Full wwPDB X-ray Structure Validation Report ⓘ

Feb 20, 2024 – 06:34 AM EST

PDB ID	:	4MOK
Title	:	Pyranose 2-oxidase H167A mutant soaked with 3-fluorinated galactose (not bound)
Authors	:	Tan, T.C.; Spadiut, O.; Gandini, R.; Haltrich, D.; Divne, C.
Deposited on	:	2013-09-12
Resolution	:	1.90 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:

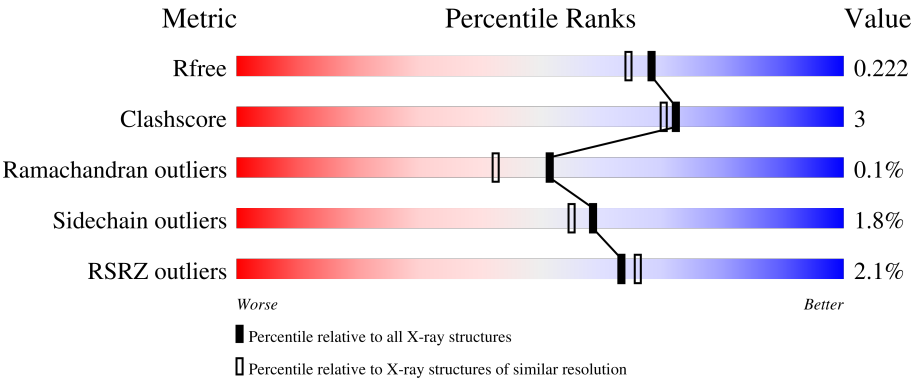
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	633	83% 8% • 9%
1	B	633	82% 8% • 9%
1	C	633	82% 8% 9%
1	D	633	81% 9% 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20179 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Pyranose 2-oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	0	0
			4537	2865	775	872	25			
1	B	575	Total	C	N	O	S	0	0	0
			4529	2860	774	871	24			
1	C	574	Total	C	N	O	S	0	0	0
			4521	2856	773	868	24			
1	D	572	Total	C	N	O	S	0	0	0
			4502	2841	771	866	24			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	SEE REMARK 999	UNP Q7ZA32
A	167	ALA	HIS	engineered mutation	UNP Q7ZA32
A	623	ALA	-	expression tag	UNP Q7ZA32
A	624	ALA	-	expression tag	UNP Q7ZA32
A	625	ALA	-	expression tag	UNP Q7ZA32
A	626	LEU	-	expression tag	UNP Q7ZA32
A	627	GLU	-	expression tag	UNP Q7ZA32
A	628	HIS	-	expression tag	UNP Q7ZA32
A	629	HIS	-	expression tag	UNP Q7ZA32
A	630	HIS	-	expression tag	UNP Q7ZA32
A	631	HIS	-	expression tag	UNP Q7ZA32
A	632	HIS	-	expression tag	UNP Q7ZA32
A	633	HIS	-	expression tag	UNP Q7ZA32
B	2	ALA	SER	SEE REMARK 999	UNP Q7ZA32
B	167	ALA	HIS	engineered mutation	UNP Q7ZA32
B	623	ALA	-	expression tag	UNP Q7ZA32
B	624	ALA	-	expression tag	UNP Q7ZA32
B	625	ALA	-	expression tag	UNP Q7ZA32
B	626	LEU	-	expression tag	UNP Q7ZA32
B	627	GLU	-	expression tag	UNP Q7ZA32
B	628	HIS	-	expression tag	UNP Q7ZA32

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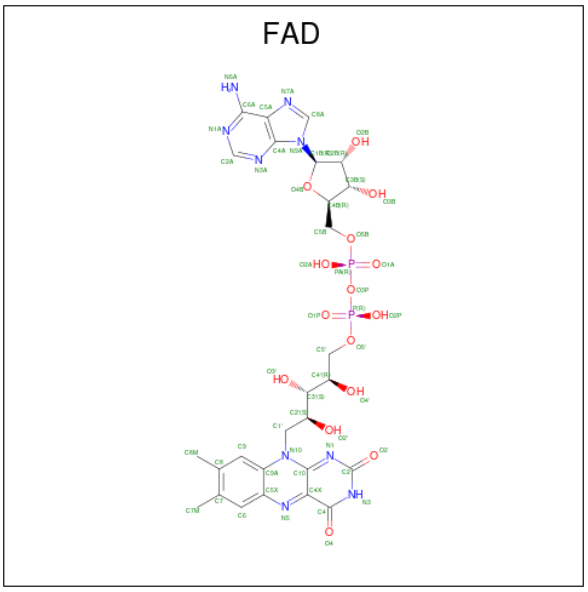
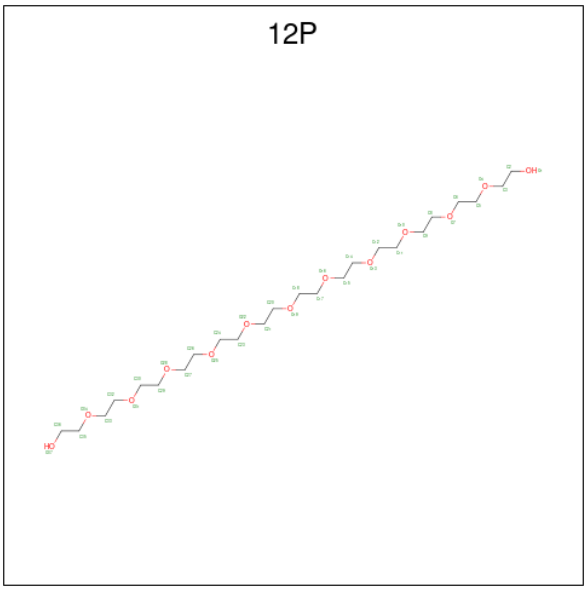
Chain	Residue	Modelled	Actual	Comment	Reference
B	629	HIS	-	expression tag	UNP Q7ZA32
B	630	HIS	-	expression tag	UNP Q7ZA32
B	631	HIS	-	expression tag	UNP Q7ZA32
B	632	HIS	-	expression tag	UNP Q7ZA32
B	633	HIS	-	expression tag	UNP Q7ZA32
C	2	ALA	SER	SEE REMARK 999	UNP Q7ZA32
C	167	ALA	HIS	engineered mutation	UNP Q7ZA32
C	623	ALA	-	expression tag	UNP Q7ZA32
C	624	ALA	-	expression tag	UNP Q7ZA32
C	625	ALA	-	expression tag	UNP Q7ZA32
C	626	LEU	-	expression tag	UNP Q7ZA32
C	627	GLU	-	expression tag	UNP Q7ZA32
C	628	HIS	-	expression tag	UNP Q7ZA32
C	629	HIS	-	expression tag	UNP Q7ZA32
C	630	HIS	-	expression tag	UNP Q7ZA32
C	631	HIS	-	expression tag	UNP Q7ZA32
C	632	HIS	-	expression tag	UNP Q7ZA32
C	633	HIS	-	expression tag	UNP Q7ZA32
D	2	ALA	SER	SEE REMARK 999	UNP Q7ZA32
D	167	ALA	HIS	engineered mutation	UNP Q7ZA32
D	623	ALA	-	expression tag	UNP Q7ZA32
D	624	ALA	-	expression tag	UNP Q7ZA32
D	625	ALA	-	expression tag	UNP Q7ZA32
D	626	LEU	-	expression tag	UNP Q7ZA32
D	627	GLU	-	expression tag	UNP Q7ZA32
D	628	HIS	-	expression tag	UNP Q7ZA32
D	629	HIS	-	expression tag	UNP Q7ZA32
D	630	HIS	-	expression tag	UNP Q7ZA32
D	631	HIS	-	expression tag	UNP Q7ZA32
D	632	HIS	-	expression tag	UNP Q7ZA32
D	633	HIS	-	expression tag	UNP Q7ZA32

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



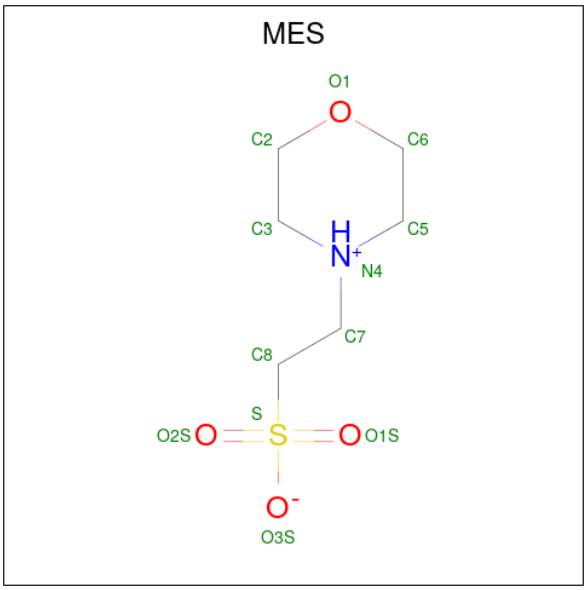
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is DODECAETHYLENE GLYCOL (three-letter code: 12P) (formula: $C_{24}H_{50}O_{13}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 16 10 6	0	0
3	B	1	Total C O 16 10 6	0	0
3	C	1	Total C O 16 10 6	0	0
3	D	1	Total C O 13 8 5	0	0

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 12 6 1 4 1	0	0
4	C	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	536	Total O 536 536	0	0
5	B	498	Total O 498 498	0	0
5	C	449	Total O 449 449	0	0

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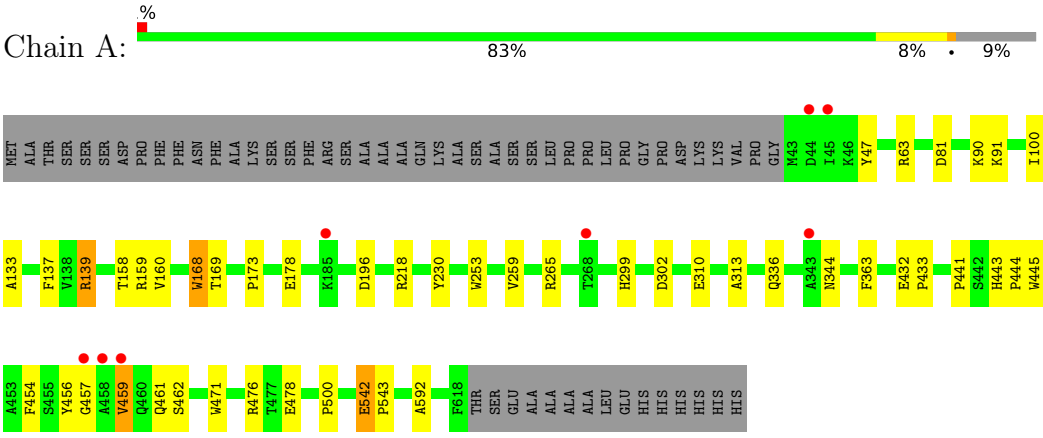
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	310	Total	O	0	0
			310	310		

