Full wwPDB X-ray Structure Validation Report (i)

Feb 20, 2024 – 03:10 AM EST

PDB ID	:	4MIH
Title	:	Pyranose 2-oxidase from Phanerochaete chrysosporium, recombinant H158A mutant
Authors	:	Hassan, N.; Tan, T.C.; Spadiut, O.; Pisanelli, I.; Fusco, L.; Haltrich, D.; Peterbauer, C.; Divne, C.
Deposited on	:	2013-08-31
Resolution	:	2.40 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

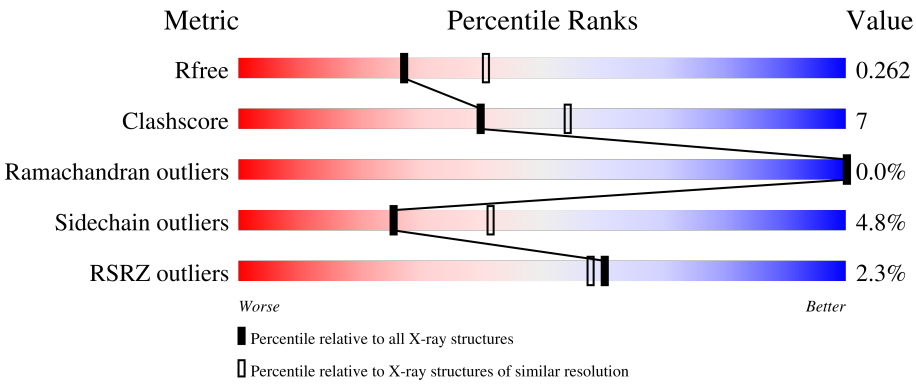
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	621	77% 14% • 7%
1	B	621	% 75% 17% • 7%
1	C	621	4% 70% 21% • 7%
1	D	621	2% 74% 18% • 7%

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Mol	Chain	Length	Quality of chain
1	E	621	2% 79% 13% • 7%
1	F	621	2% 78% 14% • 7%
1	G	621	2% 72% 19% • 7%
1	H	621	4% 71% 21% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 37799 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
			Total	C	N	O	S			
1	A	576	4548	2895	782	844	27	0	0	0
1	B	578	4568	2906	787	848	27	0	0	0
1	C	578	4568	2906	787	848	27	0	0	0
1	D	578	4568	2906	787	848	27	0	0	0
1	E	576	4548	2895	782	844	27	0	0	0
1	F	578	4568	2906	787	848	27	0	0	0
1	G	578	4568	2906	787	848	27	0	0	0
1	H	578	4568	2906	787	848	27	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q6QWR1
A	158	ALA	HIS	engineered mutation	UNP Q6QWR1
B	0	SER	-	expression tag	UNP Q6QWR1
B	158	ALA	HIS	engineered mutation	UNP Q6QWR1
C	0	SER	-	expression tag	UNP Q6QWR1
C	158	ALA	HIS	engineered mutation	UNP Q6QWR1
D	0	SER	-	expression tag	UNP Q6QWR1
D	158	ALA	HIS	engineered mutation	UNP Q6QWR1
E	0	SER	-	expression tag	UNP Q6QWR1
E	158	ALA	HIS	engineered mutation	UNP Q6QWR1
F	0	SER	-	expression tag	UNP Q6QWR1
F	158	ALA	HIS	engineered mutation	UNP Q6QWR1
G	0	SER	-	expression tag	UNP Q6QWR1

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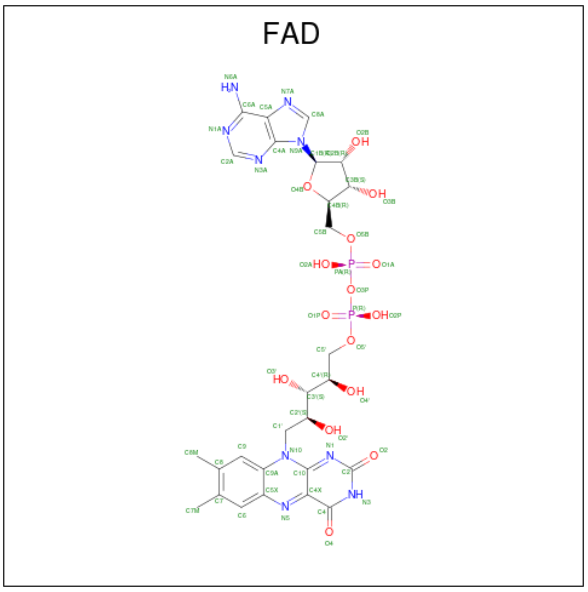
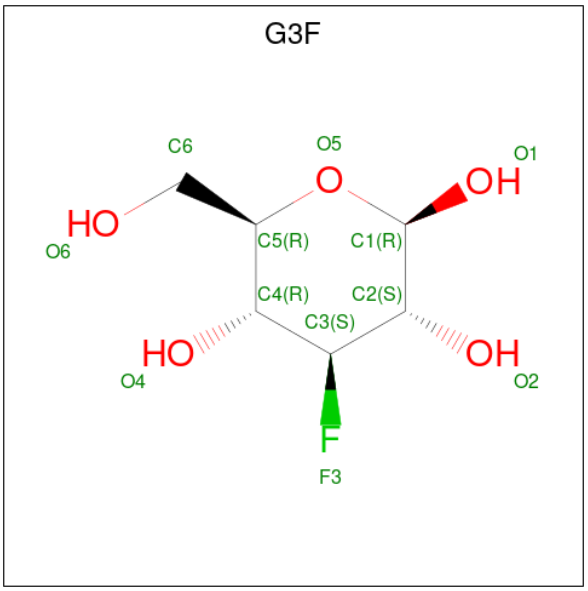
Chain	Residue	Modelled	Actual	Comment	Reference
G	158	ALA	HIS	engineered mutation	UNP Q6QWR1
H	0	SER	-	expression tag	UNP Q6QWR1
H	158	ALA	HIS	engineered mutation	UNP Q6QWR1

- 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
			Total	C	N	O	P		
2	A	1	53	27	9	15	2	0	0
2	B	1	53	27	9	15	2	0	0
2	C	1	53	27	9	15	2	0	0
2	D	1	53	27	9	15	2	0	0
2	E	1	53	27	9	15	2	0	0
2	F	1	53	27	9	15	2	0	0
2	G	1	53	27	9	15	2	0	0
2	H	1	53	27	9	15	2	0	0

- Molecule 3 is 3-deoxy-3-fluoro-beta-D-glucopyranose (three-letter code: G3F) (formula: $C_6H_{11}FO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	F	O		
3	A	1	12	6	1	5	0	0
3	B	1	12	6	1	5	0	0
3	C	1	12	6	1	5	0	0
3	D	1	12	6	1	5	0	0
3	E	1	12	6	1	5	0	0
3	F	1	12	6	1	5	0	0
3	G	1	12	6	1	5	0	0
3	H	1	12	6	1	5	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	133	133	133	0	0
4	B	109	109	109	0	0
4	C	77	77	77	0	0
4	D	59	59	59	0	0

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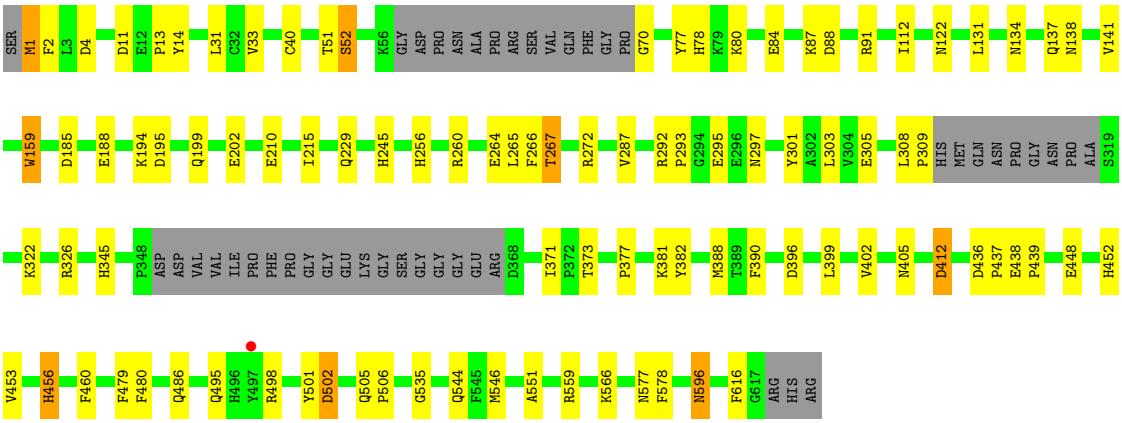
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	E	129	129	129	0	0
			Total	O		
4	F	94	94	94	0	0
			Total	O		
4	G	90	90	90	0	0
			Total	O		
4	H	84	84	84	0	0

3 Residue-property plots (i)

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

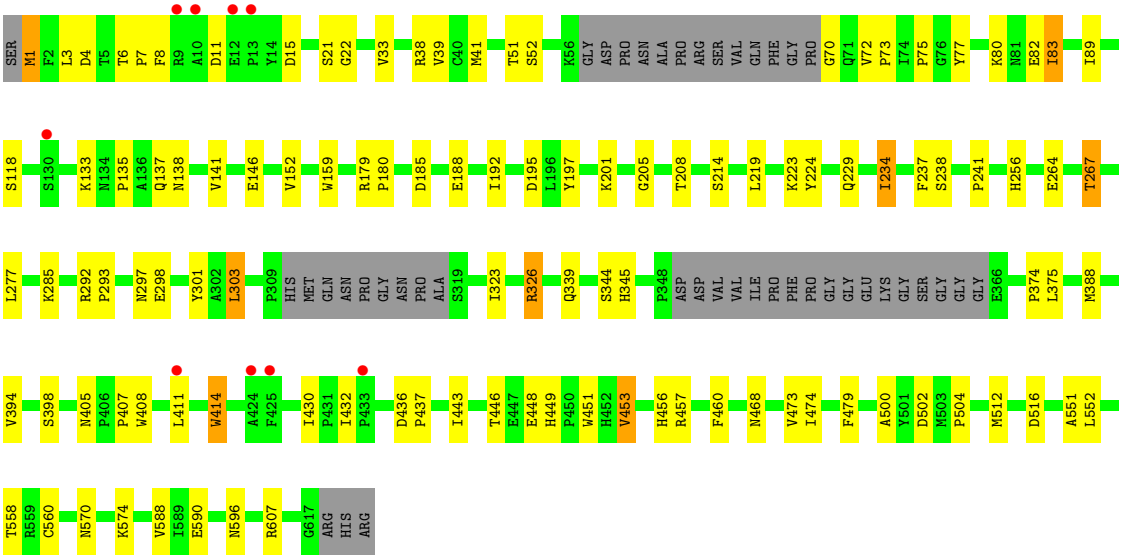
• Molecule 1: Pyranose 2-oxidase

Chain A: 77% 14% • 7%



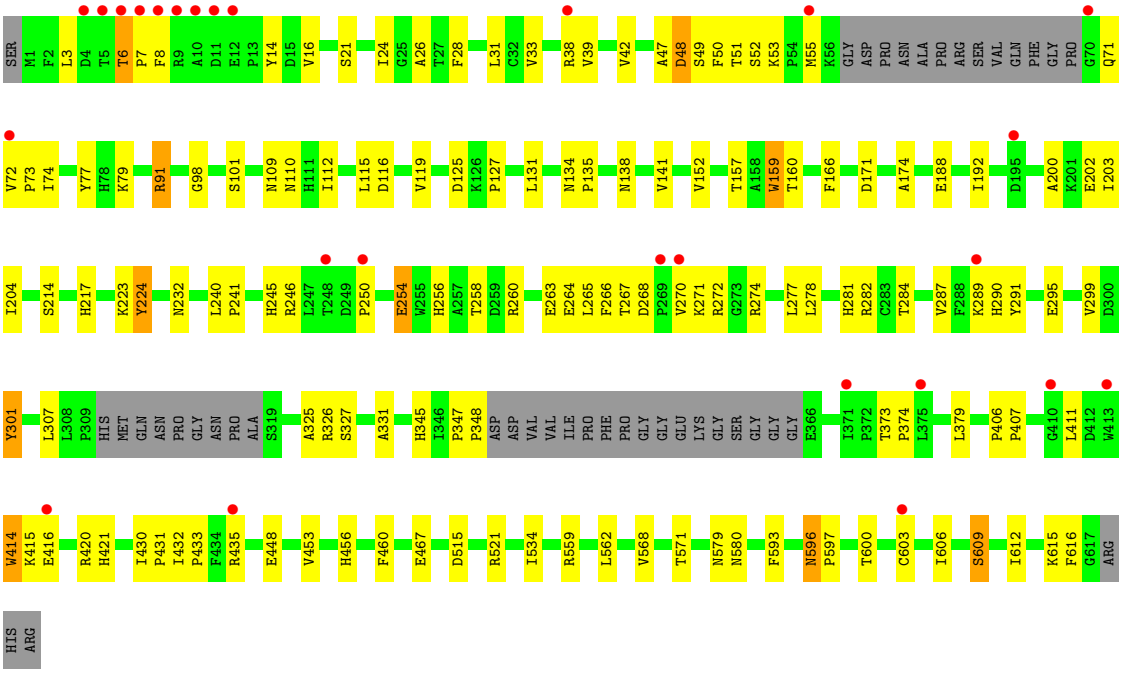
• Molecule 1: Pyranose 2-oxidase

Chain B: % 75% 17% • 7%



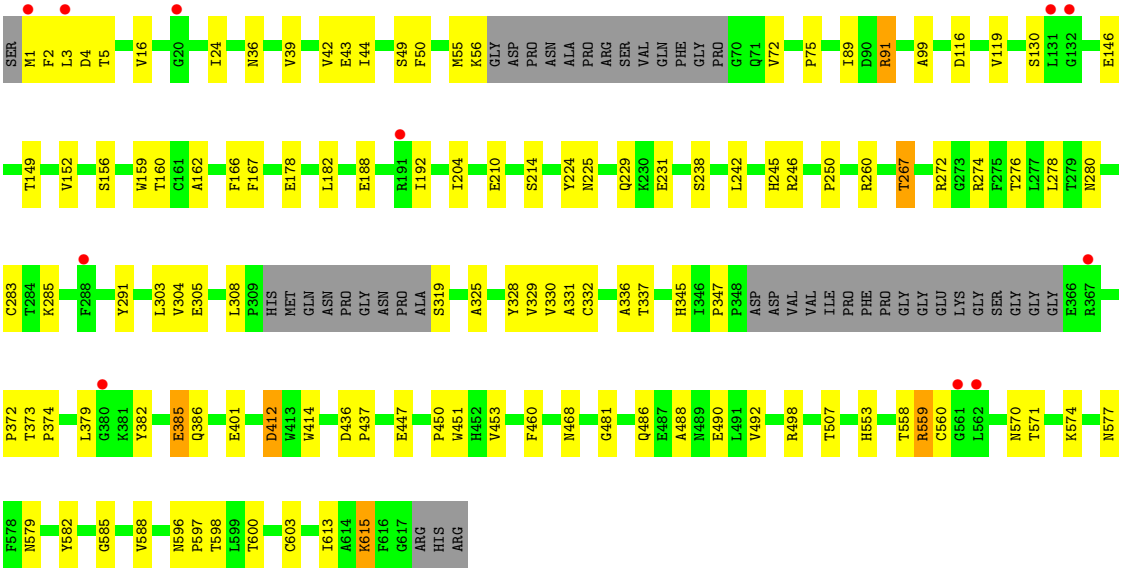
• Molecule 1: Pyranose 2-oxidase

Chain C:



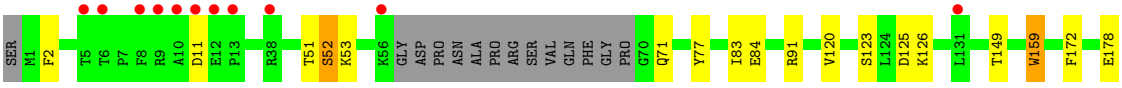
- Molecule 1: Pyranose 2-oxidase

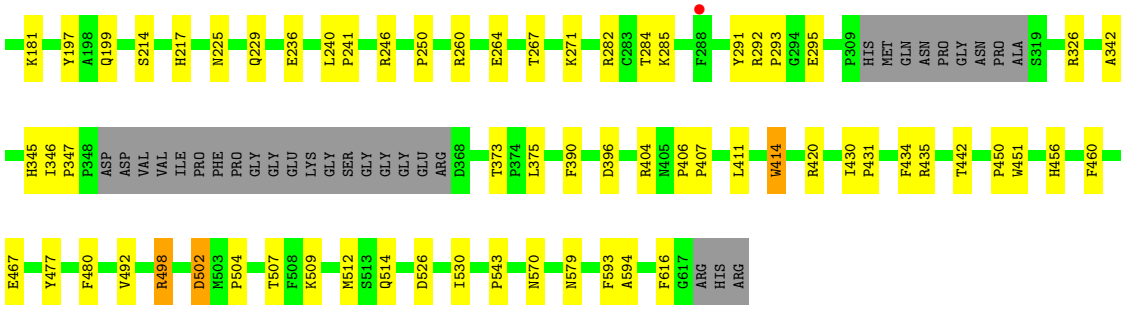
Chain D:



