



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:29 AM UTC

PDB ID : 1ZMC / pdb_00001zmc
Title : Crystal Structure of Human dihydrolipoamide dehydrogenase complexed to NAD+
Authors : Brautigam, C.A.; Chuang, J.L.; Tomchick, D.R.; Machius, M.; Chuang, D.T.
Deposited on : 2005-05-10
Resolution : 2.53 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

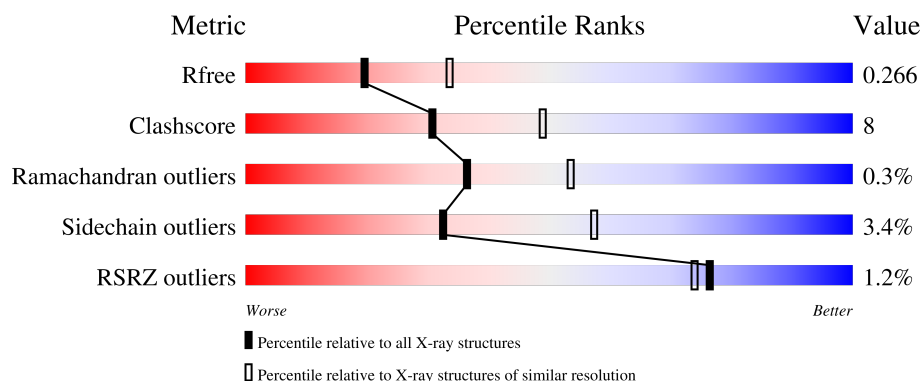
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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.



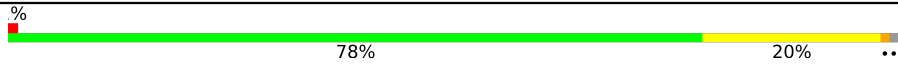
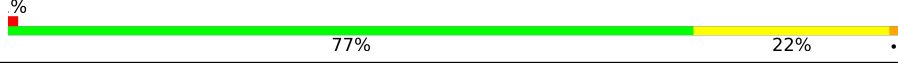
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	474	 2% 73% 24% .
1	B	474	 2% 76% 22% ..
1	C	474	 % 73% 25% ..
1	D	474	 % 72% 26% .
1	E	474	 2% 77% 21% .

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Mol	Chain	Length	Quality of chain
1	F	474	
1	G	474	
1	H	474	

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
2	SO4	A	2003	-	-	X	-
2	SO4	B	2007	-	-	X	-
2	SO4	D	2014	-	-	X	-
2	SO4	D	2016	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30312 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 Dihydrolipoyl dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	1	0
			3515	2214	609	673	19			
1	B	471	Total	C	N	O	S	0	0	0
			3496	2203	604	670	19			
1	C	471	Total	C	N	O	S	6	0	0
			3496	2203	604	670	19			
1	D	474	Total	C	N	O	S	0	1	0
			3528	2221	611	677	19			
1	E	472	Total	C	N	O	S	0	0	0
			3505	2208	606	672	19			
1	F	471	Total	C	N	O	S	4	1	0
			3506	2209	607	671	19			
1	G	472	Total	C	N	O	S	0	1	0
			3515	2214	609	673	19			
1	H	471	Total	C	N	O	S	0	0	0
			3496	2203	604	670	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	THR	LYS	conflict	UNP P09622
B	69	THR	LYS	conflict	UNP P09622
C	69	THR	LYS	conflict	UNP P09622
D	69	THR	LYS	conflict	UNP P09622
E	69	THR	LYS	conflict	UNP P09622
F	69	THR	LYS	conflict	UNP P09622
G	69	THR	LYS	conflict	UNP P09622
H	69	THR	LYS	conflict	UNP P09622

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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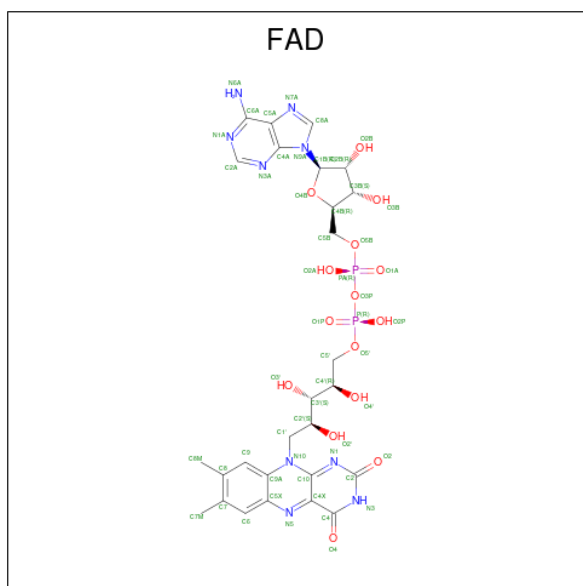
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

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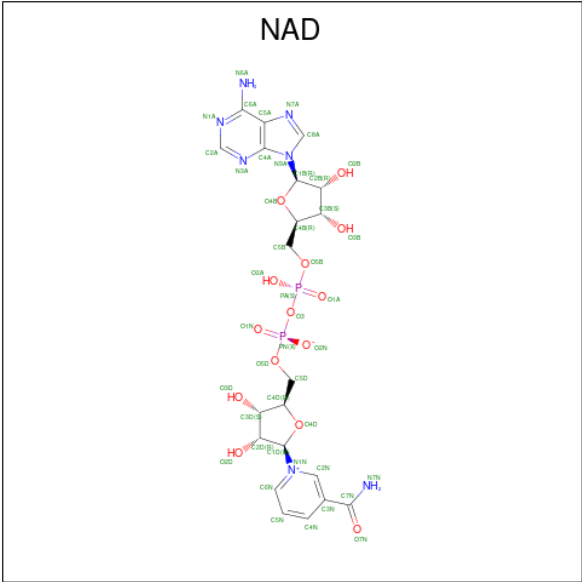
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	158	Total	O	0	0
			158	158		
5	B	137	Total	O	0	0
			137	137		
5	C	138	Total	O	0	0
			138	138		
5	D	144	Total	O	0	0
			144	144		

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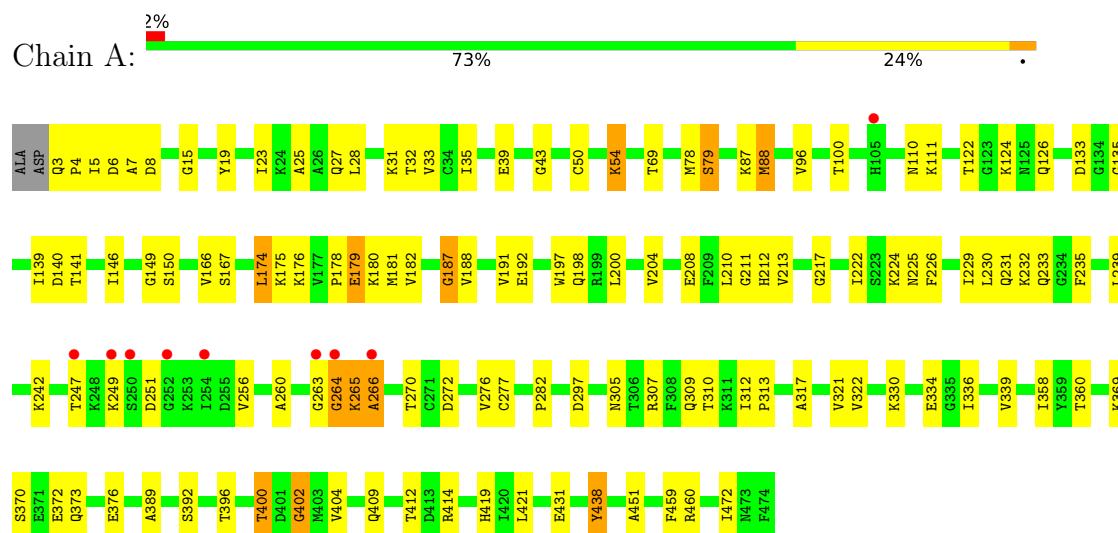
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	175	Total 175	O 175	0	0
5	F	229	Total 229	O 229	0	0
5	G	247	Total 247	O 247	0	0
5	H	173	Total 173	O 173	0	0