3 Residue-property plots (i)

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

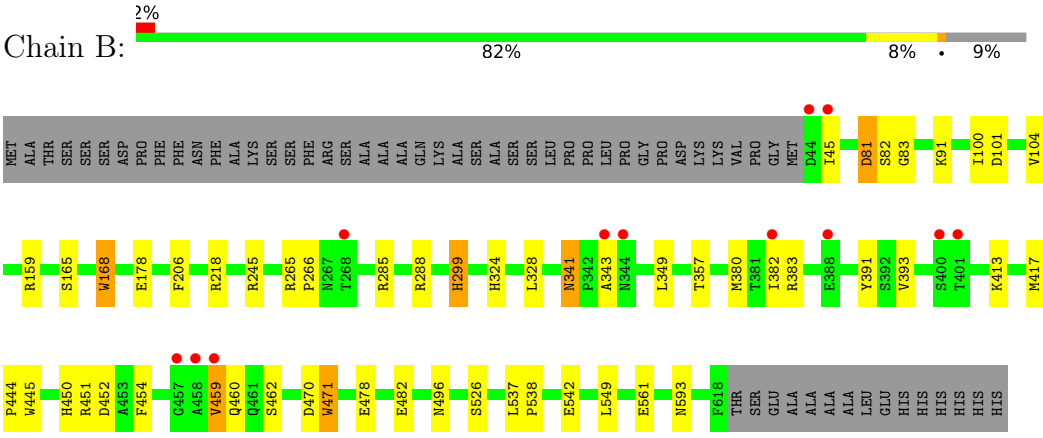
• Molecule 1: Pyranose 2-oxidase

Chain A:



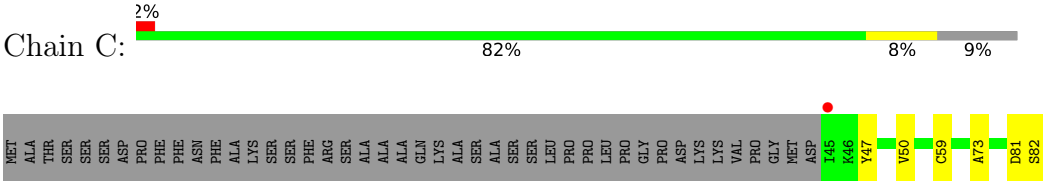
• Molecule 1: Pyranose 2-oxidase

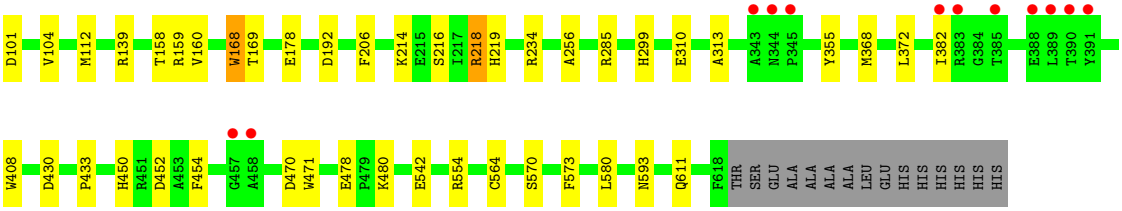
Chain B:



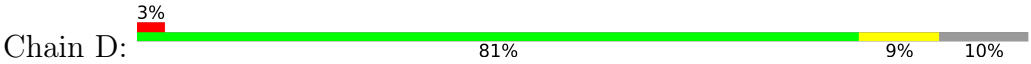
• Molecule 1: Pyranose 2-oxidase

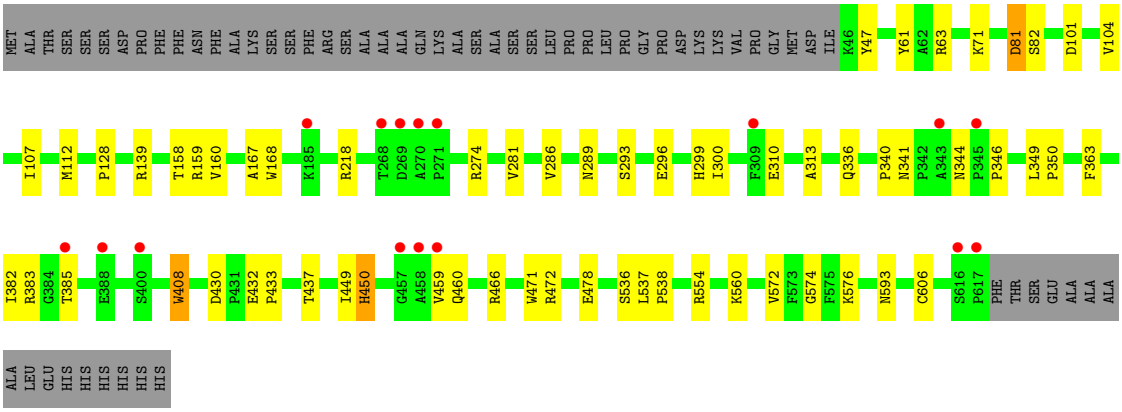
Chain C:





• Molecule 1: Pyranose 2-oxidase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	99.88Å 102.30Å 136.96Å 90.00° 90.78° 90.00°	Depositor
Resolution (Å)	47.92 – 1.90 45.65 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.92-1.90) 99.8 (45.65-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.170 , 0.214 0.177 , 0.222	Depositor DCC
R_{free} test set	1066 reflections (0.49%)	wwPDB-VP
Wilson B-factor (Å^2)	24.3	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -k,-h,-l 0.008 for k,h,-l 0.018 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	20179	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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: MES, 12P, 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	1.06	7/4652 (0.2%)	0.97	7/6325 (0.1%)
1	B	1.02	5/4644 (0.1%)	0.95	8/6315 (0.1%)
1	C	0.95	4/4636 (0.1%)	0.93	9/6304 (0.1%)
1	D	0.85	3/4616 (0.1%)	0.86	7/6277 (0.1%)
All	All	0.97	19/18548 (0.1%)	0.93	31/25221 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	478	GLU	CD-OE1	7.62	1.34	1.25
1	A	253	TRP	CD2-CE2	7.27	1.50	1.41
1	A	478	GLU	CD-OE1	7.00	1.33	1.25
1	B	471	TRP	CD2-CE2	6.35	1.49	1.41
1	C	168	TRP	CD2-CE2	6.34	1.49	1.41
1	C	478	GLU	CD-OE1	5.96	1.32	1.25
1	B	542	GLU	CD-OE1	5.80	1.32	1.25
1	A	542	GLU	CD-OE2	5.75	1.31	1.25
1	A	443	HIS	CG-CD2	5.75	1.45	1.35
1	B	482	GLU	CD-OE1	5.70	1.31	1.25
1	B	299	HIS	CG-CD2	5.69	1.45	1.35
1	D	408	TRP	CD2-CE2	5.62	1.48	1.41
1	D	536	SER	CB-OG	-5.56	1.35	1.42
1	C	542	GLU	CD-OE1	5.51	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	542	GLU	CD-OE1	5.40	1.31	1.25
1	D	478	GLU	CD-OE1	5.29	1.31	1.25
1	A	456	TYR	CE1-CZ	-5.26	1.31	1.38
1	C	471	TRP	CD2-CE2	5.26	1.47	1.41
1	A	168	TRP	CD2-CE2	5.19	1.47	1.41

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	139	ARG	NE-CZ-NH2	-11.52	114.54	120.30
1	A	139	ARG	NE-CZ-NH1	8.75	124.68	120.30
1	D	139	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	D	466	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	B	139	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	B	451	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	A	302	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	C	139	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	B	245	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	B	139	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	D	383	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	C	554	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	C	452	ASP	CB-CG-OD2	6.19	123.87	118.30
1	C	192	ASP	CB-CG-OD1	6.18	123.87	118.30
1	D	81	ASP	CB-CG-OD1	-6.18	112.74	118.30
1	A	302	ASP	CB-CG-OD1	6.04	123.74	118.30
1	B	288	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	C	470	ASP	CB-CG-OD1	5.79	123.51	118.30
1	C	368	MET	CG-SD-CE	5.74	109.39	100.20
1	B	349	LEU	CB-CG-CD2	5.73	120.74	111.00
1	C	218	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	D	383	ARG	CG-CD-NE	5.51	123.38	111.80
1	B	470	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	C	234	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	476	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	D	81	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	265	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	D	63	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	196	ASP	CB-CG-OD1	5.09	122.89	118.30
1	C	159	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	81	ASP	CB-CG-OD1	-5.04	113.76	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	230	TYR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4537	0	4386	31	0
1	B	4529	0	4377	35	0
1	C	4521	0	4373	24	0
1	D	4502	0	4353	32	0
2	A	53	0	31	1	0
2	B	53	0	30	1	0
2	C	53	0	30	0	0
2	D	53	0	29	1	0
3	A	16	0	21	0	0
3	B	16	0	21	0	0
3	C	16	0	21	0	0
3	D	13	0	16	0	0
4	A	12	0	13	4	0
4	C	12	0	13	0	0
5	A	536	0	0	2	0
5	B	498	0	0	9	0
5	C	449	0	0	3	0
5	D	310	0	0	3	0
All	All	20179	0	17714	122	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 3.