- Molecule 1: Pyranose 2-oxidase

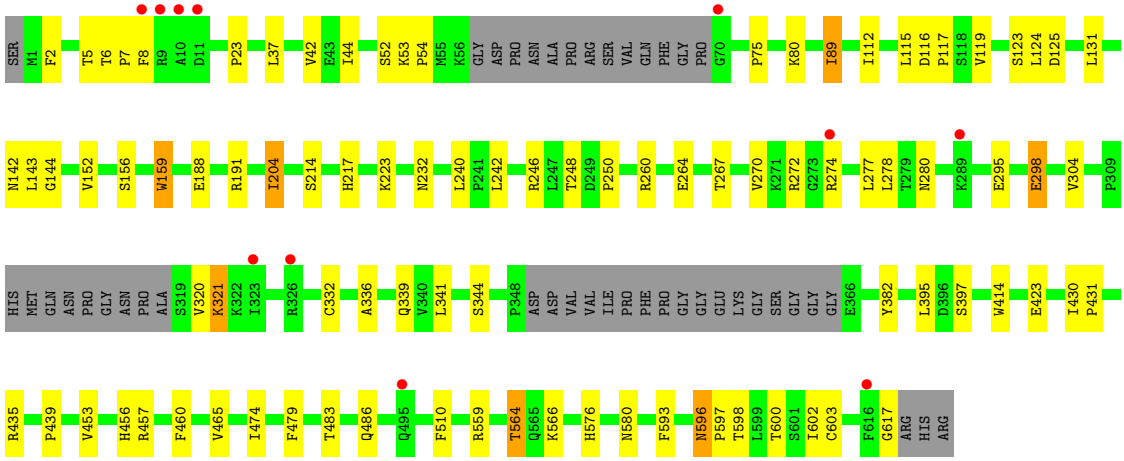
Chain E:





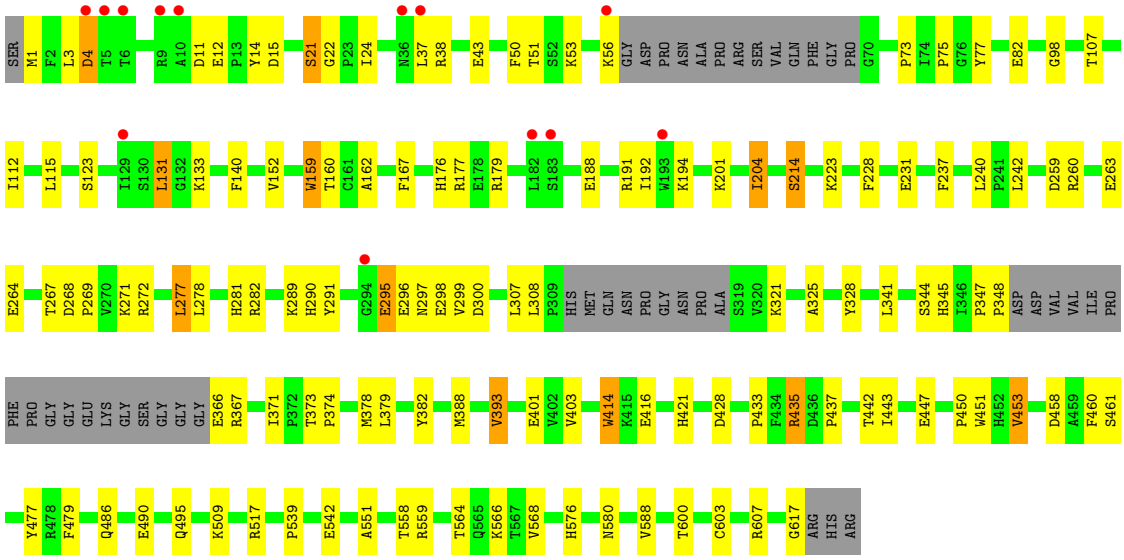
- Molecule 1: Pyranose 2-oxidase

Chain F:



- Molecule 1: Pyranose 2-oxidase

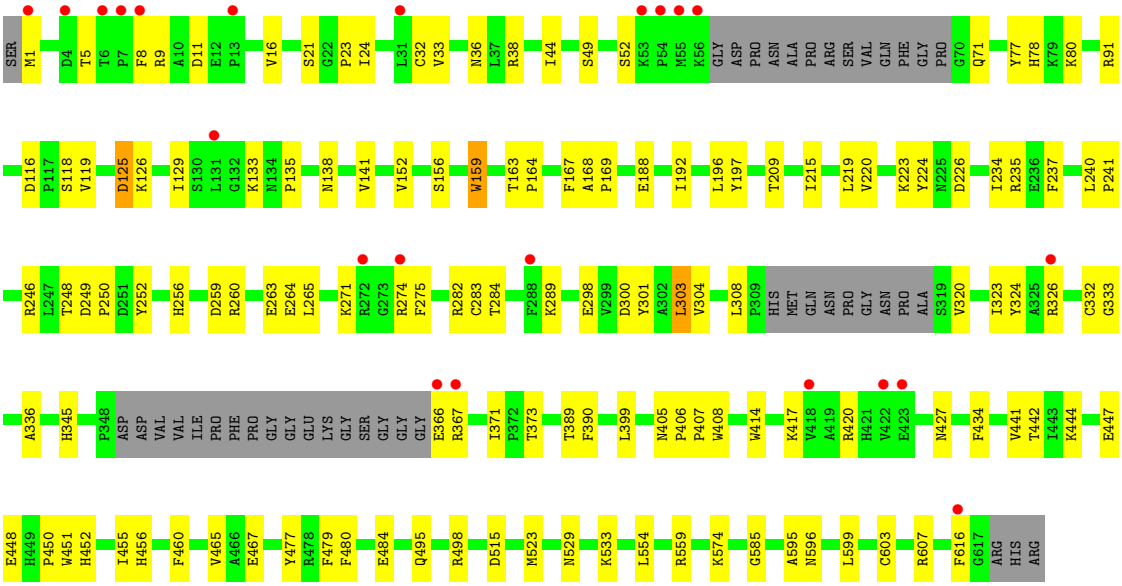
Chain G:



- Molecule 1: Pyranose 2-oxidase

Chain H:

4%
71%
21%
7%


SER M1 D4 T5 T6 P7 F8 R9 A10 D11 E12 P13 V16 S21 G22 P23 I24 L31 C32 V33 N36 L37 R38 I44 S49 S52 K53 P54 M55 K56 GLY ASP PRO ASN ALA PRO ARG SER VAL GLN PHE GLY PRO G70 Q71 Y77 H78 K79 K80 R91
D116 P117 S118 V119 D125 K126 I129 S130 L131 G132 K133 N134 P135 N138 V141 V152 S156 W159 T163 P164 F167 A168 P169 E188 I192 L196 Y197 T209 I215 L219 V220 K223 Y224 N225 D226 I234 R235 E236 F237 L240 P241
R246 L247 T248 D249 P250 D251 Y252 H256 D259 R260 E263 E264 L265 K271 R272 G273 R274 F275 R282 C283 T284 F288 K289 E298 V299 D300 Y301 A302 L303 V304 L308 P309 HIS MET GLN ASN PRO GLY ASN PRO ALA S319 V320 I323 Y324 A325 R326 C332 G333
A336 H345 P348 ASP ASP VAL VAL ILE PRO PHE PRO GLY GLY GLU LYS GLY SER GLY GLY GLY E366 R367 I371 P372 T373 T389 F390 L399 N405 P406 P407 W408 W414 K417 V418 A419 R420 H421 V422 E423 N427 F434 V441 T442 I443 K444 E447
E448 H449 P450 W451 H452 I455 H456 F460 V465 A466 E467 Y477 R478 F479 F480 E484 Q495 R498 D515 M523 N529 K533 L554 R559 K574 G585 A595 N596 L599 C603 R607 F616 G617 ARG HIS ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	110.10Å 167.10Å 168.47Å 90.00° 93.98° 90.00°	Depositor
Resolution (Å)	48.56 – 2.40 48.56 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.56-2.40) 98.4 (48.56-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.205 , 0.265 0.206 , 0.262	Depositor DCC
R_{free} test set	1500 reflections (0.64%)	wwPDB-VP
Wilson B-factor (Å^2)	44.5	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 43.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	37799	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, G3F

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	0.54	0/4670	0.63	0/6356
1	B	0.48	0/4690	0.60	0/6382
1	C	0.49	0/4690	0.61	0/6382
1	D	0.46	1/4690 (0.0%)	0.60	0/6382
1	E	0.44	0/4670	0.59	0/6356
1	F	0.41	0/4690	0.57	0/6382
1	G	0.44	0/4690	0.58	0/6382
1	H	0.42	0/4690	0.54	0/6382
All	All	0.46	1/37480 (0.0%)	0.59	0/51004

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	385	GLU	CD-OE2	-5.05	1.20	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4548	0	4440	65	0
1	B	4568	0	4459	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4568	0	4459	96	0
1	D	4568	0	4459	81	0
1	E	4548	0	4440	48	0
1	F	4568	0	4459	53	0
1	G	4568	0	4459	78	0
1	H	4568	0	4459	70	0
2	A	53	0	31	2	0
2	B	53	0	31	2	0
2	C	53	0	31	2	0
2	D	53	0	31	3	0
2	E	53	0	31	2	0
2	F	53	0	31	3	0
2	G	53	0	31	3	0
2	H	53	0	31	2	0
3	A	12	0	11	2	0
3	B	12	0	11	0	0
3	C	12	0	11	1	0
3	D	12	0	11	0	0
3	E	12	0	11	1	0
3	F	12	0	11	1	0
3	G	12	0	11	0	0
3	H	12	0	11	1	0
4	A	133	0	0	1	0
4	B	109	0	0	1	0
4	C	77	0	0	1	0
4	D	59	0	0	1	0
4	E	129	0	0	3	0
4	F	94	0	0	1	0
4	G	90	0	0	5	0
4	H	84	0	0	1	0
All	All	37799	0	35970	531	0