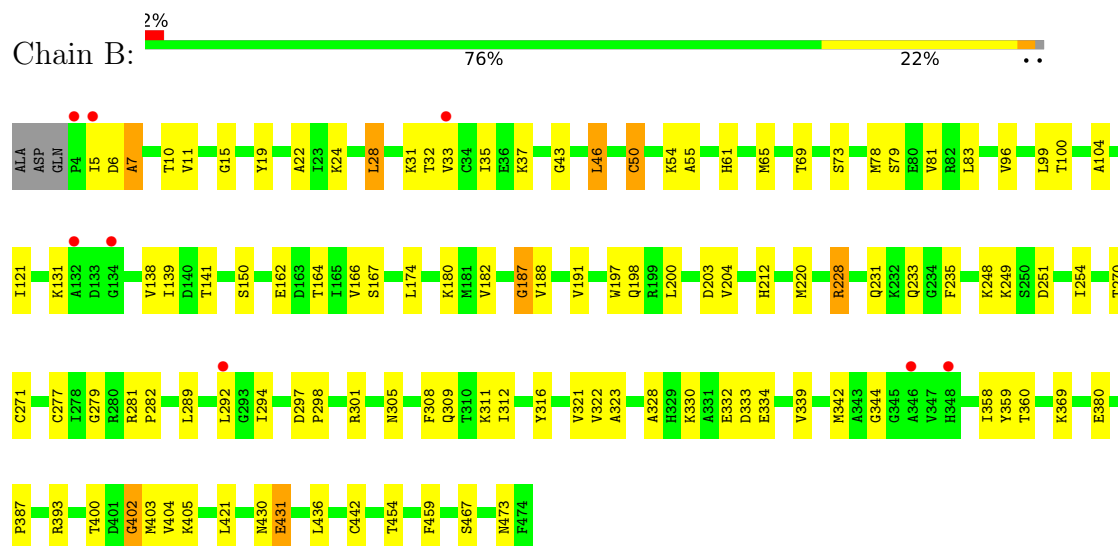
3 Residue-property plots [i](#)

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

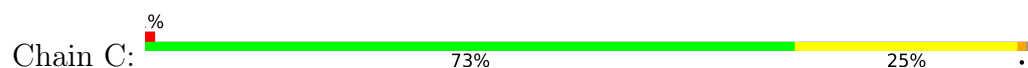
- Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial

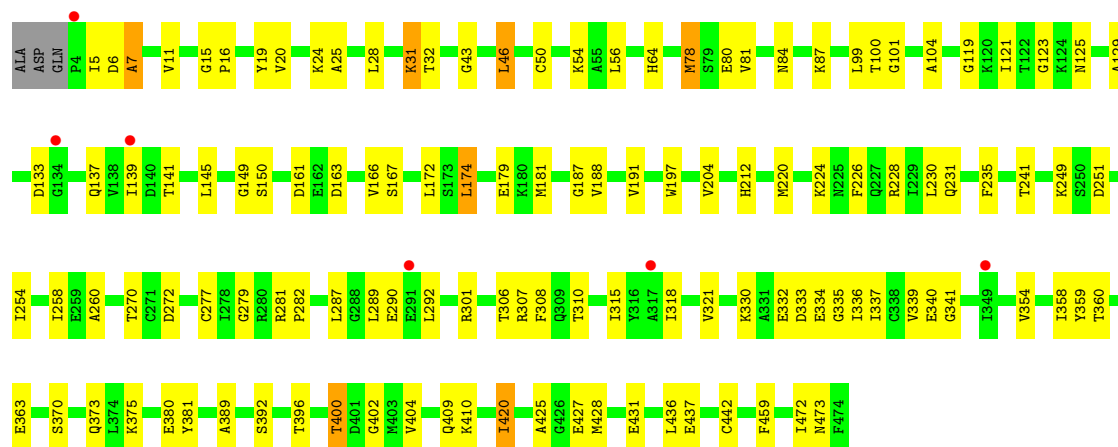


- Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial

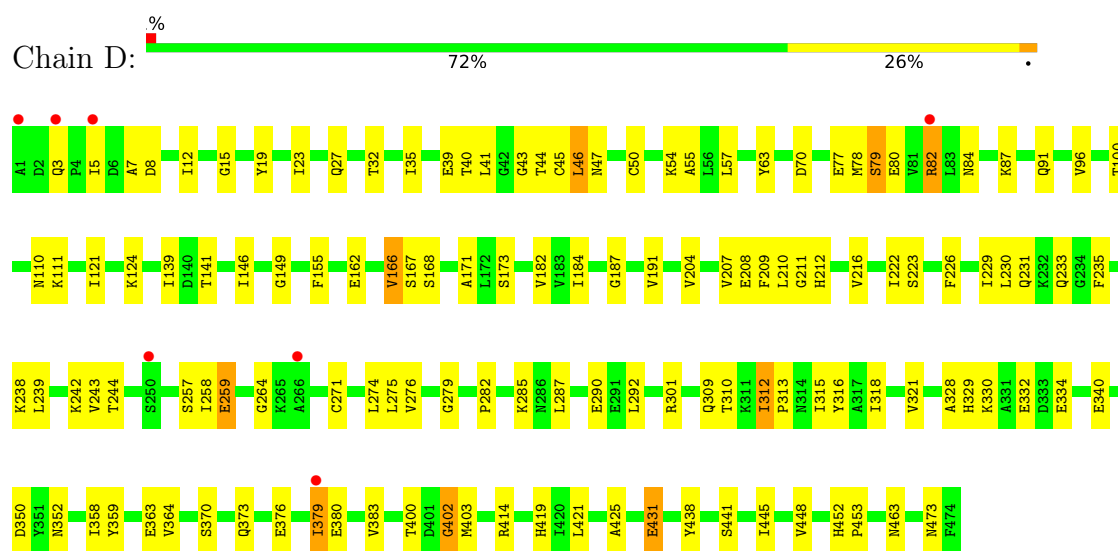


- Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial

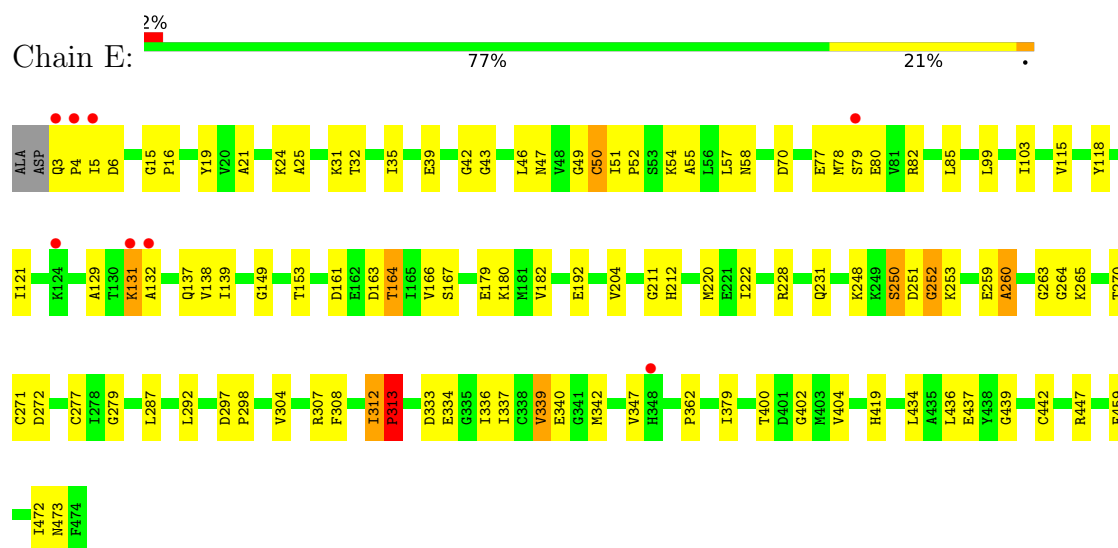




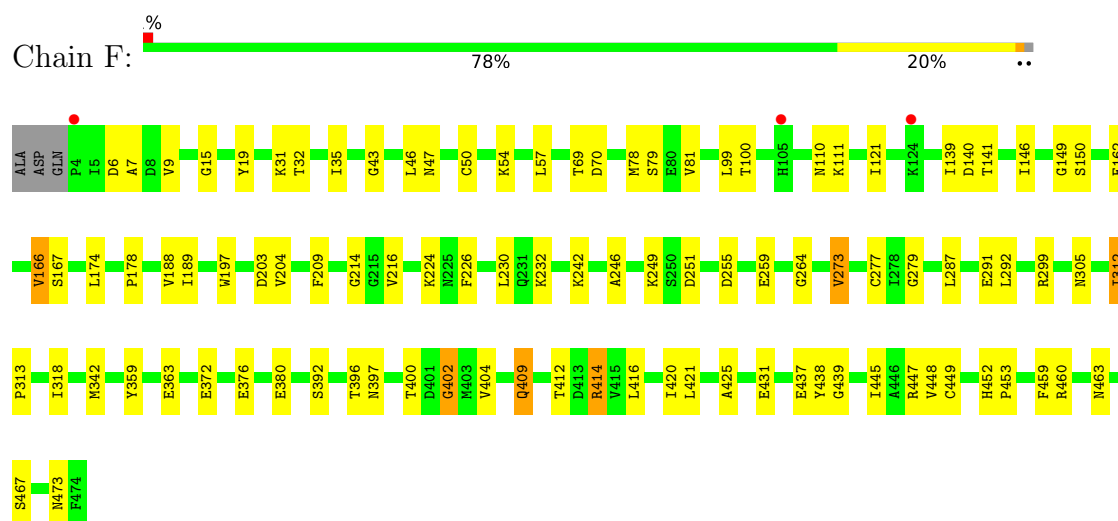
- Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial



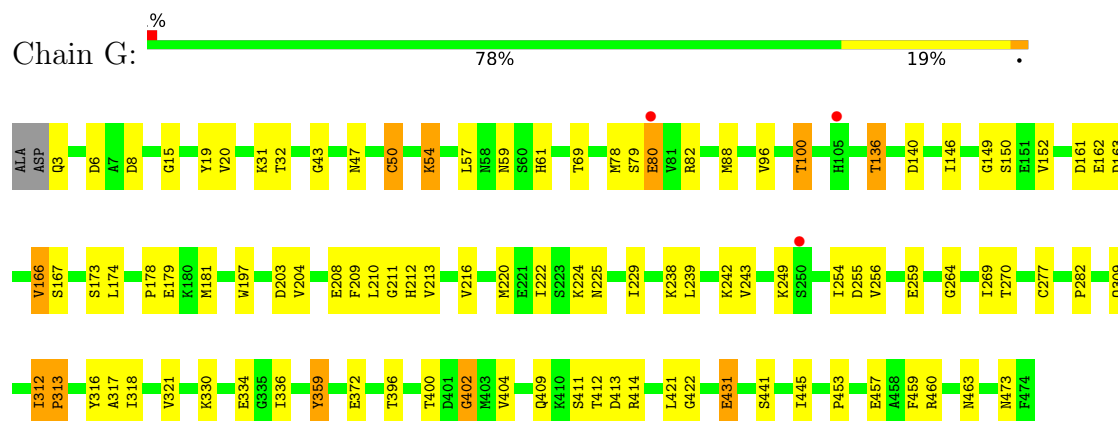
- Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial



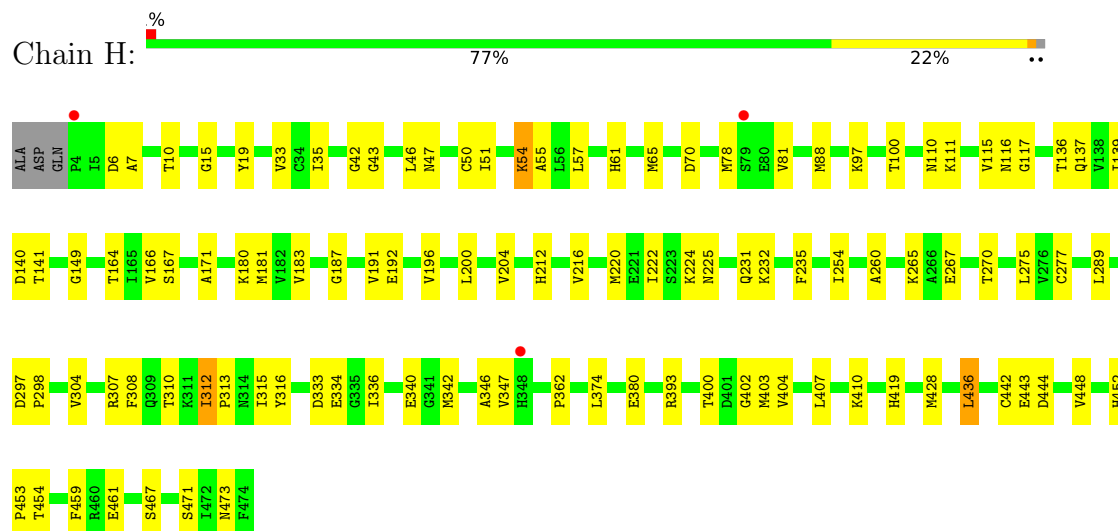
- Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial



- Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial



- Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	176.12Å 210.76Å 126.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.09 – 2.53 43.09 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.2 (43.09-2.53) 99.3 (43.09-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.54Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.211 , 0.267 0.211 , 0.266	Depositor DCC
R_{free} test set	942 reflections (0.60%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtrriage
Anisotropy	0.404	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	30312	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.36 % 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 4.2598e-05. 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: NAD, FAD, SO4

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	0.66	1/3571 (0.0%)	1.09	21/4824 (0.4%)
1	B	0.63	0/3551	1.07	21/4796 (0.4%)
1	C	0.63	0/3551	1.08	19/4796 (0.4%)
1	D	0.64	0/3584	1.09	21/4842 (0.4%)
1	E	0.66	0/3560	1.12	30/4809 (0.6%)
1	F	0.69	0/3562	1.11	19/4811 (0.4%)
1	G	0.71	0/3571	1.12	25/4824 (0.5%)
1	H	0.67	0/3551	1.07	15/4796 (0.3%)
All	All	0.66	1/28501 (0.0%)	1.09	171/38498 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	310	THR	CA-CB	5.69	1.60	1.53