All (122) 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:A:133:ALA:HB3	4:A:803:MES:H71	1.35	1.03
1:B:380:MET:HE1	1:B:413:LYS:HB2	1.49	0.94
1:A:133:ALA:CB	4:A:803:MES:H71	2.03	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ALA:HB2	4:A:803:MES:O1S	1.74	0.88
1:B:417:MET:SD	5:B:1356:HOH:O	2.38	0.81
1:B:393:VAL:HG23	5:B:1356:HOH:O	1.83	0.78
1:D:101:ASP:O	1:D:104:VAL:HG12	1.83	0.78
1:B:101:ASP:O	1:B:104:VAL:HG12	1.87	0.74
1:D:382:ILE:HD13	5:D:1057:HOH:O	1.92	0.70
1:B:285:ARG:HD2	5:B:1379:HOH:O	1.91	0.70
1:A:457:GLY:HA3	5:A:1235:HOH:O	1.93	0.68
1:C:101:ASP:HB2	5:C:1225:HOH:O	1.95	0.67
1:A:104:VAL:HG23	1:A:454:PHE:O	1.97	0.65
1:A:81:ASP:OD2	1:A:90:LYS:NZ	2.27	0.65
1:A:101:ASP:O	1:A:104:VAL:HG12	1.97	0.64
1:D:299:HIS:CD2	1:D:310:GLU:HG3	2.32	0.64
1:C:50:VAL:HG13	1:C:313:ALA:HB2	1.80	0.64
1:B:380:MET:HE1	1:B:413:LYS:CB	2.26	0.63
1:D:81:ASP:OD1	1:D:81:ASP:C	2.32	0.63
1:C:382:ILE:HD13	5:C:1265:HOH:O	2.01	0.61
1:D:299:HIS:NE2	1:D:310:GLU:HG3	2.15	0.61
1:B:91:LYS:HD2	1:B:100:ILE:HD11	1.82	0.60
1:D:450:HIS:CE1	1:D:472:ARG:HH11	2.22	0.58
1:B:178:GLU:HG3	5:B:1163:HOH:O	2.02	0.58
1:C:299:HIS:NE2	1:C:310:GLU:HG2	2.18	0.58
1:C:158:THR:HG22	1:C:160:VAL:HG22	1.87	0.56
1:A:459:VAL:HG22	1:A:461:GLN:NE2	2.21	0.56
1:C:101:ASP:O	1:C:104:VAL:HG12	2.04	0.56
1:B:299:HIS:HB3	5:B:1374:HOH:O	2.05	0.56
1:B:383:ARG:O	1:B:391:TYR:HA	2.06	0.56
1:B:81:ASP:OD1	1:B:81:ASP:N	2.36	0.55
1:A:299:HIS:NE2	1:A:310:GLU:HG3	2.22	0.54
1:D:432:GLU:HB2	1:D:433:PRO:HD2	1.90	0.54
1:A:432:GLU:HB2	1:A:433:PRO:HD2	1.90	0.54
1:A:178:GLU:OE1	1:A:441:PRO:HG3	2.08	0.53
1:C:81:ASP:N	1:C:81:ASP:OD1	2.38	0.53
1:C:564:CYS:HG	1:C:573:PHE:HE2	1.55	0.53
1:B:81:ASP:O	1:B:83:GLY:N	2.37	0.52
1:A:63:ARG:HD2	1:A:259:VAL:O	2.08	0.52
1:B:432:GLU:HB2	1:B:433:PRO:HD2	1.91	0.52
1:C:299:HIS:NE2	1:C:310:GLU:CG	2.72	0.52
1:A:81:ASP:CG	1:A:90:LYS:NZ	2.64	0.51
1:A:299:HIS:CD2	1:A:310:GLU:HG3	2.45	0.51
1:D:218:ARG:HD2	5:D:923:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ARG:HD2	5:A:1120:HOH:O	2.11	0.51
1:D:81:ASP:O	1:D:81:ASP:CG	2.47	0.50
1:B:328:LEU:HD23	1:B:328:LEU:C	2.33	0.49
1:A:169:THR:HG21	1:A:454:PHE:CZ	2.47	0.49
1:C:104:VAL:HG23	1:C:454:PHE:O	2.11	0.49
1:D:158:THR:HG22	1:D:160:VAL:HG22	1.95	0.49
1:A:158:THR:HG22	1:A:160:VAL:HG22	1.95	0.49
1:D:81:ASP:OD1	1:D:81:ASP:N	2.43	0.48
1:A:133:ALA:CB	4:A:803:MES:O1S	2.52	0.48
1:B:299:HIS:CG	5:B:1374:HOH:O	2.66	0.48
1:B:328:LEU:HD23	1:B:328:LEU:O	2.14	0.48
1:D:289:ASN:HB3	1:D:296:GLU:OE2	2.14	0.48
1:D:450:HIS:HD2	5:D:1151:HOH:O	1.96	0.48
1:A:459:VAL:O	1:A:459:VAL:CG1	2.62	0.48
1:D:293:SER:O	1:D:576:LYS:NZ	2.43	0.48
1:B:91:LYS:NZ	1:B:452:ASP:OD1	2.47	0.48
1:B:471:TRP:CH2	1:B:526:SER:HA	2.50	0.47
1:A:173:PRO:HG2	1:A:592:ALA:HB1	1.95	0.47
1:C:158:THR:CG2	1:C:160:VAL:HG22	2.43	0.47
1:D:349:LEU:HD11	1:D:572:VAL:HG13	1.96	0.47
1:C:81:ASP:OD2	1:C:90:LYS:NZ	2.31	0.47
1:A:91:LYS:HD2	1:A:100:ILE:HD11	1.96	0.47
1:B:459:VAL:CG1	1:B:460:GLN:N	2.78	0.47
1:C:218:ARG:HG3	1:C:430:ASP:OD2	2.15	0.47
1:D:437:THR:O	1:D:437:THR:HG23	2.15	0.47
1:A:47:TYR:O	1:A:313:ALA:HA	2.15	0.46
1:D:107:ILE:HG12	1:D:167:ALA:HB1	1.97	0.46
1:D:281:VAL:HG11	1:D:300:ILE:HD12	1.96	0.46
1:B:341:ASN:HD21	1:B:343:ALA:HB3	1.80	0.46
1:C:178:GLU:HB2	5:C:1086:HOH:O	2.14	0.46
1:C:216:SER:HB3	1:C:219:HIS:HB3	1.98	0.45
1:D:293:SER:HA	1:D:574:GLY:O	2.16	0.45
1:A:459:VAL:O	1:A:459:VAL:HG13	2.16	0.45
1:B:393:VAL:N	5:B:1356:HOH:O	2.50	0.45
1:A:91:LYS:NZ	1:A:452:ASP:OD1	2.49	0.45
1:B:459:VAL:CG1	1:B:460:GLN:H	2.29	0.45
1:B:380:MET:CE	1:B:413:LYS:HB2	2.34	0.45
1:B:159:ARG:HA	2:B:801:FAD:O2B	2.17	0.44
1:A:137:PHE:CE2	1:A:139:ARG:HG3	2.52	0.44
1:A:363:PHE:HA	1:A:471:TRP:O	2.18	0.44
1:B:380:MET:HE3	1:B:393:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:THR:HG21	1:C:454:PHE:CE2	2.52	0.44
1:D:159:ARG:HA	2:D:801:FAD:O2B	2.18	0.43
1:C:59:CYS:SG	1:C:256:ALA:HB1	2.58	0.43
1:B:382:ILE:O	1:B:382:ILE:HG22	2.18	0.43
1:B:444:PRO:HD2	1:B:445:TRP:CZ3	2.54	0.43
1:C:169:THR:HG21	1:C:454:PHE:CZ	2.53	0.43
1:B:104:VAL:HG23	1:B:454:PHE:O	2.18	0.43
1:B:537:LEU:HB3	1:B:538:PRO:HD2	2.00	0.43
1:B:265:ARG:HA	1:B:266:PRO:C	2.40	0.42
1:D:47:TYR:O	1:D:313:ALA:HA	2.19	0.42
1:A:542:GLU:HA	1:A:543:PRO:HD3	1.87	0.42
1:C:355:TYR:HA	1:C:480:LYS:O	2.19	0.42
1:D:81:ASP:OD1	1:D:81:ASP:O	2.37	0.42
1:D:346:PRO:HG2	1:D:350:PRO:HA	2.00	0.42
1:C:81:ASP:O	1:C:83:GLY:N	2.49	0.42
1:D:71:LYS:HB2	1:D:274:ARG:CZ	2.50	0.42
1:D:363:PHE:HA	1:D:471:TRP:O	2.18	0.42
1:A:336:GLN:NE2	1:A:344:ASN:O	2.53	0.42
1:B:324:HIS:HD2	5:B:1025:HOH:O	2.03	0.42
1:C:47:TYR:CD2	1:C:73:ALA:HB2	2.55	0.42
1:A:444:PRO:HD2	1:A:445:TRP:CZ3	2.55	0.42
1:D:341:ASN:ND2	1:D:344:ASN:ND2	2.67	0.42
1:A:159:ARG:HA	2:A:801:FAD:O2B	2.19	0.42
1:D:449:ILE:HG12	1:D:471:TRP:CZ3	2.55	0.41
1:B:165:SER:HA	1:B:168:TRP:CD1	2.55	0.41
1:B:357:THR:O	1:B:549:LEU:HD12	2.21	0.41
1:B:380:MET:HE1	1:B:413:LYS:CA	2.51	0.41
1:A:459:VAL:HG22	1:A:461:GLN:HE22	1.86	0.41
1:D:218:ARG:HG3	1:D:430:ASP:OD2	2.20	0.41
1:D:459:VAL:HG12	1:D:460:GLN:H	1.85	0.41
1:D:61:TYR:HA	1:D:606:CYS:SG	2.61	0.40
1:D:336:GLN:OE1	1:D:340:PRO:HA	2.22	0.40
1:D:537:LEU:HB3	1:D:538:PRO:HD2	2.03	0.40
1:C:47:TYR:O	1:C:313:ALA:HA	2.21	0.40
1:B:218:ARG:HD2	5:B:1124:HOH:O	2.21	0.40
1:C:372:LEU:HD23	1:C:372:LEU:HA	1.98	0.40
1:C:570:SER:HB3	1:C:580:LEU:O	2.22	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	574/633 (91%)	562 (98%)	12 (2%)	0	100	100
1	B	573/633 (90%)	553 (96%)	18 (3%)	2 (0%)	41	31
1	C	572/633 (90%)	550 (96%)	21 (4%)	1 (0%)	47	38
1	D	570/633 (90%)	549 (96%)	21 (4%)	0	100	100
All	All	2289/2532 (90%)	2214 (97%)	72 (3%)	3 (0%)	51	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	82	SER
1	C	82	SER
1	B	459	VAL

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	503/547 (92%)	498 (99%)	5 (1%)	76	76
1	B	502/547 (92%)	492 (98%)	10 (2%)	55	51
1	C	501/547 (92%)	491 (98%)	10 (2%)	55	51
1	D	499/547 (91%)	488 (98%)	11 (2%)	52	47
All	All	2005/2188 (92%)	1969 (98%)	36 (2%)	59	55

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	TRP
1	A	450	HIS
1	A	459	VAL
1	A	462	SER
1	A	500	PRO
1	B	45	ILE
1	B	112	MET
1	B	168	TRP
1	B	206	PHE
1	B	341	ASN
1	B	450	HIS
1	B	462	SER
1	B	496	ASN
1	B	561	GLU
1	B	593	ASN
1	C	112	MET
1	C	168	TRP
1	C	206	PHE
1	C	214	LYS
1	C	285	ARG
1	C	408	TRP
1	C	433	PRO
1	C	450	HIS
1	C	593	ASN
1	C	611	GLN
1	D	82	SER
1	D	112	MET
1	D	128	PRO
1	D	168	TRP
1	D	286	VAL
1	D	385	THR
1	D	408	TRP
1	D	450	HIS
1	D	554	ARG
1	D	560	LYS
1	D	593	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	B	341	ASN
1	C	224	ASN

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Mol	Chain	Res	Type
1	C	344	ASN
1	D	344	ASN
1	D	450	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

