



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:33 PM UTC

PDB ID : 8CAP / pdb_00008cap
Title : Crystal structure of dehydrogenase domain of *Cylindrospermum stagnale* NADPH-Oxidase 5 (NOX5) in complex with CB28
Authors : Reis, J.; Mattevi, A.
Deposited on : 2023-01-24
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

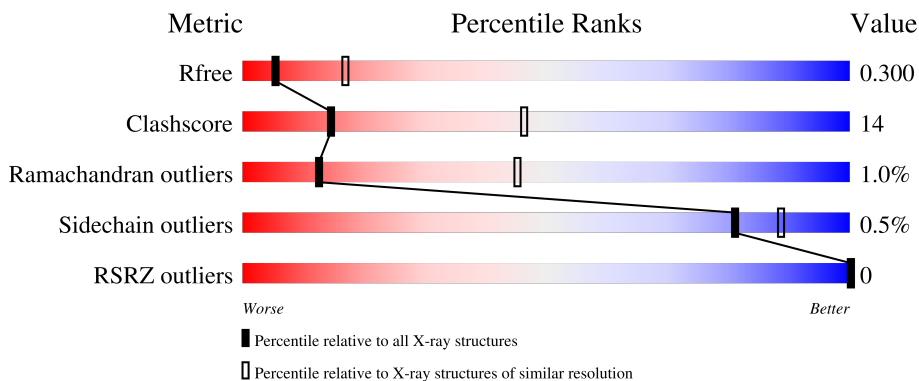
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


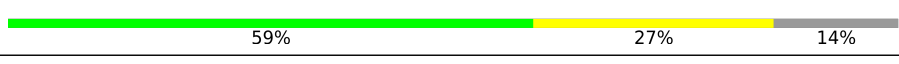
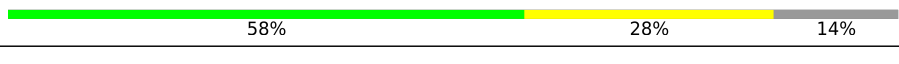

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. 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	283	 59% 26% 13%
1	B	283	 59% 27% 14%
1	C	283	 58% 28% 14%
1	E	283	 59% 27% 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8174 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 Putative ferric reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	247	1977	1286	329	356	6	0	0	0
1	B	243	1947	1269	324	348	6	0	0	0
1	C	244	1952	1272	325	349	6	0	0	0
1	E	242	1942	1266	323	347	6	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

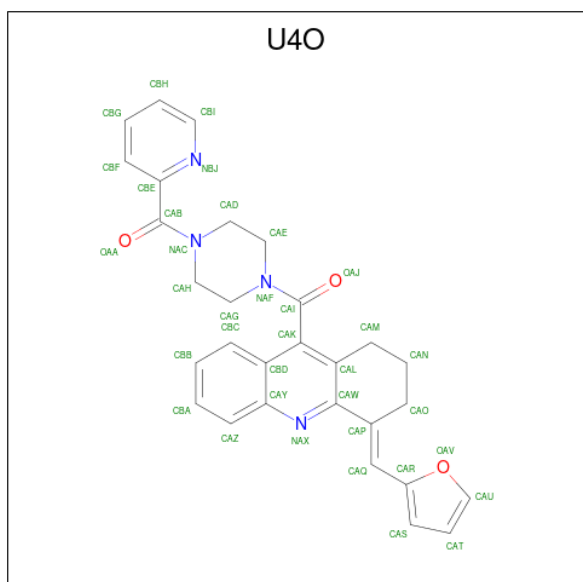
Chain	Residue	Modelled	Actual	Comment	Reference
A	411	GLY	-	expression tag	UNP K9WT99
A	412	SER	-	expression tag	UNP K9WT99
B	411	GLY	-	expression tag	UNP K9WT99
B	412	SER	-	expression tag	UNP K9WT99
C	411	GLY	-	expression tag	UNP K9WT99
C	412	SER	-	expression tag	UNP K9WT99
E	411	GLY	-	expression tag	UNP K9WT99
E	412	SER	-	expression tag	UNP K9WT99

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



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

- Molecule 3 is [4-[[[4 {E}]-4-(furan-2-ylmethylidene)-2,3-dihydro-1 {H}-acridin-9-yl]carbonyl]piperazin-1-yl]-pyridin-2-yl-methanone (CCD ID: U4O) (formula: C₂₉H₂₆N₄O₃) (labeled as "Ligand of Interest" by depositor).



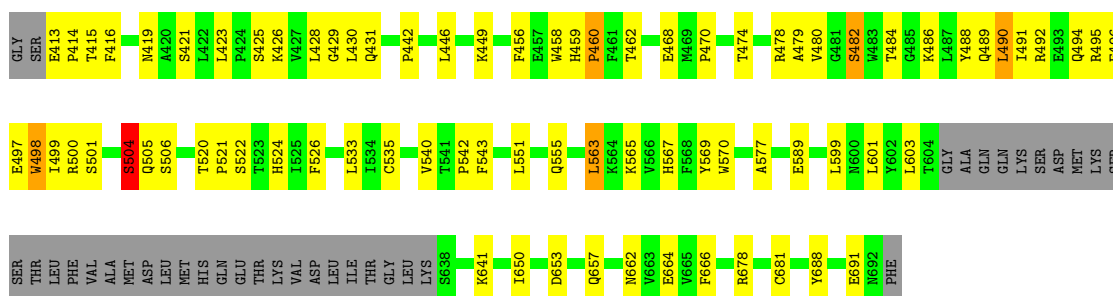
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 36	C 29	N 4	O 3	0	0
3	B	1	Total 36	C 29	N 4	O 3	0	0
3	C	1	Total 36	C 29	N 4	O 3	0	0
3	E	1	Total 36	C 29	N 4	O 3	0	0

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.

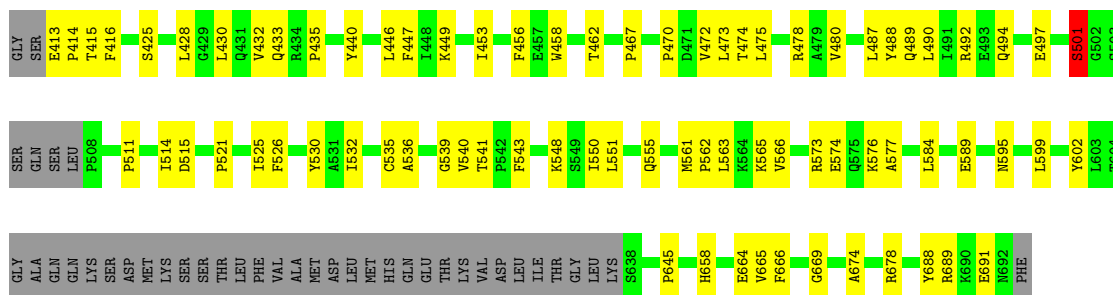
- Molecule 1: Putative ferric reductase

Chain A: 



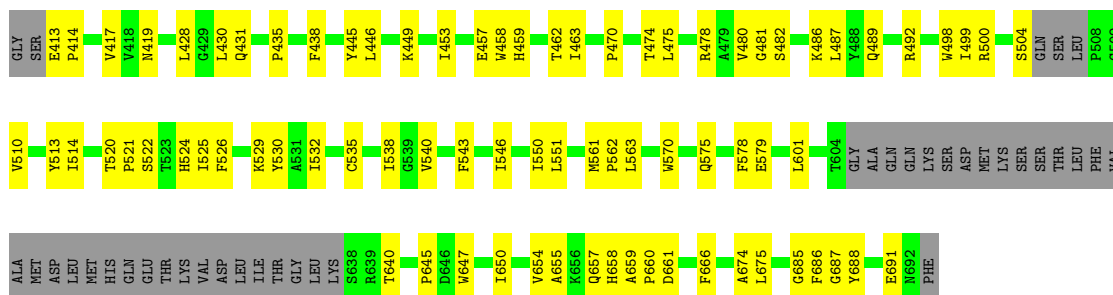
- Molecule 1: Putative ferric reductase

Chain B: 



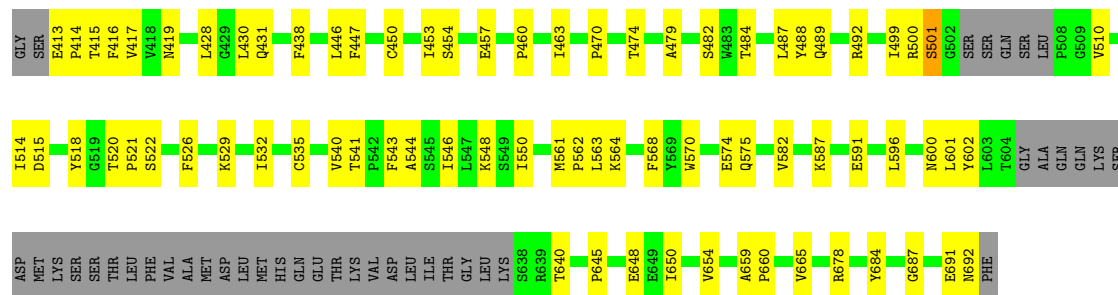
- Molecule 1: Putative ferric reductase

Chain C: 



- Molecule 1: Putative ferric reductase

Chain E:  59% 27% 14%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.83Å 88.22Å 98.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.02 – 3.00 49.02 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.1 (49.02-3.00) 96.0 (49.02-3.00)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.239 , 0.295 0.240 , 0.300	Depositor DCC
R_{free} test set	1172 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	75.1	Xtrriage
Anisotropy	0.617	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.135 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8174	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, U4O

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	0.59	0/2037	0.84	5/2772 (0.2%)
1	B	0.48	0/2006	0.78	1/2728 (0.0%)
1	C	0.52	0/2011	0.79	0/2735
1	E	0.64	1/2001 (0.0%)	0.86	2/2721 (0.1%)
All	All	0.56	1/8055 (0.0%)	0.82	8/10956 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	501	SER	CA-C	-8.79	1.45	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	504	SER	N-CA-C	8.91	123.06	110.68
1	B	501	SER	N-CA-C	-8.56	92.56	110.80
1	A	500	ARG	N-CA-C	-8.05	103.55	112.72
1	A	498	TRP	N-CA-C	-6.21	102.99	112.99
1	E	501	SER	CB-CA-C	-5.80	106.11	114.87
1	A	505	GLN	N-CA-C	-5.41	102.66	111.04
1	A	506	SER	N-CA-C	-5.30	100.68	108.79
1	E	500	ARG	N-CA-C	-5.02	106.25	112.38

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	1977	0	1931	53	1
1	B	1947	0	1899	62	0
1	C	1952	0	1901	62	0
1	E	1942	0	1897	52	3
2	A	53	0	31	2	0
2	B	53	0	31	3	0
2	C	53	0	31	4	0
2	E	53	0	31	2	2
3	A	36	0	0	0	0
3	B	36	0	0	1	0
3	C	36	0	0	0	0
3	E	36	0	0	0	0
All	All	8174	0	7752	223	3

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 14.