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	252	GLY	N-CA-C	-12.04	100.16	114.48
1	A	265	LYS	N-CA-C	-9.04	99.95	112.25
1	G	166	VAL	N-CA-C	8.47	121.32	109.29
1	E	32	THR	N-CA-C	8.30	122.44	109.07
1	F	166	VAL	N-CA-C	8.06	120.74	109.29
1	C	400	THR	N-CA-C	8.04	122.40	112.59
1	G	69	THR	N-CA-C	8.04	120.12	111.36
1	A	167	SER	N-CA-C	-8.02	98.40	109.95
1	H	70	ASP	N-CA-C	7.83	120.57	111.02
1	D	400	THR	N-CA-C	7.66	122.34	112.92
1	F	312	ILE	CA-C-N	7.65	129.40	119.84
1	F	312	ILE	C-N-CA	7.65	129.40	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	167	SER	N-CA-C	-7.64	98.94	109.95
1	E	400	THR	N-CA-C	7.61	122.65	112.30
1	H	167	SER	N-CA-C	-7.59	98.77	109.69
1	E	312	ILE	CA-C-N	7.57	129.30	119.84
1	E	312	ILE	C-N-CA	7.57	129.30	119.84
1	A	402	GLY	N-CA-C	7.54	126.41	112.77
1	F	31	LYS	N-CA-C	-7.33	98.82	109.59
1	G	402	GLY	N-CA-C	7.31	127.79	112.45
1	H	402	GLY	N-CA-C	7.29	126.24	112.62
1	C	473	ASN	N-CA-C	7.26	121.73	113.02
1	B	431	GLU	N-CA-C	-7.25	103.09	112.23
1	C	204	VAL	N-CA-C	7.11	118.85	108.53
1	H	312	ILE	CA-C-N	7.10	128.71	119.84
1	H	312	ILE	C-N-CA	7.10	128.71	119.84
1	F	47	ASN	N-CA-C	7.07	120.03	111.40
1	E	166	VAL	N-CA-C	7.06	120.15	109.20
1	E	287	LEU	N-CA-C	-7.01	104.86	113.41
1	B	359	TYR	N-CA-C	6.99	120.76	112.93
1	A	166	VAL	N-CA-C	6.98	119.21	109.29
1	A	392	SER	N-CA-C	6.98	118.54	111.07
1	C	402	GLY	N-CA-C	6.96	125.63	112.62
1	B	402	GLY	N-CA-C	6.90	125.53	112.62
1	D	166	VAL	N-CA-C	6.90	119.09	109.29
1	G	431	GLU	N-CA-C	-6.90	103.81	111.82
1	D	402	GLY	N-CA-C	6.90	125.52	112.62
1	C	166	VAL	N-CA-C	6.84	118.89	109.46
1	G	149	GLY	N-CA-C	6.81	123.18	111.47
1	D	312	ILE	CA-C-N	6.80	128.34	119.84
1	D	312	ILE	C-N-CA	6.80	128.34	119.84
1	A	312	ILE	CA-C-N	6.78	128.31	119.84
1	A	312	ILE	C-N-CA	6.78	128.31	119.84
1	D	473	ASN	N-CA-C	6.76	120.50	112.93
1	D	167	SER	N-CA-C	-6.76	100.22	109.95
1	F	473	ASN	N-CA-C	6.75	121.12	113.02
1	D	32	THR	N-CA-C	6.70	120.38	109.59
1	G	204	VAL	N-CA-C	6.70	118.13	108.48
1	F	150	SER	N-CA-C	6.68	118.27	108.86
1	B	167	SER	N-CA-C	-6.65	99.28	109.65
1	D	204	VAL	N-CA-C	6.60	117.98	108.48
1	A	149	GLY	N-CA-C	6.60	122.81	111.47
1	E	70	ASP	N-CA-C	6.53	118.99	111.02
1	A	32	THR	N-CA-C	6.53	120.10	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	32	THR	N-CA-C	6.52	120.03	109.40
1	F	214	GLY	N-CA-C	6.48	122.19	114.48
1	D	149	GLY	N-CA-C	6.46	122.75	111.50
1	A	264	GLY	N-CA-C	6.46	128.48	113.18
1	E	167	SER	N-CA-C	-6.45	100.43	110.17
1	G	359	TYR	N-CA-C	6.45	119.80	112.97
1	C	279	GLY	N-CA-C	6.42	119.55	111.85
1	G	150	SER	N-CA-C	6.42	117.91	108.86
1	G	400	THR	N-CA-C	6.39	121.87	113.30
1	F	392	SER	N-CA-C	6.39	117.91	111.07
1	F	100	THR	N-CA-C	-6.39	104.41	111.82
1	C	31	LYS	N-CA-C	-6.37	98.80	108.67
1	D	340	GLU	N-CA-C	-6.33	104.46	111.36
1	F	402	GLY	N-CA-C	6.29	125.76	112.17
1	E	279	GLY	N-CA-C	6.26	118.43	112.04
1	C	287	LEU	N-CA-C	-6.25	105.48	113.23
1	F	32	THR	N-CA-C	6.24	119.57	109.40
1	F	149	GLY	N-CA-C	6.23	122.60	111.02
1	G	473	ASN	N-CA-C	6.21	119.80	112.72
1	C	167	SER	N-CA-C	-6.20	100.16	109.96
1	H	473	ASN	N-CA-C	6.19	119.86	112.93
1	E	31	LYS	N-CA-C	-6.18	99.09	108.67
1	G	422	GLY	CA-C-N	6.17	126.12	119.76
1	G	422	GLY	C-N-CA	6.17	126.12	119.76
1	F	400	THR	N-CA-C	6.04	120.68	112.88
1	E	342	MET	N-CA-C	-6.04	104.81	111.82
1	A	31	LYS	N-CA-C	-6.02	100.49	109.15
1	C	289	LEU	N-CA-C	-6.00	104.81	111.71
1	A	204	VAL	N-CA-C	5.98	117.09	108.48
1	E	402	GLY	N-CA-C	5.96	123.77	112.62
1	H	346	ALA	N-CA-C	-5.94	102.53	110.55
1	G	47	ASN	N-CA-C	5.93	118.98	111.69
1	B	46	LEU	N-CA-C	5.92	117.81	111.36
1	G	100	THR	N-CA-C	-5.91	104.96	111.82
1	A	336	ILE	N-CA-C	5.87	116.05	110.42
1	H	400	THR	N-CA-C	5.86	120.03	112.41
1	D	70	ASP	N-CA-C	5.84	118.14	111.02
1	B	7	ALA	N-CA-C	5.83	117.00	108.14
1	E	50	CYS	N-CA-C	5.79	118.06	111.11
1	E	473	ASN	N-CA-C	5.79	119.96	113.02
1	G	243	VAL	N-CA-C	-5.77	102.14	109.58
1	G	8	ASP	N-CA-C	-5.77	104.44	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	442	CYS	N-CA-C	-5.76	105.00	111.28
1	F	204	VAL	N-CA-C	5.76	116.78	108.48
1	C	260	ALA	N-CA-C	-5.76	102.38	110.50
1	E	153	THR	CA-C-N	-5.74	113.28	120.51
1	E	153	THR	C-N-CA	-5.74	113.28	120.51
1	E	149	GLY	N-CA-C	5.72	121.31	111.47
1	F	70	ASP	N-CA-C	5.72	117.97	111.11
1	D	173	SER	N-CA-C	5.71	119.92	111.87
1	H	166	VAL	N-CA-C	5.71	117.39	109.29
1	H	47	ASN	N-CA-C	5.70	119.42	112.23
1	B	400	THR	N-CA-C	5.70	119.82	112.41
1	B	473	ASN	N-CA-C	5.68	119.83	113.02
1	H	149	GLY	N-CA-C	5.68	121.38	111.50
1	F	167	SER	N-CA-C	-5.66	101.81	109.95
1	E	204	VAL	N-CA-C	5.65	116.73	108.53
1	C	392	SER	N-CA-C	5.64	117.11	111.07
1	A	187	GLY	N-CA-C	-5.63	103.54	112.66
1	G	31	LYS	N-CA-C	-5.63	100.63	109.25
1	B	6	ASP	N-CA-C	5.62	118.23	109.52
1	E	264	GLY	N-CA-C	5.61	118.89	111.70
1	D	383	VAL	N-CA-C	5.61	116.19	108.12
1	B	31	LYS	N-CA-C	-5.59	98.15	107.99
1	C	32	THR	N-CA-C	5.59	118.07	109.07
1	A	400	THR	N-CA-C	5.57	119.77	112.92
1	D	44	THR	N-CA-C	5.56	117.78	111.11
1	B	311	LYS	N-CA-C	-5.55	105.13	111.07
1	A	69	THR	N-CA-C	5.54	120.04	113.28
1	B	344	GLY	N-CA-C	5.52	120.25	113.79
1	C	420	ILE	N-CA-C	5.50	115.91	107.77
1	B	369	LYS	N-CA-C	5.47	118.65	109.95
1	D	63	TYR	N-CA-C	-5.47	105.32	111.28
1	B	204	VAL	N-CA-C	5.46	116.45	108.53
1	B	50	CYS	CA-CB-SG	5.45	126.92	114.40
1	E	313	PRO	N-CA-C	5.44	123.68	112.47
1	E	21	ALA	N-CA-C	-5.44	105.43	111.36
1	D	8	ASP	N-CA-C	-5.42	104.92	112.45
1	B	279	GLY	N-CA-C	5.41	118.62	111.70
1	E	260	ALA	N-CA-C	-5.40	102.28	110.28
1	H	260	ALA	N-CA-C	-5.40	102.89	110.50
1	D	431	GLU	N-CA-C	-5.38	105.33	111.14
1	G	312	ILE	CA-C-N	5.37	126.56	119.84
1	G	312	ILE	C-N-CA	5.37	126.56	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	153	THR	N-CA-C	-5.36	103.31	110.07
1	E	439	GLY	N-CA-C	-5.35	106.02	114.10
1	E	379	ILE	N-CA-C	5.34	115.94	108.89
1	D	45	CYS	N-CA-C	5.33	116.78	111.07
1	A	150	SER	N-CA-C	5.32	116.36	108.86
1	F	431	GLU	N-CA-C	-5.31	105.57	111.36
1	E	47	ASN	N-CA-C	5.30	119.81	112.45
1	F	203	ASP	N-CA-C	-5.30	99.88	108.41
1	A	8	ASP	N-CA-C	-5.29	105.10	112.45
1	C	7	ALA	N-CA-C	5.28	116.87	108.79
1	G	136	THR	N-CA-C	5.28	118.03	109.06
1	G	313	PRO	N-CA-C	5.28	123.34	112.47
1	H	289	LEU	N-CA-C	5.25	116.69	111.07
1	B	233	GLN	N-CA-C	-5.25	106.72	113.23
1	G	173	SER	N-CA-C	5.25	119.44	112.30
1	B	203	ASP	N-CA-C	-5.23	99.99	108.41
1	E	77	GLU	N-CA-C	5.23	117.25	108.73
1	C	472	ILE	N-CA-C	-5.21	106.60	111.45
1	G	203	ASP	N-CA-C	-5.21	100.01	108.41
1	C	149	GLY	N-CA-C	5.20	120.41	111.47
1	H	100	THR	N-CA-C	-5.15	105.74	111.36
1	B	198	GLN	N-CA-C	-5.15	105.56	111.07
1	D	3	GLN	N-CA-C	-5.09	98.56	109.81
1	B	104	ALA	N-CA-C	-5.08	105.82	111.36
1	E	250	SER	N-CA-C	-5.08	106.34	112.54
1	B	187	GLY	N-CA-C	-5.08	104.44	112.66
1	A	198	GLN	N-CA-C	-5.07	105.02	111.11
1	A	369	LYS	N-CA-C	5.06	118.27	110.42
1	A	217	GLY	N-CA-C	5.06	121.84	115.42
1	H	204	VAL	N-CA-C	5.06	115.76	108.48
1	D	403	MET	N-CA-C	5.04	115.95	108.60
1	E	442	CYS	N-CA-C	-5.04	105.87	111.36
1	C	359	TYR	N-CA-C	5.02	118.29	112.97