10 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	12P	A	802	-	15,15,36	0.64	0	14,14,35	0.38	0
2	FAD	D	801	-	53,58,58	1.28	7 (13%)	68,89,89	1.90	21 (30%)
3	12P	C	802	-	15,15,36	0.56	0	14,14,35	0.51	0
4	MES	A	803	-	12,12,12	1.89	1 (8%)	14,16,16	2.10	5 (35%)
4	MES	C	803	-	12,12,12	2.02	1 (8%)	14,16,16	1.79	4 (28%)
3	12P	D	802	-	12,12,36	0.52	0	11,11,35	0.48	0
2	FAD	B	801	-	53,58,58	1.30	8 (15%)	68,89,89	1.86	16 (23%)
2	FAD	C	801	-	53,58,58	1.48	9 (16%)	68,89,89	1.83	18 (26%)
3	12P	B	802	-	15,15,36	0.64	0	14,14,35	0.91	1 (7%)
2	FAD	A	801	-	53,58,58	1.35	8 (15%)	68,89,89	1.94	13 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	12P	A	802	-	-	1/13/13/34	-
2	FAD	D	801	-	-	3/30/50/50	0/6/6/6
3	12P	C	802	-	-	3/13/13/34	-
4	MES	A	803	-	-	0/6/14/14	0/1/1/1
4	MES	C	803	-	-	0/6/14/14	0/1/1/1
3	12P	D	802	-	-	1/10/10/34	-
2	FAD	B	801	-	-	5/30/50/50	0/6/6/6
2	FAD	C	801	-	-	1/30/50/50	0/6/6/6
3	12P	B	802	-	-	3/13/13/34	-
2	FAD	A	801	-	-	1/30/50/50	0/6/6/6

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	803	MES	C8-S	-6.31	1.68	1.77
4	A	803	MES	C8-S	-5.39	1.69	1.77
2	A	801	FAD	C6-C5X	4.90	1.47	1.40
2	C	801	FAD	C2B-C1B	-4.16	1.47	1.53
2	D	801	FAD	C5'-C4'	3.25	1.56	1.51
2	B	801	FAD	O4B-C4B	-3.11	1.38	1.45
2	D	801	FAD	O4B-C4B	-2.86	1.38	1.45
2	C	801	FAD	C4'-C3'	2.82	1.58	1.53
2	D	801	FAD	C2A-N1A	2.82	1.39	1.33
2	A	801	FAD	C2-N3	-2.69	1.32	1.39
2	C	801	FAD	C2A-N1A	2.68	1.38	1.33
2	C	801	FAD	C10-N1	2.66	1.38	1.33
2	C	801	FAD	C5X-N5	-2.57	1.34	1.39
2	C	801	FAD	C2A-N3A	2.53	1.36	1.32
2	B	801	FAD	O4B-C1B	2.50	1.44	1.41
2	B	801	FAD	C2B-C1B	-2.49	1.50	1.53
2	B	801	FAD	O3B-C3B	-2.48	1.37	1.43
2	B	801	FAD	C6-C7	2.45	1.43	1.39
2	D	801	FAD	C2A-N3A	2.43	1.36	1.32
2	D	801	FAD	C10-N1	2.41	1.38	1.33
2	A	801	FAD	C2B-C1B	-2.39	1.50	1.53
2	B	801	FAD	C2A-N3A	2.38	1.35	1.32
2	A	801	FAD	O4B-C1B	-2.35	1.37	1.41
2	C	801	FAD	C2'-C3'	-2.33	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	FAD	C9-C8	2.28	1.42	1.39
2	A	801	FAD	O3B-C3B	-2.25	1.37	1.43
2	B	801	FAD	C10-N1	2.23	1.37	1.33
2	D	801	FAD	C6-C5X	2.16	1.43	1.40
2	B	801	FAD	C6-C5X	2.14	1.43	1.40
2	D	801	FAD	O3B-C3B	-2.13	1.38	1.43
2	A	801	FAD	C2A-N1A	2.10	1.37	1.33
2	C	801	FAD	C1'-C2'	2.09	1.55	1.52
2	A	801	FAD	C4X-N5	2.04	1.34	1.30
2	A	801	FAD	O4B-C4B	-2.03	1.40	1.45

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	FAD	O4-C4-N3	5.81	131.25	120.12
2	B	801	FAD	N3A-C2A-N1A	-5.43	120.19	128.68
2	A	801	FAD	C4-N3-C2	5.42	135.66	125.64
2	B	801	FAD	O4-C4-N3	5.30	130.28	120.12
2	C	801	FAD	O3B-C3B-C4B	5.23	126.18	111.05
4	A	803	MES	O2S-S-C8	4.99	112.92	106.92
2	D	801	FAD	N3A-C2A-N1A	-4.92	120.98	128.68
2	A	801	FAD	N3A-C2A-N1A	-4.88	121.05	128.68
2	C	801	FAD	N3A-C2A-N1A	-4.73	121.29	128.68
2	B	801	FAD	C9A-C5X-N5	-4.16	117.91	122.43
2	B	801	FAD	C4-N3-C2	4.04	133.12	125.64
2	D	801	FAD	N3-C2-N1	-4.01	111.52	119.38
2	A	801	FAD	O2B-C2B-C3B	4.00	124.77	111.82
2	A	801	FAD	N3-C2-N1	-4.00	111.54	119.38
2	D	801	FAD	O3B-C3B-C4B	3.94	122.43	111.05
2	C	801	FAD	O4-C4-N3	3.84	127.47	120.12
4	A	803	MES	O1S-S-C8	3.69	111.36	106.92
2	C	801	FAD	O2B-C2B-C1B	3.49	123.74	110.85
2	A	801	FAD	O4B-C4B-C3B	3.49	112.02	105.11
2	D	801	FAD	O2B-C2B-C3B	3.44	122.97	111.82
2	C	801	FAD	O2B-C2B-C3B	3.39	122.80	111.82
2	A	801	FAD	C3B-C2B-C1B	3.37	106.05	100.98
2	D	801	FAD	O2B-C2B-C1B	3.34	123.20	110.85
2	A	801	FAD	C10-N1-C2	3.34	123.59	116.90
4	C	803	MES	O2S-S-C8	3.31	110.90	106.92
2	C	801	FAD	O4-C4-C4X	-3.29	117.87	126.60
2	D	801	FAD	O4B-C4B-C5B	3.28	120.17	109.37
2	B	801	FAD	C5B-C4B-C3B	3.27	127.43	115.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	FAD	O2B-C2B-C3B	3.25	122.35	111.82
2	C	801	FAD	C5B-C4B-C3B	3.25	127.35	115.18
4	C	803	MES	O3S-S-C8	3.22	110.97	105.77
2	D	801	FAD	C10-C4X-N5	-3.20	118.06	124.86
2	D	801	FAD	O4-C4-N3	3.18	126.22	120.12
2	D	801	FAD	C2A-N1A-C6A	3.07	124.01	118.75
2	A	801	FAD	C5A-C6A-N6A	3.05	124.99	120.35
2	D	801	FAD	C9A-C5X-N5	-2.95	119.22	122.43
2	D	801	FAD	O4B-C1B-C2B	2.93	111.20	106.93
2	D	801	FAD	O2A-PA-O1A	2.90	126.58	112.24
2	B	801	FAD	C3B-C2B-C1B	2.88	105.31	100.98
2	B	801	FAD	N3-C2-N1	-2.84	113.80	119.38
2	B	801	FAD	O4B-C4B-C5B	2.83	118.68	109.37
2	B	801	FAD	O2B-C2B-C1B	2.80	121.19	110.85
2	B	801	FAD	C10-C4X-N5	-2.76	118.99	124.86
4	C	803	MES	C6-C5-N4	2.74	114.27	110.10
2	D	801	FAD	C5B-C4B-C3B	2.74	125.43	115.18
2	B	801	FAD	O4-C4-C4X	-2.68	119.50	126.60
2	D	801	FAD	C5A-C6A-N6A	2.67	124.41	120.35
2	C	801	FAD	O2-C2-N1	-2.61	117.51	121.83
2	A	801	FAD	C2A-N1A-C6A	2.61	123.21	118.75
2	C	801	FAD	O2A-PA-O1A	2.60	125.09	112.24
2	C	801	FAD	O4B-C4B-C5B	2.60	117.92	109.37
2	C	801	FAD	C2A-N1A-C6A	2.60	123.20	118.75
2	D	801	FAD	C5A-C6A-N1A	-2.57	114.52	120.35
2	B	801	FAD	O2-C2-N3	2.50	123.51	118.65
2	C	801	FAD	C4X-C10-N1	-2.42	119.11	124.73
4	A	803	MES	O2S-S-O1S	-2.41	105.59	113.95
2	C	801	FAD	O4B-C1B-C2B	2.41	110.45	106.93
2	D	801	FAD	C4-N3-C2	2.36	130.01	125.64
2	A	801	FAD	O4-C4-C4X	-2.35	120.38	126.60
2	D	801	FAD	O4B-C4B-C3B	2.32	109.69	105.11
2	B	801	FAD	O3B-C3B-C4B	2.27	117.61	111.05
2	B	801	FAD	C10-N1-C2	2.27	121.44	116.90
2	C	801	FAD	O2'-C2'-C1'	-2.26	104.33	109.80
2	D	801	FAD	O2P-P-O1P	2.25	123.36	112.24
2	A	801	FAD	C4X-C4-N3	-2.24	107.50	113.19
2	C	801	FAD	C9A-C5X-N5	-2.24	120.00	122.43
2	B	801	FAD	C4X-C10-N10	2.18	119.67	116.48
2	C	801	FAD	C4-C4X-N5	2.18	121.33	118.23
3	B	802	12P	C12-O13-C14	2.17	122.69	113.29
2	D	801	FAD	C4X-C10-N1	-2.13	119.78	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	803	MES	O3S-S-O1S	-2.13	106.08	111.27
2	D	801	FAD	O2-C2-N1	-2.11	118.32	121.83
4	A	803	MES	O3S-S-C8	2.11	109.19	105.77
2	C	801	FAD	C5A-C6A-N1A	-2.11	115.57	120.35
2	D	801	FAD	O3'-C3'-C4'	2.11	113.90	108.81
4	C	803	MES	O2S-S-O1S	-2.09	106.70	113.95
2	A	801	FAD	C5B-C4B-C3B	2.01	122.72	115.18
2	C	801	FAD	N3-C2-N1	-2.01	115.45	119.38

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	FAD	PA-O3P-P-O5'
2	D	801	FAD	PA-O3P-P-O5'
3	B	802	12P	O13-C14-C15-O16
3	C	802	12P	O13-C14-C15-O16
2	B	801	FAD	P-O3P-PA-O1A
3	C	802	12P	O10-C11-C12-O13
3	B	802	12P	C15-C14-O13-C12
3	D	802	12P	O10-C11-C12-O13
2	B	801	FAD	C3B-C4B-C5B-O5B
3	B	802	12P	C11-C12-O13-C14
3	C	802	12P	O7-C8-C9-O10
2	B	801	FAD	O4B-C4B-C5B-O5B
2	A	801	FAD	O4B-C4B-C5B-O5B
2	B	801	FAD	P-O3P-PA-O2A
2	D	801	FAD	P-O3P-PA-O2A
2	C	801	FAD	O4B-C4B-C5B-O5B
2	D	801	FAD	O4B-C4B-C5B-O5B
3	A	802	12P	O1-C2-C3-O4

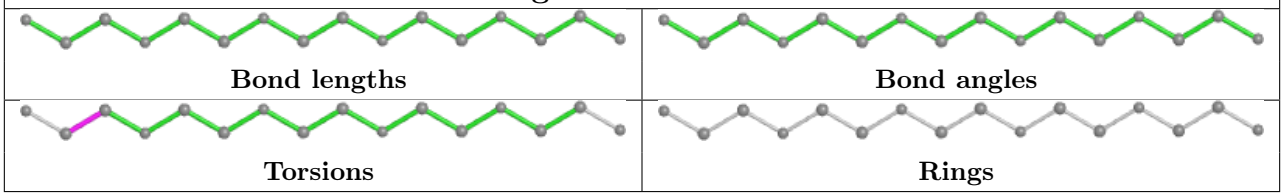
There are no ring outliers.