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

All (531) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:VAL:HG13	1:C:39:VAL:HG13	1.33	1.06
1:A:405:ASN:OD1	1:A:405:ASN:O	1.90	0.89
1:D:55:MET:HE1	1:D:272:ARG:HH11	1.38	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:264:GLU:HA	1:E:267:THR:HG22	1.60	0.84
1:D:4:ASP:O	1:D:5:THR:HG22	1.77	0.83
1:A:371:ILE:HA	1:A:495:GLN:HE21	1.42	0.83
1:D:385:GLU:HG3	1:D:386:GLN:H	1.42	0.81
1:D:4:ASP:O	1:D:5:THR:CG2	2.29	0.80
1:D:55:MET:CE	1:D:272:ARG:NH1	2.46	0.78
1:C:112:ILE:HD11	1:D:468:ASN:HB2	1.67	0.76
1:B:229:GLN:HA	1:B:234:ILE:HD13	1.68	0.76
1:H:24:ILE:HG13	1:H:585:GLY:HA2	1.69	0.73
1:D:55:MET:HE1	1:D:272:ARG:NH1	2.04	0.73
1:A:292:ARG:NE	1:A:295:GLU:OE1	2.21	0.72
1:H:326:ARG:NH2	1:H:616:PHE:O	2.21	0.72
1:D:401:GLU:OE1	1:D:401:GLU:HA	1.89	0.72
1:A:87:LYS:NZ	1:B:500:ALA:O	2.25	0.70
1:G:490:GLU:OE1	1:G:509:LYS:NZ	2.24	0.70
1:G:289:LYS:HD3	1:G:290:HIS:HD2	1.58	0.68
1:F:270:VAL:HG12	1:F:274:ARG:HH22	1.63	0.64
1:G:21:SER:HB3	1:G:43:GLU:HB2	1.78	0.64
1:D:385:GLU:HG3	1:D:386:GLN:N	2.13	0.64
1:F:42:VAL:HG12	1:F:278:LEU:HD12	1.80	0.64
1:D:16:VAL:HB	1:D:39:VAL:HG22	1.80	0.64
1:G:192:ILE:HD13	1:G:607:ARG:HH12	1.64	0.63
1:F:37:LEU:HD21	1:F:617:GLY:HA2	1.80	0.63
1:C:268:ASP:HB3	1:C:271:LYS:HB2	1.80	0.63
1:C:48:ASP:OD1	1:C:48:ASP:N	2.30	0.63
1:E:199:GLN:NE2	4:E:950:HOH:O	2.31	0.62
1:D:570:ASN:HD21	1:D:574:LYS:HB3	1.64	0.62
1:G:290:HIS:CE1	1:G:295:GLU:HG2	2.34	0.62
1:C:289:LYS:HE3	1:C:290:HIS:HD2	1.64	0.62
1:A:51:THR:HB	1:A:77:TYR:CD1	2.35	0.62
1:H:36:ASN:HA	1:H:274:ARG:HE	1.64	0.62
1:H:215:ILE:HD11	1:H:417:LYS:HD2	1.81	0.62
1:H:52:SER:HB3	1:H:71:GLN:HE21	1.64	0.61
1:A:501:TYR:CE2	1:B:83:ILE:HD11	2.35	0.61
1:C:214:SER:HB3	1:C:217:HIS:HB3	1.82	0.61
1:G:341:LEU:O	1:G:344:SER:HB2	1.99	0.61
1:A:266:PHE:O	1:A:272:ARG:NH1	2.33	0.61
1:E:2:PHE:H	1:F:52:SER:HB2	1.65	0.61
1:F:23:PRO:HG3	1:F:156:SER:HB3	1.83	0.60
1:B:15:ASP:HA	1:B:326:ARG:HG3	1.83	0.60
1:D:4:ASP:C	1:D:5:THR:CG2	2.69	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:188:GLU:OE2	1:G:191:ARG:NH1	2.33	0.60
1:C:612:ILE:O	1:C:616:PHE:HB2	2.01	0.60
1:D:385:GLU:CG	1:D:386:GLN:H	2.12	0.60
1:B:301:TYR:HE1	1:B:303:LEU:HD12	1.67	0.60
1:C:271:LYS:HA	1:C:274:ARG:HH21	1.66	0.60
1:D:4:ASP:C	1:D:5:THR:HG23	2.23	0.60
1:H:78:HIS:CE1	1:H:80:LYS:HB2	2.37	0.60
1:F:217:HIS:HA	1:F:439:PRO:HB3	1.84	0.59
1:C:596:ASN:OD1	1:C:596:ASN:N	2.26	0.59
1:F:332:CYS:O	1:F:336:ALA:HB3	2.02	0.59
1:D:42:VAL:HG12	1:D:278:LEU:HB2	1.84	0.59
1:D:55:MET:HE2	1:D:272:ARG:NH1	2.18	0.59
1:H:21:SER:OG	1:H:152:VAL:HA	2.03	0.59
1:B:33:VAL:HG23	1:B:39:VAL:HG21	1.83	0.58
1:C:98:GLY:O	1:D:91:ARG:NH1	2.36	0.58
1:D:246:ARG:NH1	1:D:250:PRO:O	2.36	0.58
1:G:345:HIS:CD2	1:G:373:THR:HA	2.38	0.58
1:C:16:VAL:HG12	1:C:39:VAL:HG22	1.85	0.58
1:B:408:TRP:HB2	1:B:411:LEU:HD11	1.86	0.58
1:A:78:HIS:CE1	1:A:80:LYS:HB2	2.39	0.58
1:C:16:VAL:CG1	1:C:39:VAL:HG22	2.33	0.58
1:D:167:PHE:CE2	1:D:447:GLU:HG2	2.39	0.57
1:A:501:TYR:HE2	1:B:83:ILE:HD11	1.68	0.57
1:G:176:HIS:ND1	1:G:447:GLU:OE2	2.25	0.57
1:B:297:ASN:OD1	1:B:298:GLU:N	2.38	0.57
1:B:339:GLN:NE2	1:B:504:PRO:O	2.28	0.57
1:D:386:GLN:HB3	1:D:481:GLY:O	2.04	0.57
1:E:411:LEU:HB3	1:E:414:TRP:HB3	1.86	0.57
1:C:21:SER:OG	1:C:152:VAL:HA	2.04	0.57
1:D:146:GLU:OE2	1:D:385:GLU:OE1	2.23	0.57
1:D:385:GLU:CG	1:D:386:GLN:N	2.68	0.57
1:C:109:ASN:ND2	1:C:127:PRO:HB3	2.20	0.56
1:D:24:ILE:HG21	1:D:585:GLY:N	2.21	0.55
1:H:219:LEU:HD21	1:H:399:LEU:HD13	1.87	0.55
1:H:371:ILE:HG12	1:H:495:GLN:HG2	1.88	0.55
1:C:73:PRO:HB3	1:D:1:MET:HE1	1.88	0.55
1:D:182:LEU:HD22	1:D:571:THR:HB	1.86	0.55
1:C:42:VAL:HG12	1:C:278:LEU:HB2	1.89	0.55
1:B:41:MET:HG2	1:B:277:LEU:HD13	1.87	0.55
1:B:75:PRO:HB2	1:B:152:VAL:HG11	1.89	0.55
1:D:75:PRO:HB2	1:D:152:VAL:HG11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:345:HIS:NE2	1:E:375:LEU:HB2	2.21	0.55
1:C:159:TRP:HA	2:C:801:FAD:C6	2.37	0.55
1:D:308:LEU:O	1:D:308:LEU:HD12	2.07	0.54
1:A:70:GLY:N	1:B:4:ASP:OD2	2.40	0.54
1:B:33:VAL:HG23	1:B:39:VAL:CG2	2.38	0.54
1:D:332:CYS:O	1:D:336:ALA:HB3	2.07	0.54
1:E:292:ARG:NE	1:E:295:GLU:OE1	2.36	0.54
1:G:98:GLY:O	1:H:91:ARG:NH1	2.41	0.54
1:F:264:GLU:HA	1:F:267:THR:HG22	1.88	0.54
1:C:116:ASP:HB3	1:C:119:VAL:HG13	1.89	0.54
1:F:483:THR:HG21	1:F:510:PHE:HZ	1.73	0.54
1:A:112:ILE:HD11	1:B:468:ASN:HB2	1.90	0.54
1:E:543:PRO:O	1:G:542:GLU:HG2	2.08	0.54
1:G:345:HIS:HD2	1:G:374:PRO:HD2	1.73	0.54
1:D:558:THR:O	1:D:588:VAL:HA	2.07	0.53
1:C:16:VAL:CG1	1:C:39:VAL:HG13	2.24	0.53
1:G:56:LYS:HB2	1:G:269:PRO:HD3	1.90	0.53
1:A:4:ASP:OD1	1:B:70:GLY:N	2.41	0.53
1:E:264:GLU:OE1	1:E:271:LYS:NZ	2.40	0.53
1:C:264:GLU:HA	1:C:267:THR:HG22	1.89	0.53
1:D:99:ALA:HB1	1:D:149:THR:HG23	1.89	0.53
1:H:125:ASP:OD1	1:H:125:ASP:N	2.40	0.53
1:H:138:ASN:HB3	1:H:141:VAL:HG22	1.88	0.53
1:F:75:PRO:HB2	1:F:152:VAL:HG11	1.89	0.53
1:F:382:TYR:HA	1:F:486:GLN:O	2.07	0.53
1:D:188:GLU:O	1:D:192:ILE:HG13	2.08	0.53
1:F:54:PRO:O	1:F:267:THR:OG1	2.26	0.53
1:C:16:VAL:HG13	1:C:39:VAL:CG1	2.24	0.53
1:G:37:LEU:HD21	1:G:617:GLY:HA2	1.91	0.53
1:E:225:ASN:O	1:E:229:GLN:HG2	2.09	0.53
1:F:159:TRP:HA	2:F:801:FAD:C6	2.39	0.53
1:C:245:HIS:CE1	1:C:254:GLU:HG2	2.44	0.52
1:G:112:ILE:HB	1:G:115:LEU:HG	1.91	0.52
1:H:407:PRO:HD2	1:H:408:TRP:CE3	2.44	0.52
1:A:210:GLU:HG3	1:A:245:HIS:HA	1.91	0.52
1:C:562:LEU:HD21	1:C:571:THR:HG21	1.90	0.52
1:G:188:GLU:O	1:G:192:ILE:HG13	2.09	0.52
1:F:8:PHE:CE2	1:F:321:LYS:HE2	2.45	0.52
1:G:296:GLU:HG3	1:G:297:ASN:N	2.24	0.52
1:C:52:SER:OG	1:D:2:PHE:N	2.41	0.52
1:D:166:PHE:HB3	1:D:178:GLU:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:441:VAL:HB	1:H:455:ILE:HB	1.91	0.52
1:E:492:VAL:HG23	1:E:507:THR:HB	1.92	0.52
1:G:177:ARG:NE	1:G:179:ARG:O	2.39	0.52
1:E:342:ALA:O	1:E:345:HIS:HB2	2.10	0.52
1:F:8:PHE:HE2	1:F:321:LYS:HE2	1.74	0.52
1:C:265:LEU:HA	1:C:271:LYS:HB3	1.91	0.52
1:F:457:ARG:HD3	1:F:474:ILE:O	2.09	0.52
1:G:228:PHE:HA	1:G:231:GLU:HG2	1.92	0.52
1:H:196:LEU:HD11	1:H:607:ARG:HD3	1.91	0.52
1:G:73:PRO:HB3	1:H:1:MET:SD	2.49	0.52
1:C:28:PHE:HA	1:C:609:SER:OG	2.10	0.51
1:E:172:PHE:CZ	1:E:181:LYS:HD3	2.45	0.51
2:E:801:FAD:N5	3:E:802:G3F:H2	2.25	0.51
1:F:188:GLU:OE1	1:F:191:ARG:NE	2.35	0.51
1:G:201:LYS:HE2	4:G:926:HOH:O	2.10	0.51
1:H:163:THR:HB	1:H:599:LEU:HB2	1.92	0.51
1:A:544:GLN:HG3	1:A:546:MET:HE2	1.92	0.51
2:C:801:FAD:N5	3:C:802:G3F:H2	2.25	0.51
1:E:84:GLU:OE2	1:E:91:ARG:NH1	2.44	0.51
1:A:297:ASN:N	1:A:577:ASN:O	2.42	0.51
1:B:345:HIS:NE2	1:B:375:LEU:HB2	2.25	0.51
1:E:498:ARG:HG2	1:E:502:ASP:HA	1.92	0.51
1:A:412:ASP:N	1:A:412:ASP:OD1	2.41	0.51
1:B:345:HIS:CD2	1:B:374:PRO:HD2	2.45	0.51
1:D:116:ASP:O	1:D:119:VAL:HG22	2.11	0.51
1:H:220:VAL:HG12	1:H:441:VAL:HG21	1.93	0.51
1:H:448:GLU:OE1	1:H:448:GLU:N	2.44	0.51
1:A:33:VAL:HG11	1:A:265:LEU:HD22	1.92	0.50
1:A:438:GLU:OE2	1:A:438:GLU:N	2.36	0.50
1:C:287:VAL:HB	1:C:301:TYR:CE2	2.46	0.50
1:A:559:ARG:NH1	1:A:566:LYS:O	2.44	0.50
1:E:420:ARG:HG2	4:E:903:HOH:O	2.10	0.50
1:C:55:MET:SD	1:C:272:ARG:NH2	2.85	0.50
1:C:138:ASN:HB3	1:C:141:VAL:HG22	1.93	0.50
1:D:44:ILE:HB	2:D:801:FAD:C2A	2.42	0.50
1:G:600:THR:O	1:G:603:CYS:HB2	2.11	0.50
1:A:256:HIS:HB3	1:A:260:ARG:HD3	1.93	0.50
1:G:268:ASP:OD2	1:G:271:LYS:HG3	2.12	0.50
1:G:378:MET:HE3	1:G:566:LYS:HA	1.92	0.50
1:B:3:LEU:HD12	1:B:277:LEU:HG	1.94	0.50
1:F:5:THR:HG21	1:F:277:LEU:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:ILE:HD11	1:D:468:ASN:CB	2.37	0.50
1:C:282:ARG:NE	1:C:284:THR:OG1	2.34	0.50
1:A:11:ASP:O	1:A:13:PRO:HD3	2.12	0.49
1:B:80:LYS:HD2	1:B:89:ILE:HD11	1.93	0.49
1:C:327:SER:HB3	1:C:616:PHE:CE2	2.47	0.49
1:D:492:VAL:HG23	1:D:507:THR:HB	1.94	0.49
1:E:512:MET:HG2	4:E:902:HOH:O	2.11	0.49
1:E:480:PHE:O	1:E:594:ALA:HB1	2.12	0.49
1:D:55:MET:HE1	1:D:272:ARG:HD2	1.94	0.49
1:D:283:CYS:HA	1:D:304:VAL:HG22	1.94	0.49
1:D:4:ASP:O	1:D:5:THR:HG23	2.13	0.49
1:F:564:THR:HG23	1:F:576:HIS:CE1	2.48	0.49
1:G:1:MET:HG2	1:G:50:PHE:HZ	1.77	0.49
1:E:240:LEU:HD13	1:E:442:THR:HB	1.94	0.49
1:C:291:TYR:CZ	1:C:347:PRO:HB3	2.48	0.49
1:H:345:HIS:CD2	1:H:373:THR:HA	2.47	0.49
1:B:453:VAL:HB	1:B:479:PHE:CE1	2.47	0.49
1:D:291:TYR:CE1	1:D:347:PRO:HB3	2.48	0.49
1:D:412:ASP:N	1:D:412:ASP:OD1	2.46	0.49
1:D:210:GLU:HG3	1:D:245:HIS:HA	1.95	0.49
1:D:488:ALA:O	1:D:490:GLU:HG3	2.12	0.48
1:A:596:ASN:OD1	1:A:596:ASN:N	2.41	0.48
1:C:204:ILE:O	1:C:256:HIS:ND1	2.38	0.48
1:D:56:LYS:HG3	1:D:267:THR:HG23	1.95	0.48
1:F:246:ARG:NH1	1:F:250:PRO:O	2.46	0.48
1:G:388:MET:HE2	1:G:551:ALA:HB2	1.95	0.48
1:C:52:SER:CB	1:D:2:PHE:H	2.27	0.48
1:F:272:ARG:HH11	1:F:272:ARG:HB3	1.79	0.48
1:H:223:LYS:HD2	1:H:223:LYS:HA	1.64	0.48
1:G:539:PRO:HA	1:G:542:GLU:OE2	2.14	0.48
1:A:396:ASP:OD1	1:A:535:GLY:HA2	2.14	0.48
1:C:110:ASN:HB2	1:D:468:ASN:OD1	2.13	0.48
1:F:270:VAL:HG12	1:F:274:ARG:NH2	2.29	0.48
1:E:246:ARG:NH1	1:E:250:PRO:O	2.47	0.48
1:E:390:PHE:HA	1:E:477:TYR:O	2.13	0.48
1:G:299:VAL:H	1:G:580:ASN:HD21	1.62	0.48
1:B:205:GLY:HA3	1:B:256:HIS:HD1	1.78	0.48
1:C:112:ILE:HB	1:C:115:LEU:HG	1.95	0.48
1:H:450:PRO:HD2	1:H:451:TRP:CZ3	2.49	0.48
1:C:38:ARG:HA	1:C:274:ARG:HB3	1.95	0.48
1:H:390:PHE:HA	1:H:477:TYR:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:ASP:HB3	1:C:174:ALA:HB2	1.95	0.47
1:D:24:ILE:HG22	1:D:331:ALA:HB1	1.96	0.47
1:E:291:TYR:CD2	1:E:347:PRO:HG3	2.49	0.47
1:G:75:PRO:HB2	1:G:152:VAL:HG11	1.96	0.47
1:A:264:GLU:HA	1:A:267:THR:HG22	1.96	0.47
1:A:287:VAL:HG21	1:A:301:TYR:CZ	2.48	0.47
2:F:801:FAD:N5	3:F:802:G3F:H2	2.29	0.47
1:G:393:VAL:HG22	1:G:477:TYR:HE1	1.78	0.47
1:D:36:ASN:HA	1:D:274:ARG:CZ	2.45	0.47
1:H:451:TRP:CG	1:H:523:MET:HG3	2.50	0.47
2:H:801:FAD:N5	3:H:802:G3F:H2	2.30	0.47
1:E:404:ARG:HH11	1:E:431:PRO:HG3	1.80	0.47
1:D:330:VAL:CG1	1:D:337:THR:HG23	2.44	0.47
1:E:285:LYS:NZ	1:E:346:ILE:O	2.42	0.47
1:G:371:ILE:HG12	1:G:495:GLN:HG3	1.97	0.47
1:H:116:ASP:O	1:H:119:VAL:HG22	2.14	0.47
1:D:329:VAL:HG22	1:D:582:TYR:HB2	1.97	0.47
1:F:217:HIS:HB2	1:F:439:PRO:HA	1.96	0.47
1:G:347:PRO:HA	1:G:348:PRO:HD2	1.80	0.47
1:H:240:LEU:HD13	1:H:442:THR:HB	1.95	0.47
1:H:529:ASN:O	1:H:533:LYS:HG2	2.15	0.47
1:D:89:ILE:HD12	1:D:89:ILE:HA	1.74	0.47
1:G:53:LYS:HG3	1:G:263:GLU:OE2	2.15	0.47
1:G:453:VAL:HB	1:G:479:PHE:CE1	2.50	0.47
1:C:411:LEU:O	1:C:415:LYS:HG3	2.14	0.47
1:H:164:PRO:HG2	1:H:595:ALA:HB1	1.96	0.47
1:A:382:TYR:OH	1:A:566:LYS:HD2	2.15	0.47
1:B:208:THR:HG22	1:B:241:PRO:HA	1.97	0.47
1:D:613:ILE:C	1:D:615:LYS:H	2.19	0.47
1:E:450:PRO:HD2	1:E:451:TRP:CZ3	2.50	0.47
1:F:112:ILE:HB	1:F:115:LEU:HG	1.97	0.47
1:G:297:ASN:OD1	1:G:298:GLU:N	2.48	0.47
1:H:38:ARG:HA	1:H:274:ARG:HB2	1.97	0.47
1:C:33:VAL:HG11	1:C:265:LEU:HD22	1.97	0.46
1:D:43:GLU:OE2	2:D:801:FAD:O2B	2.23	0.46
1:G:240:LEU:HD13	1:G:442:THR:HB	1.96	0.46
1:G:291:TYR:CZ	1:G:347:PRO:HB3	2.49	0.46
1:H:33:VAL:HG21	1:H:265:LEU:HD21	1.96	0.46
1:D:55:MET:SD	1:D:72:VAL:HG21	2.55	0.46
1:F:44:ILE:O	1:F:280:ASN:HA	2.15	0.46
1:G:435:ARG:NH1	4:G:985:HOH:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:ASP:O	1:C:119:VAL:HG22	2.15	0.46
1:C:188:GLU:O	1:C:192:ILE:HG13	2.15	0.46
1:C:91:ARG:HH11	1:C:91:ARG:HG2	1.80	0.46
1:E:326:ARG:NH2	1:E:616:PHE:O	2.49	0.46
1:G:3:LEU:HD12	1:G:277:LEU:HB3	1.98	0.46
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.74	0.46
1:G:15:ASP:OD2	1:G:38:ARG:N	2.47	0.46
1:G:167:PHE:CE2	1:G:447:GLU:HG2	2.51	0.46
1:A:439:PRO:O	1:A:456:HIS:HA	2.16	0.46
1:B:8:PHE:CZ	1:B:323:ILE:HG12	2.51	0.46
1:B:414:TRP:CD1	1:B:414:TRP:C	2.89	0.46
1:C:406:PRO:HA	1:C:407:PRO:HD3	1.86	0.46
1:D:450:PRO:HD2	1:D:451:TRP:CZ3	2.50	0.46
1:D:574:LYS:HB2	1:D:582:TYR:CE2	2.51	0.46
1:E:430:ILE:HA	1:E:431:PRO:HD3	1.76	0.46
1:C:53:LYS:HG2	1:C:263:GLU:CD	2.36	0.45
1:C:72:VAL:HG11	1:C:266:PHE:O	2.16	0.45
2:A:801:FAD:N5	3:A:802:G3F:H2	2.32	0.45
1:B:6:THR:HA	1:B:7:PRO:HD3	1.83	0.45
1:D:1:MET:CE	1:D:3:LEU:HD23	2.47	0.45
1:D:291:TYR:CZ	1:D:347:PRO:HB3	2.50	0.45