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	3515	0	3562	72	0
1	B	3496	0	3549	62	0
1	C	3496	0	3549	67	0
1	D	3528	0	3574	77	0
1	E	3505	0	3556	58	0
1	F	3506	0	3555	65	0
1	G	3515	0	3562	53	0
1	H	3496	0	3549	61	0
2	A	20	0	0	3	0
2	B	20	0	0	3	0
2	C	20	0	0	1	0
2	D	25	0	0	4	0
2	E	25	0	0	1	0
2	F	20	0	0	1	0
2	G	25	0	0	1	0
2	H	25	0	0	0	0
3	A	53	0	31	2	0
3	B	53	0	31	4	0
3	C	53	0	31	2	0
3	D	53	0	31	3	0
3	E	53	0	31	3	0
3	F	53	0	31	2	0
3	G	53	0	31	3	0
3	H	53	0	31	2	0
4	A	44	0	26	0	0
4	B	27	0	12	0	0
4	C	27	0	12	0	0
4	D	44	0	26	2	0
4	E	27	0	12	0	0
4	F	27	0	12	2	0
4	G	27	0	12	0	0
4	H	27	0	12	1	0
5	A	158	0	0	3	0
5	B	137	0	0	1	0
5	C	138	0	0	1	0
5	D	144	0	0	2	0
5	E	175	0	0	4	0
5	F	229	0	0	2	0
5	G	247	0	0	4	0
5	H	173	0	0	2	1
All	All	30312	0	28828	476	1

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 8.

