Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2021 – 05:18 am BST

PDB ID	:	7PBI
Title	:	4-ethylphenol oxidase from Gulosibacter chungangensis: isoeugenol complex
Authors	:	Alvigini, L.; Mattevi, A.
Deposited on	:	2021-08-02
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

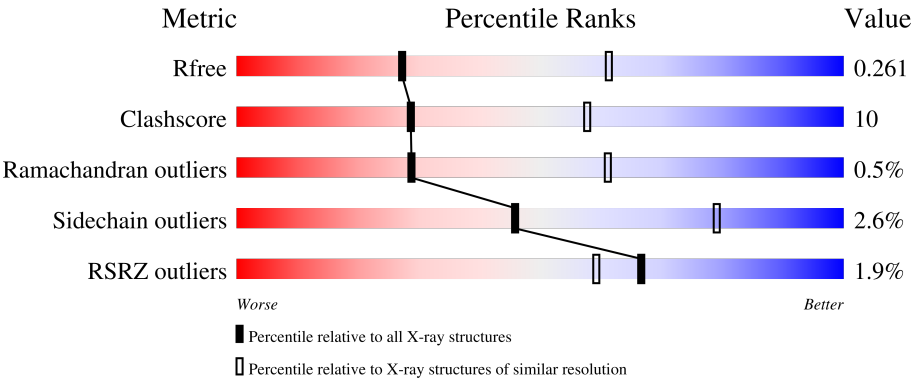
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	529	81% 17%
1	B	529	82% 17%
1	C	529	81% 18%
1	D	529	82% 17%
1	E	529	4% 78% 19%

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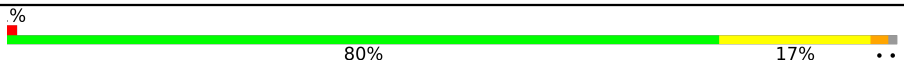
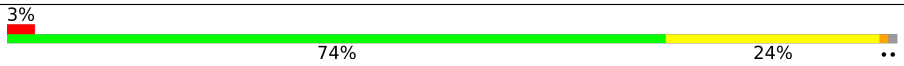
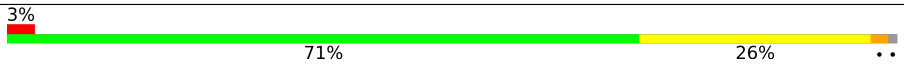
Mol	Chain	Length	Quality of chain
1	F	529	
1	G	529	
1	H	529	

2 Entry composition (i)

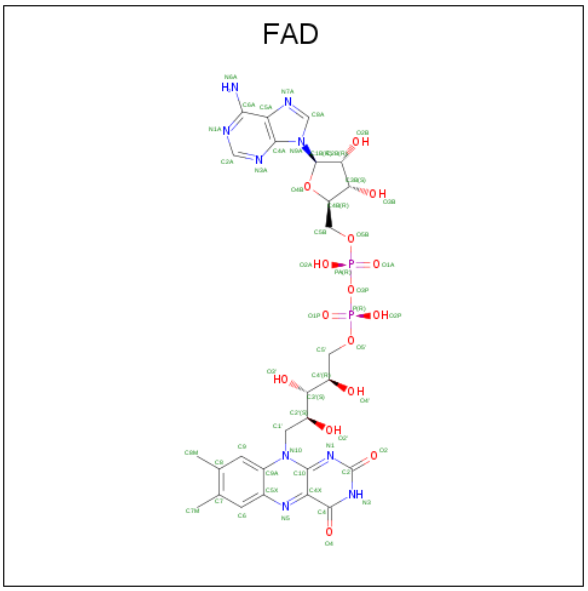
There are 3 unique types of molecules in this entry. The entry contains 33344 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FAD-binding oxidoreductase.

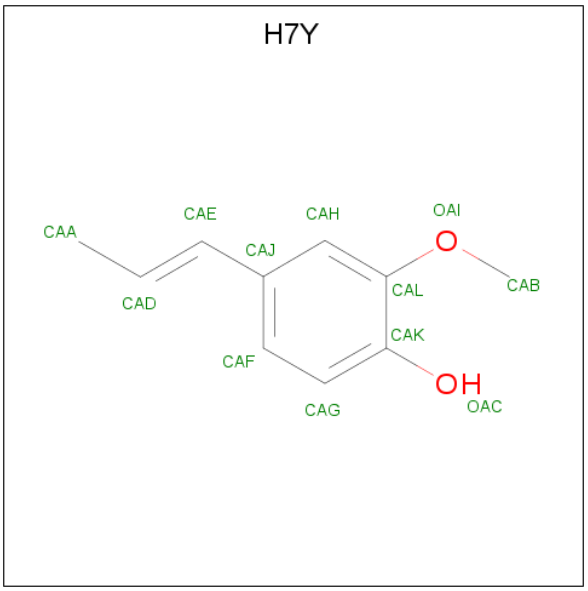
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	523	Total	C	N	O	S	0	0	0
			4095	2583	703	786	23			
1	B	525	Total	C	N	O	S	0	0	0
			4117	2598	708	788	23			
1	C	523	Total	C	N	O	S	0	0	0
			4095	2583	703	786	23			
1	D	525	Total	C	N	O	S	0	0	0
			4117	2598	708	788	23			
1	E	523	Total	C	N	O	S	0	0	0
			4095	2583	703	786	23			
1	F	525	Total	C	N	O	S	0	0	0
			4117	2598	708	788	23			
1	G	523	Total	C	N	O	S	0	0	0
			4095	2583	703	786	23			
1	H	525	Total	C	N	O	S	0	0	0
			4117	2598	708	788	23			

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



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

- Molecule 3 is ISOEUGENOL (three-letter code: H7Y) (formula: $C_{10}H_{12}O_2$) (labeled as "Ligand of Interest" by depositor).



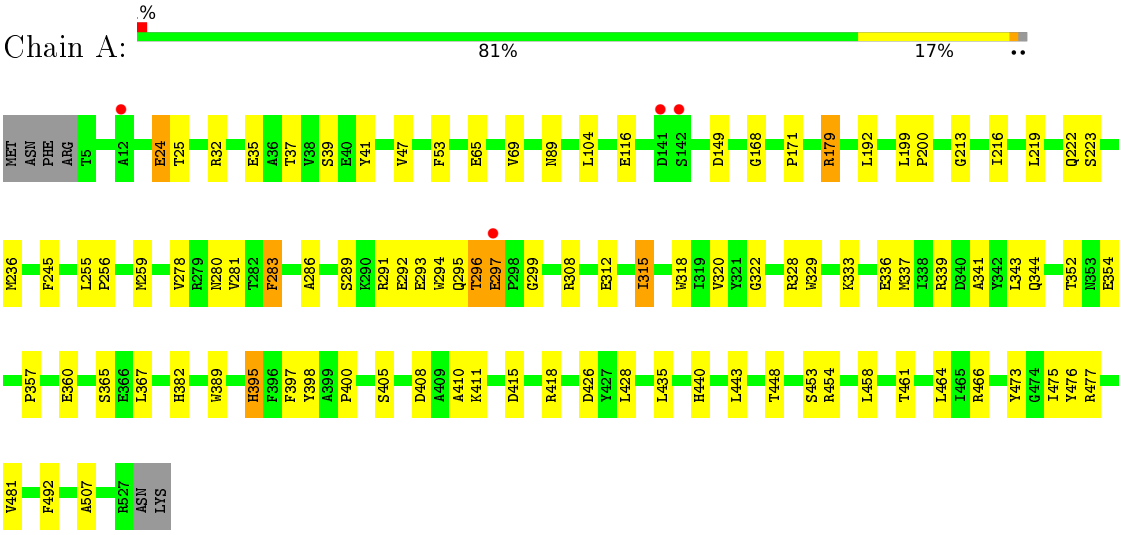
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 10 2	0	0
3	B	1	Total C O 12 10 2	0	0
3	C	1	Total C O 12 10 2	0	0
3	D	1	Total C O 12 10 2	0	0
3	E	1	Total C O 12 10 2	0	0
3	F	1	Total C O 12 10 2	0	0

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.

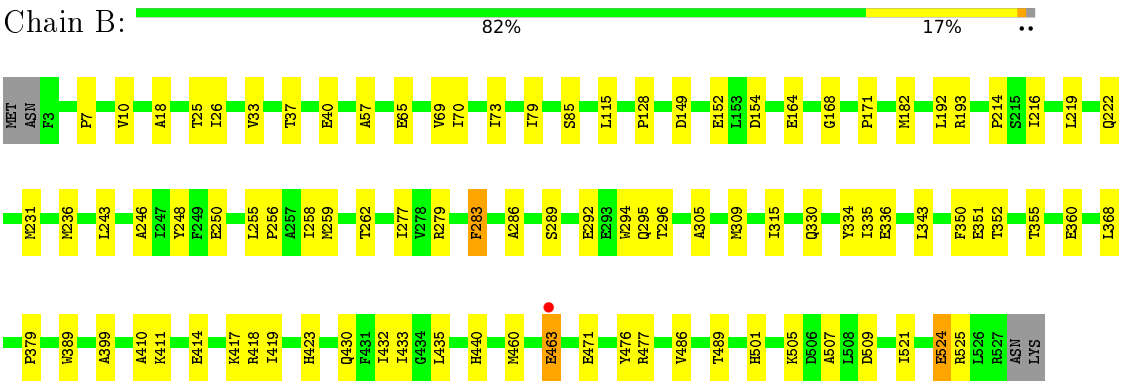
- Molecule 1: FAD-binding oxidoreductase

Chain A:



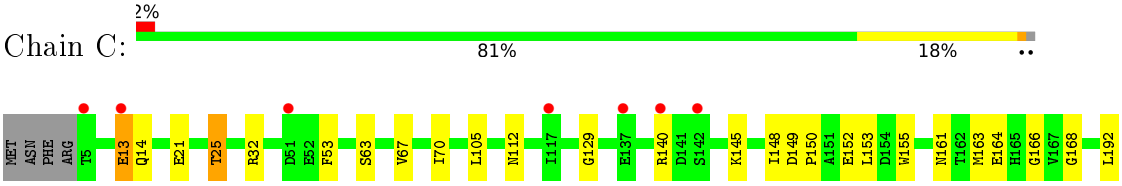
- Molecule 1: FAD-binding oxidoreductase

Chain B:

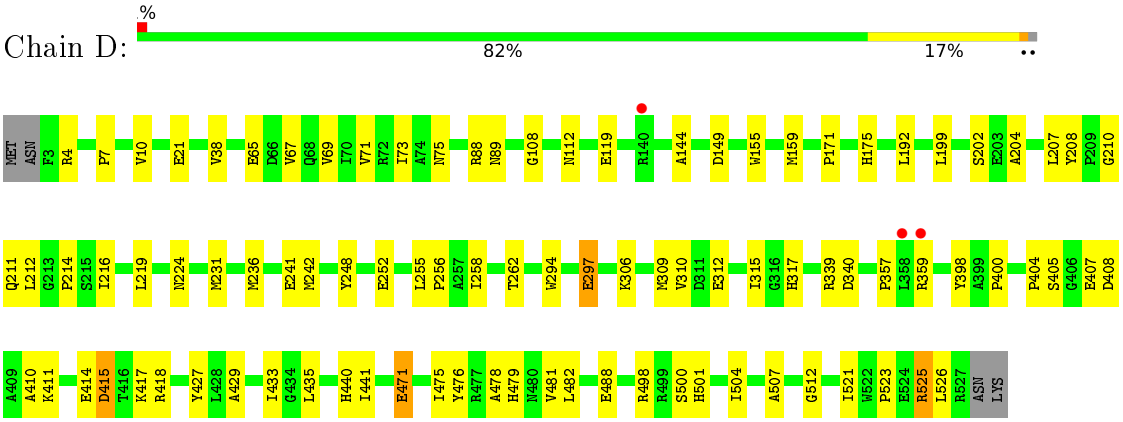


- Molecule 1: FAD-binding oxidoreductase

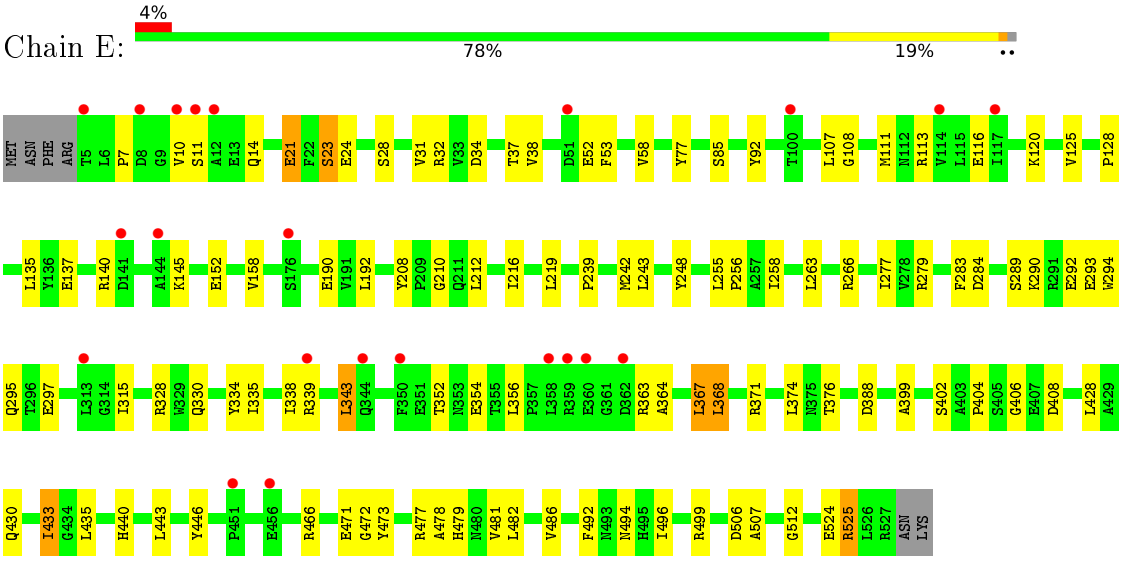
Chain C:



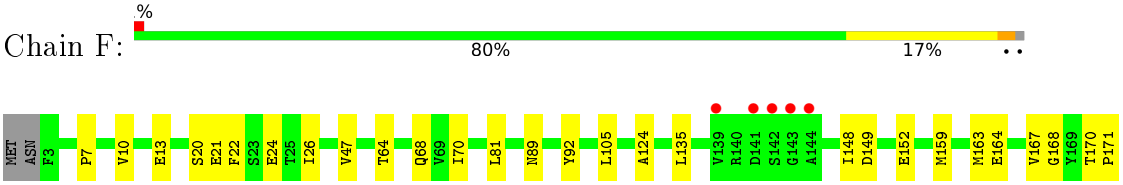
• Molecule 1: FAD-binding oxidoreductase

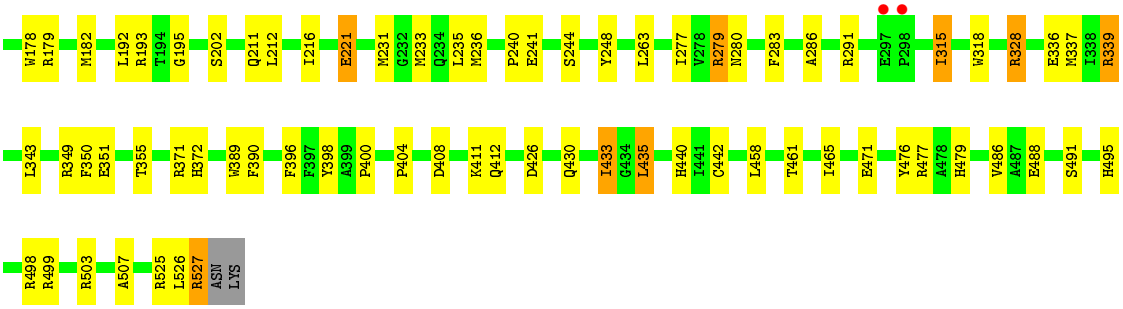


• Molecule 1: FAD-binding oxidoreductase



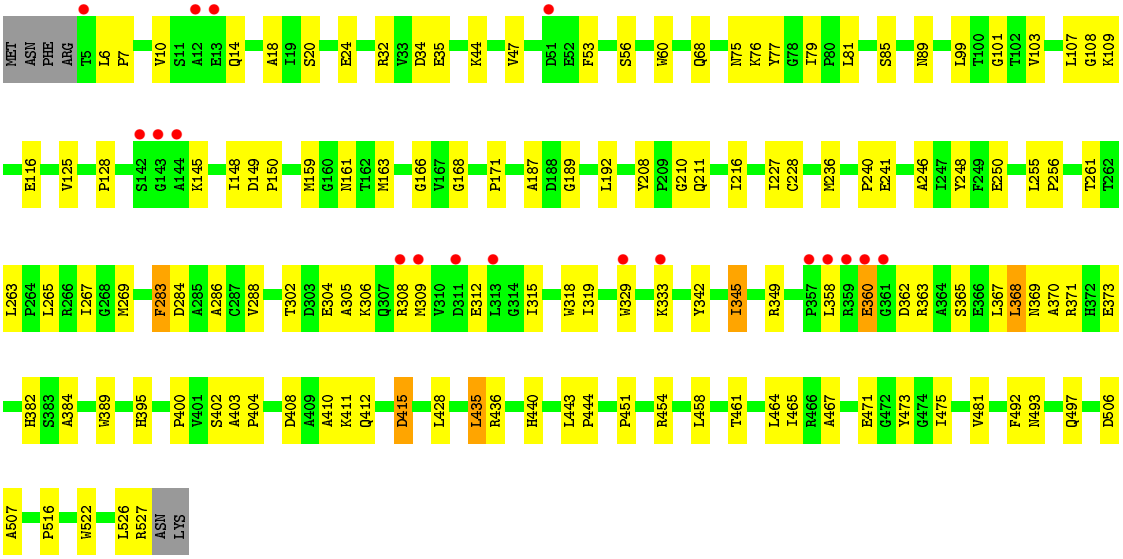
• Molecule 1: FAD-binding oxidoreductase





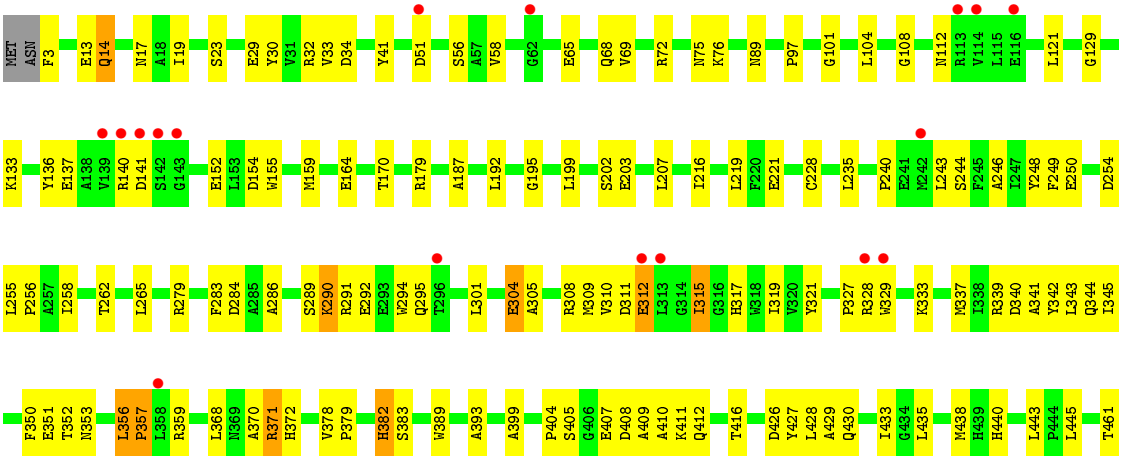
• Molecule 1: FAD-binding oxidoreductase

Chain G:



• Molecule 1: FAD-binding oxidoreductase

Chain H:




R462
I465
R477
Q485
I496
A507
P523
E524
R525
L526
R527
ASN
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.59Å 228.21Å 300.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.14 – 2.80 49.09 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.14-2.80) 99.9 (49.09-2.80)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.208 , 0.265 0.208 , 0.261	Depositor DCC
R_{free} test set	5889 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	53.3	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 32.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	33344	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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: H7Y, FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.64	0/4198	0.81	2/5703 (0.0%)
1	B	0.63	0/4221	0.82	1/5733 (0.0%)
1	C	0.64	0/4198	0.79	0/5703
1	D	0.65	0/4221	0.80	0/5733
1	E	0.65	0/4198	0.82	1/5703 (0.0%)
1	F	0.64	0/4221	0.78	0/5733
1	G	0.64	0/4198	0.79	0/5703
1	H	0.64	0/4221	0.79	0/5733
All	All	0.64	0/33676	0.80	4/45744 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	525	ARG	CG-CD-NE	-6.00	99.20	111.80
1	B	463	GLU	CB-CA-C	-5.94	98.52	110.40
1	A	297	GLU	N-CA-CB	5.41	120.33	110.60
1	A	24	GLU	N-CA-CB	5.18	119.93	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4095	0	3935	64	0
1	B	4117	0	3957	68	0
1	C	4095	0	3935	62	3
1	D	4117	0	3957	63	0
1	E	4095	0	3935	89	0
1	F	4117	0	3957	71	3
1	G	4095	0	3935	102	0
1	H	4117	0	3957	127	2
2	A	53	0	29	2	0
2	B	53	0	29	2	0
2	C	53	0	29	1	0
2	D	53	0	29	2	0
2	E	53	0	30	2	0
2	F	53	0	29	3	0
2	G	53	0	29	3	0
2	H	53	0	29	6	0
3	A	12	0	0	2	0
3	B	12	0	0	1	0
3	C	12	0	0	1	0
3	D	12	0	0	2	0
3	E	12	0	0	0	0
3	F	12	0	0	2	0
All	All	33344	0	31801	630	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (630) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:411:LYS:CE	1:D:471:GLU:OE1	1.65	1.45
1:G:342:TYR:O	1:G:345:ILE:CD1	2.00	1.09
1:G:304:GLU:O	1:G:308:ARG:HG3	1.56	1.04
1:E:152:GLU:HG3	2:E:601:FAD:N5	1.73	1.03
1:G:342:TYR:O	1:G:345:ILE:HD13	1.63	0.99
1:E:363:ARG:O	1:E:367:LEU:CD2	2.12	0.97
1:B:460:MET:O	1:B:463:GLU:HB2	1.66	0.95
1:H:294:TRP:CD1	1:H:309:MET:HG2	2.04	0.93
1:D:512:GLY:O	1:D:525:ARG:NH2	2.02	0.92
1:G:506:ASP:OD2	1:G:527:ARG:NH2	2.01	0.92
1:B:259:MET:HE1	1:B:433:ILE:HD11	1.51	0.92
1:C:21:GLU:O	1:C:25:THR:OG1	1.87	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:471:GLU:HB2	1:G:473:TYR:CE2	2.03	0.91
1:D:410:ALA:O	1:D:414:GLU:HG3	1.71	0.91
1:E:364:ALA:HA	1:E:367:LEU:HD21	1.50	0.91
1:H:427:TYR:HE1	1:H:429:ALA:HB2	1.33	0.90
1:D:411:LYS:HE2	1:D:471:GLU:CD	1.90	0.90
1:H:32:ARG:NH2	1:H:34:ASP:OD2	2.05	0.89
1:D:411:LYS:HE2	1:D:471:GLU:OE1	0.71	0.88
1:E:277:ILE:HB	1:E:430:GLN:HE21	1.38	0.88
1:G:362:ASP:O	1:G:365:SER:OG	1.92	0.88
1:F:336:GLU:OE1	1:F:339:ARG:NH2	2.06	0.88
1:B:259:MET:CE	1:B:433:ILE:HD11	2.06	0.86
1:G:471:GLU:HB2	1:G:473:TYR:CD2	2.11	0.85
1:H:289:SER:HG	1:H:294:TRP:HH2	1.20	0.85
1:H:462:ARG:HG2	1:H:485:GLN:OE1	1.79	0.83
1:A:171:PRO:HD2	1:A:236:MET:HE1	1.59	0.83
1:B:460:MET:HA	1:B:463:GLU:HG3	1.61	0.82
1:E:363:ARG:O	1:E:367:LEU:HD22	1.78	0.82
1:G:305:ALA:HA	1:G:308:ARG:HD3	1.62	0.81
1:E:367:LEU:HD23	1:E:367:LEU:H	1.44	0.81
1:D:192:LEU:HD21	1:D:216:ILE:HD11	1.62	0.81
1:D:252:GLU:OE2	1:D:417:LYS:NZ	2.14	0.80
1:F:21:GLU:HA	1:F:24:GLU:HG3	1.63	0.80
1:G:345:ILE:HD12	1:G:345:ILE:H	1.47	0.80
1:G:240:PRO:O	1:G:241:GLU:HG2	1.82	0.79
1:H:75:ASN:ND2	1:H:187:ALA:O	2.15	0.79
1:C:352:THR:HG22	1:C:354:GLU:H	1.48	0.78
1:H:409:ALA:O	1:H:412:GLN:N	2.17	0.77
1:C:223:SER:HB3	1:D:214:PRO:HG3	1.67	0.77
1:H:289:SER:OG	1:H:294:TRP:HH2	1.68	0.76
1:C:278:VAL:HG22	1:C:320:VAL:HG22	1.67	0.76
1:A:411:LYS:HD3	1:A:473:TYR:OH	1.85	0.76
1:E:11:SER:N	1:E:14:GLN:OE1	2.19	0.76
1:G:370:ALA:HB2	1:G:382:HIS:HD2	1.49	0.76
1:C:289:SER:HG	1:C:294:TRP:HH2	1.34	0.75
1:F:279:ARG:NH1	1:F:430:GLN:OE1	2.19	0.75
1:G:333:LYS:HG2	1:H:329:TRP:CZ2	2.22	0.75
1:H:427:TYR:CE1	1:H:429:ALA:HB2	2.20	0.75
1:F:476:TYR:OH	3:F:602:H7Y:OAC	2.05	0.74
1:A:53:PHE:CE2	1:A:481:VAL:HG12	2.23	0.74
1:F:461:THR:O	1:F:465:ILE:HD12	1.88	0.74
1:E:21:GLU:OE1	1:E:77:TYR:OH	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:471:GLU:CB	1:G:473:TYR:HE2	2.01	0.73
1:F:171:PRO:HB2	1:F:236:MET:HE1	1.70	0.73
1:G:342:TYR:O	1:G:345:ILE:HD12	1.87	0.73
1:B:423:HIS:CD2	1:B:463:GLU:OE1	2.41	0.72
1:C:192:LEU:HD21	1:C:216:ILE:HD11	1.71	0.72
1:F:47:VAL:CG2	1:F:458:LEU:HB2	2.19	0.72
1:B:279:ARG:HG2	1:B:430:GLN:HE21	1.55	0.71
1:E:512:GLY:O	1:E:525:ARG:NH1	2.24	0.71
1:E:10:VAL:HA	1:E:14:GLN:OE1	1.91	0.71
1:F:277:ILE:HD11	1:F:371:ARG:HD2	1.71	0.71
1:F:488:GLU:OE2	1:F:498:ARG:NH2	2.23	0.71
1:E:471:GLU:HB3	1:E:473:TYR:CE2	2.26	0.71
1:E:190:GLU:OE2	1:F:499:ARG:NH2	2.24	0.70
1:E:283:PHE:CD2	1:E:428:LEU:HB3	2.26	0.70
1:H:310:VAL:HG21	1:H:317:HIS:CD2	2.25	0.70
1:H:262:THR:HG22	1:H:342:TYR:OH	1.91	0.70
1:A:352:THR:HG22	1:A:354:GLU:H	1.57	0.70
1:G:246:ALA:HB2	1:G:368:LEU:HD22	1.74	0.70
1:H:192:LEU:HD21	1:H:216:ILE:HD11	1.74	0.69
1:A:397:PHE:CE1	1:A:443:LEU:HD13	2.27	0.69
1:G:256:PRO:HG3	1:G:410:ALA:HB2	1.73	0.69
1:H:291:ARG:NH1	1:H:426:ASP:OD1	2.26	0.69
1:C:163:MET:CE	1:C:228:CYS:HB3	2.23	0.69
1:E:352:THR:HG22	1:E:354:GLU:H	1.59	0.68
1:G:471:GLU:CB	1:G:473:TYR:CE2	2.75	0.68
1:D:256:PRO:HG3	1:D:410:ALA:HB2	1.75	0.68
1:A:291:ARG:NH1	1:A:426:ASP:OD2	2.28	0.67
1:E:356:LEU:HD23	1:E:368:LEU:HD12	1.77	0.67
1:F:343:LEU:HD21	1:F:350:PHE:HB2	1.78	0.66
1:D:488:GLU:OE2	1:D:498:ARG:NH1	2.27	0.66
1:H:291:ARG:NH1	1:H:426:ASP:OD2	2.29	0.66
1:B:259:MET:CE	1:B:433:ILE:CD1	2.74	0.66
1:G:370:ALA:HB2	1:G:382:HIS:CD2	2.30	0.66
1:H:340:ASP:O	1:H:344:GLN:HG3	1.96	0.66
1:E:364:ALA:CA	1:E:367:LEU:HD21	2.25	0.65
1:B:289:SER:OG	1:B:294:TRP:CZ3	2.49	0.65
1:D:339:ARG:NH2	1:D:340:ASP:OD1	2.29	0.65
1:C:321:TYR:OH	1:C:367:LEU:HD13	1.96	0.65
1:A:395:HIS:CD2	1:A:443:LEU:HD11	2.32	0.65
1:F:351:GLU:OE1	1:F:355:THR:HG22	1.96	0.65
1:A:223:SER:HB3	1:B:214:PRO:HG3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:367:LEU:CD2	1:E:367:LEU:H	2.10	0.65
1:E:283:PHE:HD2	1:E:428:LEU:HB3	1.61	0.64
1:G:35:GLU:HA	1:G:35:GLU:OE1	1.98	0.64
1:H:243:LEU:HD11	1:H:352:THR:HB	1.79	0.64
1:H:308:ARG:O	1:H:312:GLU:HB2	1.97	0.64
1:B:343:LEU:HD21	1:B:350:PHE:HB2	1.78	0.64
1:C:476:TYR:OH	3:C:602:H7Y:OAC	2.16	0.63
1:G:342:TYR:C	1:G:345:ILE:CD1	2.67	0.63
1:D:476:TYR:OH	3:D:602:H7Y:OAC	2.17	0.63
1:G:10:VAL:HA	1:G:14:GLN:HE21	1.63	0.63
2:E:601:FAD:H8A	2:E:601:FAD:O5B	1.98	0.63
1:E:367:LEU:HD23	1:E:367:LEU:N	2.14	0.62
1:E:339:ARG:HG2	1:E:343:LEU:CD2	2.29	0.62
1:E:507:ALA:HB2	1:F:507:ALA:HB2	1.82	0.62
1:E:334:TYR:O	1:E:338:ILE:HG13	1.98	0.62
1:E:494:ASN:HB2	1:E:499:ARG:HH21	1.64	0.62
1:H:294:TRP:CD1	1:H:312:GLU:OE1	2.53	0.62
1:D:415:ASP:OD1	1:D:418:ARG:NH2	2.33	0.62
1:F:411:LYS:HE3	1:F:471:GLU:OE2	1.99	0.61
1:G:159:MET:HE3	1:G:228:CYS:O	2.00	0.61
1:B:258:ILE:O	1:B:262:THR:OG1	2.17	0.61
1:C:163:MET:HE1	1:C:228:CYS:HB3	1.82	0.61
1:G:288:VAL:HG13	1:G:367:LEU:HD21	1.82	0.61
1:E:492:PHE:CE2	1:F:193:ARG:HG3	2.36	0.61
1:H:152:GLU:OE1	1:H:383:SER:OG	2.19	0.60
1:A:256:PRO:HG3	1:A:410:ALA:HB2	1.82	0.60
1:B:289:SER:HG	1:B:294:TRP:HH2	1.40	0.60
1:A:24:GLU:O	1:A:24:GLU:HG2	1.99	0.60
1:G:284:ASP:HB3	1:G:367:LEU:HD13	1.82	0.60
1:A:289:SER:HB2	1:A:293:GLU:OE1	2.02	0.60
1:G:367:LEU:O	1:G:371:ARG:HG2	2.01	0.60
1:B:26:ILE:HG13	1:B:70:ILE:HD11	1.83	0.60
1:B:192:LEU:HD21	1:B:216:ILE:HD11	1.84	0.60
1:F:526:LEU:C	1:F:527:ARG:HG3	2.22	0.60
1:H:290:LYS:O	1:H:294:TRP:CZ3	2.54	0.60
1:B:154:ASP:HB3	1:B:379:PRO:HB2	1.83	0.59
1:C:277:ILE:HD11	1:C:371:ARG:HD2	1.83	0.59
1:H:152:GLU:HG3	2:H:601:FAD:N5	2.18	0.59
1:B:37:THR:O	1:B:40:GLU:HB2	2.02	0.59
1:E:289:SER:OG	1:E:294:TRP:CH2	2.55	0.59
1:H:461:THR:O	1:H:465:ILE:HG13	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:342:TYR:HA	1:G:345:ILE:HD11	1.84	0.59
1:E:471:GLU:CB	1:E:473:TYR:CE2	2.86	0.59
1:A:149:ASP:OD1	1:A:168:GLY:HA3	2.02	0.58
1:A:171:PRO:CD	1:A:236:MET:HE1	2.30	0.58
1:D:398:TYR:CE1	1:D:475:ILE:HD11	2.39	0.58
1:F:192:LEU:HD21	1:F:216:ILE:HD11	1.85	0.58
1:D:255:LEU:HB3	1:D:256:PRO:HD3	1.86	0.58
1:G:507:ALA:HB2	1:H:507:ALA:HB2	1.86	0.58
2:B:601:FAD:H8A	2:B:601:FAD:O5B	2.02	0.58
1:F:286:ALA:HA	1:F:389:TRP:CE3	2.39	0.58
1:G:461:THR:HA	1:G:464:LEU:HD12	1.86	0.58
1:H:291:ARG:NH1	1:H:426:ASP:CG	2.57	0.58
1:A:476:TYR:OH	3:A:602:H7Y:OAC	2.21	0.58
1:B:360:GLU:CD	1:B:360:GLU:H	2.07	0.57
1:E:263:LEU:HD12	1:E:404:PRO:HG2	1.85	0.57
1:H:279:ARG:HH22	1:H:371:ARG:HH21	1.53	0.57
1:H:339:ARG:HH11	1:H:343:LEU:HD12	1.69	0.57
1:H:370:ALA:HB2	1:H:382:HIS:CD2	2.39	0.57
1:A:25:THR:HB	1:A:69:VAL:HG11	1.85	0.57
1:E:363:ARG:O	1:E:367:LEU:HD23	2.03	0.57
1:A:295:GLN:O	1:A:296:THR:HG23	2.05	0.57
1:B:460:MET:CA	1:B:463:GLU:HG3	2.35	0.57
1:D:67:VAL:O	1:D:71:VAL:HG23	2.05	0.57
1:G:261:THR:O	1:G:265:LEU:HD23	2.05	0.57
1:G:402:SER:HB3	1:G:473:TYR:CD1	2.40	0.57
1:C:339:ARG:HD3	1:C:350:PHE:CD2	2.40	0.57
1:E:32:ARG:HD3	1:E:37:THR:HG21	1.87	0.56
1:C:488:GLU:OE1	1:C:498:ARG:NH2	2.38	0.56
1:H:154:ASP:HB3	1:H:379:PRO:HB2	1.88	0.56
1:H:309:MET:CA	1:H:312:GLU:HB2	2.35	0.56
1:B:277:ILE:HG22	1:B:432:ILE:HG12	1.87	0.56
1:F:20:SER:O	1:F:24:GLU:HG3	2.05	0.56
1:F:152:GLU:HG3	2:F:601:FAD:N5	2.21	0.56
1:H:279:ARG:NH2	1:H:371:ARG:HH21	2.03	0.56
2:D:601:FAD:H8A	2:D:601:FAD:O5B	2.06	0.56
2:C:601:FAD:H8A	2:C:601:FAD:O5B	2.06	0.56
1:B:279:ARG:CG	1:B:430:GLN:HE21	2.19	0.55
1:C:400:PRO:HD2	1:C:440:HIS:O	2.07	0.55
1:H:89:ASN:HA	2:H:601:FAD:H5'2	1.88	0.55
1:B:7:PRO:HG2	1:B:10:VAL:HB	1.89	0.55
1:H:248:TYR:CE1	1:H:315:ILE:HG22	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:292:GLU:HA	1:H:295:GLN:O	2.07	0.55
1:B:259:MET:HE1	1:B:433:ILE:CD1	2.29	0.55
1:C:332:ASP:O	1:C:336:GLU:HB2	2.06	0.55
1:F:244:SER:HG	1:F:372:HIS:HD1	0.59	0.55
1:C:397:PHE:CE1	1:C:443:LEU:HD13	2.42	0.55
1:G:20:SER:O	1:G:24:GLU:CG	2.55	0.55
1:D:306:LYS:HA	1:D:309:MET:CE	2.37	0.55
1:E:266:ARG:HG2	1:E:433:ILE:HG22	1.89	0.55
1:F:152:GLU:OE1	1:F:371:ARG:NH2	2.40	0.55
1:E:212:LEU:HD22	1:F:486:VAL:HG12	1.88	0.55
1:G:149:ASP:OD1	1:G:168:GLY:HA3	2.07	0.55
1:H:159:MET:CE	2:H:601:FAD:N6A	2.70	0.55
1:H:408:ASP:O	1:H:412:GLN:HG3	2.07	0.55
1:C:507:ALA:HB2	1:D:507:ALA:HB2	1.88	0.55
1:D:21:GLU:HA	1:D:21:GLU:OE1	2.06	0.55
1:H:68:GLN:O	1:H:72:ARG:HG3	2.06	0.54
1:B:259:MET:HE3	1:B:433:ILE:CD1	2.36	0.54
1:C:333:LYS:O	1:C:336:GLU:HB3	2.08	0.54
1:A:461:THR:HA	1:A:464:LEU:HD12	1.89	0.54
1:H:13:GLU:OE2	1:H:17:ASN:OD1	2.26	0.54
1:A:405:SER:HB3	1:A:408:ASP:HB2	1.90	0.54
1:E:239:PRO:HD2	1:E:242:MET:HE2	1.90	0.54
1:H:416:THR:HG22	1:H:427:TYR:CE2	2.42	0.54
1:B:255:LEU:HB3	1:B:256:PRO:HD3	1.89	0.54
1:G:333:LYS:HG2	1:H:329:TRP:CE2	2.43	0.54
1:C:241:GLU:HG2	1:C:328:ARG:HD2	1.90	0.54
2:F:601:FAD:H8A	2:F:601:FAD:O5B	2.07	0.54
1:H:3:PHE:CD1	1:H:33:VAL:HG11	2.43	0.54
1:H:309:MET:HA	1:H:312:GLU:HB2	1.90	0.54
1:A:278:VAL:HG22	1:A:320:VAL:HG22	1.89	0.53
1:E:7:PRO:HG2	1:E:10:VAL:HB	1.90	0.53
1:E:293:GLU:O	1:E:293:GLU:HG2	2.09	0.53
1:G:161:ASN:ND2	1:G:166:GLY:HA3	2.24	0.53
1:H:294:TRP:NE1	1:H:312:GLU:OE1	2.41	0.53
1:H:409:ALA:O	1:H:411:LYS:N	2.41	0.53
1:G:497:GLN:NE2	1:H:195:GLY:O	2.41	0.53
1:H:339:ARG:HG3	1:H:350:PHE:CG	2.43	0.53
1:B:524:GLU:HG2	1:B:525:ARG:N	2.24	0.53
1:E:279:ARG:NH2	1:E:430:GLN:CD	2.62	0.53
1:F:404:PRO:HB3	1:F:433:ILE:CD1	2.39	0.53
1:D:400:PRO:HD2	1:D:440:HIS:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:20:SER:O	1:G:24:GLU:HG2	2.09	0.53
1:G:465:ILE:HG12	1:G:475:ILE:CD1	2.38	0.53
1:A:308:ARG:O	1:A:312:GLU:HG3	2.08	0.53
1:A:395:HIS:CG	1:A:443:LEU:HD11	2.43	0.53
1:E:38:VAL:HG22	1:E:58:VAL:HG23	1.91	0.53
1:G:288:VAL:HG13	1:G:367:LEU:CD2	2.39	0.53
1:H:244:SER:OG	1:H:372:HIS:ND1	2.28	0.53
1:F:400:PRO:HD2	1:F:440:HIS:O	2.08	0.52
1:H:248:TYR:HE1	1:H:315:ILE:HG22	1.74	0.52
1:A:179:ARG:O	1:A:179:ARG:HG2	2.09	0.52
1:C:277:ILE:HG22	1:C:432:ILE:HG12	1.91	0.52
1:G:68:GLN:HG2	1:G:189:GLY:O	2.10	0.52
1:E:289:SER:HG	1:E:294:TRP:HZ3	1.53	0.52
1:G:85:SER:O	1:G:108:GLY:HA3	2.10	0.52
1:C:289:SER:OG	1:C:294:TRP:CH2	2.53	0.52
1:D:405:SER:HB2	1:D:408:ASP:H	1.75	0.52
1:A:281:VAL:HG23	1:A:315:ILE:HD11	1.91	0.52
1:E:496:ILE:HG23	1:F:192:LEU:HD12	1.92	0.52
1:F:277:ILE:HD12	1:F:279:ARG:HD3	1.91	0.51
1:G:471:GLU:HB3	1:G:473:TYR:HE2	1.73	0.51
1:H:265:LEU:HD11	1:H:341:ALA:CB	2.40	0.51
1:E:34:ASP:OD1	1:E:34:ASP:N	2.41	0.51
1:D:208:TYR:CE2	1:D:210:GLY:HA3	2.45	0.51
1:H:305:ALA:O	1:H:309:MET:HG3	2.10	0.51
1:B:279:ARG:NH1	1:B:430:GLN:NE2	2.57	0.51
1:C:112:ASN:HB3	1:C:129:GLY:HA3	1.93	0.51
1:G:286:ALA:HA	1:G:389:TRP:CE3	2.44	0.51
1:B:289:SER:OG	1:B:294:TRP:HZ3	1.92	0.51
1:E:23:SER:HB3	1:E:28:SER:HA	1.92	0.51
1:E:284:ASP:CG	1:E:367:LEU:HD12	2.31	0.51
1:F:408:ASP:O	1:F:412:GLN:HG3	2.11	0.51
1:D:357:PRO:O	1:D:359:ARG:HG3	2.10	0.51
1:H:351:GLU:OE1	1:H:356:LEU:HD12	2.11	0.51
1:B:152:GLU:HG3	2:B:601:FAD:N5	2.25	0.51
1:D:500:SER:O	1:D:504:ILE:HG13	2.11	0.51
1:H:179:ARG:NH1	1:H:221:GLU:OE1	2.44	0.51
1:H:121:LEU:HD13	1:H:207:LEU:HD21	1.93	0.51
1:H:243:LEU:HD12	1:H:353:ASN:OD1	2.10	0.51
1:G:345:ILE:HD12	1:G:345:ILE:N	2.21	0.51
1:E:85:SER:O	1:E:108:GLY:HA3	2.11	0.51
1:E:279:ARG:NH2	1:E:430:GLN:OE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:258:ILE:O	1:H:262:THR:HG23	2.11	0.51
1:E:242:MET:SD	1:E:376:THR:HG22	2.51	0.50
1:A:89:ASN:HA	2:A:601:FAD:H5'2	1.92	0.50
1:G:192:LEU:HD12	1:H:496:ILE:HG23	1.94	0.50
1:A:293:GLU:O	1:A:293:GLU:HG2	2.10	0.50
1:D:89:ASN:HA	2:D:601:FAD:H5'2	1.94	0.50
1:F:81:LEU:HD22	1:F:105:LEU:HD21	1.93	0.50
1:F:124:ALA:HB2	1:F:235:LEU:HD11	1.94	0.50
1:D:297:GLU:H	1:D:297:GLU:CD	2.14	0.50
1:E:107:LEU:HD13	1:E:111:MET:CE	2.41	0.50
1:C:256:PRO:O	1:C:260:GLU:HG3	2.11	0.50
1:C:259:MET:HE3	1:C:433:ILE:HD11	1.93	0.50
1:G:269:MET:HG3	1:G:435:LEU:HD11	1.93	0.50
1:C:525:ARG:NH2	1:C:526:LEU:HD21	2.26	0.50
1:E:11:SER:OG	1:E:14:GLN:HG3	2.12	0.50
1:G:411:LYS:O	1:G:415:ASP:HB2	2.10	0.50
1:C:204:ALA:HA	1:C:207:LEU:HD12	1.92	0.50
1:C:486:VAL:HG12	1:D:212:LEU:HD22	1.94	0.50
1:F:70:ILE:HG21	1:F:105:LEU:HD11	1.94	0.50
1:G:315:ILE:HD12	1:G:319:ILE:HD11	1.93	0.50
1:G:471:GLU:HB2	1:G:473:TYR:HD2	1.70	0.50
1:H:159:MET:HE1	1:H:228:CYS:O	2.11	0.50
1:H:246:ALA:HB2	1:H:368:LEU:HD12	1.93	0.50
1:A:448:THR:O	1:A:454:ARG:NH2	2.44	0.50
1:G:408:ASP:O	1:G:412:GLN:HB2	2.11	0.50
1:F:21:GLU:CA	1:F:24:GLU:HG3	2.39	0.49
1:G:436:ARG:O	1:H:207:LEU:HD23	2.11	0.49
1:H:327:PRO:HB2	1:H:329:TRP:CD1	2.47	0.49
1:B:524:GLU:CG	1:B:525:ARG:N	2.74	0.49
1:E:433:ILE:HG22	1:E:433:ILE:O	2.11	0.49
1:H:290:LYS:O	1:H:294:TRP:HZ3	1.95	0.49
1:C:306:LYS:HA	1:C:309:MET:CE	2.42	0.49
1:G:283:PHE:CZ	1:G:443:LEU:HD13	2.48	0.49
1:C:395:HIS:HB2	1:C:443:LEU:HD12	1.94	0.49
1:G:467:ALA:O	1:G:471:GLU:HG2	2.12	0.49
1:A:286:ALA:HA	1:A:389:TRP:CE3	2.47	0.49
1:C:163:MET:HE1	1:C:228:CYS:CB	2.41	0.49
1:F:7:PRO:HG2	1:F:10:VAL:HG21	1.94	0.49
1:H:279:ARG:NH1	1:H:430:GLN:OE1	2.46	0.49