1:D:373:THR:HG21	1:D:379:LEU:HD23	1.98	0.45
1:A:195:ASP:OD2	1:A:199:GLN:NE2	2.46	0.45
1:A:287:VAL:HG21	1:A:301:TYR:CE1	2.52	0.45
1:C:593:PHE:CE1	1:C:597:PRO:HB3	2.52	0.45
1:F:596:ASN:OD1	1:F:596:ASN:N	2.49	0.45
1:G:21:SER:OG	1:G:152:VAL:HA	2.17	0.45
1:H:8:PHE:CZ	1:H:323:ILE:HG12	2.51	0.45
1:A:134:ASN:ND2	1:A:137:GLN:HB2	2.32	0.45
1:D:345:HIS:CD2	1:D:373:THR:HA	2.51	0.45
1:H:167:PHE:CE2	1:H:447:GLU:HG2	2.51	0.45
1:H:452:HIS:HB3	1:H:480:PHE:HB2	1.98	0.45
1:C:51:THR:HB	1:C:77:TYR:CD1	2.51	0.45
1:E:52:SER:O	1:E:53:LYS:HD3	2.16	0.45
1:H:125:ASP:O	1:H:126:LYS:HG2	2.17	0.45
1:H:389:THR:OG1	1:H:479:PHE:HB2	2.17	0.45
1:A:185:ASP:OD2	1:A:188:GLU:N	2.50	0.45
1:A:194:LYS:HB2	1:A:194:LYS:HE3	1.76	0.45
1:H:192:ILE:HG21	1:H:607:ARG:HD2	1.99	0.45
1:B:72:VAL:HA	1:B:73:PRO:HD2	1.89	0.45
1:E:159:TRP:HA	2:E:801:FAD:C6	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:453:VAL:HB	1:F:479:PHE:CE1	2.51	0.45
1:H:196:LEU:HD13	1:H:603:CYS:HB3	1.99	0.45
1:H:495:GLN:O	1:H:498:ARG:NH1	2.49	0.45
1:B:192:ILE:HD13	1:B:607:ARG:HH12	1.82	0.45
1:C:299:VAL:HB	1:C:580:ASN:HD21	1.82	0.45
1:H:133:LYS:O	1:H:135:PRO:HD3	2.16	0.45
1:C:270:VAL:HG12	1:C:274:ARG:NH2	2.32	0.45
1:D:1:MET:HG2	1:D:50:PHE:CZ	2.52	0.45
1:A:138:ASN:HB3	1:A:141:VAL:HG22	1.98	0.45
1:D:600:THR:O	1:D:603:CYS:HB2	2.17	0.45
1:G:414:TRP:CD1	1:G:414:TRP:C	2.91	0.45
1:B:407:PRO:HD2	1:B:408:TRP:CE3	2.52	0.44
1:F:42:VAL:HG11	1:F:304:VAL:HG11	1.99	0.44
1:H:283:CYS:HA	1:H:304:VAL:HG22	1.98	0.44
1:H:574:LYS:HE2	1:H:574:LYS:HB3	1.88	0.44
1:A:436:ASP:HA	1:A:437:PRO:HD3	1.77	0.44
1:C:31:LEU:HD11	1:C:606:ILE:HG12	1.98	0.44
1:F:430:ILE:HA	1:F:431:PRO:HD3	1.72	0.44
1:F:600:THR:O	1:F:603:CYS:HB2	2.16	0.44
1:A:122:ASN:OD1	1:A:122:ASN:N	2.50	0.44
1:A:377:PRO:O	1:A:381:LYS:HE2	2.17	0.44
1:A:390:PHE:CD2	1:A:546:MET:HE3	2.53	0.44
2:B:801:FAD:H1'1	2:B:801:FAD:H9	1.69	0.44
1:C:246:ARG:NH1	1:C:250:PRO:O	2.48	0.44
1:G:263:GLU:O	1:G:267:THR:HG22	2.18	0.44
1:H:259:ASP:OD1	1:H:260:ARG:N	2.51	0.44
1:H:284:THR:HB	1:H:303:LEU:HD23	1.99	0.44
1:A:301:TYR:CE1	1:A:322:LYS:HE3	2.52	0.44
1:C:301:TYR:H	1:C:301:TYR:HD2	1.64	0.44
1:D:55:MET:CE	1:D:272:ARG:HD2	2.48	0.44
1:A:390:PHE:HB3	1:A:546:MET:CE	2.47	0.44
1:B:133:LYS:O	1:B:135:PRO:HD3	2.18	0.44
1:C:224:TYR:CZ	1:C:534:ILE:HG12	2.53	0.44
1:E:52:SER:HB3	1:E:71:GLN:HE21	1.83	0.44
1:G:107:THR:HG22	1:G:133:LYS:HB2	1.98	0.44
1:G:450:PRO:HD2	1:G:451:TRP:CZ3	2.53	0.44
1:H:78:HIS:ND1	1:H:80:LYS:HB2	2.33	0.44
1:A:159:TRP:HA	2:A:801:FAD:C6	2.47	0.44
1:G:382:TYR:HA	1:G:486:GLN:O	2.18	0.44
1:A:303:LEU:HD12	1:A:303:LEU:HA	1.72	0.44
1:C:373:THR:HG21	1:C:379:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:HIS:ND1	1:C:433:PRO:HA	2.33	0.44
1:D:325:ALA:N	1:D:328:TYR:OH	2.36	0.44
1:C:414:TRP:CD1	1:C:414:TRP:C	2.92	0.44
1:E:240:LEU:HA	1:E:241:PRO:HD3	1.75	0.44
1:H:301:TYR:HB3	1:H:324:TYR:CE2	2.53	0.44
1:A:202:GLU:O	1:A:260:ARG:NH2	2.51	0.43
1:C:301:TYR:CD2	1:C:301:TYR:N	2.85	0.43
1:A:1:MET:SD	1:A:2:PHE:N	2.91	0.43
1:B:22:GLY:HA3	2:B:801:FAD:O1P	2.18	0.43
1:G:214:SER:HB2	1:G:437:PRO:HB2	2.00	0.43
1:A:390:PHE:HB3	1:A:546:MET:HE3	1.99	0.43
1:C:432:ILE:HA	1:C:433:PRO:HD3	1.80	0.43
1:D:225:ASN:O	1:D:229:GLN:HG2	2.19	0.43
1:G:11:ASP:OD2	1:G:12:GLU:HG3	2.18	0.43
1:G:564:THR:HG23	1:G:576:HIS:CE1	2.53	0.43
1:A:292:ARG:HA	1:A:293:PRO:HD3	1.87	0.43
1:C:14:TYR:HB2	1:C:325:ALA:HB2	2.01	0.43
1:C:166:PHE:CZ	1:C:597:PRO:HA	2.54	0.43
1:C:430:ILE:HA	1:C:431:PRO:HD2	1.88	0.43
1:D:345:HIS:HD2	1:D:374:PRO:HD2	1.83	0.43
1:G:282:ARG:HB2	1:G:307:LEU:HD11	2.01	0.43
1:G:291:TYR:CE1	1:G:347:PRO:HB3	2.54	0.43
1:G:442:THR:OG1	1:G:443:ILE:N	2.51	0.43
1:H:246:ARG:NH1	1:H:250:PRO:O	2.51	0.43
1:A:84:GLU:HG2	4:A:933:HOH:O	2.19	0.43
1:B:51:THR:HB	1:B:77:TYR:CD1	2.53	0.43
1:B:394:VAL:HA	1:B:473:VAL:O	2.19	0.43
1:B:560:CYS:HB3	1:B:570:ASN:O	2.18	0.43
1:C:24:ILE:HG22	1:C:331:ALA:HB1	1.99	0.43
1:E:52:SER:HB2	1:F:2:PHE:H	1.84	0.43
1:E:282:ARG:NE	1:E:284:THR:OG1	2.51	0.43
1:F:80:LYS:HD2	1:F:89:ILE:HD11	2.01	0.43
1:F:341:LEU:O	1:F:344:SER:HB2	2.17	0.43
1:G:237:PHE:CE2	1:G:443:ILE:HD11	2.53	0.43
1:H:447:GLU:O	1:H:450:PRO:HG3	2.18	0.43
1:A:505:GLN:OE1	1:A:506:PRO:HD2	2.19	0.43
1:H:23:PRO:HD3	1:H:156:SER:HB3	2.01	0.43
1:B:205:GLY:HA3	1:B:256:HIS:ND1	2.34	0.43
1:C:345:HIS:HD2	1:C:374:PRO:HD2	1.84	0.43
1:C:596:ASN:HA	1:C:597:PRO:HD3	1.92	0.43
1:E:84:GLU:HG3	4:F:925:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6:THR:HA	1:F:7:PRO:HD3	1.88	0.43
2:G:801:FAD:O4'	2:G:801:FAD:O2'	2.35	0.43
1:H:249:ASP:HB3	1:H:252:TYR:HD1	1.84	0.43
1:A:14:TYR:CE2	1:A:40:CYS:HB2	2.54	0.43
1:C:26:ALA:HB2	1:C:258:THR:HG23	1.99	0.43
1:C:55:MET:HG3	1:C:267:THR:O	2.18	0.43
1:D:385:GLU:OE2	1:D:553:HIS:N	2.51	0.43
1:F:123:SER:HA	1:G:140:PHE:CD2	2.53	0.43
1:G:568:VAL:HA	4:G:933:HOH:O	2.18	0.43
1:C:134:ASN:HA	1:C:135:PRO:HD3	1.85	0.43
1:C:240:LEU:HA	1:C:241:PRO:HD3	1.93	0.43
1:C:287:VAL:HG11	1:C:301:TYR:HE2	1.84	0.43
1:F:143:LEU:HD23	1:F:143:LEU:HA	1.86	0.43
1:G:4:ASP:O	1:G:272:ARG:NH2	2.52	0.43
1:H:264:GLU:OE1	1:H:271:LYS:HE2	2.19	0.43
1:A:11:ASP:OD2	1:E:570:ASN:HB2	2.18	0.43
1:C:326:ARG:NH2	1:C:616:PHE:HD1	2.17	0.43
1:C:347:PRO:HA	1:C:348:PRO:HD3	1.89	0.43
1:D:330:VAL:HG11	1:D:337:THR:HG23	2.00	0.43
1:E:292:ARG:HA	1:E:293:PRO:HD2	1.82	0.43
1:B:138:ASN:HB3	1:B:141:VAL:HG22	2.00	0.42
1:B:443:ILE:HD12	1:B:453:VAL:HG21	2.00	0.42
1:D:182:LEU:HD23	1:D:182:LEU:HA	1.71	0.42
1:E:396:ASP:HA	1:F:119:VAL:HA	2.01	0.42
1:G:204:ILE:HD12	1:G:204:ILE:HA	1.77	0.42
1:B:21:SER:OG	1:B:152:VAL:HA	2.19	0.42
1:D:598:THR:HG1	2:D:801:FAD:C2	2.32	0.42
1:H:224:TYR:HB3	1:H:237:PHE:CD1	2.54	0.42
1:H:289:LYS:HD3	1:H:298:GLU:HB2	2.01	0.42
1:H:399:LEU:HD23	1:H:399:LEU:HA	1.80	0.42
1:B:446:THR:HB	1:B:448:GLU:HG2	2.00	0.42
1:C:416:GLU:O	1:C:420:ARG:HG3	2.18	0.42
1:D:204:ILE:HD12	1:D:204:ILE:HA	1.74	0.42
1:H:5:THR:HB	1:H:275:PHE:O	2.19	0.42
1:H:49:SER:OG	1:H:77:TYR:O	2.30	0.42
1:A:297:ASN:O	1:A:578:PHE:HA	2.19	0.42
1:A:551:ALA:O	3:A:802:G3F:O1	2.26	0.42
1:B:449:HIS:O	1:B:451:TRP:N	2.47	0.42
1:G:228:PHE:CD2	1:G:231:GLU:HG3	2.54	0.42
1:H:159:TRP:HA	2:H:801:FAD:C6	2.48	0.42
1:A:308:LEU:HA	1:A:309:PRO:HD2	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:LEU:HD23	1:F:242:LEU:HD21	2.00	0.42
1:F:321:LYS:HD3	1:F:321:LYS:HA	1.66	0.42
1:G:379:LEU:HD11	1:G:558:THR:HG22	2.01	0.42
1:A:88:ASP:OD2	1:A:91:ARG:HG3	2.20	0.42
1:A:326:ARG:NH2	1:A:616:PHE:HB3	2.35	0.42
1:C:50:PHE:HA	1:C:74:ILE:O	2.20	0.42
1:E:120:VAL:HG23	1:F:395:LEU:O	2.19	0.42
1:E:414:TRP:CD1	1:E:414:TRP:C	2.93	0.42
1:H:16:VAL:HG21	1:H:32:CYS:SG	2.60	0.42
1:A:452:HIS:HB3	1:A:480:PHE:HB2	2.00	0.42
1:B:237:PHE:CE2	1:B:443:ILE:HD11	2.55	0.42
1:B:264:GLU:HA	1:B:267:THR:HG22	2.02	0.42
1:B:285:LYS:HB2	1:B:344:SER:HA	2.02	0.42
1:D:43:GLU:O	1:D:280:ASN:N	2.52	0.42
1:G:159:TRP:HA	2:G:801:FAD:C6	2.50	0.42
1:H:332:CYS:O	1:H:336:ALA:HB3	2.19	0.42
1:H:444:LYS:HE3	1:H:444:LYS:HB2	1.85	0.42
1:A:345:HIS:CD2	1:A:373:THR:HA	2.55	0.42
1:A:448:GLU:OE1	1:A:448:GLU:N	2.53	0.42
1:B:197:TYR:O	1:B:201:LYS:HG3	2.20	0.42
1:B:457:ARG:HD3	1:B:474:ILE:O	2.20	0.42
1:C:448:GLU:N	1:C:448:GLU:OE2	2.53	0.42
1:D:319:SER:O	1:D:319:SER:OG	2.33	0.42
1:E:120:VAL:HA	1:F:397:SER:HB3	2.02	0.42
1:F:124:LEU:HD12	1:F:124:LEU:HA	1.62	0.42
1:F:559:ARG:NH1	1:F:566:LYS:O	2.52	0.42
1:G:328:TYR:N	1:G:580:ASN:O	2.52	0.42
1:B:179:ARG:HA	1:B:180:PRO:HD3	1.82	0.42
1:B:185:ASP:HB3	1:B:188:GLU:HB3	2.01	0.42
1:C:223:LYS:HD2	1:C:223:LYS:HA	1.90	0.42
1:F:204:ILE:HD12	1:F:204:ILE:HA	1.66	0.42
1:H:406:PRO:HA	1:H:407:PRO:HD3	1.94	0.42
1:B:512:MET:HG2	1:B:516:ASP:HB3	2.02	0.42
1:D:162:ALA:HA	1:D:242:LEU:HD23	2.01	0.42
1:D:436:ASP:HA	1:D:437:PRO:HD3	1.89	0.42
1:D:560:CYS:SG	1:D:588:VAL:HB	2.60	0.42
1:H:240:LEU:HD12	1:H:241:PRO:HD2	2.01	0.42
1:C:299:VAL:HB	1:C:580:ASN:ND2	2.35	0.41
1:D:382:TYR:HB2	1:D:559:ARG:HD2	2.02	0.41
1:F:142:ASN:ND2	1:F:144:GLY:HA2	2.35	0.41
1:G:131:LEU:HG	1:H:434:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:PRO:C	1:D:374:PRO:HD3	2.39	0.41
1:F:336:ALA:HA	1:F:339:GLN:HB3	2.02	0.41
1:G:403:VAL:HA	1:G:414:TRP:HZ2	1.83	0.41
1:H:44:ILE:HD12	1:H:282:ARG:HG3	2.02	0.41
1:A:388:MET:HA	1:A:479:PHE:O	2.20	0.41
1:B:430:ILE:HD13	1:B:473:VAL:HG13	2.01	0.41
1:C:8:PHE:HA	1:C:14:TYR:OH	2.20	0.41
1:C:200:ALA:HA	1:C:203:ILE:HD12	2.02	0.41
1:D:486:GLN:N	4:D:949:HOH:O	2.47	0.41
1:F:117:PRO:O	1:G:517:ARG:NH1	2.52	0.41
1:B:345:HIS:HD2	1:B:374:PRO:HD2	1.84	0.41
1:E:178:GLU:HG2	1:E:593:PHE:HA	2.03	0.41
1:F:116:ASP:O	1:F:119:VAL:HG22	2.20	0.41
1:F:116:ASP:HA	1:F:117:PRO:HD3	1.95	0.41
2:F:801:FAD:H9	2:F:801:FAD:H1'1	1.85	0.41
1:G:428:ASP:HB2	1:H:129:ILE:HD12	2.01	0.41
1:A:301:TYR:CZ	1:A:322:LYS:HE3	2.55	0.41
1:A:399:LEU:O	1:A:402:VAL:HB	2.20	0.41
1:A:498:ARG:HG2	1:A:502:ASP:C	2.40	0.41
1:E:526:ASP:O	1:E:530:ILE:HG13	2.20	0.41
1:H:234:ILE:O	1:H:235:ARG:HD2	2.20	0.41
1:H:256:HIS:HB3	1:H:260:ARG:HD3	2.02	0.41
1:B:292:ARG:HA	1:B:293:PRO:HD3	1.75	0.41
1:C:282:ARG:HB2	1:C:307:LEU:HD11	2.02	0.41
1:C:327:SER:HA	1:C:580:ASN:HB2	2.02	0.41
1:F:598:THR:O	1:F:602:ILE:HG13	2.21	0.41
1:G:22:GLY:HA3	2:G:801:FAD:O1P	2.20	0.41
1:C:3:LEU:HD13	1:C:277:LEU:HG	2.03	0.41
1:C:48:ASP:HB2	1:C:79:LYS:HE2	2.03	0.41
1:B:146:GLU:OE1	1:B:552:LEU:HA	2.21	0.41
1:C:47:ALA:HB1	1:C:50:PHE:CZ	2.55	0.41
1:E:123:SER:OG	1:E:126:LYS:HB2	2.21	0.41
1:G:421:HIS:ND1	1:G:433:PRO:HA	2.35	0.41
1:A:52:SER:HB2	1:B:1:MET:HA	2.03	0.41
1:B:118:SER:HB2	1:C:521:ARG:NH2	2.36	0.41
1:B:219:LEU:O	1:B:223:LYS:HB2	2.20	0.41
1:B:388:MET:HE2	1:B:551:ALA:HB2	2.01	0.41
1:C:26:ALA:CB	1:C:258:THR:HG23	2.51	0.41
1:C:203:ILE:HA	4:C:937:HOH:O	2.21	0.41
1:C:204:ILE:HD12	1:C:204:ILE:HA	1.96	0.41
1:C:278:LEU:O	1:C:281:HIS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:600:THR:O	1:C:603:CYS:HB2	2.21	0.41
1:G:82:GLU:HA	4:G:921:HOH:O	2.21	0.41
1:B:430:ILE:HG22	1:B:432:ILE:H	1.85	0.41
1:C:52:SER:HB3	1:C:71:GLN:OE1	2.20	0.41
1:E:214:SER:HB3	1:E:217:HIS:HB3	2.03	0.41
1:E:406:PRO:HG3	1:E:414:TRP:CE2	2.56	0.41
1:E:434:PHE:CD1	1:F:131:LEU:HG	2.55	0.41
1:B:137:GLN:NE2	4:B:926:HOH:O	2.54	0.40
1:C:6:THR:HA	1:C:7:PRO:HD3	1.80	0.40
1:C:282:ARG:HE	1:C:284:THR:HG1	1.63	0.40
1:D:1:MET:HE3	1:D:3:LEU:HD23	2.02	0.40
1:E:498:ARG:HH21	1:E:504:PRO:HB3	1.85	0.40
1:H:417:LYS:HG2	1:H:420:ARG:NH2	2.36	0.40
1:H:417:LYS:HG2	1:H:420:ARG:HH21	1.86	0.40
1:A:215:ILE:N	1:A:436:ASP:OD1	2.53	0.40
1:A:382:TYR:HA	1:A:486:GLN:O	2.21	0.40
1:B:558:THR:O	1:B:588:VAL:HA	2.21	0.40
1:B:570:ASN:ND2	1:B:574:LYS:HB3	2.36	0.40
1:C:301:TYR:HD2	1:C:301:TYR:N	2.19	0.40
1:F:593:PHE:CE1	1:F:597:PRO:HB3	2.56	0.40
1:G:4:ASP:OD2	1:G:4:ASP:N	2.50	0.40
1:H:333:GLY:HA2	4:H:952:HOH:O	2.21	0.40
1:E:51:THR:HB	1:E:77:TYR:CD1	2.56	0.40
1:F:298:GLU:HG2	1:F:580:ASN:ND2	2.36	0.40
1:G:14:TYR:O	1:G:325:ALA:HA	2.21	0.40
1:G:51:THR:HB	1:G:77:TYR:CD1	2.57	0.40
1:G:264:GLU:HA	1:G:267:THR:HG22	2.02	0.40
1:G:290:HIS:HE1	1:G:295:GLU:HG2	1.80	0.40
1:B:436:ASP:HA	1:B:437:PRO:HD3	1.82	0.40
1:G:162:ALA:HA	1:G:242:LEU:HD23	2.03	0.40
1:G:223:LYS:HD2	1:G:223:LYS:HA	1.90	0.40
1:C:345:HIS:CD2	1:C:373:THR:HA	2.57	0.40
1:E:345:HIS:CD2	1:E:373:THR:HA	2.57	0.40
1:G:278:LEU:HB3	1:G:281:HIS:CD2	2.57	0.40
1:G:461:SER:HB2	4:G:987:HOH:O	2.22	0.40
1:H:168:ALA:HA	1:H:169:PRO:HD2	1.96	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	568/621 (92%)	548 (96%)	20 (4%)	0	100	100
1	B	570/621 (92%)	547 (96%)	23 (4%)	0	100	100
1	C	570/621 (92%)	539 (95%)	31 (5%)	0	100	100
1	D	570/621 (92%)	530 (93%)	39 (7%)	1 (0%)	47	62
1	E	568/621 (92%)	545 (96%)	22 (4%)	1 (0%)	47	62
1	F	570/621 (92%)	552 (97%)	18 (3%)	0	100	100
1	G	570/621 (92%)	546 (96%)	24 (4%)	0	100	100
1	H	570/621 (92%)	545 (96%)	25 (4%)	0	100	100
All	All	4556/4968 (92%)	4352 (96%)	202 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	407	PRO
1	D	597	PRO