All (476) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:GLU:HG3	1:D:448:VAL:HG22	1.37	1.05
1:B:228:ARG:HG2	1:B:228:ARG:HH11	1.27	0.98
1:F:9:VAL:HG22	1:F:342:MET:HE1	1.54	0.88
1:C:78:MET:HG2	1:D:78:MET:HG2	1.53	0.88
1:B:228:ARG:HG2	1:B:228:ARG:NH1	1.94	0.79
1:E:297:ASP:HB2	1:E:298:PRO:HD2	1.65	0.79
1:H:180:LYS:HE3	1:H:270:THR:O	1.83	0.79
1:C:212:HIS:HB3	1:C:220:MET:HE1	1.68	0.75
1:A:79:SER:OG	1:B:79:SER:HB2	1.86	0.75
1:D:207:VAL:HG12	1:D:238:LYS:HB2	1.71	0.73
1:A:28:LEU:HD12	1:A:339:VAL:HG12	1.71	0.72
1:E:437:GLU:HG3	1:F:448:VAL:HG22	1.72	0.72
1:G:59:ASN:HB3	1:G:88:MET:HE2	1.71	0.72
1:B:212:HIS:HB3	1:B:220:MET:HE1	1.71	0.71
1:B:228:ARG:HH11	1:B:228:ARG:CG	2.01	0.71
1:C:121:ILE:HG21	1:C:292:LEU:HD11	1.73	0.71
1:B:10:THR:HG23	1:B:33:VAL:HG13	1.75	0.69
1:C:28:LEU:HD12	1:C:339:VAL:HG12	1.75	0.69
1:E:251:ASP:HB3	1:E:253:LYS:H	1.59	0.68
1:A:88:MET:HE1	1:A:200:LEU:HD21	1.75	0.68
1:B:297:ASP:HB2	1:B:298:PRO:HD2	1.74	0.68
1:E:180:LYS:HE3	1:E:270:THR:O	1.94	0.67
1:E:42:GLY:HA3	1:E:46:LEU:HD23	1.77	0.67
1:F:363:GLU:HB2	1:F:425:ALA:HB3	1.76	0.67
1:G:15:GLY:HA3	3:G:480:FAD:H52A	1.77	0.66
1:G:402:GLY:HA3	1:G:421:LEU:O	1.94	0.66
1:D:379:ILE:HG23	2:D:2014:SO4:O2	1.96	0.66
1:A:212:HIS:ND1	2:A:2003:SO4:O3	2.29	0.65
1:C:43:GLY:HA2	3:C:480:FAD:O3B	1.97	0.65
1:A:232:LYS:O	1:A:232:LYS:HD3	1.96	0.65
1:B:289:LEU:HB3	1:B:294:ILE:HB	1.78	0.64
1:B:15:GLY:HA3	3:B:480:FAD:H52A	1.79	0.64
1:D:43:GLY:HA2	3:D:480:FAD:O3B	1.98	0.64
1:D:121:ILE:HG21	1:D:292:LEU:HD11	1.81	0.63
1:F:43:GLY:HA2	3:F:480:FAD:O3B	1.98	0.63
1:G:43:GLY:HA2	3:G:480:FAD:O3B	1.99	0.63
1:H:15:GLY:HA3	3:H:480:FAD:H52A	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:249:LYS:HD2	1:G:255:ASP:OD1	1.98	0.62
1:D:40:THR:HG22	1:D:41:LEU:O	2.00	0.62
1:C:181:MET:HE1	1:C:197:TRP:HB2	1.82	0.62
1:E:118:TYR:O	1:E:129:ALA:HA	2.00	0.62
1:G:249:LYS:HD2	1:G:255:ASP:CG	2.24	0.62
1:A:33:VAL:HG11	1:A:139:ILE:HD13	1.81	0.62
1:E:15:GLY:HA3	3:E:480:FAD:H52A	1.82	0.61
1:B:212:HIS:ND1	2:B:2007:SO4:O1	2.33	0.61
1:E:212:HIS:HB3	1:E:220:MET:HE1	1.80	0.61
1:A:305:ASN:HB2	1:F:438:TYR:O	2.00	0.61
1:E:57:LEU:HD11	1:E:192:GLU:HB3	1.82	0.61
1:E:434:LEU:HD12	1:F:448:VAL:HG21	1.82	0.61
1:F:9:VAL:HG22	1:F:342:MET:CE	2.30	0.61
1:G:78:MET:HG2	1:H:81:VAL:HG22	1.80	0.61
1:C:307:ARG:O	1:C:308:PHE:HB2	2.01	0.61
1:H:297:ASP:HB2	1:H:298:PRO:HD2	1.80	0.61
1:D:182:VAL:HG23	1:D:271:CYS:HB3	1.82	0.61
1:B:69:THR:HG22	2:B:2004:SO4:O1	2.01	0.61
1:E:43:GLY:HA2	3:E:480:FAD:O3B	2.01	0.61
1:A:263:GLY:HA3	1:H:97:LYS:NZ	2.16	0.61
1:A:15:GLY:HA3	3:A:480:FAD:H52A	1.83	0.60
1:D:370:SER:OG	1:D:373:GLN:HG3	2.01	0.60
1:D:110:ASN:O	1:D:111:LYS:HB2	2.02	0.60
1:H:231:GLN:HA	1:H:235:PHE:O	2.02	0.59
1:C:241:THR:HG21	1:C:258:ILE:HD12	1.84	0.59
1:E:362:PRO:HA	5:E:2157:HOH:O	2.03	0.59
1:B:231:GLN:HA	1:B:235:PHE:O	2.03	0.58
1:E:35:ILE:HD12	1:E:115:VAL:HB	1.85	0.58
1:A:3:GLN:N	1:A:4:PRO:HD3	2.19	0.58
1:E:49:GLY:O	1:E:52:PRO:HD2	2.04	0.58
1:H:43:GLY:HA2	3:H:480:FAD:O3B	2.02	0.58
1:H:42:GLY:HA3	1:H:46:LEU:HD23	1.85	0.58
1:C:15:GLY:HA3	3:C:480:FAD:H52A	1.86	0.58
1:D:96:VAL:O	1:D:100:THR:HG23	2.04	0.58
1:C:46:LEU:HD21	1:C:99:LEU:HB2	1.86	0.58
1:H:10:THR:HB	1:H:141:THR:HG21	1.86	0.58
1:G:396:THR:CG2	1:H:55:ALA:HB2	2.34	0.57
1:B:43:GLY:HA2	3:B:480:FAD:O3B	2.05	0.57
1:D:208:GLU:HG3	1:D:210:LEU:H	1.69	0.57
1:F:279:GLY:HA2	4:F:481:NAD:O1A	2.04	0.57
1:B:96:VAL:O	1:B:100:THR:HG23	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:110:ASN:O	1:F:111:LYS:HB2	2.04	0.56
1:D:40:THR:HG23	1:D:100:THR:HB	1.87	0.56
1:H:116:ASN:HD22	1:H:117:GLY:N	2.03	0.56
1:D:309:GLN:HG2	1:D:316:TYR:CE2	2.40	0.56
1:E:15:GLY:HA2	1:E:43:GLY:HA3	1.88	0.56
1:G:254:ILE:O	1:G:270:THR:HA	2.05	0.56
1:A:211:GLY:O	1:A:239:LEU:HD13	2.06	0.56
1:B:150:SER:HB2	1:B:281:ARG:O	2.06	0.56
1:D:380:GLU:HB2	2:D:2014:SO4:O4	2.06	0.56
1:G:259:GLU:HB2	1:G:264:GLY:O	2.06	0.56
1:B:212:HIS:CE1	2:B:2007:SO4:O1	2.58	0.55
1:D:244:THR:OG1	1:D:257:SER:HB2	2.05	0.55
1:A:122:THR:OG1	1:A:126:GLN:HG2	2.06	0.55
1:D:229:ILE:O	1:D:233:GLN:HG3	2.06	0.55
1:A:414:ARG:HH21	1:F:305:ASN:HA	1.71	0.55
1:D:7:ALA:O	1:D:141:THR:HA	2.05	0.55
1:D:226:PHE:CZ	1:D:230:LEU:HD11	2.41	0.55
1:A:451:ALA:H	1:B:430:ASN:HD21	1.52	0.55
1:A:78:MET:HG3	1:B:81:VAL:HG22	1.88	0.55
1:G:256:VAL:HB	1:G:269:ILE:HG13	1.89	0.54
1:C:363:GLU:HB2	1:C:425:ALA:HB3	1.88	0.54
1:E:78:MET:HG3	1:F:81:VAL:HG22	1.88	0.54
1:C:187:GLY:O	1:C:191:VAL:HG23	2.06	0.54
1:F:404:VAL:HG22	1:F:420:ILE:HG23	1.90	0.54
1:G:404:VAL:HG11	1:G:459:PHE:HA	1.89	0.54
1:D:5:ILE:HG23	1:D:139:ILE:HG23	1.89	0.54
1:E:79:SER:HB2	1:F:79:SER:OG	2.08	0.54
1:C:427:GLU:HG2	5:D:2035:HOH:O	2.07	0.54
1:D:328:ALA:O	1:D:332:GLU:HG3	2.08	0.54
1:E:137:GLN:HE21	1:E:138:VAL:N	2.05	0.54
1:F:372:GLU:CD	1:F:372:GLU:H	2.16	0.54
1:C:16:PRO:O	1:C:332:GLU:HG2	2.08	0.53
1:A:370:SER:OG	1:A:373:GLN:HG3	2.08	0.53
1:H:336:ILE:O	1:H:340:GLU:HG3	2.08	0.53
1:A:260:ALA:HB3	1:A:263:GLY:O	2.08	0.53
1:B:404:VAL:HG11	1:B:459:PHE:HA	1.90	0.53
1:H:212:HIS:HB3	1:H:220:MET:HE1	1.89	0.53
1:G:212:HIS:CG	1:G:220:MET:HE1	2.44	0.53
1:G:412:THR:O	1:G:413:ASP:HB3	2.09	0.53
1:A:305:ASN:ND2	1:A:309:GLN:HB2	2.23	0.53
1:B:35:ILE:HD11	1:B:139:ILE:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:MET:HE3	1:D:78:MET:HE3	1.90	0.53
1:E:248:LYS:HE2	1:E:252:GLY:O	2.09	0.52
1:E:336:ILE:O	1:E:339:VAL:HG12	2.09	0.52
1:C:150:SER:HB2	1:C:281:ARG:O	2.10	0.52
1:D:182:VAL:O	1:D:274:LEU:HD12	2.08	0.52
1:F:57:LEU:HD13	1:F:359:TYR:HB2	1.92	0.52
1:C:174:LEU:HB2	1:C:197:TRP:CZ2	2.45	0.52
1:D:46:LEU:HD13	1:D:100:THR:HG22	1.90	0.52
1:G:445:ILE:HG21	1:G:463:ASN:ND2	2.25	0.52
1:E:80:GLU:OE1	1:E:82:ARG:HD2	2.10	0.52
