



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:16 PM UTC

PDB ID : 5LNX / pdb_00005lnx
Title : Crystal structure of MmgC, an acyl-CoA dehydrogenase from bacillus subtilis.
Authors : Baker, G.E.; Race, P.R.
Deposited on : 2016-08-07
Resolution : 2.60 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

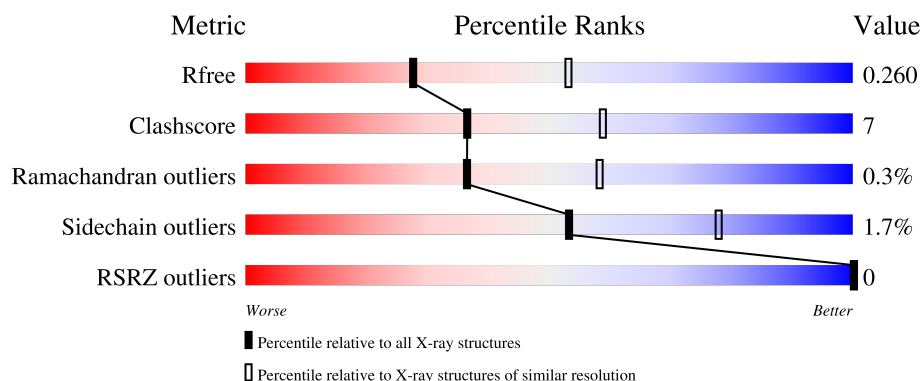
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

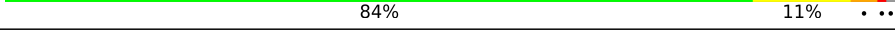
The reported resolution of this entry is 2.60 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	379	
1	B	379	
1	C	379	
1	D	379	
1	E	379	

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Mol	Chain	Length	Quality of chain
1	F	379	83% 12% • •
1	G	379	79% 15% • • •
1	H	379	84% 13% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22225 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 Acyl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2713	1727	472	503	11			
1	B	372	Total	C	N	O	S	0	0	0
			2702	1715	466	511	10			
1	C	364	Total	C	N	O	S	0	0	0
			2627	1666	460	490	11			
1	D	374	Total	C	N	O	S	0	0	0
			2743	1736	479	517	11			
1	E	368	Total	C	N	O	S	0	0	0
			2623	1663	446	505	9			
1	F	372	Total	C	N	O	S	0	0	0
			2663	1682	464	506	11			
1	G	367	Total	C	N	O	S	0	0	0
			2621	1661	461	491	8			
1	H	374	Total	C	N	O	S	0	0	0
			2698	1712	469	508	9			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total	O	0	0
			43	43		
4	B	54	Total	O	0	0
			54	54		
4	C	26	Total	O	0	0
			26	26		
4	D	52	Total	O	0	0
			52	52		

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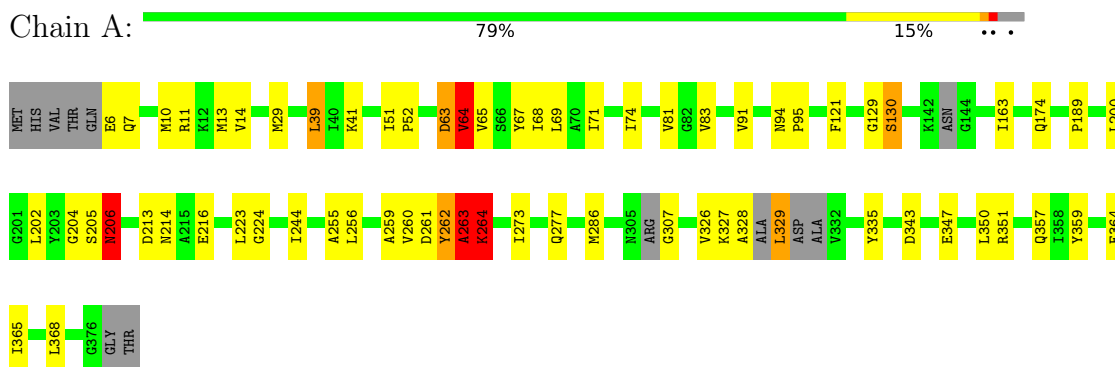
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	32	Total 32	O 32	0	0
4	F	50	Total 50	O 50	0	0
4	G	44	Total 44	O 44	0	0
4	H	44	Total 44	O 44	0	0

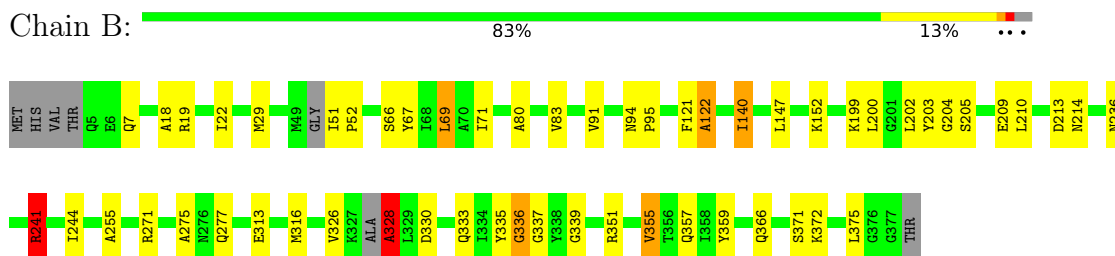
3 Residue-property plots

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.

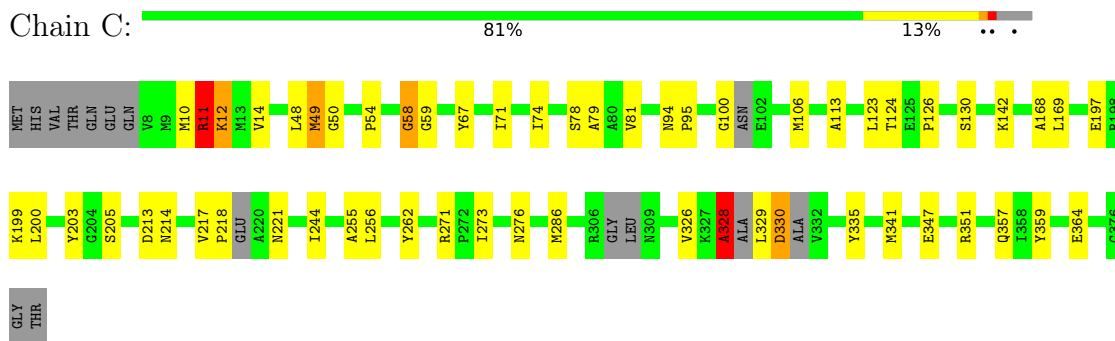
- Molecule 1: Acyl-CoA dehydrogenase



- Molecule 1: Acyl-CoA dehydrogenase

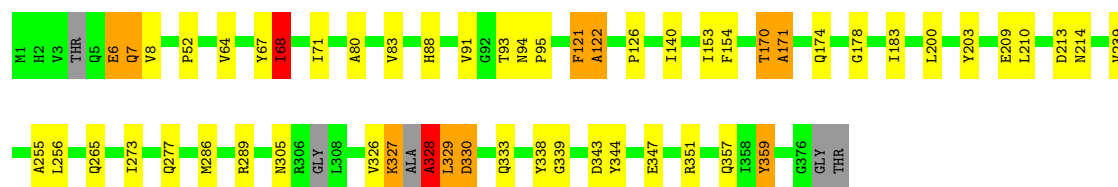


- Molecule 1: Acyl-CoA dehydrogenase



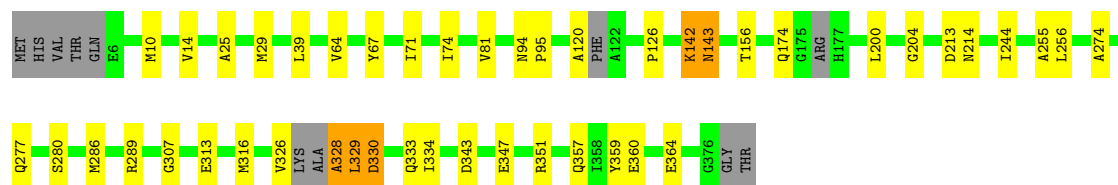
- Molecule 1: Acyl-CoA dehydrogenase

Chain D:  84% 11% . .



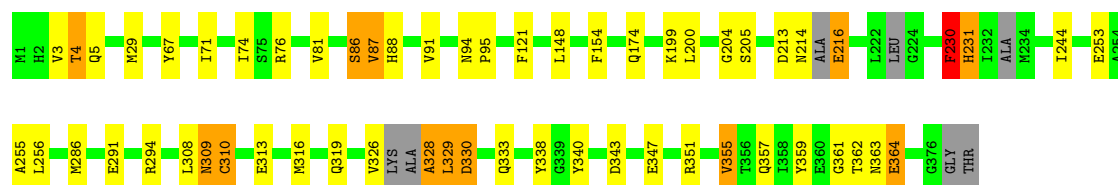
• Molecule 1: Acyl-CoA dehydrogenase

Chain E:  85% 11% . .



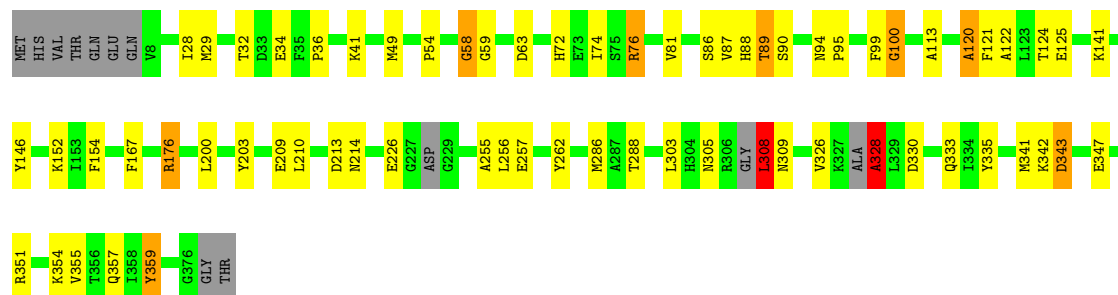
• Molecule 1: Acyl-CoA dehydrogenase

Chain F:  83% 12% . .



• Molecule 1: Acyl-CoA dehydrogenase

Chain G:  79% 15% . . .



• Molecule 1: Acyl-CoA dehydrogenase

Chain H:  84% 13% . .





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.17Å 279.27Å 78.19Å 90.00° 101.40° 90.00°	Depositor
Resolution (Å)	48.76 – 2.60 48.76 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.76-2.60) 99.9 (48.76-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.247 , 0.285 0.224 , 0.260	Depositor DCC
R_{free} test set	4985 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.821	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 13.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.390 for l,-k,h	Xtriage
Reported twinning fraction	0.481 for H, K, L 0.519 for L, -K, H	Depositor
Outliers	0 of 100323 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22225	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.04% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	5/2761 (0.2%)	1.23	21/3725 (0.6%)
1	B	0.84	1/2751 (0.0%)	1.12	11/3728 (0.3%)
1	C	0.80	3/2672 (0.1%)	1.27	19/3612 (0.5%)
1	D	0.84	2/2793 (0.1%)	1.27	25/3775 (0.7%)
1	E	0.78	0/2666	1.19	11/3617 (0.3%)
1	F	0.79	0/2706	1.23	14/3663 (0.4%)
1	G	0.80	0/2667	1.15	14/3616 (0.4%)
1	H	0.95	2/2747 (0.1%)	1.16	10/3721 (0.3%)
All	All	0.83	13/21763 (0.1%)	1.20	125/29457 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	3
1	C	0	5
1	D	0	3
1	E	1	4
1	F	0	3
1	G	0	4
1	H	0	3
All	All	1	30

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	307	GLY	C-N	-22.96	1.02	1.33
1	H	308	LEU	C-N	16.87	1.57	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	170	THR	CA-C	10.41	1.66	1.52
1	D	327	LYS	C-N	-9.80	1.20	1.34
1	C	11	ARG	C-N	-6.28	1.25	1.33
1	A	263	ALA	C-O	-6.21	1.16	1.24
1	A	63	ASP	C-O	-5.67	1.16	1.23
1	C	217	VAL	C-O	-5.63	1.18	1.24
1	A	130	SER	N-CA	5.61	1.53	1.46
1	C	168	ALA	N-CA	5.56	1.53	1.46
1	A	224	GLY	N-CA	5.31	1.52	1.45
1	B	337	GLY	N-CA	5.29	1.54	1.45
1	A	329	LEU	CA-C	-5.03	1.42	1.52