All (223) 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:B:550:ILE:HG23	1:B:561:MET:HE1	1.63	0.79
1:C:561:MET:HE2	1:C:563:LEU:HB3	1.64	0.79
1:E:532:ILE:HB	1:E:665:VAL:HG22	1.64	0.79
1:E:521:PRO:HG2	1:E:691:GLU:HG2	1.68	0.76
1:A:479:ALA:HA	1:A:484:THR:HB	1.68	0.76
1:E:453:ILE:HD11	1:E:487:LEU:HD13	1.68	0.76
1:E:601:LEU:HB2	1:E:640:THR:HB	1.68	0.75
1:B:521:PRO:HG2	1:B:691:GLU:HG2	1.69	0.74
1:B:453:ILE:HD11	1:B:487:LEU:HD13	1.69	0.74
1:E:550:ILE:HG23	1:E:561:MET:HE1	1.70	0.74
1:E:419:ASN:HB3	1:E:431:GLN:HG3	1.68	0.74
1:C:521:PRO:HG2	1:C:691:GLU:HG2	1.70	0.72
1:E:546:ILE:O	1:E:550:ILE:HG13	1.91	0.71
1:A:492:ARG:NH1	1:A:496:GLU:OE2	2.24	0.71
1:A:478:ARG:HG2	1:A:480:VAL:HG13	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:529:LYS:NZ	1:C:661:ASP:OD2	2.20	0.70
1:C:449:LYS:HB3	1:C:513:TYR:HB2	1.74	0.70
1:B:532:ILE:HB	1:B:665:VAL:HG22	1.75	0.69
1:C:478:ARG:HG2	1:C:480:VAL:HG13	1.72	0.69
1:C:462:THR:HG23	2:C:801:FAD:H6	1.76	0.68
1:E:532:ILE:HD11	1:E:654:VAL:HG11	1.75	0.68
1:E:522:SER:OG	1:E:691:GLU:OE2	2.10	0.68
1:C:459:HIS:HD1	2:C:801:FAD:HO4'	1.36	0.68
1:C:535:CYS:HB2	1:C:543:PHE:CE2	2.28	0.68
1:A:551:LEU:O	1:A:555:GLN:HG2	1.95	0.67
1:C:538:ILE:HB	1:C:578:PHE:HZ	1.61	0.66
1:B:413:GLU:HB3	1:B:414:PRO:HD3	1.77	0.66
1:B:489:GLN:OE1	1:B:492:ARG:NH2	2.29	0.66
1:E:561:MET:HE2	1:E:563:LEU:HB3	1.77	0.66
1:E:526:PHE:O	1:E:562:PRO:HG2	1.96	0.66
2:A:801:FAD:O1P	1:E:678:ARG:NH1	2.28	0.65
1:C:482:SER:O	1:C:486:LYS:HE2	1.96	0.65
1:C:413:GLU:HB3	1:C:414:PRO:HD3	1.79	0.64
1:B:551:LEU:O	1:B:555:GLN:HG2	1.96	0.64
1:A:456:PHE:HB3	1:E:687:GLY:HA2	1.81	0.63
1:E:430:LEU:O	1:E:474:THR:HA	1.98	0.63
1:C:535:CYS:HB2	1:C:543:PHE:HE2	1.64	0.62
1:A:491:ILE:O	1:A:495:ARG:N	2.32	0.62
1:B:602:TYR:CD2	1:B:645:PRO:HG3	2.33	0.62
1:A:489:GLN:O	1:A:491:ILE:N	2.34	0.61
1:C:489:GLN:OE1	1:C:492:ARG:NH2	2.27	0.61
1:C:532:ILE:HD11	1:C:654:VAL:HG11	1.82	0.60
1:E:529:LYS:HG3	1:E:564:LYS:HG3	1.84	0.60
1:A:569:TYR:CE2	1:A:650:ILE:HD13	2.36	0.60
1:C:445:TYR:HA	1:C:462:THR:HA	1.82	0.59
1:A:489:GLN:C	1:A:491:ILE:H	2.10	0.59
1:A:413:GLU:HB3	1:A:414:PRO:HD3	1.83	0.59
1:A:522:SER:OG	1:A:691:GLU:OE2	2.20	0.59
1:B:478:ARG:HG2	1:B:480:VAL:HG13	1.82	0.59
1:C:535:CYS:SG	1:C:540:VAL:HG12	2.44	0.58
1:A:415:THR:OG1	1:A:416:PHE:N	2.38	0.57
1:B:428:LEU:HD11	1:B:488:TYR:HA	1.86	0.57
1:E:529:LYS:HA	1:E:562:PRO:O	2.05	0.56
1:A:662:ASN:ND2	1:A:664:GLU:OE2	2.39	0.56
1:B:462:THR:HG23	2:B:801:FAD:H6	1.88	0.55
1:A:653:ASP:OD2	1:A:657:GLN:NE2	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:GLN:C	1:A:491:ILE:N	2.64	0.55
1:C:453:ILE:HD11	1:C:487:LEU:HD13	1.88	0.55
1:B:430:LEU:O	1:B:474:THR:HA	2.06	0.55
1:B:447:PHE:HB2	1:B:515:ASP:HB3	1.88	0.54
1:C:525:ILE:O	1:C:563:LEU:HD22	2.06	0.54
1:A:521:PRO:HG2	1:A:691:GLU:HG2	1.90	0.54
1:B:530:TYR:CG	1:B:658:HIS:ND1	2.75	0.54
1:B:563:LEU:HD11	1:B:566:VAL:HG22	1.90	0.54
1:A:462:THR:HG21	1:A:542:PRO:HB3	1.88	0.54
1:B:490:LEU:O	1:B:494:GLN:HB2	2.08	0.54
1:E:535:CYS:SG	1:E:540:VAL:HG12	2.47	0.54
1:B:678:ARG:NE	1:C:457:GLU:OE1	2.41	0.53
1:C:522:SER:HB3	1:C:546:ILE:HD11	1.89	0.53
1:E:574:GLU:OE2	1:E:575:GLN:N	2.39	0.53
1:B:456:PHE:HB3	1:C:687:GLY:HA2	1.90	0.53
1:A:449:LYS:HE3	1:A:458:TRP:CE2	2.44	0.53
1:C:570:TRP:HE3	1:C:601:LEU:HD22	1.73	0.53
1:A:421:SER:HB3	1:A:423:LEU:HD21	1.91	0.53
1:B:526:PHE:O	1:B:562:PRO:HG2	2.09	0.53
1:B:440:TYR:CZ	1:B:467:PRO:HA	2.44	0.52
1:E:450:CYS:HB3	1:E:453:ILE:HD12	1.91	0.52
1:A:482:SER:O	1:A:486:LYS:HD2	2.09	0.52
1:A:681:CYS:SG	1:A:688:TYR:HB2	2.49	0.52
1:E:413:GLU:HB3	1:E:414:PRO:HD3	1.91	0.52
1:B:678:ARG:NH1	2:C:801:FAD:O1P	2.31	0.52
1:E:544:ALA:O	1:E:548:LYS:HG3	2.10	0.52
1:A:419:ASN:HB3	1:A:431:GLN:HG3	1.93	0.51
1:B:416:PHE:HE1	1:B:511:PRO:HG3	1.76	0.51
1:B:526:PHE:CE1	1:B:550:ILE:HG12	2.45	0.51
1:E:535:CYS:HB2	1:E:543:PHE:CE2	2.45	0.51
1:A:446:LEU:O	1:A:460:PRO:HA	2.10	0.51
1:C:538:ILE:HG22	1:C:578:PHE:HE2	1.76	0.51
1:B:535:CYS:HB2	1:B:543:PHE:CE2	2.46	0.51
1:A:442:PRO:HG2	1:A:526:PHE:CZ	2.46	0.50
1:C:446:LEU:HG	1:C:463:ILE:HD11	1.92	0.50
1:B:664:GLU:OE1	1:B:689:ARG:NH1	2.42	0.50
1:C:525:ILE:HG12	1:C:666:PHE:CE2	2.46	0.50
1:B:530:TYR:CD2	1:B:658:HIS:HB3	2.46	0.50
1:C:601:LEU:HB2	1:C:640:THR:HB	1.93	0.50
1:A:570:TRP:HB3	1:A:601:LEU:HD22	1.92	0.50
1:C:435:PRO:HG2	1:C:514:ILE:HD11	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:568:PHE:CZ	1:E:570:TRP:HB2	2.47	0.50
1:B:674:ALA:HB1	1:B:688:TYR:OH	2.11	0.50
1:C:520:THR:C	1:C:522:SER:H	2.19	0.50
1:A:430:LEU:O	1:A:474:THR:HA	2.12	0.50
1:B:535:CYS:HB2	1:B:543:PHE:CD2	2.47	0.50
1:A:535:CYS:SG	1:A:540:VAL:HG12	2.52	0.49
1:C:499:ILE:HG13	1:C:500:ARG:N	2.25	0.49
1:C:645:PRO:HB3	1:C:650:ILE:HD11	1.95	0.49
1:E:520:THR:C	1:E:522:SER:H	2.21	0.49
1:A:460:PRO:HD2	2:A:801:FAD:O2'	2.13	0.48
1:C:645:PRO:HG2	1:C:647:TRP:CZ2	2.48	0.48
1:B:415:THR:OG1	1:B:433:GLN:HB3	2.13	0.48
1:E:479:ALA:HA	1:E:484:THR:HB	1.94	0.48
1:C:428:LEU:HD13	1:C:430:LEU:HD11	1.96	0.48
1:C:538:ILE:HG22	1:C:578:PHE:CE2	2.48	0.48
1:B:526:PHE:HE1	1:B:550:ILE:HG12	1.79	0.48
1:A:589:GLU:HG3	1:A:599:LEU:HD12	1.95	0.48
1:C:551:LEU:HD23	1:C:551:LEU:HA	1.72	0.48
1:C:520:THR:HB	1:C:521:PRO:HD2	1.96	0.48
1:C:674:ALA:HB1	1:C:688:TYR:OH	2.14	0.48
1:A:486:LYS:HD2	1:A:486:LYS:H	1.78	0.48
1:B:565:LYS:HB3	1:B:658:HIS:CE1	2.49	0.48
1:C:550:ILE:HG23	1:C:561:MET:HE1	1.96	0.48
1:B:449:LYS:HE3	1:B:458:TRP:NE1	2.28	0.47
1:A:428:LEU:HD11	1:A:488:TYR:HA	1.96	0.47
1:A:496:GLU:HA	1:A:499:ILE:HG12	1.96	0.47
1:E:438:PHE:CZ	1:E:446:LEU:HD21	2.50	0.47
1:C:529:LYS:HA	1:C:562:PRO:O	2.14	0.47
1:C:499:ILE:HG13	1:C:500:ARG:H	1.78	0.47
1:E:600:ASN:O	1:E:601:LEU:HD23	2.15	0.47
1:A:462:THR:HG21	1:A:542:PRO:CB	2.45	0.47
1:B:415:THR:OG1	1:B:416:PHE:N	2.48	0.47
1:B:535:CYS:SG	1:B:540:VAL:HG12	2.54	0.47
1:C:419:ASN:HB3	1:C:431:GLN:HG3	1.96	0.46
1:E:587:LYS:HE3	1:E:591:GLU:OE1	2.15	0.46
1:C:521:PRO:CG	1:C:691:GLU:HG2	2.43	0.46
1:E:417:VAL:HB	1:E:510:VAL:HB	1.97	0.46
1:E:691:GLU:O	1:E:692:ASN:HB3	2.15	0.46
1:B:462:THR:OG1	1:B:541:THR:HB	2.14	0.46
1:A:524:HIS:NE2	1:E:515:ASP:OD1	2.49	0.46
1:B:561:MET:HE2	1:B:563:LEU:HD23	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:GLU:OE2	1:A:468:GLU:N	2.49	0.46
1:A:520:THR:HB	1:A:521:PRO:HD2	1.98	0.46
1:E:648:GLU:OE2	1:E:684:TYR:OH	2.23	0.46
1:A:449:LYS:HE3	1:A:458:TRP:NE1	2.31	0.46
1:E:515:ASP:OD2	1:E:518:TYR:OH	2.16	0.46
1:C:481:GLY:HA3	2:C:801:FAD:O3P	2.15	0.45
1:B:515:ASP:OD1	1:C:524:HIS:CE1	2.70	0.45
1:B:458:TRP:CZ3	1:B:515:ASP:HB2	2.52	0.45
1:B:602:TYR:CG	1:B:645:PRO:HG3	2.51	0.45
1:C:417:VAL:HB	1:C:510:VAL:HB	1.98	0.45
1:C:659:ALA:HA	1:C:660:PRO:HA	1.74	0.45
1:C:575:GLN:O	1:C:579:GLU:HG3	2.17	0.45
1:C:657:GLN:C	1:C:658:HIS:HD2	2.24	0.45
1:B:432:VAL:O	1:B:472:VAL:HA	2.16	0.45
1:E:446:LEU:O	1:E:460:PRO:HA	2.16	0.45
1:A:567:HIS:HB3	1:A:569:TYR:HE1	1.83	0.44
1:B:433:GLN:O	1:B:435:PRO:HD3	2.17	0.44
1:C:446:LEU:HD12	1:C:475:LEU:HD21	1.99	0.44
1:C:530:TYR:CG	1:C:658:HIS:ND1	2.84	0.44
1:B:478:ARG:HG2	1:B:480:VAL:CG1	2.48	0.44
1:B:497:GLU:O	1:B:501:SER:HB3	2.17	0.44
1:B:541:THR:HG21	2:B:801:FAD:O4	2.18	0.44
1:B:689:ARG:HB3	1:C:458:TRP:HB2	2.00	0.44
1:A:428:LEU:HB3	1:A:430:LEU:CD1	2.48	0.44
1:A:641:LYS:HB3	1:A:641:LYS:HE3	1.57	0.44
1:E:575:GLN:OE1	1:E:582:VAL:HG21	2.16	0.44
1:B:548:LYS:HD3	1:B:584:LEU:HD11	2.00	0.44
1:E:489:GLN:OE1	1:E:492:ARG:NH2	2.49	0.44
1:E:602:TYR:CD2	1:E:645:PRO:HG3	2.53	0.44
1:A:535:CYS:HB2	1:A:543:PHE:CD2	2.52	0.44
1:C:521:PRO:HG2	1:C:691:GLU:CG	2.45	0.44
1:C:535:CYS:HB2	1:C:543:PHE:CD2	2.52	0.44
1:A:540:VAL:HG11	1:A:570:TRP:CE2	2.53	0.43
1:B:447:PHE:O	1:B:514:ILE:HA	2.18	0.43
1:E:447:PHE:O	1:E:514:ILE:HA	2.18	0.43
1:B:536:ALA:HB3	1:B:669:GLY:HA3	2.00	0.43
1:C:453:ILE:HG23	1:C:486:LYS:HB3	1.99	0.43
1:A:551:LEU:HA	1:A:551:LEU:HD23	1.78	0.43
2:B:801:FAD:H8A	1:C:675:LEU:HD11	2.00	0.43
2:E:801:FAD:H9	2:E:801:FAD:H1'1	1.80	0.43
1:B:573:ARG:HE	1:B:574:GLU:HB2	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:GLU:OE2	1:B:576:LYS:N	2.51	0.43
1:C:655:ALA:HB2	1:C:686:PHE:HZ	1.84	0.43
1:E:428:LEU:HD11	1:E:488:TYR:HA	1.99	0.43
1:A:678:ARG:HD2	1:A:688:TYR:CE2	2.53	0.43
1:C:430:LEU:O	1:C:474:THR:HA	2.19	0.43
1:C:438:PHE:CE2	1:C:514:ILE:HD12	2.53	0.43
1:A:459:HIS:HA	1:A:460:PRO:HD3	1.73	0.43
1:E:541:THR:HG21	2:E:801:FAD:O4	2.19	0.43
1:E:522:SER:HB3	1:E:546:ILE:HD11	1.99	0.42
1:B:413:GLU:HB3	1:B:414:PRO:CD	2.48	0.42
1:E:659:ALA:HA	1:E:660:PRO:HA	1.80	0.42
1:B:453:ILE:HD11	1:B:487:LEU:CD1	2.43	0.42
1:B:456:PHE:CZ	1:C:685:GLY:HA2	2.53	0.42
1:B:539:GLY:HA2	3:B:802:U4O:CAZ	2.50	0.42
1:E:454:SER:OG	1:E:457:GLU:HG3	2.20	0.42
1:E:550:ILE:HG22	1:E:596:LEU:HD21	2.01	0.42
1:A:425:SER:HB3	1:A:577:ALA:HA	1.99	0.42
1:C:445:TYR:HB3	1:C:462:THR:HG22	2.00	0.42
1:C:428:LEU:HB3	1:C:430:LEU:CD1	2.50	0.42
1:C:526:PHE:O	1:C:562:PRO:HG2	2.20	0.42
1:E:446:LEU:HA	1:E:446:LEU:HD23	1.72	0.42
1:E:529:LYS:CG	1:E:564:LYS:HG3	2.49	0.42
1:A:490:LEU:O	1:A:494:GLN:HB2	2.20	0.42
1:B:432:VAL:HB	1:B:473:LEU:HB2	2.01	0.42
1:E:446:LEU:HG	1:E:463:ILE:HD11	2.02	0.42
1:B:525:ILE:HG12	1:B:666:PHE:CE2	2.55	0.41
1:B:446:LEU:HA	1:B:446:LEU:HD23	1.83	0.41
1:B:521:PRO:HG2	1:B:691:GLU:OE2	2.21	0.41
1:A:563:LEU:HD12	1:A:563:LEU:HA	1.83	0.41
1:B:425:SER:HB3	1:B:577:ALA:HA	2.03	0.41
1:B:589:GLU:HG3	1:B:599:LEU:HD12	2.03	0.41
1:E:650:ILE:O	1:E:654:VAL:HG23	2.20	0.41
1:B:474:THR:O	1:B:475:LEU:HD23	2.21	0.41
1:C:498:TRP:CZ2	1:C:504:SER:HA	2.56	0.40
1:E:526:PHE:HD1	1:E:561:MET:HE3	1.86	0.40
1:A:426:LYS:HA	1:A:488:TYR:CE2	2.56	0.40
1:A:429:GLY:O	1:A:430:LEU:HD12	2.22	0.40
1:E:415:THR:OG1	1:E:416:PHE:N	2.54	0.40
1:E:499:ILE:C	1:E:501:SER:N	2.78	0.40
1:A:533:LEU:HD23	1:A:666:PHE:HB2	2.02	0.40
1:A:565:LYS:HD2	1:A:565:LYS:HA	1.89	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:LYS:NZ	1:B:595:ASN:O	2.43	0.40
1:A:603:LEU:HA	1:A:603:LEU:HD22	1.81	0.40
1:E:691:GLU:O	1:E:692:ASN:CB	2.69	0.40

