



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:33 AM UTC

PDB ID : 3PM9 / pdb_00003pm9
Title : Crystal structure of a Putative dehydrogenase (RPA1076) from Rhodopseudomonas palustris CGA009 at 2.57 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2010-11-16
Resolution : 2.57 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)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

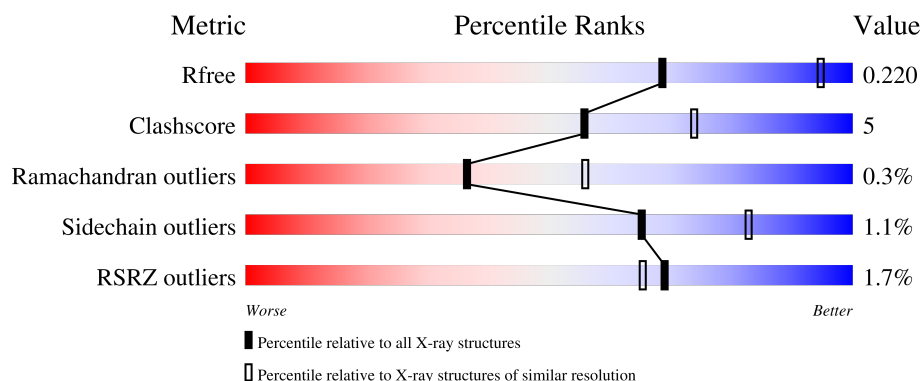
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	476	0% 88% 10% .
1	B	476	0% 86% 12% .
1	C	476	2% 88% 10% .
1	D	476	0% 87% 11% ..
1	E	476	2% 88% 9% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	476	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	UNL	A	477	-	-	X	-
3	UNL	B	477	-	-	X	-
3	UNL	C	477	-	-	X	-
3	UNL	D	477	-	-	X	-
3	UNL	E	477	-	-	X	-
3	UNL	F	477	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22350 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 oxidoreductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	Se	0	3	0
			3487	2208	600	671	2	6			
1	B	465	Total	C	N	O	S	Se	0	4	0
			3493	2212	602	671	2	6			
1	C	465	Total	C	N	O	S	Se	0	5	0
			3499	2215	602	674	2	6			
1	D	465	Total	C	N	O	S	Se	0	5	0
			3501	2216	609	668	2	6			
1	E	465	Total	C	N	O	S	Se	0	6	0
			3509	2220	608	673	2	6			
1	F	465	Total	C	N	O	S	Se	0	4	0
			3498	2213	605	672	2	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q6NAV4
B	0	GLY	-	expression tag	UNP Q6NAV4
C	0	GLY	-	expression tag	UNP Q6NAV4
D	0	GLY	-	expression tag	UNP Q6NAV4
E	0	GLY	-	expression tag	UNP Q6NAV4
F	0	GLY	-	expression tag	UNP Q6NAV4

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



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

- Molecule 3 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

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

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		

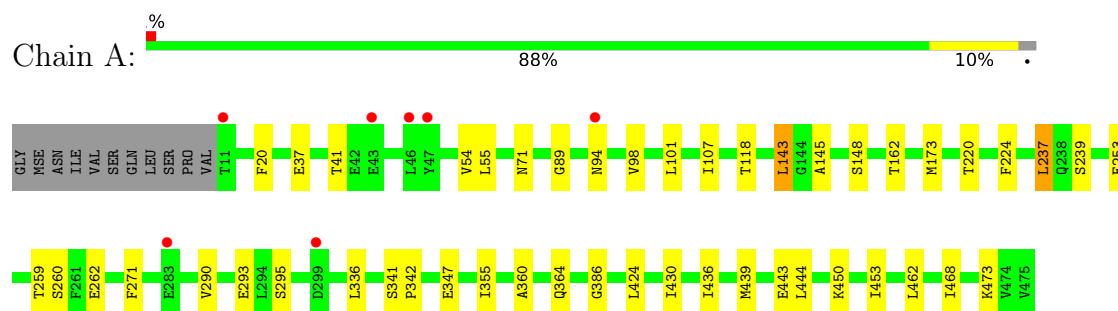
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	203	Total	O	0	0
			203	203		
5	B	168	Total	O	0	0
			168	168		
5	C	126	Total	O	0	0
			126	126		
5	D	143	Total	O	0	0
			143	143		
5	E	145	Total	O	0	0
			145	145		
5	F	134	Total	O	0	0
			134	134		

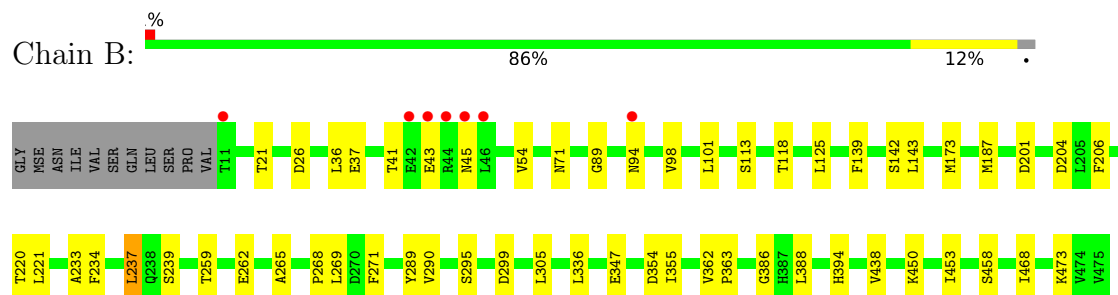
3 Residue-property plots [i](#)

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.

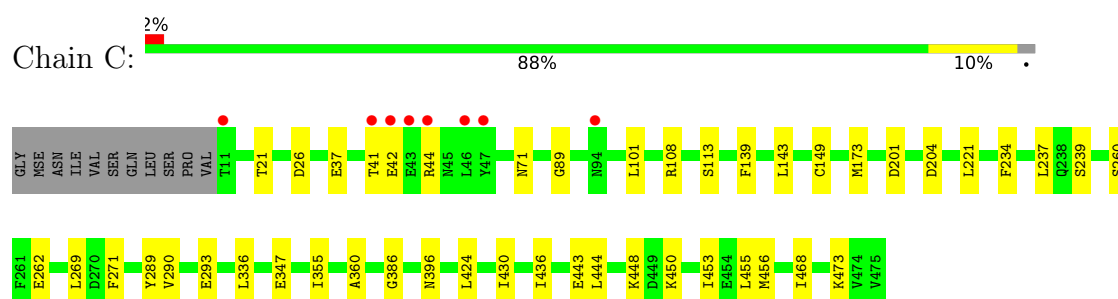
• Molecule 1: Putative oxidoreductase



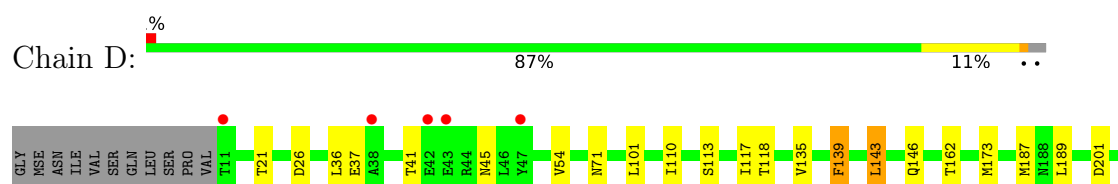
• Molecule 1: Putative oxidoreductase

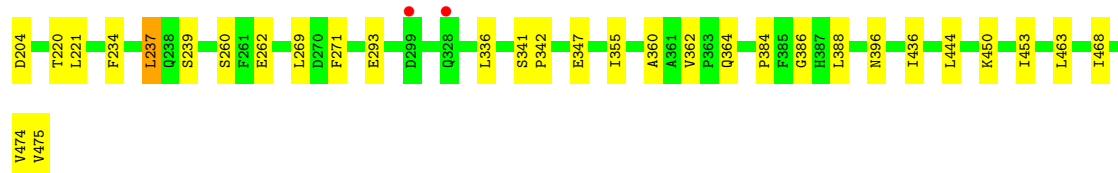


• Molecule 1: Putative oxidoreductase

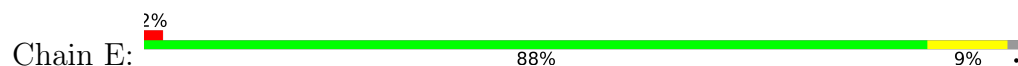


• Molecule 1: Putative oxidoreductase

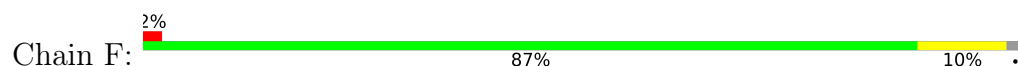




● Molecule 1: Putative oxidoreductase



● Molecule 1: Putative oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	146.09Å 250.73Å 251.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.36 – 2.57 49.36 – 2.57	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.36-2.57) 98.9 (49.36-2.57)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.193 , 0.227 0.190 , 0.220	Depositor DCC
R_{free} test set	7270 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 29.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22350	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.01 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.3365e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UNL, PO4, FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.85	0/3549	0.84	6/4814 (0.1%)
1	B	0.84	1/3558 (0.0%)	0.83	4/4826 (0.1%)
1	C	0.85	0/3567	0.84	3/4838 (0.1%)
1	D	0.84	0/3569	0.85	4/4840 (0.1%)
1	E	0.85	0/3580	0.85	3/4855 (0.1%)
1	F	0.84	0/3563	0.83	1/4833 (0.0%)
All	All	0.84	1/21386 (0.0%)	0.84	21/29006 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	43	GLU	N-CA	5.04	1.52	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	239	SER	N-CA-C	7.36	114.84	108.22
1	E	239	SER	N-CA-C	7.29	114.78	108.22
1	A	239	SER	N-CA-C	7.03	114.55	108.22
1	B	94	ASN	N-CA-C	6.81	119.12	110.61
1	D	239	SER	N-CA-C	6.70	114.25	108.22
1	B	386	GLY	N-CA-C	6.05	118.74	110.69
1	A	94	ASN	N-CA-C	5.93	118.53	110.06
1	B	239	SER	N-CA-C	5.90	113.53	108.22
1	E	386	GLY	N-CA-C	5.75	118.34	110.69
1	C	386	GLY	N-CA-C	5.66	118.21	110.69
1	D	386	GLY	N-CA-C	5.59	118.69	110.80
1	E	107	ILE	N-CA-C	-5.52	99.79	108.23
1	A	386	GLY	N-CA-C	5.46	118.50	110.80
1	C	239	SER	N-CA-C	5.42	113.10	108.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	108	ARG	N-CA-C	5.32	117.16	111.36
1	A	107	ILE	N-CA-C	-5.28	100.29	107.99
1	A	439	MSE	N-CA-C	5.17	116.61	111.07
1	A	143	LEU	N-CA-CB	-5.16	103.41	111.56
1	D	139	PHE	CA-C-N	5.11	124.72	119.56
1	D	139	PHE	C-N-CA	5.11	124.72	119.56
1	B	394	HIS	N-CA-C	-5.07	100.82	108.67

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3487	0	3506	29	0
1	B	3493	0	3516	32	0
1	C	3499	0	3520	30	0
1	D	3501	0	3539	31	0
1	E	3509	0	3540	24	0
1	F	3498	0	3522	31	0
2	A	53	0	31	3	0
2	B	53	0	31	3	0
2	C	53	0	31	4	0
2	D	53	0	31	3	0
2	E	53	0	31	2	0
2	F	53	0	31	2	0
3	A	6	0	0	3	0
3	B	6	0	0	4	0
3	C	6	0	0	4	0
3	D	6	0	0	4	0
3	E	6	0	0	3	0
3	F	6	0	0	2	0
4	A	15	0	0	0	0
4	B	15	0	0	0	0
4	C	15	0	0	1	0
4	D	15	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	15	0	0	0	0
4	F	15	0	0	0	0
5	A	203	0	0	3	0
5	B	168	0	0	2	0
5	C	126	0	0	2	0
5	D	143	0	0	1	0
5	E	145	0	0	2	0
5	F	134	0	0	0	0
All	All	22350	0	21329	201	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 5.