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	142	LYS	CB-CA-C	-19.98	70.66	110.42
1	F	362	THR	N-CA-C	-17.64	82.18	109.52
1	D	327	LYS	CA-C-N	16.80	144.85	121.33
1	D	327	LYS	C-N-CA	16.80	144.85	121.33
1	D	8	VAL	N-CA-C	-16.40	96.56	112.96
1	C	49	MET	N-CA-C	-15.98	87.42	110.59
1	C	11	ARG	CA-C-N	15.12	140.10	120.44
1	C	11	ARG	C-N-CA	15.12	140.10	120.44
1	H	330	ASP	N-CA-C	-14.83	93.73	112.72
1	H	308	LEU	O-C-N	13.28	140.24	123.10
1	F	330	ASP	N-CA-C	-12.84	96.29	112.72
1	D	330	ASP	N-CA-C	-12.72	96.44	112.72
1	A	63	ASP	CA-C-N	12.44	144.09	121.70
1	A	63	ASP	C-N-CA	12.44	144.09	121.70
1	C	12	LYS	N-CA-C	-12.24	97.97	111.07
1	F	4	THR	CB-CA-C	11.73	126.02	109.71
1	F	361	GLY	CA-C-O	-11.65	114.19	122.23
1	E	330	ASP	N-CA-C	-11.57	97.91	112.72
1	F	4	THR	N-CA-C	-11.18	94.09	110.42
1	G	343	ASP	N-CA-C	-10.46	101.01	113.88
1	F	361	GLY	N-CA-C	-10.39	100.65	112.29
1	E	143	ASN	N-CA-C	10.37	129.56	113.28
1	H	329	LEU	CB-CA-C	-10.10	90.90	110.10
1	D	170	THR	N-CA-C	10.05	124.20	111.24
1	H	307	GLY	CA-C-N	10.04	140.59	122.92
1	H	307	GLY	C-N-CA	10.04	140.59	122.92
1	C	11	ARG	CB-CA-C	9.99	130.29	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	78	SER	N-CA-C	9.99	125.50	112.12
1	A	205	SER	N-CA-C	9.93	121.79	110.97
1	F	329	LEU	CB-CA-C	-9.89	91.30	110.10
1	C	197	GLU	N-CA-C	9.83	123.23	111.82
1	C	168	ALA	N-CA-C	9.42	130.87	110.80
1	E	329	LEU	CB-CA-C	-9.39	92.25	110.10
1	A	206	ASN	N-CA-CB	9.24	126.11	110.49
1	B	122	ALA	N-CA-C	9.19	124.55	113.16
1	A	264	LYS	N-CA-C	-9.19	91.24	110.80
1	G	120	ALA	N-CA-C	9.04	130.06	110.80
1	C	100	GLY	N-CA-C	8.84	138.93	113.30
1	B	328	ALA	N-CA-C	-8.64	100.21	110.41
1	C	169	LEU	N-CA-C	8.42	121.54	111.02
1	C	328	ALA	N-CA-C	-8.37	100.54	110.41
1	D	327	LYS	N-CA-C	-8.36	96.10	109.39
1	C	50	GLY	N-CA-C	8.34	132.95	113.18
1	D	329	LEU	CB-CA-C	-8.30	94.32	110.10
1	A	64	VAL	N-CA-CB	8.25	125.53	111.50
1	G	308	LEU	CB-CA-C	8.23	125.75	110.10
1	B	19	ARG	N-CA-C	8.13	120.22	111.36
1	H	328	ALA	N-CA-C	8.13	123.63	107.62
1	G	343	ASP	N-CA-CB	-8.00	99.96	110.59
1	G	89	THR	N-CA-C	-7.82	100.44	110.53
1	D	7	GLN	CB-CA-C	-7.79	95.30	110.10
1	F	174	GLN	N-CA-C	-7.75	97.69	110.17
1	C	330	ASP	N-CA-C	-7.65	89.57	111.00
1	D	170	THR	CA-C-N	7.62	135.41	121.70
1	D	170	THR	C-N-CA	7.62	135.41	121.70
1	F	230	PHE	CB-CA-C	-7.61	95.65	110.10
1	D	327	LYS	O-C-N	-7.59	112.61	122.56
1	A	174	GLN	N-CA-C	-7.55	98.72	110.42
1	A	65	VAL	N-CA-C	-7.49	103.55	110.82
1	A	130	SER	N-CA-CB	7.49	123.14	110.49
1	C	328	ALA	N-CA-CB	7.46	120.74	111.79
1	F	87	VAL	N-CA-C	-7.36	103.50	110.42
1	D	68	ILE	CG1-CB-CG2	-7.33	88.71	110.70
1	D	68	ILE	CB-CG1-CD1	7.19	128.90	113.80
1	A	39	LEU	N-CA-CB	7.11	122.50	110.49
1	B	336	GLY	CA-C-N	7.01	134.31	121.70
1	B	336	GLY	C-N-CA	7.01	134.31	121.70
1	A	63	ASP	N-CA-C	-6.81	99.89	110.17
1	E	120	ALA	N-CA-C	6.80	130.04	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	TYR	N-CA-C	6.71	122.45	111.37
1	G	58	GLY	O-C-N	-6.71	115.05	122.50
1	F	355	VAL	CB-CA-C	-6.69	101.79	112.16
1	G	203	TYR	N-CA-C	6.68	122.40	111.37
1	C	12	LYS	N-CA-CB	6.67	119.68	110.01
1	C	58	GLY	O-C-N	-6.54	115.24	122.50
1	H	307	GLY	O-C-N	-6.54	114.36	122.34
1	A	63	ASP	O-C-N	-6.53	114.20	122.43
1	G	309	ASN	N-CA-C	-6.46	98.68	108.96
1	B	69	LEU	CA-CB-CG	6.45	138.87	116.30
1	A	130	SER	N-CA-C	-6.45	97.07	110.80
1	A	343	ASP	N-CA-CB	-6.43	100.31	110.28
1	F	362	THR	N-CA-CB	6.42	122.72	111.55
1	D	6	GLU	CA-C-N	6.42	133.25	121.70
1	D	6	GLU	C-N-CA	6.42	133.25	121.70
1	D	170	THR	O-C-N	-6.41	114.67	122.11
1	B	328	ALA	N-CA-CB	6.40	119.47	111.79
1	B	241	ARG	CG-CD-NE	6.40	126.08	112.00
1	D	328	ALA	N-CA-C	6.32	117.94	107.20
1	A	63	ASP	CA-C-O	-6.22	113.79	121.88
1	F	5	GLN	N-CA-CB	-6.17	99.08	110.18
1	A	263	ALA	O-C-N	-6.16	114.17	122.43
1	D	121	PHE	N-CA-C	6.05	123.16	114.39
1	G	90	SER	N-CA-CB	5.98	120.59	110.49
1	H	329	LEU	N-CA-C	5.97	127.71	111.00
1	E	313	GLU	CB-CG-CD	5.96	122.73	112.60
1	D	171	ALA	CB-CA-C	-5.92	101.63	110.50
1	C	11	ARG	N-CA-C	-5.88	98.27	110.80
1	D	122	ALA	N-CA-C	5.82	123.19	110.80
1	C	79	ALA	N-CA-CB	5.75	120.21	110.49
1	E	329	LEU	N-CA-C	5.75	127.09	111.00
1	A	189	PRO	N-CA-C	5.71	124.22	112.47
1	D	7	GLN	N-CA-C	5.68	126.92	111.00
1	G	328	ALA	CB-CA-C	5.63	118.14	111.22
1	F	329	LEU	N-CA-C	5.62	126.74	111.00
1	A	264	LYS	CA-CB-CG	-5.51	103.08	114.10
1	G	328	ALA	N-CA-C	5.50	120.20	112.72
1	G	99	PHE	N-CA-C	-5.36	105.09	111.69
1	G	100	GLY	CA-C-N	5.35	131.33	121.70
1	G	100	GLY	C-N-CA	5.35	131.33	121.70
1	A	329	LEU	CA-CB-CG	5.32	134.92	116.30
1	E	142	LYS	CA-C-N	-5.32	117.03	126.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	142	LYS	C-N-CA	-5.32	117.03	126.45
1	D	329	LEU	N-CA-C	5.23	125.63	111.00
1	E	360	GLU	CB-CG-CD	5.18	121.41	112.60
1	H	188	THR	CA-C-N	5.16	125.41	119.83
1	H	188	THR	C-N-CA	5.16	125.41	119.83
1	A	205	SER	CB-CA-C	5.13	118.86	110.96
1	A	39	LEU	N-CA-C	-5.11	99.92	110.80
1	B	51	ILE	CG1-CB-CG2	-5.09	95.44	110.70
1	E	174	GLN	N-CA-C	-5.08	99.99	110.80
1	D	328	ALA	CA-C-N	5.07	130.82	121.70
1	D	328	ALA	C-N-CA	5.07	130.82	121.70
1	C	168	ALA	CB-CA-C	-5.07	100.34	110.42
1	D	183	ILE	CB-CA-C	-5.06	106.44	111.80
1	B	336	GLY	CA-C-O	-5.00	115.98	121.94

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	E	143	ASN	CA

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	206	ASN	Mainchain
1	A	223	LEU	Peptide
1	A	262	TYR	Peptide
1	A	263	ALA	Peptide
1	A	307	GLY	Peptide
1	B	241	ARG	Sidechain
1	B	328	ALA	Peptide
1	B	335	TYR	Peptide
1	C	11	ARG	Peptide
1	C	142	LYS	Peptide
1	C	203	TYR	Peptide
1	C	328	ALA	Peptide
1	C	58	GLY	Peptide
1	D	203	TYR	Peptide
1	D	327	LYS	Peptide
1	D	328	ALA	Peptide
1	E	142	LYS	Peptide
1	E	143	ASN	Peptide
1	E	307	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	E	328	ALA	Peptide
1	F	216	GLU	Peptide
1	F	230	PHE	Mainchain
1	F	328	ALA	Peptide
1	G	100	GLY	Peptide
1	G	328	ALA	Peptide
1	G	342	LYS	Peptide
1	G	58	GLY	Peptide
1	H	328	ALA	Peptide
1	H	4	THR	Peptide
1	H	7	GLN	Peptide

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	2713	0	2653	48	0
1	B	2702	0	2583	41	0
1	C	2627	0	2477	35	0
1	D	2743	0	2613	47	0
1	E	2623	0	2446	27	0
1	F	2663	0	2483	39	0
1	G	2621	0	2464	44	0
1	H	2698	0	2554	40	0
2	A	18	0	24	1	0
2	C	18	0	24	0	0
2	D	6	0	8	0	0
2	F	6	0	8	0	0
2	G	12	0	16	0	0
2	H	6	0	8	0	0
3	A	53	0	31	2	0
3	B	53	0	31	2	0
3	C	53	0	31	5	0
3	D	53	0	31	2	0
3	E	53	0	31	2	0
3	F	53	0	31	2	0
3	G	53	0	31	5	0
3	H	53	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	43	0	0	0	0
4	B	54	0	0	1	0
4	C	26	0	0	0	0
4	D	52	0	0	0	0
4	E	32	0	0	0	0
4	F	50	0	0	0	0
4	G	44	0	0	0	0
4	H	44	0	0	0	0
All	All	22225	0	20609	306	0