1:B:292:GLU:HA	1:B:295:GLN:O	2.12	0.49
1:C:363:ARG:HA	1:C:366:GLU:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:277:ILE:HB	1:E:430:GLN:NE2	2.18	0.49
1:G:18:ALA:CB	1:G:79:ILE:HD12	2.43	0.49
1:E:279:ARG:NH1	1:E:430:GLN:HB2	2.28	0.49
1:G:283:PHE:CD2	1:G:428:LEU:HB3	2.48	0.49
1:H:199:LEU:HD22	1:H:202:SER:HB2	1.95	0.49
1:H:428:LEU:HB2	1:H:443:LEU:O	2.13	0.49
1:B:279:ARG:NH1	1:B:430:GLN:HE22	2.11	0.49
1:E:399:ALA:HA	1:E:440:HIS:O	2.12	0.49
1:G:255:LEU:HD22	1:G:318:TRP:CZ2	2.48	0.49
1:H:283:PHE:CD2	1:H:428:LEU:HB3	2.48	0.49
1:A:53:PHE:HE2	1:A:481:VAL:HG12	1.73	0.48
1:C:149:ASP:OD1	1:C:168:GLY:HA3	2.13	0.48
1:D:88:ARG:HD3	1:D:155:TRP:CD1	2.48	0.48
1:D:108:GLY:O	1:D:112:ASN:HB3	2.13	0.48
1:H:370:ALA:CB	1:H:382:HIS:CD2	2.95	0.48
1:A:398:TYR:CE1	1:A:475:ILE:HD11	2.48	0.48
1:E:506:ASP:OD2	1:E:524:GLU:HG3	2.13	0.48
1:G:369:ASN:O	1:G:373:GLU:HG3	2.13	0.48
1:H:308:ARG:O	1:H:312:GLU:CB	2.60	0.48
1:H:339:ARG:NH1	1:H:343:LEU:HD12	2.28	0.48
1:A:35:GLU:O	1:A:39:SER:OG	2.26	0.48
1:B:256:PRO:HG3	1:B:410:ALA:HB2	1.95	0.48
1:D:306:LYS:HA	1:D:309:MET:HE3	1.95	0.48
1:G:208:TYR:CE2	1:G:210:GLY:HA3	2.47	0.48
1:B:171:PRO:HB2	1:B:236:MET:HE3	1.96	0.48
1:C:289:SER:OG	1:C:294:TRP:HH2	1.92	0.48
1:D:479:HIS:ND1	1:D:481:VAL:HG12	2.29	0.48
1:H:41:TYR:CE2	1:H:58:VAL:HG21	2.48	0.48
1:H:353:ASN:HB3	1:H:368:LEU:HD21	1.95	0.48
1:A:255:LEU:HB3	1:A:256:PRO:HD3	1.94	0.48
1:A:395:HIS:HB2	1:A:443:LEU:HD12	1.96	0.48
1:F:7:PRO:O	1:F:10:VAL:HB	2.13	0.48
1:G:6:LEU:HG	1:G:7:PRO:HD2	1.93	0.48
1:H:29:GLU:HG3	1:H:30:TYR:CE2	2.48	0.48
1:B:69:VAL:O	1:B:73:ILE:HG12	2.13	0.48
1:D:171:PRO:HB2	1:D:236:MET:HE1	1.95	0.48
1:D:411:LYS:CD	1:D:471:GLU:OE1	2.54	0.48
1:B:501:HIS:HB3	1:B:521:ILE:HG12	1.95	0.48
1:B:164:GLU:HG3	1:B:477:ARG:NE	2.28	0.48
1:E:135:LEU:HD22	1:E:158:VAL:HG21	1.96	0.48
1:G:53:PHE:CE2	1:G:481:VAL:HG12	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:333:LYS:O	1:H:337:MET:HG3	2.14	0.48
1:B:289:SER:CB	1:B:294:TRP:CH2	2.97	0.48
1:G:329:TRP:CE2	1:H:333:LYS:HD3	2.49	0.48
1:B:18:ALA:CB	1:B:79:ILE:HD12	2.44	0.47
1:B:351:GLU:OE1	1:B:355:THR:HG22	2.14	0.47
1:D:65:GLU:O	1:D:69:VAL:HG23	2.13	0.47
1:F:488:GLU:O	1:F:495:HIS:NE2	2.42	0.47
1:H:404:PRO:HA	1:H:438:MET:HB2	1.96	0.47
1:B:330:GLN:HE21	1:B:334:TYR:HE2	1.59	0.47
1:G:288:VAL:CG1	1:G:367:LEU:HD21	2.44	0.47
1:H:405:SER:OG	1:H:407:GLU:HG3	2.14	0.47
1:E:248:TYR:CD1	1:E:315:ILE:HA	2.49	0.47
1:E:486:VAL:HG12	1:F:212:LEU:HD22	1.96	0.47
1:E:283:PHE:CE2	1:E:443:LEU:HD13	2.49	0.47
1:G:75:ASN:ND2	1:G:187:ALA:O	2.41	0.47
1:A:344:GLN:OE1	1:H:524:GLU:OE1	2.31	0.47
1:B:419:ILE:HG23	1:B:463:GLU:OE1	2.14	0.47
1:C:13:GLU:HG2	1:C:14:GLN:OE1	2.13	0.47
1:E:53:PHE:CE2	1:E:481:VAL:HG22	2.49	0.47
1:G:89:ASN:HA	2:G:601:FAD:H5'2	1.95	0.47
1:A:222:GLN:NE2	1:A:477:ARG:HG3	2.29	0.47
1:A:280:ASN:HB3	1:A:318:TRP:CZ3	2.49	0.47
1:E:208:TYR:CE2	1:E:210:GLY:HA3	2.49	0.47
1:E:266:ARG:HG2	1:E:433:ILE:CG2	2.44	0.47
1:G:263:LEU:HD11	1:G:267:ILE:HD12	1.97	0.47
1:H:154:ASP:CB	1:H:379:PRO:HB2	2.45	0.47
1:A:294:TRP:HZ3	1:A:312:GLU:HG3	1.79	0.47
1:C:164:GLU:HG3	1:C:477:ARG:NE	2.29	0.47
1:G:304:GLU:O	1:G:308:ARG:CG	2.46	0.47
1:H:262:THR:OG1	1:H:433:ILE:HD12	2.15	0.47
1:C:395:HIS:CD2	1:C:443:LEU:HD11	2.50	0.47
1:C:13:GLU:CG	1:C:14:GLN:OE1	2.63	0.46
1:H:356:LEU:N	1:H:357:PRO:CD	2.77	0.46
1:H:399:ALA:HA	1:H:440:HIS:O	2.15	0.46
1:A:47:VAL:HG22	1:A:458:LEU:HB2	1.97	0.46
1:A:400:PRO:HD2	1:A:440:HIS:O	2.14	0.46
1:D:441:ILE:HD13	3:D:602:H7Y:CAH	2.45	0.46
1:D:523:PRO:HG2	1:D:526:LEU:HD12	1.97	0.46
1:G:56:SER:HB3	1:G:101:GLY:HA2	1.98	0.46
1:H:133:LYS:O	1:H:137:GLU:HG3	2.16	0.46
1:A:507:ALA:HB2	1:B:507:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:LEU:O	1:B:259:MET:HG2	2.15	0.46
1:F:22:PHE:O	1:F:26:ILE:HG12	2.15	0.46
1:H:65:GLU:O	1:H:69:VAL:HG23	2.15	0.46
1:H:286:ALA:HA	1:H:389:TRP:CE3	2.51	0.46
1:C:291:ARG:NH1	1:C:301:LEU:HG	2.30	0.46
1:D:405:SER:HB2	1:D:408:ASP:HB2	1.96	0.46
1:E:479:HIS:CE1	1:E:481:VAL:HG23	2.50	0.46
1:H:321:TYR:CD2	1:H:371:ARG:HG3	2.50	0.46
1:A:65:GLU:O	1:A:69:VAL:HG23	2.15	0.46
1:F:328:ARG:HD2	1:F:328:ARG:HA	1.40	0.46
1:G:44:LYS:HD3	1:G:44:LYS:HA	1.67	0.46
1:F:149:ASP:OD1	1:F:168:GLY:HA3	2.15	0.46
1:H:203:GLU:O	1:H:207:LEU:HD13	2.15	0.46
1:C:359:ARG:HG3	1:C:359:ARG:HH11	1.80	0.46
1:C:398:TYR:CE1	1:C:475:ILE:HD11	2.51	0.46
1:E:330:GLN:HE21	1:E:334:TYR:HE2	1.60	0.46
1:H:3:PHE:HD1	1:H:33:VAL:HG11	1.78	0.46
1:H:416:THR:HB	1:H:427:TYR:CE2	2.51	0.46
1:A:492:PHE:CE2	1:B:193:ARG:HG3	2.51	0.46
1:B:292:GLU:OE1	1:B:296:THR:HA	2.16	0.46
1:B:410:ALA:O	1:B:414:GLU:HG2	2.16	0.46
1:F:178:TRP:HB2	1:F:233:MET:CE	2.46	0.46
1:H:136:TYR:OH	1:H:378:VAL:HG22	2.16	0.46
1:H:408:ASP:O	1:H:411:LYS:HB3	2.15	0.46
1:H:524:GLU:HA	1:H:527:ARG:HH21	1.81	0.46
1:B:289:SER:OG	1:B:294:TRP:CH2	2.55	0.45
1:D:410:ALA:O	1:D:414:GLU:CG	2.54	0.45
2:H:601:FAD:H8A	2:H:601:FAD:O5B	2.17	0.45
1:E:92:TYR:CE1	1:E:477:ARG:HG2	2.51	0.45
1:E:279:ARG:NH1	1:E:283:PHE:CZ	2.84	0.45
1:F:21:GLU:HA	1:F:24:GLU:CG	2.42	0.45
1:F:171:PRO:HB2	1:F:236:MET:CE	2.41	0.45
1:G:240:PRO:C	1:G:241:GLU:HG2	2.37	0.45
1:A:291:ARG:NH1	1:A:426:ASP:CG	2.70	0.45
1:G:192:LEU:HD21	1:G:216:ILE:HD11	1.99	0.45
2:H:601:FAD:O2P	2:H:601:FAD:O4'	2.28	0.45
1:A:341:ALA:O	1:A:344:GLN:HG2	2.16	0.45
1:G:382:HIS:O	1:G:384:ALA:N	2.49	0.45
1:A:213:GLY:HA2	1:B:222:GLN:O	2.17	0.45
1:G:163:MET:HE3	2:G:601:FAD:C8A	2.46	0.45
1:H:248:TYR:CD1	1:H:315:ILE:HA	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:60:TRP:CG	1:G:109:LYS:HG2	2.52	0.45
1:G:81:LEU:HA	1:G:103:VAL:O	2.17	0.45
1:A:245:PHE:CZ	1:A:322:GLY:HA3	2.51	0.45
1:A:405:SER:CB	1:A:408:ASP:HB2	2.47	0.45
1:A:428:LEU:HB2	1:A:443:LEU:O	2.17	0.45
1:C:148:ILE:HG13	1:C:150:PRO:HD3	1.97	0.45
1:C:255:LEU:HB3	1:C:256:PRO:HD3	1.99	0.45
1:E:279:ARG:NH2	1:E:430:GLN:NE2	2.65	0.45
1:H:33:VAL:HG12	1:H:33:VAL:O	2.17	0.45
1:H:351:GLU:HG3	1:H:356:LEU:CD1	2.46	0.45
1:B:246:ALA:HB2	1:B:368:LEU:HD13	1.98	0.45
1:C:152:GLU:HG2	1:C:371:ARG:HH22	1.81	0.45
1:H:409:ALA:HB2	1:H:438:MET:HE1	1.98	0.45
1:A:216:ILE:O	1:A:219:LEU:HB2	2.17	0.45
1:D:171:PRO:CG	1:D:236:MET:HE1	2.47	0.45
1:E:85:SER:HB3	1:E:128:PRO:O	2.16	0.45
1:A:41:TYR:HB3	1:A:104:LEU:HD23	1.99	0.45
1:D:159:MET:HE2	1:D:231:MET:HB2	2.00	0.45
1:D:294:TRP:HH2	1:D:312:GLU:HG2	1.82	0.45
1:E:290:LYS:HG3	1:E:388:ASP:O	2.18	0.45
1:G:107:LEU:HD11	1:G:227:ILE:HG23	1.99	0.45
1:C:351:GLU:OE2	1:C:355:THR:OG1	2.23	0.44
1:E:116:GLU:HB3	1:E:125:VAL:HG23	1.99	0.44
1:E:243:LEU:HD23	1:E:335:ILE:HG13	1.98	0.44
1:E:289:SER:OG	1:E:294:TRP:HH2	1.95	0.44
1:E:292:GLU:HB3	1:E:295:GLN:O	2.17	0.44
1:F:89:ASN:HA	2:F:601:FAD:H5'2	1.97	0.44
1:G:20:SER:O	1:G:24:GLU:HG3	2.17	0.44
1:G:451:PRO:HA	1:G:454:ARG:HD2	1.99	0.44
1:H:291:ARG:HH11	1:H:426:ASP:CG	2.15	0.44
1:F:179:ARG:NH1	1:F:221:GLU:OE2	2.51	0.44
1:C:221:GLU:OE1	1:C:221:GLU:HA	2.18	0.44
2:A:601:FAD:H8A	2:A:601:FAD:O5B	2.18	0.44
1:D:7:PRO:HG2	1:D:10:VAL:HB	1.98	0.44
1:D:69:VAL:O	1:D:73:ILE:HG12	2.17	0.44
1:A:283:PHE:HZ	3:A:602:H7Y:CAA	2.30	0.44
1:A:291:ARG:NH1	1:A:426:ASP:OD1	2.50	0.44
1:F:47:VAL:HG11	1:F:396:PHE:CE1	2.53	0.44
1:F:149:ASP:OD2	1:F:170:THR:OG1	2.34	0.44
1:C:13:GLU:HG3	1:C:14:GLN:N	2.33	0.44
1:E:192:LEU:HD21	1:E:216:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:99:LEU:HD21	1:G:522:TRP:HZ3	1.82	0.44
1:H:284:ASP:OD2	1:H:319:ILE:HD13	2.18	0.44
1:B:85:SER:HB3	1:B:128:PRO:O	2.18	0.44
1:E:137:GLU:O	1:E:140:ARG:HB3	2.18	0.44
1:G:10:VAL:HG13	1:G:14:GLN:HG3	1.99	0.44
1:G:76:LYS:HE2	1:G:77:TYR:CZ	2.53	0.44
1:H:289:SER:CB	1:H:294:TRP:HH2	2.31	0.44
1:B:182:MET:HG2	1:B:231:MET:HG3	2.00	0.43
1:C:70:ILE:HG21	1:C:105:LEU:HD21	2.00	0.43
1:E:256:PRO:HA	1:E:406:GLY:CA	2.48	0.43
1:G:32:ARG:NH2	1:G:34:ASP:OD2	2.51	0.43
1:H:216:ILE:O	1:H:219:LEU:HB2	2.18	0.43
1:C:304:GLU:O	1:C:308:ARG:HG3	2.17	0.43
1:G:53:PHE:CZ	1:G:481:VAL:HG12	2.52	0.43
1:G:412:GLN:HE21	1:G:440:HIS:HB2	1.82	0.43
1:F:7:PRO:HG2	1:F:10:VAL:HG11	2.00	0.43
1:F:47:VAL:HG22	1:F:47:VAL:O	2.19	0.43
1:G:400:PRO:HB2	1:G:473:TYR:HB3	2.00	0.43
1:G:412:GLN:HE21	1:G:440:HIS:CB	2.31	0.43
1:A:192:LEU:CD2	1:A:216:ILE:HD11	2.49	0.43
1:C:291:ARG:HD2	1:C:426:ASP:OD2	2.18	0.43
1:G:395:HIS:HA	1:G:444:PRO:O	2.18	0.43
1:H:301:LEU:HD23	1:H:301:LEU:HA	1.86	0.43
1:G:148:ILE:HG13	1:G:150:PRO:HD3	2.00	0.43
1:H:19:ILE:O	1:H:23:SER:HB2	2.18	0.43
1:D:216:ILE:HB	1:D:219:LEU:HD12	2.01	0.43
1:E:23:SER:HA	1:E:31:VAL:HG21	2.00	0.43
1:F:171:PRO:CB	1:F:236:MET:HE1	2.44	0.43
1:F:182:MET:HG2	1:F:231:MET:HG3	2.00	0.43
1:A:199:LEU:HD23	1:A:200:PRO:O	2.19	0.43
1:B:216:ILE:HB	1:B:219:LEU:HD12	2.01	0.43
1:D:71:VAL:O	1:D:75:ASN:ND2	2.52	0.43
1:C:411:LYS:HE2	1:C:411:LYS:HB2	1.62	0.43
1:F:64:THR:O	1:F:68:GLN:HG3	2.18	0.43
1:G:171:PRO:HB2	1:G:236:MET:HE3	2.01	0.43
1:G:47:VAL:HG22	1:G:458:LEU:HB2	1.99	0.43
1:G:116:GLU:HB3	1:G:125:VAL:HB	2.00	0.43
1:B:149:ASP:OD1	1:B:168:GLY:HA3	2.19	0.43
1:B:33:VAL:HG12	1:B:57:ALA:HB2	2.01	0.42
1:C:153:LEU:HD13	1:C:155:TRP:CZ2	2.53	0.42
1:D:199:LEU:HD23	1:D:202:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:159:MET:O	1:F:163:MET:HG3	2.18	0.42
1:H:416:THR:HB	1:H:427:TYR:HE2	1.84	0.42
1:D:204:ALA:HA	1:D:207:LEU:HD12	2.00	0.42
1:H:240:PRO:HG2	1:H:327:PRO:HG3	2.00	0.42
1:A:336:GLU:OE2	1:A:339:ARG:NH2	2.53	0.42
1:A:339:ARG:O	1:A:343:LEU:HG	2.19	0.42
1:C:32:ARG:HD3	1:C:32:ARG:HA	1.78	0.42
1:D:258:ILE:O	1:D:262:THR:OG1	2.25	0.42
1:E:52:GLU:HB3	1:E:53:PHE:CE2	2.55	0.42
1:E:120:LYS:O	1:F:263:LEU:HD21	2.19	0.42
1:E:216:ILE:O	1:E:219:LEU:HB2	2.19	0.42
1:F:280:ASN:HB3	1:F:318:TRP:CZ3	2.54	0.42
1:H:351:GLU:CG	1:H:356:LEU:CD1	2.97	0.42
1:C:63:SER:O	1:C:67:VAL:HG23	2.19	0.42
1:H:294:TRP:NE1	1:H:312:GLU:CD	2.73	0.42
1:F:248:TYR:CD1	1:F:315:ILE:HA	2.54	0.42
1:F:435:LEU:HD12	1:F:435:LEU:HA	1.94	0.42
1:H:97:PRO:HG3	1:H:104:LEU:HD21	2.02	0.42
1:B:243:LEU:HD23	1:B:335:ILE:HG13	2.01	0.42
1:C:398:TYR:HB3	1:C:442:CYS:HB3	2.02	0.42
1:G:403:ALA:HA	1:G:404:PRO:HD3	1.89	0.42
1:H:249:PHE:HB3	1:H:254:ASP:OD2	2.19	0.42
1:H:416:THR:CG2	1:H:427:TYR:CE2	3.02	0.42
1:A:336:GLU:OE2	1:A:339:ARG:NE	2.51	0.42
1:B:411:LYS:HE2	1:B:471:GLU:OE1	2.20	0.42
1:C:53:PHE:CE2	1:C:481:VAL:CG1	3.03	0.42
1:D:216:ILE:O	1:D:219:LEU:HB2	2.18	0.42
1:D:501:HIS:HB3	1:D:521:ILE:HG12	2.00	0.42
1:G:246:ALA:HB2	1:G:368:LEU:CD2	2.47	0.42
1:H:409:ALA:C	1:H:411:LYS:N	2.72	0.42
1:D:306:LYS:HA	1:D:309:MET:HE2	2.01	0.42
1:E:402:SER:HB3	1:E:473:TYR:CD1	2.55	0.42
1:F:491:SER:HA	1:F:495:HIS:CD2	2.55	0.42
1:G:342:TYR:C	1:G:345:ILE:HD12	2.37	0.42
1:H:356:LEU:N	1:H:357:PRO:HD3	2.34	0.42
1:B:399:ALA:HA	1:B:440:HIS:O	2.20	0.42
1:B:476:TYR:OH	3:B:602:H7Y:OAC	2.38	0.42
1:C:161:ASN:OD1	1:C:166:GLY:HA3	2.20	0.42
1:C:306:LYS:HA	1:C:309:MET:HE3	2.02	0.42
1:D:224:ASN:OD1	1:D:224:ASN:N	2.52	0.42
1:E:255:LEU:HA	1:E:258:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:92:TYR:HA	1:F:479:HIS:HA	2.02	0.42
1:H:249:PHE:CE2	1:H:345:ILE:HD12	2.55	0.42
1:E:428:LEU:HB2	1:E:443:LEU:O	2.20	0.41
1:F:178:TRP:HB2	1:F:233:MET:HE1	2.02	0.41
1:H:112:ASN:CB	1:H:129:GLY:HA3	2.50	0.41
1:B:286:ALA:HA	1:B:389:TRP:CE3	2.55	0.41
1:D:404:PRO:HB3	1:D:433:ILE:CD1	2.50	0.41
1:E:292:GLU:HA	1:E:295:GLN:O	2.20	0.41
1:A:291:ARG:NH2	1:A:299:GLY:O	2.52	0.41
1:B:486:VAL:O	1:B:489:THR:OG1	2.29	0.41
1:D:119:GLU:OE2	1:D:144:ALA:HA	2.21	0.41
1:F:70:ILE:HD13	1:F:105:LEU:HD11	2.02	0.41
1:F:164:GLU:HG3	1:F:477:ARG:NE	2.35	0.41
1:F:277:ILE:CD1	1:F:371:ARG:HD2	2.48	0.41
1:F:339:ARG:HE	1:F:339:ARG:HB3	1.68	0.41
1:G:211:GLN:N	1:G:211:GLN:OE1	2.54	0.41
1:F:291:ARG:NH1	1:F:426:ASP:OD2	2.53	0.41
1:F:398:TYR:HB3	1:F:442:CYS:HB3	2.02	0.41
1:G:492:PHE:CE1	1:G:493:ASN:HB2	2.56	0.41
1:A:32:ARG:HG3	1:A:37:THR:HG21	2.02	0.41
1:C:243:LEU:HD11	1:C:354:GLU:HG3	2.03	0.41
1:D:248:TYR:CE1	1:D:315:ILE:HG22	2.56	0.41
1:F:167:VAL:CG2	3:F:602:H7Y:CAB	2.99	0.41
1:D:478:ALA:HB1	1:D:482:LEU:HB2	2.03	0.41
1:F:349:ARG:HG2	1:F:350:PHE:N	2.35	0.41
1:G:412:GLN:OE1	1:G:473:TYR:CE1	2.73	0.41
1:H:56:SER:HB3	1:H:101:GLY:HA2	2.01	0.41
1:H:164:GLU:HG3	1:H:477:ARG:NE	2.36	0.41
1:A:329:TRP:O	1:A:333:LYS:HG2	2.21	0.41
1:A:333:LYS:O	1:A:337:MET:HG3	2.21	0.41
1:A:395:HIS:HB2	1:A:443:LEU:CD1	2.51	0.41
1:E:371:ARG:NH1	1:E:374:LEU:HD12	2.35	0.41
1:H:294:TRP:NE1	1:H:309:MET:HG2	2.31	0.41
1:B:25:THR:HB	1:B:69:VAL:HG11	2.02	0.41
1:B:505:LYS:NZ	1:B:509:ASP:OD2	2.41	0.41
1:D:171:PRO:HD2	1:D:236:MET:CE	2.50	0.41
1:G:99:LEU:HD11	1:G:516:PRO:HB2	2.02	0.41
1:G:248:TYR:CD1	1:G:315:ILE:HA	2.56	0.41
1:G:302:THR:O	1:G:306:LYS:HG3	2.21	0.41
1:H:136:TYR:CZ	1:H:378:VAL:HG22	2.55	0.41
1:H:523:PRO:HD2	1:H:526:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:LEU:HD11	1:A:259:MET:HE2	2.03	0.41
1:A:357:PRO:O	1:A:365:SER:HB2	2.21	0.41
1:B:279:ARG:NH1	1:B:283:PHE:CE1	2.89	0.41
1:B:279:ARG:HD3	1:B:283:PHE:CG	2.56	0.41
1:B:305:ALA:O	1:B:309:MET:HG3	2.20	0.41
1:B:350:PHE:HE1	1:B:352:THR:HG22	1.86	0.41
1:C:321:TYR:CD1	1:C:371:ARG:HG3	2.56	0.41
1:C:362:ASP:OD2	1:C:365:SER:HB3	2.21	0.41
1:D:149:ASP:OD2	1:D:175:HIS:NE2	2.53	0.41
1:D:427:TYR:CZ	1:D:429:ALA:HB2	2.55	0.41
1:E:107:LEU:HD13	1:E:111:MET:HE1	2.02	0.41
1:E:471:GLU:HB2	1:E:473:TYR:CD2	2.56	0.41
1:G:436:ARG:NH2	1:H:235:LEU:O	2.53	0.41
1:H:159:MET:CE	2:H:601:FAD:H61A	2.34	0.41
1:H:304:GLU:H	1:H:304:GLU:HG3	1.62	0.41
1:H:393:ALA:HB1	1:H:445:LEU:HD22	2.03	0.41
1:H:416:THR:CB	1:H:427:TYR:HE2	2.33	0.41
1:B:115:LEU:HD23	1:B:115:LEU:HA	1.94	0.41
1:B:248:TYR:CE1	1:B:315:ILE:HG22	2.56	0.41
1:D:310:VAL:HG21	1:D:317:HIS:CD2	2.56	0.41
1:D:523:PRO:CG	1:D:526:LEU:HD12	2.51	0.41
1:E:248:TYR:CE1	1:E:315:ILE:HG22	2.56	0.41
1:H:255:LEU:HB3	1:H:256:PRO:HD3	2.03	0.41
1:H:321:TYR:CG	1:H:371:ARG:HG3	2.56	0.41
1:E:428:LEU:HD22	1:E:443:LEU:HD22	2.02	0.40
1:H:309:MET:C	1:H:312:GLU:HB2	2.42	0.40
1:E:478:ALA:HB1	1:E:482:LEU:HB2	2.03	0.40
1:F:135:LEU:HG	1:F:148:ILE:HG21	2.02	0.40
1:G:128:PRO:HG3	1:G:159:MET:HE1	2.04	0.40
1:A:308:ARG:O	1:A:312:GLU:CG	2.69	0.40
1:E:472:GLY:O	1:F:202:SER:HA	2.21	0.40
1:G:288:VAL:CG1	1:G:367:LEU:CD2	2.99	0.40
1:H:112:ASN:HB3	1:H:129:GLY:HA3	2.02	0.40
1:D:4:ARG:HH11	1:D:38:VAL:HG12	1.87	0.40
1:D:427:TYR:CE1	1:D:429:ALA:HB2	2.57	0.40
1:E:506:ASP:CG	1:E:524:GLU:HG3	2.42	0.40
1:F:240:PRO:O	1:F:241:GLU:HG3	2.22	0.40
1:H:291:ARG:HB2	1:H:389:TRP:CE2	2.56	0.40
1:C:339:ARG:O	1:C:343:LEU:HG	2.21	0.40
1:C:403:ALA:HA	1:C:404:PRO:HD3	1.96	0.40
1:E:339:ARG:HG2	1:E:343:LEU:HD23	1.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:195:GLY:HA2	1:F:211:GLN:OE1	2.22	0.40
1:G:163:MET:HE1	2:G:601:FAD:C5A	2.51	0.40
1:H:108:GLY:O	1:H:112:ASN:HB3	2.21	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:ASP:OD1	1:F:13:GLU:OE2[1_655]	1.66	0.54
1:C:362:ASP:CG	1:F:13:GLU:OE2[1_655]	1.67	0.53
1:H:14:GLN:NE2	1:H:311:ASP:CG[1_655]	1.99	0.21
1:C:362:ASP:OD2	1:F:13:GLU:OE2[1_655]	2.06	0.14
1:H:14:GLN:NE2	1:H:311:ASP:OD2[1_655]	2.07	0.13