All (201) 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)
3:F:477:UNL:O1	3:F:477:UNL:O3	1.64	1.15
3:B:477:UNL:O2	3:B:477:UNL:O3	1.66	1.12
3:C:477:UNL:O2	3:C:477:UNL:O3	1.68	1.11
3:D:477:UNL:O3	3:D:477:UNL:O4	1.78	0.99
3:A:477:UNL:O5	3:A:477:UNL:O6	1.85	0.95
3:D:477:UNL:O3	3:D:477:UNL:O2	1.90	0.89
3:E:477:UNL:O4	3:E:477:UNL:O6	1.93	0.86
3:E:477:UNL:O4	3:E:477:UNL:O5	1.96	0.84
3:B:477:UNL:O2	3:B:477:UNL:O1	1.97	0.82
1:A:173:MSE:HA	1:A:173:MSE:HE2	1.72	0.72
3:C:477:UNL:O2	3:C:477:UNL:O1	2.08	0.70
1:D:271:PHE:CZ	1:D:347:GLU:HG2	2.28	0.69
1:E:271:PHE:CZ	1:E:347:GLU:HG2	2.28	0.69
1:F:173:MSE:HA	1:F:173:MSE:HE2	1.75	0.69
1:D:173:MSE:HE2	1:D:173:MSE:HA	1.74	0.68
1:C:355:ILE:C	1:C:355:ILE:HD12	2.19	0.68
1:F:101:LEU:HD13	2:F:476:FAD:N6A	2.10	0.67
1:D:101:LEU:HD13	2:D:476:FAD:N6A	2.08	0.67
1:F:355:ILE:HD12	1:F:355:ILE:C	2.19	0.66
1:A:271:PHE:CZ	1:A:347:GLU:HG2	2.31	0.65
2:F:476:FAD:N1	2:F:476:FAD:H2'	2.11	0.65
2:A:476:FAD:H2'	2:A:476:FAD:N1	2.11	0.64
3:B:477:UNL:O4	3:B:477:UNL:O6	2.15	0.64
1:B:173:MSE:HA	1:B:173:MSE:HE2	1.80	0.64
1:F:271:PHE:CZ	1:F:347:GLU:HG2	2.33	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:191:SER:H	1:F:220[B]:THR:HG21	1.62	0.63
1:A:101:LEU:HD13	2:A:476:FAD:N6A	2.12	0.63
1:C:271:PHE:CZ	1:C:347:GLU:HG2	2.34	0.62
1:C:450:LYS:O	1:C:453:ILE:HG22	2.00	0.62
2:C:476:FAD:N1	2:C:476:FAD:H2'	2.14	0.62
3:C:477:UNL:O4	3:C:477:UNL:O5	2.17	0.62
1:C:336:LEU:C	1:C:336:LEU:HD23	2.24	0.62
1:E:173:MSE:HA	1:E:173:MSE:HE2	1.82	0.61
2:B:476:FAD:H2'	2:B:476:FAD:N1	2.16	0.61
1:F:269:LEU:C	1:F:269:LEU:HD23	2.25	0.61
1:D:436:ILE:HG13	1:D:444:LEU:HD22	1.83	0.61
1:A:355:ILE:C	1:A:355:ILE:HD12	2.27	0.60
2:D:476:FAD:H2'	2:D:476:FAD:N1	2.16	0.60
1:F:450:LYS:O	1:F:453:ILE:HG22	2.02	0.60
1:B:101:LEU:HD13	2:B:476:FAD:N6A	2.16	0.60
2:E:476:FAD:H2'	2:E:476:FAD:N1	2.16	0.59
1:B:89:GLY:HA2	1:B:473:LYS:HD3	1.84	0.59
1:A:162:THR:HG23	1:A:262:GLU:OE2	2.02	0.58
1:A:450:LYS:O	1:A:453:ILE:HG22	2.04	0.58
1:B:355:ILE:HD12	1:B:355:ILE:C	2.28	0.58
3:F:477:UNL:O3	3:F:477:UNL:O4	2.21	0.58
1:C:473:LYS:NZ	5:C:1051:HOH:O	2.36	0.58
1:D:355:ILE:C	1:D:355:ILE:HD12	2.28	0.58
1:F:190:LEU:HD22	1:F:220[A]:THR:HG23	1.85	0.57
1:A:336:LEU:C	1:A:336:LEU:HD23	2.30	0.57
1:B:237:LEU:HD12	1:B:237:LEU:N	2.20	0.57
1:C:37:GLU:O	1:C:41:THR:HG22	2.05	0.57
1:D:396:ASN:ND2	4:D:493:PO4:O2	2.38	0.56
1:D:36:LEU:CD2	1:D:54:VAL:HG23	2.35	0.56
1:E:424[B]:LEU:HD12	5:E:858:HOH:O	2.05	0.56
1:D:187:MSE:HE3	1:D:189:LEU:HD12	1.87	0.56
1:C:139:PHE:CZ	1:C:221:LEU:HD13	2.41	0.55
1:A:462:LEU:HD21	1:B:458:SER:HB3	1.88	0.55
1:A:54:VAL:HG22	1:A:98:VAL:HB	1.89	0.55
1:A:118:THR:OG1	1:A:220:THR:HG22	2.07	0.55
1:E:269:LEU:HD13	1:E:289:TYR:CE1	2.42	0.55
1:F:71:ASN:HA	1:F:468:ILE:HD13	1.89	0.55
1:E:89:GLY:HA2	1:E:473:LYS:HD3	1.89	0.54
1:F:36:LEU:CD2	1:F:54:VAL:HG23	2.36	0.54
1:A:143:LEU:HD23	1:A:145:ALA:H	1.72	0.54
1:F:474:VAL:HG12	1:F:475:VAL:HG13	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:GLY:HA2	1:C:473:LYS:HD3	1.89	0.54
3:D:477:UNL:O3	3:D:477:UNL:O5	2.26	0.54
1:B:139:PHE:CZ	1:B:221:LEU:HD13	2.43	0.54
1:D:139:PHE:CZ	1:D:221:LEU:HD13	2.43	0.54
3:B:477:UNL:O3	3:B:477:UNL:O4	2.25	0.53
1:E:450:LYS:O	1:E:453:ILE:HG22	2.08	0.53
1:C:269:LEU:HD13	1:C:289:TYR:CE1	2.43	0.53
1:E:21:THR:HG23	1:E:26:ASP:HA	1.90	0.53
1:B:336:LEU:C	1:B:336:LEU:HD23	2.35	0.52
1:C:396:ASN:ND2	4:C:492:PO4:O3	2.42	0.52
1:F:336:LEU:C	1:F:336:LEU:HD23	2.35	0.52
1:D:260:SER:HB2	1:D:293:GLU:HB3	1.92	0.52
1:E:11:THR:HG23	5:E:938:HOH:O	2.08	0.51
1:E:101:LEU:HD13	2:E:476:FAD:N6A	2.25	0.51
1:E:355:ILE:HD12	1:E:355:ILE:C	2.34	0.51
1:F:143:LEU:HD11	1:F:149:CYS:SG	2.51	0.51
1:F:293:GLU:C	1:F:294:LEU:HD12	2.36	0.51
1:A:89:GLY:HA2	1:A:473:LYS:HD3	1.94	0.50
1:A:37:GLU:O	1:A:41:THR:HG22	2.11	0.50
1:F:237:LEU:HD12	1:F:237:LEU:N	2.26	0.50
3:E:477:UNL:O1	3:E:477:UNL:O3	2.30	0.50
1:C:42[B]:GLU:OE1	1:C:44:ARG:N	2.43	0.50
1:E:336:LEU:C	1:E:336:LEU:HD23	2.37	0.50
1:A:473:LYS:NZ	5:A:845:HOH:O	2.45	0.50
1:E:448:LYS:HE2	1:E:456:MSE:HE1	1.93	0.50
1:D:118:THR:OG1	1:D:220[A]:THR:HG22	2.12	0.50
1:B:125:LEU:CD2	1:B:143:LEU:HD13	2.41	0.49
1:E:37:GLU:O	1:E:41:THR:HG22	2.12	0.49
1:B:362:VAL:HG11	1:B:388:LEU:HD13	1.93	0.49
1:D:450:LYS:O	1:D:453:ILE:HG22	2.12	0.49
1:F:201:ASP:OD1	1:F:201:ASP:C	2.56	0.49
1:A:424[B]:LEU:HD12	5:A:1088:HOH:O	2.12	0.49
1:B:269:LEU:C	1:B:269:LEU:HD23	2.36	0.49
1:C:143:LEU:HD11	1:C:149:CYS:SG	2.53	0.49
1:F:191:SER:O	1:F:220[B]:THR:HG21	2.13	0.49
1:F:37:GLU:O	1:F:41:THR:HG22	2.12	0.49
1:F:430:ILE:HD13	1:F:443:GLU:HG3	1.95	0.49
1:B:262:GLU:O	1:B:290:VAL:HA	2.13	0.48
1:D:71:ASN:HA	1:D:468:ILE:HD13	1.96	0.48
1:C:101:LEU:HD13	2:C:476:FAD:N6A	2.29	0.48
1:D:201:ASP:OD2	1:D:204:ASP:OD2	2.32	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:430:ILE:HD13	1:C:443:GLU:HG3	1.96	0.47
1:B:201:ASP:OD2	1:B:204:ASP:OD2	2.33	0.47
3:D:477:UNL:O4	3:D:477:UNL:O6	2.32	0.47
3:A:477:UNL:O2	3:A:477:UNL:O4	2.32	0.47
1:B:36:LEU:CD2	1:B:54:VAL:HG23	2.44	0.47
1:B:71:ASN:HA	1:B:468:ILE:HD13	1.96	0.47
1:F:448:LYS:HE2	1:F:456:MSE:HE1	1.95	0.47
1:A:71:ASN:HA	1:A:468:ILE:HD13	1.96	0.47
1:D:162:THR:HG23	1:D:262:GLU:OE2	2.15	0.47
1:A:259:THR:HG21	1:A:295:SER:HB2	1.98	0.46
1:C:262:GLU:O	1:C:290:VAL:HA	2.15	0.46
1:C:424[B]:LEU:HD12	5:C:1032:HOH:O	2.15	0.46
1:C:336:LEU:HD23	1:C:336:LEU:O	2.15	0.46
1:F:201:ASP:OD2	1:F:204:ASP:OD2	2.33	0.46
1:B:37:GLU:O	1:B:41:THR:HG22	2.16	0.46
1:D:237:LEU:HD12	1:D:237:LEU:N	2.30	0.46
1:D:101:LEU:CD1	2:D:476:FAD:N6A	2.79	0.46
1:F:259:THR:HG21	1:F:295:SER:HB2	1.97	0.46
1:E:269:LEU:C	1:E:269:LEU:HD23	2.40	0.46
1:E:430:ILE:HD13	1:E:443:GLU:HG3	1.98	0.46
1:B:362:VAL:HB	1:B:363:PRO:HD3	1.97	0.46
1:F:262:GLU:O	1:F:290:VAL:HA	2.16	0.45
1:D:364:GLN:HG3	5:D:516:HOH:O	2.17	0.45
1:E:143:LEU:HD11	1:E:149:CYS:SG	2.56	0.45
1:E:143:LEU:O	1:E:146:GLN:HG3	2.17	0.45
1:E:260:SER:HB2	1:E:293:GLU:HB3	1.98	0.45
1:A:341:SER:HB3	1:A:342:PRO:CD	2.47	0.45
1:A:237:LEU:HD12	1:A:237:LEU:N	2.32	0.45
1:B:473:LYS:NZ	5:B:1320:HOH:O	2.50	0.45
1:D:21:THR:HG23	1:D:26:ASP:HA	1.97	0.45
1:C:201:ASP:OD2	1:C:204:ASP:OD2	2.35	0.45
1:C:113:SER:HB2	1:D:360:ALA:HB2	1.99	0.45
1:B:259:THR:HG21	1:B:295:SER:HB2	1.99	0.44
1:C:201:ASP:OD1	1:C:201:ASP:C	2.60	0.44
1:E:269:LEU:HD13	1:E:289:TYR:CD1	2.53	0.44
1:A:20:PHE:HB3	1:A:55:LEU:HD11	1.99	0.44
1:F:372:ALA:HB1	1:F:418:VAL:CG1	2.47	0.44
1:C:71:ASN:HA	1:C:468:ILE:HD13	1.99	0.44
1:C:448:LYS:HE2	1:C:456:MSE:HE1	1.98	0.44
2:C:476:FAD:N1	2:C:476:FAD:C2'	2.80	0.44
1:A:262:GLU:O	1:A:290:VAL:HA	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:MSE:HE1	1:A:224:PHE:CZ	2.53	0.44
1:B:118:THR:OG1	1:B:220[A]:THR:HG22	2.17	0.44
1:B:54:VAL:HG22	1:B:98:VAL:HB	1.98	0.44
1:B:143:LEU:N	1:B:143:LEU:HD12	2.33	0.44
1:B:269:LEU:HD13	1:B:289:TYR:CE1	2.53	0.44
1:D:336:LEU:C	1:D:336:LEU:HD23	2.42	0.44
1:A:260:SER:HB2	1:A:293:GLU:HB3	1.99	0.43
1:C:260:SER:HB2	1:C:293:GLU:HB3	2.00	0.43
1:D:37:GLU:O	1:D:41:THR:HG22	2.18	0.43
2:B:476:FAD:N1	2:B:476:FAD:C2'	2.80	0.43
1:D:362:VAL:HG11	1:D:388:LEU:HD13	2.00	0.43
1:F:436:ILE:HG13	1:F:444:LEU:HD22	1.99	0.43
1:F:276:ALA:HB1	1:F:339:GLU:OE1	2.17	0.43
1:C:455:LEU:HD22	1:D:463:LEU:HD11	2.01	0.43
1:D:143:LEU:O	1:D:146:GLN:HG3	2.18	0.43
1:C:355:ILE:C	1:C:355:ILE:CD1	2.86	0.43
3:C:477:UNL:O3	3:C:477:UNL:O4	2.37	0.43
1:D:110:ILE:HD13	1:D:117:ILE:HG13	2.01	0.43
1:E:314[A]:GLU:HA	1:E:314[A]:GLU:OE1	2.19	0.42
1:F:54:VAL:HG22	1:F:98:VAL:HB	2.01	0.42
1:A:430:ILE:HD13	1:A:443:GLU:HG3	2.00	0.42
1:B:187:MSE:HE1	1:B:206:PHE:CE2	2.55	0.42
1:E:372:ALA:HB1	1:E:418:VAL:CG1	2.50	0.42
1:F:53:LEU:HD21	1:F:55:LEU:HD21	2.01	0.42
1:A:360:ALA:HB2	1:B:113:SER:HB2	2.01	0.42
1:B:271:PHE:CZ	1:B:347:GLU:HG2	2.54	0.42
1:A:173:MSE:HE1	1:A:224:PHE:CE1	2.54	0.42
1:A:364:GLN:HG3	5:A:537:HOH:O	2.18	0.42
1:B:450:LYS:O	1:B:453:ILE:HG22	2.20	0.42
1:A:173:MSE:HE2	1:A:173:MSE:CA	2.47	0.42
1:B:265:ALA:O	1:B:268:PRO:HG2	2.20	0.42
1:C:436:ILE:HG13	1:C:444:LEU:HD22	2.02	0.41
1:B:142:SER:C	1:B:143:LEU:HD12	2.44	0.41
1:E:143:LEU:HD12	1:E:145:ALA:H	1.84	0.41
1:B:233:ALA:HB2	1:B:305:LEU:HD21	2.02	0.41
1:F:355:ILE:C	1:F:355:ILE:CD1	2.88	0.41
1:D:269:LEU:C	1:D:269:LEU:HD23	2.46	0.41
1:D:474:VAL:HG12	1:D:475:VAL:HG13	2.02	0.41
1:B:21:THR:HG23	1:B:26:ASP:HA	2.02	0.41
1:A:436:ILE:HG13	1:A:444:LEU:HD22	2.03	0.41
1:C:101:LEU:CD1	2:C:476:FAD:N6A	2.82	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:LEU:C	1:C:336:LEU:CD2	2.92	0.41
1:C:21:THR:HG23	1:C:26:ASP:HA	2.02	0.41
1:C:360:ALA:HB2	1:D:113:SER:HB2	2.03	0.41
1:E:57:PRO:HD2	1:E:100:SER:O	2.21	0.41
1:F:143:LEU:O	1:F:146:GLN:HG3	2.21	0.41
2:A:476:FAD:N1	2:A:476:FAD:C2'	2.79	0.41
1:D:110:ILE:HG21	1:D:135:VAL:HG21	2.03	0.41
1:E:443:GLU:O	1:E:447:VAL:HG22	2.21	0.41
1:D:341:SER:HB3	1:D:342:PRO:CD	2.50	0.40
1:B:354:ASP:HB3	5:B:1236:HOH:O	2.20	0.40
1:F:452:ALA:O	1:F:456:MSE:HG3	2.22	0.40
3:A:477:UNL:O5	3:A:477:UNL:O4	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	466/476 (98%)	453 (97%)	13 (3%)	0	100	100
1	B	467/476 (98%)	454 (97%)	12 (3%)	1 (0%)	43	63
1	C	468/476 (98%)	456 (97%)	12 (3%)	0	100	100
1	D	468/476 (98%)	450 (96%)	16 (3%)	2 (0%)	30	49
1	E	469/476 (98%)	456 (97%)	11 (2%)	2 (0%)	30	49
1	F	467/476 (98%)	453 (97%)	12 (3%)	2 (0%)	30	49
All	All	2805/2856 (98%)	2722 (97%)	76 (3%)	7 (0%)	36	63