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

All (306) 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:H:7:GLN:HB3	1:H:10:MET:H	1.25	1.00
1:B:355:VAL:HG13	1:B:359:TYR:HE2	1.29	0.98
1:D:88:HIS:O	1:D:93:THR:HG23	1.67	0.94
1:G:29:MET:HE2	1:G:36:PRO:HB3	1.50	0.93
1:G:176:ARG:HG3	1:G:176:ARG:HH11	1.34	0.93
1:F:3:VAL:O	1:F:4:THR:C	2.14	0.89
1:B:66:SER:HA	1:B:69:LEU:HG	1.53	0.89
1:G:32:THR:HG23	1:G:34:GLU:H	1.38	0.88
1:A:328:ALA:N	1:A:329:LEU:O	2.07	0.87
1:G:28:ILE:O	1:G:32:THR:HG22	1.77	0.85
1:A:260:VAL:O	1:A:263:ALA:HB3	1.79	0.83
1:H:78:SER:HB3	1:H:81:VAL:HG12	1.59	0.83
1:B:355:VAL:HG13	1:B:359:TYR:CE2	2.13	0.81
1:B:313:GLU:HA	1:B:316:MET:CE	2.11	0.81
1:D:171:ALA:CB	1:D:178:GLY:O	2.29	0.80
1:D:171:ALA:HB3	1:D:178:GLY:O	1.82	0.79
1:B:355:VAL:CG1	1:B:359:TYR:HE2	1.96	0.77
1:B:122:ALA:O	1:B:152:LYS:HD2	1.84	0.76
1:G:86:SER:O	1:G:89:THR:O	2.04	0.75
1:G:303:LEU:O	1:G:308:LEU:HB3	1.85	0.75
1:C:199:LYS:NZ	1:C:205:SER:O	2.21	0.74
1:C:364:GLU:HB2	3:C:404:FAD:O2B	1.88	0.73
3:B:401:FAD:HM71	4:B:714:HOH:O	1.89	0.72
1:H:199:LYS:NZ	1:H:205:SER:O	2.23	0.72
1:B:199:LYS:NZ	1:B:205:SER:O	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:199:LYS:NZ	1:F:205:SER:O	2.23	0.72
1:A:83:VAL:HG11	1:A:359:TYR:OH	1.90	0.71
1:A:129:GLY:O	3:A:404:FAD:O5'	2.08	0.71
1:H:329:LEU:O	1:H:329:LEU:HG	1.90	0.71
1:A:259:ALA:O	1:A:263:ALA:HB2	1.91	0.71
1:F:319:GLN:HA	1:F:363:ASN:HD21	1.56	0.70
1:H:4:THR:OG1	1:H:5:GLN:HA	1.92	0.70
1:A:328:ALA:CA	1:A:329:LEU:C	2.65	0.69
1:H:7:GLN:HB3	1:H:10:MET:N	2.03	0.69
1:G:29:MET:HE2	1:G:36:PRO:CB	2.21	0.69
1:D:171:ALA:HB1	1:D:178:GLY:CA	2.23	0.69
1:A:328:ALA:HA	1:A:329:LEU:C	2.18	0.69
1:C:200:LEU:HB2	1:D:347:GLU:HG3	1.76	0.68
1:H:78:SER:CB	1:H:81:VAL:HG12	2.23	0.67
1:B:202:LEU:HD11	1:B:355:VAL:HG11	1.77	0.67
1:B:313:GLU:HA	1:B:316:MET:HE3	1.76	0.67
1:C:10:MET:C	1:C:12:LYS:H	2.02	0.66
1:B:313:GLU:HA	1:B:316:MET:HE2	1.77	0.66
3:G:403:FAD:O1P	3:G:403:FAD:O3'	2.13	0.65
1:A:6:GLU:HG3	1:A:7:GLN:HG3	1.79	0.65
1:B:95:PRO:HG3	1:B:236:ASN:OD1	1.97	0.65
1:F:329:LEU:O	1:F:329:LEU:HG	1.95	0.65
1:H:7:GLN:CB	1:H:10:MET:H	2.06	0.65
1:A:328:ALA:CA	1:A:329:LEU:O	2.45	0.65
1:B:326:VAL:HG21	1:B:357:GLN:CD	2.23	0.65
1:A:260:VAL:O	1:A:263:ALA:CB	2.44	0.64
1:A:10:MET:O	1:A:13:MET:HG2	1.97	0.64
1:G:303:LEU:O	1:G:308:LEU:CB	2.46	0.64
1:E:29:MET:HE2	1:E:204:GLY:HA3	1.80	0.63
1:A:29:MET:HE2	1:A:204:GLY:HA3	1.81	0.63
1:A:83:VAL:HG21	1:A:202:LEU:HD13	1.79	0.63
1:F:29:MET:HE2	1:F:204:GLY:HA3	1.81	0.62
1:H:112:LEU:HD11	1:H:163:ILE:CD1	2.30	0.62
1:C:200:LEU:HB2	1:D:347:GLU:CG	2.29	0.62
1:H:29:MET:HE2	1:H:204:GLY:HA3	1.81	0.62
1:G:141:LYS:HE2	1:G:146:TYR:CZ	2.35	0.62
1:H:112:LEU:HD11	1:H:163:ILE:HD13	1.81	0.61
1:F:291:GLU:OE1	1:F:294:ARG:NH2	2.32	0.61
1:A:329:LEU:HG	1:A:350:LEU:HD13	1.82	0.61
1:F:319:GLN:HA	1:F:363:ASN:ND2	2.15	0.61
1:E:329:LEU:HG	1:E:329:LEU:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:326:VAL:HG21	1:F:357:GLN:CD	2.26	0.61
1:E:326:VAL:HG21	1:E:357:GLN:CD	2.25	0.61
1:C:326:VAL:O	1:C:329:LEU:HD22	2.02	0.59
1:E:200:LEU:HD23	1:F:340:TYR:CE1	2.37	0.59
1:H:4:THR:CB	1:H:5:GLN:HA	2.32	0.59
1:A:260:VAL:O	1:A:264:LYS:HB2	2.03	0.59
1:G:76:ARG:NH2	1:G:257:GLU:OE2	2.35	0.59
1:H:326:VAL:HG21	1:H:357:GLN:CD	2.28	0.59
1:G:124:THR:OG1	3:G:403:FAD:N1	2.35	0.58
1:G:326:VAL:HG21	1:G:357:GLN:CD	2.28	0.58
1:B:355:VAL:HG22	1:B:359:TYR:CD2	2.38	0.58
1:D:171:ALA:HB1	1:D:178:GLY:O	2.03	0.58
1:D:326:VAL:HG21	1:D:357:GLN:CD	2.29	0.58
1:C:218:PRO:HG2	1:C:221:ASN:CG	2.29	0.58
1:A:326:VAL:HG21	1:A:357:GLN:CD	2.28	0.58
1:F:308:LEU:O	1:F:309:ASN:O	2.22	0.57
1:C:326:VAL:HG21	1:C:357:GLN:CD	2.29	0.57
1:D:170:THR:N	1:D:171:ALA:HB3	2.19	0.57
1:D:171:ALA:HB1	1:D:178:GLY:HA3	1.86	0.57
1:B:29:MET:HE2	1:B:204:GLY:HA3	1.85	0.57
1:E:274:ALA:O	1:E:280:SER:OG	2.23	0.57
1:F:3:VAL:O	1:F:4:THR:O	2.22	0.57
1:G:49:MET:HE3	1:G:88:HIS:CE1	2.39	0.57
1:D:6:GLU:HA	1:D:7:GLN:HB2	1.86	0.56
1:G:354:LYS:HD3	1:H:329:LEU:HD12	1.88	0.56
1:C:11:ARG:O	1:C:14:VAL:N	2.39	0.56
1:H:78:SER:HB3	1:H:81:VAL:CG1	2.33	0.56
1:A:91:VAL:HB	1:A:121:PHE:CD1	2.40	0.56
1:C:59:GLY:H	1:C:113:ALA:HB1	1.71	0.55
1:G:59:GLY:H	1:G:113:ALA:HB1	1.71	0.55
1:B:66:SER:CA	1:B:69:LEU:HG	2.29	0.55
1:B:91:VAL:HB	1:B:121:PHE:CD1	2.41	0.55
1:H:91:VAL:HB	1:H:121:PHE:CD1	2.42	0.55
1:F:91:VAL:HB	1:F:121:PHE:CD1	2.41	0.55
1:A:277:GLN:OE1	1:C:276:ASN:HB3	2.06	0.55
1:D:91:VAL:HB	1:D:121:PHE:CD1	2.42	0.55
1:D:347:GLU:OE2	1:D:351:ARG:NE	2.39	0.55
1:D:329:LEU:O	1:D:329:LEU:HG	2.07	0.54
1:B:202:LEU:HD12	1:B:202:LEU:N	2.22	0.54
1:F:319:GLN:HG2	1:F:363:ASN:ND2	2.22	0.54
1:H:291:GLU:OE1	1:H:294:ARG:NH2	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:230:PHE:CE2	1:H:234:MET:SD	3.01	0.54
1:B:66:SER:HA	1:B:69:LEU:CG	2.34	0.54
1:B:371:SER:O	1:B:375:LEU:HD13	2.08	0.54
1:F:364:GLU:N	1:F:364:GLU:OE2	2.41	0.53
1:G:124:THR:HG21	3:G:403:FAD:H1'1	1.89	0.53
1:G:32:THR:HG23	1:G:34:GLU:N	2.18	0.53
1:D:140:ILE:HG23	1:D:140:ILE:O	2.08	0.53
1:C:326:VAL:C	1:C:328:ALA:H	2.17	0.53
1:H:91:VAL:HG23	1:H:121:PHE:HB2	1.91	0.52
1:D:213:ASP:O	1:D:214:ASN:C	2.52	0.51
1:G:141:LYS:HE2	1:G:146:TYR:OH	2.11	0.51
1:G:328:ALA:HA	1:G:330:ASP:H	1.76	0.51
1:A:364:GLU:HB2	3:A:404:FAD:O2B	2.09	0.51
1:C:328:ALA:HA	1:C:330:ASP:O	2.10	0.51
1:A:261:ASP:C	1:A:263:ALA:H	2.18	0.51
1:A:263:ALA:O	1:A:273:ILE:HG13	2.11	0.51
1:B:241:ARG:HD3	1:B:366:GLN:HE22	1.75	0.51
1:E:213:ASP:O	1:E:214:ASN:C	2.54	0.51
1:C:124:THR:OG1	3:C:404:FAD:H1'1	2.10	0.51
1:F:74:ILE:HG21	1:F:81:VAL:HG12	1.93	0.51
1:G:213:ASP:O	1:G:214:ASN:C	2.54	0.51
1:D:343:ASP:OD1	1:D:344:TYR:HD2	1.94	0.51
1:A:326:VAL:C	1:A:328:ALA:H	2.19	0.50
1:F:148:LEU:H	1:F:216:GLU:CB	2.24	0.50
1:A:64:VAL:H	1:A:67:TYR:HB3	1.77	0.50
1:A:213:ASP:O	1:A:214:ASN:C	2.54	0.50
1:A:327:LYS:C	1:A:329:LEU:O	2.55	0.50
1:B:326:VAL:C	1:B:328:ALA:H	2.20	0.50
1:G:122:ALA:HB1	1:G:152:LYS:HG3	1.94	0.50
1:G:355:VAL:HG12	1:G:359:TYR:CE2	2.46	0.50
1:H:213:ASP:O	1:H:214:ASN:C	2.55	0.50
1:E:74:ILE:HG21	1:E:81:VAL:HG12	1.94	0.49
1:C:54:PRO:O	1:C:59:GLY:HA3	2.12	0.49
1:A:74:ILE:HG21	1:A:81:VAL:HG12	1.95	0.49
1:D:200:LEU:O	1:D:351:ARG:HD2	2.13	0.49
1:A:6:GLU:CG	1:A:7:GLN:HG3	2.40	0.49
1:B:213:ASP:O	1:B:214:ASN:C	2.56	0.49
1:F:326:VAL:O	1:F:329:LEU:HB2	2.13	0.49
1:F:355:VAL:CB	1:F:359:TYR:HE2	2.26	0.49
1:G:54:PRO:O	1:G:59:GLY:HA3	2.12	0.49
1:A:94:ASN:N	1:A:95:PRO:CD	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:326:VAL:O	1:E:329:LEU:HB2	2.13	0.49
1:F:88:HIS:C	1:F:88:HIS:CD2	2.90	0.49
1:C:200:LEU:O	1:C:351:ARG:HD2	2.13	0.48
1:G:200:LEU:O	1:G:351:ARG:HD2	2.13	0.48
1:D:121:PHE:O	1:D:122:ALA:C	2.57	0.48
1:C:273:ILE:HG22	3:D:402:FAD:C8A	2.42	0.48
1:H:326:VAL:O	1:H:329:LEU:HB2	2.14	0.48
1:C:218:PRO:HG2	1:C:221:ASN:ND2	2.28	0.48
1:C:213:ASP:O	1:C:214:ASN:C	2.56	0.48
1:F:213:ASP:O	1:F:214:ASN:C	2.57	0.48
1:D:126:PRO:HA	1:D:153:ILE:HD13	1.96	0.48
1:E:25:ALA:CB	1:E:39:LEU:HD22	2.43	0.48
1:D:328:ALA:HA	1:D:330:ASP:H	1.78	0.48
1:B:52:PRO:HG3	1:B:67:TYR:CG	2.48	0.47
1:F:200:LEU:O	1:F:351:ARG:HD2	2.13	0.47
1:E:277:GLN:HE21	1:H:368:LEU:HD13	1.79	0.47
1:C:74:ILE:HG21	1:C:81:VAL:HG12	1.95	0.47
1:D:67:TYR:CD2	1:D:68:ILE:HD12	2.49	0.47
1:G:308:LEU:HD13	1:G:308:LEU:HA	1.78	0.47
1:A:261:ASP:C	1:A:263:ALA:N	2.72	0.47
1:B:200:LEU:O	1:B:351:ARG:HD2	2.14	0.47
1:D:339:GLY:O	1:D:347:GLU:HB2	2.14	0.47
1:E:364:GLU:HB2	3:E:401:FAD:O2B	2.13	0.47
1:G:32:THR:OG1	1:G:34:GLU:HG3	2.15	0.47
1:A:200:LEU:O	1:A:351:ARG:HD2	2.14	0.47
1:A:273:ILE:HG22	3:B:401:FAD:C8A	2.45	0.47
1:D:170:THR:CA	1:D:171:ALA:HB3	2.44	0.47
1:D:326:VAL:O	1:D:329:LEU:HB2	2.15	0.47
1:E:244:ILE:HD12	1:E:359:TYR:CE1	2.50	0.47
1:B:271:ARG:HD3	1:B:275:ALA:CB	2.45	0.47
1:G:74:ILE:HG21	1:G:81:VAL:HG12	1.95	0.47
3:G:403:FAD:C6A	1:H:276:ASN:OD1	2.63	0.47
1:C:123:LEU:HB3	3:C:404:FAD:O2	2.14	0.47
1:E:328:ALA:HA	1:E:330:ASP:H	1.80	0.47
1:F:76:ARG:NE	1:F:253:GLU:OE1	2.48	0.47
1:A:365:ILE:HG21	2:A:401:GOL:H11	1.96	0.46
1:H:200:LEU:O	1:H:351:ARG:HD2	2.14	0.46
1:C:271:ARG:HA	1:H:140:ILE:HG23	1.97	0.46
1:H:7:GLN:C	1:H:9:MET:N	2.72	0.46
1:B:355:VAL:HG22	1:B:359:TYR:HD2	1.79	0.46
1:E:64:VAL:HA	1:E:67:TYR:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:THR:OG1	3:E:401:FAD:H6	2.16	0.46
1:B:244:ILE:HD12	1:B:359:TYR:CE1	2.51	0.46
1:E:255:ALA:HB1	1:E:328:ALA:HB1	1.98	0.46
1:C:262:TYR:CE1	1:C:335:TYR:HA	2.51	0.46
1:F:255:ALA:HB1	1:F:328:ALA:HB1	1.98	0.46
1:A:67:TYR:CZ	1:A:71:ILE:HD11	2.51	0.46
1:F:310:CYS:HA	1:F:313:GLU:OE1	2.16	0.46
1:E:94:ASN:N	1:E:95:PRO:CD	2.80	0.45
1:H:112:LEU:HD21	1:H:163:ILE:HD12	1.99	0.45
1:F:244:ILE:HD12	1:F:359:TYR:CE1	2.51	0.45
1:G:341:MET:C	1:G:343:ASP:H	2.23	0.45
1:C:326:VAL:C	1:C:328:ALA:N	2.75	0.45
1:G:141:LYS:HE3	1:G:226:GLU:OE2	2.16	0.45
1:A:63:ASP:HB2	1:A:64:VAL:HB	1.98	0.45
1:A:255:ALA:HB1	1:A:328:ALA:HB1	1.98	0.45
1:B:7:GLN:HB3	1:B:69:LEU:HD21	1.99	0.45
1:H:255:ALA:HB1	1:H:328:ALA:HB1	1.98	0.45
1:C:244:ILE:HD12	1:C:359:TYR:CE1	2.52	0.45
1:D:255:ALA:HB1	1:D:328:ALA:HB1	1.98	0.45
1:C:67:TYR:CZ	1:C:71:ILE:HD11	2.52	0.45
1:D:170:THR:H	1:D:171:ALA:HB3	1.80	0.45
1:F:154:PHE:O	3:F:402:FAD:C4X	2.65	0.45
1:A:52:PRO:HG3	1:A:67:TYR:CG	2.52	0.44
1:F:76:ARG:HE	1:F:253:GLU:HB3	1.82	0.44
1:C:126:PRO:HA	1:D:338:TYR:OH	2.17	0.44
1:D:171:ALA:HB1	1:D:178:GLY:C	2.42	0.44
1:G:154:PHE:O	3:G:403:FAD:C4X	2.65	0.44
1:A:11:ARG:HD3	1:A:69:LEU:HD11	2.00	0.44
1:G:262:TYR:CE1	1:G:335:TYR:HA	2.52	0.44
1:A:244:ILE:HD12	1:A:359:TYR:CE1	2.52	0.44
1:A:329:LEU:O	1:A:329:LEU:HD12	2.17	0.44
1:B:29:MET:CE	1:B:204:GLY:HA3	2.48	0.44
1:C:94:ASN:N	1:C:95:PRO:CD	2.81	0.44
1:D:6:GLU:HA	1:D:7:GLN:CB	2.47	0.44
1:G:256:LEU:HA	1:G:286:MET:HE2	2.00	0.44
1:H:67:TYR:CZ	1:H:71:ILE:HD11	2.53	0.44
1:H:72:HIS:HE2	1:H:253:GLU:CD	2.26	0.44
1:B:277:GLN:HB2	1:D:277:GLN:HB2	1.99	0.44
1:D:80:ALA:O	1:D:83:VAL:HG12	2.18	0.43
1:D:347:GLU:C	1:D:347:GLU:CD	2.85	0.43
1:G:330:ASP:O	1:G:333:GLN:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ALA:O	1:B:22:ILE:HB	2.18	0.43
1:C:130:SER:HB2	3:C:404:FAD:O2A	2.18	0.43
1:E:126:PRO:HA	1:F:338:TYR:OH	2.17	0.43
1:D:52:PRO:HG3	1:D:67:TYR:CG	2.54	0.43
1:E:333:GLN:HG2	1:F:364:GLU:OE1	2.18	0.43
1:G:94:ASN:N	1:G:95:PRO:CD	2.81	0.43
1:H:256:LEU:HA	1:H:286:MET:HE2	2.00	0.43
1:B:255:ALA:HB1	1:B:328:ALA:HB1	2.00	0.43
1:H:328:ALA:HA	1:H:330:ASP:H	1.83	0.43
1:A:83:VAL:CG1	1:A:359:TYR:OH	2.62	0.43
1:B:80:ALA:O	1:B:83:VAL:HG12	2.19	0.43
1:C:255:ALA:HB1	1:C:328:ALA:HB1	2.01	0.43
1:F:67:TYR:CZ	1:F:71:ILE:HD11	2.54	0.43
1:C:48:LEU:C	1:C:49:MET:O	2.51	0.43
1:E:256:LEU:HA	1:E:286:MET:HE2	2.01	0.43
1:E:67:TYR:CZ	1:E:71:ILE:HD11	2.53	0.43
1:F:256:LEU:HA	1:F:286:MET:HE2	2.01	0.43
1:F:330:ASP:O	1:F:333:GLN:HB3	2.19	0.43
1:H:330:ASP:O	1:H:333:GLN:HB3	2.19	0.43
1:H:52:PRO:HG3	1:H:67:TYR:CG	2.54	0.43
1:E:200:LEU:O	1:E:351:ARG:HD2	2.18	0.42
1:E:316:MET:HG2	1:H:288:THR:OG1	2.18	0.42
1:E:330:ASP:O	1:E:333:GLN:HB3	2.19	0.42
1:H:94:ASN:N	1:H:95:PRO:CD	2.82	0.42
1:A:64:VAL:O	1:A:68:ILE:HG12	2.19	0.42
1:C:341:MET:HE3	1:D:154:PHE:CD1	2.54	0.42
1:D:94:ASN:N	1:D:95:PRO:CD	2.82	0.42
1:D:256:LEU:HA	1:D:286:MET:HE2	2.01	0.42
1:D:330:ASP:O	1:D:333:GLN:HB3	2.20	0.42
1:F:328:ALA:HA	1:F:330:ASP:H	1.84	0.42
1:B:209:GLU:HG2	1:B:210:LEU:N	2.34	0.42
1:C:256:LEU:HA	1:C:286:MET:HE2	2.01	0.42
1:D:67:TYR:CZ	1:D:71:ILE:HD11	2.54	0.42
1:F:71:ILE:HD13	1:F:86:SER:OG	2.19	0.42
1:B:94:ASN:N	1:B:95:PRO:CD	2.83	0.42
1:D:174:GLN:HG3	1:H:176:ARG:NH1	2.35	0.42
1:A:368:LEU:HD13	1:D:277:GLN:HE21	1.84	0.42
1:E:289:ARG:HH21	1:E:289:ARG:HD3	1.72	0.42
1:G:72:HIS:CD2	1:G:72:HIS:C	2.98	0.42
1:A:262:TYR:CE2	1:A:335:TYR:HA	2.55	0.42
1:G:63:ASP:CG	1:G:305:ASN:OD1	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:LEU:HA	1:A:286:MET:HE2	2.01	0.42
1:D:359:TYR:HD2	3:D:402:FAD:C6	2.33	0.42
1:H:22:ILE:HG23	1:H:81:VAL:HG11	2.01	0.42
1:H:209:GLU:HG2	1:H:210:LEU:N	2.34	0.42
1:D:343:ASP:OD1	1:D:344:TYR:CD2	2.73	0.41
1:F:310:CYS:O	1:F:310:CYS:SG	2.78	0.41
1:F:316:MET:HG2	1:G:288:THR:OG1	2.20	0.41
1:G:87:VAL:O	1:G:89:THR:O	2.38	0.41
1:G:121:PHE:CE1	1:G:167:PHE:HE2	2.37	0.41
1:B:330:ASP:O	1:B:333:GLN:HB3	2.20	0.41
1:F:94:ASN:N	1:F:95:PRO:CD	2.83	0.41
1:F:309:ASN:O	1:F:310:CYS:SG	2.79	0.41
1:G:121:PHE:CE1	1:G:167:PHE:CE2	3.08	0.41
1:A:10:MET:HE3	1:A:14:VAL:CG2	2.51	0.41
1:F:230:PHE:O	1:F:231:HIS:CB	2.68	0.41
1:G:255:ALA:HB1	1:G:328:ALA:HB1	2.03	0.41
1:B:336:GLY:HA2	1:B:339:GLY:H	1.85	0.41
1:B:140:ILE:HD11	1:B:147:LEU:HD23	2.03	0.41
3:C:404:FAD:C8A	1:D:273:ILE:HG22	2.51	0.41
1:G:125:GLU:HG2	1:G:152:LYS:HD3	2.03	0.41
1:G:209:GLU:HG2	1:G:210:LEU:N	2.36	0.41
1:H:124:THR:OG1	3:H:402:FAD:N1	2.34	0.41
1:B:326:VAL:HG21	1:B:357:GLN:OE1	2.22	0.40
1:B:326:VAL:C	1:B:328:ALA:N	2.79	0.40
1:D:209:GLU:HG2	1:D:210:LEU:N	2.35	0.40
1:G:120:ALA:O	1:G:121:PHE:CB	2.68	0.40
1:C:341:MET:HE3	1:D:154:PHE:CE1	2.56	0.40
1:A:51:ILE:N	1:A:52:PRO:CD	2.84	0.40
1:A:326:VAL:C	1:A:328:ALA:N	2.80	0.40
1:D:64:VAL:CG1	1:D:305:ASN:HB2	2.51	0.40
1:E:10:MET:HE3	1:E:14:VAL:CG2	2.51	0.40
1:A:41:LYS:HE3	1:A:41:LYS:HB2	2.00	0.40
1:B:67:TYR:CZ	1:B:71:ILE:HD11	2.55	0.40
1:C:326:VAL:HG21	1:C:357:GLN:OE1	2.22	0.40
1:E:334:ILE:O	3:F:402:FAD:H4B	2.22	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	359/379 (95%)	340 (95%)	14 (4%)	5 (1%)	9	19
1	B	368/379 (97%)	355 (96%)	13 (4%)	0	100	100
1	C	354/379 (93%)	332 (94%)	22 (6%)	0	100	100
1	D	368/379 (97%)	345 (94%)	23 (6%)	0	100	100
1	E	360/379 (95%)	339 (94%)	21 (6%)	0	100	100
1	F	362/379 (96%)	343 (95%)	16 (4%)	3 (1%)	16	34
1	G	361/379 (95%)	340 (94%)	21 (6%)	0	100	100
1	H	372/379 (98%)	353 (95%)	19 (5%)	0	100	100
All	All	2904/3032 (96%)	2747 (95%)	149 (5%)	8 (0%)	36	58

