/19	0.72	0.19	35,50,64,68	0
3	B3P	B	602	19/19	0.75	0.17	33,42,63,69	0
3	B3P	E	602	19/19	0.77	0.15	30,38,44,47	0
3	B3P	C	602	19/19	0.79	0.15	34,42,49,50	0
5	MRD	A	605	8/8	0.79	0.19	32,37,44,48	0
4	MPD	B	603	8/8	0.80	0.17	25,29,34,35	0
4	MPD	A	604	8/8	0.81	0.17	24,30,36,41	0
3	B3P	A	603	19/19	0.85	0.13	24,30,36,37	0
3	B3P	F	602	19/19	0.85	0.12	23,29,32,35	0
4	MPD	E	603	8/8	0.87	0.15	20,27,35,45	0
3	B3P	D	604	19/19	0.88	0.15	20,33,70,73	0
4	MPD	F	603	8/8	0.91	0.13	23,27,38,44	0
3	B3P	A	602	19/19	0.91	0.09	17,23,25,26	0
6	CL	A	606	1/1	0.96	0.11	26,26,26,26	0
6	CL	C	603	1/1	0.97	0.07	27,27,27,27	0
6	CL	D	602	1/1	0.97	0.08	23,23,23,23	0
6	CL	E	604	1/1	0.97	0.09	24,24,24,24	0
2	FAD	G	601	53/53	0.98	0.05	11,13,17,18	0
2	FAD	A	601	53/53	0.98	0.04	7,9,12,13	0

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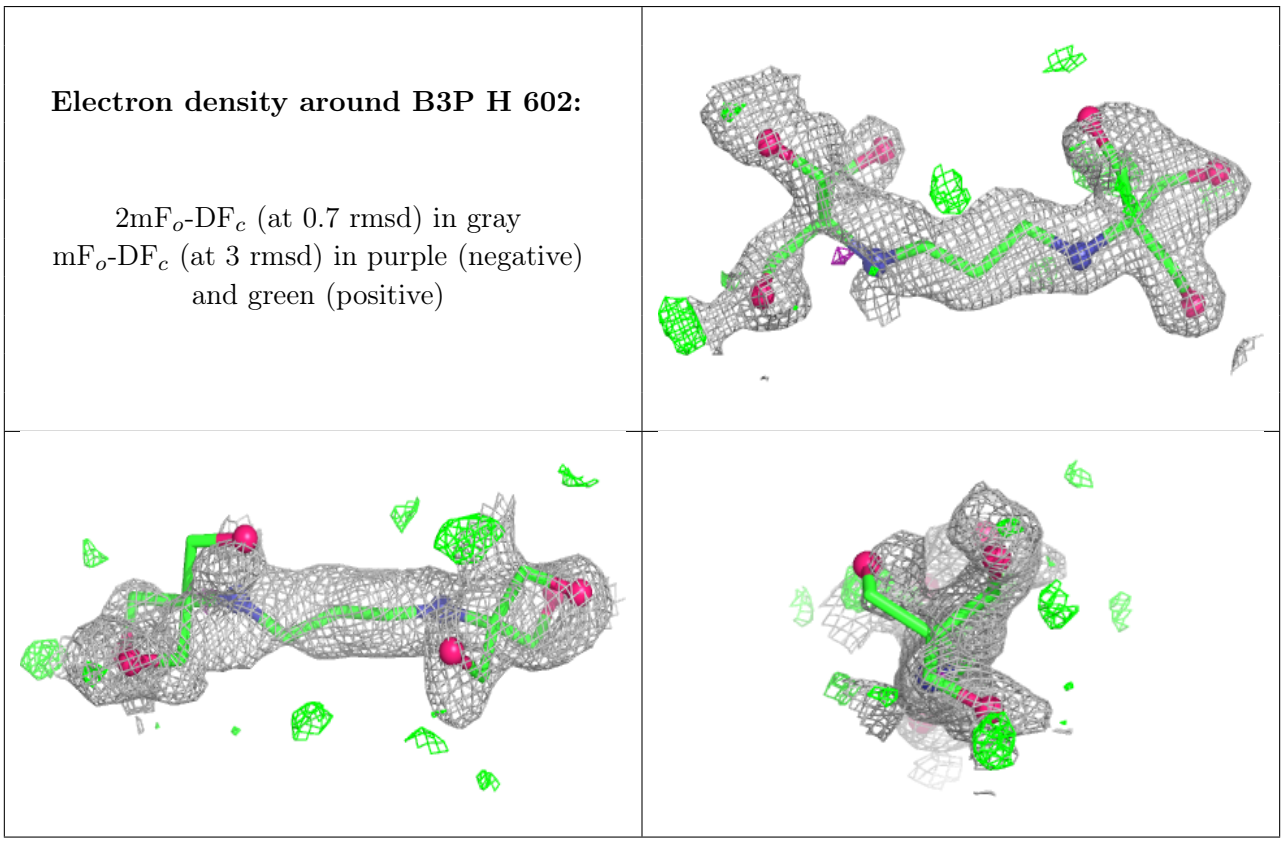
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CL	D	603	1/1	0.98	0.10	18,18,18,18	0
2	FAD	B	601	53/53	0.98	0.04	9,11,13,15	0
6	CL	H	603	1/1	0.98	0.05	24,24,24,24	0
6	CL	B	604	1/1	0.99	0.06	19,19,19,19	0
2	FAD	H	601	53/53	0.99	0.04	10,11,14,15	0
2	FAD	D	601	53/53	0.99	0.04	9,10,13,14	0
2	FAD	E	601	53/53	0.99	0.04	7,10,11,13	0
2	FAD	F	601	53/53	0.99	0.04	8,10,12,14	0
6	CL	F	604	1/1	0.99	0.04	19,19,19,19	0
6	CL	G	602	1/1	0.99	0.05	22,22,22,22	0
2	FAD	C	601	53/53	0.99	0.04	10,11,14,15	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.