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	495/529 (94%)	482 (97%)	13 (3%)	46	66
1	B	497/529 (94%)	473 (95%)	24 (5%)	25	41
1	C	497/529 (94%)	467 (94%)	30 (6%)	19	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	497/529 (94%)	471 (95%)	26 (5%)	23	38
1	E	495/529 (94%)	476 (96%)	19 (4%)	33	51
1	F	497/529 (94%)	475 (96%)	22 (4%)	28	45
1	G	497/529 (94%)	468 (94%)	29 (6%)	20	32
1	H	497/529 (94%)	468 (94%)	29 (6%)	20	32
All	All	3972/4232 (94%)	3780 (95%)	192 (5%)	25	41

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	31	LEU
1	A	52	SER
1	A	159	TRP
1	A	229	GLN
1	A	267	THR
1	A	305	GLU
1	A	412	ASP
1	A	453	VAL
1	A	456	HIS
1	A	460	PHE
1	A	502	ASP
1	A	596	ASN
1	B	1	MET
1	B	11	ASP
1	B	38	ARG
1	B	52	SER
1	B	82	GLU
1	B	83	ILE
1	B	159	TRP
1	B	195	ASP
1	B	214	SER
1	B	224	TYR
1	B	234	ILE
1	B	238	SER
1	B	267	THR
1	B	303	LEU
1	B	326	ARG
1	B	398	SER
1	B	405	ASN

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Mol	Chain	Res	Type
1	B	414	TRP
1	B	453	VAL
1	B	456	HIS
1	B	460	PHE
1	B	502	ASP
1	B	590	GLU
1	B	596	ASN
1	C	6	THR
1	C	48	ASP
1	C	49	SER
1	C	91	ARG
1	C	101	SER
1	C	125	ASP
1	C	131	LEU
1	C	157	THR
1	C	159	TRP
1	C	160	THR
1	C	202	GLU
1	C	224	TYR
1	C	232	ASN
1	C	254	GLU
1	C	260	ARG
1	C	295	GLU
1	C	301	TYR
1	C	414	TRP
1	C	435	ARG
1	C	453	VAL
1	C	456	HIS
1	C	460	PHE
1	C	467	GLU
1	C	515	ASP
1	C	559	ARG
1	C	568	VAL
1	C	579	ASN
1	C	596	ASN
1	C	609	SER
1	C	615	LYS
1	D	49	SER
1	D	91	ARG
1	D	130	SER
1	D	156	SER
1	D	159	TRP

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Mol	Chain	Res	Type
1	D	160	THR
1	D	214	SER
1	D	224	TYR
1	D	231	GLU
1	D	238	SER
1	D	260	ARG
1	D	267	THR
1	D	276	THR
1	D	285	LYS
1	D	303	LEU
1	D	305	GLU
1	D	412	ASP
1	D	414	TRP
1	D	453	VAL
1	D	460	PHE
1	D	498	ARG
1	D	559	ARG
1	D	577	ASN
1	D	579	ASN
1	D	596	ASN
1	D	615	LYS
1	E	11	ASP
1	E	52	SER
1	E	83	ILE
1	E	125	ASP
1	E	149	THR
1	E	159	TRP
1	E	197	TYR
1	E	236	GLU
1	E	260	ARG
1	E	414	TRP
1	E	435	ARG
1	E	456	HIS
1	E	460	PHE
1	E	467	GLU
1	E	498	ARG
1	E	502	ASP
1	E	509	LYS
1	E	514	GLN
1	E	579	ASN
1	F	53	LYS
1	F	89	ILE

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Mol	Chain	Res	Type
1	F	125	ASP
1	F	159	TRP
1	F	204	ILE
1	F	214	SER
1	F	223	LYS
1	F	232	ASN
1	F	248	THR
1	F	260	ARG
1	F	295	GLU
1	F	298	GLU
1	F	320	VAL
1	F	321	LYS
1	F	414	TRP
1	F	423	GLU
1	F	435	ARG
1	F	456	HIS
1	F	460	PHE
1	F	465	VAL
1	F	564	THR
1	F	596	ASN
1	G	4	ASP
1	G	21	SER
1	G	24	ILE
1	G	123	SER
1	G	131	LEU
1	G	159	TRP
1	G	160	THR
1	G	194	LYS
1	G	204	ILE
1	G	214	SER
1	G	259	ASP
1	G	260	ARG
1	G	277	LEU
1	G	295	GLU
1	G	300	ASP
1	G	308	LEU
1	G	321	LYS
1	G	366	GLU
1	G	367	ARG
1	G	393	VAL
1	G	401	GLU
1	G	414	TRP

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Mol	Chain	Res	Type
1	G	416	GLU
1	G	435	ARG
1	G	453	VAL
1	G	458	ASP
1	G	460	PHE
1	G	559	ARG
1	G	588	VAL
1	H	9	ARG
1	H	11	ASP
1	H	118	SER
1	H	125	ASP
1	H	159	TRP
1	H	188	GLU
1	H	197	TYR
1	H	209	THR
1	H	226	ASP
1	H	248	THR
1	H	263	GLU
1	H	300	ASP
1	H	303	LEU
1	H	308	LEU
1	H	320	VAL
1	H	366	GLU
1	H	367	ARG
1	H	405	ASN
1	H	414	TRP
1	H	427	ASN
1	H	456	HIS
1	H	460	PHE
1	H	465	VAL
1	H	467	GLU
1	H	484	GLU
1	H	515	ASP
1	H	554	LEU
1	H	559	ARG
1	H	596	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	GLN
1	A	405	ASN

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Mol	Chain	Res	Type
1	A	495	GLN
1	B	494	GLN
1	E	71	GLN
1	G	345	HIS
1	G	495	GLN
1	G	576	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	G3F	H	802	-	12,12,12	1.93	4 (33%)	17,17,17	0.85	1 (5%)
2	FAD	A	801	-	53,58,58	1.12	5 (9%)	68,89,89	1.46	13 (19%)
2	FAD	B	801	-	53,58,58	1.24	5 (9%)	68,89,89	1.42	11 (16%)
3	G3F	G	802	-	12,12,12	2.16	5 (41%)	17,17,17	1.29	2 (11%)
3	G3F	C	802	-	12,12,12	1.91	5 (41%)	17,17,17	1.42	2 (11%)
3	G3F	F	802	-	12,12,12	1.84	4 (33%)	17,17,17	1.18	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FAD	D	801	-	53,58,58	1.11	3 (5%)	68,89,89	1.36	9 (13%)
3	G3F	D	802	-	12,12,12	1.96	5 (41%)	17,17,17	1.75	3 (17%)
3	G3F	E	802	-	12,12,12	2.05	6 (50%)	17,17,17	1.31	2 (11%)
2	FAD	E	801	-	53,58,58	1.13	5 (9%)	68,89,89	1.30	7 (10%)
3	G3F	A	802	-	12,12,12	2.49	7 (58%)	17,17,17	1.57	2 (11%)
2	FAD	G	801	-	53,58,58	1.15	4 (7%)	68,89,89	1.39	9 (13%)
3	G3F	B	802	-	12,12,12	2.16	5 (41%)	17,17,17	1.58	3 (17%)
2	FAD	C	801	-	53,58,58	1.15	4 (7%)	68,89,89	1.48	9 (13%)
2	FAD	H	801	-	53,58,58	1.15	4 (7%)	68,89,89	1.31	8 (11%)
2	FAD	F	801	-	53,58,58	1.19	5 (9%)	68,89,89	1.43	12 (17%)

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	G3F	H	802	-	-	0/2/22/22	0/1/1/1
2	FAD	A	801	-	-	2/30/50/50	0/6/6/6
2	FAD	B	801	-	-	1/30/50/50	0/6/6/6
3	G3F	G	802	-	-	0/2/22/22	0/1/1/1
3	G3F	C	802	-	-	0/2/22/22	0/1/1/1
3	G3F	F	802	-	-	0/2/22/22	0/1/1/1
2	FAD	D	801	-	-	3/30/50/50	0/6/6/6
3	G3F	D	802	-	-	0/2/22/22	0/1/1/1
3	G3F	E	802	-	-	0/2/22/22	0/1/1/1
2	FAD	E	801	-	-	2/30/50/50	0/6/6/6
3	G3F	A	802	-	-	0/2/22/22	0/1/1/1
2	FAD	G	801	-	-	1/30/50/50	0/6/6/6
3	G3F	B	802	-	-	0/2/22/22	0/1/1/1
2	FAD	C	801	-	-	4/30/50/50	0/6/6/6
2	FAD	H	801	-	-	2/30/50/50	0/6/6/6
2	FAD	F	801	-	-	3/30/50/50	0/6/6/6

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	G3F	C3-C2	-4.81	1.48	1.52
2	B	801	FAD	C4X-N5	4.77	1.40	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	801	FAD	C2A-N3A	4.19	1.38	1.32
3	B	802	G3F	C3-C2	-4.15	1.48	1.52
2	B	801	FAD	C2A-N3A	4.04	1.38	1.32
2	G	801	FAD	C2A-N3A	3.83	1.38	1.32
2	D	801	FAD	C2A-N3A	3.82	1.38	1.32
2	G	801	FAD	C4X-N5	3.78	1.38	1.30
2	H	801	FAD	C2A-N3A	3.76	1.38	1.32
2	F	801	FAD	C4X-N5	3.72	1.38	1.30
2	H	801	FAD	C4X-N5	3.71	1.38	1.30
2	D	801	FAD	C4X-N5	3.70	1.37	1.30
2	A	801	FAD	C2A-N3A	3.65	1.38	1.32
2	E	801	FAD	C2A-N3A	3.61	1.37	1.32
2	C	801	FAD	C2A-N3A	3.57	1.37	1.32
2	E	801	FAD	C4X-N5	3.56	1.37	1.30
3	A	802	G3F	F3-C3	-3.55	1.32	1.40
2	C	801	FAD	C4X-N5	3.46	1.37	1.30
3	G	802	G3F	C3-C2	-3.43	1.49	1.52
3	E	802	G3F	F3-C3	-3.37	1.32	1.40
3	G	802	G3F	F3-C3	-3.29	1.33	1.40
2	A	801	FAD	C4X-N5	3.28	1.37	1.30
3	D	802	G3F	F3-C3	-3.27	1.33	1.40
3	F	802	G3F	F3-C3	-3.23	1.33	1.40
3	A	802	G3F	C3-C4	-3.20	1.49	1.52
3	C	802	G3F	F3-C3	-3.20	1.33	1.40
3	H	802	G3F	F3-C3	-3.14	1.33	1.40
3	F	802	G3F	O5-C5	-3.04	1.37	1.44
3	B	802	G3F	F3-C3	-3.03	1.33	1.40
3	B	802	G3F	O5-C5	-3.01	1.37	1.44
3	E	802	G3F	O5-C5	-2.94	1.37	1.44
3	A	802	G3F	O5-C5	-2.86	1.37	1.44
3	G	802	G3F	O5-C5	-2.84	1.37	1.44
3	G	802	G3F	C3-C4	-2.78	1.50	1.52
3	D	802	G3F	O5-C5	-2.75	1.37	1.44
3	C	802	G3F	O5-C5	-2.74	1.37	1.44
3	H	802	G3F	C3-C2	-2.70	1.50	1.52
2	H	801	FAD	C2A-N1A	2.69	1.38	1.33
3	H	802	G3F	O5-C5	-2.68	1.37	1.44
2	C	801	FAD	C2A-N1A	2.65	1.38	1.33
3	E	802	G3F	C3-C2	-2.58	1.50	1.52
2	D	801	FAD	C2A-N1A	2.57	1.38	1.33
2	G	801	FAD	C10-N1	2.56	1.38	1.33
3	C	802	G3F	C3-C2	-2.55	1.50	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	FAD	C2A-N1A	2.52	1.38	1.33
2	B	801	FAD	C2B-C1B	-2.46	1.50	1.53
3	D	802	G3F	O4-C4	-2.46	1.37	1.43
3	D	802	G3F	C3-C4	-2.45	1.50	1.52
3	E	802	G3F	O2-C2	-2.41	1.37	1.43
3	A	802	G3F	O4-C4	-2.36	1.37	1.43
2	B	801	FAD	C2A-N1A	2.35	1.38	1.33
2	F	801	FAD	C2A-N1A	2.34	1.38	1.33
3	B	802	G3F	O2-C2	-2.33	1.37	1.43
3	H	802	G3F	C3-C4	-2.31	1.50	1.52
2	H	801	FAD	C10-N1	2.31	1.37	1.33
3	A	802	G3F	O5-C1	-2.29	1.37	1.42
2	B	801	FAD	C10-N1	2.28	1.37	1.33
2	G	801	FAD	C2A-N1A	2.26	1.38	1.33
3	A	802	G3F	O2-C2	-2.25	1.37	1.43
3	C	802	G3F	O4-C4	-2.25	1.37	1.43
3	E	802	G3F	O5-C1	-2.14	1.37	1.42
3	G	802	G3F	O2-C2	-2.14	1.37	1.43
3	C	802	G3F	O2-C2	-2.14	1.37	1.43
3	F	802	G3F	O4-C4	-2.11	1.38	1.43
3	D	802	G3F	O2-C2	-2.08	1.38	1.43
2	E	801	FAD	C10-N1	2.07	1.37	1.33
2	C	801	FAD	C9A-N10	-2.06	1.37	1.41
2	E	801	FAD	C2A-N1A	2.05	1.37	1.33
3	E	802	G3F	C3-C4	-2.05	1.50	1.52
2	F	801	FAD	C2'-C3'	-2.04	1.49	1.53
2	F	801	FAD	C10-N1	2.04	1.37	1.33
2	E	801	FAD	C5'-C4'	2.04	1.54	1.51
3	B	802	G3F	O4-C4	-2.03	1.38	1.43
2	A	801	FAD	C4X-C4	-2.02	1.37	1.44
3	F	802	G3F	O5-C1	-2.01	1.37	1.42
2	A	801	FAD	C10-N1	2.01	1.37	1.33