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	64	VAL
1	A	130	SER
1	F	309	ASN
1	A	206	ASN
1	A	264	LYS
1	F	230	PHE
1	F	231	HIS

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	259/291 (89%)	255 (98%)	4 (2%)	57	80
1	B	252/291 (87%)	248 (98%)	4 (2%)	55	79
1	C	238/291 (82%)	236 (99%)	2 (1%)	73	88
1	D	259/291 (89%)	254 (98%)	5 (2%)	50	75
1	E	240/291 (82%)	238 (99%)	2 (1%)	73	88
1	F	242/291 (83%)	235 (97%)	7 (3%)	37	65
1	G	233/291 (80%)	227 (97%)	6 (3%)	40	68
1	H	247/291 (85%)	244 (99%)	3 (1%)	63	83
All	All	1970/2328 (85%)	1937 (98%)	33 (2%)	53	78

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	ILE
1	A	206	ASN
1	A	216	GLU
1	A	347	GLU
1	B	140	ILE
1	B	241	ARG
1	B	355	VAL
1	B	372	LYS
1	C	106	MET
1	C	347	GLU
1	D	68	ILE
1	D	239	VAL
1	D	265	GLN
1	D	289	ARG
1	D	359	TYR
1	E	343	ASP
1	E	347	GLU
1	F	86	SER
1	F	87	VAL
1	F	230	PHE
1	F	310	CYS
1	F	343	ASP
1	F	347	GLU
1	F	364	GLU
1	G	41	LYS
1	G	76	ARG
1	G	176	ARG

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Mol	Chain	Res	Type
1	G	308	LEU
1	G	347	GLU
1	G	359	TYR
1	H	89	THR
1	H	271	ARG
1	H	347	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	B	127	HIS
1	B	363	ASN
1	C	127	HIS
1	D	111	ASN
1	D	177	HIS
1	F	127	HIS
1	F	174	GLN
1	F	363	ASN
1	G	363	ASN
1	H	7	GLN
1	H	187	ASN
1	H	231	HIS
1	H	236	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

19 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
2	GOL	G	402	-	5,5,5	0.65	0	5,5,5	0.58	0
3	FAD	A	404	-	58,58,58	1.50	9 (15%)	85,89,89	1.93	27 (31%)
2	GOL	H	401	-	5,5,5	0.46	0	5,5,5	0.12	0
2	GOL	C	402	-	5,5,5	0.42	0	5,5,5	0.31	0
2	GOL	G	401	-	5,5,5	0.74	0	5,5,5	0.61	0
2	GOL	D	401	-	5,5,5	0.32	0	5,5,5	0.46	0
3	FAD	F	402	-	58,58,58	1.84	11 (18%)	85,89,89	1.65	19 (22%)
2	GOL	A	402	-	5,5,5	0.44	0	5,5,5	0.72	0
2	GOL	C	403	-	5,5,5	0.27	0	5,5,5	0.64	0
3	FAD	D	402	-	58,58,58	1.62	13 (22%)	85,89,89	1.84	24 (28%)
2	GOL	C	401	-	5,5,5	0.82	0	5,5,5	0.96	0
3	FAD	C	404	-	58,58,58	1.50	8 (13%)	85,89,89	1.63	18 (21%)
2	GOL	F	401	-	5,5,5	0.51	0	5,5,5	0.18	0
3	FAD	B	401	-	58,58,58	1.65	8 (13%)	85,89,89	1.83	24 (28%)
3	FAD	G	403	-	58,58,58	1.58	11 (18%)	85,89,89	2.06	28 (32%)
2	GOL	A	403	-	5,5,5	0.40	0	5,5,5	0.61	0
3	FAD	H	402	-	58,58,58	1.61	10 (17%)	85,89,89	1.91	24 (28%)
2	GOL	A	401	-	5,5,5	0.45	0	5,5,5	0.88	0
3	FAD	E	401	-	58,58,58	1.65	12 (20%)	85,89,89	1.89	22 (25%)

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	GOL	G	402	-	-	2/4/4/4	-
3	FAD	A	404	-	-	6/34/50/50	0/6/6/6
2	GOL	H	401	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	C	402	-	-	2/4/4/4	-
2	GOL	G	401	-	-	0/4/4/4	-
2	GOL	D	401	-	-	2/4/4/4	-
3	FAD	F	402	-	-	3/34/50/50	0/6/6/6
2	GOL	A	402	-	-	2/4/4/4	-
2	GOL	C	403	-	-	2/4/4/4	-
3	FAD	D	402	-	-	4/34/50/50	0/6/6/6
2	GOL	C	401	-	-	1/4/4/4	-
3	FAD	C	404	-	-	4/34/50/50	0/6/6/6
2	GOL	F	401	-	-	4/4/4/4	-
3	FAD	B	401	-	-	4/34/50/50	0/6/6/6
3	FAD	G	403	-	-	11/34/50/50	0/6/6/6
2	GOL	A	403	-	-	2/4/4/4	-
3	FAD	H	402	-	-	10/34/50/50	0/6/6/6
2	GOL	A	401	-	-	0/4/4/4	-
3	FAD	E	401	-	-	4/34/50/50	0/6/6/6

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	402	FAD	P-O3P	6.07	1.66	1.59
3	H	402	FAD	C9A-C5X	5.69	1.50	1.41
3	B	401	FAD	C1'-C2'	5.69	1.60	1.52
3	F	402	FAD	C9A-C5X	5.61	1.50	1.41
3	G	403	FAD	C5A-C4A	5.35	1.48	1.39
3	E	401	FAD	P-O3P	5.33	1.65	1.59
3	A	404	FAD	C5A-C4A	5.31	1.48	1.39
3	C	404	FAD	C9A-C5X	5.28	1.49	1.41
3	F	402	FAD	C5A-C4A	4.99	1.48	1.39
3	B	401	FAD	C9A-C5X	4.93	1.49	1.41
3	D	402	FAD	C9A-C5X	4.82	1.48	1.41
3	E	401	FAD	C9A-C5X	4.76	1.48	1.41
3	D	402	FAD	C5A-C4A	4.70	1.47	1.39
3	A	404	FAD	C9A-C5X	4.61	1.48	1.41
3	C	404	FAD	C5A-C4A	4.51	1.47	1.39
3	B	401	FAD	C5A-C4A	4.45	1.47	1.39
3	H	402	FAD	C5A-C4A	4.38	1.46	1.39
3	E	401	FAD	C5A-C4A	4.19	1.46	1.39
3	F	402	FAD	C1'-C2'	4.16	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	402	FAD	C8-C7	3.88	1.50	1.40
3	G	403	FAD	C9A-N10	3.68	1.47	1.41
3	E	401	FAD	C4A-N9A	-3.66	1.30	1.37
3	E	401	FAD	PA-O3P	3.55	1.63	1.59
3	G	403	FAD	C9A-C5X	3.45	1.46	1.41
3	D	402	FAD	C8-C7	3.44	1.49	1.40
3	F	402	FAD	C8-C7	3.35	1.49	1.40
3	G	403	FAD	C5X-N5	-3.22	1.33	1.39
3	B	401	FAD	C8-C7	3.22	1.48	1.40
3	E	401	FAD	C8-C7	3.08	1.48	1.40
3	H	402	FAD	C8A-N7A	3.04	1.37	1.31
3	C	404	FAD	P-O3P	2.97	1.62	1.59
3	D	402	FAD	C8A-N7A	2.95	1.37	1.31
3	A	404	FAD	C8-C7	2.95	1.48	1.40
3	B	401	FAD	C4A-N9A	-2.92	1.31	1.37
3	H	402	FAD	C4-N3	-2.89	1.33	1.38
3	A	404	FAD	C5A-C6A	2.88	1.49	1.41
3	A	404	FAD	C5X-N5	-2.84	1.34	1.39
3	G	403	FAD	C8A-N7A	2.77	1.37	1.31
3	D	402	FAD	PA-O3P	2.76	1.62	1.59
3	G	403	FAD	C5A-C6A	2.75	1.48	1.41
3	G	403	FAD	C8-C7	2.70	1.47	1.40
3	H	402	FAD	C5A-C6A	2.68	1.48	1.41
3	F	402	FAD	C5A-C6A	2.67	1.48	1.41
3	D	402	FAD	C5'-C4'	2.64	1.55	1.51
3	F	402	FAD	C5'-C4'	2.59	1.55	1.51
3	A	404	FAD	C8A-N7A	2.54	1.36	1.31
3	C	404	FAD	C4A-N9A	-2.51	1.32	1.37
3	F	402	FAD	C8A-N7A	2.51	1.36	1.31
3	C	404	FAD	C8-C7	2.50	1.47	1.40
3	C	404	FAD	C4-N3	-2.49	1.34	1.38
3	G	403	FAD	C4A-N9A	-2.47	1.32	1.37
3	A	404	FAD	C4A-N9A	-2.46	1.32	1.37
3	D	402	FAD	P-O3P	2.43	1.62	1.59
3	B	401	FAD	C5A-N7A	-2.42	1.34	1.39
3	E	401	FAD	O4-C4	2.42	1.28	1.23
3	C	404	FAD	C5A-C6A	2.41	1.47	1.41
3	D	402	FAD	C4-N3	-2.40	1.34	1.38
3	G	403	FAD	C2-N3	-2.37	1.33	1.39
3	H	402	FAD	C5X-N5	-2.35	1.35	1.39
3	H	402	FAD	C4A-N9A	-2.32	1.32	1.37
3	F	402	FAD	C2-N3	-2.32	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	404	FAD	C8A-N7A	2.30	1.36	1.31
3	H	402	FAD	P-O3P	2.27	1.62	1.59
3	E	401	FAD	C4X-N5	2.26	1.35	1.30
3	F	402	FAD	PA-O3P	2.25	1.61	1.59
3	G	403	FAD	C4-N3	-2.25	1.34	1.38
3	E	401	FAD	C8A-N7A	2.24	1.36	1.31
3	E	401	FAD	C1'-C2'	2.22	1.55	1.52
3	D	402	FAD	C10-N10	2.22	1.42	1.37
3	A	404	FAD	PA-O3P	2.18	1.61	1.59
3	D	402	FAD	C4X-N5	2.18	1.35	1.30
3	F	402	FAD	C10-N10	2.17	1.42	1.37
3	D	402	FAD	C5A-C6A	2.16	1.47	1.41
3	B	401	FAD	C5A-C6A	2.14	1.47	1.41
3	G	403	FAD	C10-N10	2.13	1.41	1.37
3	D	402	FAD	C4A-N9A	-2.12	1.33	1.37
3	A	404	FAD	C4-N3	-2.11	1.34	1.38
3	H	402	FAD	C5A-N7A	-2.07	1.35	1.39
3	E	401	FAD	C5A-C6A	2.04	1.46	1.41
3	D	402	FAD	C5X-N5	-2.03	1.35	1.39
3	B	401	FAD	C8A-N7A	2.03	1.35	1.31
3	E	401	FAD	C5A-N7A	-2.01	1.35	1.39