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	521/529 (98%)	495 (95%)	22 (4%)	4 (1%)	19	49
1	B	523/529 (99%)	503 (96%)	19 (4%)	1 (0%)	47	78
1	C	521/529 (98%)	494 (95%)	23 (4%)	4 (1%)	19	49
1	D	523/529 (99%)	500 (96%)	21 (4%)	2 (0%)	34	66
1	E	521/529 (98%)	498 (96%)	22 (4%)	1 (0%)	47	78
1	F	523/529 (99%)	501 (96%)	20 (4%)	2 (0%)	34	66
1	G	521/529 (98%)	495 (95%)	23 (4%)	3 (1%)	25	56
1	H	523/529 (99%)	492 (94%)	27 (5%)	4 (1%)	19	49
All	All	4176/4232 (99%)	3978 (95%)	177 (4%)	21 (0%)	29	61

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	296	THR
1	B	435	LEU
1	E	435	LEU
1	F	435	LEU
1	H	410	ALA
1	C	13	GLU
1	C	435	LEU
1	G	358	LEU
1	H	435	LEU
1	D	211	GLN
1	G	360	GLU
1	G	435	LEU
1	H	357	PRO
1	A	435	LEU
1	D	435	LEU
1	A	292	GLU
1	H	315	ILE
1	F	315	ILE
1	A	315	ILE
1	C	315	ILE
1	C	515	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	431/437 (99%)	418 (97%)	13 (3%)	41	75
1	B	433/437 (99%)	426 (98%)	7 (2%)	62	88
1	C	431/437 (99%)	423 (98%)	8 (2%)	57	85
1	D	433/437 (99%)	426 (98%)	7 (2%)	62	88
1	E	431/437 (99%)	417 (97%)	14 (3%)	39	73
1	F	433/437 (99%)	422 (98%)	11 (2%)	47	80
1	G	431/437 (99%)	419 (97%)	12 (3%)	43	77
1	H	433/437 (99%)	416 (96%)	17 (4%)	32	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3456/3496 (99%)	3367 (97%)	89 (3%)	46 79

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

Mol	Chain	Res	Type
1	A	116	GLU
1	A	179	ARG
1	A	283	PHE
1	A	297	GLU
1	A	328	ARG
1	A	360	GLU
1	A	367	LEU
1	A	382	HIS
1	A	395	HIS
1	A	415	ASP
1	A	418	ARG
1	A	453	SER
1	A	466	ARG
1	B	65	GLU
1	B	250	GLU
1	B	283	PHE
1	B	336	GLU
1	B	417	LYS
1	B	418	ARG
1	B	524	GLU
1	C	25	THR
1	C	140	ARG
1	C	145	LYS
1	C	283	PHE
1	C	304	GLU
1	C	359	ARG
1	C	360	GLU
1	C	466	ARG
1	D	241	GLU
1	D	242	MET
1	D	297	GLU
1	D	407	GLU
1	D	415	ASP
1	D	471	GLU
1	D	525	ARG
1	E	21	GLU
1	E	23	SER

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Mol	Chain	Res	Type
1	E	24	GLU
1	E	113	ARG
1	E	145	LYS
1	E	297	GLU
1	E	328	ARG
1	E	343	LEU
1	E	367	LEU
1	E	368	LEU
1	E	408	ASP
1	E	433	ILE
1	E	446	TYR
1	E	466	ARG
1	F	221	GLU
1	F	279	ARG
1	F	283	PHE
1	F	328	ARG
1	F	337	MET
1	F	339	ARG
1	F	390	PHE
1	F	433	ILE
1	F	503	ARG
1	F	525	ARG
1	F	527	ARG
1	G	145	LYS
1	G	250	GLU
1	G	283	PHE
1	G	309	MET
1	G	312	GLU
1	G	345	ILE
1	G	349	ARG
1	G	360	GLU
1	G	363	ARG
1	G	368	LEU
1	G	415	ASP
1	G	526	LEU
1	H	14	GLN
1	H	51	ASP
1	H	76	LYS
1	H	140	ARG
1	H	141	ASP
1	H	155	TRP
1	H	170	THR

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Mol	Chain	Res	Type
1	H	250	GLU
1	H	290	LYS
1	H	304	GLU
1	H	312	GLU
1	H	328	ARG
1	H	356	LEU
1	H	359	ARG
1	H	371	ARG
1	H	382	HIS
1	H	524	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	430	GLN
1	E	430	GLN
1	E	439	HIS
1	F	412	GLN
1	G	14	GLN
1	G	161	ASN
1	G	165	HIS
1	G	330	GLN
1	G	382	HIS
1	G	412	GLN
1	H	307	GLN
1	H	382	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 (i)

14 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	H7Y	A	602	-	12,12,12	1.56	2 (16%)	15,15,15	1.79	4 (26%)
3	H7Y	E	602	-	12,12,12	1.43	2 (16%)	15,15,15	1.13	1 (6%)
2	FAD	B	601	1	51,58,58	1.14	2 (3%)	60,89,89	1.80	7 (11%)
3	H7Y	C	602	-	12,12,12	1.61	2 (16%)	15,15,15	1.48	3 (20%)
2	FAD	D	601	1	51,58,58	1.18	2 (3%)	60,89,89	1.76	7 (11%)
2	FAD	A	601	1	51,58,58	1.17	2 (3%)	60,89,89	1.83	6 (10%)
2	FAD	G	601	1	51,58,58	1.12	2 (3%)	60,89,89	1.81	7 (11%)
3	H7Y	D	602	-	12,12,12	1.60	2 (16%)	15,15,15	1.51	3 (20%)
2	FAD	C	601	1	51,58,58	1.15	2 (3%)	60,89,89	1.76	7 (11%)
3	H7Y	F	602	-	12,12,12	1.52	2 (16%)	15,15,15	1.34	2 (13%)
2	FAD	E	601	1	51,58,58	1.10	2 (3%)	60,89,89	1.74	7 (11%)
2	FAD	H	601	1	51,58,58	1.08	3 (5%)	60,89,89	1.69	6 (10%)
2	FAD	F	601	1	51,58,58	1.10	2 (3%)	60,89,89	1.77	7 (11%)
3	H7Y	B	602	-	12,12,12	1.58	2 (16%)	15,15,15	1.53	3 (20%)

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	H7Y	A	602	-	-	0/5/5/5	0/1/1/1
3	H7Y	E	602	-	-	0/5/5/5	0/1/1/1
2	FAD	B	601	1	-	5/30/50/50	0/6/6/6
3	H7Y	C	602	-	-	1/5/5/5	0/1/1/1
2	FAD	D	601	1	-	4/30/50/50	0/6/6/6
2	FAD	A	601	1	-	3/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	G	601	1	-	5/30/50/50	0/6/6/6
3	H7Y	D	602	-	-	0/5/5/5	0/1/1/1
2	FAD	C	601	1	-	6/30/50/50	0/6/6/6
3	H7Y	F	602	-	-	2/5/5/5	0/1/1/1
2	FAD	E	601	1	-	14/30/50/50	0/6/6/6
2	FAD	H	601	1	-	7/30/50/50	0/6/6/6
2	FAD	F	601	1	-	5/30/50/50	0/6/6/6
3	H7Y	B	602	-	-	0/5/5/5	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	FAD	C4X-C10	6.20	1.45	1.38
2	A	601	FAD	C4X-C10	6.18	1.45	1.38
2	C	601	FAD	C4X-C10	6.17	1.45	1.38
2	B	601	FAD	C4X-C10	6.01	1.44	1.38
2	H	601	FAD	C4X-C10	5.73	1.44	1.38
2	G	601	FAD	C4X-C10	5.57	1.44	1.38
2	E	601	FAD	C4X-C10	5.55	1.44	1.38
2	F	601	FAD	C4X-C10	5.47	1.44	1.38
3	C	602	H7Y	CAE-CAD	3.99	1.54	1.30
3	B	602	H7Y	CAE-CAD	3.91	1.54	1.30
3	F	602	H7Y	CAE-CAD	3.87	1.53	1.30
3	E	602	H7Y	CAE-CAD	3.83	1.53	1.30
3	D	602	H7Y	CAE-CAD	3.79	1.53	1.30
3	A	602	H7Y	CAE-CAD	3.60	1.52	1.30
3	A	602	H7Y	CAJ-CAE	-3.36	1.37	1.47
3	D	602	H7Y	CAJ-CAE	-3.22	1.38	1.47
3	B	602	H7Y	CAJ-CAE	-3.01	1.38	1.47
2	C	601	FAD	C4-N3	2.93	1.38	1.33
3	C	602	H7Y	CAJ-CAE	-2.87	1.39	1.47
3	E	602	H7Y	CAJ-CAE	-2.85	1.39	1.47
3	F	602	H7Y	CAJ-CAE	-2.75	1.39	1.47
2	E	601	FAD	C4-N3	2.74	1.37	1.33
2	D	601	FAD	C4-N3	2.74	1.37	1.33
2	H	601	FAD	C4-N3	2.70	1.37	1.33
2	A	601	FAD	C4-N3	2.66	1.37	1.33
2	G	601	FAD	C4-N3	2.59	1.37	1.33
2	F	601	FAD	C4-N3	2.59	1.37	1.33
2	B	601	FAD	C4-N3	2.30	1.37	1.33
2	H	601	FAD	C4X-N5	-2.03	1.30	1.33

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	FAD	C4-N3-C2	8.49	122.31	115.14
2	A	601	FAD	C4-N3-C2	8.43	122.26	115.14
2	G	601	FAD	C4-N3-C2	8.16	122.03	115.14
2	D	601	FAD	C4-N3-C2	8.15	122.02	115.14
2	F	601	FAD	C4-N3-C2	8.11	121.99	115.14
2	C	601	FAD	C4-N3-C2	8.06	121.95	115.14
2	E	601	FAD	C4-N3-C2	7.88	121.79	115.14
2	H	601	FAD	C4-N3-C2	7.70	121.64	115.14
2	H	601	FAD	C10-C4X-N5	5.58	125.11	121.26
2	D	601	FAD	C4-C4X-C10	-5.50	116.31	119.95
2	B	601	FAD	C4-C4X-C10	-5.31	116.43	119.95
2	G	601	FAD	C10-C4X-N5	5.31	124.93	121.26
2	G	601	FAD	C4-C4X-C10	-5.26	116.47	119.95
2	A	601	FAD	C4-C4X-C10	-4.99	116.65	119.95
2	E	601	FAD	C10-C4X-N5	4.97	124.69	121.26
2	B	601	FAD	C10-C4X-N5	4.97	124.69	121.26
2	F	601	FAD	C10-C4X-N5	4.96	124.69	121.26
2	F	601	FAD	C4-C4X-C10	-4.94	116.68	119.95
2	A	601	FAD	C10-C4X-N5	4.93	124.67	121.26
2	E	601	FAD	C4-C4X-C10	-4.87	116.73	119.95
2	C	601	FAD	C10-C4X-N5	4.82	124.59	121.26
2	D	601	FAD	C10-C4X-N5	4.80	124.58	121.26
2	A	601	FAD	C4X-C4-N3	-4.65	117.07	123.43
2	C	601	FAD	C4X-C4-N3	-4.59	117.15	123.43
2	C	601	FAD	C4-C4X-C10	-4.55	116.94	119.95
2	B	601	FAD	C4X-C4-N3	-4.47	117.32	123.43
3	A	602	H7Y	OAI-CAL-CAK	4.44	121.00	114.57
2	D	601	FAD	C4X-C4-N3	-4.33	117.51	123.43
2	H	601	FAD	C4-C4X-C10	-4.29	117.11	119.95
2	E	601	FAD	C4X-C4-N3	-4.15	117.75	123.43
2	G	601	FAD	C4X-C4-N3	-4.11	117.81	123.43
2	F	601	FAD	C4X-C4-N3	-4.07	117.86	123.43
2	E	601	FAD	C4X-C10-N10	-3.94	116.26	120.30
2	H	601	FAD	C4X-C4-N3	-3.87	118.14	123.43
2	H	601	FAD	C4X-C10-N10	-3.79	116.40	120.30
2	C	601	FAD	C4X-C10-N10	-3.79	116.41	120.30
2	A	601	FAD	C4X-C10-N10	-3.75	116.45	120.30
3	B	602	H7Y	OAI-CAL-CAK	3.68	119.90	114.57
2	F	601	FAD	C1'-N10-C9A	3.55	121.09	118.29
2	D	601	FAD	C4X-C10-N10	-3.54	116.66	120.30
2	G	601	FAD	C1'-N10-C9A	3.52	121.06	118.29
2	B	601	FAD	C4X-C10-N10	-3.52	116.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	602	H7Y	OAI-CAL-CAK	3.45	119.56	114.57
2	F	601	FAD	C4X-C10-N10	-3.43	116.78	120.30
2	G	601	FAD	C4X-C10-N10	-3.38	116.83	120.30
3	C	602	H7Y	OAI-CAL-CAK	3.30	119.35	114.57
2	A	601	FAD	C1'-N10-C9A	3.27	120.87	118.29
2	C	601	FAD	C1'-N10-C9A	2.89	120.56	118.29
2	D	601	FAD	C1'-N10-C9A	2.84	120.53	118.29
3	F	602	H7Y	OAI-CAL-CAK	2.82	118.65	114.57
3	C	602	H7Y	CAJ-CAE-CAD	-2.65	117.42	126.97
2	B	601	FAD	C1'-N10-C9A	2.55	120.30	118.29
3	D	602	H7Y	CAJ-CAE-CAD	-2.47	118.08	126.97
3	C	602	H7Y	OAI-CAL-CAH	-2.45	119.90	124.12
2	C	601	FAD	C5A-C6A-N6A	2.44	124.06	120.35
2	E	601	FAD	C1'-N10-C9A	2.41	120.19	118.29
3	E	602	H7Y	OAI-CAL-CAK	2.41	118.05	114.57
3	A	602	H7Y	OAI-CAL-CAH	-2.38	120.02	124.12
3	F	602	H7Y	CAB-OAI-CAL	-2.36	113.96	117.53
3	B	602	H7Y	OAI-CAL-CAH	-2.28	120.19	124.12
3	D	602	H7Y	CAB-OAI-CAL	2.23	120.89	117.53
3	A	602	H7Y	CAA-CAD-CAE	-2.13	117.05	125.59
2	F	601	FAD	C5A-C6A-N6A	2.12	123.58	120.35
2	H	601	FAD	C5A-C6A-N6A	2.12	123.57	120.35
2	D	601	FAD	C5A-C6A-N6A	2.12	123.57	120.35
3	A	602	H7Y	CAF-CAJ-CAH	2.08	121.30	118.71
2	E	601	FAD	C1'-C2'-C3'	2.07	115.56	109.79
3	B	602	H7Y	CAJ-CAE-CAD	-2.04	119.62	126.97
2	B	601	FAD	C5A-C6A-N6A	2.04	123.45	120.35
2	G	601	FAD	C1'-C2'-C3'	2.01	115.40	109.79

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	601	FAD	N10-C1'-C2'-O2'
2	E	601	FAD	C1'-C2'-C3'-O3'
2	E	601	FAD	C1'-C2'-C3'-C4'
2	H	601	FAD	N10-C1'-C2'-C3'
2	E	601	FAD	O2'-C2'-C3'-O3'
2	E	601	FAD	O2'-C2'-C3'-C4'
2	E	601	FAD	C2'-C3'-C4'-O4'
2	B	601	FAD	O4'-C4'-C5'-O5'
2	C	601	FAD	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	G	601	FAD	O4'-C4'-C5'-O5'
2	E	601	FAD	C2'-C3'-C4'-C5'
2	E	601	FAD	O3'-C3'-C4'-O4'
2	D	601	FAD	C2'-C3'-C4'-O4'
2	H	601	FAD	C2'-C3'-C4'-O4'
2	H	601	FAD	O3'-C3'-C4'-O4'
2	C	601	FAD	C2'-C3'-C4'-O4'
2	B	601	FAD	C3'-C4'-C5'-O5'
2	C	601	FAD	C3'-C4'-C5'-O5'
2	F	601	FAD	C3'-C4'-C5'-O5'
2	G	601	FAD	C3'-C4'-C5'-O5'
2	D	601	FAD	C2'-C3'-C4'-C5'
2	H	601	FAD	C2'-C3'-C4'-C5'
2	G	601	FAD	O4B-C4B-C5B-O5B
2	F	601	FAD	C4'-C5'-O5'-P
2	H	601	FAD	C4'-C5'-O5'-P
2	F	601	FAD	O4'-C4'-C5'-O5'
2	C	601	FAD	C2'-C3'-C4'-C5'
2	E	601	FAD	C4'-C5'-O5'-P
2	H	601	FAD	O3'-C3'-C4'-C5'
3	F	602	H7Y	CAK-CAL-OAI-CAB
2	A	601	FAD	C4'-C5'-O5'-P
2	C	601	FAD	C4'-C5'-O5'-P
2	D	601	FAD	C4'-C5'-O5'-P
2	B	601	FAD	C4'-C5'-O5'-P
2	G	601	FAD	C4'-C5'-O5'-P
2	E	601	FAD	N10-C1'-C2'-C3'
2	D	601	FAD	O3'-C3'-C4'-O4'
3	F	602	H7Y	CAH-CAL-OAI-CAB
2	A	601	FAD	C2'-C3'-C4'-O4'
2	B	601	FAD	C2'-C3'-C4'-O4'
2	G	601	FAD	C3B-C4B-C5B-O5B
2	E	601	FAD	O3'-C3'-C4'-C5'
2	C	601	FAD	O3'-C3'-C4'-O4'
3	C	602	H7Y	CAD-CAE-CAJ-CAF
2	E	601	FAD	PA-O3P-P-O1P
2	E	601	FAD	PA-O3P-P-O2P
2	F	601	FAD	O2'-C2'-C3'-O3'
2	A	601	FAD	C3'-C4'-C5'-O5'
2	E	601	FAD	C3'-C4'-C5'-O5'
2	B	601	FAD	C1'-C2'-C3'-O3'
2	F	601	FAD	C1'-C2'-C3'-O3'

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Mol	Chain	Res	Type	Atoms
2	H	601	FAD	C1'-C2'-C3'-O3'

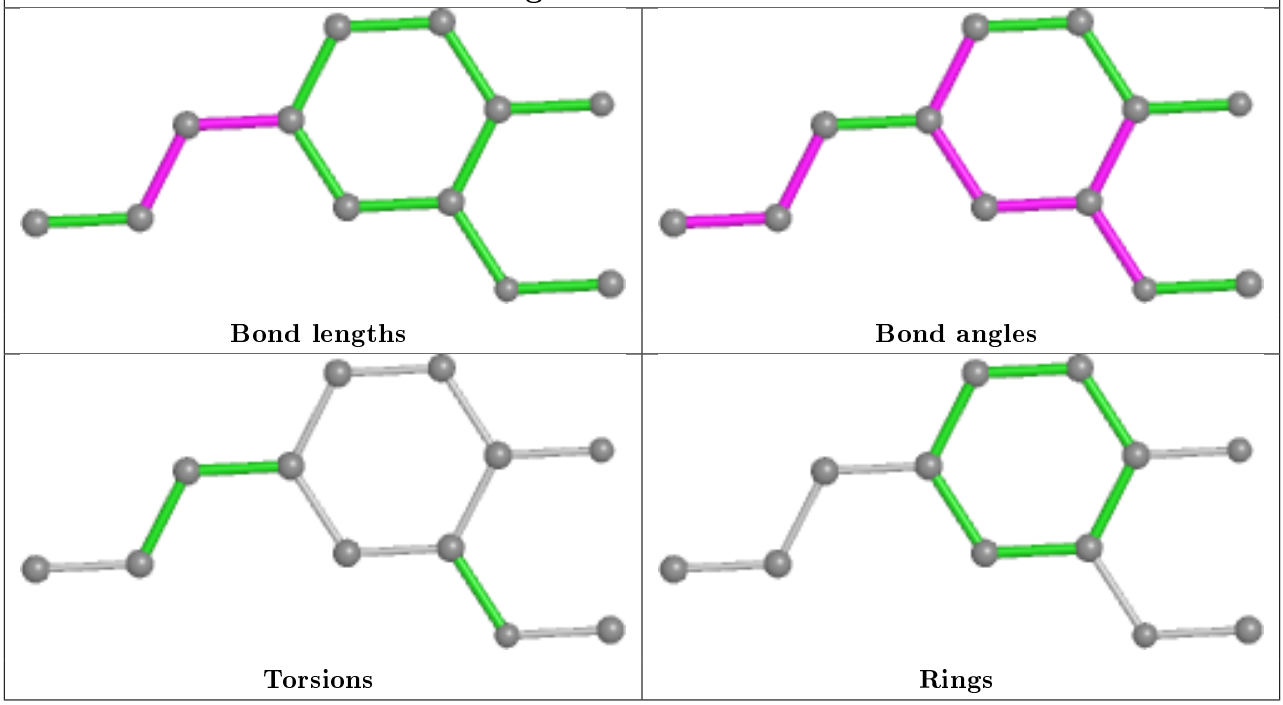
There are no ring outliers.