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	45	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	45	ASN
1	F	146	GLN
1	D	45	ASN
1	D	384	PRO
1	E	384	PRO
1	F	384	PRO

5.3.2 Protein sidechains ⓘ

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	362/372 (97%)	358 (99%)	4 (1%)	65	83
1	B	363/372 (98%)	359 (99%)	4 (1%)	65	83
1	C	365/372 (98%)	362 (99%)	3 (1%)	73	87
1	D	365/372 (98%)	362 (99%)	3 (1%)	73	87
1	E	366/372 (98%)	358 (98%)	8 (2%)	45	70
1	F	364/372 (98%)	361 (99%)	3 (1%)	73	87
All	All	2185/2232 (98%)	2160 (99%)	25 (1%)	65	83

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	SER
1	A	237	LEU
1	A	253[A]	GLU
1	A	253[B]	GLU
1	B	234	PHE
1	B	237	LEU
1	B	299	ASP
1	B	438	VAL
1	C	173	MSE
1	C	234	PHE
1	C	237	LEU
1	D	143	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	234	PHE
1	D	237	LEU
1	E	94	ASN
1	E	173	MSE
1	E	228[A]	ARG
1	E	228[B]	ARG
1	E	234	PHE
1	E	237	LEU
1	E	283	GLU
1	E	299	ASP
1	F	94	ASN
1	F	234	PHE
1	F	237	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	GLN
1	A	154	ASN
1	B	154	ASN
1	C	94	ASN
1	D	330	GLN
1	D	344	GLN
1	D	396	ASN
1	E	251	GLN
1	E	330	GLN
1	F	251	GLN
1	F	396	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 30 ligands modelled in this entry, 6 are unknown - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PO4	A	478	-	4,4,4	0.96	0	6,6,6	0.53	0
4	PO4	E	494	-	4,4,4	0.87	0	6,6,6	0.48	0
2	FAD	A	476	-	58,58,58	1.37	11 (18%)	85,89,89	1.63	20 (23%)
2	FAD	C	476	-	58,58,58	1.23	7 (12%)	85,89,89	1.70	20 (23%)
4	PO4	B	479	-	4,4,4	0.87	0	6,6,6	0.37	0
4	PO4	C	480	-	4,4,4	0.80	0	6,6,6	0.53	0
2	FAD	D	476	-	58,58,58	1.28	8 (13%)	85,89,89	1.66	18 (21%)
4	PO4	B	485	-	4,4,4	0.73	0	6,6,6	0.70	0
4	PO4	D	487	-	4,4,4	0.89	0	6,6,6	0.64	0
4	PO4	C	492	-	4,4,4	1.08	0	6,6,6	0.56	0
4	PO4	F	495	-	4,4,4	1.01	0	6,6,6	0.63	0
4	PO4	A	484	-	4,4,4	0.86	0	6,6,6	0.42	0
4	PO4	E	482	-	4,4,4	0.97	0	6,6,6	0.43	0
4	PO4	C	486	-	4,4,4	0.82	0	6,6,6	0.70	0
2	FAD	B	476	-	58,58,58	1.20	8 (13%)	85,89,89	1.65	19 (22%)
4	PO4	B	491	-	4,4,4	1.24	0	6,6,6	0.63	0
2	FAD	F	476	-	58,58,58	1.20	7 (12%)	85,89,89	1.63	19 (22%)
4	PO4	E	488	-	4,4,4	0.84	0	6,6,6	0.42	0
4	PO4	D	493	-	4,4,4	0.92	0	6,6,6	0.60	0
2	FAD	E	476	-	58,58,58	1.30	9 (15%)	85,89,89	1.62	21 (24%)
4	PO4	D	481	-	4,4,4	0.88	0	6,6,6	0.48	0
4	PO4	F	489	-	4,4,4	0.73	0	6,6,6	0.49	0
4	PO4	F	483	-	4,4,4	0.85	0	6,6,6	0.63	0
4	PO4	A	490	-	4,4,4	1.00	0	6,6,6	0.61	0