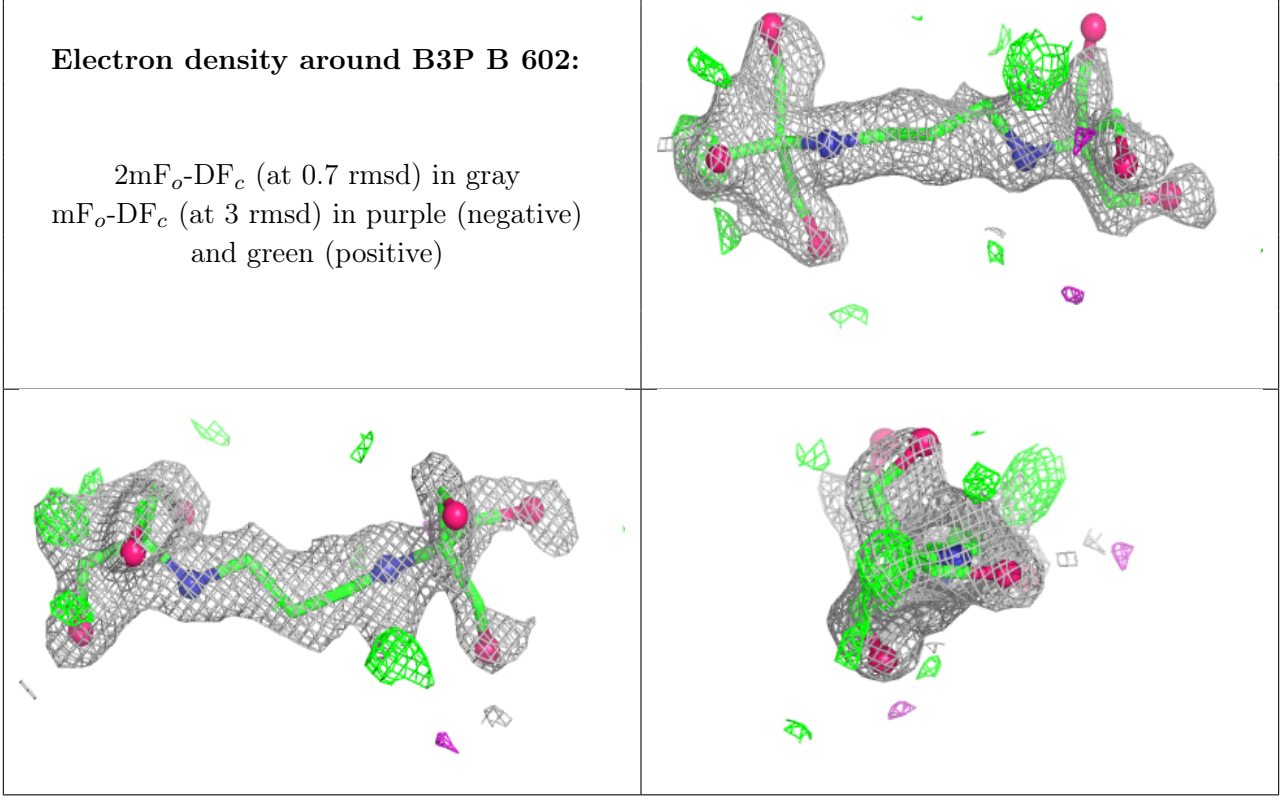
Electron density around B3P H 602:

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



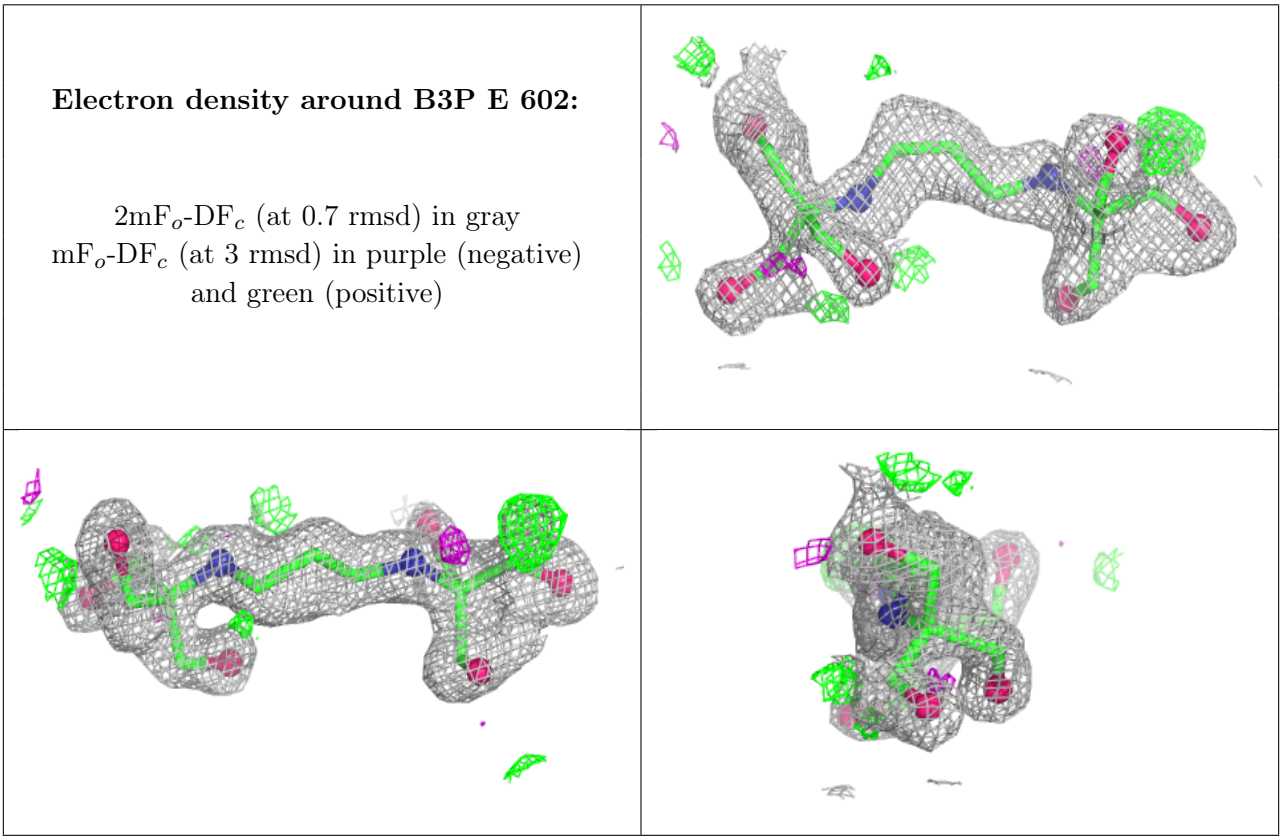
Electron density around B3P B 602:

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



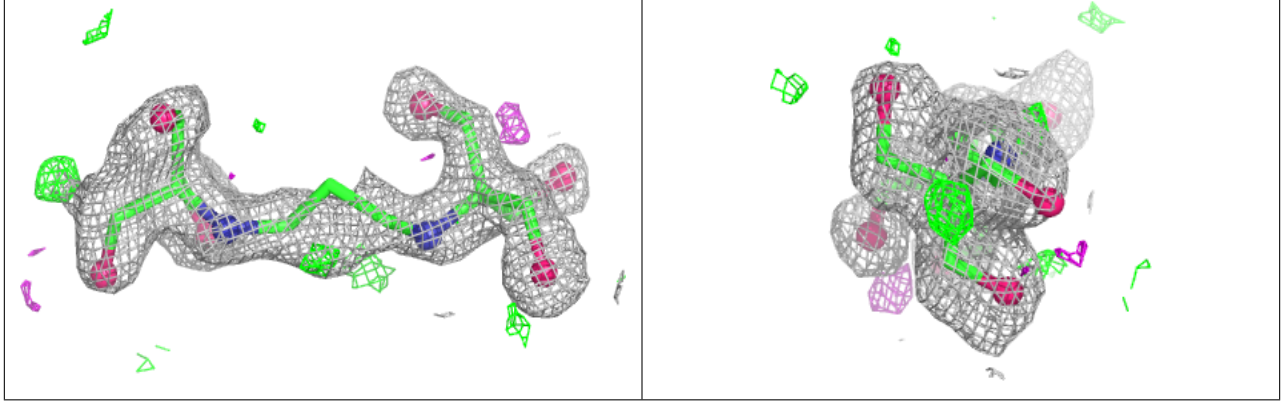
Electron density around B3P E 602:

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



Electron density around B3P C 602:

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



Electron density around B3P A 603:

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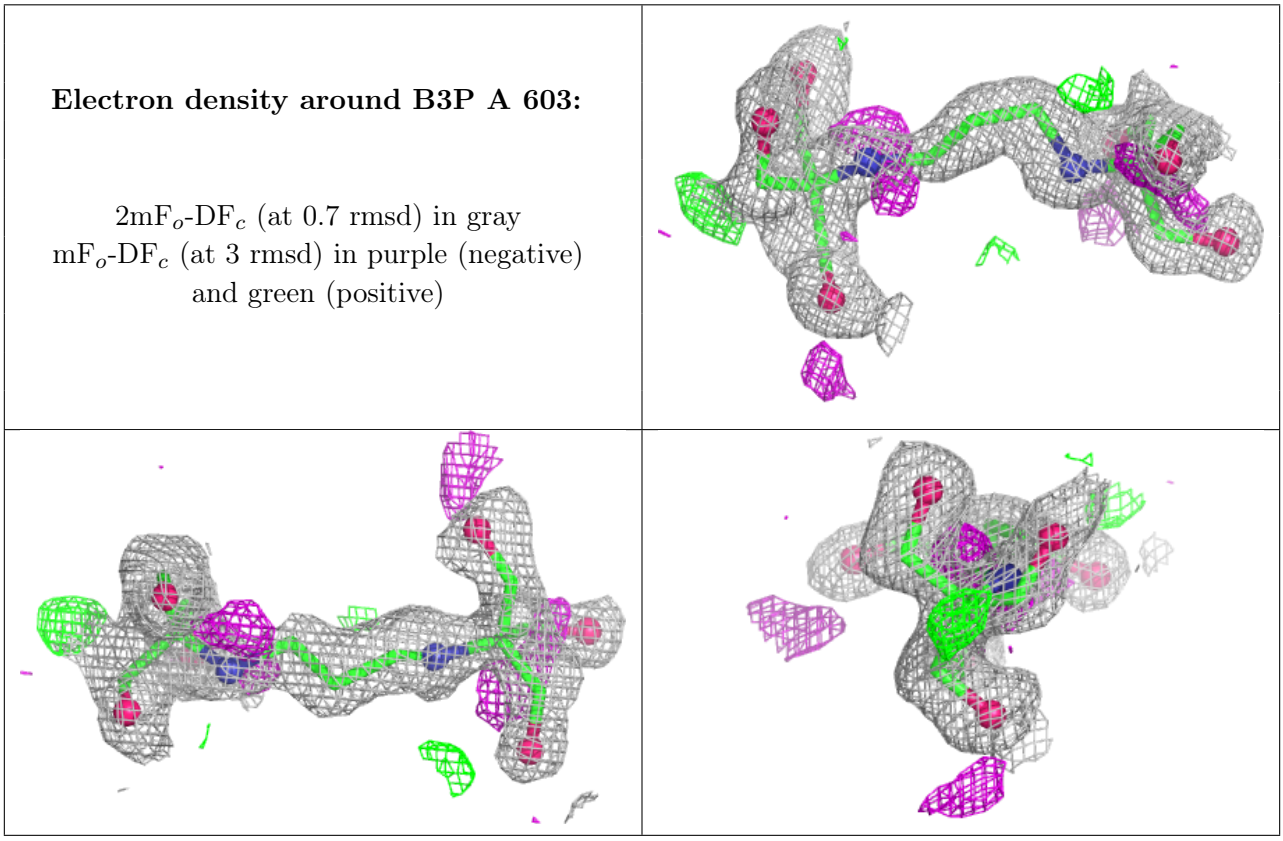
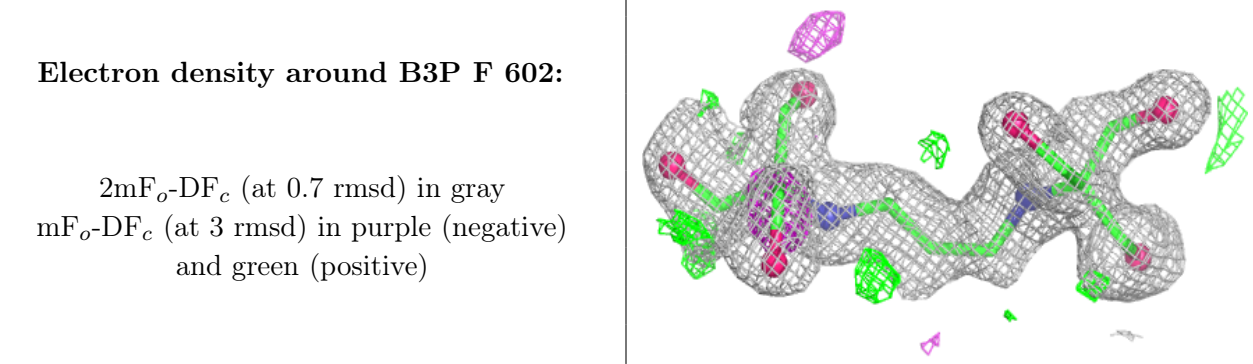
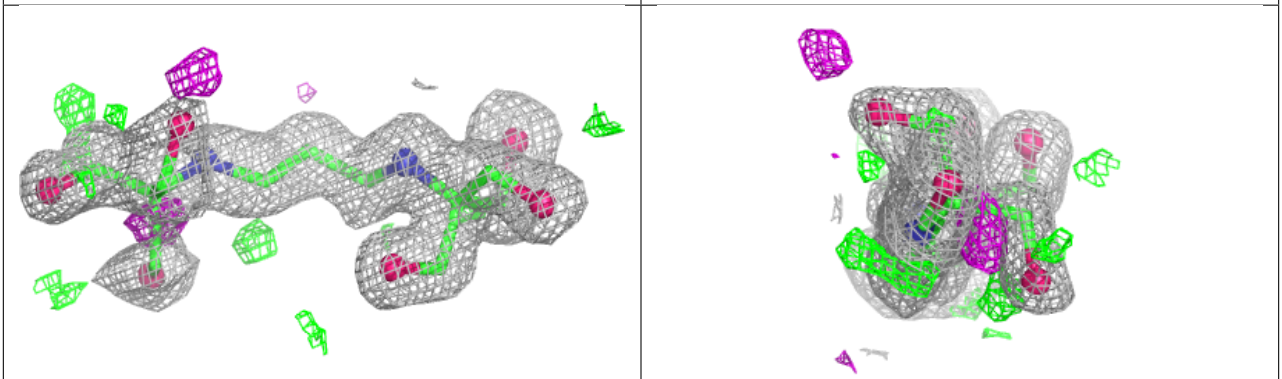
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around B3P F 602:

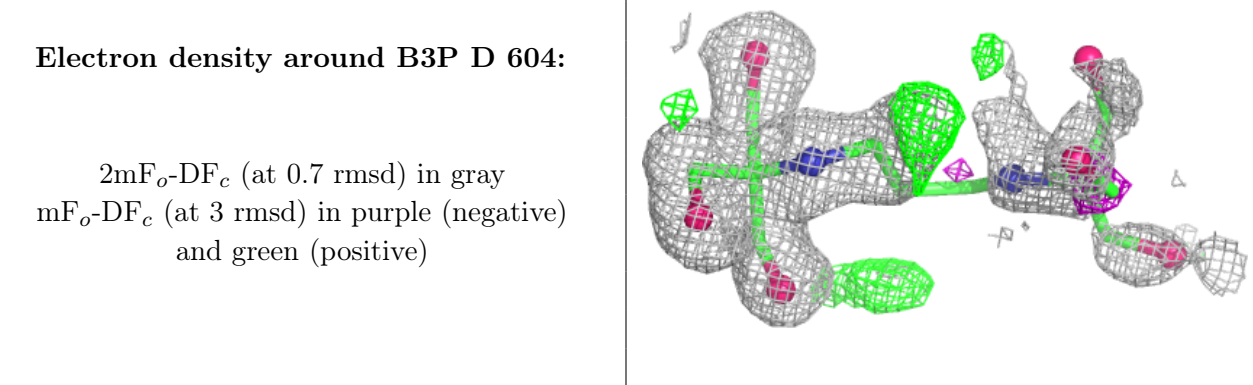
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