All (186) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	401	FAD	C4A-N9A-C8A	5.93	111.96	105.74
3	F	402	FAD	C5A-C4A-N3A	-5.39	119.29	126.72
3	D	402	FAD	N3A-C2A-N1A	-5.35	120.48	128.58
3	G	403	FAD	N3A-C2A-N1A	-5.27	120.60	128.58
3	E	401	FAD	N3A-C2A-N1A	-5.25	120.64	128.58
3	H	402	FAD	N3A-C2A-N1A	-5.06	120.92	128.58
3	C	404	FAD	C5A-C4A-N3A	-4.64	120.33	126.72
3	G	403	FAD	C2A-N1A-C6A	4.62	126.33	118.73
3	H	402	FAD	C4A-N9A-C8A	4.59	110.56	105.74
3	F	402	FAD	N3A-C4A-N9A	4.58	134.96	127.17
3	A	404	FAD	C5A-C4A-N3A	-4.48	120.55	126.72
3	D	402	FAD	C5A-C4A-N3A	-4.44	120.61	126.72
3	H	402	FAD	O4B-C1B-N9A	4.43	116.60	108.09
3	C	404	FAD	N3A-C2A-N1A	-4.34	122.02	128.58
3	G	403	FAD	O4B-C1B-N9A	4.32	116.38	108.09
3	D	402	FAD	C4A-N9A-C8A	4.28	110.23	105.74
3	D	402	FAD	O3P-P-O1P	-4.26	97.90	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	FAD	C5A-C4A-N3A	-4.26	120.86	126.72
3	C	404	FAD	N3A-C4A-N9A	4.25	134.40	127.17
3	B	401	FAD	N3A-C2A-N1A	-4.24	122.16	128.58
3	A	404	FAD	N3A-C2A-N1A	-4.15	122.31	128.58
3	G	403	FAD	C4'-C3'-C2'	4.13	120.45	113.57
3	B	401	FAD	O4'-C4'-C5'	-4.08	100.98	109.99
3	H	402	FAD	C5A-C4A-N3A	-4.03	121.17	126.72
3	F	402	FAD	C2A-N3A-C4A	4.03	121.67	111.83
3	H	402	FAD	C2A-N3A-C4A	4.01	121.62	111.83
3	E	401	FAD	C4A-N9A-C1B	-4.00	117.28	126.63
3	D	402	FAD	C2A-N3A-C4A	3.97	121.52	111.83
3	C	404	FAD	C4A-N9A-C8A	3.92	109.85	105.74
3	C	404	FAD	C2A-N3A-C4A	3.91	121.37	111.83
3	H	402	FAD	N9A-C8A-N7A	-3.86	108.46	113.94
3	D	402	FAD	N3A-C4A-N9A	3.85	133.72	127.17
3	B	401	FAD	O2-C2-N1	-3.85	115.41	121.80
3	F	402	FAD	N3A-C2A-N1A	-3.79	122.85	128.58
3	B	401	FAD	C4'-C3'-C2'	3.78	119.86	113.57
3	G	403	FAD	C6A-C5A-N7A	3.77	139.36	132.09
3	A	404	FAD	C2A-N3A-C4A	3.76	121.00	111.83
3	E	401	FAD	C4-C4X-N5	3.74	123.38	118.21
3	A	404	FAD	C2B-C1B-N9A	3.71	122.52	113.30
3	G	403	FAD	C2A-N3A-C4A	3.67	120.79	111.83
3	A	404	FAD	C4A-N9A-C8A	3.66	109.59	105.74
3	A	404	FAD	O4-C4-C4X	-3.66	116.88	126.53
3	A	404	FAD	N3A-C4A-N9A	3.64	133.35	127.17
3	H	402	FAD	N3A-C4A-N9A	3.61	133.31	127.17
3	G	403	FAD	O4-C4-C4X	-3.57	117.10	126.53
3	G	403	FAD	C5A-C4A-N3A	-3.57	121.80	126.72
3	B	401	FAD	C2A-N3A-C4A	3.56	120.53	111.83
3	A	404	FAD	C4A-C5A-N7A	-3.53	106.54	110.58
3	B	401	FAD	N3A-C4A-N9A	3.53	133.17	127.17
3	E	401	FAD	N9A-C8A-N7A	-3.52	108.94	113.94
3	E	401	FAD	C2A-N3A-C4A	3.50	120.37	111.83
3	A	404	FAD	O2-C2-N1	-3.49	116.00	121.80
3	E	401	FAD	O2-C2-N1	-3.47	116.03	121.80
3	G	403	FAD	C6-C5X-C9A	3.45	123.78	119.05
3	B	401	FAD	C4X-C10-N10	3.43	121.39	116.48
3	E	401	FAD	N3A-C4A-N9A	3.42	132.98	127.17
3	G	403	FAD	C4A-N9A-C1B	-3.39	118.70	126.63
3	D	402	FAD	C2A-N1A-C6A	3.38	124.29	118.73
3	G	403	FAD	C4X-C10-N1	-3.36	116.34	124.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	404	FAD	C4'-C3'-C2'	3.33	119.11	113.57
3	G	403	FAD	C9A-C5X-N5	-3.33	118.92	122.45
3	H	402	FAD	C4A-N9A-C1B	-3.29	118.94	126.63
3	A	404	FAD	O4'-C4'-C5'	-3.28	102.76	109.99
3	A	404	FAD	C6A-C5A-N7A	3.26	138.37	132.09
3	E	401	FAD	C6A-C5A-N7A	3.25	138.35	132.09
3	D	402	FAD	C4A-C5A-N7A	-3.21	106.91	110.58
3	D	402	FAD	C6A-C5A-N7A	3.20	138.27	132.09
3	H	402	FAD	C5'-C4'-C3'	-3.18	106.22	112.22
3	H	402	FAD	C6A-C5A-N7A	3.10	138.07	132.09
3	G	403	FAD	C4A-C5A-N7A	-3.10	107.03	110.58
3	E	401	FAD	C6A-C5A-C4A	-3.01	113.07	117.18
3	G	403	FAD	C4-N3-C2	-3.01	120.30	125.64
3	E	401	FAD	C4'-C3'-C2'	3.01	118.57	113.57
3	D	402	FAD	N9A-C8A-N7A	-2.99	109.70	113.94
3	B	401	FAD	C4A-N9A-C8A	2.98	108.87	105.74
3	G	403	FAD	C5X-C9A-N10	2.98	120.66	117.97
3	B	401	FAD	O4'-C4'-C3'	2.96	116.19	109.25
3	G	403	FAD	C4A-N9A-C8A	2.96	108.85	105.74
3	H	402	FAD	O2A-PA-O1A	2.96	126.21	112.44
3	H	402	FAD	C4X-C10-N10	2.95	120.71	116.48
3	E	401	FAD	C4X-C10-N10	2.93	120.68	116.48
3	H	402	FAD	C5A-N7A-C8A	2.92	108.04	103.45
3	D	402	FAD	C4X-C10-N1	-2.89	117.51	124.59
3	B	401	FAD	C2A-N1A-C6A	2.88	123.47	118.73
3	B	401	FAD	O2A-PA-O1A	2.88	125.83	112.44
3	F	402	FAD	C4-C4X-N5	2.83	122.12	118.21
3	E	401	FAD	C2A-N1A-C6A	2.82	123.37	118.73
3	E	401	FAD	C5A-C4A-N3A	-2.79	122.88	126.72
3	G	403	FAD	C5X-N5-C4X	2.79	122.60	118.09
3	H	402	FAD	C4A-C5A-N7A	-2.78	107.41	110.58
3	B	401	FAD	C4-C4X-N5	2.77	122.03	118.21
3	H	402	FAD	O3'-C3'-C4'	-2.77	102.64	108.93
3	G	403	FAD	C9-C9A-C5X	-2.76	115.15	120.03
3	A	404	FAD	N9A-C8A-N7A	-2.75	110.03	113.94
3	A	404	FAD	O3'-C3'-C2'	-2.74	102.70	108.93
3	D	402	FAD	O5'-C5'-C4'	2.73	116.66	109.36
3	G	403	FAD	N3A-C4A-N9A	2.73	131.81	127.17
3	F	402	FAD	C4A-N9A-C8A	2.72	108.60	105.74
3	A	404	FAD	O4-C4-N3	2.67	125.14	120.11
3	A	404	FAD	C9A-N10-C10	-2.67	116.68	120.75
3	G	403	FAD	C9A-N10-C10	-2.64	116.73	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	401	FAD	C10-C4X-N5	-2.63	119.43	124.81
3	G	403	FAD	C6A-C5A-C4A	-2.63	113.59	117.18
3	B	401	FAD	C4X-C10-N1	-2.62	118.16	124.59
3	B	401	FAD	C4A-C5A-N7A	-2.60	107.61	110.58
3	C	404	FAD	C4A-C5A-N7A	-2.59	107.62	110.58
3	A	404	FAD	C4X-C10-N1	-2.59	118.25	124.59
3	A	404	FAD	C5A-N7A-C8A	2.59	107.51	103.45
3	F	402	FAD	C4X-C10-N1	-2.58	118.25	124.59
3	D	402	FAD	C4A-N9A-C1B	-2.58	120.60	126.63
3	F	402	FAD	C4'-C3'-C2'	2.58	117.86	113.57
3	C	404	FAD	C9A-C5X-N5	-2.57	119.73	122.45
3	A	404	FAD	C1'-N10-C9A	2.57	125.62	120.63
3	H	402	FAD	C4X-C10-N1	-2.56	118.32	124.59
3	D	402	FAD	O2-C2-N1	-2.56	117.56	121.80
3	B	401	FAD	C4-N3-C2	-2.55	121.12	125.64
3	G	403	FAD	O5B-C5B-C4B	2.53	117.60	108.99
3	C	404	FAD	C4X-C10-N1	-2.53	118.40	124.59
3	D	402	FAD	C5A-N7A-C8A	2.52	107.42	103.45
3	G	403	FAD	O4B-C4B-C5B	-2.52	101.27	109.33
3	H	402	FAD	O2-C2-N1	-2.51	117.64	121.80
3	C	404	FAD	C5X-C9A-N10	2.51	120.23	117.97
3	F	402	FAD	C4A-C5A-N7A	-2.50	107.72	110.58
3	F	402	FAD	C6A-C5A-N7A	2.47	136.85	132.09
3	G	403	FAD	N10-C10-N1	2.47	125.78	118.51
3	E	401	FAD	C10-N1-C2	2.47	122.19	116.85
3	A	404	FAD	O2A-PA-O1A	2.46	123.90	112.44
3	C	404	FAD	O2A-PA-O1A	2.46	123.89	112.44
3	A	404	FAD	C6-C5X-C9A	2.46	122.43	119.05
3	A	404	FAD	C2A-N1A-C6A	2.45	122.75	118.73
3	F	402	FAD	O2P-P-O3P	2.45	113.89	107.27
3	B	401	FAD	O3P-P-O1P	-2.44	103.35	110.70
3	D	402	FAD	O2A-PA-O1A	2.44	123.79	112.44
3	H	402	FAD	C2A-N1A-C6A	2.43	122.72	118.73
3	E	401	FAD	C5X-N5-C4X	2.43	122.01	118.09
3	C	404	FAD	C6A-C5A-N7A	2.42	136.75	132.09
3	A	404	FAD	C4X-C10-N10	2.42	119.94	116.48
3	B	401	FAD	C9A-N10-C10	-2.41	117.07	120.75
3	F	402	FAD	O5B-PA-O1A	-2.39	99.48	108.94
3	E	401	FAD	C4X-C10-N1	-2.37	118.78	124.59
3	G	403	FAD	C1B-N9A-C8A	2.37	132.35	127.09
3	B	401	FAD	O4-C4-C4X	-2.35	120.34	126.53
3	D	402	FAD	C4X-C10-N10	2.35	119.84	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	FAD	C6A-C5A-N7A	2.33	136.58	132.09
3	F	402	FAD	C4X-C10-N10	2.32	119.81	116.48
3	F	402	FAD	C5X-N5-C4X	2.32	121.84	118.09
3	A	404	FAD	C4A-N9A-C1B	-2.31	121.22	126.63
3	G	403	FAD	C4X-C4-N3	2.29	119.08	113.25
3	F	402	FAD	O2B-C2B-C1B	2.26	117.89	110.10
3	B	401	FAD	O3'-C3'-C2'	-2.25	103.82	108.93
3	D	402	FAD	C4-N3-C2	-2.24	121.66	125.64
3	B	401	FAD	C10-N1-C2	2.24	121.69	116.85
3	C	404	FAD	O4-C4-C4X	-2.21	120.69	126.53
3	C	404	FAD	C2A-N1A-C6A	2.21	122.35	118.73
3	F	402	FAD	C9A-C5X-N5	-2.20	120.11	122.45
3	H	402	FAD	C9A-N10-C10	-2.19	117.41	120.75
3	C	404	FAD	N9A-C8A-N7A	-2.19	110.83	113.94
3	C	404	FAD	C10-N1-C2	2.19	121.59	116.85
3	A	404	FAD	O2P-P-O1P	2.19	122.61	112.44
3	F	402	FAD	C10-N1-C2	2.18	121.56	116.85
3	H	402	FAD	C4'-C3'-C2'	2.17	117.17	113.57
3	F	402	FAD	O4B-C1B-N9A	2.16	112.24	108.09
3	G	403	FAD	O3P-P-O1P	-2.16	104.20	110.70
3	D	402	FAD	O4-C4-C4X	-2.16	120.83	126.53
3	A	404	FAD	C2B-C3B-C4B	2.16	106.78	102.61
3	E	401	FAD	O4'-C4'-C3'	2.16	114.29	109.25
3	F	402	FAD	C9A-N10-C10	-2.11	117.53	120.75
3	D	402	FAD	C7M-C7-C8	2.11	125.06	120.76
3	B	401	FAD	O2'-C2'-C1'	2.10	118.84	110.20
3	E	401	FAD	O2A-PA-O1A	2.10	122.22	112.44
3	B	401	FAD	C10-C4X-N5	-2.10	120.52	124.81
3	A	404	FAD	C4-N3-C2	-2.10	121.92	125.64
3	D	402	FAD	C9A-N10-C10	-2.09	117.56	120.75
3	H	402	FAD	C2B-C1B-N9A	-2.07	108.15	113.30
3	G	403	FAD	C1'-C2'-C3'	2.06	115.24	109.66
3	C	404	FAD	C9A-N10-C10	-2.05	117.62	120.75
3	E	401	FAD	O4'-C4'-C5'	-2.04	105.50	109.99
3	D	402	FAD	N3-C2-N1	2.04	123.83	119.50
3	C	404	FAD	C4X-C4-N3	2.03	118.43	113.25
3	E	401	FAD	O4-C4-C4X	-2.03	121.17	126.53
3	D	402	FAD	C10-N1-C2	2.03	121.24	116.85
3	H	402	FAD	O2B-C2B-C1B	2.02	117.07	110.10
3	H	402	FAD	N3-C2-N1	2.02	123.80	119.50
3	H	402	FAD	O2P-P-O1P	2.02	121.83	112.44
3	C	404	FAD	C4X-C10-N10	2.00	119.35	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	FAD	C7M-C7-C6	-2.00	116.05	119.57

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	403	GOL	O1-C1-C2-C3
2	D	401	GOL	C1-C2-C3-O3
2	F	401	GOL	C1-C2-C3-O3
2	G	402	GOL	O1-C1-C2-C3
2	H	401	GOL	O1-C1-C2-C3
3	A	404	FAD	C5B-O5B-PA-O1A
3	A	404	FAD	PA-O3P-P-O5'
3	C	404	FAD	C3'-C4'-C5'-O5'
3	C	404	FAD	O4'-C4'-C5'-O5'
3	C	404	FAD	C5'-O5'-P-O1P
3	C	404	FAD	C5'-O5'-P-O3P
3	G	403	FAD	C5B-O5B-PA-O3P
3	G	403	FAD	C5'-O5'-P-O1P
3	G	403	FAD	C5'-O5'-P-O3P
3	G	403	FAD	PA-O3P-P-O5'
3	E	401	FAD	O4B-C4B-C5B-O5B
3	H	402	FAD	O4B-C4B-C5B-O5B
3	B	401	FAD	O2'-C2'-C3'-C4'
3	D	402	FAD	O2'-C2'-C3'-C4'
2	A	402	GOL	O1-C1-C2-C3
2	F	401	GOL	O1-C1-C2-C3
2	H	401	GOL	O1-C1-C2-O2
3	H	402	FAD	O4'-C4'-C5'-O5'
3	E	401	FAD	C3B-C4B-C5B-O5B
3	F	402	FAD	O2'-C2'-C3'-C4'
3	H	402	FAD	C3B-C4B-C5B-O5B
3	B	401	FAD	C3'-C4'-C5'-O5'
3	H	402	FAD	C3'-C4'-C5'-O5'
2	A	402	GOL	O1-C1-C2-O2
2	A	403	GOL	O1-C1-C2-O2
2	D	401	GOL	O2-C2-C3-O3
2	F	401	GOL	O2-C2-C3-O3
2	G	402	GOL	O1-C1-C2-O2
3	B	401	FAD	O4'-C4'-C5'-O5'
3	A	404	FAD	C2'-C3'-C4'-O4'
3	B	401	FAD	O2'-C2'-C3'-O3'

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Mol	Chain	Res	Type	Atoms
3	D	402	FAD	PA-O3P-P-O5'
2	C	401	GOL	O1-C1-C2-O2
2	C	402	GOL	O2-C2-C3-O3
2	C	403	GOL	O2-C2-C3-O3
2	C	403	GOL	O1-C1-C2-C3
3	D	402	FAD	O2'-C2'-C3'-O3'
3	F	402	FAD	O2'-C2'-C3'-O3'
3	G	403	FAD	O4B-C4B-C5B-O5B
3	G	403	FAD	C4'-C5'-O5'-P
3	G	403	FAD	C5'-O5'-P-O2P
3	H	402	FAD	C5'-O5'-P-O3P
2	F	401	GOL	O1-C1-C2-O2
3	H	402	FAD	C2'-C3'-C4'-C5'
3	E	401	FAD	PA-O3P-P-O1P
3	E	401	FAD	PA-O3P-P-O2P
3	G	403	FAD	P-O3P-PA-O1A
3	G	403	FAD	P-O3P-PA-O2A
3	H	402	FAD	O2'-C2'-C3'-O3'
3	D	402	FAD	C4'-C5'-O5'-P
2	C	402	GOL	C1-C2-C3-O3
3	F	402	FAD	C4'-C5'-O5'-P
3	A	404	FAD	O3'-C3'-C4'-O4'
3	A	404	FAD	P-O3P-PA-O1A
3	G	403	FAD	PA-O3P-P-O1P
3	H	402	FAD	C2'-C3'-C4'-O4'
3	A	404	FAD	C2'-C3'-C4'-C5'
3	H	402	FAD	O3'-C3'-C4'-C5'
3	G	403	FAD	PA-O3P-P-O2P
3	H	402	FAD	PA-O3P-P-O2P

There are no ring outliers.