4 monomers are involved in 7 short contacts:

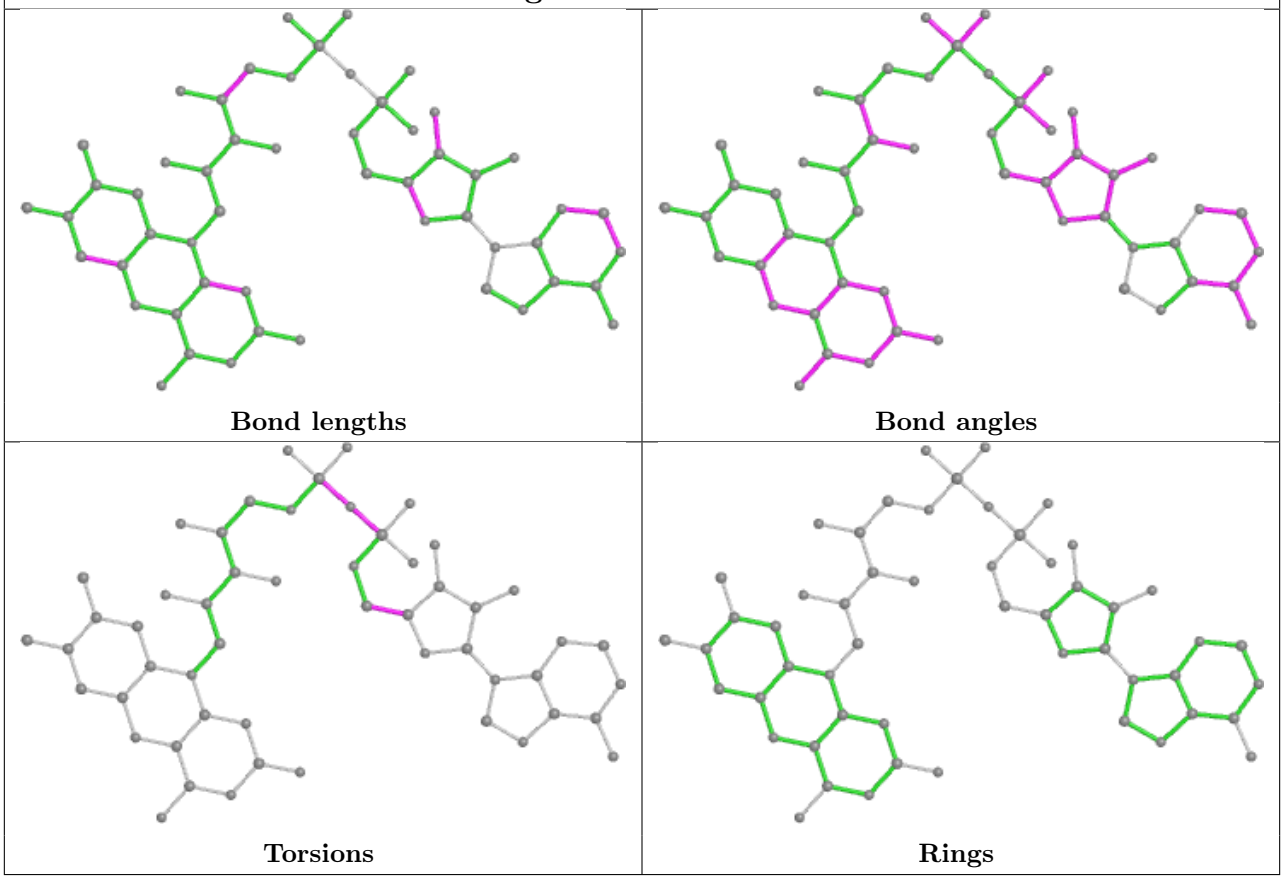
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	801	FAD	1	0
4	A	803	MES	4	0
2	B	801	FAD	1	0
2	A	801	FAD	1	0

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.