All (3) 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:E:564:LYS:NZ	2:E:801:FAD:C2B[2_645]	1.44	0.76
1:A:504:SER:OG	1:E:419:ASN:ND2[1_455]	1.75	0.45
1:E:564:LYS:NZ	2:E:801:FAD:O2B[2_645]	2.15	0.05

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	243/283 (86%)	222 (91%)	16 (7%)	5 (2%)	5	27
1	B	237/283 (84%)	225 (95%)	10 (4%)	2 (1%)	16	50
1	C	238/283 (84%)	226 (95%)	11 (5%)	1 (0%)	30	65
1	E	236/283 (83%)	225 (95%)	9 (4%)	2 (1%)	16	50
All	All	954/1132 (84%)	898 (94%)	46 (5%)	10 (1%)	12	45

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	470	PRO
1	A	470	PRO
1	A	482	SER
1	A	490	LEU
1	E	470	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	460	PRO
1	A	563	LEU
1	E	482	SER
1	B	501	SER
1	C	470	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	214/250 (86%)	210 (98%)	4 (2%)	50	76
1	B	209/250 (84%)	209 (100%)	0	100	100
1	C	209/250 (84%)	209 (100%)	0	100	100
1	E	209/250 (84%)	209 (100%)	0	100	100
All	All	841/1000 (84%)	837 (100%)	4 (0%)	81	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	497	GLU
1	A	498	TRP
1	A	501	SER
1	A	504	SER

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

Mol	Chain	Res	Type
1	A	441	GLN
1	A	489	GLN
1	B	600	ASN
1	C	555	GLN
1	C	572	ASN
1	C	575	GLN
1	C	600	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	657	GLN
1	C	679	HIS
1	E	524	HIS
1	E	600	ASN
1	E	657	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	U4O	B	802	-	41,41,41	3.61	12 (29%)	57,58,58	1.70	13 (22%)
3	U4O	E	802	-	41,41,41	3.58	13 (31%)	57,58,58	1.58	11 (19%)
2	FAD	B	801	-	58,58,58	0.78	1 (1%)	85,89,89	0.71	2 (2%)
2	FAD	E	801	-	58,58,58	0.82	2 (3%)	85,89,89	0.65	1 (1%)
2	FAD	C	801	-	58,58,58	0.58	1 (1%)	85,89,89	0.62	3 (3%)
3	U4O	C	802	-	41,41,41	3.18	11 (26%)	57,58,58	1.69	16 (28%)
2	FAD	A	801	-	58,58,58	0.71	2 (3%)	85,89,89	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	U4O	A	802	-	41,41,41	3.38	14 (34%)	57,58,58	1.63	12 (21%)

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	U4O	B	802	-	-	3/20/40/40	0/6/6/6
3	U4O	E	802	-	-	2/20/40/40	0/6/6/6
2	FAD	B	801	-	-	15/34/50/50	0/6/6/6
2	FAD	E	801	-	-	11/34/50/50	0/6/6/6
2	FAD	C	801	-	-	9/34/50/50	0/6/6/6
3	U4O	C	802	-	-	4/20/40/40	0/6/6/6
2	FAD	A	801	-	-	15/34/50/50	0/6/6/6
3	U4O	A	802	-	-	4/20/40/40	0/6/6/6

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	U4O	CAK-CAI	-14.14	1.40	1.51
3	E	802	U4O	CAW-CAP	-12.67	1.39	1.49
3	A	802	U4O	CAW-CAP	-12.65	1.39	1.49
3	C	802	U4O	CAK-CAI	-12.62	1.42	1.51
3	E	802	U4O	CAK-CAI	-12.32	1.42	1.51
3	A	802	U4O	CAK-CAI	-11.04	1.43	1.51
3	B	802	U4O	CAW-CAP	-11.01	1.40	1.49
3	C	802	U4O	CAW-CAP	-9.79	1.41	1.49
3	E	802	U4O	CAM-CAL	-7.66	1.39	1.51
3	B	802	U4O	CAM-CAL	-6.92	1.40	1.51
3	E	802	U4O	CBE-CAB	-6.70	1.39	1.50
3	B	802	U4O	CBE-CAB	-6.46	1.39	1.50
3	A	802	U4O	CAM-CAL	-5.74	1.42	1.51
3	A	802	U4O	CBE-CAB	-5.50	1.41	1.50
3	C	802	U4O	CBE-CAB	-5.18	1.41	1.50
3	C	802	U4O	CAM-CAL	-5.03	1.43	1.51
2	B	801	FAD	P-O3P	-5.00	1.54	1.59
3	A	802	U4O	CAQ-CAR	-4.93	1.33	1.43
3	B	802	U4O	OAV-CAR	4.76	1.45	1.37
2	E	801	FAD	P-O3P	-4.44	1.54	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	802	U4O	CAQ-CAR	-4.33	1.34	1.43
3	E	802	U4O	CAQ-CAP	4.25	1.42	1.34
3	B	802	U4O	CAQ-CAR	-4.01	1.35	1.43
3	C	802	U4O	CBI-NBJ	3.74	1.42	1.34
3	A	802	U4O	CAK-CAL	3.67	1.43	1.38
2	A	801	FAD	P-O3P	-3.65	1.55	1.59
3	B	802	U4O	CAQ-CAP	3.53	1.41	1.34
3	E	802	U4O	CAO-CAP	-3.45	1.39	1.50
3	C	802	U4O	CAQ-CAP	3.43	1.41	1.34
3	B	802	U4O	CAK-CAL	3.30	1.42	1.38
3	E	802	U4O	CBI-NBJ	3.26	1.41	1.34
3	A	802	U4O	CAO-CAP	-3.21	1.40	1.50
3	C	802	U4O	CAK-CAL	3.20	1.42	1.38
3	A	802	U4O	CBI-NBJ	3.18	1.41	1.34
3	E	802	U4O	CAQ-CAR	-3.18	1.36	1.43
2	A	801	FAD	P-O2P	-3.17	1.40	1.55
3	B	802	U4O	CAO-CAP	-3.16	1.40	1.50
3	E	802	U4O	CAD-NAC	3.09	1.52	1.47
3	B	802	U4O	CBI-NBJ	2.86	1.40	1.34
3	A	802	U4O	OAV-CAR	2.85	1.41	1.37
3	B	802	U4O	CAD-NAC	2.84	1.52	1.47
3	C	802	U4O	CAD-NAC	2.78	1.52	1.47
2	C	801	FAD	P-O2P	-2.69	1.42	1.55
3	C	802	U4O	CAO-CAP	-2.64	1.42	1.50
3	A	802	U4O	CAG-NAF	2.46	1.51	1.47
3	B	802	U4O	CAW-NAX	2.42	1.35	1.32
2	E	801	FAD	P-O2P	-2.34	1.44	1.55
3	A	802	U4O	CAQ-CAP	2.25	1.38	1.34
3	E	802	U4O	OAV-CAR	2.19	1.40	1.37
3	E	802	U4O	CAK-CAL	2.17	1.41	1.38
3	A	802	U4O	CAD-NAC	2.16	1.50	1.47
3	A	802	U4O	CAH-NAC	2.15	1.50	1.47
3	C	802	U4O	CAW-NAX	2.12	1.35	1.32
3	A	802	U4O	CAY-NAX	-2.02	1.34	1.37
3	E	802	U4O	CAY-NAX	-2.02	1.34	1.37
3	E	802	U4O	CAW-NAX	2.01	1.35	1.32