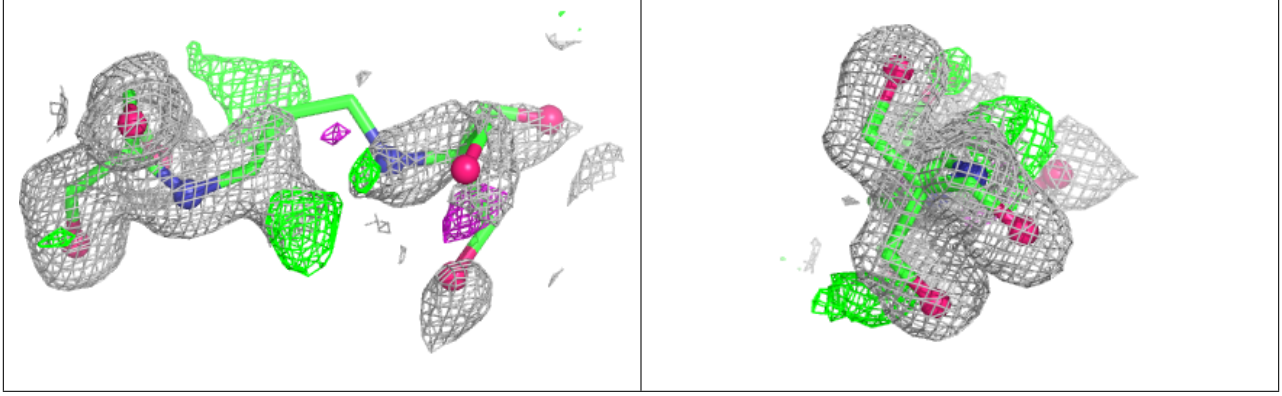




Electron density around B3P D 604:

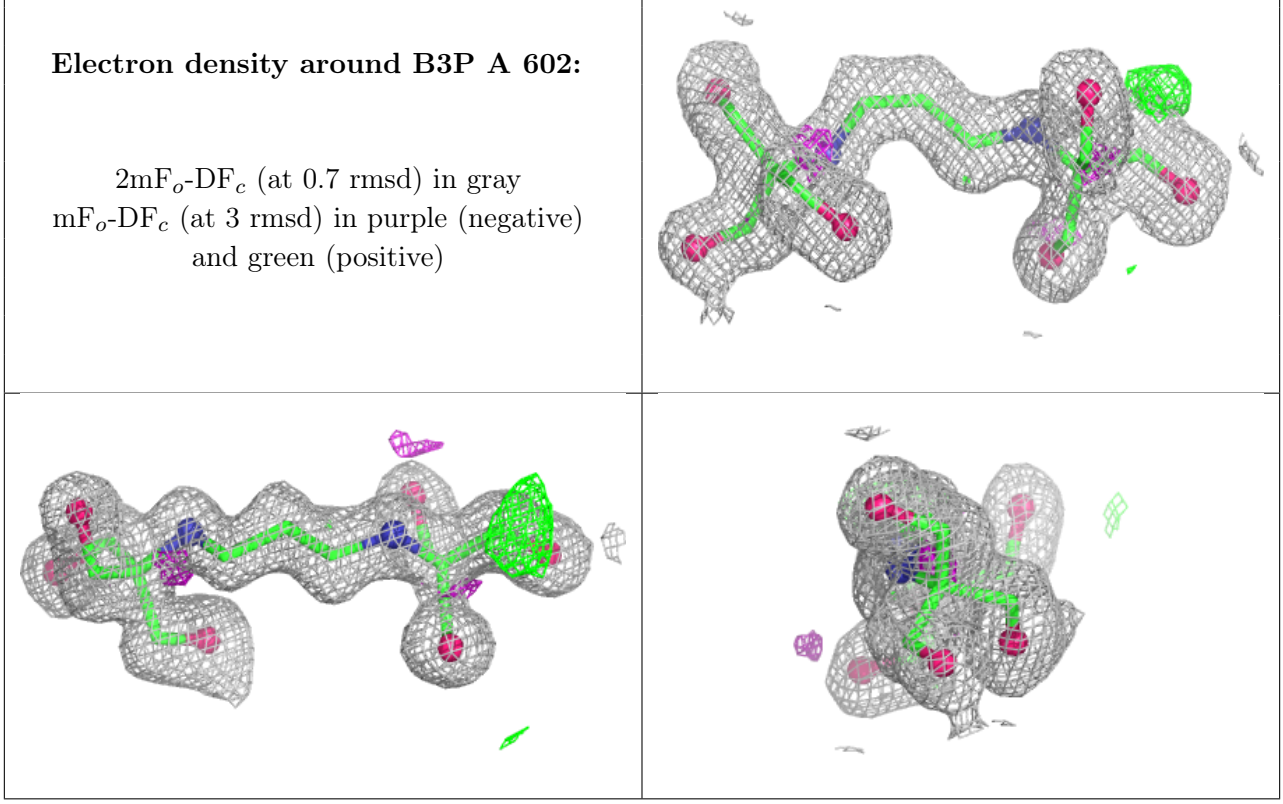
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