1:A:229:ILE:O	1:A:233:GLN:HG3	2.09	0.52
1:H:57:LEU:HD11	1:H:192:GLU:HB3	1.92	0.52
1:B:330:LYS:HE2	1:B:334:GLU:OE2	2.10	0.52
1:B:380:GLU:HG2	5:B:2037:HOH:O	2.10	0.52
1:C:56:LEU:HD12	1:C:172:LEU:HD23	1.91	0.52
1:C:333:ASP:O	1:C:337:ILE:HG12	2.10	0.52
1:E:99:LEU:O	1:E:103:ILE:HG12	2.09	0.52
1:E:307:ARG:HA	1:E:347:VAL:HG11	1.91	0.52
1:B:305:ASN:HD21	1:B:309:GLN:CG	2.24	0.51
1:G:15:GLY:CA	3:G:480:FAD:H52A	2.40	0.51
1:D:258:ILE:O	1:D:259:GLU:HB3	2.11	0.51
1:A:43:GLY:HA2	3:A:480:FAD:O3B	2.10	0.51
1:C:46:LEU:HD13	1:C:100:THR:HG22	1.93	0.51
1:G:330:LYS:O	1:G:334:GLU:HG3	2.10	0.51
1:H:216:VAL:HG22	4:H:481:NAD:O5D	2.10	0.51
1:H:308:PHE:CZ	1:H:334:GLU:HG2	2.45	0.51
1:A:360:THR:HB	5:A:2032:HOH:O	2.11	0.51
1:F:174:LEU:HD12	1:F:197:TRP:CE2	2.46	0.51
1:G:178:PRO:HG3	1:G:181:MET:HE2	1.93	0.51
1:A:226:PHE:CZ	1:A:230:LEU:HD11	2.45	0.51
1:D:23:ILE:O	1:D:27:GLN:HG3	2.11	0.51
1:B:188:VAL:HG22	1:B:358:ILE:CD1	2.41	0.51
1:F:178:PRO:HB3	1:F:273:VAL:HG13	1.92	0.51
1:D:40:THR:HG21	1:D:100:THR:HG21	1.93	0.51
1:A:187:GLY:O	1:A:191:VAL:HG23	2.11	0.50
1:E:25:ALA:HB2	1:E:339:VAL:HG21	1.92	0.50
1:C:318:ILE:HD13	1:C:335:GLY:HA2	1.92	0.50
1:B:5:ILE:HG22	1:B:138:VAL:O	2.11	0.50
1:C:310:THR:HG23	1:C:315:ILE:O	2.12	0.50
1:D:363:GLU:HB3	1:D:425:ALA:HB3	1.94	0.50
1:E:222:ILE:HG13	1:E:419:HIS:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ASN:O	1:A:111:LYS:HB2	2.11	0.50
1:D:168:SER:HB2	3:D:480:FAD:HM71	1.94	0.50
1:E:137:GLN:HE21	1:E:138:VAL:H	1.60	0.50
1:H:181:MET:HE3	1:H:183:VAL:HG22	1.93	0.50
1:D:216:VAL:HG23	4:D:481:NAD:O1N	2.12	0.50
1:A:23:ILE:O	1:A:27:GLN:HG3	2.12	0.49
1:A:409:GLN:HB3	1:A:412:THR:OG1	2.12	0.49
1:A:54:LYS:CA	1:A:54:LYS:HE3	2.42	0.49
1:C:375:LYS:HE3	1:C:381:TYR:OH	2.12	0.49
1:G:96:VAL:O	1:G:100:THR:HG23	2.13	0.49
1:G:409:GLN:OE1	1:G:411:SER:N	2.45	0.49
1:B:339:VAL:O	1:B:342:MET:HB2	2.13	0.49
1:C:5:ILE:HB	1:C:139:ILE:CD1	2.42	0.49
1:E:35:ILE:CD1	1:E:115:VAL:HB	2.42	0.49
1:E:131:LYS:O	1:E:132:ALA:HB3	2.11	0.49
1:F:15:GLY:HA3	3:F:480:FAD:H52A	1.94	0.49
1:H:116:ASN:HD22	1:H:117:GLY:H	1.60	0.49
1:H:232:LYS:NZ	5:H:2106:HOH:O	2.37	0.49
1:E:434:LEU:CD1	1:F:448:VAL:HG21	2.43	0.49
1:A:305:ASN:HD21	1:A:309:GLN:HB2	1.77	0.49
1:A:358:ILE:HG22	1:A:360:THR:HG23	1.93	0.49
1:B:393:ARG:HD2	1:B:454:THR:HA	1.93	0.49
1:E:3:GLN:N	1:E:4:PRO:HD3	2.28	0.49
1:C:5:ILE:HG12	1:C:137:GLN:NE2	2.28	0.49
1:C:28:LEU:HD12	1:C:339:VAL:CG1	2.41	0.49
1:G:460:ARG:HH22	1:H:333:ASP:CG	2.21	0.49
1:H:57:LEU:HD23	1:H:196:VAL:HG23	1.94	0.49
1:A:96:VAL:O	1:A:100:THR:HG23	2.12	0.49
1:A:174:LEU:HB2	1:A:197:TRP:CZ2	2.48	0.49
1:B:403:MET:HE3	1:B:405:LYS:HB2	1.94	0.49
1:C:228:ARG:HG3	1:C:228:ARG:HH11	1.78	0.49
1:G:453:PRO:HA	1:G:457:GLU:OE2	2.13	0.49
1:A:404:VAL:HG11	1:A:459:PHE:HA	1.95	0.49
1:B:164:THR:HG21	1:B:248:LYS:NZ	2.27	0.49
1:C:6:ASP:O	1:C:31:LYS:HE3	2.13	0.49
1:C:7:ALA:O	1:C:141:THR:HA	2.13	0.49
1:C:24:LYS:O	1:C:28:LEU:HG	2.13	0.49
1:B:7:ALA:O	1:B:141:THR:HA	2.13	0.48
1:B:322:VAL:CG1	1:B:323:ALA:N	2.76	0.48
1:E:131:LYS:NZ	1:E:137:GLN:HB2	2.27	0.48
1:B:294:ILE:HD11	1:B:312:ILE:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:THR:HG23	1:D:315:ILE:O	2.13	0.48
1:H:362:PRO:HA	5:H:2103:HOH:O	2.13	0.48
1:C:5:ILE:HB	1:C:139:ILE:HD13	1.95	0.48
1:A:402:GLY:HA3	1:A:421:LEU:O	2.13	0.48
1:E:333:ASP:O	1:E:337:ILE:HG12	2.13	0.48
1:H:35:ILE:HA	1:H:115:VAL:O	2.13	0.48
1:A:224:LYS:HD2	5:A:2053:HOH:O	2.14	0.48
1:C:254:ILE:O	1:C:270:THR:HA	2.13	0.48
1:E:78:MET:HG2	1:F:78:MET:SD	2.54	0.48
1:A:414:ARG:NH2	1:F:305:ASN:HA	2.29	0.48
1:G:225:ASN:O	1:G:229:ILE:HG13	2.13	0.48
1:A:211:GLY:HA3	2:A:2003:SO4:O4	2.13	0.48
1:C:20:VAL:HG12	1:C:336:ILE:HG13	1.94	0.48
1:C:370:SER:OG	1:C:373:GLN:HG3	2.13	0.48
1:D:57:LEU:HD13	1:D:359:TYR:HB2	1.96	0.48
1:F:249:LYS:HD2	1:F:255:ASP:OD1	2.13	0.48
1:G:460:ARG:NH1	5:G:2132:HOH:O	2.46	0.48
1:A:35:ILE:HD11	1:A:139:ILE:HD12	1.95	0.48
1:B:11:VAL:HG11	1:B:22:ALA:HB2	1.96	0.48
1:D:155:PHE:HZ	1:D:243:VAL:O	1.97	0.48
1:D:187:GLY:O	1:D:191:VAL:HG23	2.14	0.48
1:H:110:ASN:O	1:H:111:LYS:HB2	2.12	0.48
1:B:328:ALA:O	1:B:332:GLU:HG3	2.13	0.48
1:D:208:GLU:HG3	1:D:210:LEU:N	2.28	0.48
1:H:225:ASN:HD22	1:H:403:MET:HE2	1.77	0.48
1:A:307:ARG:HH12	1:F:437:GLU:HG3	1.79	0.48
1:G:61:HIS:HD2	5:G:2083:HOH:O	1.96	0.48
1:G:242:LYS:NZ	5:G:2247:HOH:O	2.47	0.48
1:A:54:LYS:HE3	1:A:54:LYS:N	2.28	0.47
1:F:414:ARG:CG	1:F:414:ARG:HH11	2.27	0.47
1:D:222:ILE:HG13	1:D:419:HIS:HB3	1.97	0.47
1:F:7:ALA:O	1:F:141:THR:HA	2.14	0.47
1:G:161:ASP:OD1	1:G:163:ASP:HB3	2.14	0.47
1:H:393:ARG:HD2	1:H:454:THR:HA	1.96	0.47
1:E:260:ALA:HB2	1:E:265:LYS:HG2	1.95	0.47
1:G:6:ASP:HA	1:G:140:ASP:O	2.13	0.47
1:E:5:ILE:O	1:E:139:ILE:HA	2.15	0.47
1:E:179:GLU:HB3	1:E:272:ASP:OD2	2.15	0.47
1:F:409:GLN:HB2	1:F:416:LEU:HD11	1.97	0.47
1:G:372:GLU:H	1:G:372:GLU:CD	2.21	0.47
1:H:88:MET:HE1	1:H:200:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:THR:HG21	1:E:248:LYS:NZ	2.29	0.47
1:A:208:GLU:HG3	1:A:210:LEU:H	1.78	0.47
1:A:264:GLY:C	1:A:266:ALA:H	2.23	0.47
1:F:414:ARG:HD2	1:F:439:GLY:O	2.15	0.47
5:E:2076:HOH:O	1:F:449:CYS:HB3	2.15	0.47
1:F:121:ILE:HG21	1:F:292:LEU:HD11	1.96	0.47
1:C:64:HIS:O	1:C:64:HIS:CD2	2.68	0.46
1:F:299:ARG:NH1	5:F:2186:HOH:O	2.47	0.46
1:D:279:GLY:HA2	4:D:481:NAD:O1A	2.15	0.46
1:H:139:ILE:N	1:H:139:ILE:HD12	2.31	0.46
1:B:61:HIS:O	1:B:65:MET:HG2	2.15	0.46
1:B:37:LYS:HE2	3:B:480:FAD:O2B	2.15	0.46
1:G:162:GLU:HA	1:G:166:VAL:HG12	1.97	0.46
1:F:226:PHE:CZ	1:F:230:LEU:HD11	2.50	0.46
1:F:409:GLN:HG2	5:F:2227:HOH:O	2.15	0.46
1:A:460:ARG:HH22	1:B:333:ASP:CG	2.23	0.46
1:C:431:GLU:HA	1:D:431:GLU:HG3	1.98	0.46
1:D:318:ILE:C	1:D:318:ILE:HD12	2.41	0.46