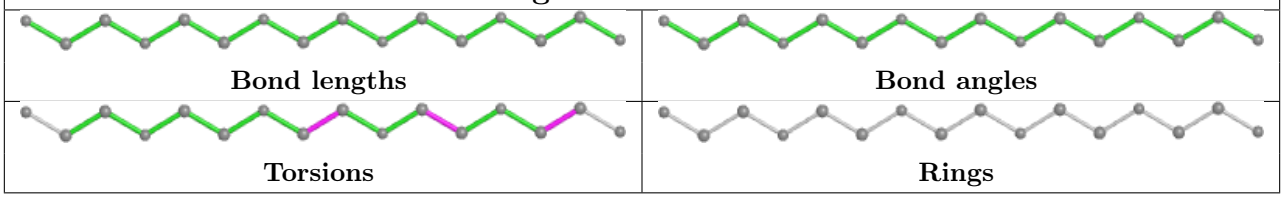
Ligand 12P A 802



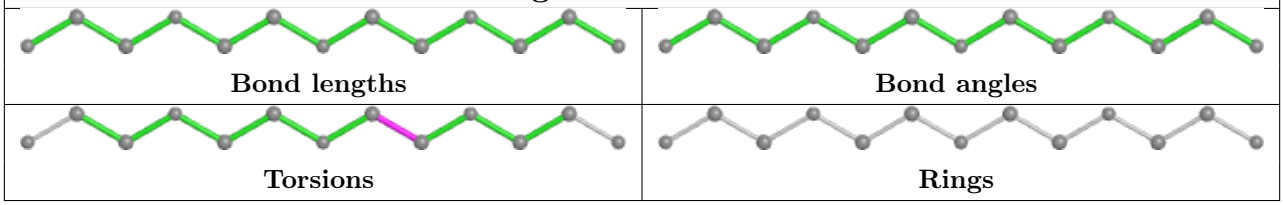
Ligand FAD D 801



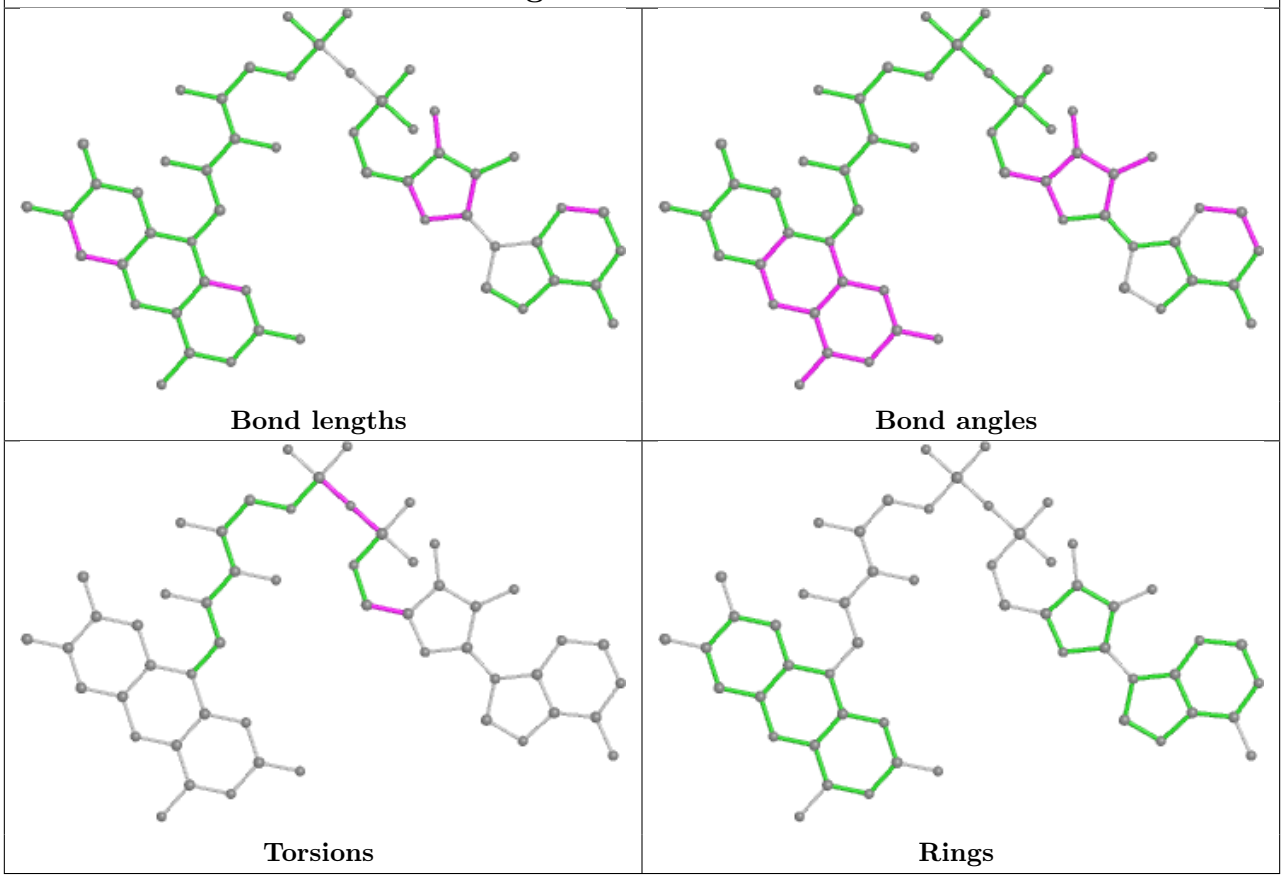
Ligand 12P C 802



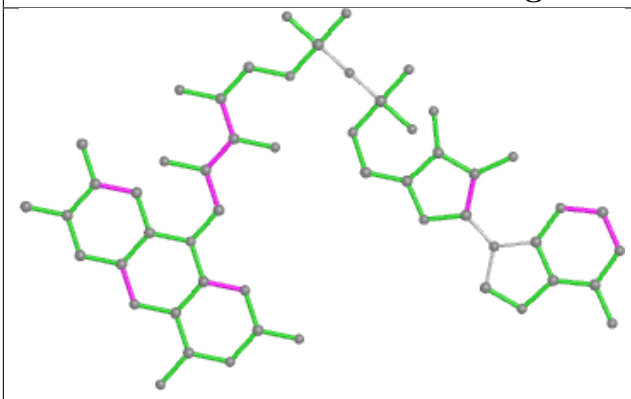
Ligand 12P D 802



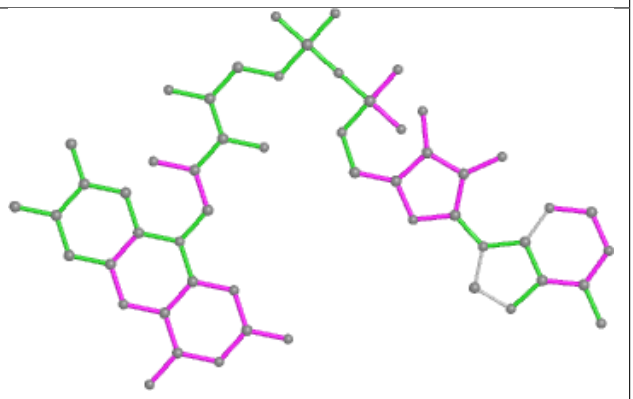
Ligand FAD B 801



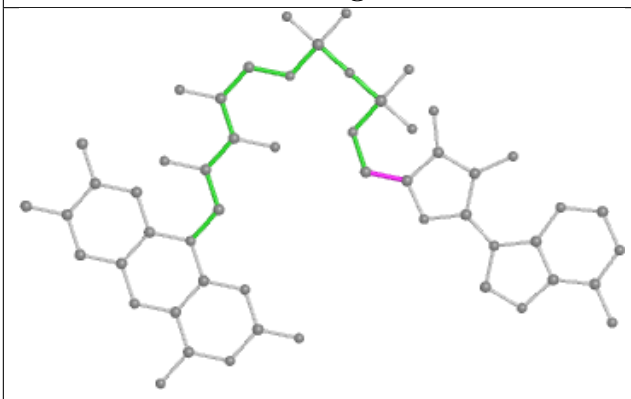
Ligand FAD C 801



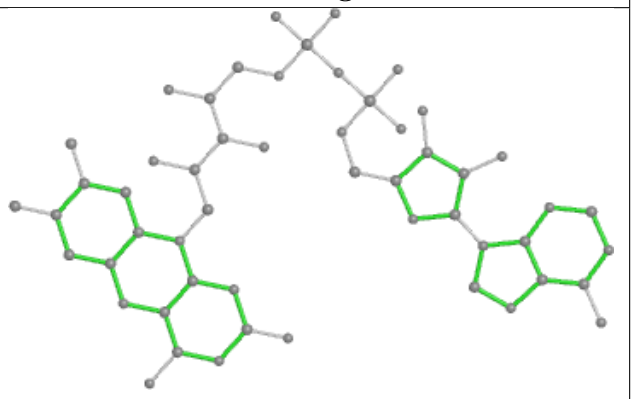
Bond lengths



Bond angles

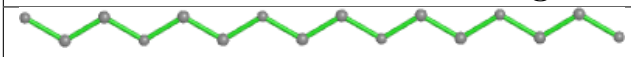


Torsions

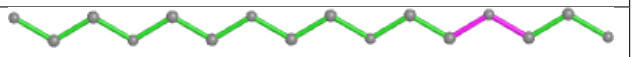


Rings

Ligand 12P B 802



Bond lengths

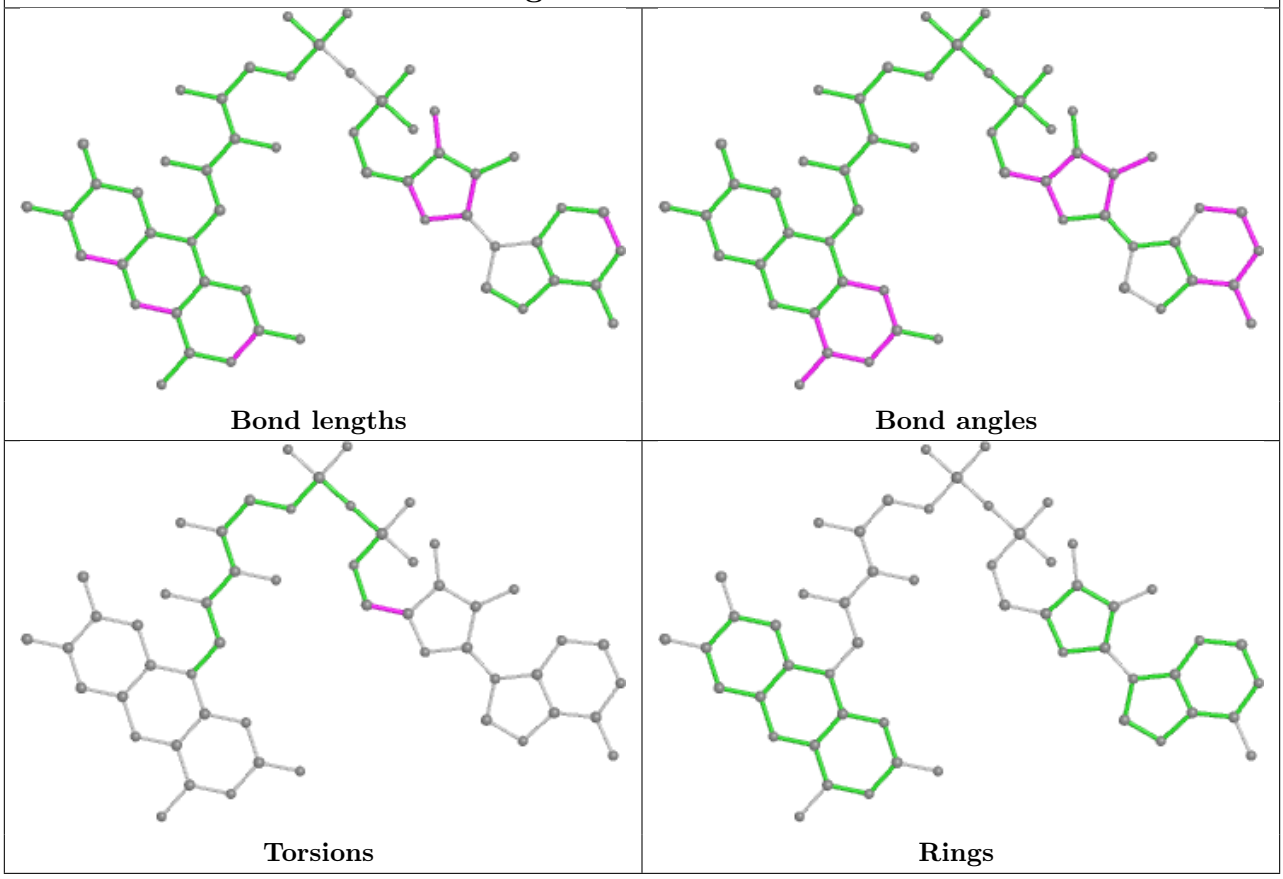


Bond angles

Torsions

Rings

Ligand FAD A 801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	576/633 (90%)	-0.37	8 (1%)	75	77	17, 23, 45, 83	0
1	B	575/633 (90%)	-0.29	12 (2%)	63	66	18, 25, 51, 90	0
1	C	574/633 (90%)	-0.28	13 (2%)	60	63	19, 29, 53, 89	0
1	D	572/633 (90%)	-0.07	16 (2%)	53	56	22, 39, 65, 97	0
All	All	2297/2532 (90%)	-0.25	49 (2%)	63	66	17, 29, 58, 97	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	458	ALA	12.2
1	D	458	ALA	9.1
1	C	457	GLY	7.5
1	D	457	GLY	5.9
1	A	459	VAL	4.8
1	B	459	VAL	4.8
1	D	343	ALA	4.6
1	A	45	ILE	4.5
1	C	458	ALA	4.4
1	C	389	LEU	4.2
1	C	390	THR	3.9
1	D	459	VAL	3.8
1	A	458	ALA	3.7
1	C	343	ALA	3.2
1	D	385	THR	3.2
1	C	385	THR	3.1
1	A	457	GLY	3.1
1	B	45	ILE	3.1
1	B	457	GLY	3.0
1	C	345	PRO	3.0
1	B	382	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	383	ARG	2.8
1	D	309	PHE	2.8
1	D	185	LYS	2.8
1	B	343	ALA	2.7
1	D	616	SER	2.7
1	B	44	ASP	2.6
1	C	45	ILE	2.6
1	C	382	ILE	2.6
1	D	269	ASP	2.5
1	D	270	ALA	2.5
1	D	400	SER	2.4
1	D	388	GLU	2.3
1	B	401	THR	2.3
1	D	345	PRO	2.3
1	D	268	THR	2.3
1	B	388	GLU	2.3
1	D	271	PRO	2.2
1	A	44	ASP	2.2
1	A	185	LYS	2.2
1	A	268	THR	2.2
1	B	268	THR	2.2
1	C	388	GLU	2.2
1	A	343	ALA	2.1
1	B	400	SER	2.1
1	B	344	ASN	2.1
1	C	344	ASN	2.0
1	D	617	PRO	2.0
1	C	391	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