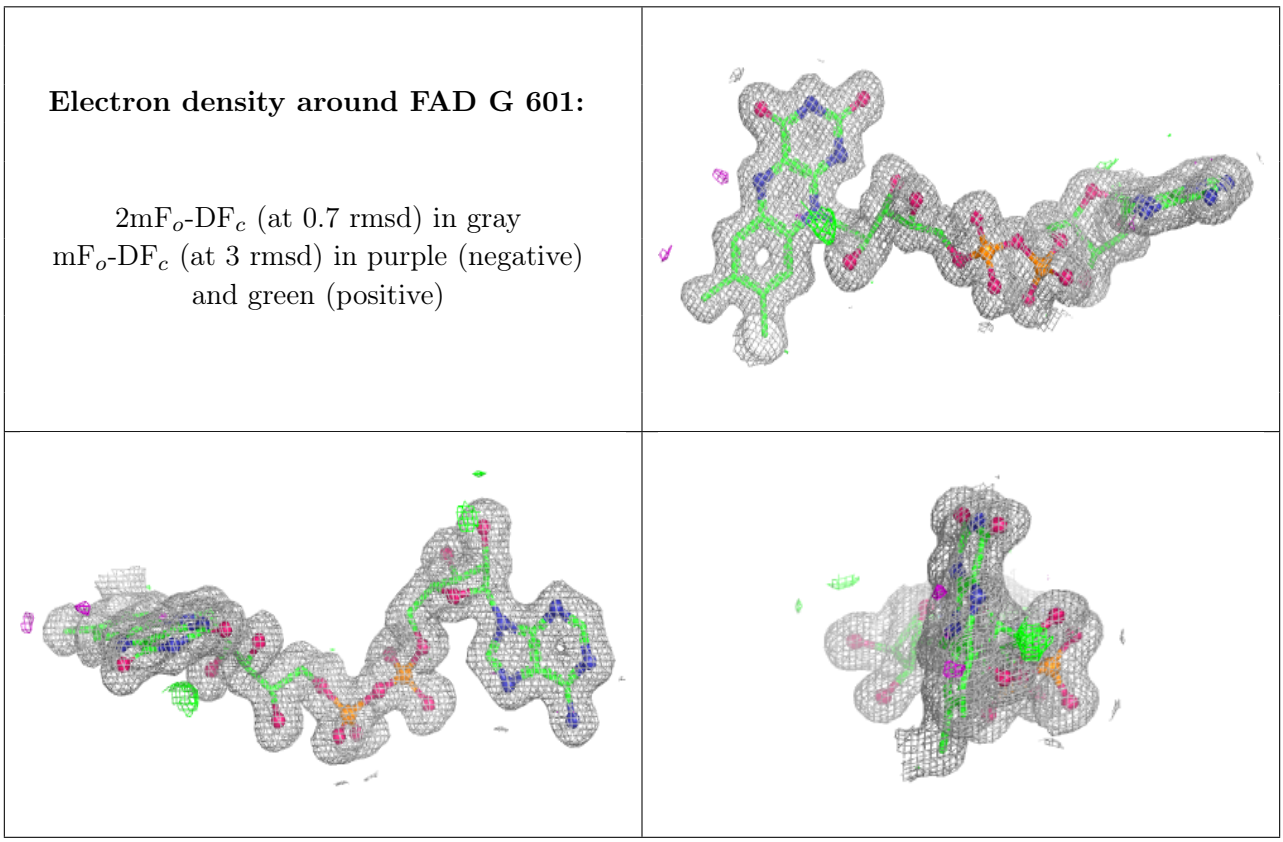
Electron density around B3P A 602:

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



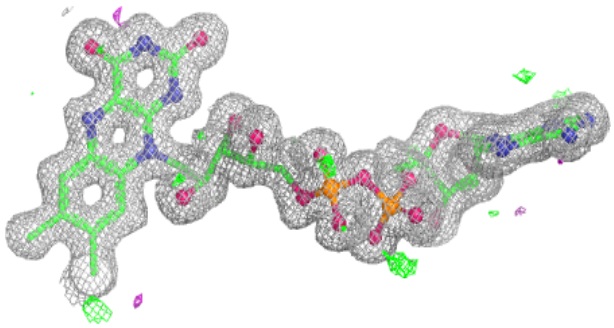
Electron density around FAD G 601:

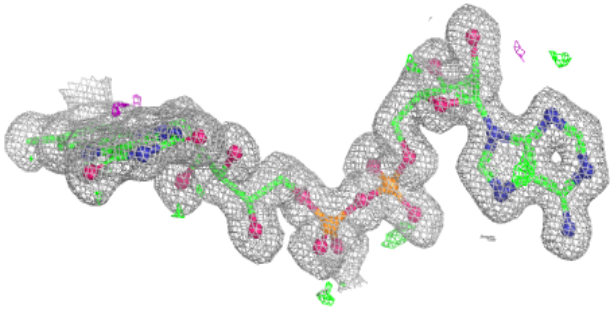
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

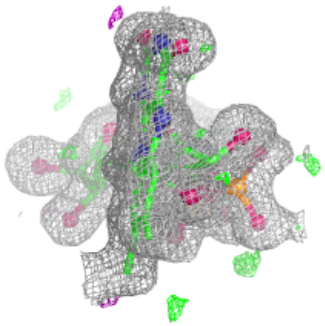


Electron density around FAD A 601:

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

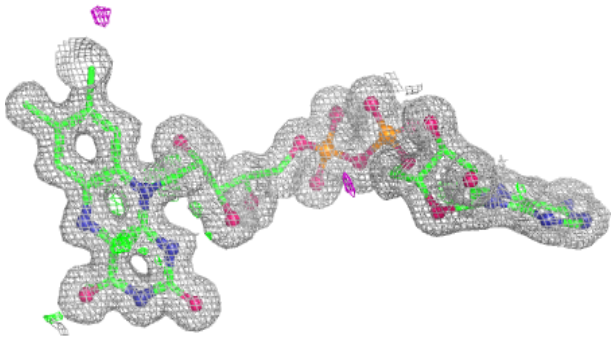


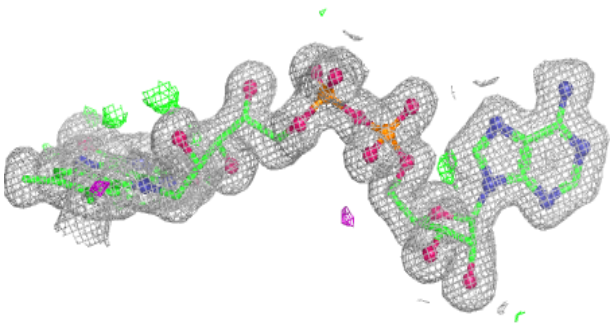


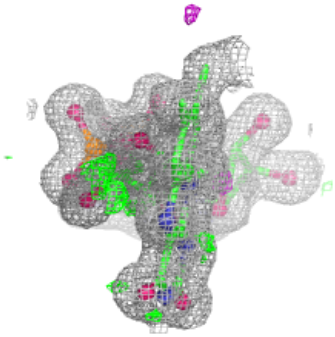


Electron density around FAD B 601:

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

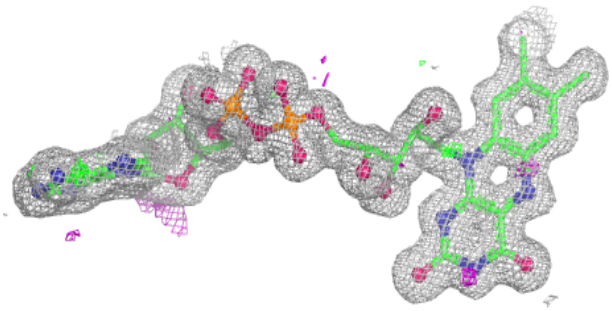


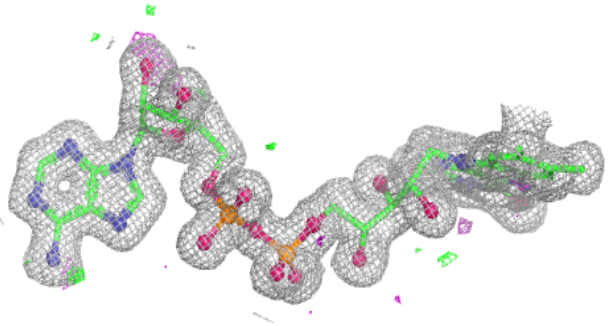


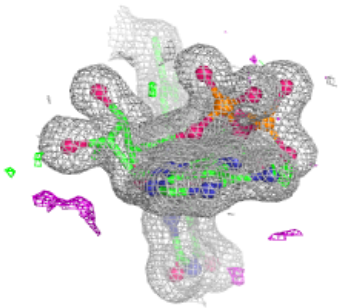


Electron density around FAD H 601:

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

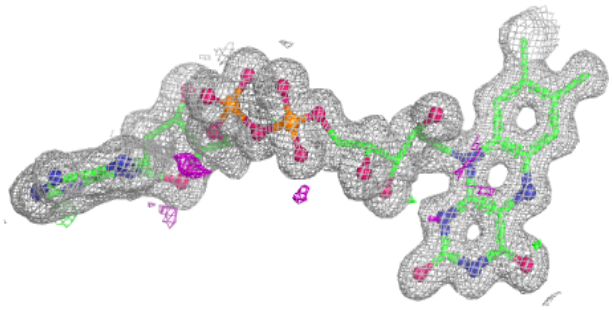


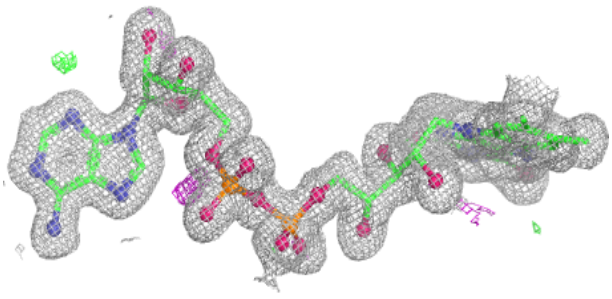


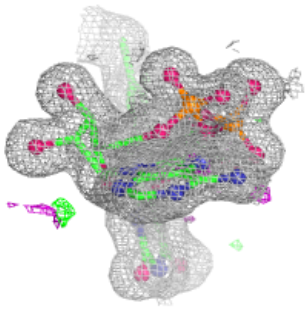


Electron density around FAD D 601:

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

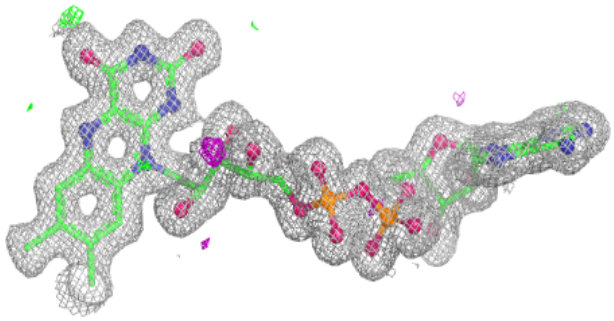


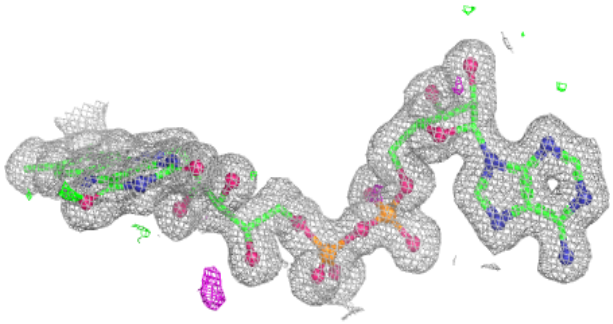


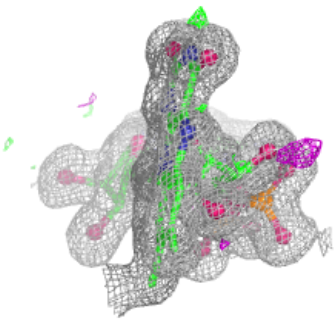


Electron density around FAD E 601:

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

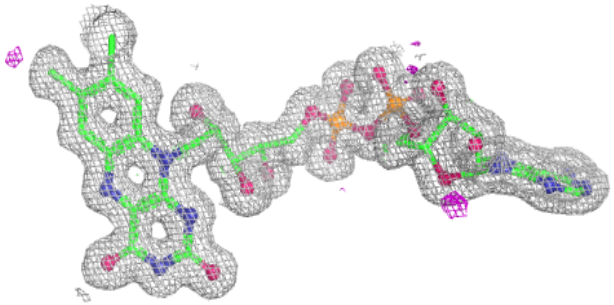


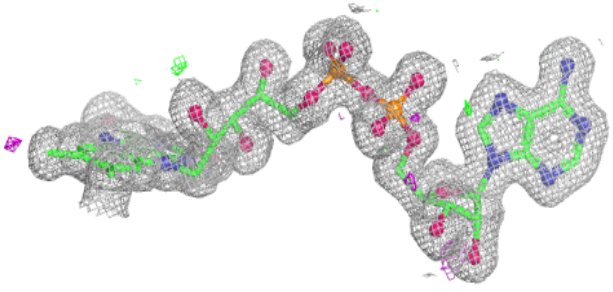


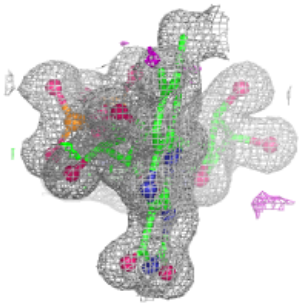


Electron density around FAD F 601:

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

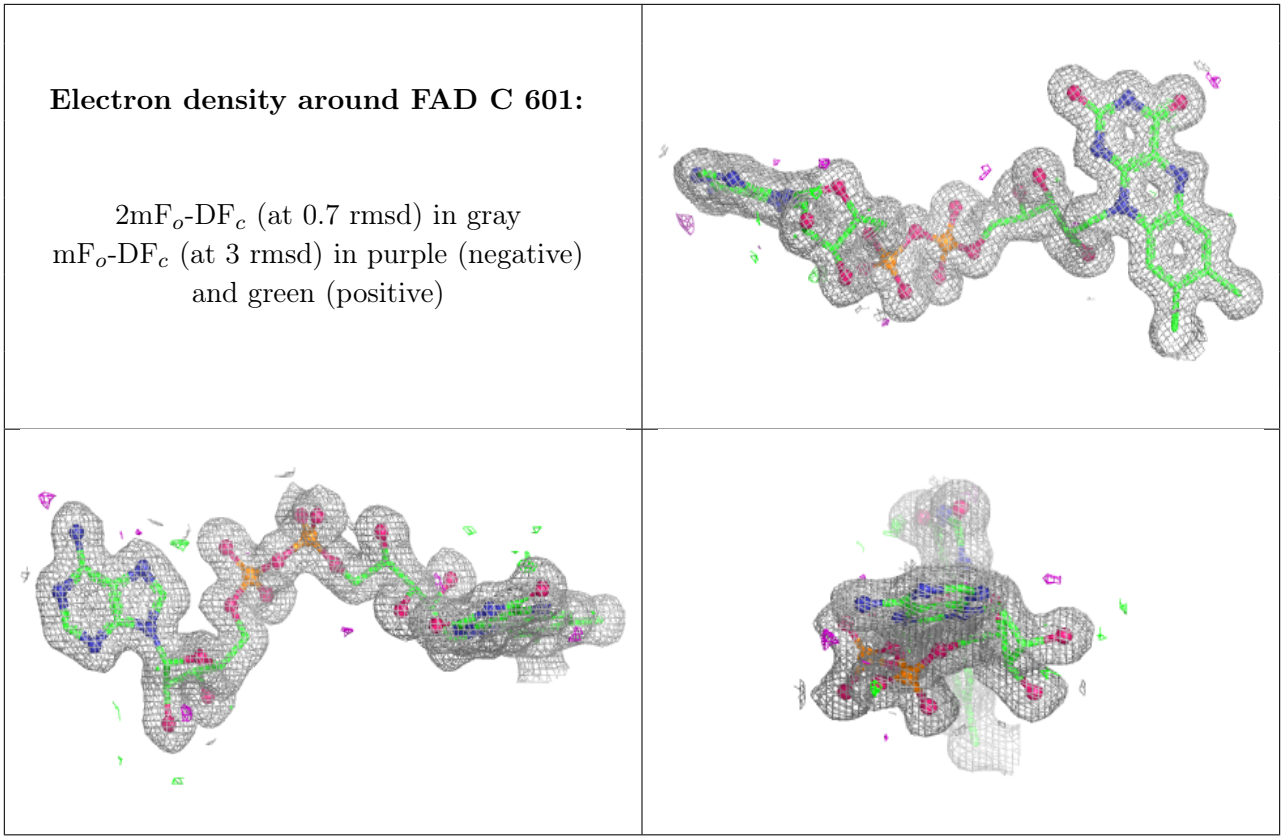






Electron density around FAD C 601:

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



6.5 Other polymers

There are no such residues in this entry.