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	801	FAD	N3A-C2A-N1A	-5.71	119.75	128.68
2	C	801	FAD	N3A-C2A-N1A	-5.68	119.80	128.68
2	E	801	FAD	N3A-C2A-N1A	-5.68	119.80	128.68
2	G	801	FAD	N3A-C2A-N1A	-5.67	119.81	128.68
2	F	801	FAD	N3A-C2A-N1A	-5.33	120.35	128.68
2	D	801	FAD	N3A-C2A-N1A	-5.23	120.50	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	FAD	N3A-C2A-N1A	-5.19	120.57	128.68
2	B	801	FAD	N3A-C2A-N1A	-5.09	120.73	128.68
3	A	802	G3F	F3-C3-C4	4.89	113.19	108.85
3	D	802	G3F	C4-C3-C2	-4.54	105.96	111.34
3	B	802	G3F	F3-C3-C4	3.96	112.37	108.85
3	C	802	G3F	F3-C3-C4	3.68	112.11	108.85
3	G	802	G3F	C4-C3-C2	-3.59	107.08	111.34
3	D	802	G3F	F3-C3-C2	3.55	112.01	108.85
2	C	801	FAD	C4X-C10-N10	3.53	121.64	116.48
2	C	801	FAD	P-O3P-PA	-3.41	121.11	132.83
3	E	802	G3F	C4-C3-C2	-3.39	107.32	111.34
2	F	801	FAD	C4X-C10-N10	3.22	121.19	116.48
2	G	801	FAD	P-O3P-PA	-3.18	121.90	132.83
2	A	801	FAD	O4-C4-C4X	-3.15	118.25	126.60
2	A	801	FAD	C5'-C4'-C3'	-3.14	106.14	112.20
2	F	801	FAD	C4-N3-C2	-3.13	119.86	125.64
2	E	801	FAD	P-O3P-PA	-3.08	122.27	132.83
2	B	801	FAD	C4X-C10-N10	2.95	120.80	116.48
3	E	802	G3F	F3-C3-C4	2.94	111.47	108.85
2	G	801	FAD	C4-N3-C2	-2.92	120.25	125.64
2	G	801	FAD	C9A-C5X-N5	-2.90	119.28	122.43
2	C	801	FAD	C10-C4X-N5	-2.87	118.76	124.86
2	C	801	FAD	C5A-C6A-N6A	-2.87	115.99	120.35
3	C	802	G3F	C4-C3-C2	-2.87	107.94	111.34
2	B	801	FAD	C4X-C4-N3	2.81	120.33	113.19
2	B	801	FAD	P-O3P-PA	-2.79	123.27	132.83
2	B	801	FAD	C4A-C5A-N7A	-2.76	106.52	109.40
2	D	801	FAD	C4X-C10-N10	2.76	120.51	116.48
2	G	801	FAD	C4X-C4-N3	2.76	120.19	113.19
2	D	801	FAD	O4-C4-C4X	-2.75	119.30	126.60
2	D	801	FAD	C4-N3-C2	-2.72	120.62	125.64
2	A	801	FAD	C4X-C10-N10	2.70	120.42	116.48
2	B	801	FAD	C4-N3-C2	-2.69	120.67	125.64
2	B	801	FAD	C4-C4X-N5	2.68	122.04	118.23
3	B	802	G3F	C4-C3-C2	-2.68	108.17	111.34
2	D	801	FAD	P-O3P-PA	-2.67	123.67	132.83
2	H	801	FAD	C4X-C10-N10	2.66	120.37	116.48
2	C	801	FAD	C4-C4X-N5	2.64	122.00	118.23
2	F	801	FAD	P-O3P-PA	-2.64	123.76	132.83
2	H	801	FAD	C4-N3-C2	-2.63	120.77	125.64
2	C	801	FAD	C4-N3-C2	-2.62	120.80	125.64
2	A	801	FAD	O2-C2-N1	-2.59	117.53	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	FAD	C9A-C5X-N5	-2.59	119.62	122.43
2	E	801	FAD	C4X-C10-N10	2.59	120.26	116.48
3	F	802	G3F	O5-C1-C2	-2.58	105.68	110.28
2	B	801	FAD	C10-C4X-N5	-2.55	119.44	124.86
2	A	801	FAD	P-O3P-PA	-2.55	124.08	132.83
2	A	801	FAD	C4-N3-C2	-2.54	120.96	125.64
2	D	801	FAD	C5X-C9A-N10	2.50	120.54	117.95
2	B	801	FAD	C9-C9A-N10	-2.50	118.45	121.84
2	D	801	FAD	C9A-C5X-N5	-2.50	119.72	122.43
2	B	801	FAD	C5X-C9A-N10	2.49	120.53	117.95
2	F	801	FAD	C5'-C4'-C3'	-2.49	107.39	112.20
2	G	801	FAD	C10-C4X-N5	-2.49	119.58	124.86
2	C	801	FAD	C4X-C4-N3	2.48	119.50	113.19
2	D	801	FAD	C4X-C4-N3	2.41	119.30	113.19
2	E	801	FAD	O4-C4-C4X	-2.40	120.23	126.60
2	A	801	FAD	C4-C4X-C10	2.39	120.81	116.79
2	G	801	FAD	C4X-C10-N1	-2.38	119.20	124.73
2	F	801	FAD	C4A-C5A-N7A	-2.37	106.93	109.40
2	F	801	FAD	C4X-C4-N3	2.36	119.17	113.19
2	H	801	FAD	C10-C4X-N5	-2.35	119.88	124.86
2	E	801	FAD	C4A-C5A-N7A	-2.34	106.96	109.40
2	H	801	FAD	C4X-C4-N3	2.34	119.13	113.19
2	F	801	FAD	C10-C4X-N5	-2.33	119.91	124.86
2	H	801	FAD	C9A-C5X-N5	-2.32	119.91	122.43
2	H	801	FAD	O4-C4-C4X	-2.31	120.47	126.60
3	D	802	G3F	C6-C5-C4	-2.26	107.71	113.00
3	F	802	G3F	F3-C3-C4	2.23	110.83	108.85
3	H	802	G3F	C4-C3-C2	-2.23	108.69	111.34
2	F	801	FAD	C5X-C9A-N10	2.22	120.25	117.95
2	D	801	FAD	O4'-C4'-C3'	2.20	114.44	109.10
3	A	802	G3F	C3-C2-C1	-2.19	107.12	110.95
2	G	801	FAD	C4X-C10-N10	2.18	119.67	116.48
2	H	801	FAD	P-O3P-PA	-2.18	125.35	132.83
2	A	801	FAD	O2-C2-N3	2.17	122.87	118.65
2	E	801	FAD	C9A-C5X-N5	-2.16	120.09	122.43
2	F	801	FAD	O4-C4-C4X	-2.15	120.89	126.60
3	B	802	G3F	F3-C3-C2	-2.12	106.97	108.85
2	A	801	FAD	C4X-C4-N3	2.12	118.57	113.19
2	F	801	FAD	O2-C2-N1	-2.10	118.35	121.83
2	F	801	FAD	C9A-C5X-N5	-2.10	120.16	122.43
2	A	801	FAD	C10-C4X-N5	-2.07	120.47	124.86
2	E	801	FAD	C4X-C4-N3	2.07	118.44	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	801	FAD	C5X-N5-C4X	2.07	121.51	118.07
2	A	801	FAD	C4X-C10-N1	-2.06	119.94	124.73
2	C	801	FAD	O5'-C5'-C4'	-2.04	103.92	109.36
2	A	801	FAD	O4B-C1B-C2B	-2.01	103.99	106.93
3	G	802	G3F	C1-O5-C5	2.01	117.45	113.66

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	FAD	PA-O3P-P-O5'
2	C	801	FAD	C3'-C4'-C5'-O5'
2	C	801	FAD	O4'-C4'-C5'-O5'
2	F	801	FAD	O4B-C4B-C5B-O5B
2	F	801	FAD	C3B-C4B-C5B-O5B
2	D	801	FAD	O4B-C4B-C5B-O5B
2	D	801	FAD	C3B-C4B-C5B-O5B
2	F	801	FAD	PA-O3P-P-O5'
2	H	801	FAD	PA-O3P-P-O5'
2	D	801	FAD	O4'-C4'-C5'-O5'
2	E	801	FAD	O4B-C4B-C5B-O5B
2	A	801	FAD	O4B-C4B-C5B-O5B
2	G	801	FAD	O4B-C4B-C5B-O5B
2	H	801	FAD	O4B-C4B-C5B-O5B
2	C	801	FAD	C5'-O5'-P-O3P
2	B	801	FAD	O4B-C4B-C5B-O5B
2	C	801	FAD	O4B-C4B-C5B-O5B
2	E	801	FAD	O4'-C4'-C5'-O5'

There are no ring outliers.

13 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	802	G3F	1	0
2	A	801	FAD	2	0
2	B	801	FAD	2	0
3	C	802	G3F	1	0
3	F	802	G3F	1	0
2	D	801	FAD	3	0
3	E	802	G3F	1	0
2	E	801	FAD	2	0

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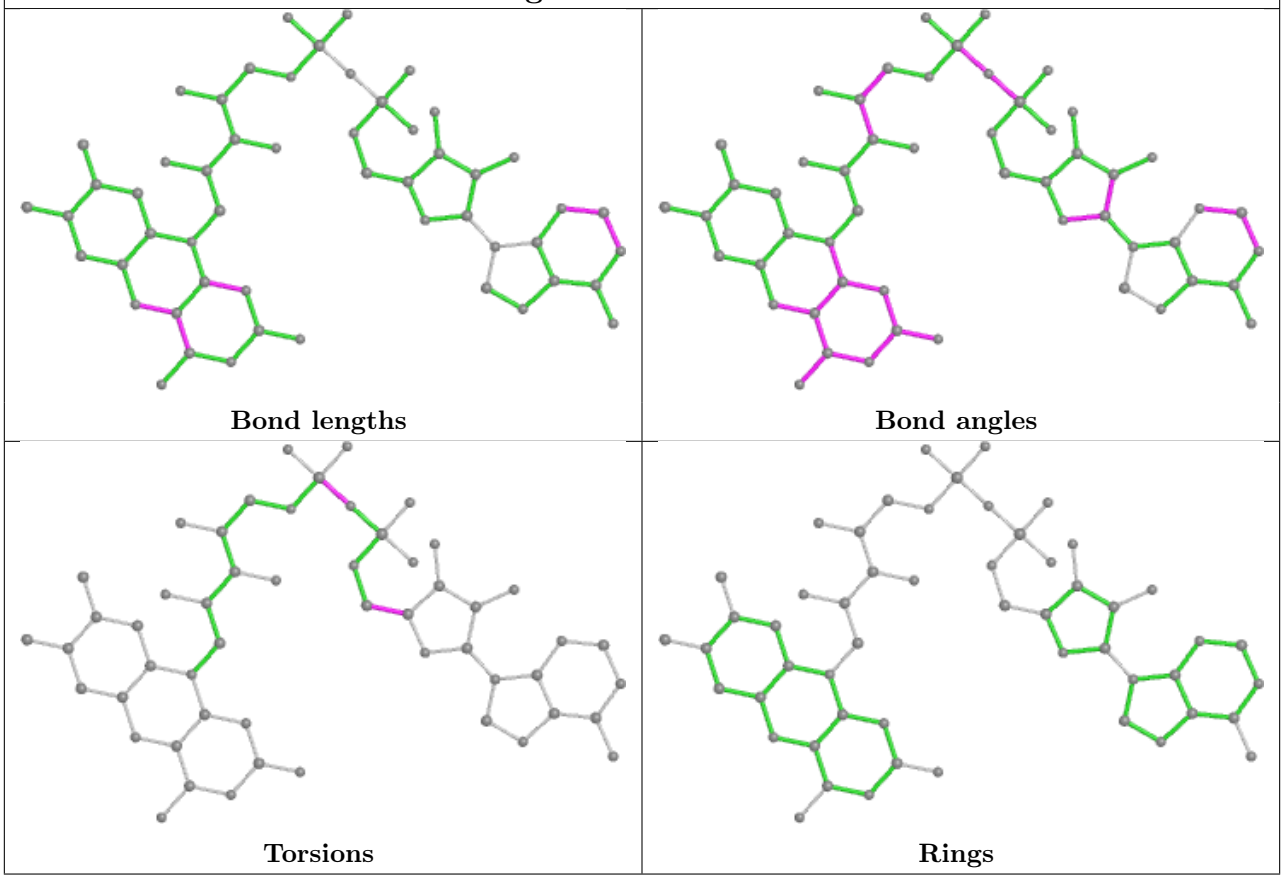
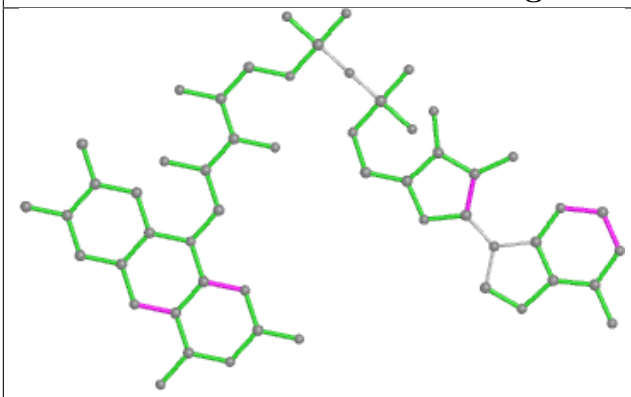
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	G3F	2	0
2	G	801	FAD	3	0
2	C	801	FAD	2	0
2	H	801	FAD	2	0
2	F	801	FAD	3	0

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

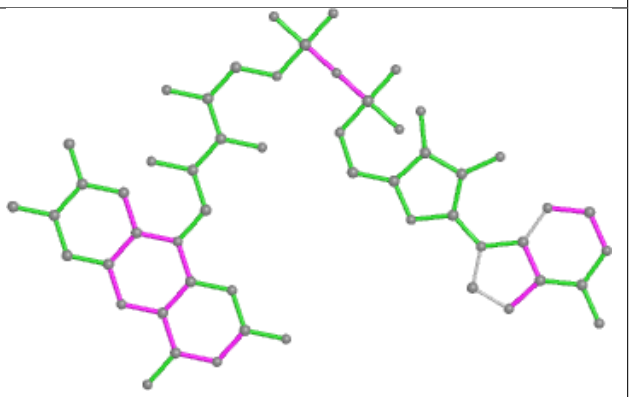
Ligand FAD A 801



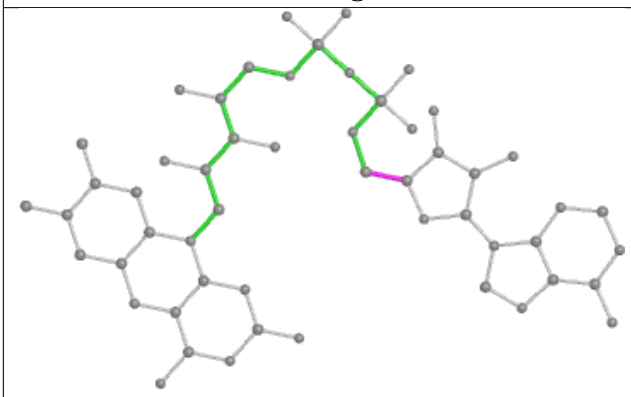
Ligand FAD B 801



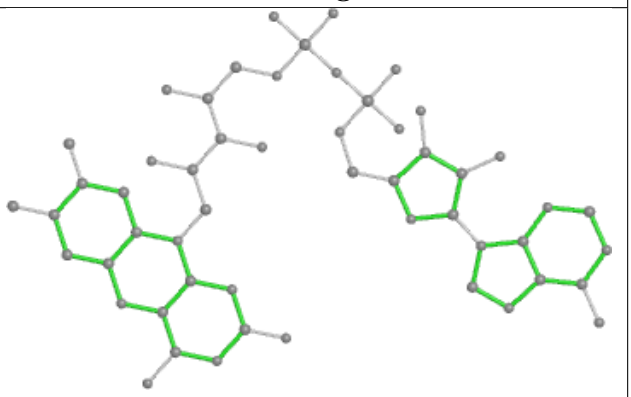
Bond lengths



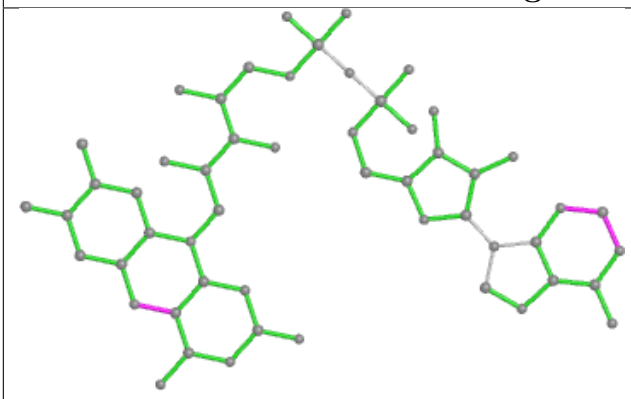
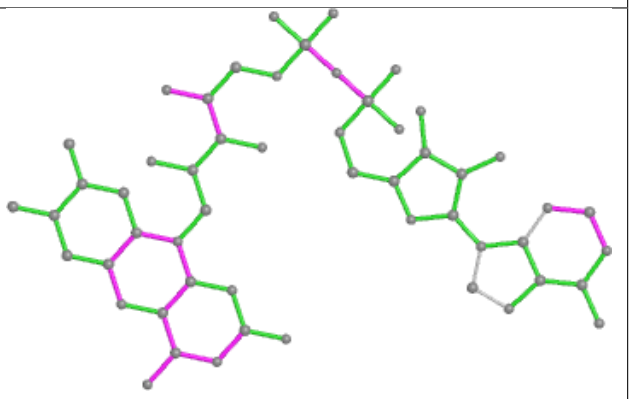
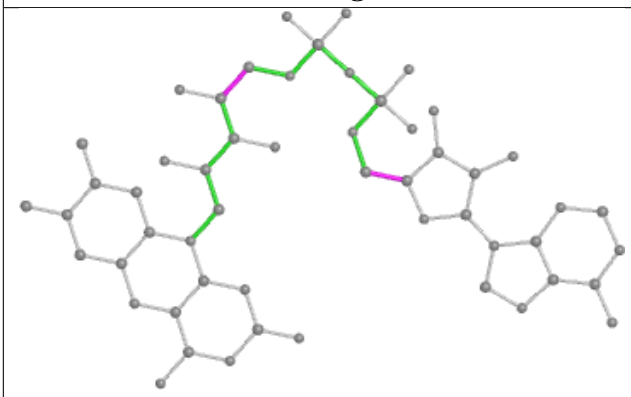
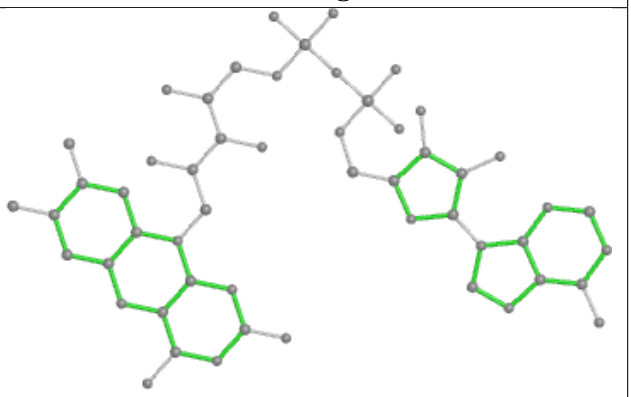
Bond angles