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
2	FAD	D	476	-	-	9/34/50/50	0/6/6/6
2	FAD	E	476	-	-	11/34/50/50	0/6/6/6
2	FAD	A	476	-	-	11/34/50/50	0/6/6/6
2	FAD	C	476	-	-	9/34/50/50	0/6/6/6
2	FAD	F	476	-	-	11/34/50/50	0/6/6/6
2	FAD	B	476	-	-	11/34/50/50	0/6/6/6

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	476	FAD	C4X-N5	4.23	1.39	1.30
2	C	476	FAD	C4X-N5	4.16	1.39	1.30
2	D	476	FAD	C4X-N5	3.72	1.38	1.30
2	A	476	FAD	C2'-C3'	-3.69	1.47	1.53
2	B	476	FAD	C4X-N5	3.58	1.38	1.30
2	A	476	FAD	C2A-N1A	3.28	1.39	1.33
2	A	476	FAD	C4X-N5	3.27	1.37	1.30
2	E	476	FAD	C2'-C3'	-3.27	1.47	1.53
2	E	476	FAD	C4X-N5	3.21	1.37	1.30
2	E	476	FAD	C2A-N1A	3.10	1.39	1.33
2	B	476	FAD	C2'-C3'	-3.05	1.48	1.53
2	D	476	FAD	C2A-N1A	3.00	1.39	1.33
2	E	476	FAD	C10-N1	2.93	1.39	1.33
2	D	476	FAD	C8A-N7A	2.93	1.37	1.31
2	C	476	FAD	C2A-N1A	2.84	1.39	1.33
2	A	476	FAD	C10-N1	2.80	1.38	1.33
2	D	476	FAD	C10-N1	2.78	1.38	1.33
2	D	476	FAD	C2'-C3'	-2.76	1.48	1.53
2	D	476	FAD	C1'-N10	2.73	1.54	1.47
2	A	476	FAD	C5A-N7A	-2.73	1.34	1.39
2	F	476	FAD	C2'-C3'	-2.72	1.48	1.53
2	A	476	FAD	C1'-N10	2.65	1.54	1.47
2	E	476	FAD	C1'-N10	2.65	1.54	1.47
2	F	476	FAD	C10-N1	2.61	1.38	1.33
2	C	476	FAD	C10-N1	2.57	1.38	1.33
2	B	476	FAD	C5A-N7A	-2.46	1.34	1.39
2	B	476	FAD	C2A-N1A	2.46	1.38	1.33
2	C	476	FAD	C5A-N7A	-2.45	1.34	1.39
2	F	476	FAD	C8A-N7A	2.38	1.36	1.31
2	F	476	FAD	C1'-N10	2.34	1.53	1.47
2	E	476	FAD	C5A-N7A	-2.33	1.34	1.39
2	E	476	FAD	C2A-N3A	2.33	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	476	FAD	C1'-C2'	2.31	1.55	1.52
2	D	476	FAD	C2A-N3A	2.30	1.38	1.33
2	B	476	FAD	C10-N1	2.28	1.37	1.33
2	A	476	FAD	P-O3P	2.28	1.62	1.59
2	A	476	FAD	C2A-N3A	2.28	1.38	1.33
2	C	476	FAD	C1'-N10	2.27	1.53	1.47
2	B	476	FAD	C8A-N7A	2.22	1.35	1.31
2	A	476	FAD	PA-O3P	2.17	1.61	1.59
2	C	476	FAD	C2A-N3A	2.16	1.37	1.33
2	B	476	FAD	C1'-C2'	2.11	1.55	1.52
2	B	476	FAD	C1'-N10	2.11	1.53	1.47
2	C	476	FAD	C2'-C3'	-2.11	1.49	1.53
2	A	476	FAD	C8A-N7A	2.10	1.35	1.31
2	A	476	FAD	C1'-C2'	2.09	1.55	1.52
2	E	476	FAD	O4B-C4B	-2.09	1.40	1.45
2	E	476	FAD	PA-O3P	2.07	1.61	1.59
2	F	476	FAD	C2A-N1A	2.06	1.37	1.33
2	F	476	FAD	C4'-C3'	2.05	1.57	1.53

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	476	FAD	N3A-C2A-N1A	-6.05	119.42	128.58
2	F	476	FAD	N3A-C2A-N1A	-5.85	119.72	128.58
2	A	476	FAD	N3A-C2A-N1A	-5.84	119.73	128.58
2	E	476	FAD	N3A-C2A-N1A	-5.76	119.87	128.58
2	D	476	FAD	N3A-C2A-N1A	-5.50	120.26	128.58
2	B	476	FAD	N3A-C2A-N1A	-5.28	120.59	128.58
2	D	476	FAD	C5A-C4A-N3A	-4.37	120.70	126.72
2	B	476	FAD	C5A-C4A-N3A	-4.33	120.76	126.72
2	C	476	FAD	N9A-C8A-N7A	-4.15	108.05	113.94
2	C	476	FAD	C5A-C4A-N3A	-4.06	121.12	126.72
2	E	476	FAD	N9A-C8A-N7A	-3.93	108.35	113.94
2	F	476	FAD	C5A-C4A-N3A	-3.92	121.32	126.72
2	D	476	FAD	N9A-C8A-N7A	-3.84	108.48	113.94
2	C	476	FAD	C4X-C10-N10	3.80	121.92	116.48
2	A	476	FAD	C5A-C4A-N3A	-3.80	121.49	126.72
2	F	476	FAD	N9A-C8A-N7A	-3.69	108.70	113.94
2	F	476	FAD	C2A-N3A-C4A	3.60	120.63	111.83
2	A	476	FAD	N9A-C8A-N7A	-3.56	108.89	113.94
2	E	476	FAD	C5A-C4A-N3A	-3.54	121.83	126.72
2	D	476	FAD	C4X-C10-N10	3.53	121.53	116.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	476	FAD	N9A-C8A-N7A	-3.51	108.95	113.94
2	C	476	FAD	C5A-N7A-C8A	3.43	108.85	103.45
2	A	476	FAD	C4X-C10-N10	3.34	121.26	116.48
2	D	476	FAD	C2A-N3A-C4A	3.32	119.93	111.83
2	E	476	FAD	C4X-C10-N10	3.28	121.18	116.48
2	C	476	FAD	C2A-N3A-C4A	3.26	119.79	111.83
2	B	476	FAD	C4X-C10-N10	3.23	121.11	116.48
2	B	476	FAD	C2A-N3A-C4A	3.20	119.64	111.83
2	D	476	FAD	C5A-N7A-C8A	3.19	108.47	103.45
2	B	476	FAD	C5A-N7A-C8A	3.17	108.43	103.45
2	A	476	FAD	C2A-N3A-C4A	3.15	119.52	111.83
2	F	476	FAD	C4X-C10-N10	3.12	120.95	116.48
2	B	476	FAD	C4-N3-C2	-3.04	120.24	125.64
2	E	476	FAD	C5A-N7A-C8A	3.03	108.21	103.45
2	C	476	FAD	C4-N3-C2	-3.02	120.28	125.64
2	A	476	FAD	C5A-N7A-C8A	3.01	108.18	103.45
2	E	476	FAD	O2A-PA-O3P	2.91	115.14	107.27
2	F	476	FAD	C4-N3-C2	-2.91	120.47	125.64
2	E	476	FAD	C2A-N3A-C4A	2.90	118.91	111.83
2	A	476	FAD	C4-N3-C2	-2.87	120.54	125.64
2	E	476	FAD	C4-N3-C2	-2.87	120.55	125.64
2	C	476	FAD	C10-C4X-N5	-2.87	118.96	124.81
2	D	476	FAD	C4-N3-C2	-2.83	120.62	125.64
2	F	476	FAD	O4'-C4'-C3'	2.80	115.79	109.25
2	D	476	FAD	O3'-C3'-C4'	2.80	115.28	108.93
2	C	476	FAD	N3A-C4A-N9A	2.79	131.91	127.17
2	F	476	FAD	C5A-N7A-C8A	2.78	107.82	103.45
2	C	476	FAD	C4-C4X-N5	2.74	121.99	118.21
2	B	476	FAD	O3'-C3'-C4'	2.70	115.06	108.93
2	B	476	FAD	C4A-C5A-N7A	-2.66	107.53	110.58
2	D	476	FAD	C4A-C5A-N7A	-2.66	107.54	110.58
2	A	476	FAD	O2A-PA-O3P	2.65	114.44	107.27
2	A	476	FAD	C4'-C3'-C2'	-2.62	109.20	113.57
2	E	476	FAD	O3'-C3'-C4'	2.62	114.89	108.93
2	B	476	FAD	C4'-C3'-C2'	-2.62	109.21	113.57
2	B	476	FAD	O2A-PA-O3P	2.60	114.30	107.27
2	C	476	FAD	C4'-C3'-C2'	-2.56	109.31	113.57
2	B	476	FAD	O4'-C4'-C3'	2.54	115.18	109.25
2	B	476	FAD	O4-C4-C4X	-2.51	119.90	126.53
2	E	476	FAD	C4X-C4-N3	2.51	119.64	113.25
2	A	476	FAD	O3'-C3'-C4'	2.49	114.59	108.93
2	A	476	FAD	C4X-C4-N3	2.49	119.58	113.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	476	FAD	C4A-N9A-C8A	2.49	108.35	105.74
2	D	476	FAD	C10-C4X-N5	-2.48	119.75	124.81
2	C	476	FAD	O4'-C4'-C3'	2.47	115.04	109.25
2	A	476	FAD	N3A-C4A-N9A	2.46	131.35	127.17
2	E	476	FAD	C4'-C3'-C2'	-2.43	109.53	113.57
2	C	476	FAD	O2A-PA-O3P	2.43	113.84	107.27
2	D	476	FAD	N3A-C4A-N9A	2.42	131.29	127.17
2	F	476	FAD	O3'-C3'-C4'	2.42	114.44	108.93
2	C	476	FAD	C4X-C4-N3	2.41	119.38	113.25
2	F	476	FAD	C10-C4X-N5	-2.40	119.90	124.81
2	D	476	FAD	C4X-C4-N3	2.40	119.36	113.25
2	C	476	FAD	O3'-C3'-C4'	2.39	114.36	108.93
2	F	476	FAD	C4X-C4-N3	2.39	119.33	113.25
2	C	476	FAD	C10-N1-C2	2.38	122.01	116.85
2	E	476	FAD	C6A-C5A-C4A	2.37	120.41	117.18
2	B	476	FAD	C4X-C4-N3	2.36	119.25	113.25
2	F	476	FAD	C4A-C5A-N7A	-2.33	107.92	110.58
2	E	476	FAD	N3A-C4A-N9A	2.32	131.11	127.17
2	A	476	FAD	C10-C4X-N5	-2.31	120.10	124.81
2	A	476	FAD	O4'-C4'-C3'	2.30	114.63	109.25
2	E	476	FAD	O4-C4-C4X	-2.29	120.50	126.53
2	F	476	FAD	N3A-C4A-N9A	2.27	131.03	127.17
2	B	476	FAD	N3A-C4A-N9A	2.26	131.00	127.17
2	C	476	FAD	C4A-N9A-C8A	2.25	108.10	105.74
2	E	476	FAD	C4X-C10-N1	-2.24	119.10	124.59
2	B	476	FAD	C10-C4X-N5	-2.23	120.26	124.81
2	B	476	FAD	C5A-C4A-N9A	2.23	108.24	105.81
2	F	476	FAD	O2A-PA-O3P	2.23	113.29	107.27
2	C	476	FAD	C4A-C5A-N7A	-2.22	108.04	110.58
2	E	476	FAD	C4A-C5A-N7A	-2.22	108.04	110.58
2	F	476	FAD	O4-C4-C4X	-2.21	120.69	126.53
2	A	476	FAD	C4X-C10-N1	-2.18	119.25	124.59
2	D	476	FAD	C4X-C10-N1	-2.18	119.26	124.59
2	B	476	FAD	C1'-N10-C9A	2.18	124.86	120.63
2	E	476	FAD	O4'-C4'-C3'	2.17	114.34	109.25
2	C	476	FAD	O2-C2-N1	-2.16	118.21	121.80
2	A	476	FAD	C1'-N10-C9A	2.14	124.80	120.63
2	A	476	FAD	O4-C4-C4X	-2.14	120.88	126.53
2	F	476	FAD	C5X-C9A-N10	2.14	119.91	117.97
2	D	476	FAD	O2A-PA-O3P	2.14	113.05	107.27
2	E	476	FAD	C10-C4X-N5	-2.13	120.47	124.81
2	D	476	FAD	C10-N1-C2	2.12	121.43	116.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	476	FAD	C4A-C5A-N7A	-2.11	108.17	110.58
2	C	476	FAD	C4X-C10-N1	-2.11	119.42	124.59
2	D	476	FAD	O4-C4-C4X	-2.11	120.97	126.53
2	D	476	FAD	O4'-C4'-C3'	2.09	114.15	109.25
2	F	476	FAD	C10-N1-C2	2.09	121.36	116.85
2	A	476	FAD	C10-N1-C2	2.08	121.36	116.85
2	F	476	FAD	C4A-N9A-C8A	2.07	107.91	105.74
2	B	476	FAD	C10-N1-C2	2.06	121.30	116.85
2	E	476	FAD	C9A-N10-C10	-2.04	117.64	120.75
2	D	476	FAD	C5A-C4A-N9A	2.02	108.01	105.81
2	A	476	FAD	C6A-C5A-C4A	2.00	119.91	117.18
2	E	476	FAD	C10-N1-C2	2.00	121.18	116.85
2	F	476	FAD	C4X-C10-N1	-2.00	119.69	124.59