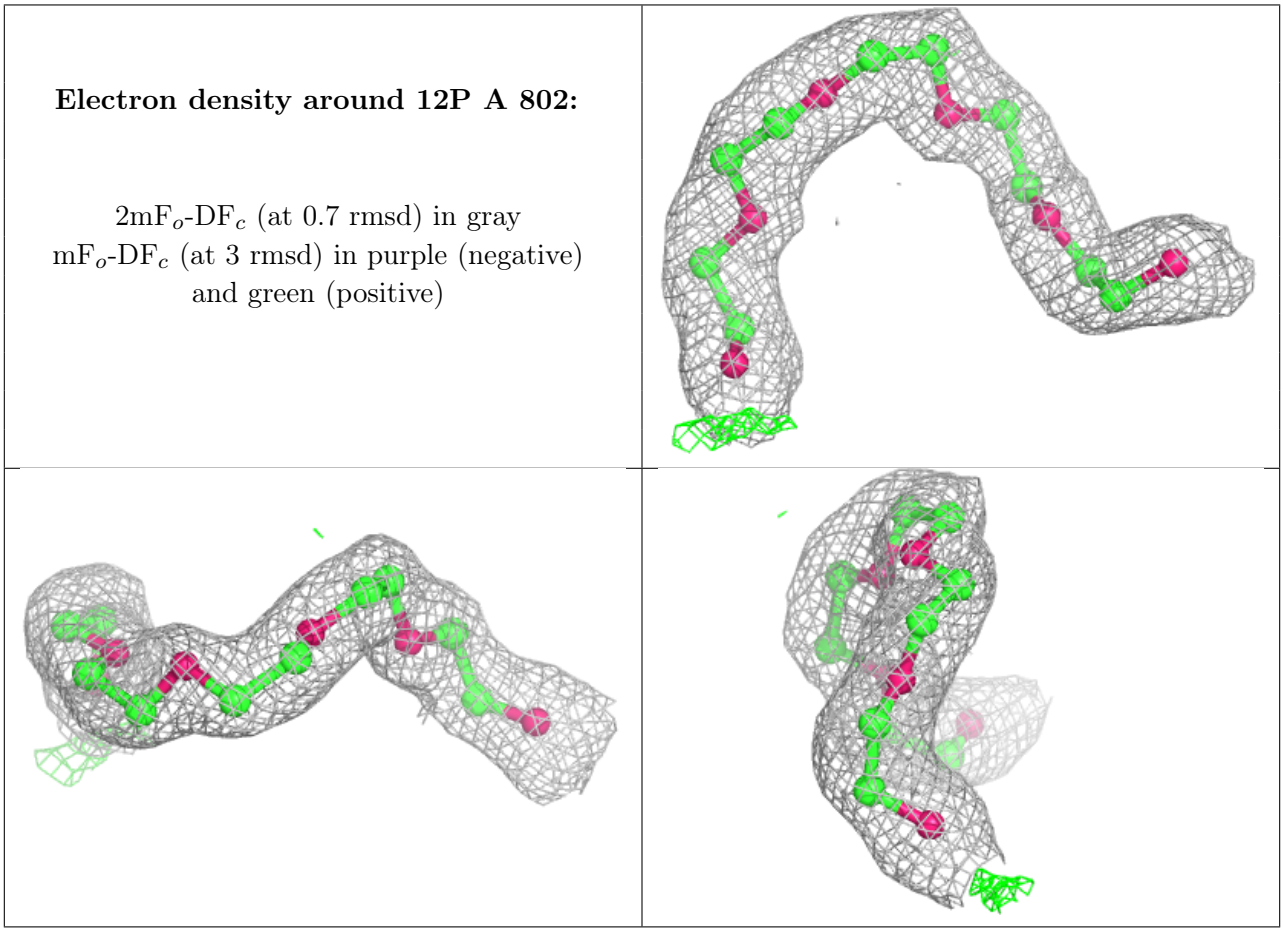
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	12P	A	802	16/37	0.92	0.11	35,38,50,51	0
4	MES	A	803	12/12	0.92	0.23	45,58,60,62	0
3	12P	B	802	16/37	0.93	0.11	31,37,50,59	0
3	12P	C	802	16/37	0.94	0.12	28,36,52,55	0
3	12P	D	802	13/37	0.95	0.12	39,41,51,57	0
4	MES	C	803	12/12	0.96	0.10	42,44,49,50	0
2	FAD	D	801	53/53	0.97	0.09	26,32,36,38	0
2	FAD	B	801	53/53	0.98	0.10	16,19,23,24	0
2	FAD	C	801	53/53	0.98	0.09	19,24,28,29	0
2	FAD	A	801	53/53	0.98	0.10	14,18,21,22	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.

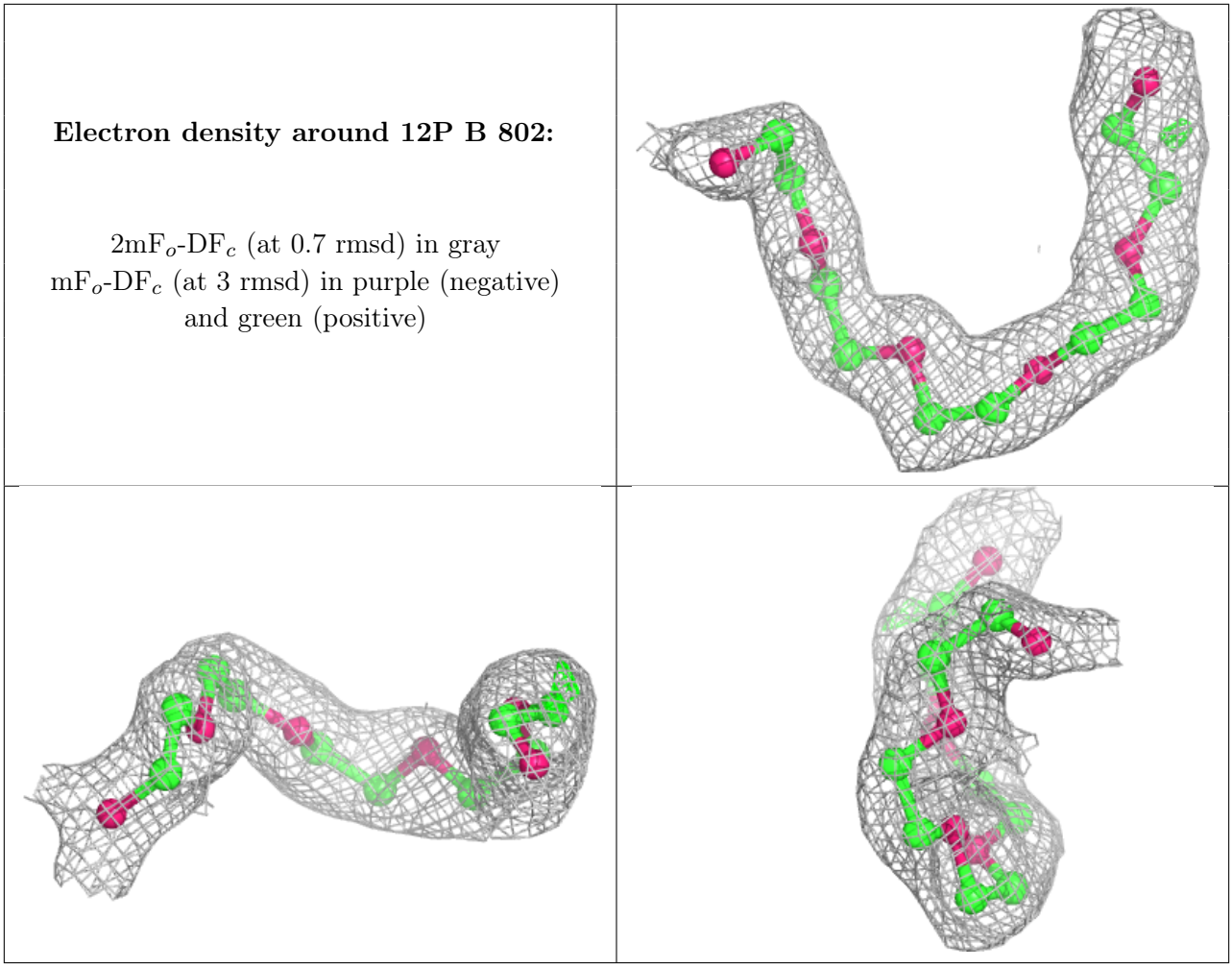
Electron density around 12P A 802:

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



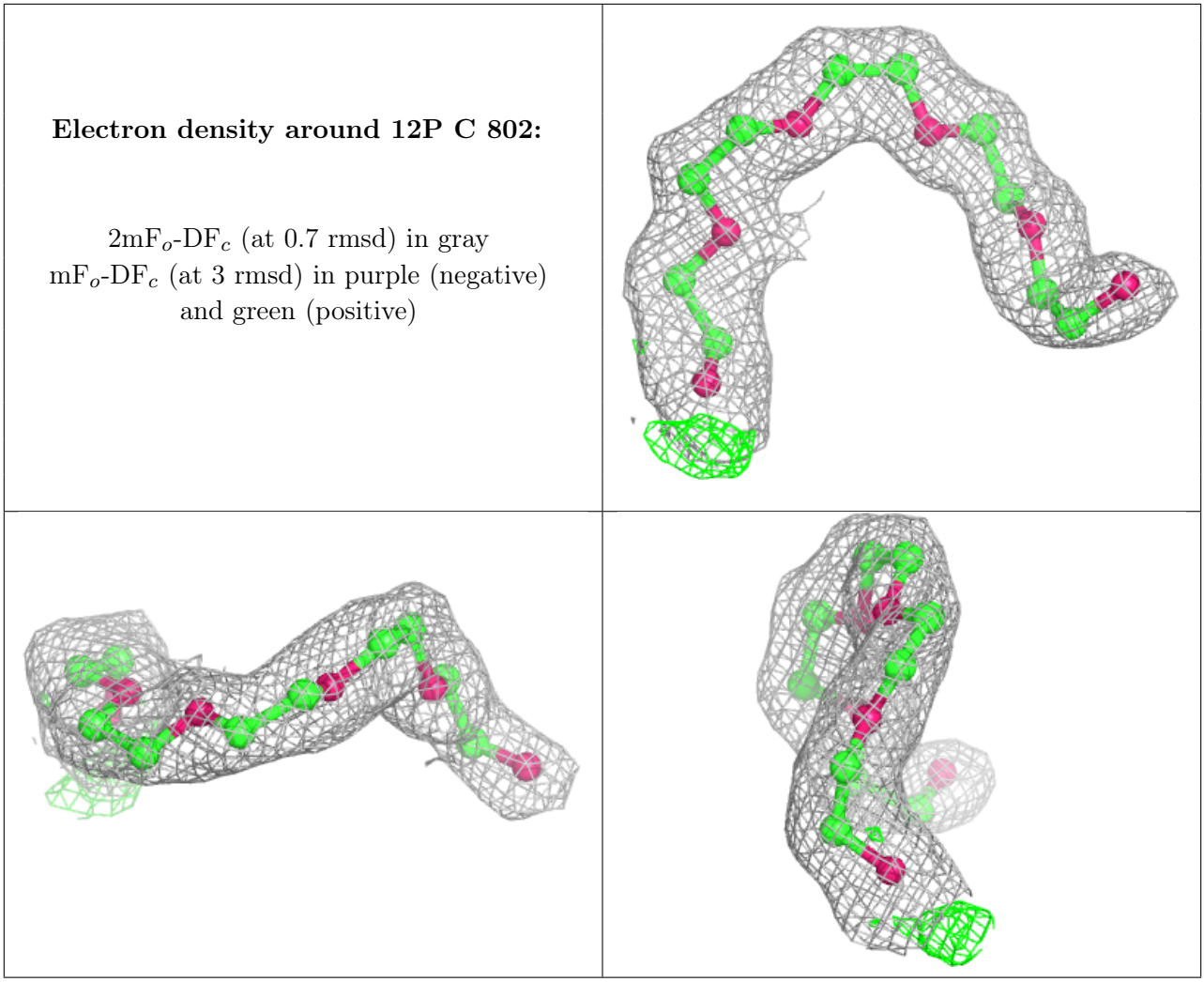
Electron density around 12P B 802:

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



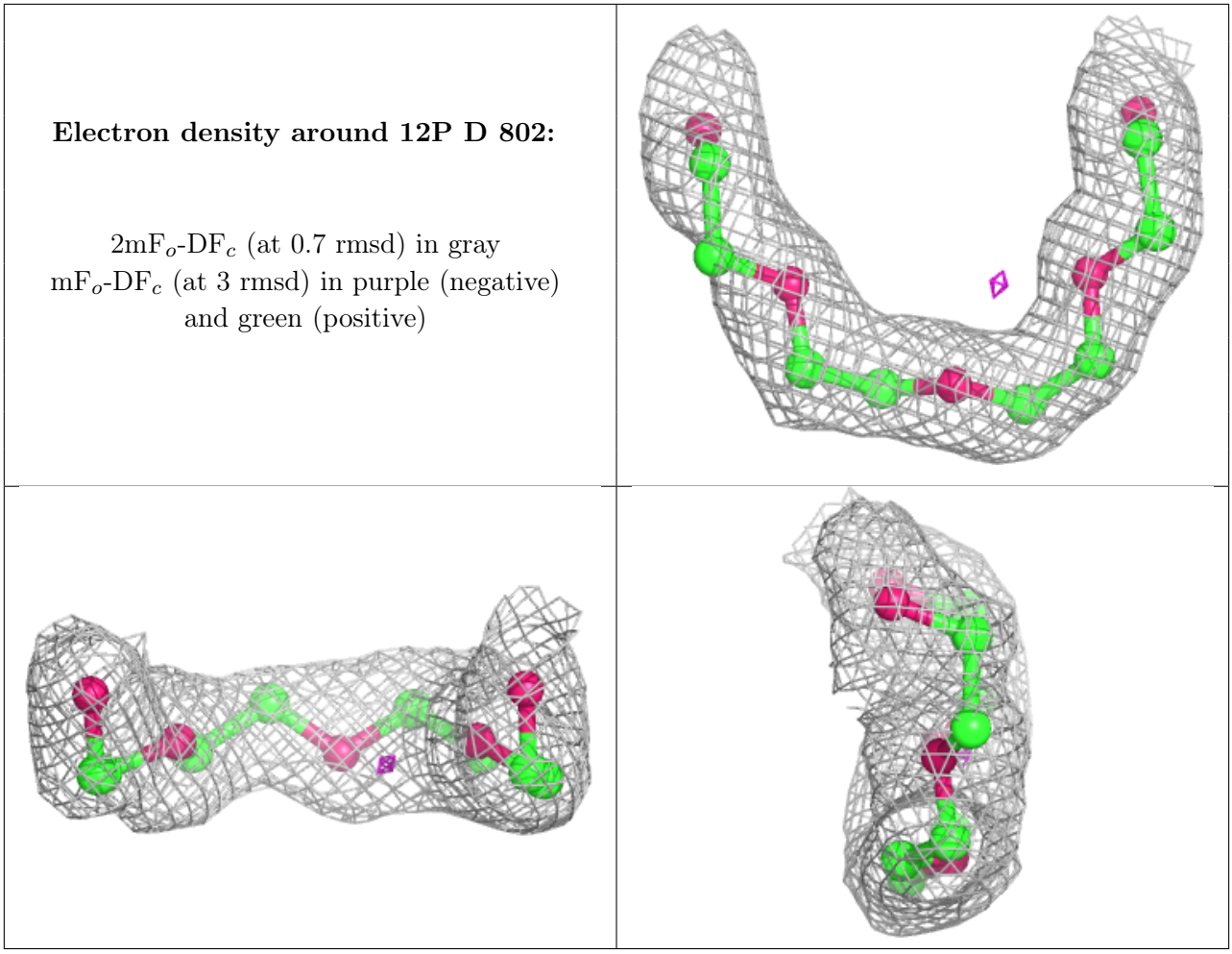
Electron density around 12P C 802:

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



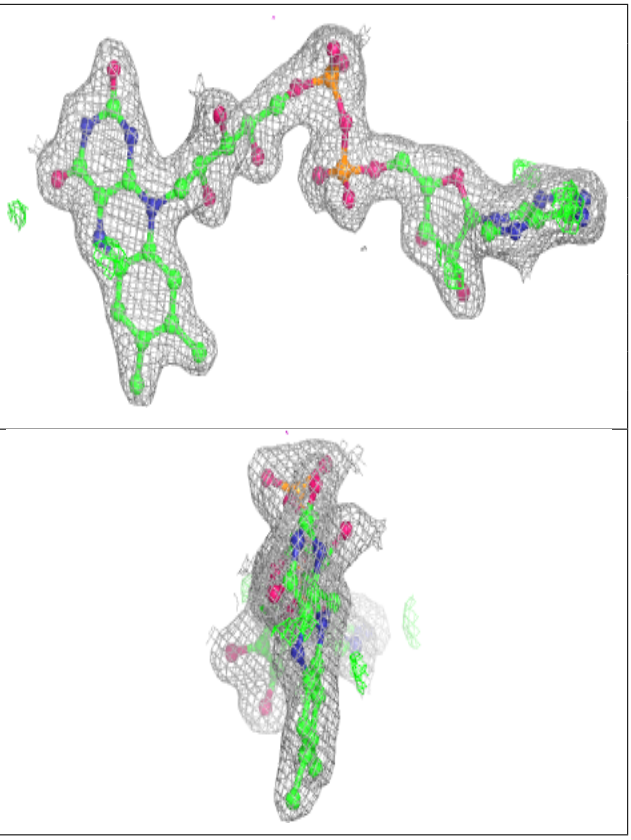
Electron density around 12P D 802:

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



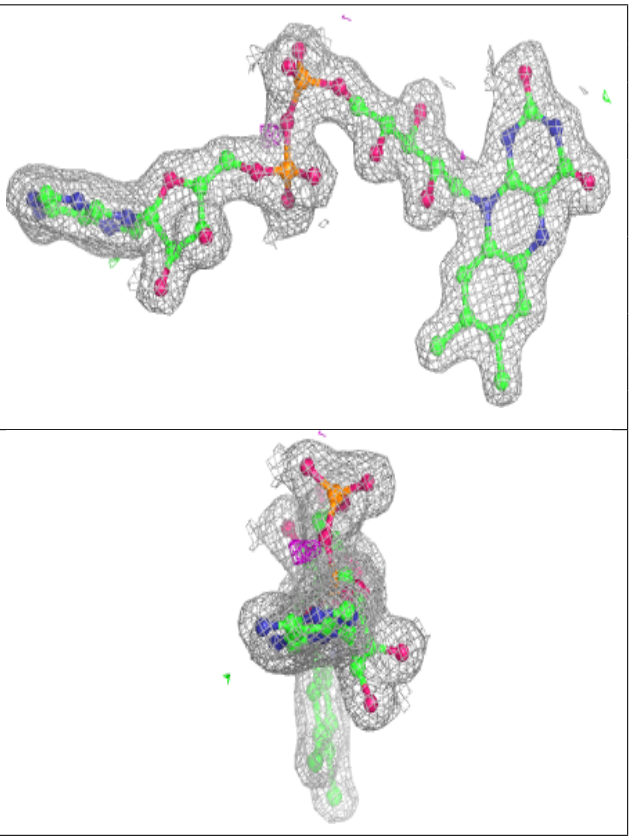
Electron density around FAD D 801:

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



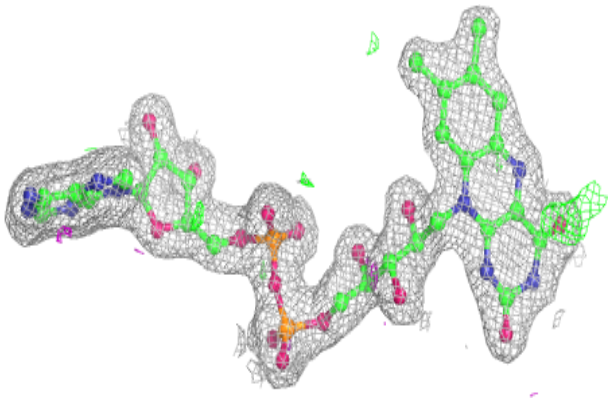
Electron density around FAD B 801:

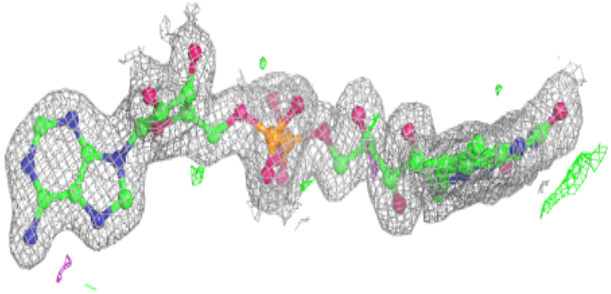
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

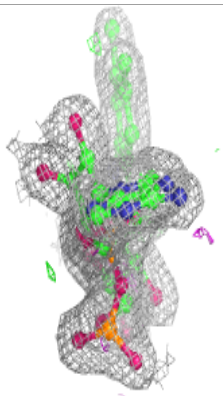


Electron density around FAD C 801:

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

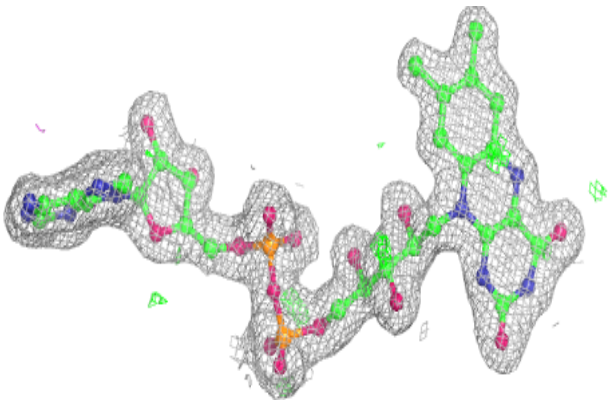


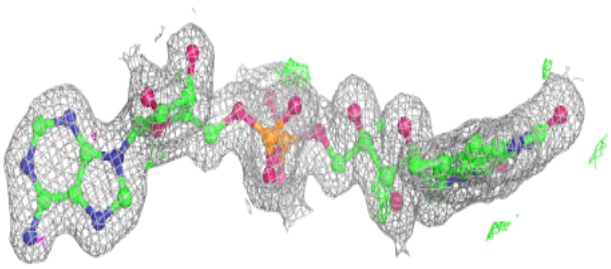


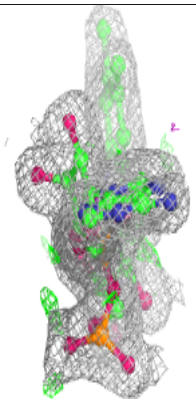


Electron density around FAD A 801:

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







6.5 Other polymers (i)

There are no such residues in this entry.