13 monomers are involved in 29 short contacts:

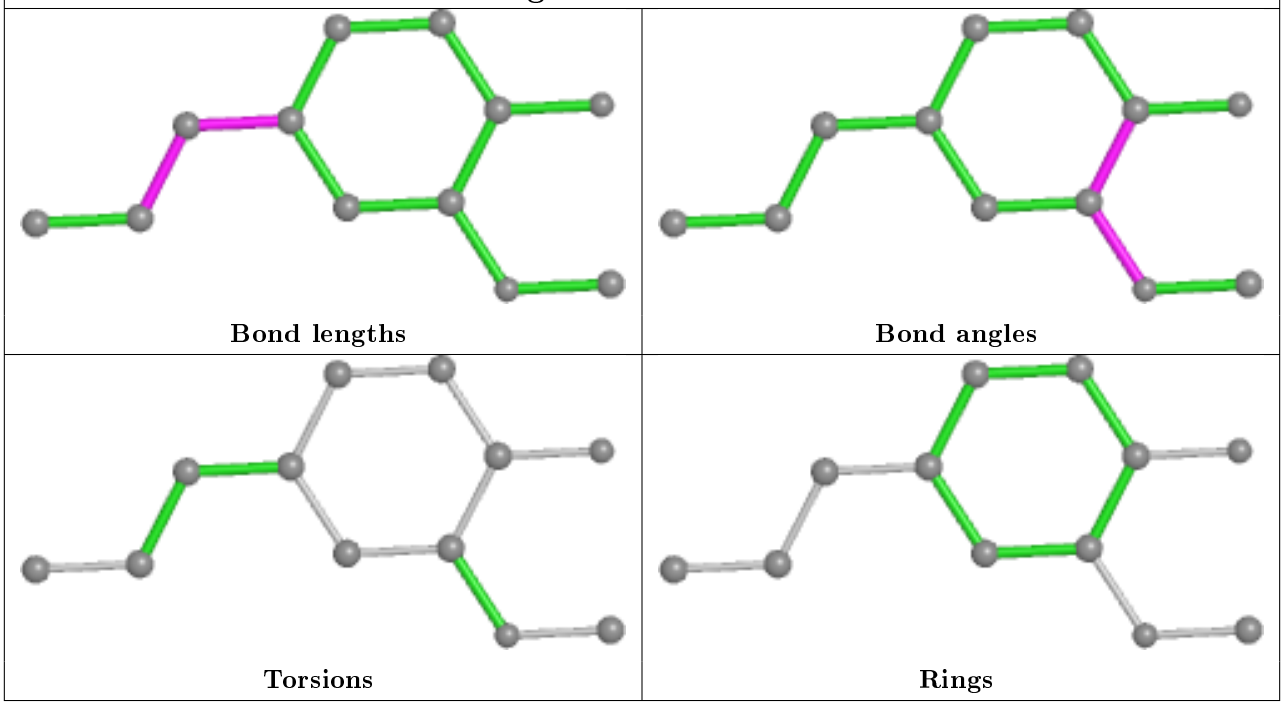
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	H7Y	2	0
2	B	601	FAD	2	0
3	C	602	H7Y	1	0
2	D	601	FAD	2	0
2	A	601	FAD	2	0
2	G	601	FAD	3	0
3	D	602	H7Y	2	0
2	C	601	FAD	1	0
3	F	602	H7Y	2	0
2	E	601	FAD	2	0
2	H	601	FAD	6	0
2	F	601	FAD	3	0
3	B	602	H7Y	1	0

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.

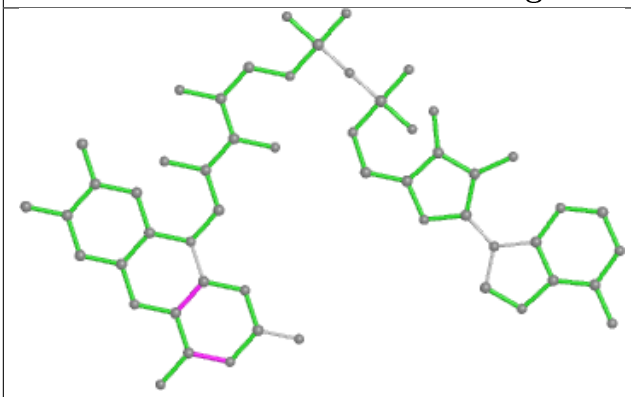
Ligand H7Y A 602



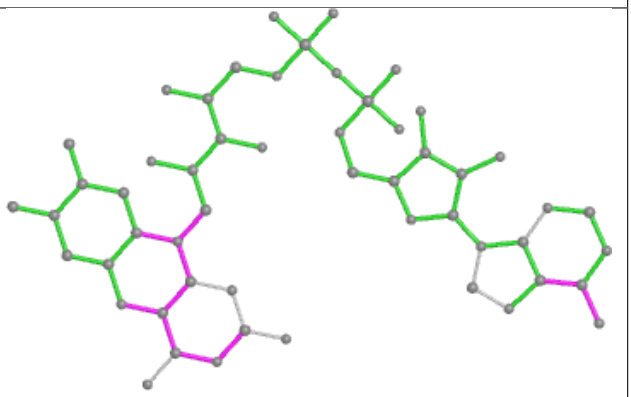
Ligand H7Y E 602



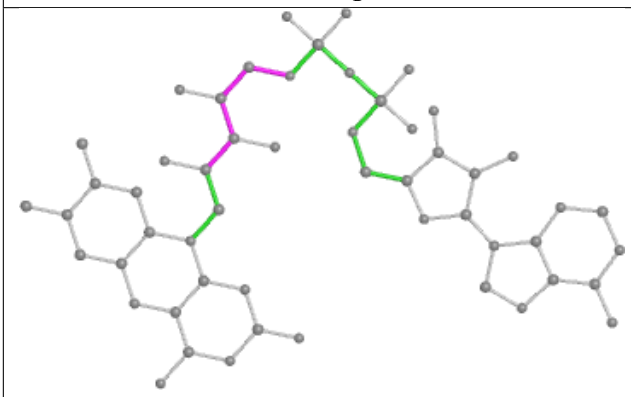
Ligand FAD B 601



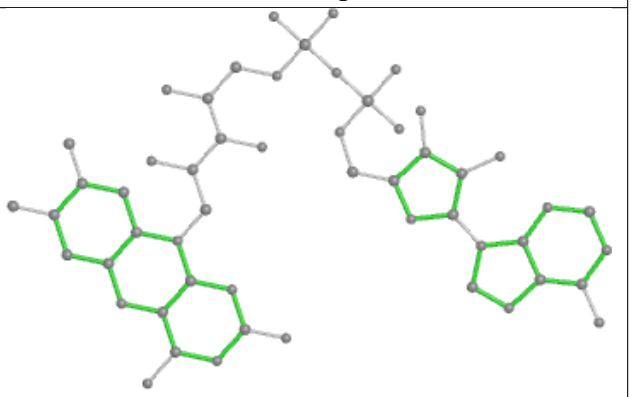
Bond lengths



Bond angles

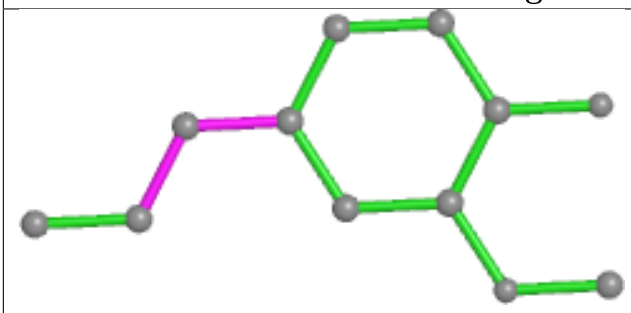


Torsions



Rings

Ligand H7Y C 602



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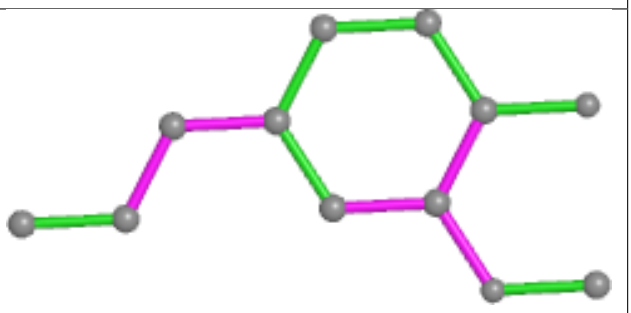
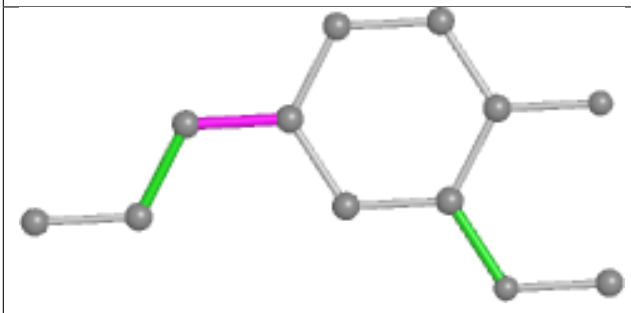


Bond angles



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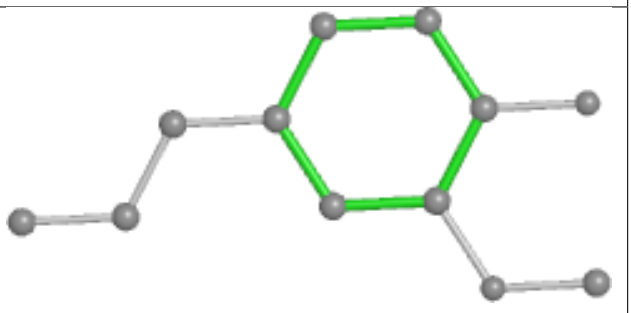
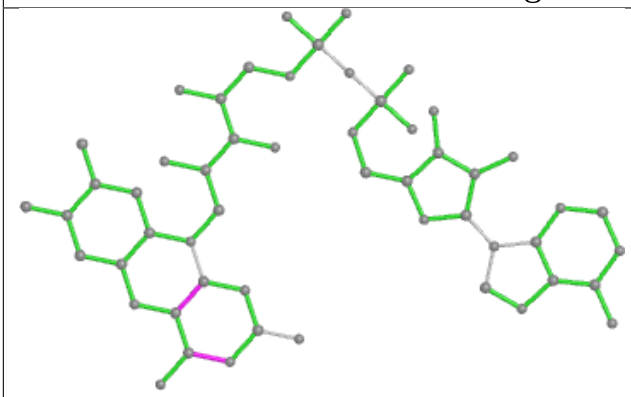


Rings

Ligand FAD D 601



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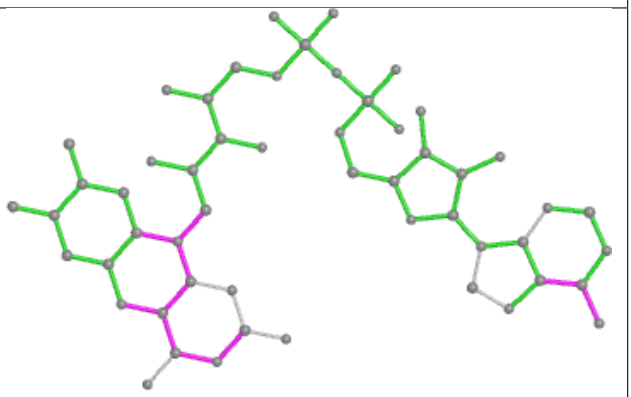

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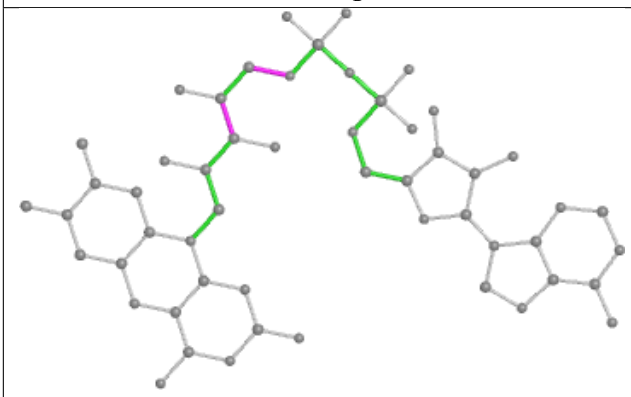

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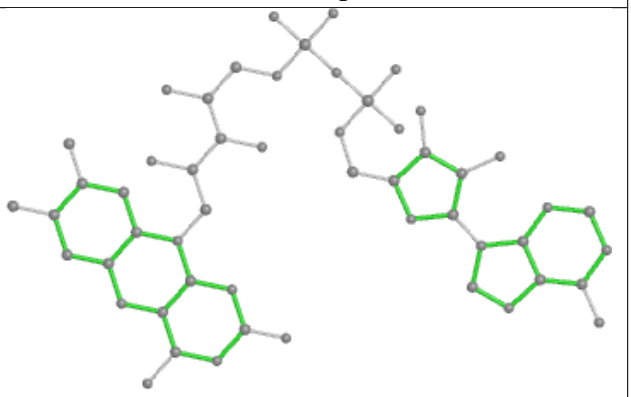
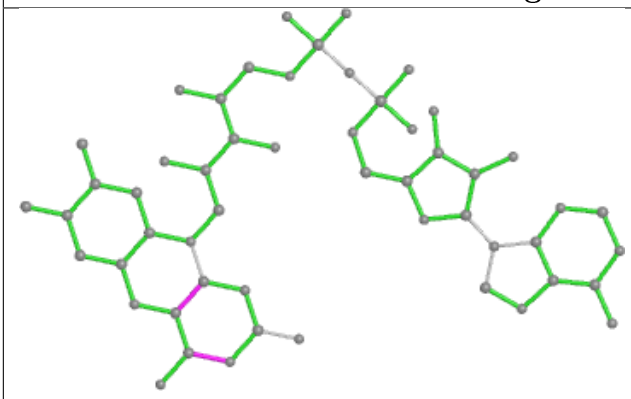


Rings

Ligand FAD A 601



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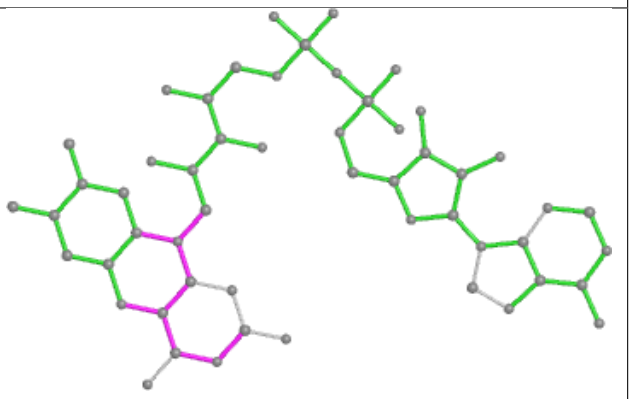
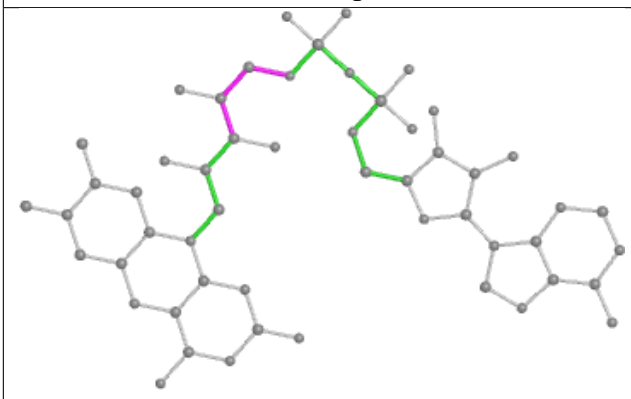
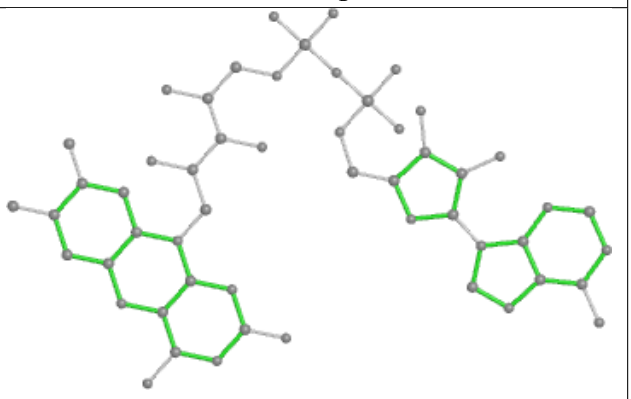


Bond angles

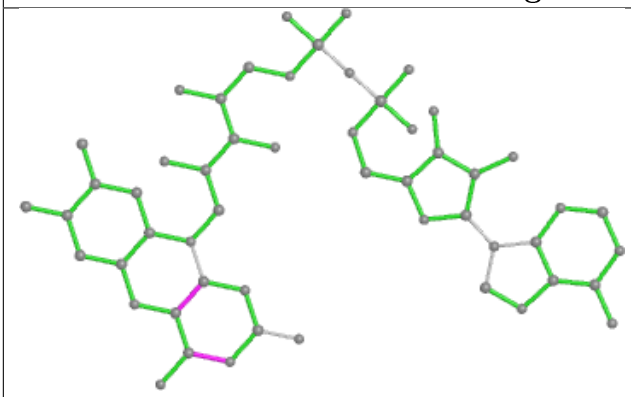


Torsions



Rings

Ligand FAD G 601



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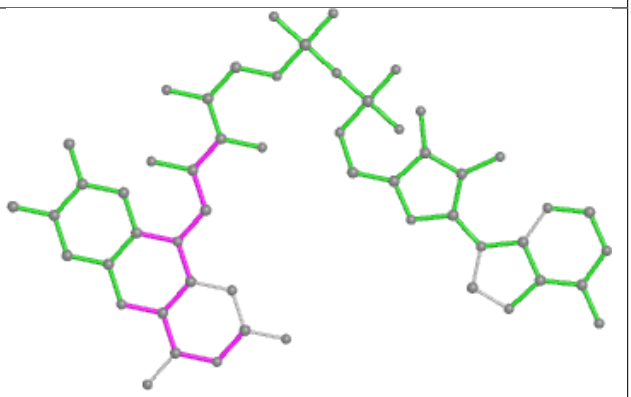
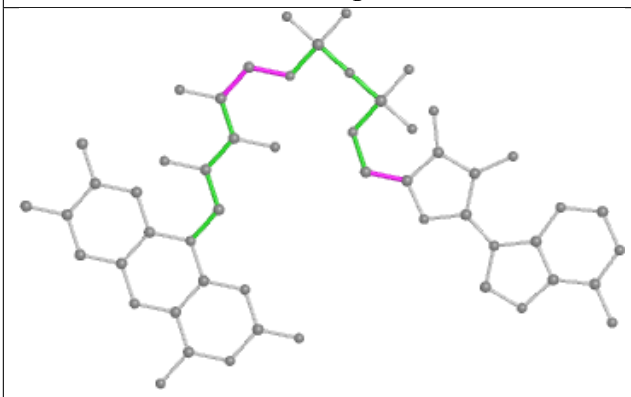


Bond angles



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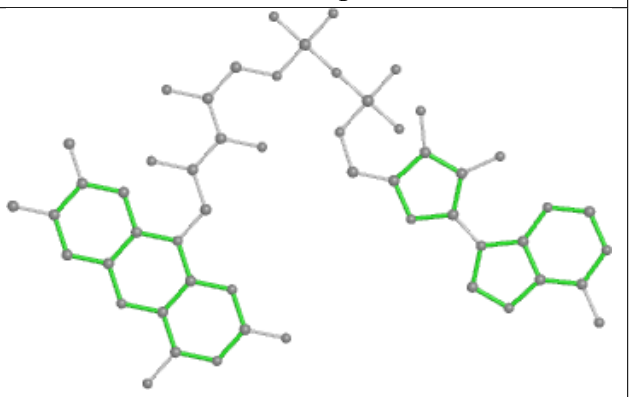
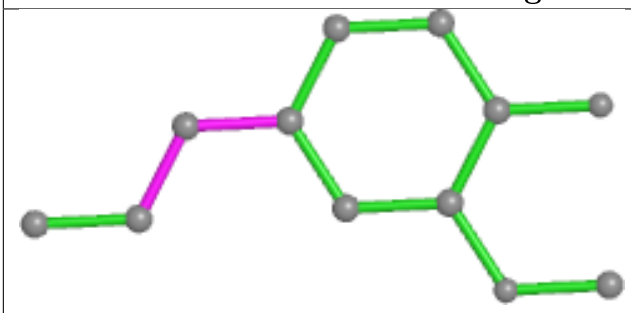