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	476	FAD	C2'-C1'-N10-C10
2	A	476	FAD	N10-C1'-C2'-O2'
2	A	476	FAD	N10-C1'-C2'-C3'
2	A	476	FAD	C2'-C3'-C4'-O4'
2	A	476	FAD	O3'-C3'-C4'-O4'
2	A	476	FAD	C3'-C4'-C5'-O5'
2	A	476	FAD	O4'-C4'-C5'-O5'
2	B	476	FAD	N10-C1'-C2'-O2'
2	B	476	FAD	N10-C1'-C2'-C3'
2	B	476	FAD	C2'-C3'-C4'-O4'
2	B	476	FAD	O3'-C3'-C4'-O4'
2	B	476	FAD	C3'-C4'-C5'-O5'
2	B	476	FAD	O4'-C4'-C5'-O5'
2	C	476	FAD	C2'-C1'-N10-C10
2	C	476	FAD	N10-C1'-C2'-O2'
2	C	476	FAD	N10-C1'-C2'-C3'
2	C	476	FAD	C2'-C3'-C4'-O4'
2	C	476	FAD	O3'-C3'-C4'-O4'
2	C	476	FAD	C3'-C4'-C5'-O5'
2	C	476	FAD	O4'-C4'-C5'-O5'
2	D	476	FAD	C2'-C1'-N10-C10
2	D	476	FAD	N10-C1'-C2'-O2'
2	D	476	FAD	N10-C1'-C2'-C3'
2	D	476	FAD	C2'-C3'-C4'-O4'

Continued on next page...

Continued from previous page...

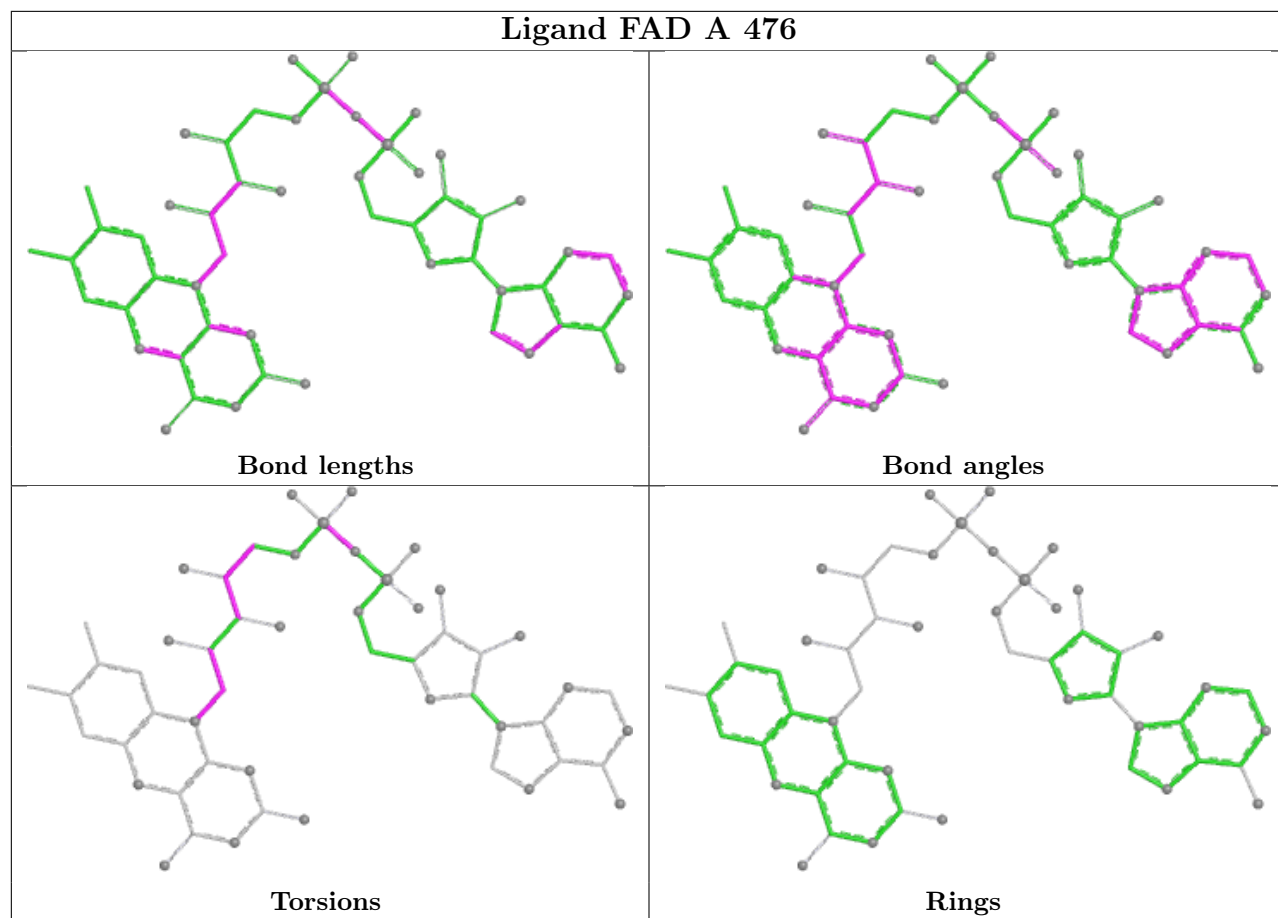
Mol	Chain	Res	Type	Atoms
2	D	476	FAD	O3'-C3'-C4'-O4'
2	D	476	FAD	C3'-C4'-C5'-O5'
2	D	476	FAD	O4'-C4'-C5'-O5'
2	E	476	FAD	C2'-C1'-N10-C10
2	E	476	FAD	N10-C1'-C2'-O2'
2	E	476	FAD	N10-C1'-C2'-C3'
2	E	476	FAD	C2'-C3'-C4'-O4'
2	E	476	FAD	O3'-C3'-C4'-O4'
2	E	476	FAD	C3'-C4'-C5'-O5'
2	E	476	FAD	O4'-C4'-C5'-O5'
2	F	476	FAD	C2'-C1'-N10-C10
2	F	476	FAD	N10-C1'-C2'-O2'
2	F	476	FAD	N10-C1'-C2'-C3'
2	F	476	FAD	C2'-C3'-C4'-O4'
2	F	476	FAD	O3'-C3'-C4'-O4'
2	F	476	FAD	C3'-C4'-C5'-O5'
2	F	476	FAD	O4'-C4'-C5'-O5'
2	A	476	FAD	O3'-C3'-C4'-C5'
2	B	476	FAD	O3'-C3'-C4'-C5'
2	C	476	FAD	O3'-C3'-C4'-C5'
2	D	476	FAD	O3'-C3'-C4'-C5'
2	E	476	FAD	O3'-C3'-C4'-C5'
2	F	476	FAD	O3'-C3'-C4'-C5'
2	A	476	FAD	C2'-C3'-C4'-C5'
2	B	476	FAD	C2'-C3'-C4'-C5'
2	C	476	FAD	C2'-C3'-C4'-C5'
2	D	476	FAD	C2'-C3'-C4'-C5'
2	E	476	FAD	C2'-C3'-C4'-C5'
2	F	476	FAD	C2'-C3'-C4'-C5'
2	B	476	FAD	C2'-C1'-N10-C10
2	B	476	FAD	PA-O3P-P-O2P
2	A	476	FAD	PA-O3P-P-O1P
2	A	476	FAD	PA-O3P-P-O2P
2	E	476	FAD	PA-O3P-P-O1P
2	E	476	FAD	PA-O3P-P-O2P
2	F	476	FAD	PA-O3P-P-O2P
2	B	476	FAD	PA-O3P-P-O1P
2	F	476	FAD	PA-O3P-P-O1P