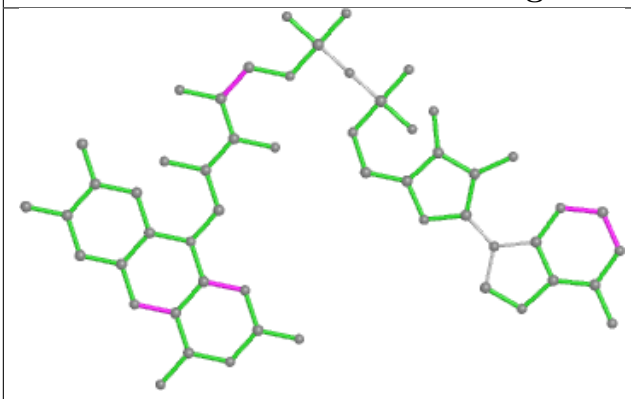
Torsions



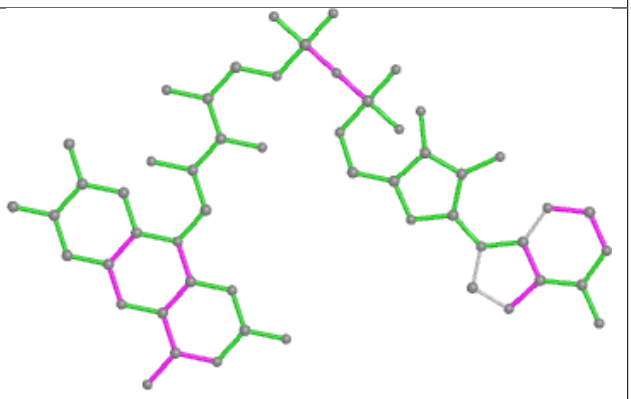
Rings

Ligand FAD D 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

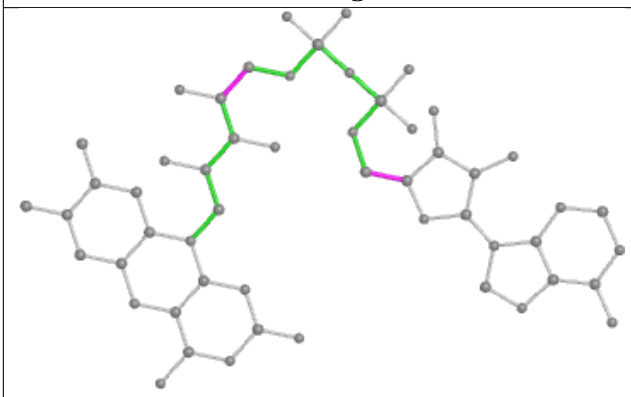
Ligand FAD E 801



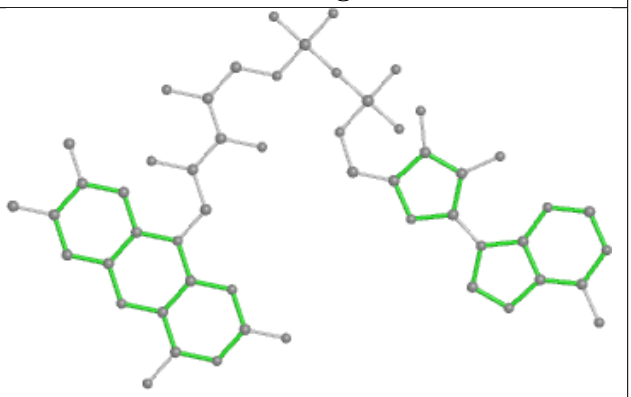
Bond lengths



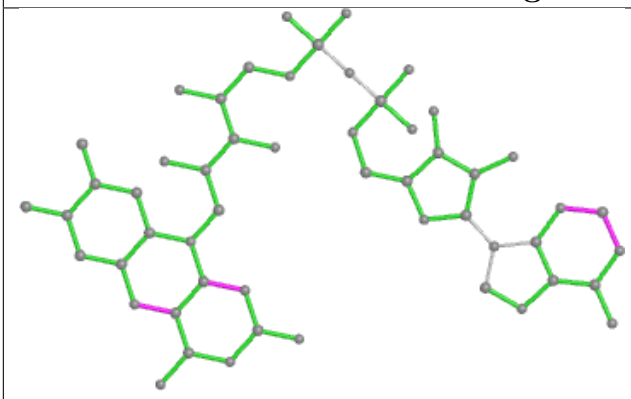
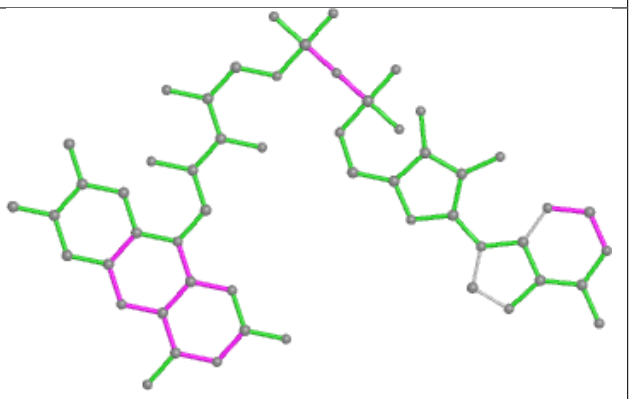
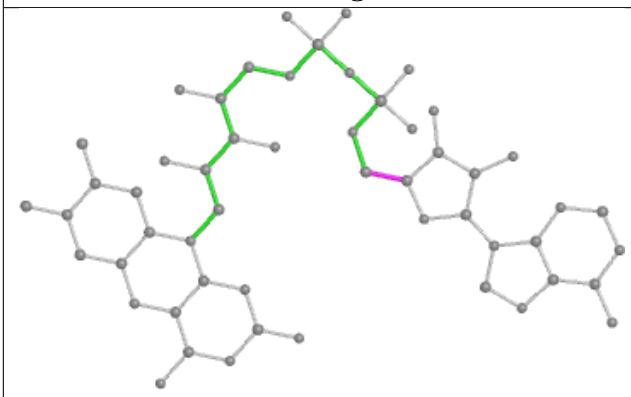
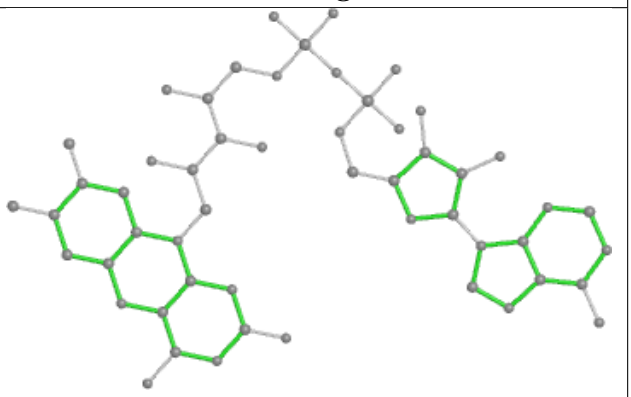
Bond angles



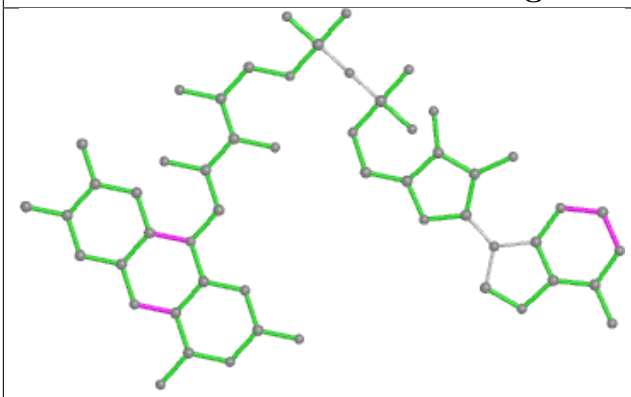
Torsions



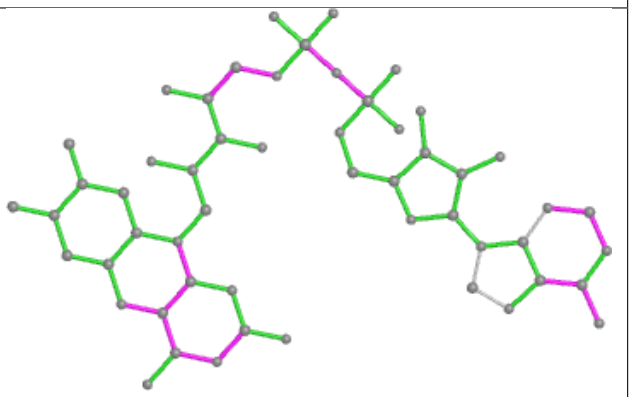
Rings

Ligand FAD G 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

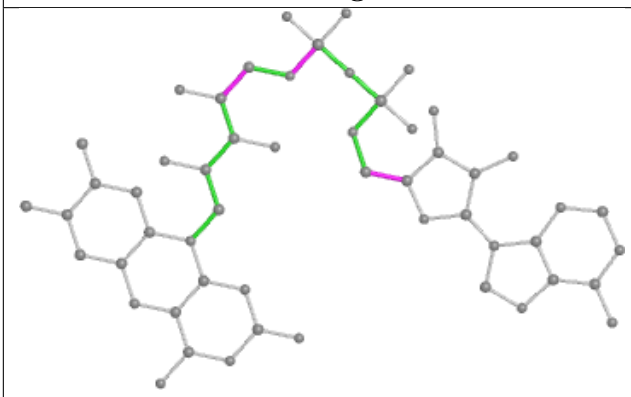
Ligand FAD C 801



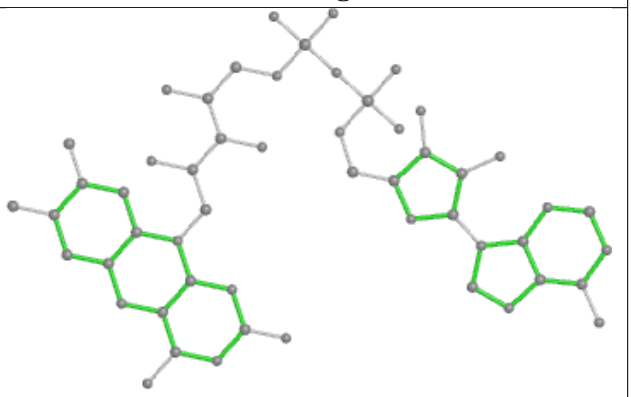
Bond lengths



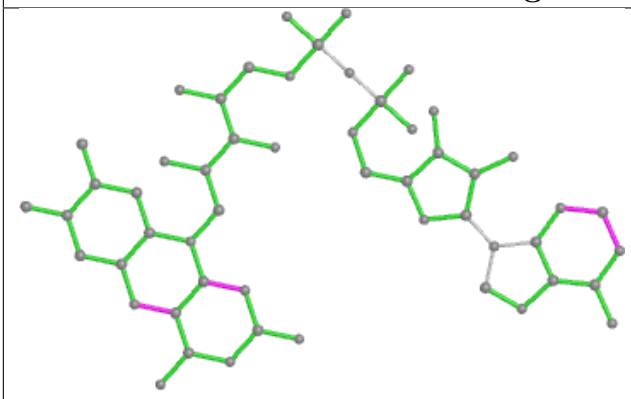
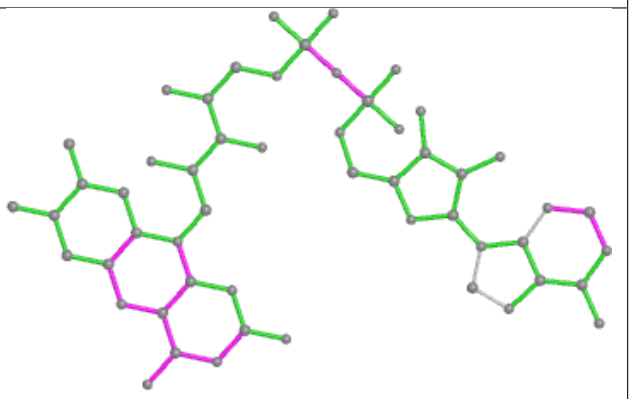
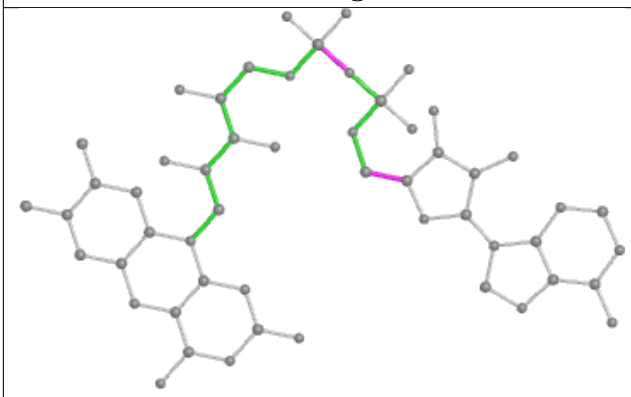
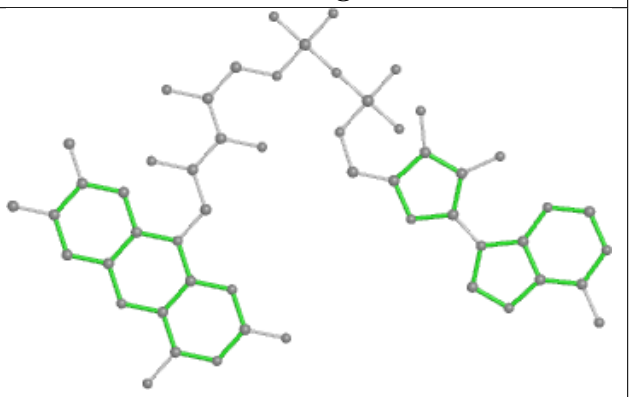
Bond angles



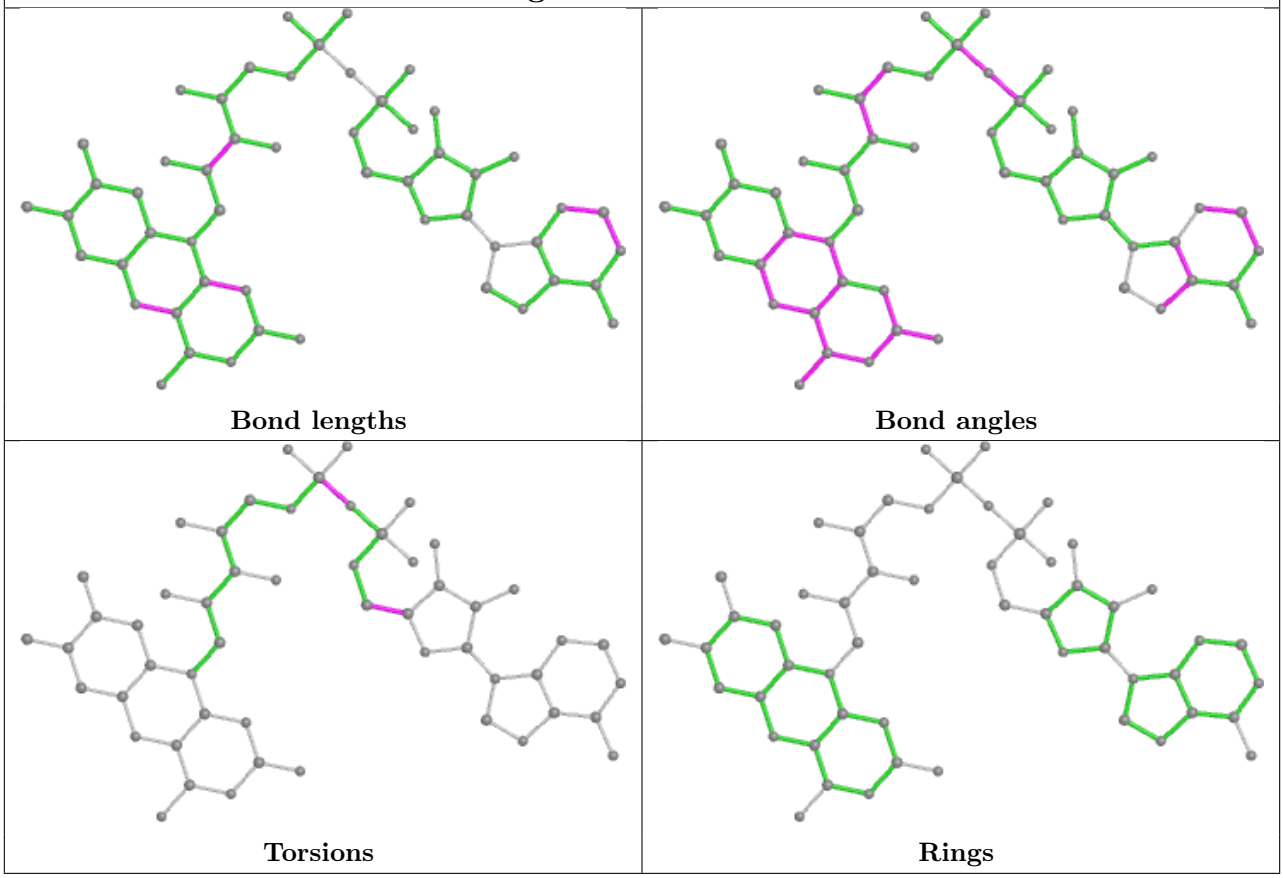
Torsions



Rings

Ligand FAD H 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FAD F 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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	576/621 (92%)	-0.38	1 (0%)	95	94	10, 26, 47, 59	0
1	B	578/621 (93%)	-0.13	9 (1%)	72	70	14, 30, 57, 85	0
1	C	578/621 (93%)	0.15	26 (4%)	33	31	14, 43, 73, 113	0
1	D	578/621 (93%)	0.02	11 (1%)	66	64	18, 42, 68, 98	0
1	E	576/621 (92%)	-0.28	12 (2%)	63	61	12, 26, 52, 94	0
1	F	578/621 (93%)	-0.19	11 (1%)	66	64	19, 33, 57, 86	0
1	G	578/621 (93%)	-0.09	13 (2%)	62	60	15, 38, 66, 97	0
1	H	578/621 (93%)	0.01	22 (3%)	40	39	15, 41, 69, 96	0
All	All	4620/4968 (92%)	-0.11	105 (2%)	60	58	10, 34, 64, 113	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	7	PRO	8.1
1	G	4	ASP	6.4
1	C	6	THR	6.3
1	E	9	ARG	5.8
1	E	11	ASP	5.5
1	H	6	THR	4.9
1	C	8	PHE	4.8
1	H	367	ARG	4.6
1	C	250	PRO	4.3
1	F	8	PHE	4.3
1	H	7	PRO	4.1
1	C	11	ASP	4.0
1	D	561	GLY	4.0
1	H	31	LEU	3.9
1	B	10	ALA	3.7
1	H	8	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	9	ARG	3.5
1	C	270	VAL	3.5
1	H	418	VAL	3.5
1	C	371	ILE	3.5
1	C	413	TRP	3.4
1	H	4	ASP	3.4
1	H	54	PRO	3.3
1	C	410	GLY	3.3
1	F	11	ASP	3.2
1	G	129	ILE	3.2
1	C	5	THR	3.2
1	D	191	ARG	3.1
1	H	616	PHE	3.1
1	E	12	GLU	3.1
1	G	5	THR	3.1
1	C	12	GLU	3.0
1	H	274	ARG	3.0
1	E	38	ARG	3.0
1	C	10	ALA	3.0
1	E	8	PHE	2.9
1	E	56	LYS	2.8
1	H	422	VAL	2.8
1	E	13	PRO	2.8
1	D	562	LEU	2.8
1	H	272	ARG	2.8
1	G	183	SER	2.8
1	C	375	LEU	2.7
1	G	182	LEU	2.7
1	G	10	ALA	2.7
1	C	70	GLY	2.7
1	G	56	LYS	2.7
1	C	435	ARG	2.6
1	E	5	THR	2.6
1	G	9	ARG	2.6
1	G	294	GLY	2.6
1	D	288	PHE	2.5
1	E	131	LEU	2.5
1	H	1	MET	2.5
1	B	411	LEU	2.5
1	C	38	ARG	2.5
1	F	70	GLY	2.5
1	C	72	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	193	TRP	2.5
1	B	424	ALA	2.5
1	G	36	ASN	2.4
1	H	56	LYS	2.4
1	C	55	MET	2.4
1	A	497	TYR	2.4
1	E	288	PHE	2.3
1	H	326	ARG	2.3
1	B	433	PRO	2.3
1	C	289	LYS	2.3
1	D	380	GLY	2.3
1	H	423	GLU	2.3
1	H	53	LYS	2.3
1	F	274	ARG	2.3
1	D	3	LEU	2.3
1	G	6	THR	2.2
1	F	9	ARG	2.2
1	H	131	LEU	2.2
1	C	603	CYS	2.2
1	D	1	MET	2.2
1	E	6	THR	2.2
1	C	248	THR	2.2
1	B	12	GLU	2.2
1	F	495	GLN	2.2
1	H	13	PRO	2.2
1	D	367	ARG	2.2
1	E	10	ALA	2.1
1	H	366	GLU	2.1
1	F	289	LYS	2.1
1	C	195	ASP	2.1
1	F	616	PHE	2.1
1	F	10	ALA	2.1
1	B	130	SER	2.1
1	C	416	GLU	2.1
1	C	269	PRO	2.1
1	F	326	ARG	2.1
1	C	4	ASP	2.1
1	B	13	PRO	2.1
1	H	288	PHE	2.1
1	B	9	ARG	2.1
1	D	20	GLY	2.1
1	F	323	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	131	LEU	2.0
1	B	425	PHE	2.0
1	D	132	GLY	2.0
1	G	37	LEU	2.0
1	H	55	MET	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, 95th 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.