9 monomers are involved in 22 short contacts:

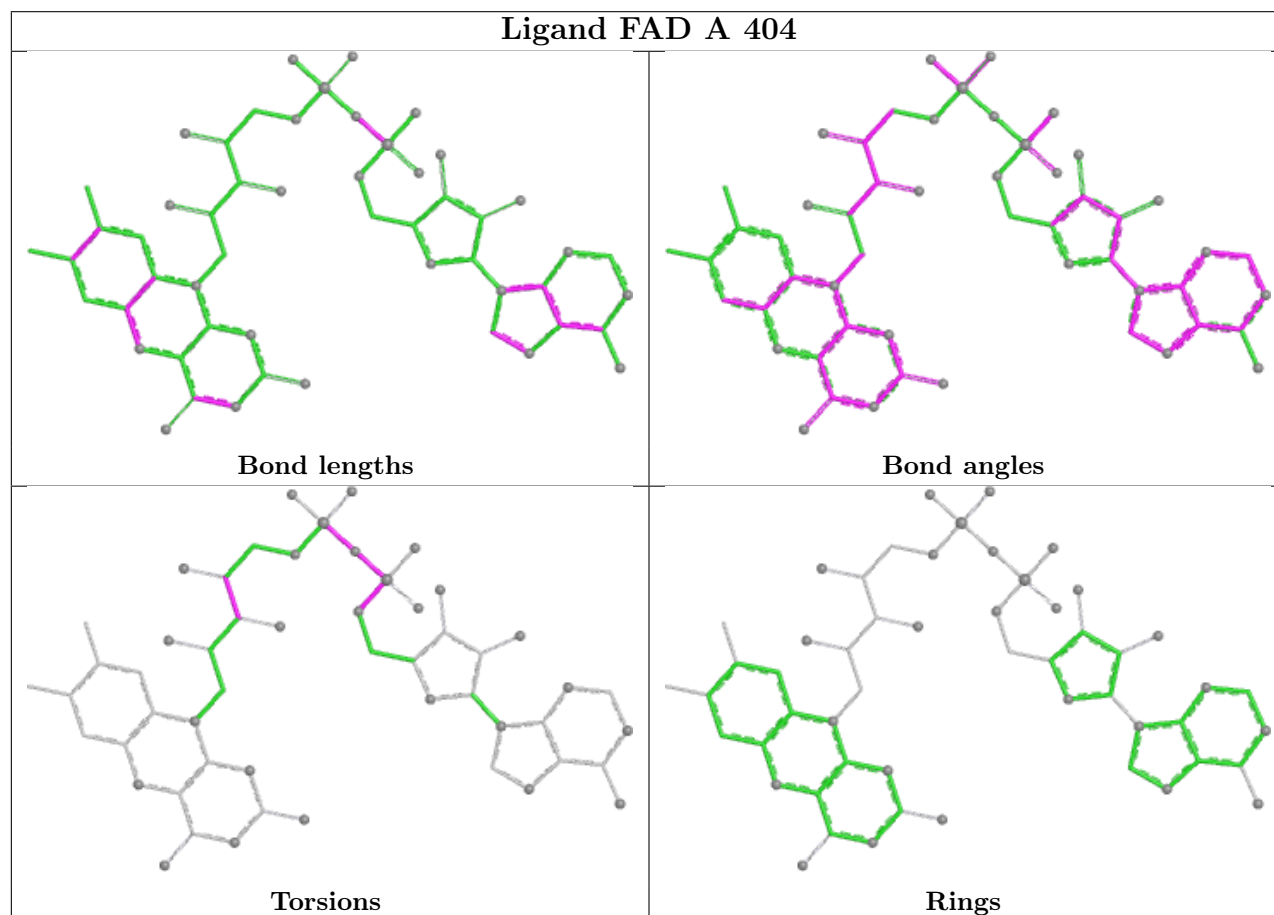
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	404	FAD	2	0
3	F	402	FAD	2	0
3	D	402	FAD	2	0
3	C	404	FAD	5	0
3	B	401	FAD	2	0
3	G	403	FAD	5	0
3	H	402	FAD	1	0
2	A	401	GOL	1	0

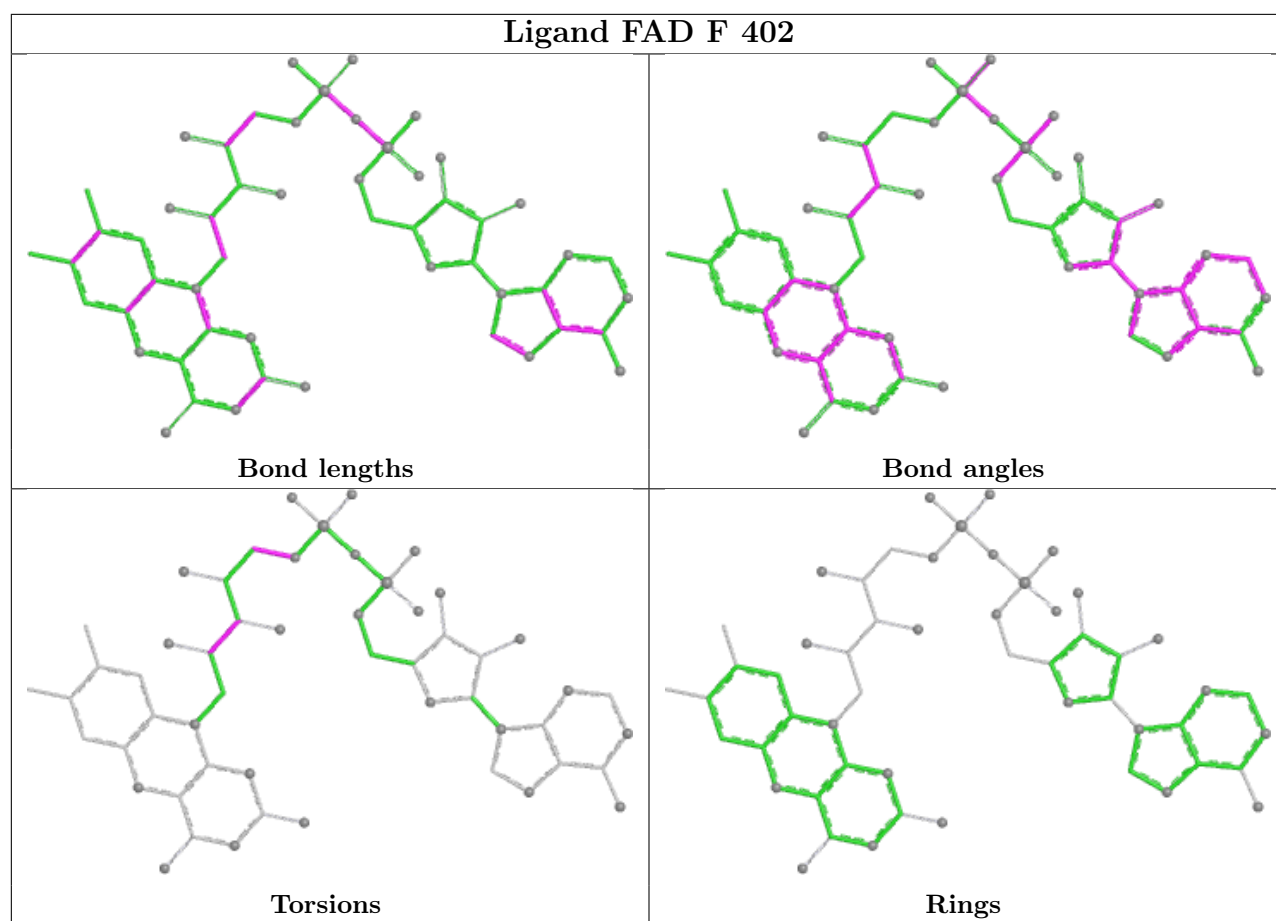
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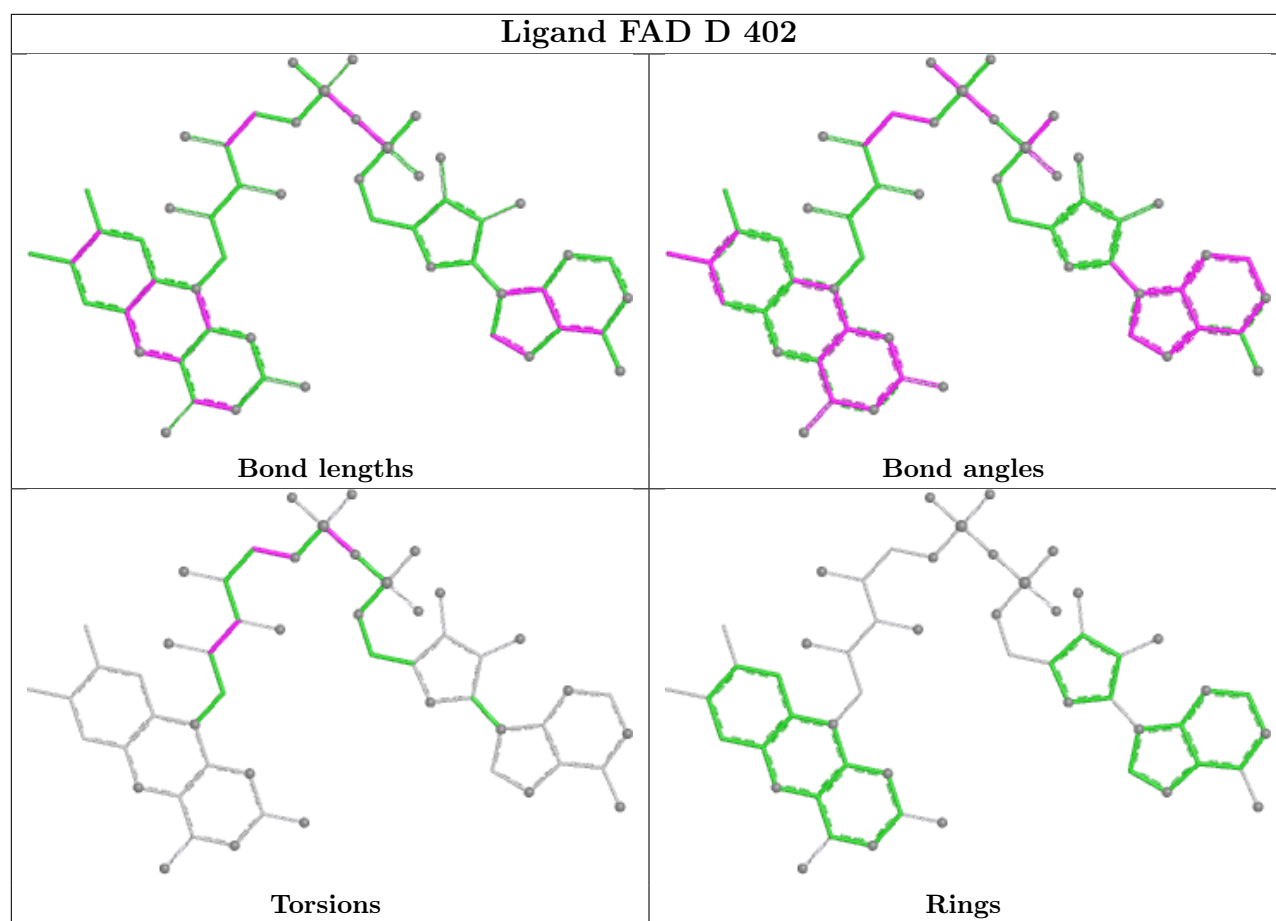
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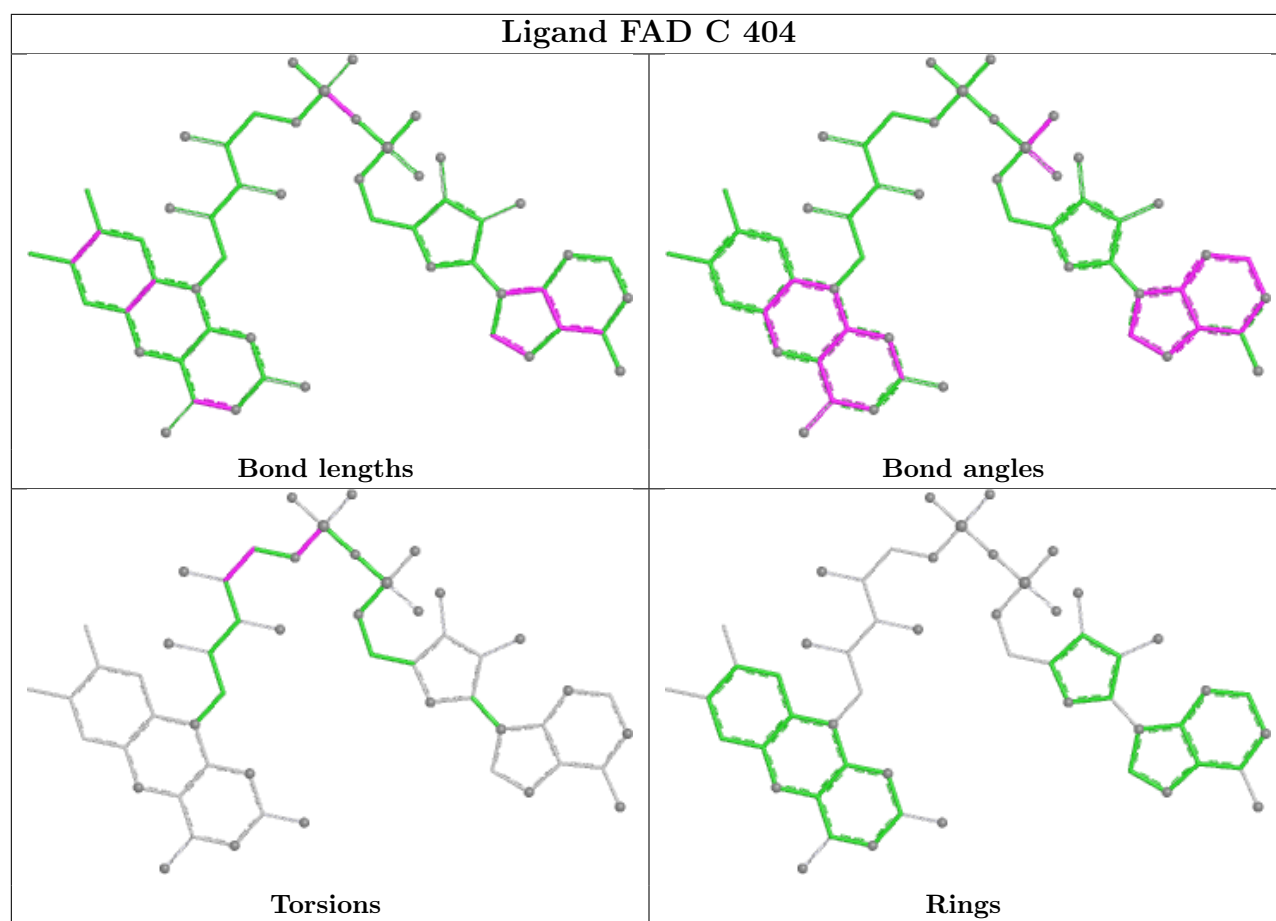
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	401	FAD	2	0