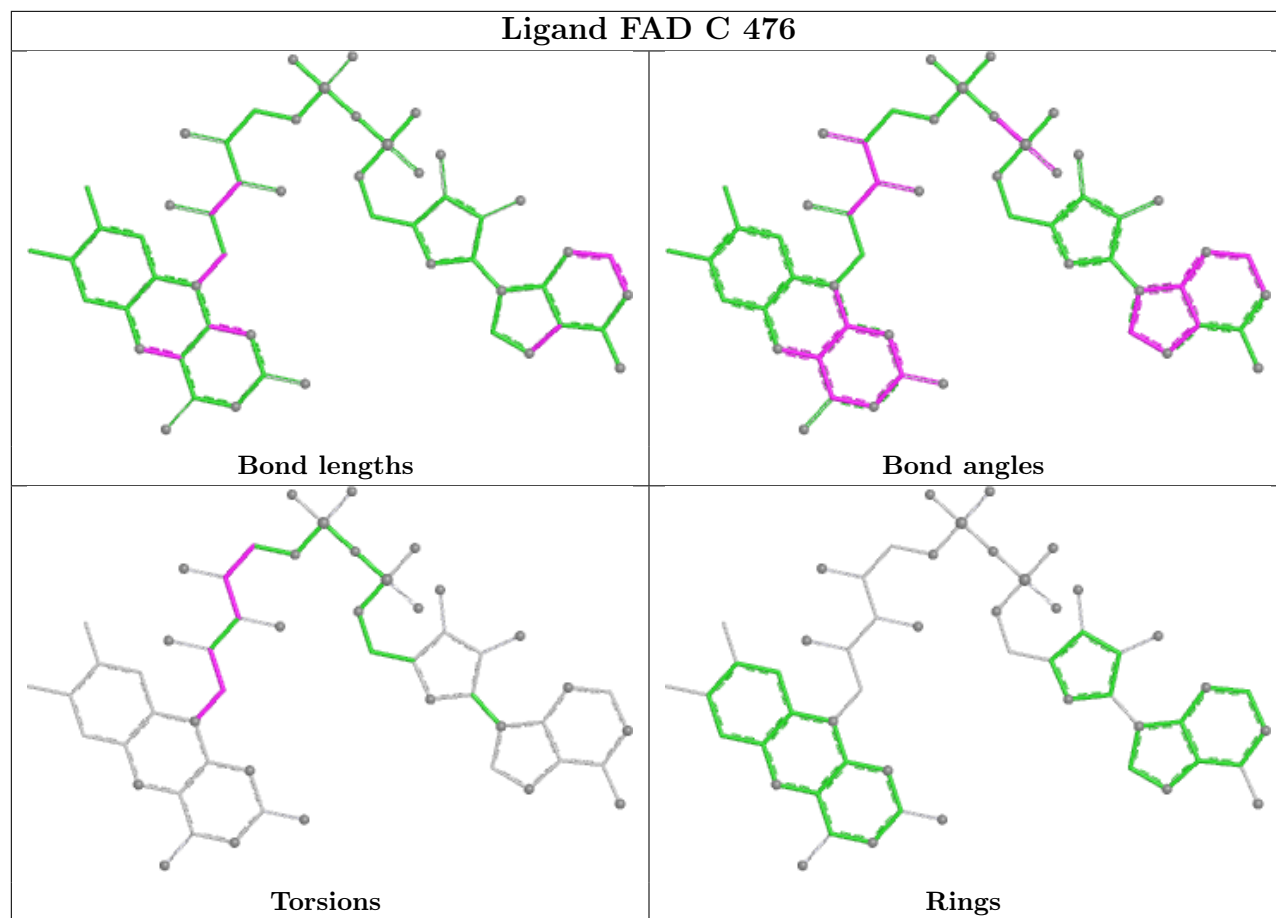
There are no ring outliers.

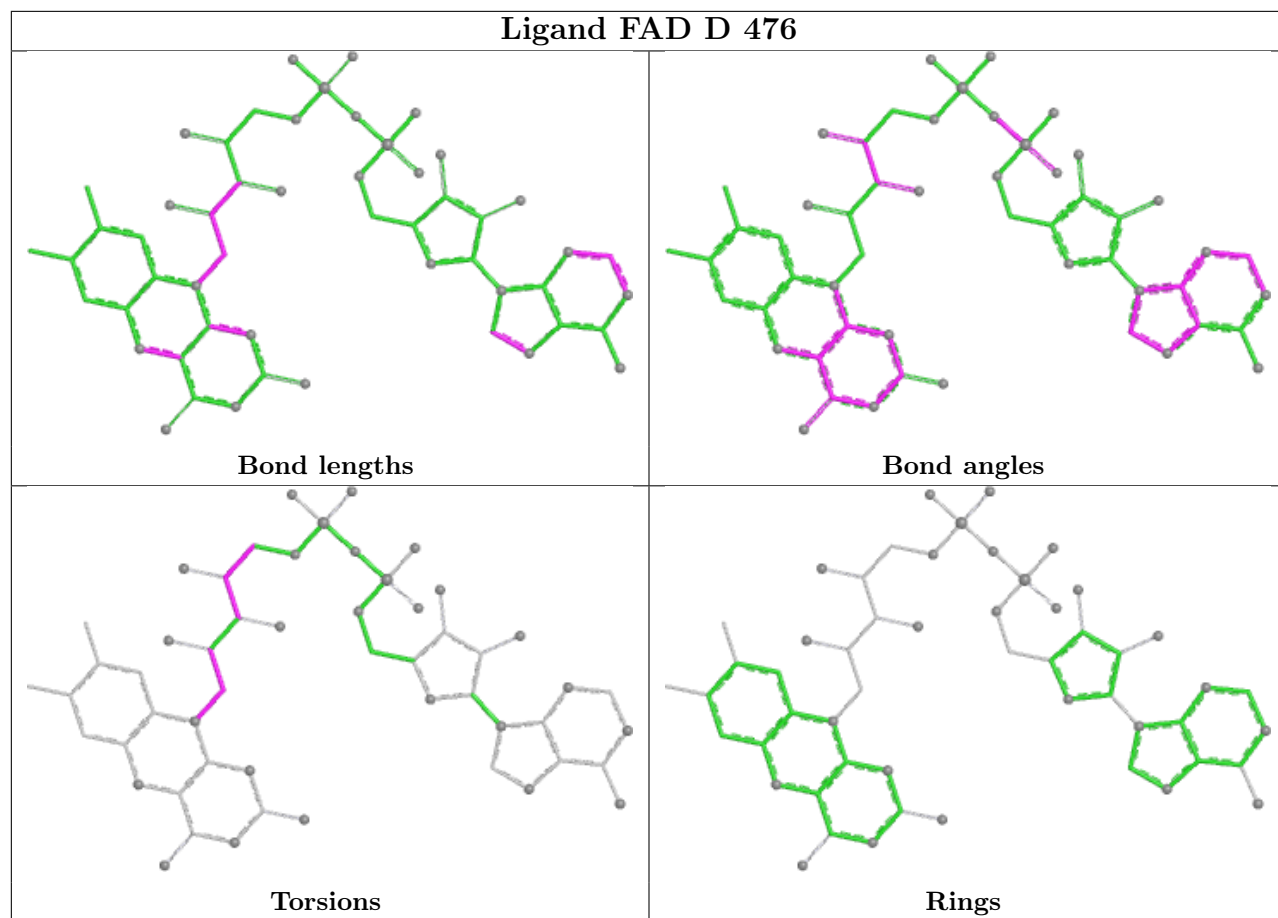
8 monomers are involved in 19 short contacts:

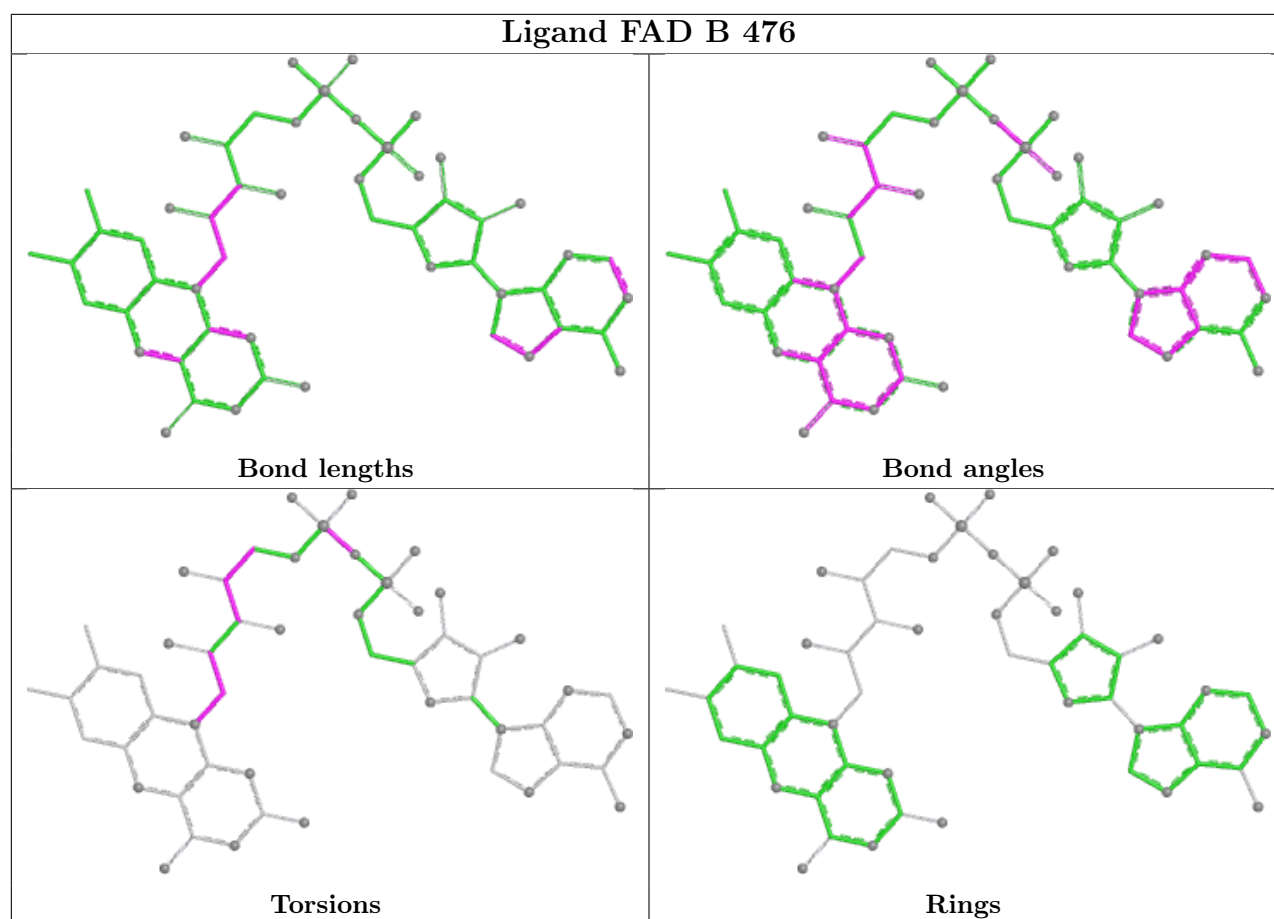
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	476	FAD	3	0
2	C	476	FAD	4	0
2	D	476	FAD	3	0
4	C	492	PO4	1	0
2	B	476	FAD	3	0
2	F	476	FAD	2	0
4	D	493	PO4	1	0
2	E	476	FAD	2	0

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.