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	U4O	CAR-CAQ-CAP	-5.17	120.70	128.61
3	B	802	U4O	OAJ-CAI-CAK	4.41	125.61	118.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	U4O	CAW-CAP-CAQ	-4.38	110.80	119.60
3	E	802	U4O	CAH-NAC-CAD	4.24	121.34	112.68
3	B	802	U4O	CAG-NAF-CAE	4.15	121.15	112.68
3	E	802	U4O	CAR-CAQ-CAP	-4.05	122.41	128.61
3	C	802	U4O	CBI-NBJ-CBE	4.02	122.11	116.93
3	E	802	U4O	CAG-NAF-CAE	3.93	120.69	112.68
3	C	802	U4O	CAG-NAF-CAE	3.52	119.87	112.68
3	B	802	U4O	CAH-NAC-CAD	3.50	119.83	112.68
3	C	802	U4O	CAH-NAC-CAD	3.47	119.77	112.68
3	A	802	U4O	CBI-NBJ-CBE	3.45	121.38	116.93
3	A	802	U4O	CAK-CBD-CAY	2.95	121.06	116.60
3	A	802	U4O	CAR-CAQ-CAP	-2.90	124.17	128.61
3	A	802	U4O	CAM-CAL-CAW	-2.89	117.03	119.33
3	C	802	U4O	CBH-CBI-NBJ	-2.89	118.84	123.42
3	C	802	U4O	CAW-NAX-CAY	2.81	122.65	117.15
3	C	802	U4O	CAW-CAP-CAQ	-2.78	114.01	119.60
3	C	802	U4O	CAP-CAW-NAX	2.73	119.08	116.76
3	A	802	U4O	CAL-CAK-CBD	-2.70	116.97	120.58
3	A	802	U4O	CBD-CAY-NAX	-2.70	119.94	122.80
3	A	802	U4O	CAS-CAT-CAU	2.61	111.33	106.94
3	C	802	U4O	CBF-CBE-NBJ	-2.59	119.26	122.74
3	B	802	U4O	CAS-CAT-CAU	2.56	111.24	106.94
3	C	802	U4O	OAV-CAR-CAQ	2.56	125.56	116.89
3	C	802	U4O	CAR-CAQ-CAP	-2.53	124.74	128.61
3	E	802	U4O	CBD-CAY-NAX	-2.51	120.15	122.80
3	A	802	U4O	CBF-CBE-NBJ	-2.49	119.39	122.74
2	C	801	FAD	O2A-PA-O1A	2.48	123.97	112.44
3	E	802	U4O	CAW-NAX-CAY	2.43	121.91	117.15
2	B	801	FAD	O5'-P-O1P	2.41	118.48	108.94
3	C	802	U4O	CAB-CBE-NBJ	2.40	121.99	117.47
3	C	802	U4O	CAL-CAW-NAX	-2.40	119.99	123.40
3	C	802	U4O	CAS-CAR-CAQ	-2.36	124.35	132.73
3	C	802	U4O	CBD-CAY-NAX	-2.31	120.35	122.80
3	B	802	U4O	CAW-NAX-CAY	2.29	121.64	117.15
3	B	802	U4O	OAJ-CAI-NAF	-2.28	118.76	122.35
3	A	802	U4O	CAG-NAF-CAE	2.25	117.27	112.68
3	B	802	U4O	CAL-CAK-CAI	2.23	123.83	120.51
3	A	802	U4O	CBH-CBI-NBJ	-2.23	119.90	123.42
3	B	802	U4O	CBH-CBI-NBJ	-2.22	119.90	123.42
3	E	802	U4O	CAP-CAW-NAX	2.22	118.64	116.76
2	C	801	FAD	O5B-PA-O1A	-2.21	100.17	108.94
3	B	802	U4O	CAL-CAW-NAX	-2.20	120.27	123.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	802	U4O	CAK-CBD-CAY	2.19	119.91	116.60
3	C	802	U4O	CBD-CAK-CAI	2.18	121.31	118.31
3	E	802	U4O	CAT-CAS-CAR	2.16	110.47	106.73
3	A	802	U4O	CAW-NAX-CAY	2.14	121.34	117.15
3	E	802	U4O	CAH-NAC-CAB	-2.14	116.18	122.79
3	C	802	U4O	OAJ-CAI-CAK	2.13	122.03	118.70
3	B	802	U4O	CAK-CBD-CAY	2.12	119.79	116.60
3	E	802	U4O	CAN-CAM-CAL	-2.09	108.60	112.84
2	C	801	FAD	O5'-P-O1P	2.08	117.20	108.94
3	B	802	U4O	CBD-CAY-NAX	-2.06	120.62	122.80
2	B	801	FAD	O4'-C4'-C5'	-2.04	105.48	109.99
3	B	802	U4O	OAV-CAR-CAQ	2.04	123.80	116.89
2	E	801	FAD	O2A-PA-O1A	2.02	121.85	112.44
3	E	802	U4O	CBD-CAK-CAI	2.00	121.07	118.31

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	FAD	C5B-O5B-PA-O1A
2	A	801	FAD	C5B-O5B-PA-O2A
2	A	801	FAD	C5B-O5B-PA-O3P
2	A	801	FAD	O4B-C4B-C5B-O5B
2	A	801	FAD	C2'-C3'-C4'-O4'
2	A	801	FAD	O3'-C3'-C4'-O4'
2	A	801	FAD	O3'-C3'-C4'-C5'
2	A	801	FAD	C5'-O5'-P-O3P
2	B	801	FAD	C5B-O5B-PA-O1A
2	B	801	FAD	C5B-O5B-PA-O3P
2	B	801	FAD	C2'-C3'-C4'-C5'
2	B	801	FAD	O3'-C3'-C4'-C5'
2	B	801	FAD	C3'-C4'-C5'-O5'
2	B	801	FAD	O4'-C4'-C5'-O5'
2	B	801	FAD	C5'-O5'-P-O1P
2	C	801	FAD	C5B-O5B-PA-O3P
2	C	801	FAD	C3'-C4'-C5'-O5'
2	C	801	FAD	O4'-C4'-C5'-O5'
2	C	801	FAD	C5'-O5'-P-O1P
2	C	801	FAD	C5'-O5'-P-O3P
2	E	801	FAD	C2'-C3'-C4'-O4'
2	E	801	FAD	O3'-C3'-C4'-O4'
2	E	801	FAD	O3'-C3'-C4'-C5'

Continued on next page...

Continued from previous page...

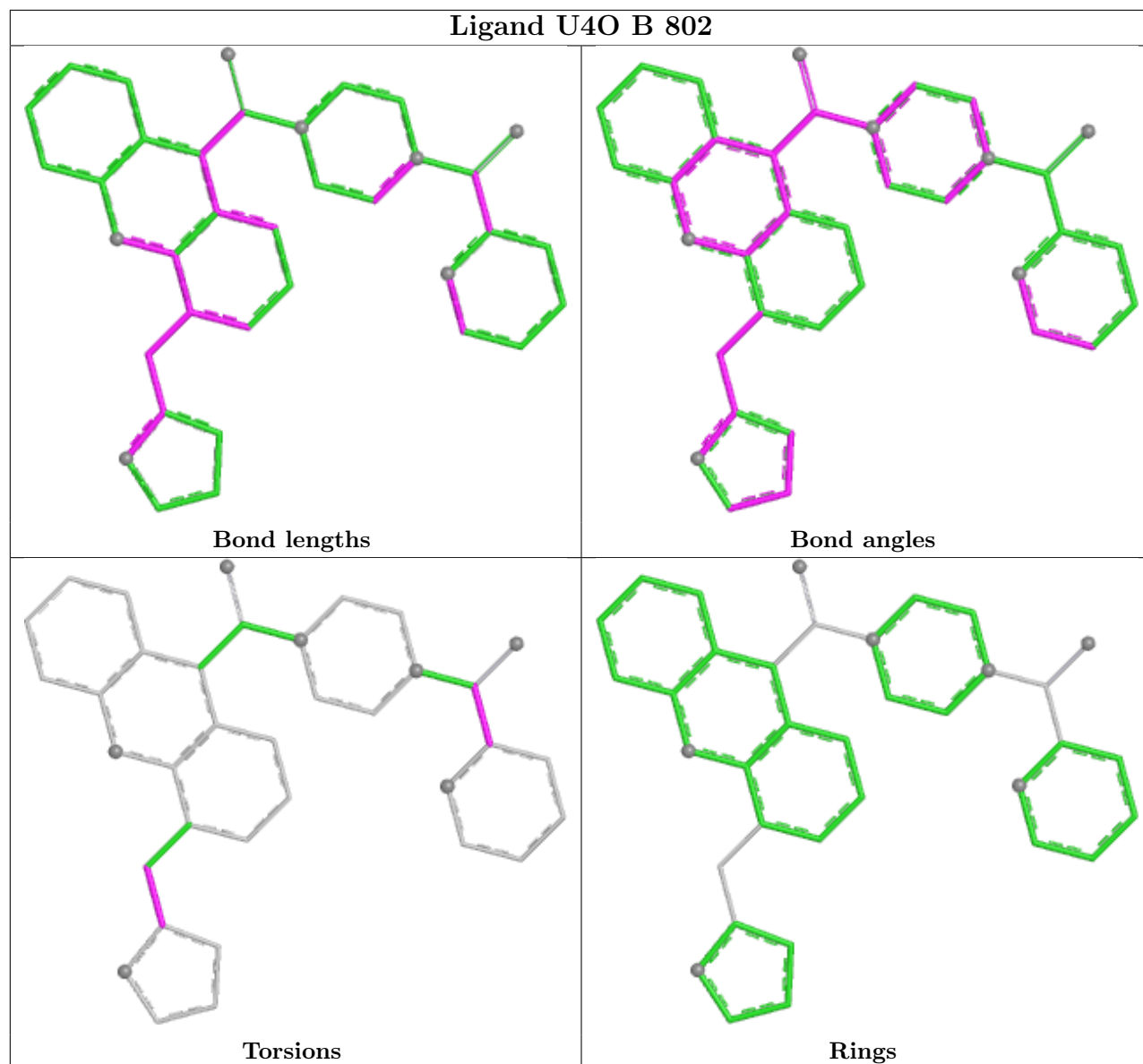
Mol	Chain	Res	Type	Atoms
2	E	801	FAD	C3'-C4'-C5'-O5'
2	E	801	FAD	O4'-C4'-C5'-O5'
2	E	801	FAD	C5'-O5'-P-O1P
3	A	802	U4O	CAP-CAQ-CAR-CAS
3	A	802	U4O	CAP-CAQ-CAR-OAV
3	B	802	U4O	CAP-CAQ-CAR-CAS
3	B	802	U4O	CAP-CAQ-CAR-OAV
3	C	802	U4O	CAP-CAQ-CAR-CAS
3	C	802	U4O	CAP-CAQ-CAR-OAV
3	E	802	U4O	CAP-CAQ-CAR-CAS
3	E	802	U4O	CAP-CAQ-CAR-OAV
2	B	801	FAD	O3'-C3'-C4'-O4'
2	A	801	FAD	C2'-C3'-C4'-C5'
2	E	801	FAD	C2'-C3'-C4'-C5'
2	B	801	FAD	C2'-C3'-C4'-O4'
2	A	801	FAD	C3B-C4B-C5B-O5B
2	B	801	FAD	O4B-C4B-C5B-O5B
2	B	801	FAD	C3B-C4B-C5B-O5B
2	E	801	FAD	O2'-C2'-C3'-C4'
2	A	801	FAD	C3'-C4'-C5'-O5'
2	B	801	FAD	O2'-C2'-C3'-C4'
2	B	801	FAD	C1'-C2'-C3'-O3'
3	A	802	U4O	NAF-CAI-CAK-CAL
3	A	802	U4O	OAJ-CAI-CAK-CAL
2	C	801	FAD	C3B-C4B-C5B-O5B
2	A	801	FAD	O4'-C4'-C5'-O5'
2	A	801	FAD	C2B-C1B-N9A-C4A
2	A	801	FAD	C5'-O5'-P-O1P
2	B	801	FAD	C5B-O5B-PA-O2A
2	C	801	FAD	C5'-O5'-P-O2P
2	A	801	FAD	C2B-C1B-N9A-C8A
2	E	801	FAD	C1'-C2'-C3'-O3'
2	E	801	FAD	O2'-C2'-C3'-O3'
2	B	801	FAD	C1'-C2'-C3'-C4'
3	B	802	U4O	OAA-CAB-CBE-CBF
2	C	801	FAD	P-O3P-PA-O1A
2	C	801	FAD	P-O3P-PA-O2A
3	C	802	U4O	OAA-CAB-CBE-CBF
3	C	802	U4O	OAA-CAB-CBE-NBJ
2	E	801	FAD	P-O3P-PA-O2A