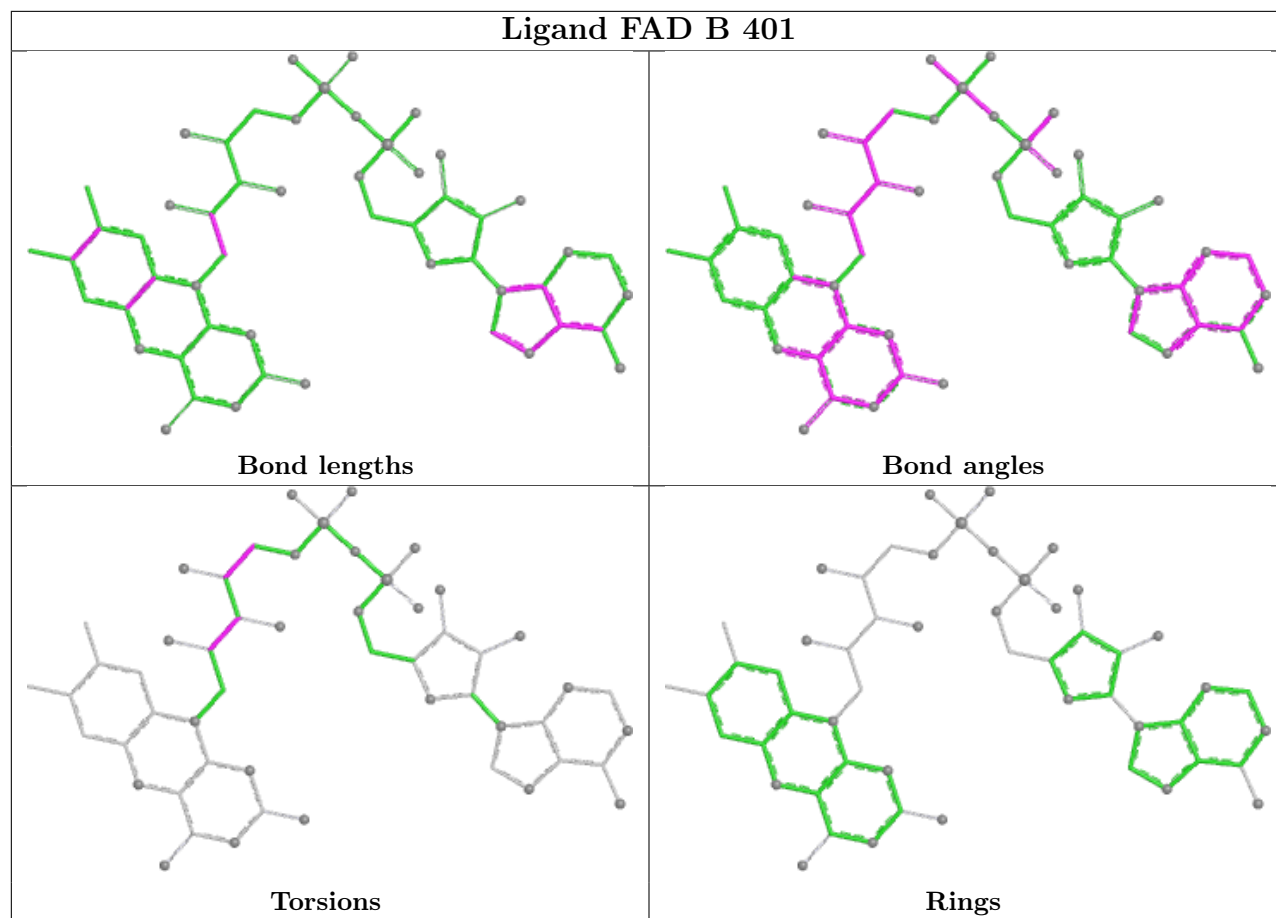
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

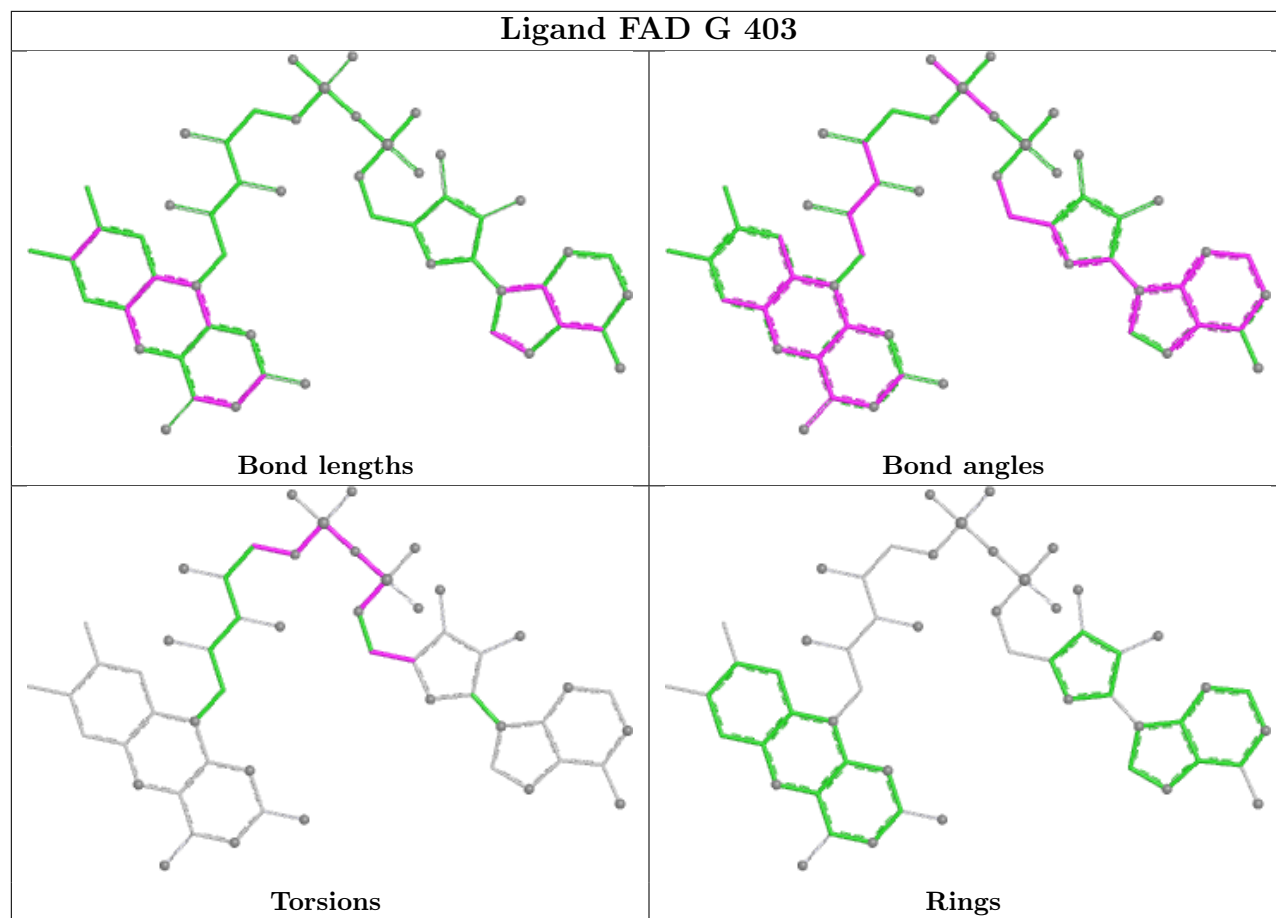


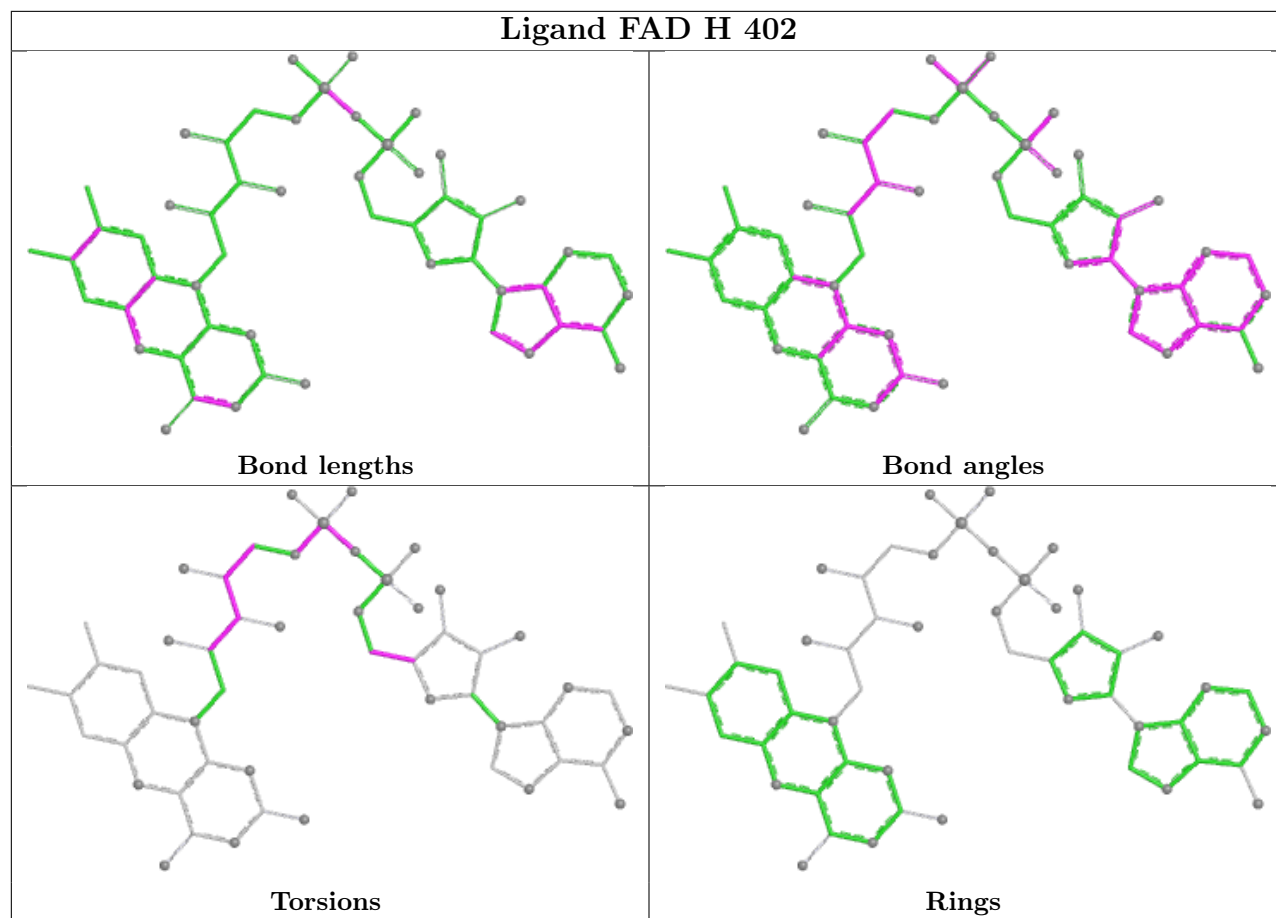


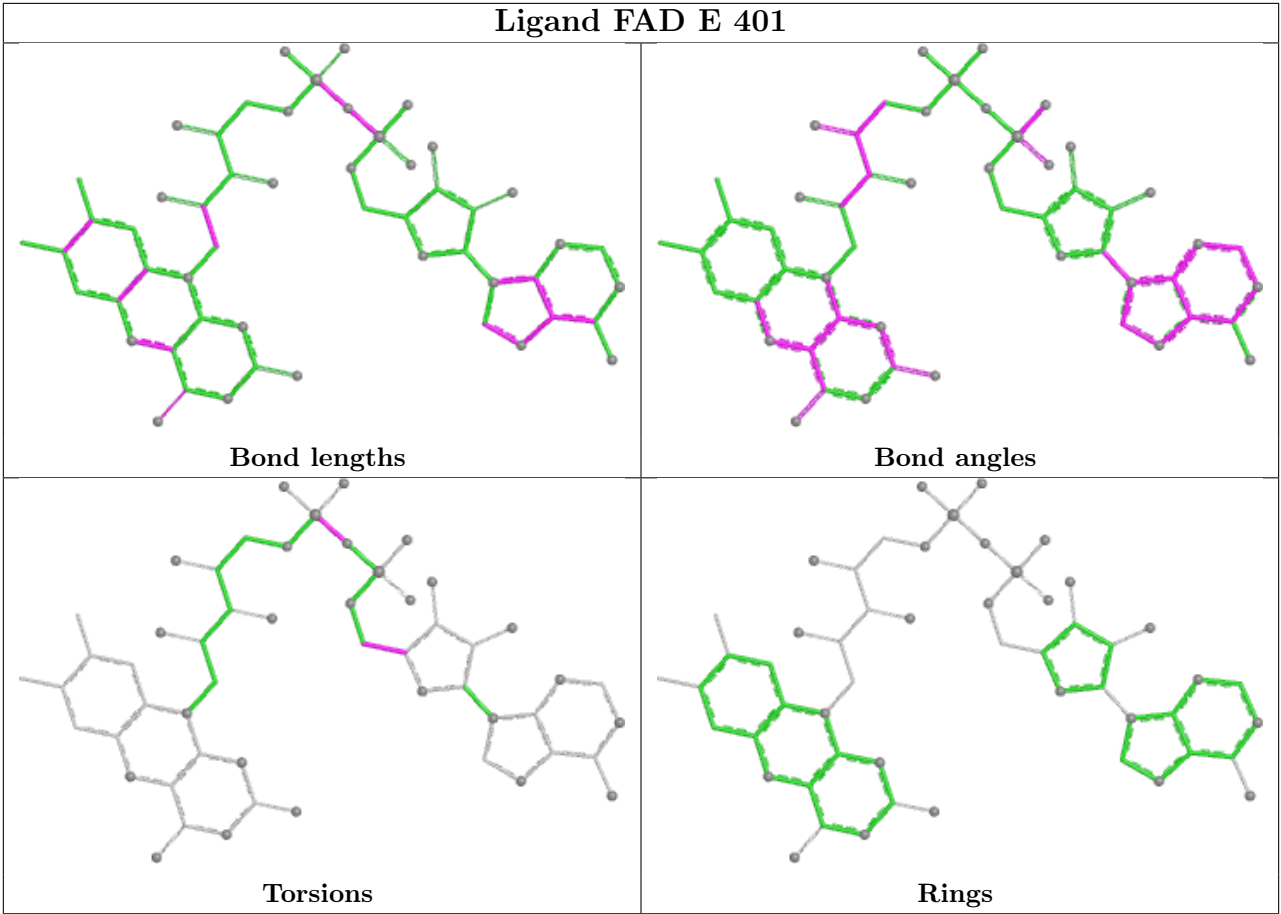












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	307:GLY	C	308:LEU	N	1.02

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	367/379 (96%)	-0.85	0 100 100	14, 30, 47, 65	0
1	B	372/379 (98%)	-0.75	0 100 100	14, 34, 58, 73	0
1	C	364/379 (96%)	-0.71	0 100 100	14, 36, 70, 95	0
1	D	374/379 (98%)	-0.77	0 100 100	15, 33, 50, 72	0
1	E	368/379 (97%)	-0.75	0 100 100	12, 34, 62, 89	0
1	F	372/379 (98%)	-0.76	0 100 100	15, 35, 58, 82	0
1	G	367/379 (96%)	-0.69	0 100 100	14, 38, 70, 98	0
1	H	374/379 (98%)	-0.81	0 100 100	14, 32, 52, 70	0
All	All	2958/3032 (97%)	-0.76	0 100 100	12, 34, 61, 98	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](#)