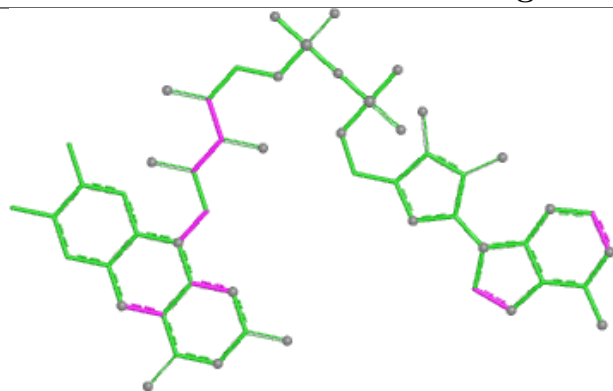




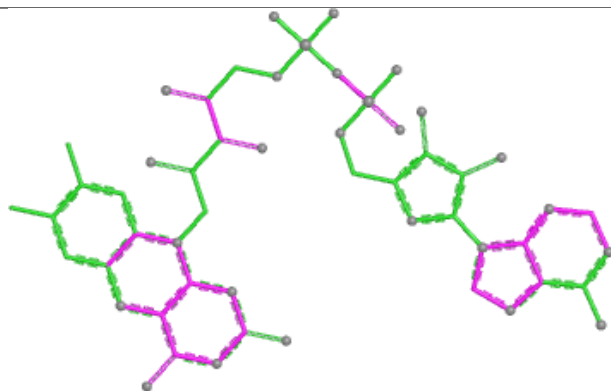




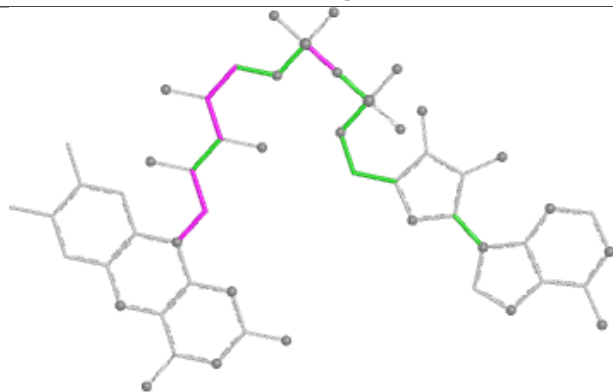
Ligand FAD F 476



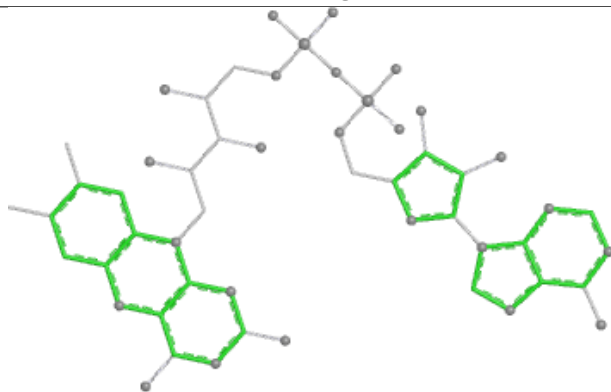
Bond lengths



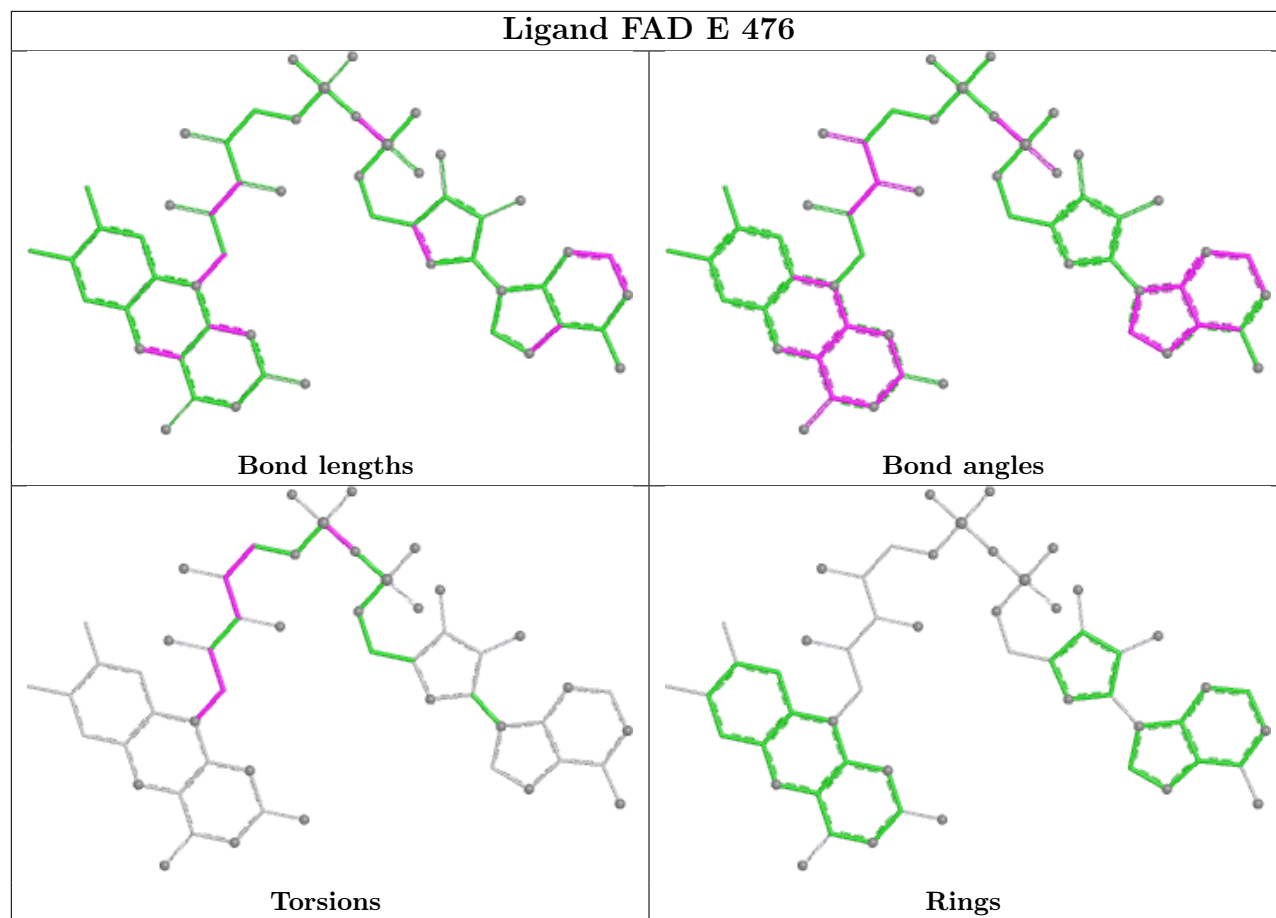
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	459/476 (96%)	-0.25	7 (1%) 72 69	17, 35, 54, 72	3 (0%)
1	B	459/476 (96%)	-0.22	7 (1%) 72 69	17, 36, 56, 73	4 (0%)
1	C	459/476 (96%)	-0.11	8 (1%) 69 65	18, 38, 58, 76	5 (1%)
1	D	459/476 (96%)	-0.17	7 (1%) 72 69	18, 37, 57, 75	5 (1%)
1	E	459/476 (96%)	-0.20	10 (2%) 62 58	17, 36, 55, 72	6 (1%)
1	F	459/476 (96%)	-0.11	9 (1%) 65 61	17, 38, 59, 77	4 (0%)
All	All	2754/2856 (96%)	-0.18	48 (1%) 69 65	17, 37, 57, 77	27 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	43	GLU	7.9
1	F	43	GLU	6.9
1	D	43	GLU	6.5
1	E	43	GLU	6.5
1	C	43	GLU	5.8
1	B	43	GLU	5.5
1	B	11	THR	4.4
1	C	11	THR	4.1
1	B	44	ARG	3.9
1	C	46	LEU	3.9
1	A	11	THR	3.5
1	F	46	LEU	3.5
1	E	45	ASN	3.5
1	B	46	LEU	3.4
1	E	11	THR	3.3
1	E	47	TYR	3.1
1	E	46	LEU	3.0
1	B	94	ASN	3.0
1	F	11	THR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	44	ARG	2.8
1	A	47	TYR	2.8
1	C	94	ASN	2.7
1	C	47	TYR	2.7
1	F	47	TYR	2.7
1	F	42[A]	GLU	2.6
1	A	46	LEU	2.5
1	E	42[A]	GLU	2.5
1	E	94	ASN	2.5
1	C	42[A]	GLU	2.5
1	A	94	ASN	2.4
1	A	299	ASP	2.3
1	B	45	ASN	2.3
1	B	42[A]	GLU	2.3
1	D	47	TYR	2.3
1	F	298	ARG	2.3
1	E	44	ARG	2.3
1	F	34	LEU	2.2
1	A	283	GLU	2.2
1	C	41	THR	2.1
1	D	42[A]	GLU	2.1
1	D	299	ASP	2.1
1	E	424[A]	LEU	2.1
1	D	328	GLN	2.0
1	D	11	THR	2.0
1	C	44	ARG	2.0
1	D	38	ALA	2.0
1	F	147	GLY	2.0
1	E	404[A]	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

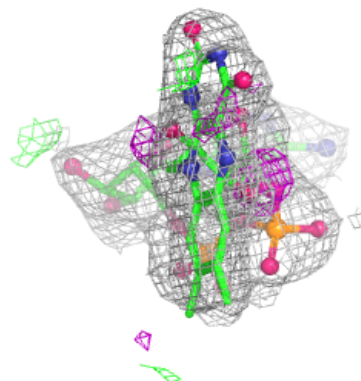
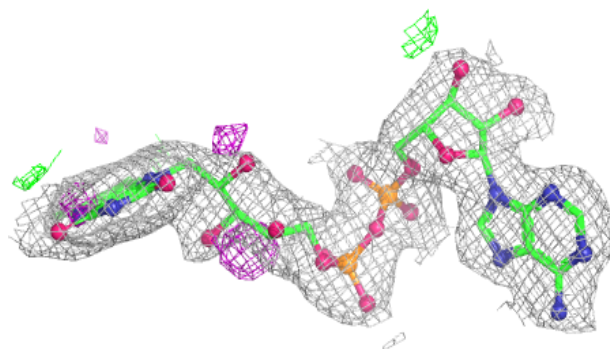
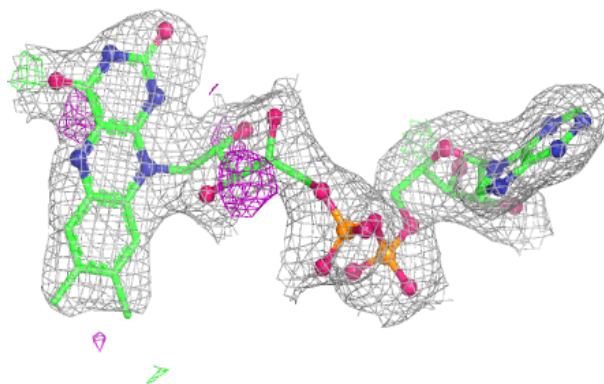
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PO4	F	489	5/5	0.83	0.32	42,42,43,43	5
4	PO4	D	487	5/5	0.86	0.28	41,42,43,43	5
4	PO4	C	486	5/5	0.86	0.25	33,34,34,34	5
4	PO4	C	492	5/5	0.88	0.17	40,40,41,41	5
4	PO4	B	485	5/5	0.88	0.28	35,35,35,36	5
4	PO4	E	488	5/5	0.88	0.30	36,37,38,38	5
4	PO4	A	484	5/5	0.88	0.26	32,32,33,34	5
4	PO4	F	495	5/5	0.88	0.19	43,44,44,44	5
4	PO4	E	494	5/5	0.89	0.23	43,43,44,44	5
3	UNL	A	477	6/-	0.90	0.18	36,52,57,67	0
3	UNL	B	477	6/-	0.90	0.14	38,44,50,56	0
3	UNL	F	477	6/-	0.90	0.18	30,49,54,55	0
4	PO4	B	491	5/5	0.91	0.14	29,29,30,31	5
3	UNL	E	477	6/-	0.91	0.18	25,50,56,57	0
4	PO4	A	490	5/5	0.92	0.17	35,35,36,37	5
3	UNL	D	477	6/-	0.92	0.17	29,48,51,53	0
3	UNL	C	477	6/-	0.92	0.15	33,47,51,54	0
4	PO4	D	493	5/5	0.92	0.13	40,40,41,41	5
4	PO4	E	482	5/5	0.94	0.16	50,51,51,52	0
4	PO4	C	480	5/5	0.95	0.14	51,51,52,53	0
4	PO4	D	481	5/5	0.95	0.13	54,54,54,55	0
4	PO4	A	478	5/5	0.95	0.13	53,54,54,55	0
4	PO4	B	479	5/5	0.96	0.17	49,49,50,50	0
2	FAD	F	476	53/53	0.97	0.07	26,33,45,48	0
2	FAD	A	476	53/53	0.97	0.06	24,29,42,44	0
2	FAD	B	476	53/53	0.97	0.07	25,32,43,45	0
2	FAD	C	476	53/53	0.97	0.07	28,35,45,48	0
4	PO4	F	483	5/5	0.97	0.14	46,46,47,48	0
2	FAD	D	476	53/53	0.97	0.07	28,33,44,46	0
2	FAD	E	476	53/53	0.97	0.07	26,32,43,45	0