Rings

Ligand H7Y D 602



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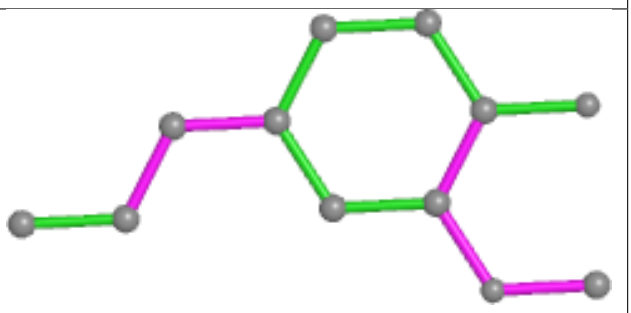
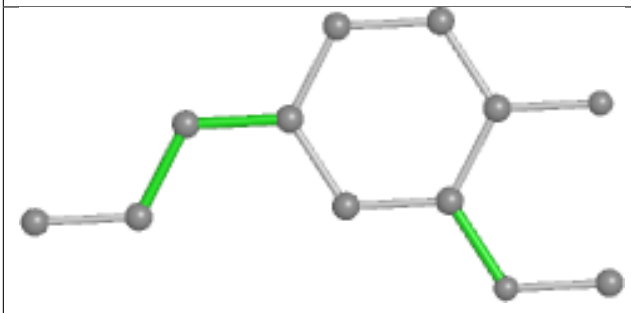


Bond angles



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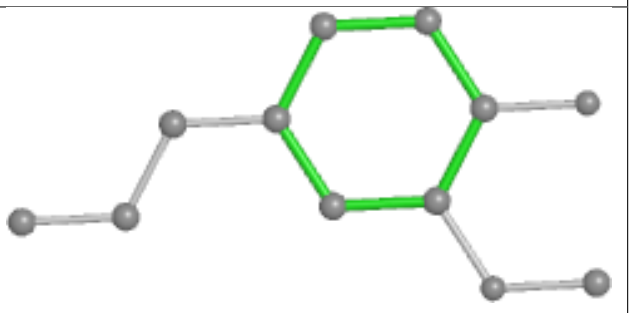
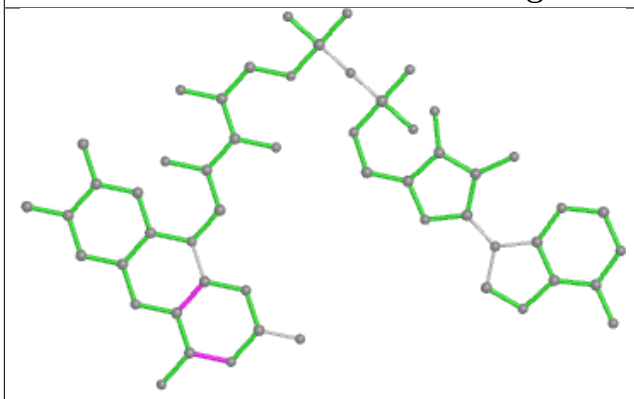


Rings

Ligand FAD C 601



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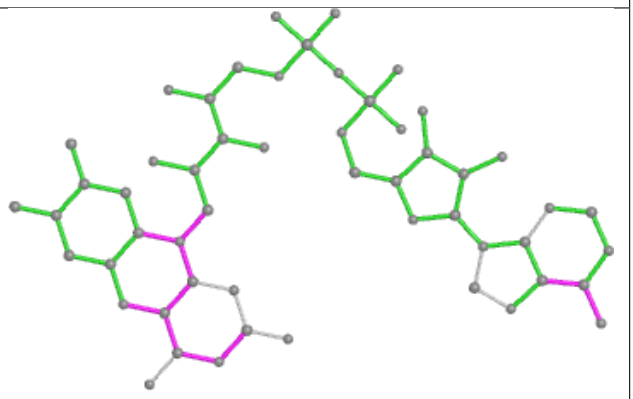

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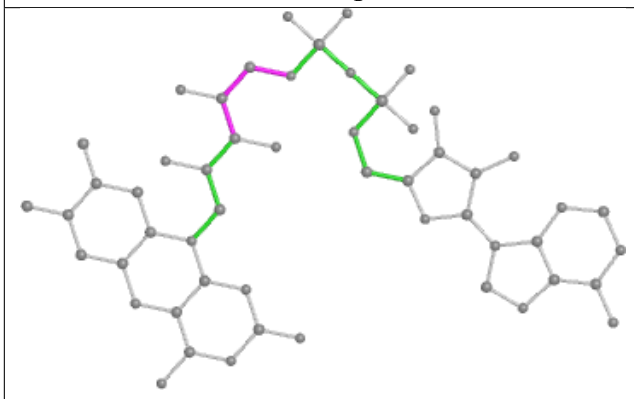

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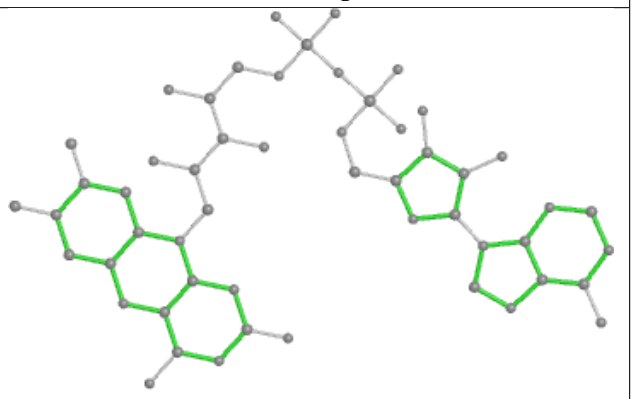
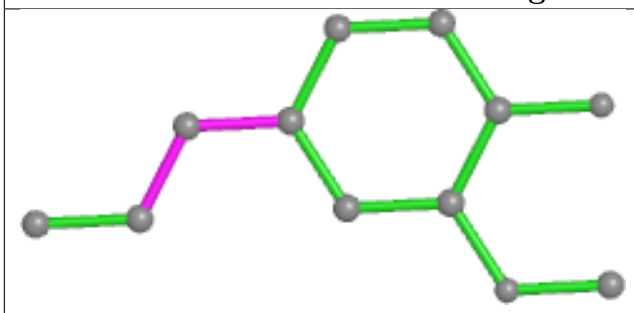


Rings

Ligand H7Y F 602



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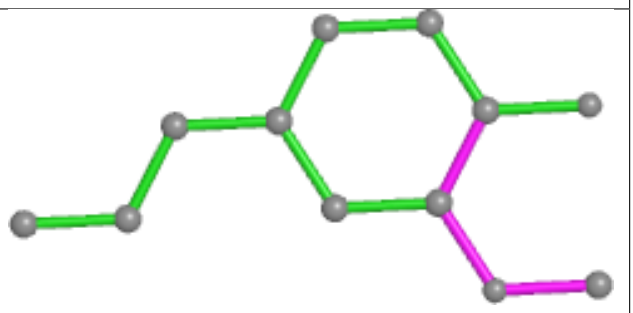
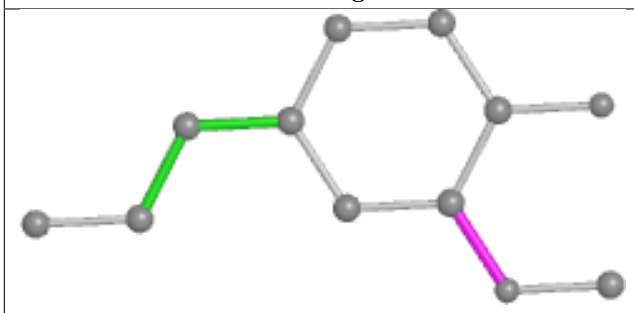
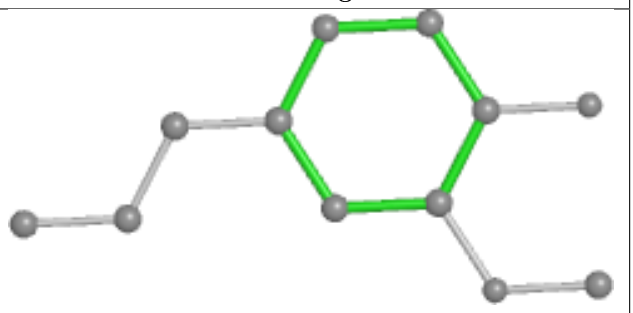


Bond angles

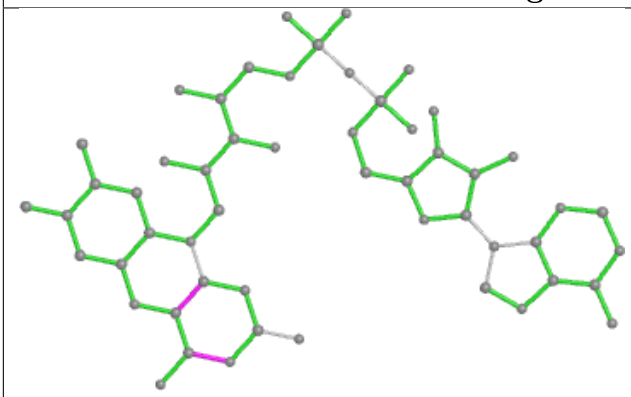


Torsions

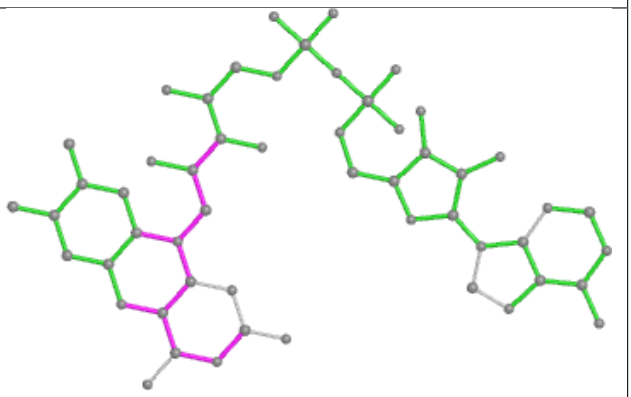


Rings

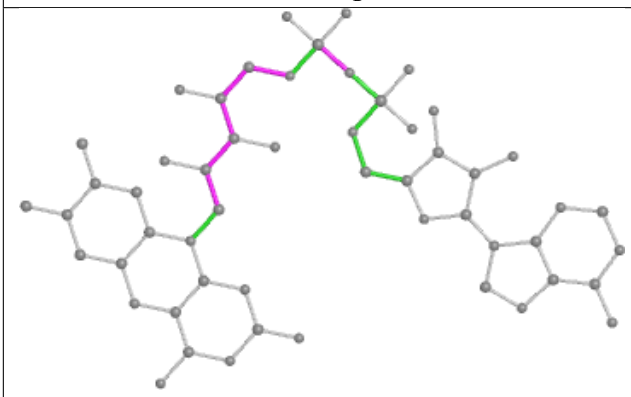
Ligand FAD E 601



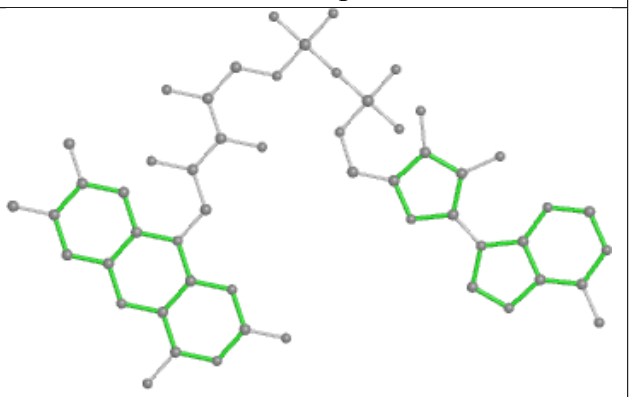
Bond lengths



Bond angles

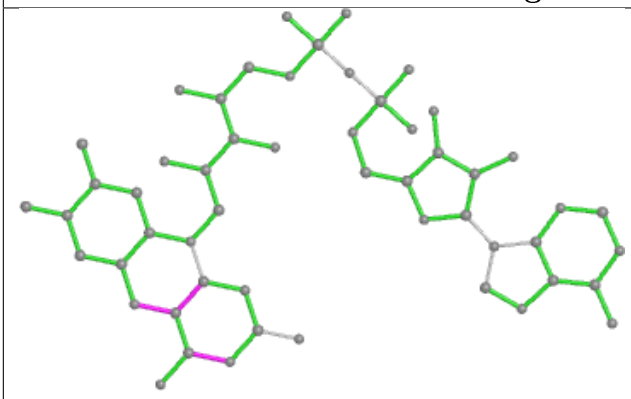


Torsions

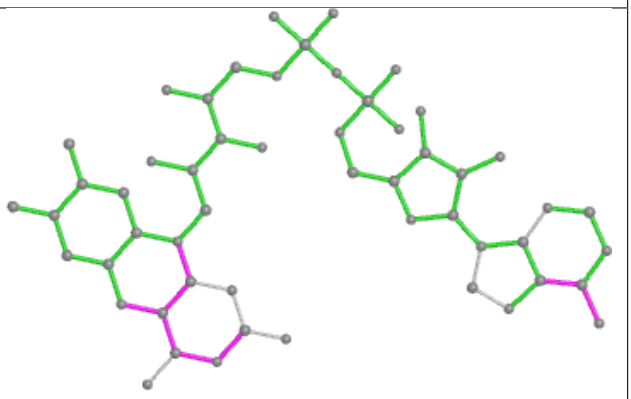


Rings

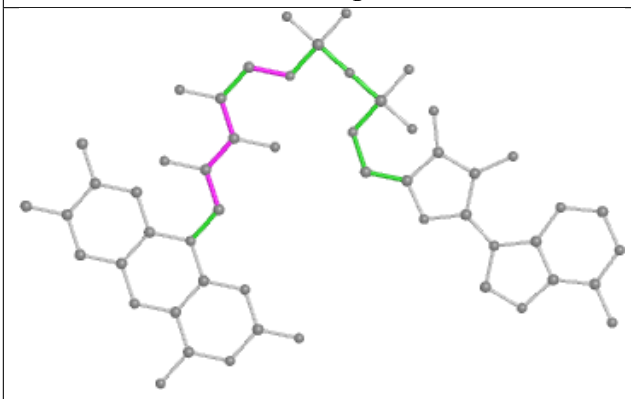
Ligand FAD H 601



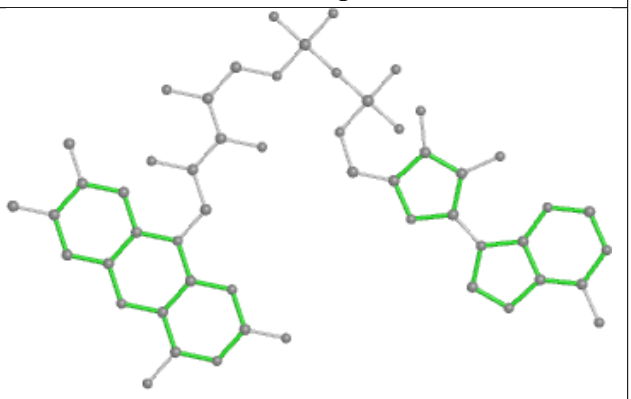
Bond lengths



Bond angles

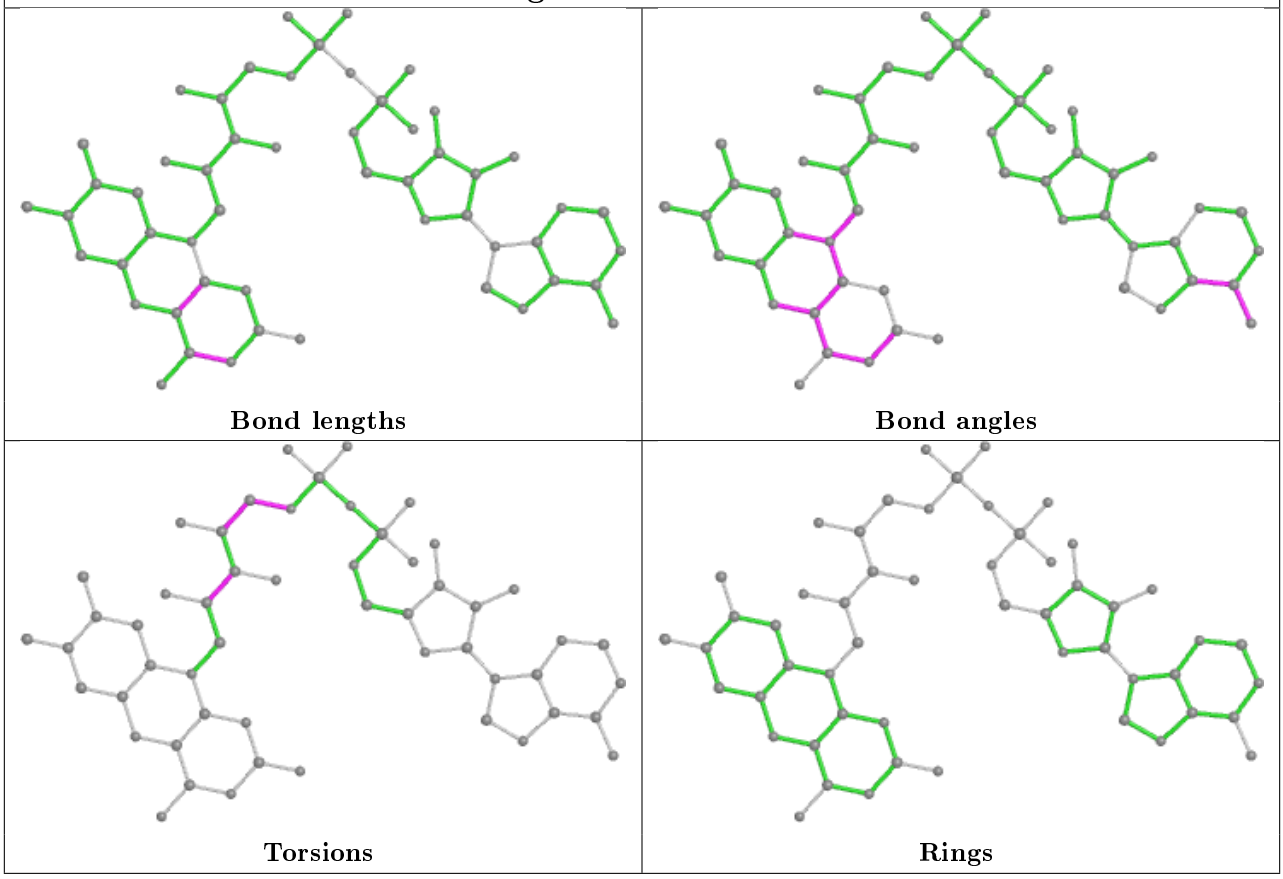


Torsions

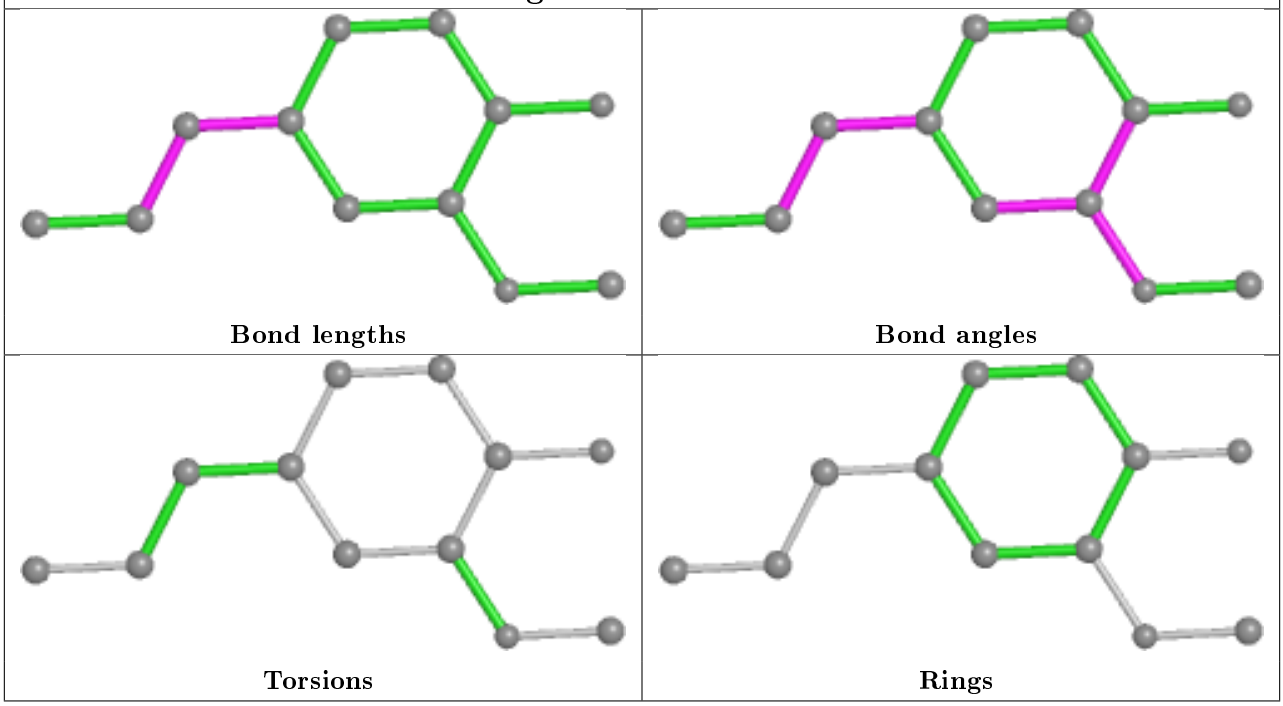


Rings

Ligand FAD F 601



Ligand H7Y B 602



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	523/529 (98%)	-0.18	4 (0%)	86 81	33, 47, 66, 96	0
1	B	525/529 (99%)	-0.27	1 (0%)	95 94	33, 43, 61, 88	0
1	C	523/529 (98%)	-0.06	8 (1%)	73 68	37, 51, 75, 106	0
1	D	525/529 (99%)	-0.16	3 (0%)	89 86	29, 47, 67, 97	0
1	E	523/529 (98%)	0.24	22 (4%)	36 26	45, 60, 83, 104	0
1	F	525/529 (99%)	-0.05	7 (1%)	77 72	39, 54, 74, 93	0
1	G	523/529 (98%)	0.15	18 (3%)	45 35	39, 63, 91, 106	0
1	H	525/529 (99%)	0.13	17 (3%)	47 37	42, 67, 92, 118	0
All	All	4192/4232 (99%)	-0.03	80 (1%)	66 59	29, 53, 83, 118	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	360	GLU	4.4
1	H	141	ASP	4.3
1	D	359	ARG	4.2
1	G	12	ALA	4.1
1	E	12	ALA	3.9
1	B	463	GLU	3.9
1	H	328	ARG	3.8
1	E	144	ALA	3.7
1	H	142	SER	3.7
1	H	143	GLY	3.6
1	G	358	LEU	3.5
1	H	358	LEU	3.3
1	E	451	PRO	3.2
1	H	114	VAL	3.2
1	G	142	SER	3.1
1	E	11	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	359	ARG	3.1
1	E	359	ARG	3.1
1	D	358	LEU	3.0
1	G	360	GLU	3.0
1	G	313	LEU	3.0
1	F	141	ASP	2.9
1	E	313	LEU	2.9
1	F	143	GLY	2.9
1	C	51	ASP	2.9
1	A	142	SER	2.8
1	E	358	LEU	2.8
1	H	313	LEU	2.8
1	G	309	MET	2.8
1	H	140	ARG	2.8
1	A	141	ASP	2.8
1	H	329	TRP	2.7
1	E	350	PHE	2.7
1	E	5	THR	2.7
1	E	339	ARG	2.7
1	E	176	SER	2.6
1	F	297	GLU	2.5
1	E	100	THR	2.5
1	E	51	ASP	2.5
1	E	141	ASP	2.5
1	H	139	VAL	2.5
1	C	137	GLU	2.5
1	H	296	THR	2.5
1	H	242	MET	2.4
1	C	142	SER	2.4
1	H	116	GLU	2.4
1	H	113	ARG	2.4
1	C	140	ARG	2.4
1	G	143	GLY	2.3
1	C	5	THR	2.3
1	G	13	GLU	2.3
1	C	470	GLU	2.3
1	E	456	GLU	2.3
1	E	114	VAL	2.3
1	G	5	THR	2.3
1	G	333	LYS	2.3
1	H	51	ASP	2.3
1	C	13	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	144	ALA	2.3
1	E	8	ASP	2.2
1	F	298	PRO	2.2
1	H	62	GLY	2.2
1	A	12	ALA	2.2
1	E	117	ILE	2.2
1	G	329	TRP	2.2
1	G	144	ALA	2.2
1	G	357	PRO	2.1
1	E	362	ASP	2.1
1	F	139	VAL	2.1
1	G	311	ASP	2.1
1	A	297	GLU	2.1
1	C	117	ILE	2.1
1	H	312	GLU	2.1
1	E	344	GLN	2.1
1	G	361	GLY	2.1
1	G	51	ASP	2.1
1	F	142	SER	2.0
1	E	10	VAL	2.0
1	G	308	ARG	2.0
1	D	140	ARG	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	H7Y	E	602	12/12	0.85	0.35	83,88,94,96	0