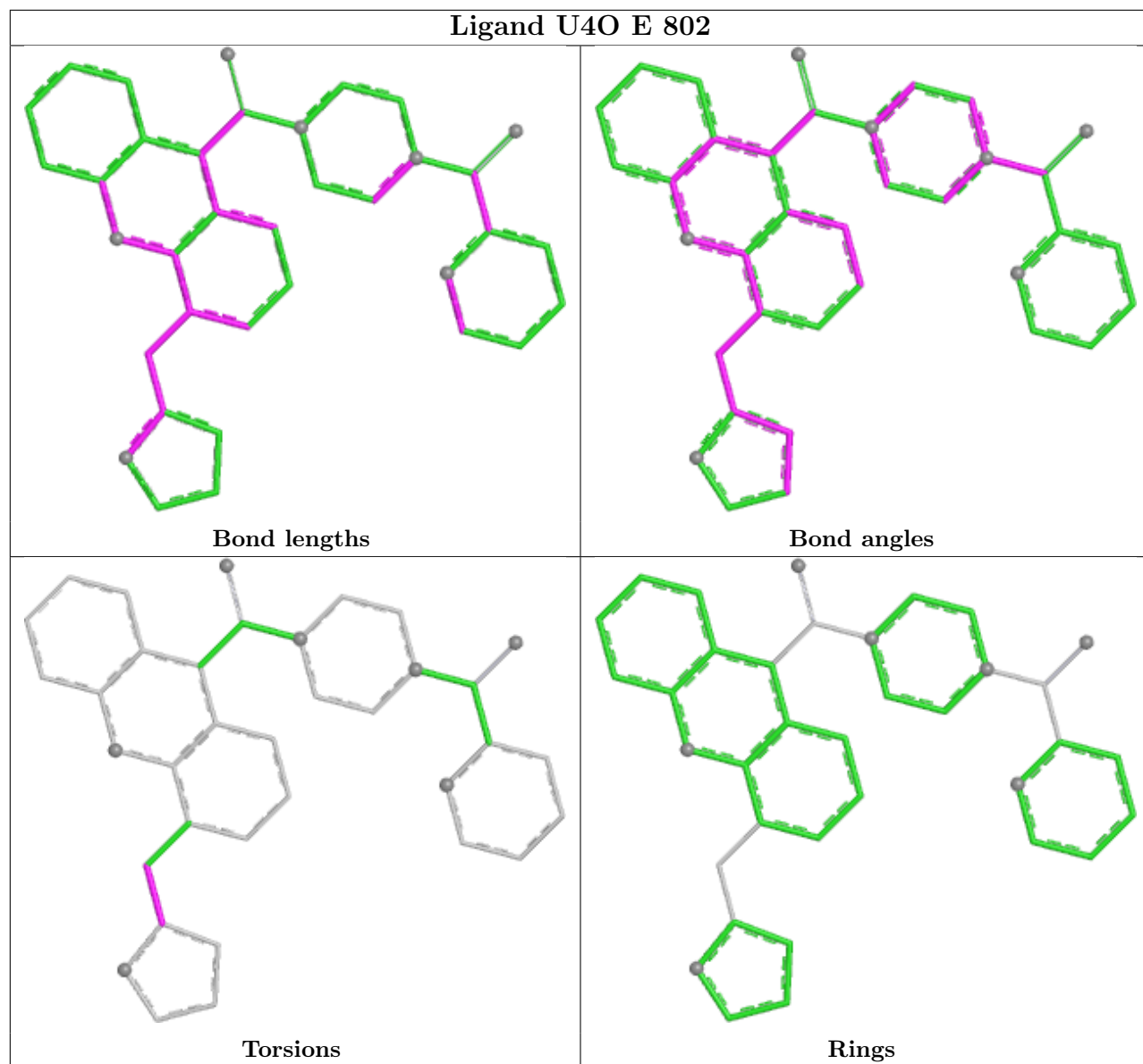
There are no ring outliers.

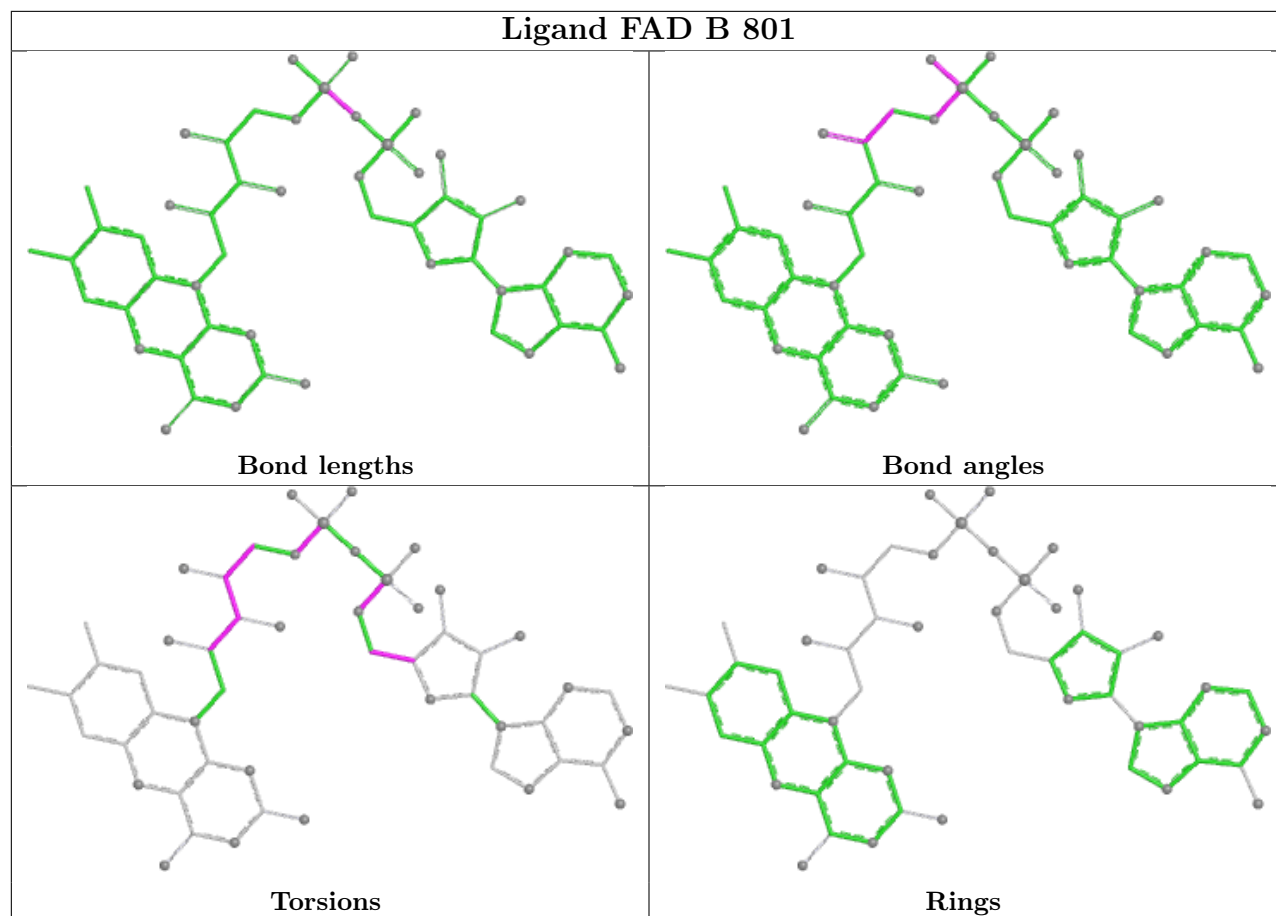
5 monomers are involved in 14 short contacts:

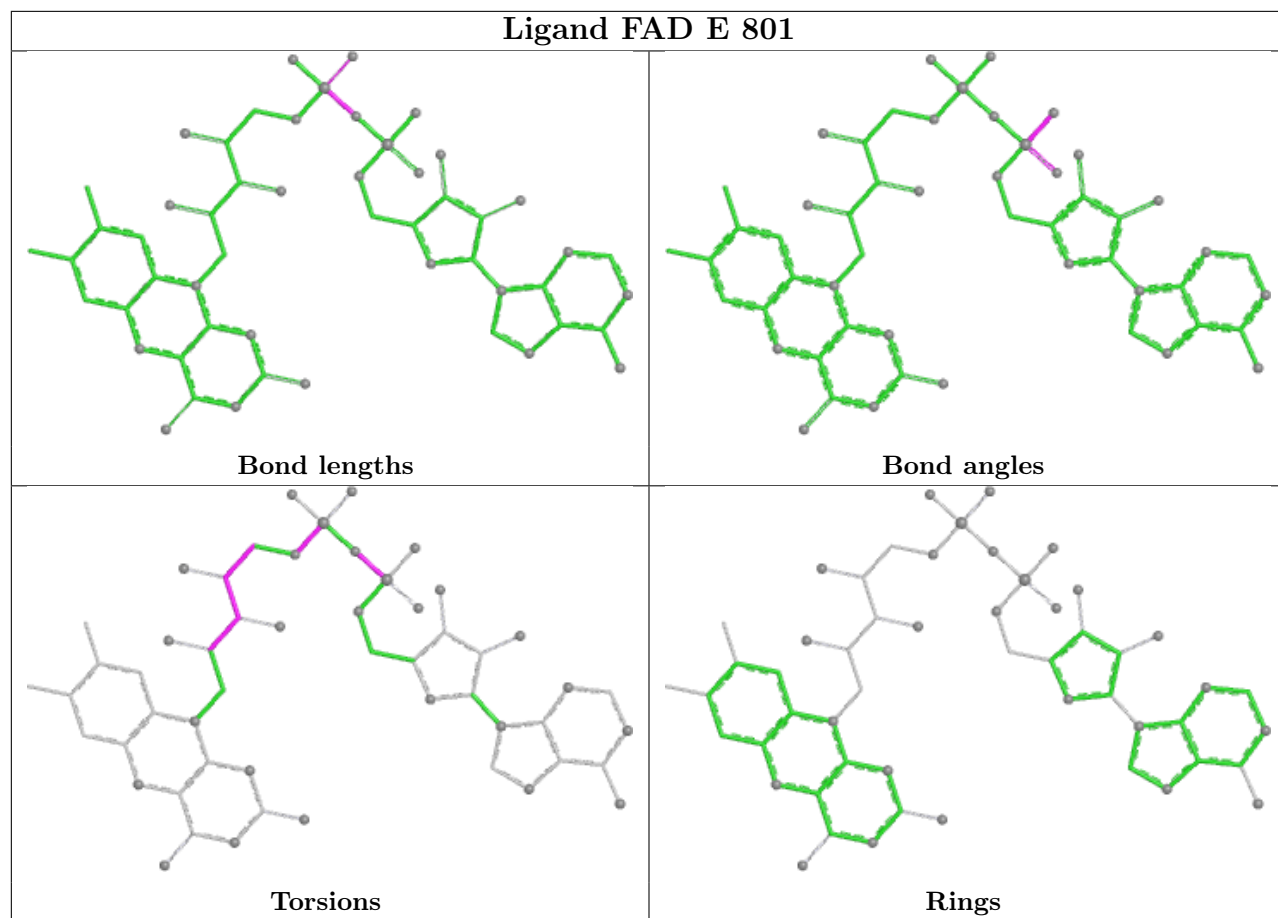
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	802	U4O	1	0
2	B	801	FAD	3	0
2	E	801	FAD	2	2
2	C	801	FAD	4	0
2	A	801	FAD	2	0

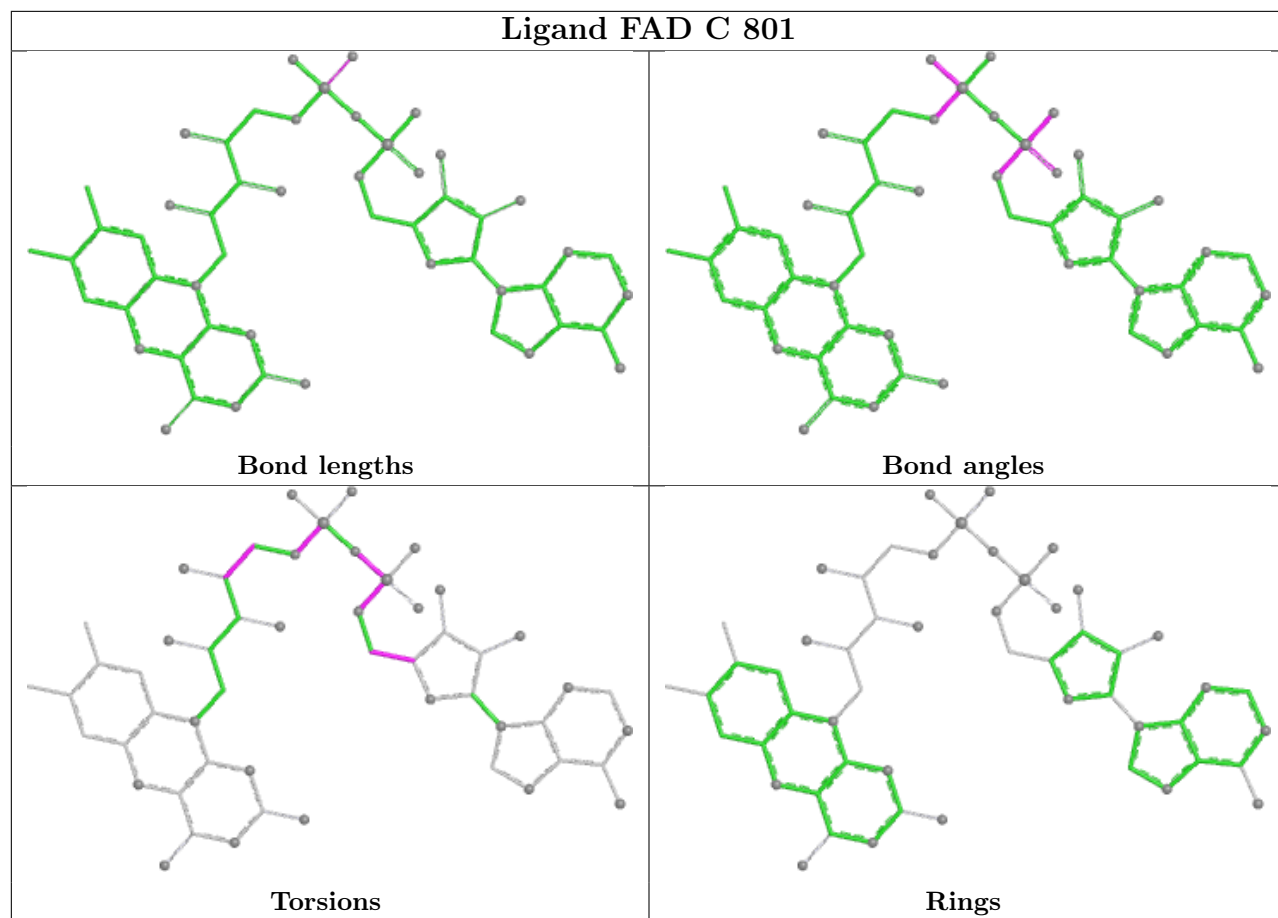
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