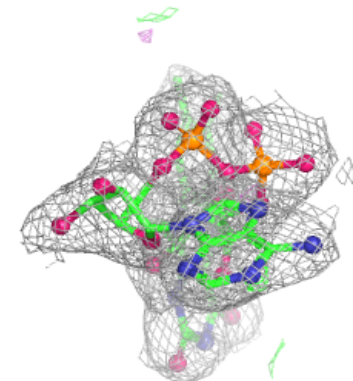
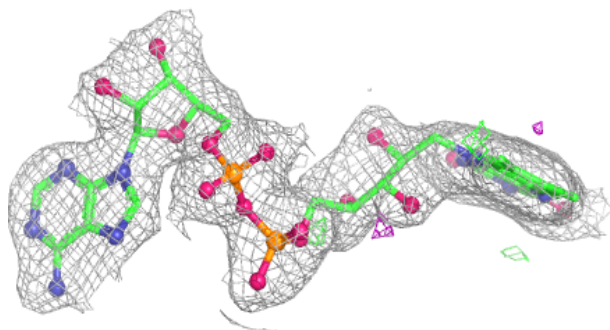
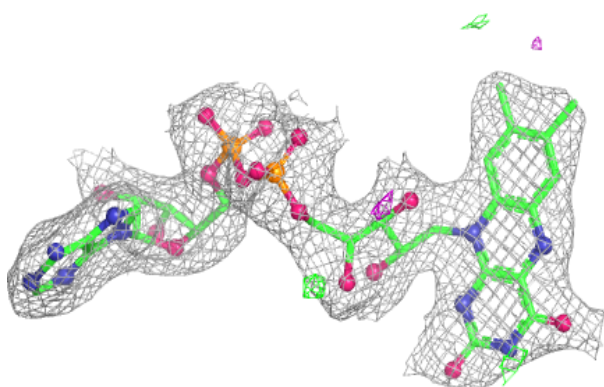
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD F 476:

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

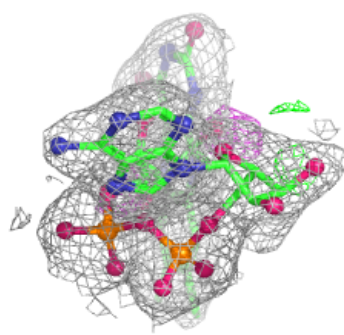
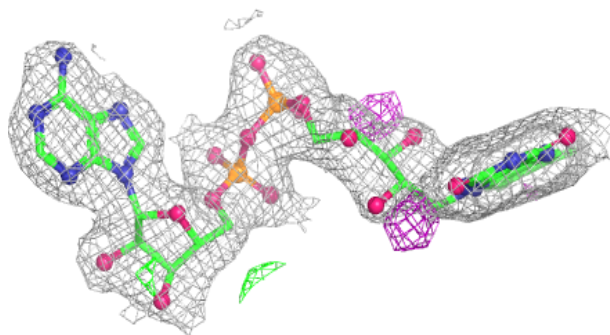
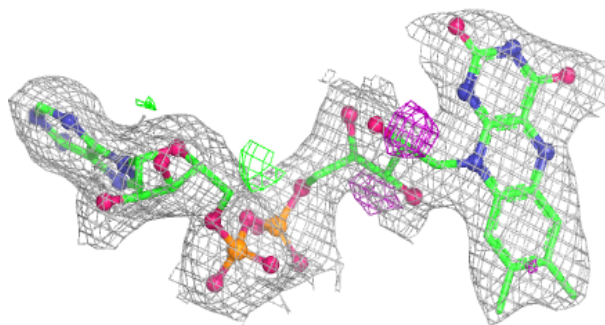
**Electron density around FAD A 476:**

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

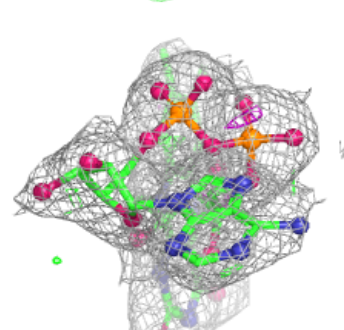
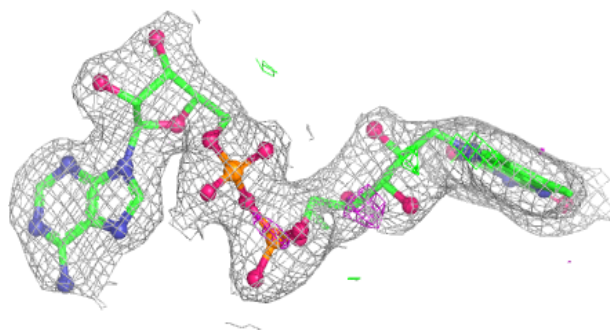
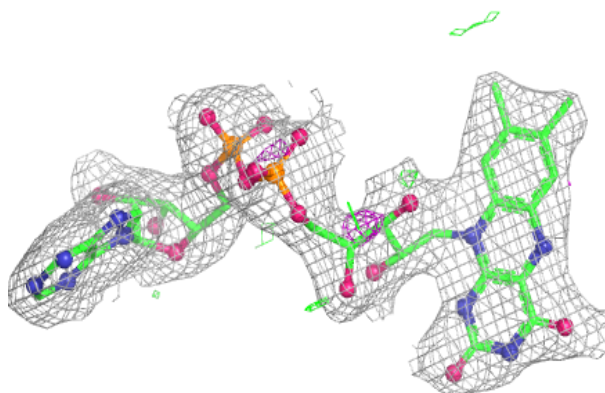


Electron density around FAD B 476:

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

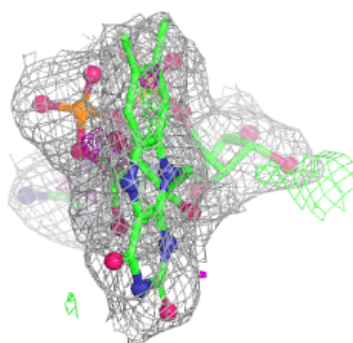
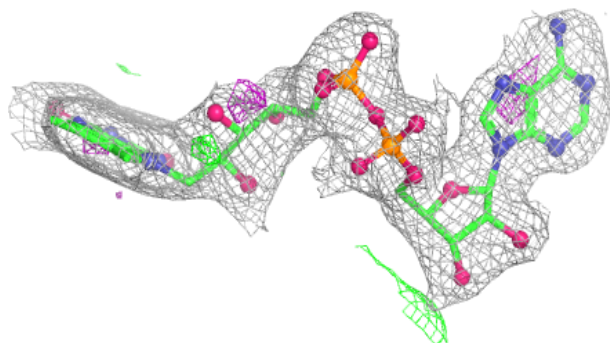
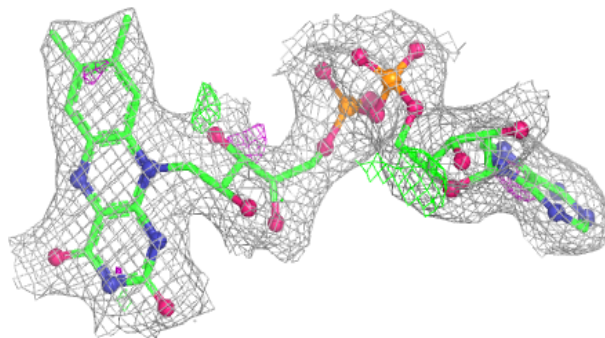
**Electron density around FAD C 476:**

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

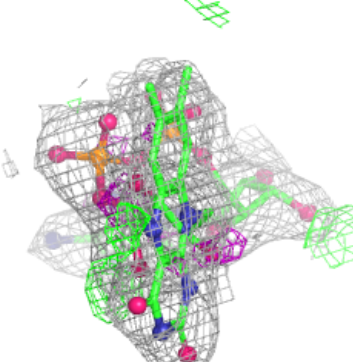
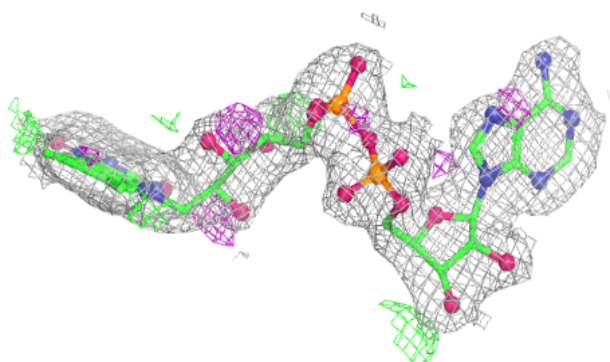
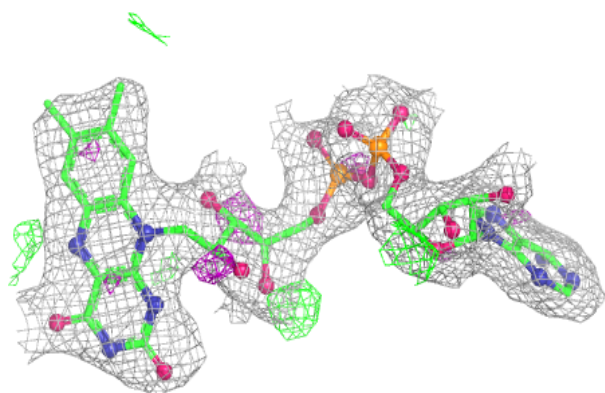


Electron density around FAD D 476:

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

**Electron density around FAD E 476:**

$2mF_o-DF_c$ (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.