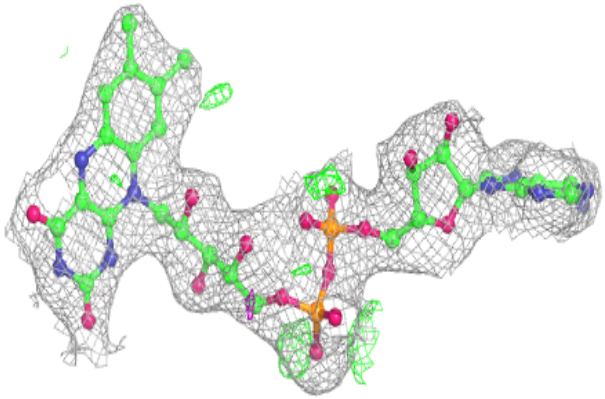
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	G3F	D	802	12/12	0.91	0.12	25,35,43,46	0
2	FAD	C	801	53/53	0.94	0.16	9,23,51,55	0
3	G3F	F	802	12/12	0.94	0.13	23,35,41,41	0
2	FAD	D	801	53/53	0.95	0.17	17,34,44,61	0
3	G3F	B	802	12/12	0.96	0.19	18,24,27,35	0
3	G3F	C	802	12/12	0.96	0.12	24,32,39,40	0
2	FAD	H	801	53/53	0.96	0.15	15,28,37,44	0
3	G3F	A	802	12/12	0.96	0.12	8,16,22,26	0
3	G3F	G	802	12/12	0.96	0.14	30,33,37,40	0
3	G3F	H	802	12/12	0.96	0.14	24,31,33,35	0
2	FAD	B	801	53/53	0.97	0.14	7,18,29,37	0
3	G3F	E	802	12/12	0.97	0.14	15,19,24,35	0
2	FAD	E	801	53/53	0.97	0.16	10,17,25,29	0
2	FAD	F	801	53/53	0.97	0.14	5,23,31,45	0
2	FAD	G	801	53/53	0.97	0.15	17,29,35,41	0
2	FAD	A	801	53/53	0.98	0.12	2,12,20,23	0

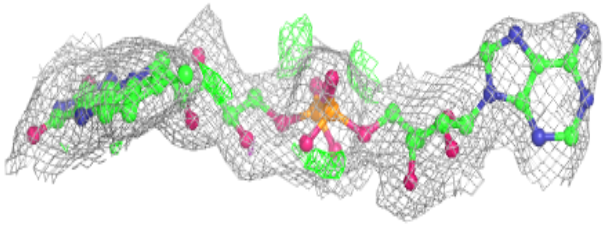
The following is a graphical depiction of the model fit to experimental electron density of all

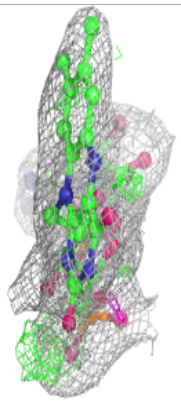
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FAD C 801:

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

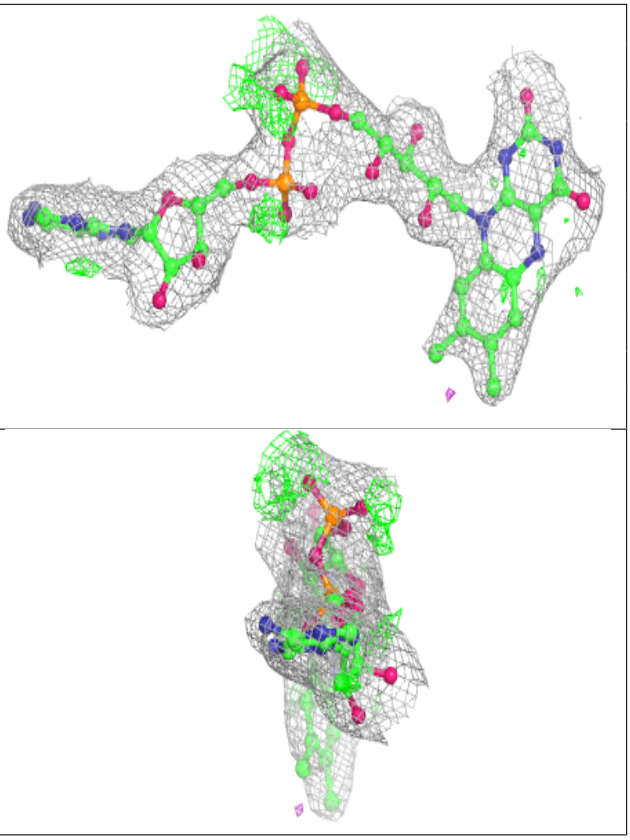


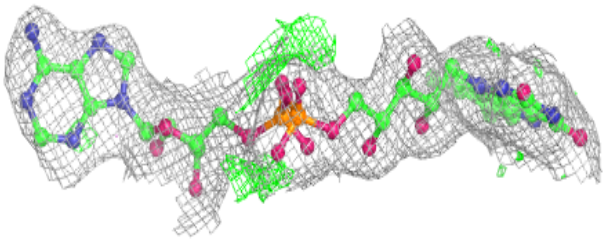




Electron density around FAD D 801:

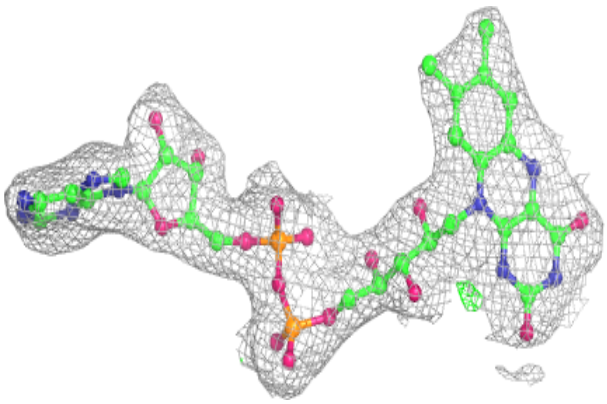
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

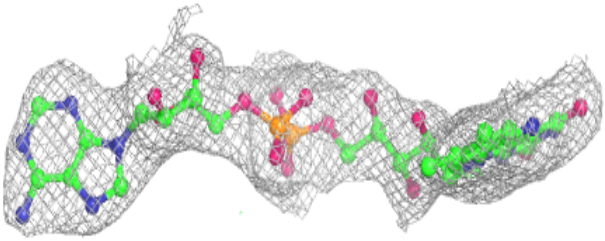


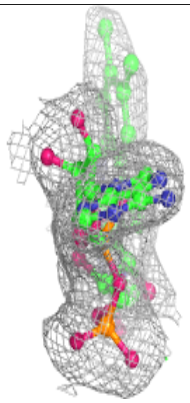


Electron density around FAD H 801:

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

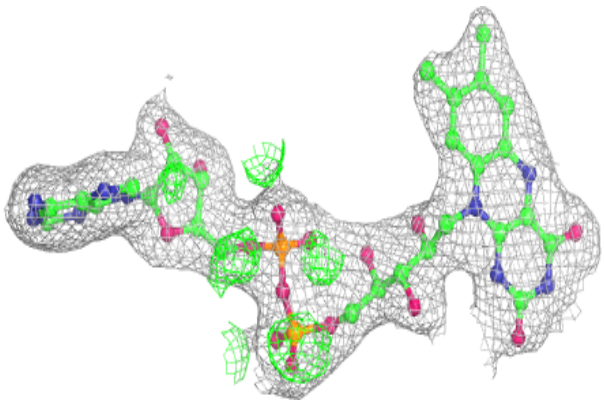


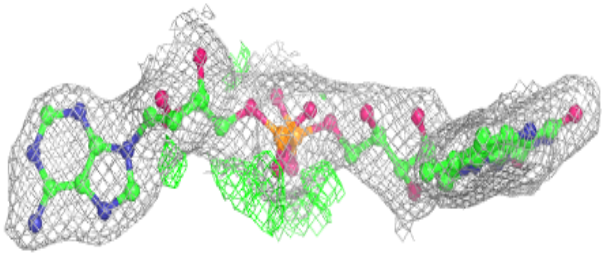


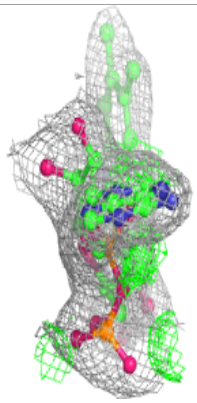


Electron density around FAD B 801:

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

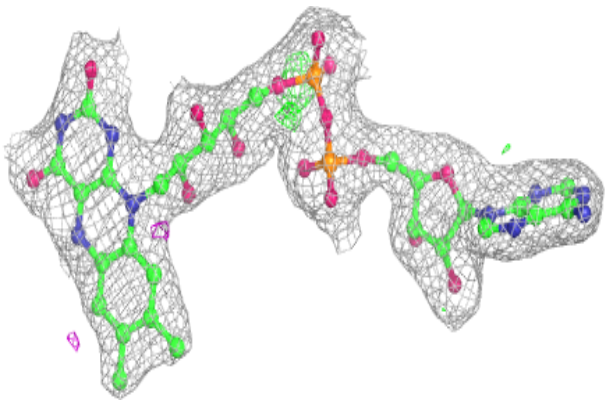


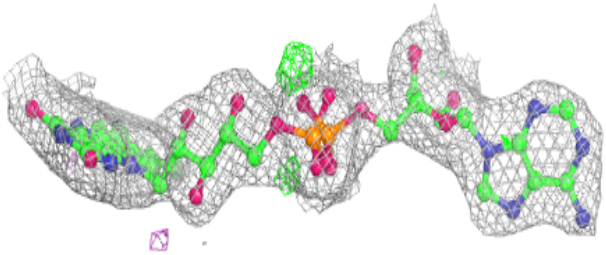


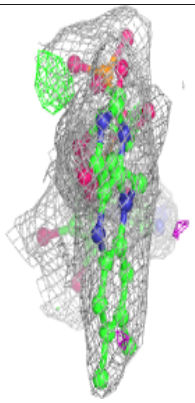


Electron density around FAD E 801:

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

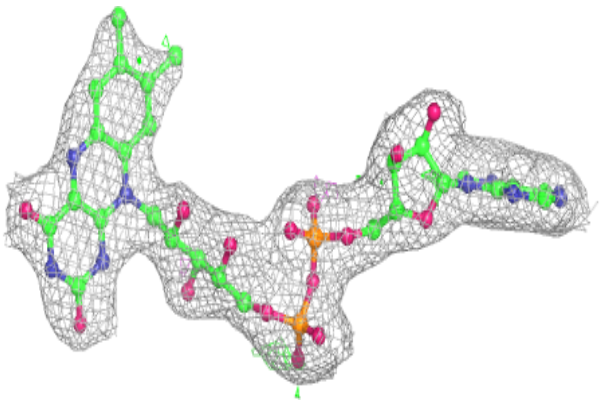


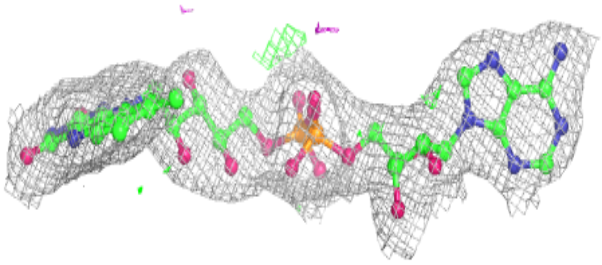


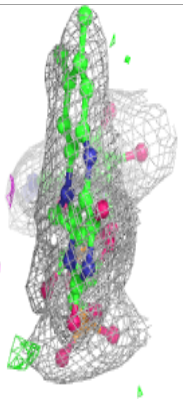


Electron density around FAD F 801:

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

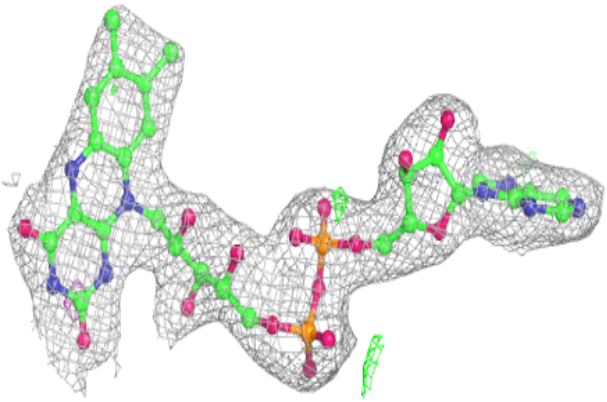


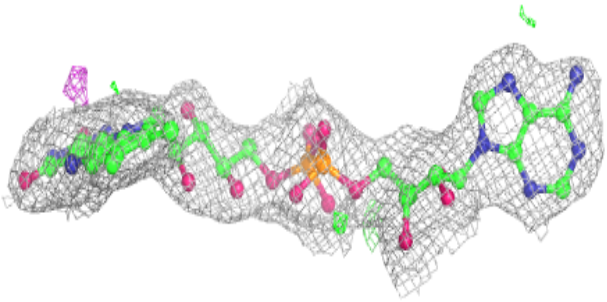


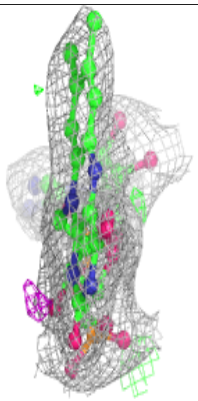


Electron density around FAD G 801:

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

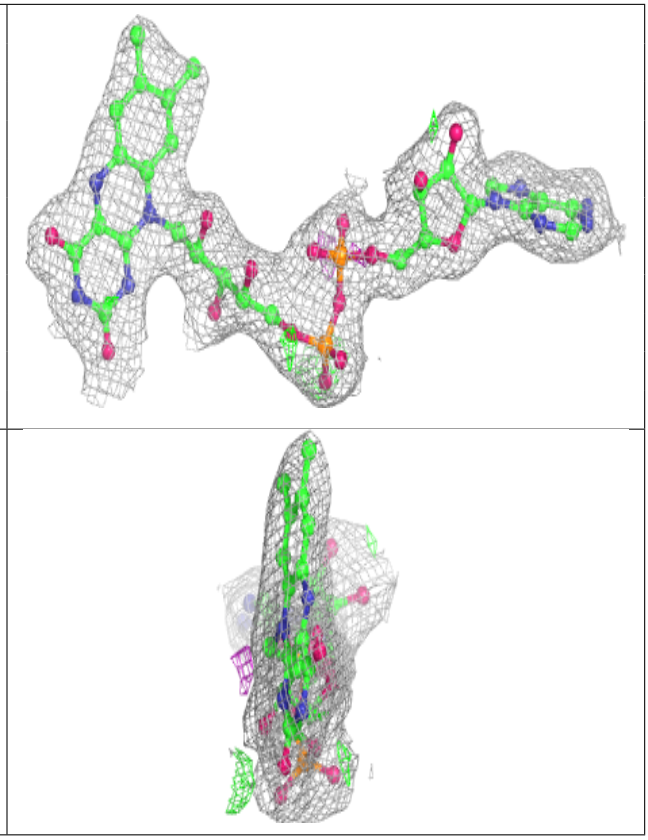






Electron density around FAD A 801:

$2mF_o$-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.