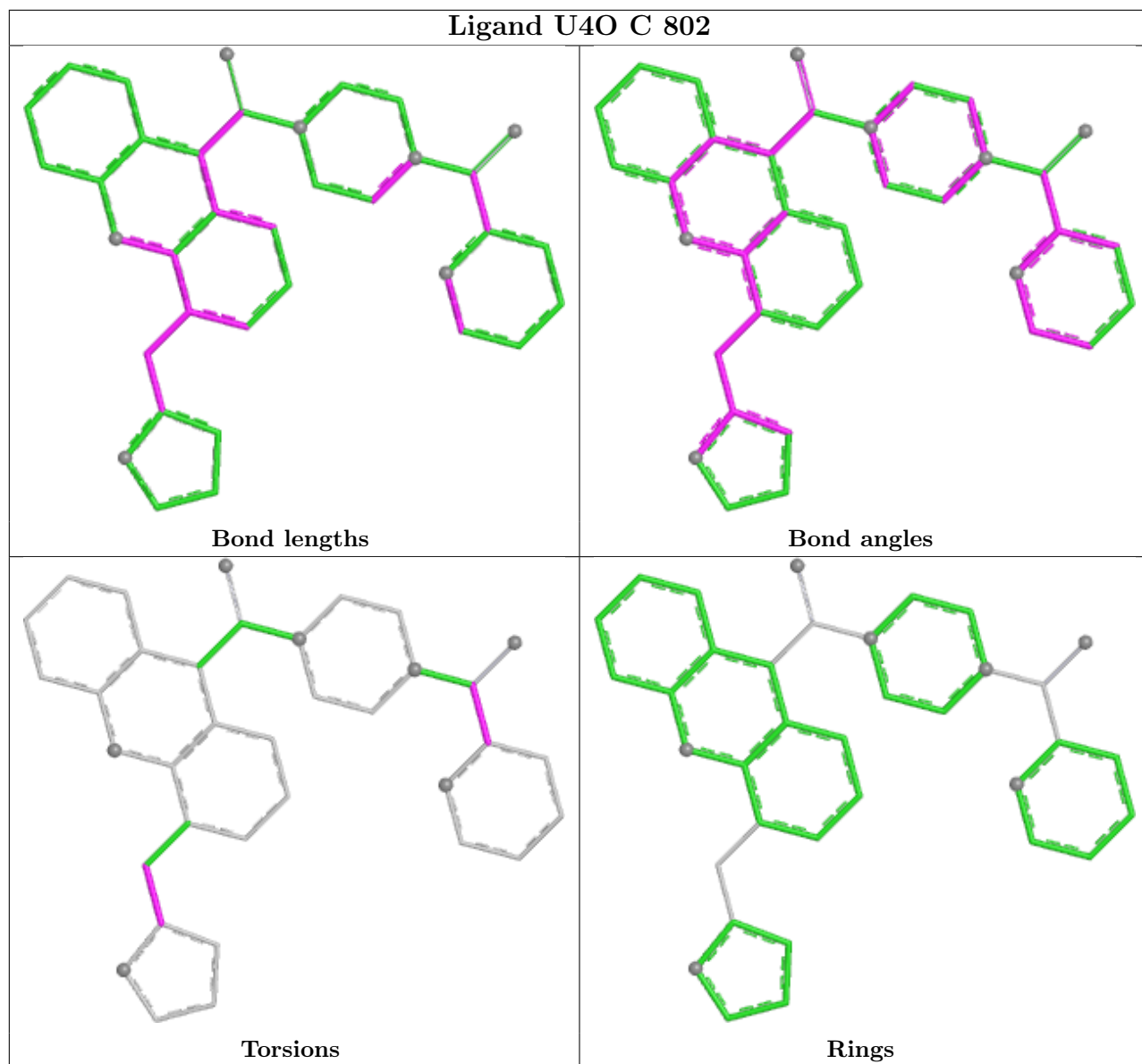


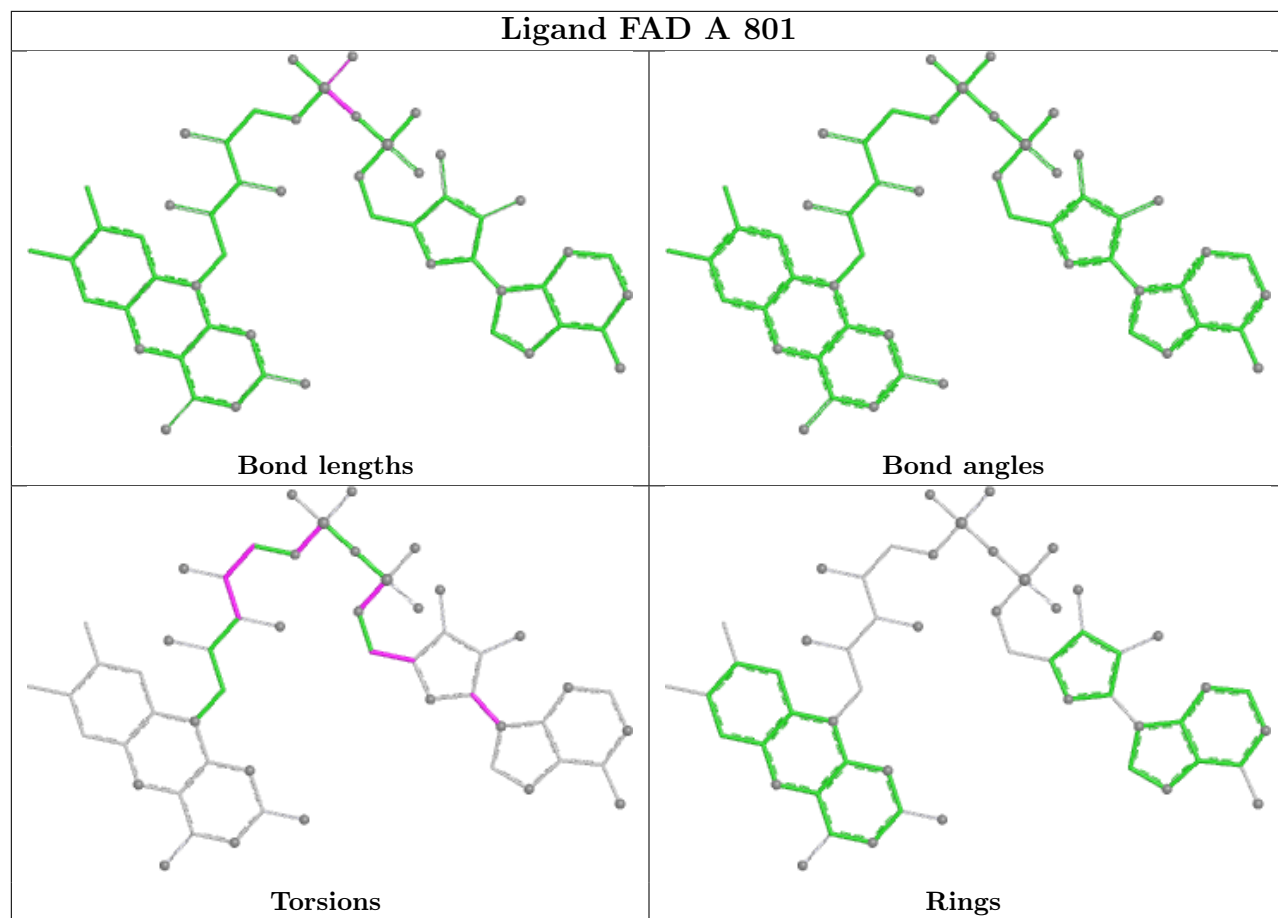


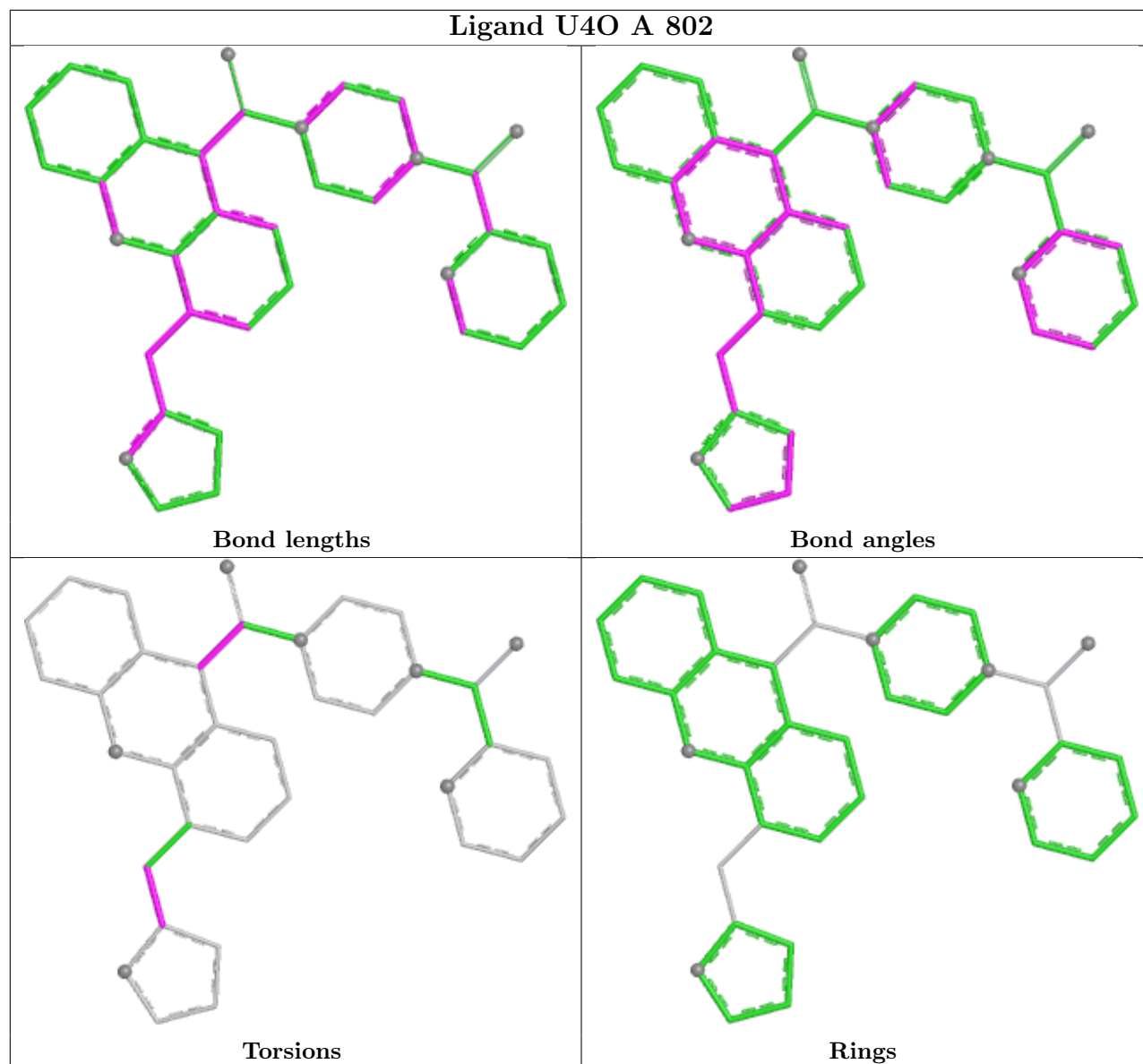












5.7 Other polymers [i](#)

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	247/283 (87%)	-1.31	0 100 100	41, 63, 99, 124	0
1	B	243/283 (85%)	-1.26	0 100 100	56, 80, 106, 128	0
1	C	244/283 (86%)	-1.34	0 100 100	49, 70, 104, 131	0
1	E	242/283 (85%)	-1.26	0 100 100	41, 62, 96, 124	0
All	All	976/1132 (86%)	-1.29	0 100 100	41, 69, 102, 131	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

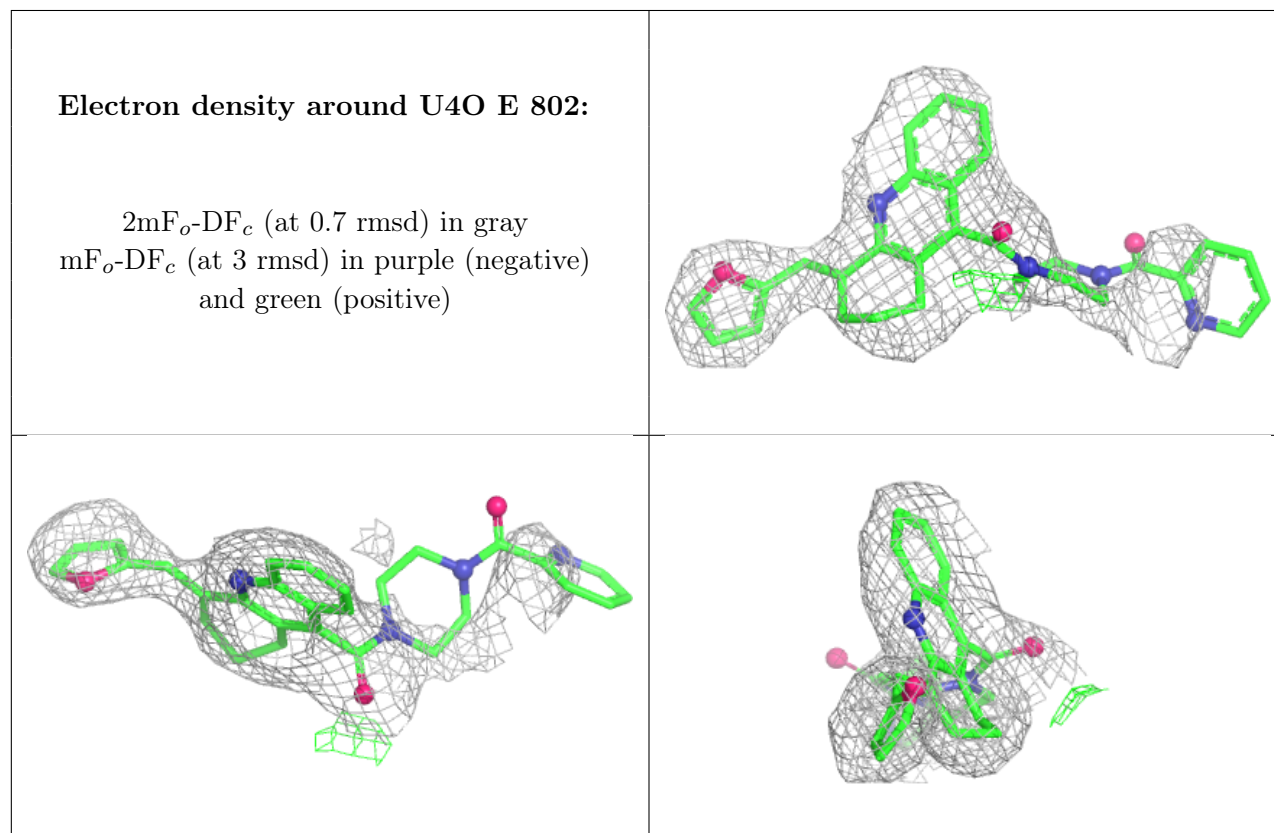
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	U4O	E	802	36/36	0.98	0.05	50,67,103,109	0
2	FAD	B	801	53/53	0.99	0.04	57,70,104,117	0
2	FAD	C	801	53/53	0.99	0.04	51,66,105,112	0
2	FAD	E	801	53/53	0.99	0.04	38,51,107,109	0

Continued on next page...

Continued from previous page...

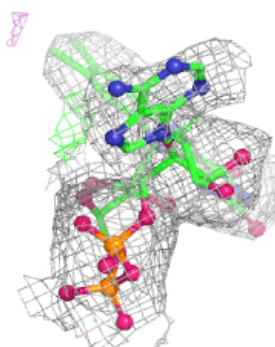
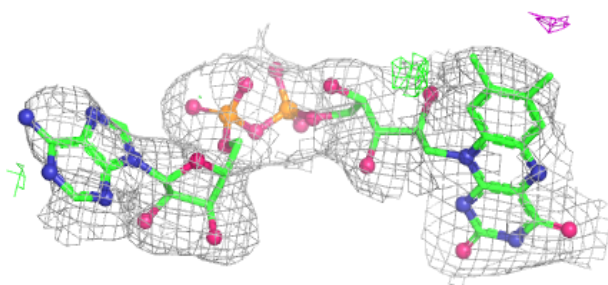
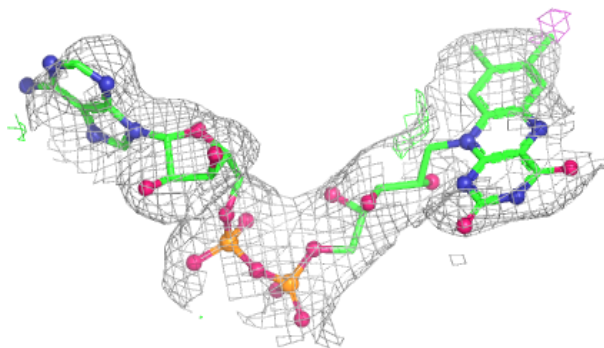
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	U4O	A	802	36/36	0.99	0.05	56,70,85,90	0
3	U4O	B	802	36/36	0.99	0.06	70,79,98,102	0
3	U4O	C	802	36/36	0.99	0.05	64,74,95,98	0
2	FAD	A	801	53/53	0.99	0.04	37,59,93,105	0

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.