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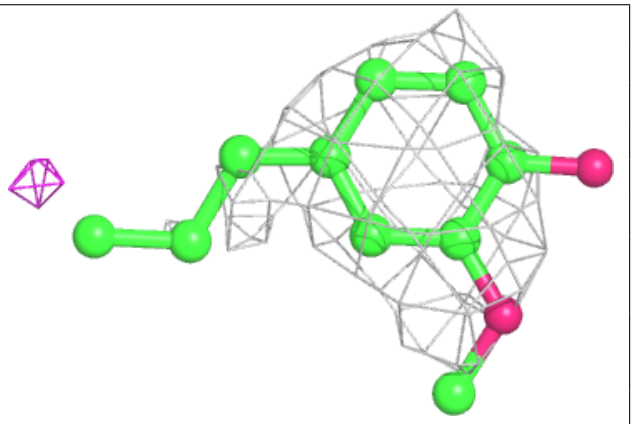
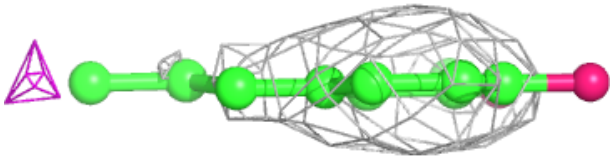
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	H7Y	C	602	12/12	0.88	0.28	67,71,83,86	0
3	H7Y	B	602	12/12	0.89	0.30	63,69,81,84	0
3	H7Y	A	602	12/12	0.91	0.28	72,74,85,87	0
3	H7Y	F	602	12/12	0.91	0.29	73,80,102,104	0
3	H7Y	D	602	12/12	0.92	0.28	65,72,83,84	0
2	FAD	E	601	53/53	0.96	0.19	39,56,67,77	0
2	FAD	G	601	53/53	0.96	0.16	44,53,66,67	0
2	FAD	H	601	53/53	0.96	0.15	45,52,57,72	0
2	FAD	D	601	53/53	0.97	0.16	28,39,49,51	0
2	FAD	F	601	53/53	0.97	0.16	39,45,51,56	0
2	FAD	C	601	53/53	0.98	0.16	38,43,49,56	0
2	FAD	A	601	53/53	0.98	0.16	36,41,46,48	0
2	FAD	B	601	53/53	0.98	0.16	31,35,42,47	0

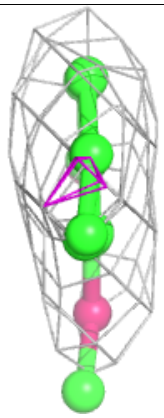
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around H7Y 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)

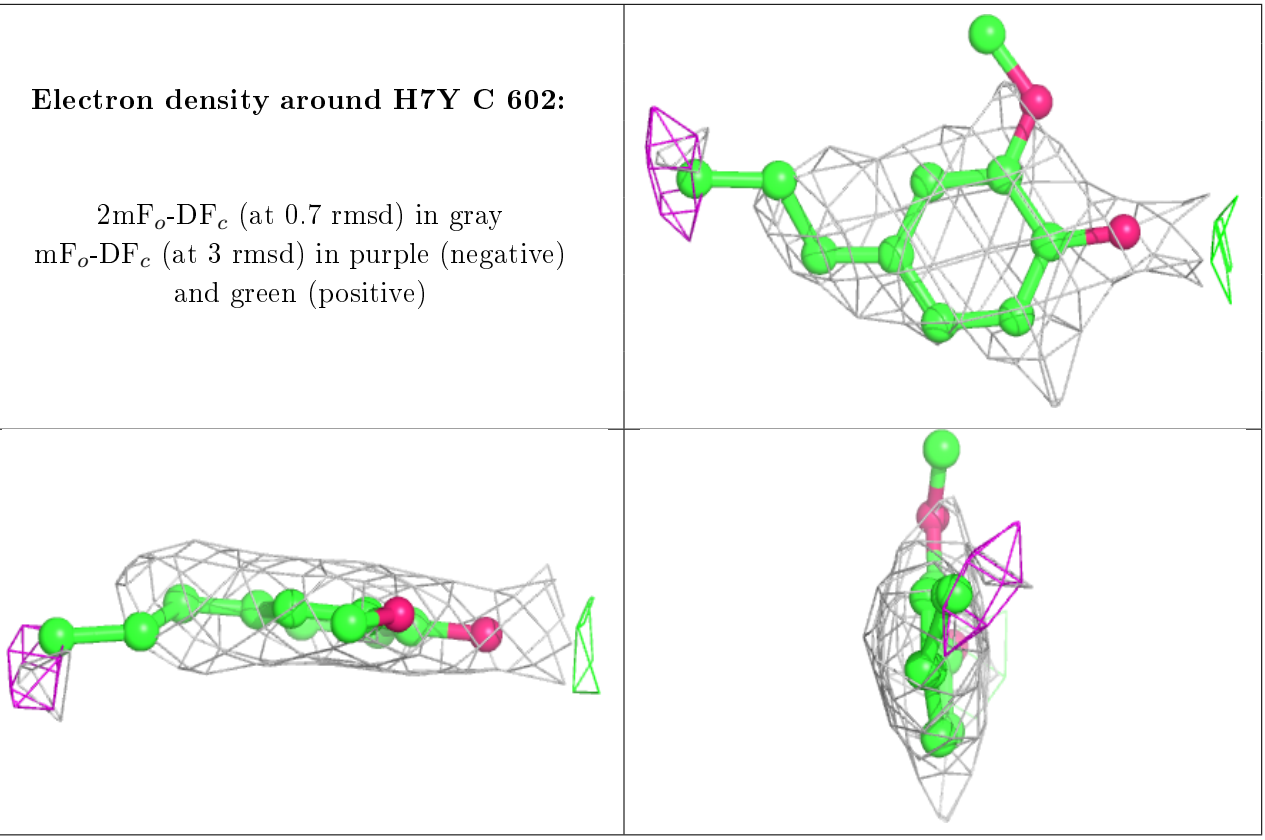






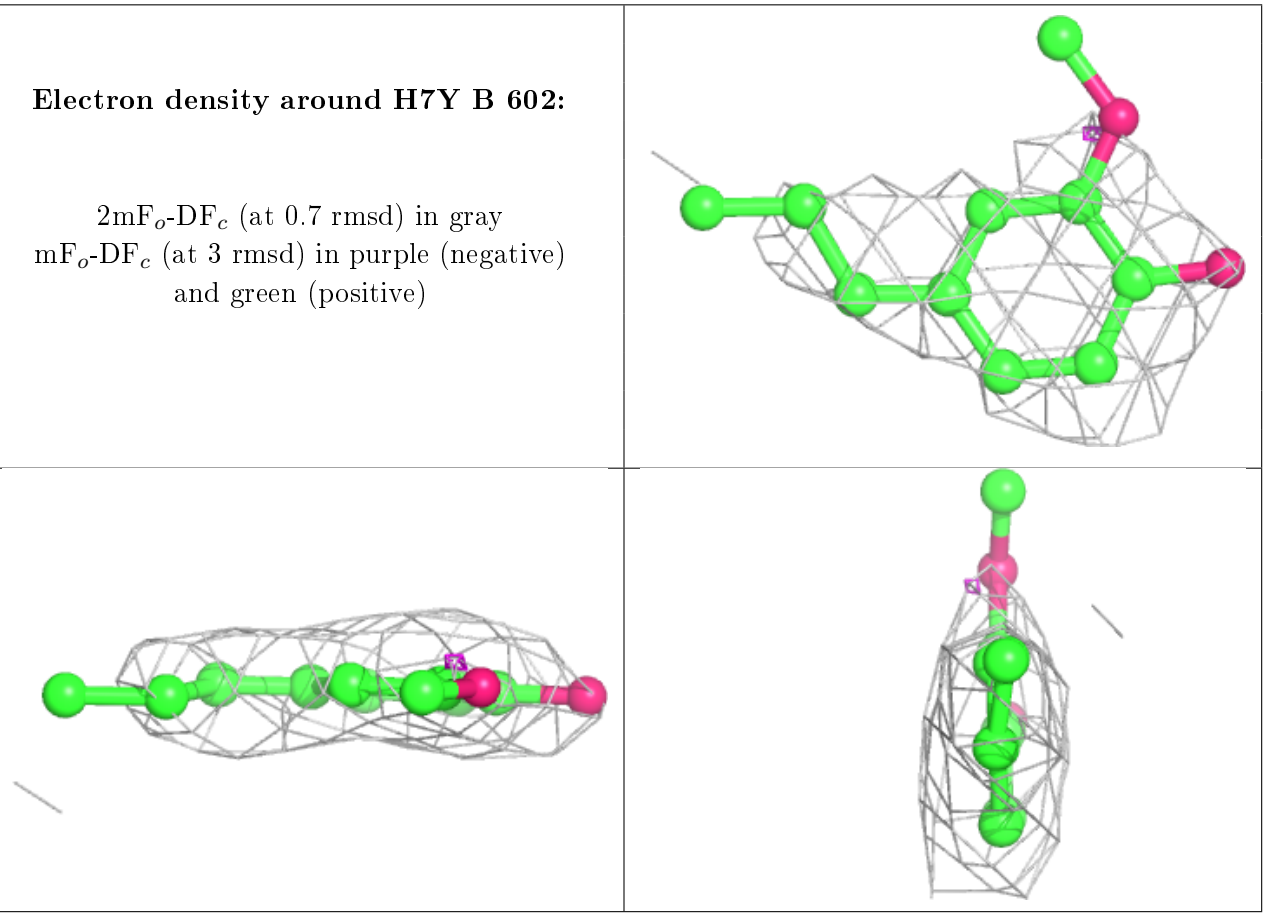
Electron density around H7Y C 602:

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



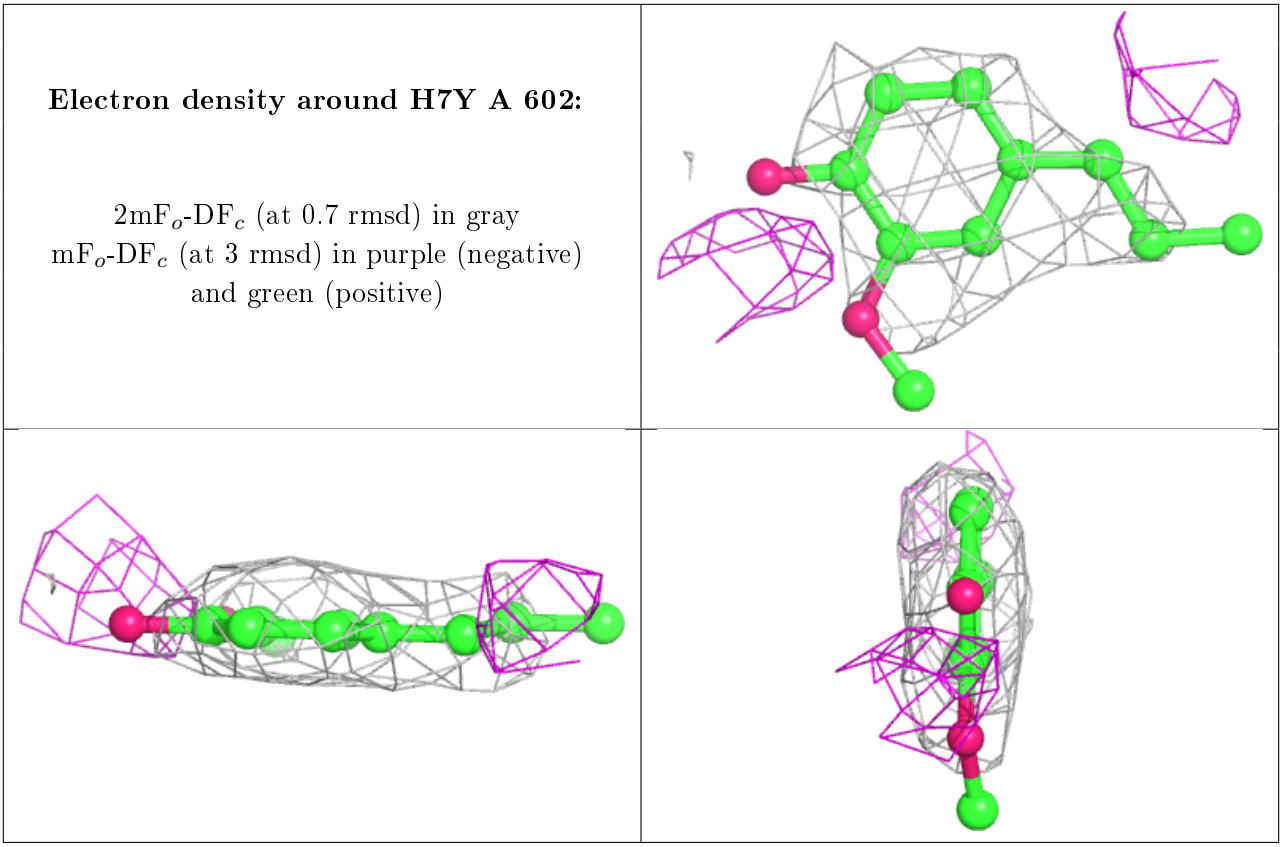
Electron density around H7Y B 602:

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



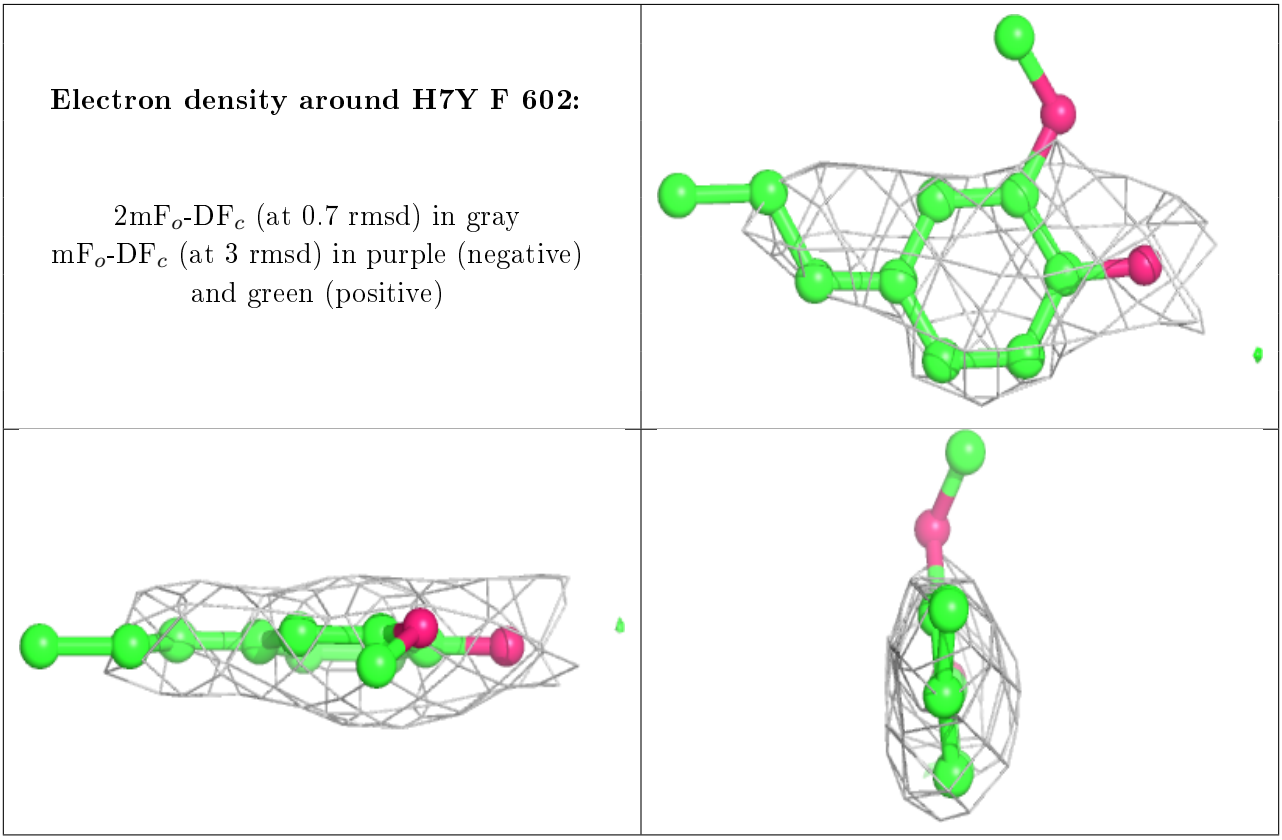
Electron density around H7Y A 602:

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



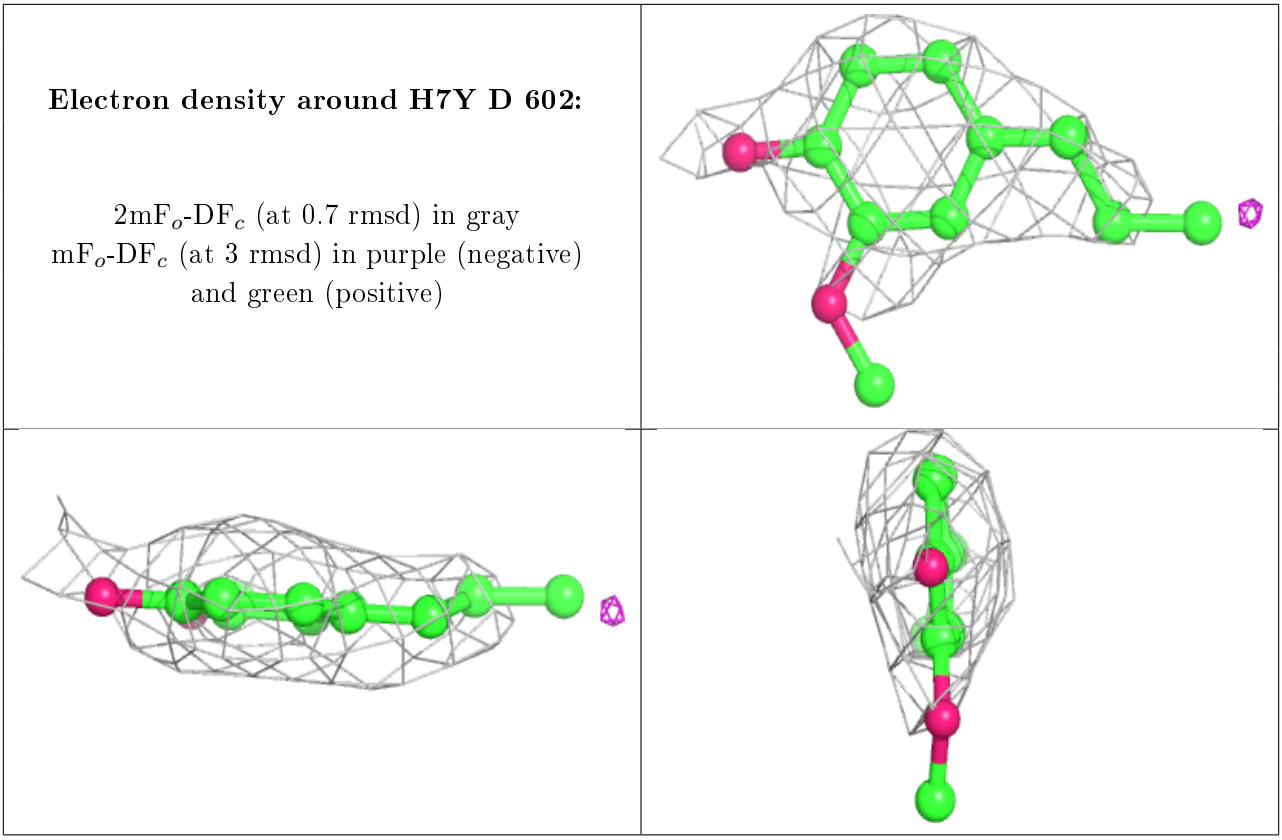
Electron density around H7Y F 602:

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



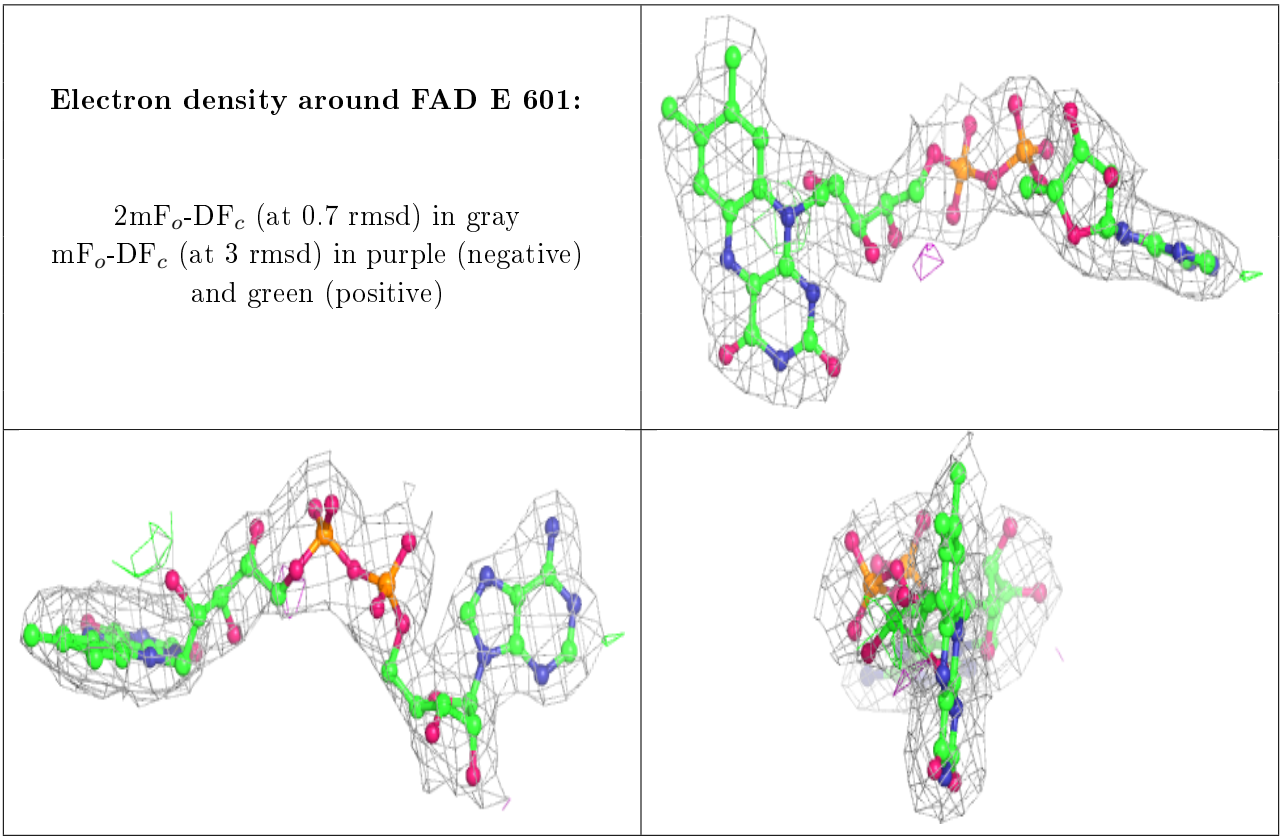
Electron density around H7Y D 602:

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



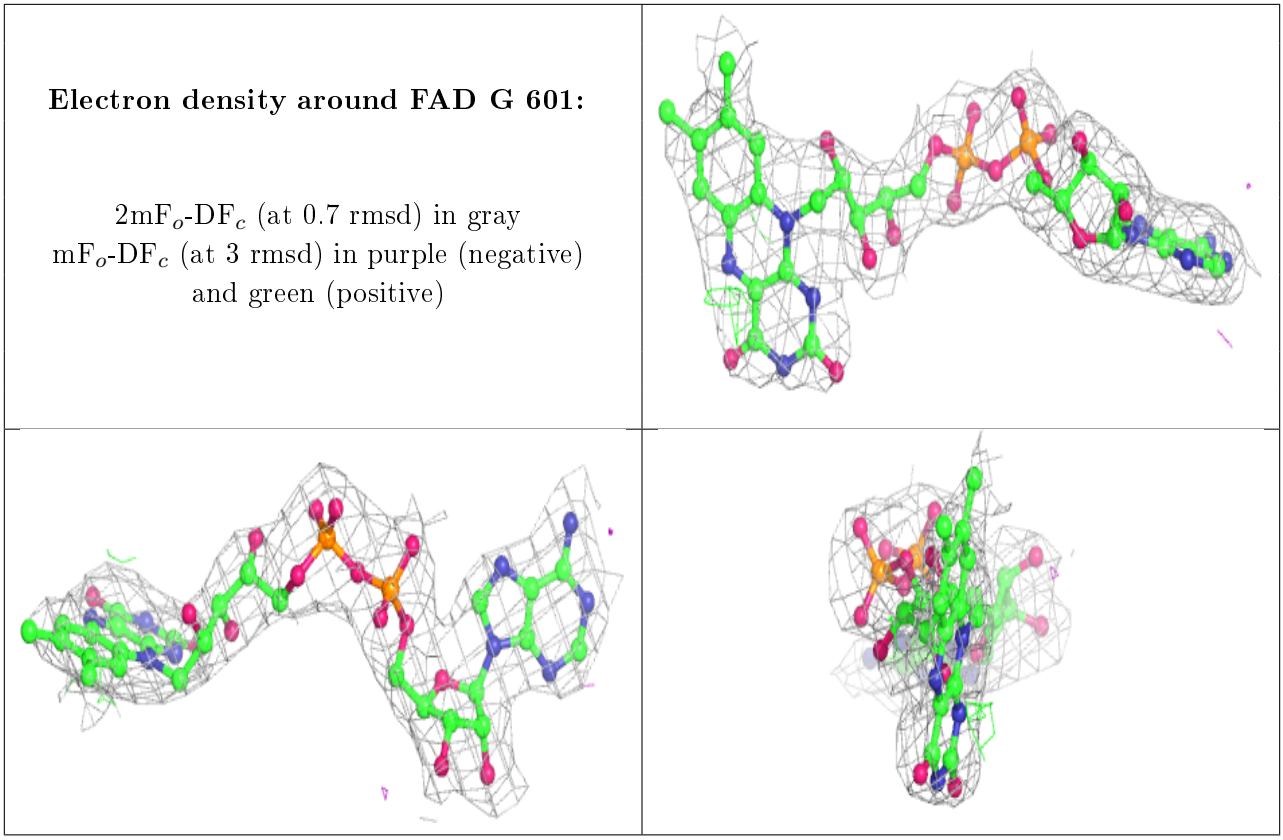
Electron density around FAD E 601:

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



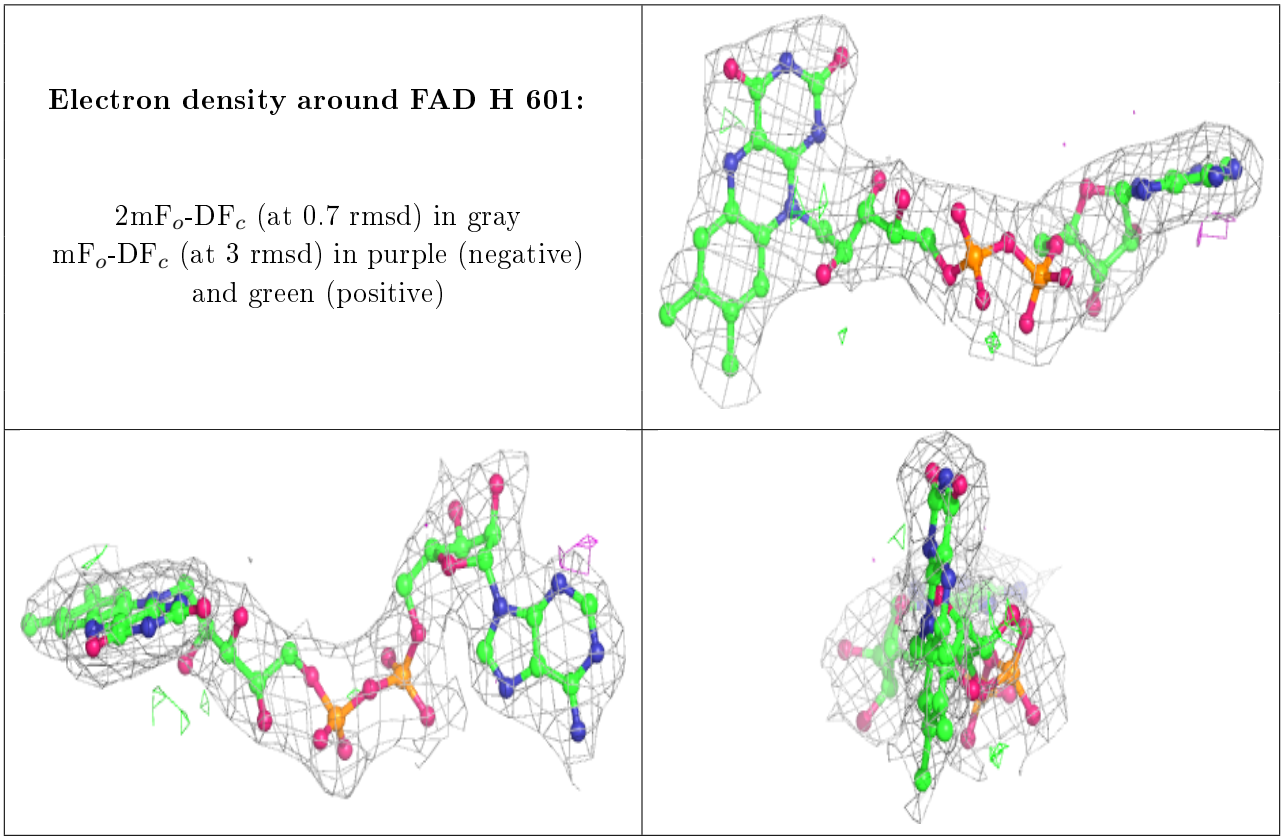
Electron density around FAD G 601:

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



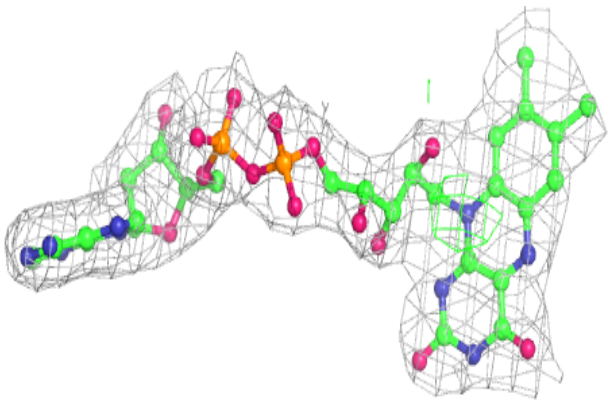
Electron density around FAD H 601:

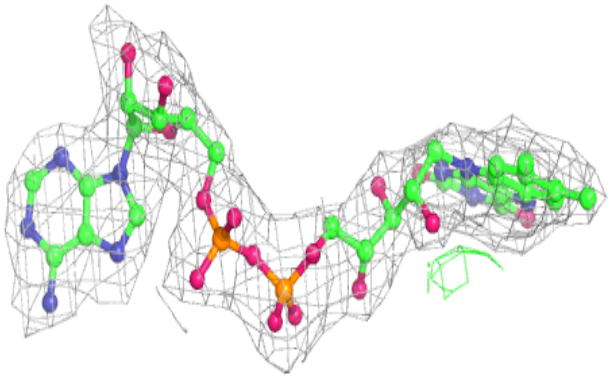
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

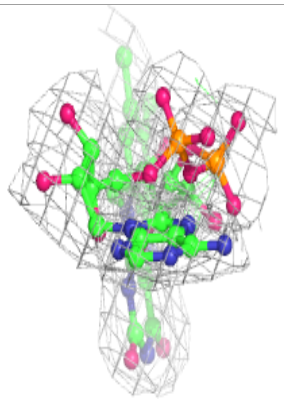


Electron density around FAD D 601:

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

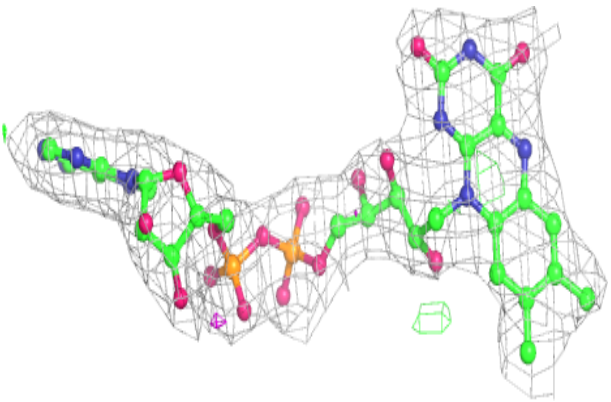


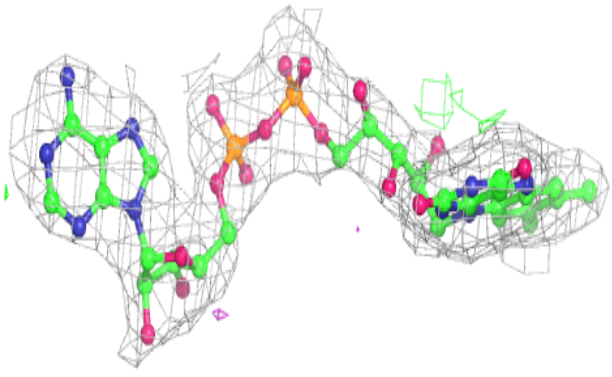


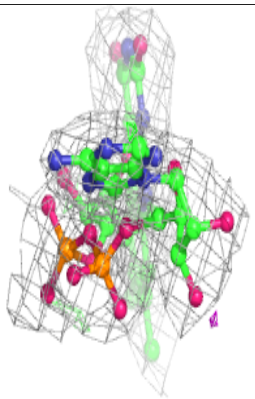


Electron density around FAD F 601:

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

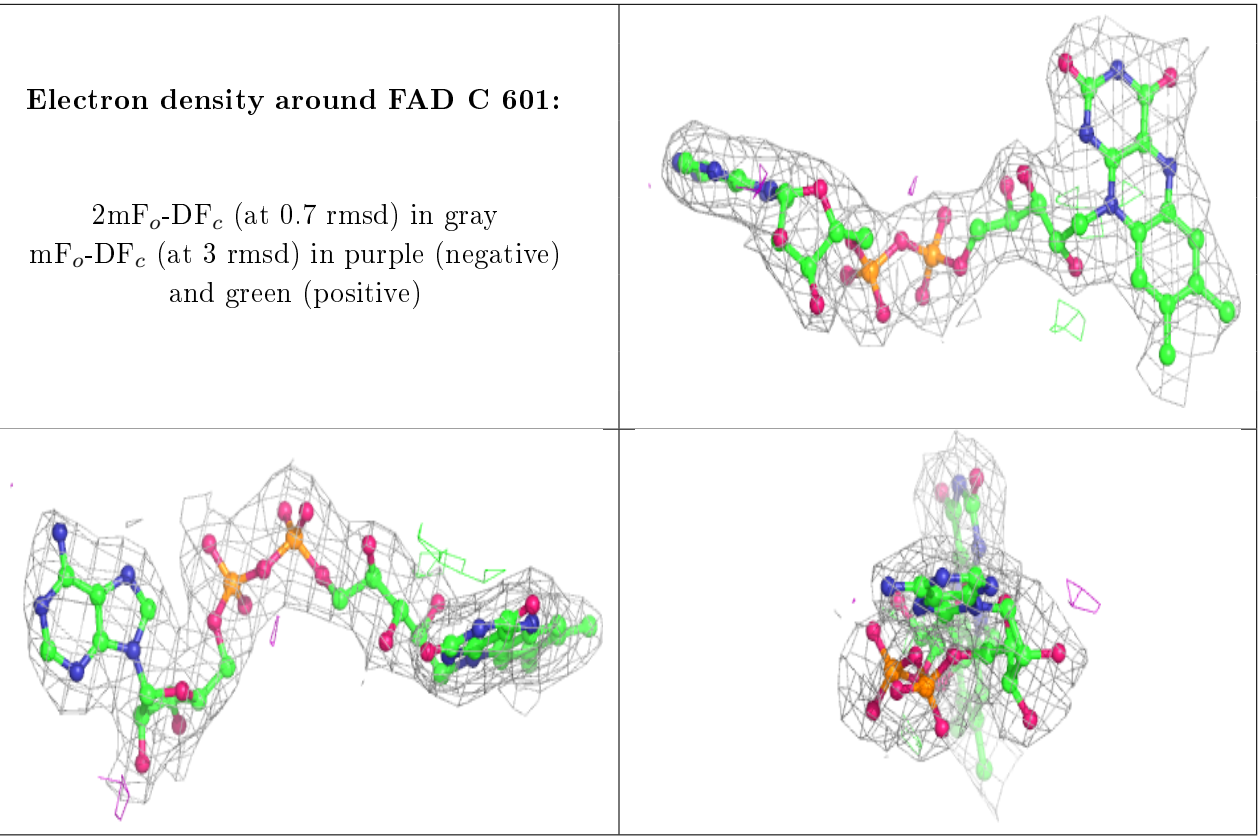






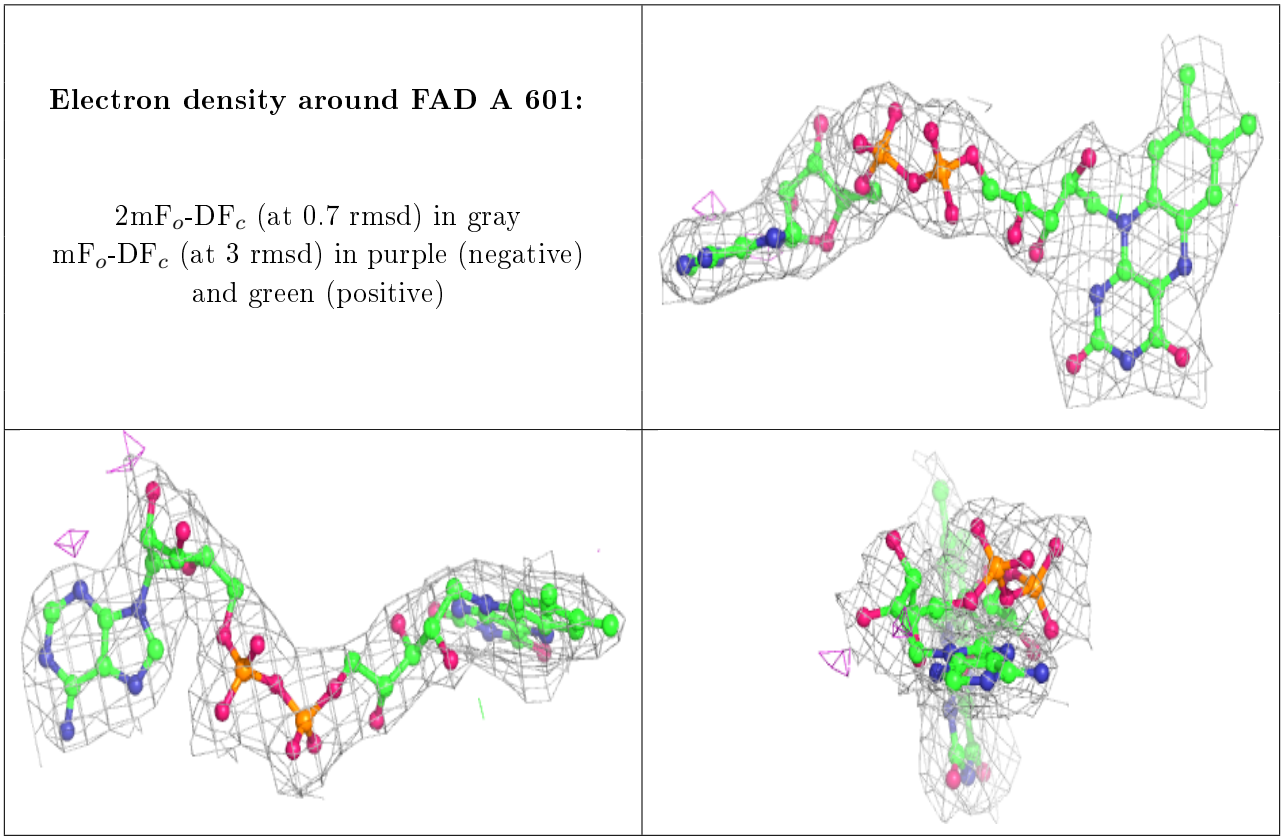
Electron density around FAD C 601:

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



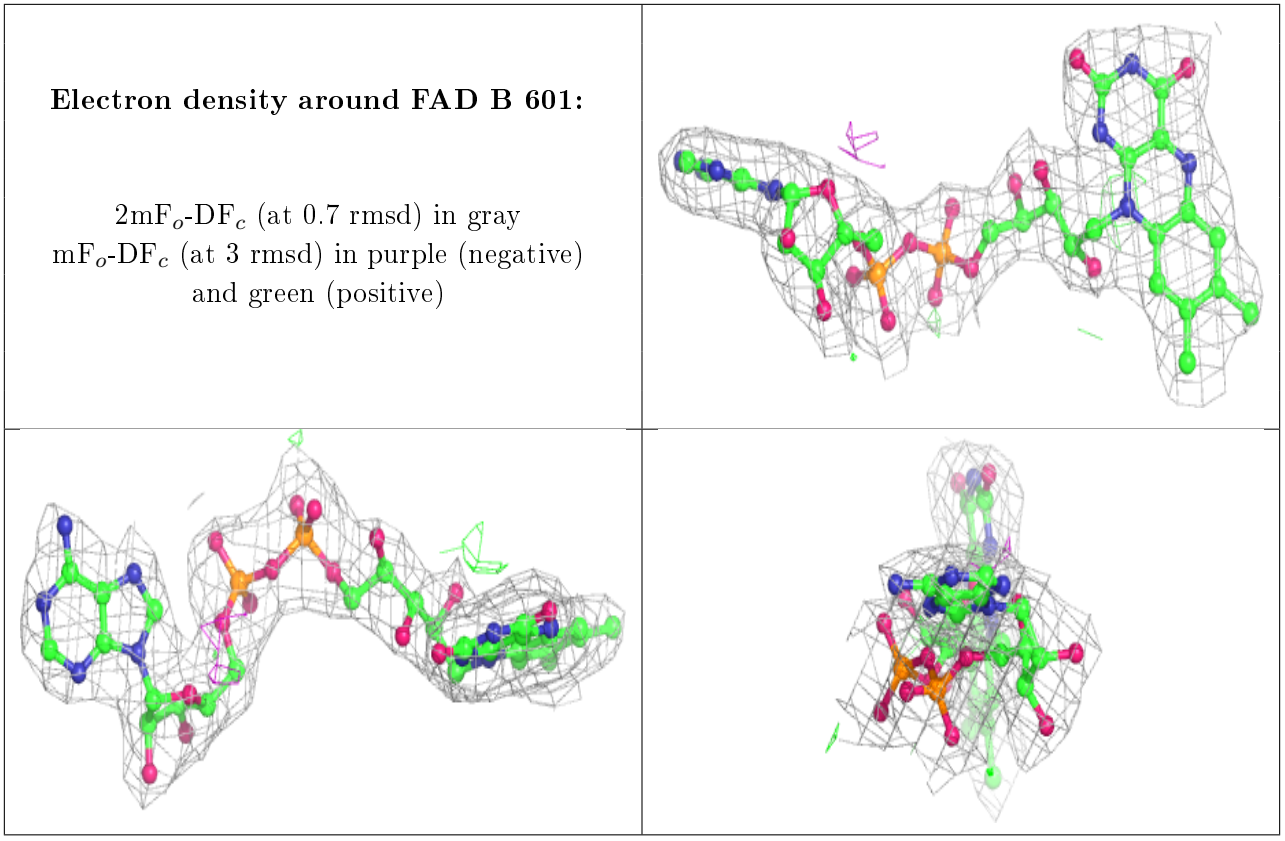
Electron density around FAD A 601:

$2mF_o$-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)



6.5 Other polymers

There are no such residues in this entry.