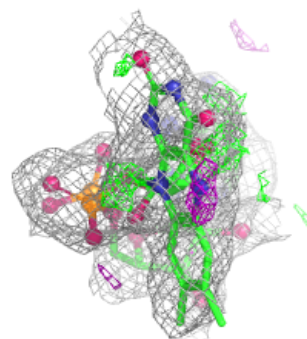
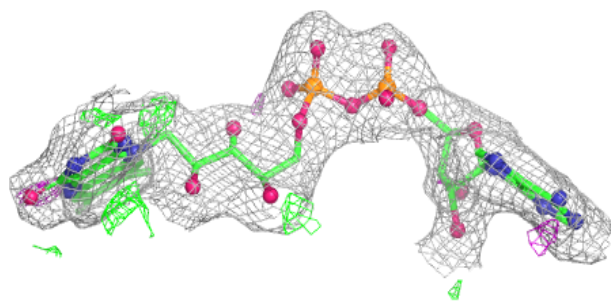
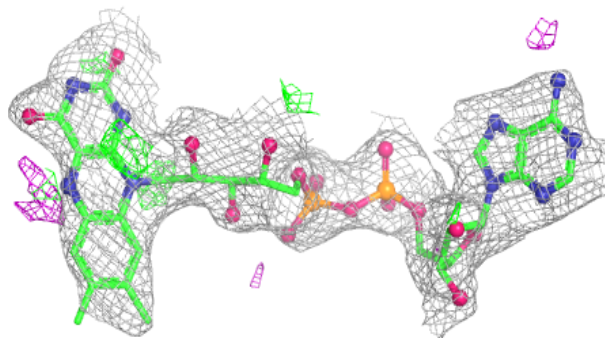
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	C	402	6/6	0.93	0.08	39,51,55,57	0
2	GOL	G	401	6/6	0.93	0.08	29,33,34,34	0
2	GOL	F	401	6/6	0.94	0.07	26,31,34,35	0
2	GOL	H	401	6/6	0.95	0.07	31,38,39,40	0
2	GOL	A	403	6/6	0.97	0.06	35,42,47,47	0
3	FAD	E	401	53/53	0.97	0.06	18,22,29,30	0
2	GOL	D	401	6/6	0.98	0.06	32,35,39,46	0
2	GOL	A	401	6/6	0.98	0.05	16,18,18,21	0
2	GOL	C	401	6/6	0.98	0.05	17,19,21,21	0
2	GOL	G	402	6/6	0.98	0.07	32,42,43,43	0
2	GOL	A	402	6/6	0.98	0.05	24,25,26,27	0
3	FAD	A	404	53/53	0.98	0.05	14,18,24,28	0
3	FAD	C	404	53/53	0.98	0.06	16,27,36,40	0
3	FAD	D	402	53/53	0.98	0.04	11,21,26,29	0
2	GOL	C	403	6/6	0.98	0.05	17,18,19,20	0
3	FAD	F	402	53/53	0.98	0.05	16,25,36,42	0
3	FAD	G	403	53/53	0.98	0.05	12,22,31,37	0
3	FAD	H	402	53/53	0.98	0.06	14,21,34,36	0
3	FAD	B	401	53/53	0.99	0.06	14,19,33,34	0

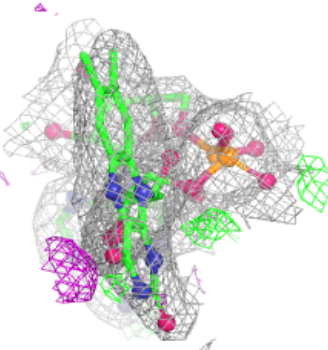
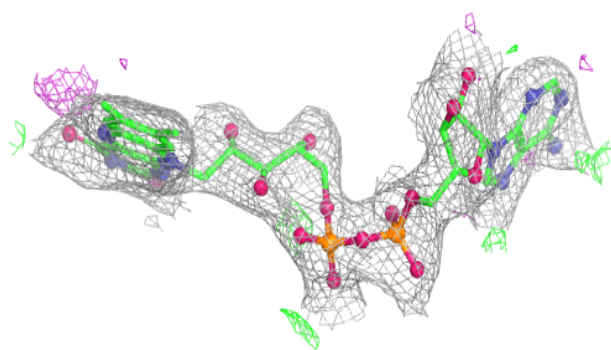
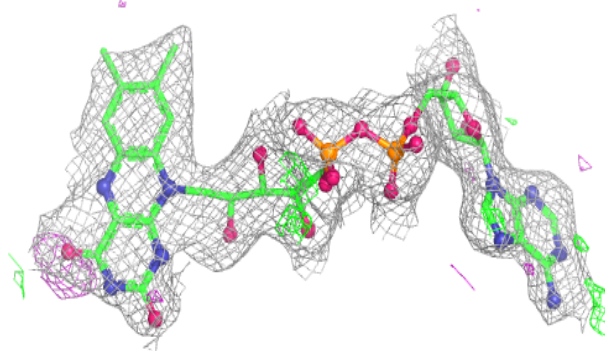
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD E 401:

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

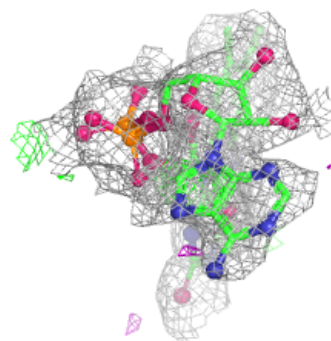
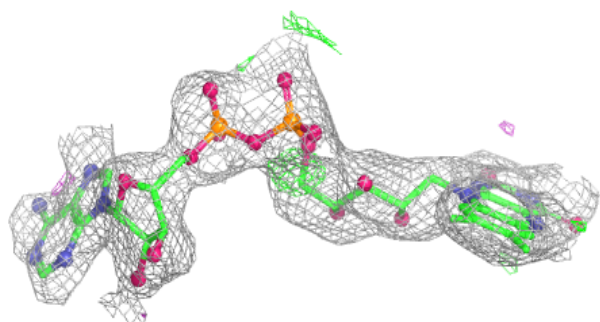
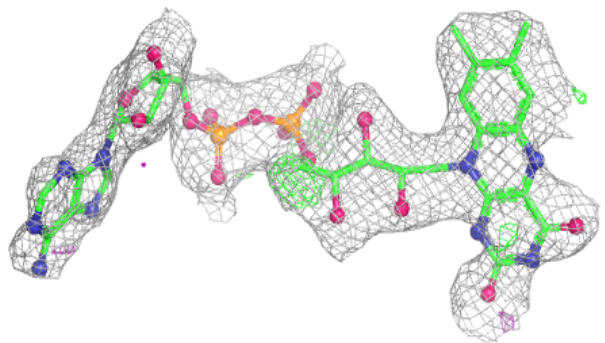
**Electron density around FAD A 404:**

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

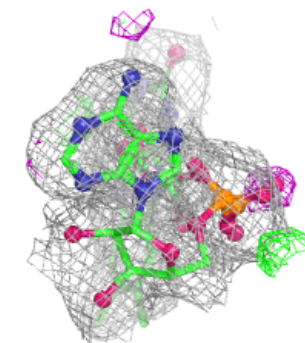
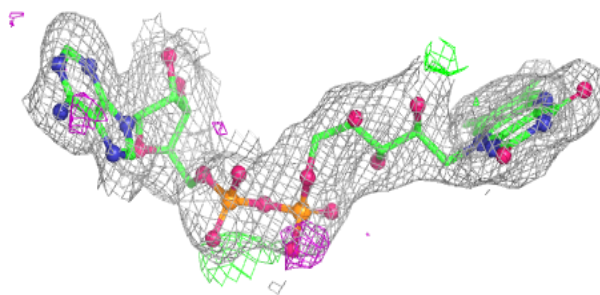
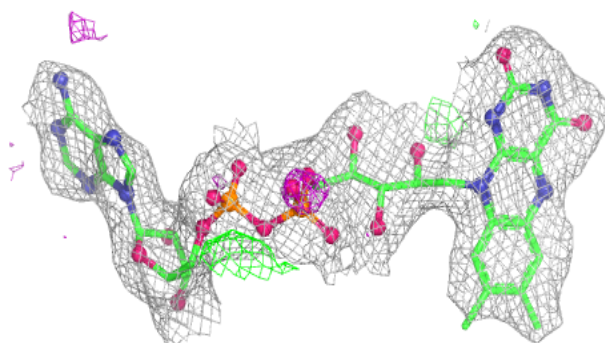


Electron density around FAD C 404:

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

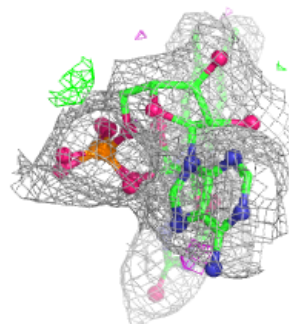
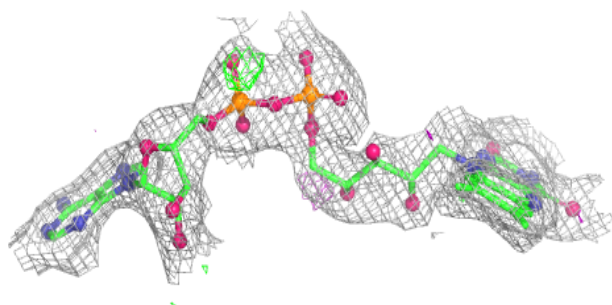
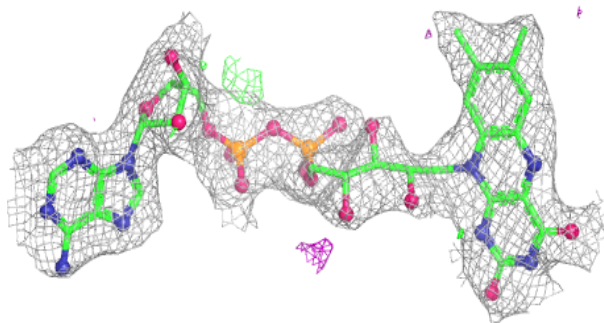
**Electron density around FAD D 402:**

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

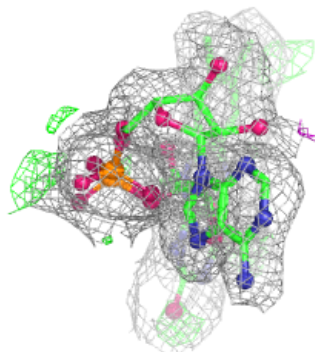
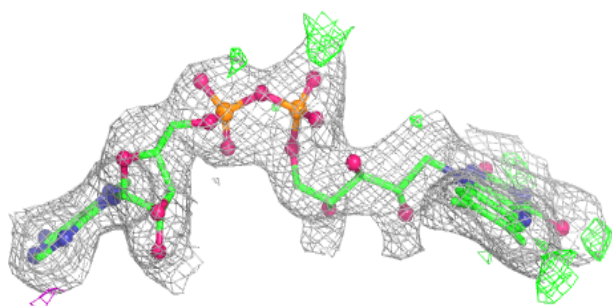
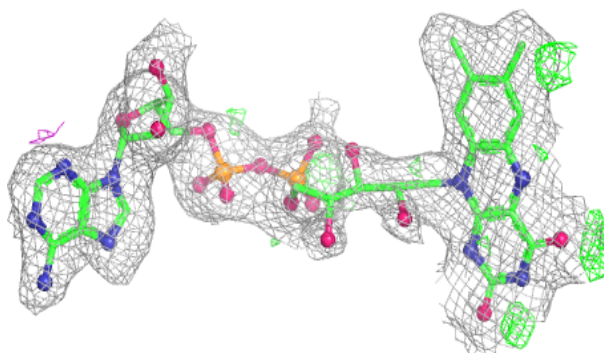


Electron density around FAD F 402:

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

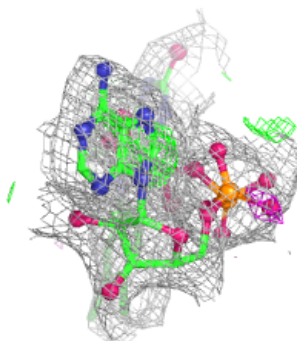
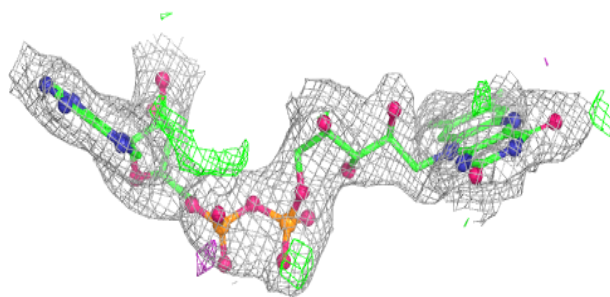
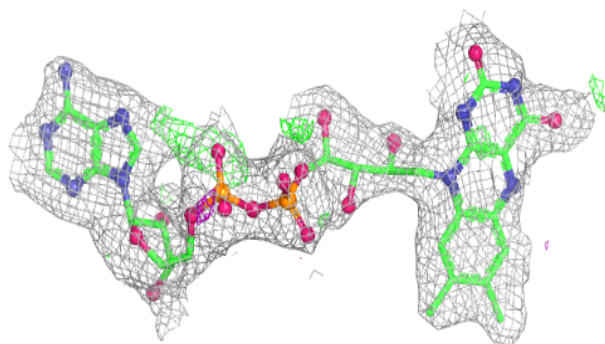
**Electron density around FAD G 403:**

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

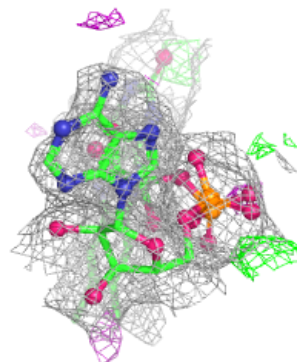
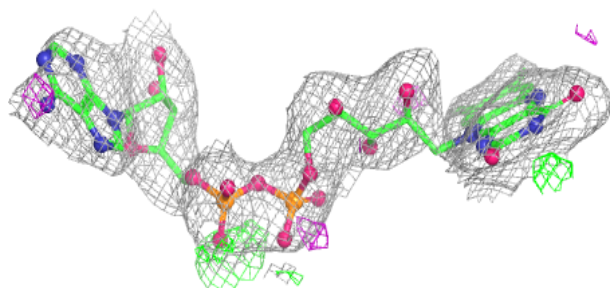
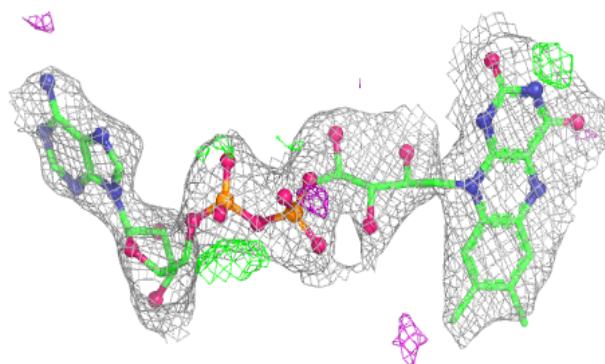


Electron density around FAD H 402:

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

**Electron density around FAD B 401:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.