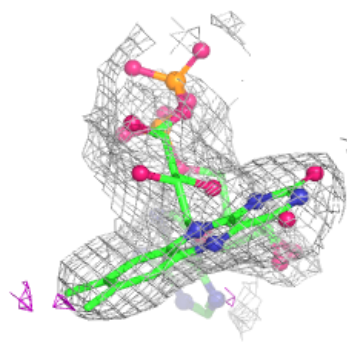
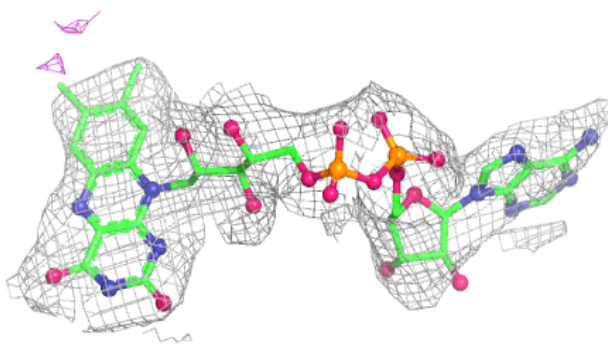
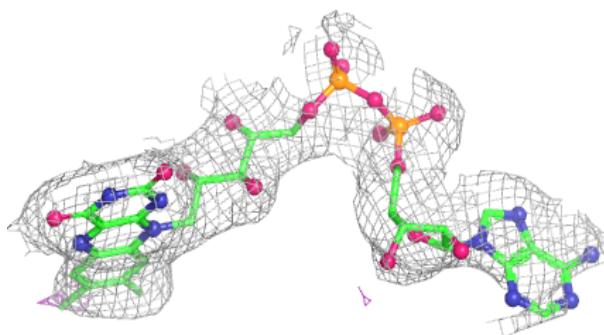


Electron density around FAD B 801:

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

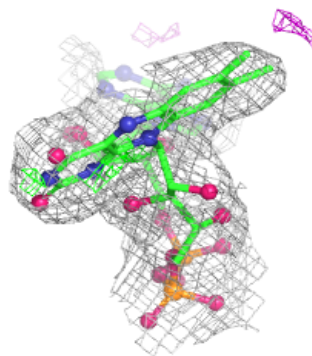
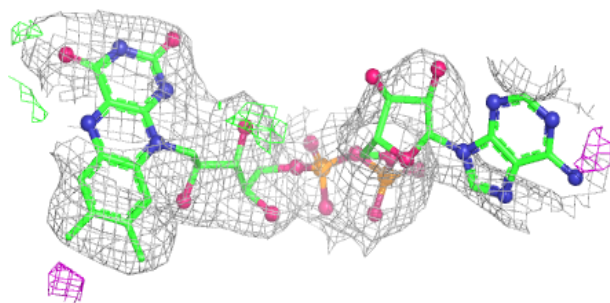
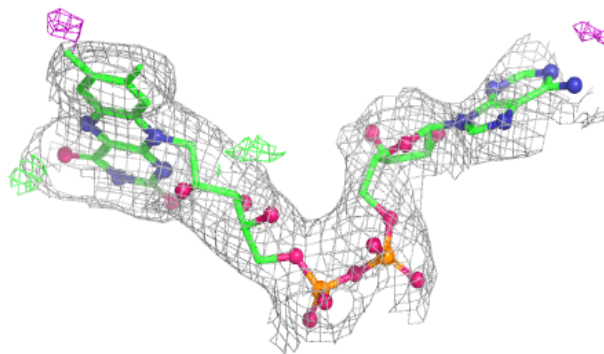
**Electron density around FAD C 801:**

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

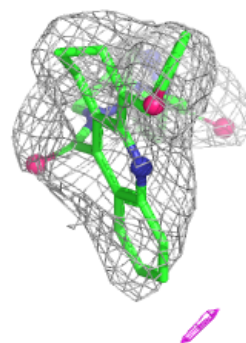
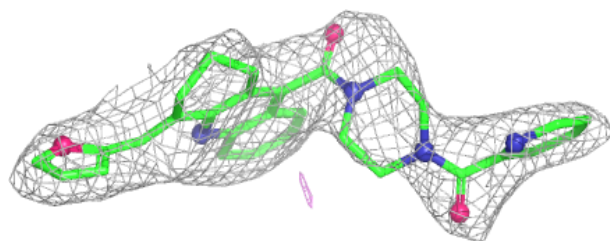
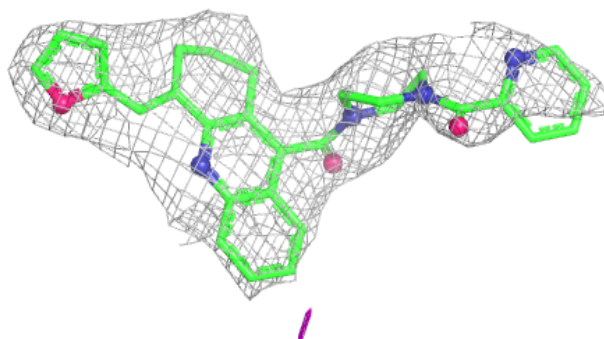


Electron density around FAD E 801:

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

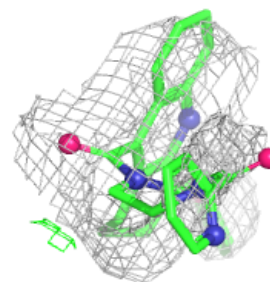
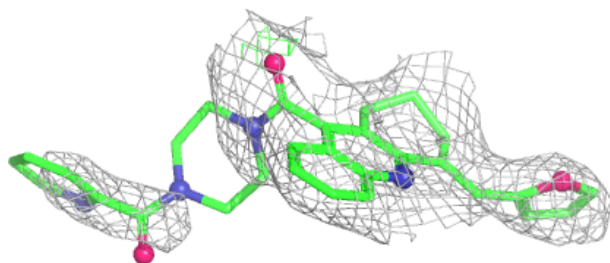
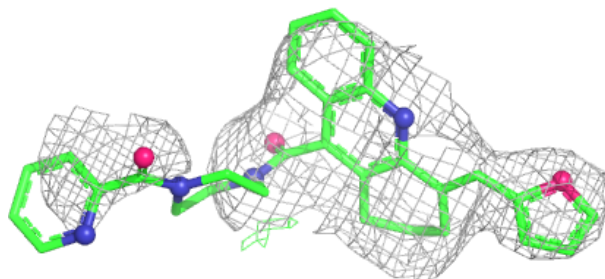
**Electron density around U4O A 802:**

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

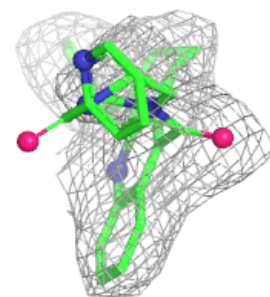
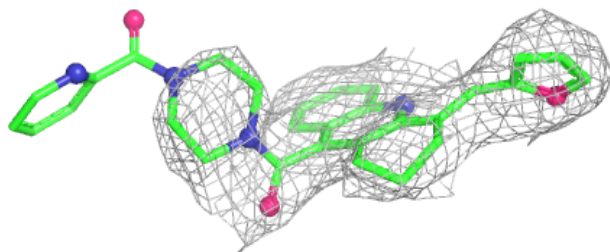
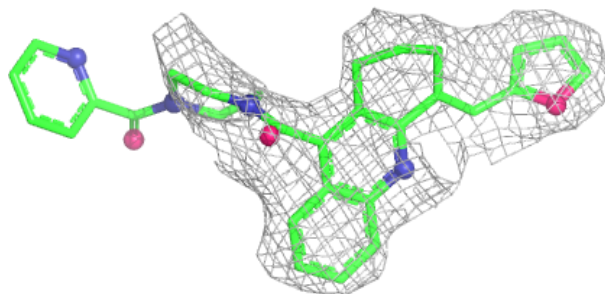


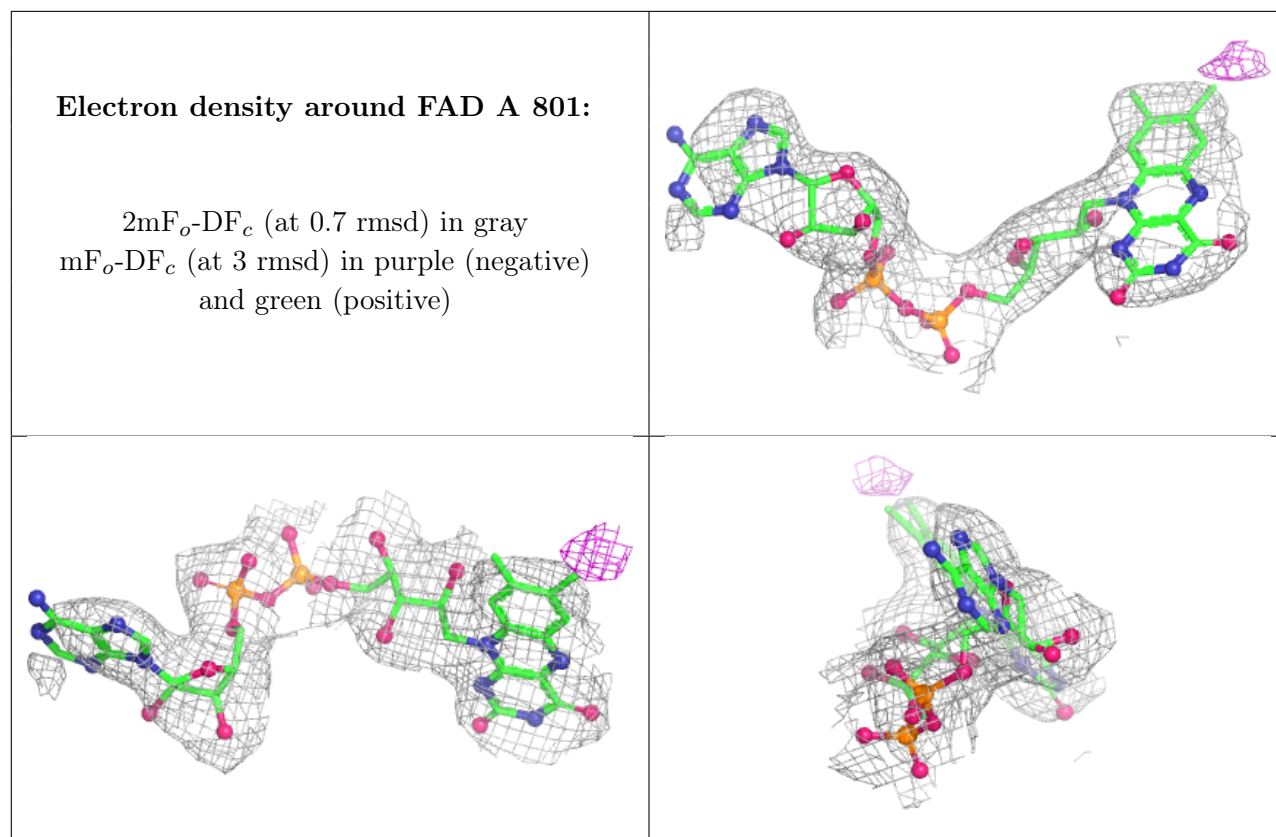
Electron density around U4O B 802:

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

**Electron density around U4O C 802:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.