1:G:220:MET:O	1:G:224:LYS:HG2	2.15	0.46
1:F:69:THR:O	1:F:69:THR:HG22	2.16	0.46
1:F:249:LYS:HB2	1:F:251:ASP:OD1	2.16	0.46
1:H:442:CYS:HB2	1:H:467:SER:HB2	1.98	0.46
1:C:11:VAL:HG22	1:C:145:LEU:HD23	1.98	0.46
1:C:78:MET:CE	1:D:78:MET:HE3	2.46	0.46
1:E:55:ALA:HB2	1:F:396:THR:HG23	1.98	0.46
1:A:188:VAL:O	1:A:192:GLU:HG3	2.16	0.46
1:A:321:VAL:HG23	1:A:322:VAL:HG13	1.98	0.46
1:B:282:PRO:HB3	1:B:321:VAL:HA	1.97	0.46
1:F:162:GLU:HA	1:F:166:VAL:HG12	1.97	0.46
1:G:179:GLU:HG3	5:G:2263:HOH:O	2.15	0.46
1:D:80:GLU:HG2	1:D:82:ARG:HH11	1.81	0.46
1:D:212:HIS:HB2	1:D:223:SER:OG	2.16	0.46
1:H:164:THR:HB	1:H:254:ILE:HD11	1.97	0.46
1:A:5:ILE:HG23	1:A:139:ILE:HG23	1.97	0.45
1:C:389:ALA:HA	1:C:400:THR:HB	1.97	0.45
1:E:312:ILE:HA	1:E:313:PRO:HD2	1.73	0.45
1:C:81:VAL:HG22	1:D:78:MET:HG2	1.97	0.45
1:H:225:ASN:ND2	1:H:403:MET:HE2	2.32	0.45
1:A:78:MET:HG2	1:B:78:MET:SD	2.55	0.45
1:D:211:GLY:O	1:D:239:LEU:HD13	2.16	0.45
1:D:212:HIS:ND1	2:D:2016:SO4:O4	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:ILE:HG21	1:E:292:LEU:HD21	1.99	0.45
1:F:380:GLU:HB2	2:F:2024:SO4:O2	2.16	0.45
1:H:116:ASN:ND2	1:H:117:GLY:N	2.65	0.45
1:A:438:TYR:O	1:F:305:ASN:HB2	2.16	0.45
1:B:182:VAL:HG23	1:B:271:CYS:HB3	1.99	0.45
1:H:187:GLY:O	1:H:191:VAL:HG23	2.16	0.45
1:C:84:ASN:ND2	1:D:77:GLU:OE2	2.49	0.45
1:D:80:GLU:HG3	1:D:82:ARG:HD3	1.98	0.45
1:F:372:GLU:CD	1:F:372:GLU:N	2.74	0.45
1:G:209:PHE:CD1	1:G:209:PHE:C	2.95	0.45
1:H:297:ASP:C	1:H:297:ASP:OD1	2.59	0.45
1:D:414:ARG:HA	1:D:441:SER:HA	1.97	0.45
1:H:452:HIS:HA	1:H:453:PRO:HA	1.71	0.45
1:A:282:PRO:HB3	1:A:321:VAL:HA	1.97	0.45
1:B:162:GLU:HA	1:B:166:VAL:HG12	1.99	0.45
1:D:231:GLN:HA	1:D:235:PHE:O	2.16	0.45
1:E:404:VAL:HG11	1:E:459:PHE:HA	1.98	0.45
5:E:2075:HOH:O	1:F:397:ASN:HB3	2.17	0.45
1:H:61:HIS:O	1:H:65:MET:HG2	2.17	0.45
1:E:447:ARG:HG2	1:E:447:ARG:HH11	1.82	0.45
1:C:81:VAL:HG22	1:D:78:MET:CG	2.46	0.45
1:C:404:VAL:HG11	1:C:459:PHE:HA	1.99	0.45
1:B:174:LEU:HD12	1:B:197:TRP:CE2	2.51	0.44
1:F:246:ALA:HA	1:F:255:ASP:O	2.16	0.44
1:F:414:ARG:NH1	1:F:414:ARG:HG2	2.32	0.44
1:A:175:LYS:O	1:A:176:LYS:HG2	2.18	0.44
1:B:282:PRO:HG3	1:B:301:ARG:HG3	1.99	0.44
1:G:57:LEU:HD13	1:G:359:TYR:HB2	1.99	0.44
1:A:389:ALA:HA	1:A:400:THR:HB	1.99	0.44
1:G:181:MET:HE1	1:G:197:TRP:CG	2.52	0.44
1:G:181:MET:HE1	1:G:197:TRP:CD1	2.52	0.44
1:E:24:LYS:HB3	1:E:339:VAL:HG11	1.99	0.44
1:G:20:VAL:HG12	1:G:336:ILE:HG13	1.99	0.44
1:C:330:LYS:O	1:C:334:GLU:HG3	2.17	0.44
1:D:350:ASP:OD2	1:D:352:ASN:HB3	2.18	0.44
1:D:452:HIS:HA	1:D:453:PRO:HA	1.76	0.44
1:E:211:GLY:N	2:E:2021:SO4:O1	2.48	0.44
1:H:310:THR:HG23	1:H:315:ILE:O	2.17	0.44
1:B:297:ASP:CB	1:B:298:PRO:HD2	2.46	0.44
1:B:402:GLY:HA3	1:B:421:LEU:O	2.17	0.44
1:D:244:THR:HG1	1:D:257:SER:HB2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:162:GLU:HA	1:F:162:GLU:OE1	2.18	0.44
1:F:216:VAL:HG22	4:F:481:NAD:O2N	2.18	0.44
1:A:263:GLY:HA3	1:H:97:LYS:CE	2.47	0.44
1:B:164:THR:OG1	1:B:254:ILE:HD11	2.18	0.44
1:D:15:GLY:HA3	3:D:480:FAD:H52A	2.00	0.44
1:F:291:GLU:H	1:F:291:GLU:CD	2.25	0.44
1:H:316:TYR:CD1	1:H:342:MET:HE2	2.53	0.44
1:H:374:LEU:HD12	1:H:407:LEU:HD13	1.98	0.44
1:B:442:CYS:HB2	1:B:467:SER:HB2	2.00	0.43
1:C:25:ALA:HA	1:C:339:VAL:HG11	2.00	0.43
1:H:461:GLU:OE2	1:H:471:SER:HB2	2.18	0.43
1:C:28:LEU:CD1	1:C:339:VAL:HG12	2.46	0.43
1:H:171:ALA:HB2	1:H:275:LEU:HD13	2.00	0.43
1:A:222:ILE:HG13	1:A:419:HIS:HB3	2.00	0.43
1:H:312:ILE:HA	1:H:313:PRO:HD3	1.83	0.43
1:A:181:MET:HE1	1:A:197:TRP:CD1	2.53	0.43
1:A:330:LYS:O	1:A:334:GLU:HG3	2.18	0.43
1:E:182:VAL:HG23	1:E:271:CYS:HB3	2.00	0.43
1:F:35:ILE:HD11	1:F:139:ILE:HD13	2.01	0.43
1:D:91:GLN:NE2	5:D:2099:HOH:O	2.50	0.43
1:F:209:PHE:HD1	1:F:242:LYS:HB3	1.83	0.43
1:C:341:GLY:HA3	5:C:2144:HOH:O	2.18	0.43
1:H:307:ARG:HA	1:H:347:VAL:HG11	2.01	0.43
1:B:180:LYS:HD3	1:B:270:THR:O	2.18	0.43
1:C:249:LYS:HB2	1:C:251:ASP:OD1	2.19	0.43
1:G:211:GLY:N	2:G:2030:SO4:O3	2.47	0.43
1:H:404:VAL:HG11	1:H:459:PHE:HA	2.00	0.43
1:A:7:ALA:O	1:A:141:THR:HA	2.17	0.43
1:B:121:ILE:HG21	1:B:292:LEU:HD22	2.01	0.43
1:D:40:THR:HG21	1:D:100:THR:CG2	2.47	0.43
1:D:330:LYS:O	1:D:334:GLU:HG3	2.18	0.43
1:G:209:PHE:CE1	1:G:210:LEU:HG	2.53	0.43
1:A:297:ASP:OD1	1:A:297:ASP:C	2.62	0.43
1:D:146:ILE:HG23	1:D:287:LEU:HD21	2.00	0.43
1:D:162:GLU:HA	1:D:166:VAL:HG12	2.00	0.43
1:F:404:VAL:HG11	1:F:459:PHE:HA	2.01	0.43
1:G:208:GLU:O	1:G:239:LEU:HA	2.19	0.43
1:H:304:VAL:HB	1:H:308:PHE:HA	2.01	0.43
1:C:78:MET:SD	1:D:78:MET:HE3	2.59	0.43
1:D:171:ALA:HB2	1:D:275:LEU:HD13	2.01	0.43
1:H:222:ILE:HG13	1:H:419:HIS:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ASN:O	1:A:229:ILE:HG13	2.19	0.42
1:C:80:GLU:HG2	1:C:81:VAL:N	2.33	0.42
1:C:123:GLY:C	1:C:125:ASN:N	2.74	0.42
1:D:445:ILE:HG21	1:D:463:ASN:ND2	2.33	0.42
1:E:46:LEU:HD12	1:E:46:LEU:O	2.19	0.42
1:H:6:ASP:HB2	1:H:140:ASP:O	2.19	0.42
1:H:46:LEU:HA	1:H:51:ILE:CG1	2.49	0.42
1:A:25:ALA:CA	1:A:339:VAL:HG11	2.49	0.42
1:A:179:GLU:HB2	1:A:272:ASP:OD2	2.18	0.42
1:A:431:GLU:HA	1:B:431:GLU:HG3	2.01	0.42
1:B:187:GLY:O	1:B:191:VAL:HG23	2.19	0.42
1:D:40:THR:HG21	1:D:47:ASN:OD1	2.19	0.42
1:D:79:SER:O	1:D:80:GLU:HB3	2.19	0.42
1:F:146:ILE:HG23	1:F:287:LEU:HD11	2.02	0.42
1:A:87:LYS:HE2	1:B:73:SER:HA	2.00	0.42
1:B:15:GLY:CA	3:B:480:FAD:H52A	2.47	0.42
1:D:184:ILE:HD12	1:D:276:VAL:HG22	2.01	0.42
1:D:402:GLY:HA3	1:D:421:LEU:O	2.19	0.42
1:E:51:ILE:HB	1:E:52:PRO:HD3	2.01	0.42
1:F:6:ASP:HA	1:F:140:ASP:O	2.19	0.42
1:E:333:ASP:OD1	1:F:460:ARG:NH2	2.49	0.42
1:G:309:GLN:HG2	1:G:316:TYR:CE2	2.54	0.42
1:A:211:GLY:CA	2:A:2003:SO4:O4	2.67	0.42
1:C:380:GLU:HG3	1:C:410:LYS:HD3	2.01	0.42
1:F:35:ILE:HD11	1:F:139:ILE:CD1	2.50	0.42
1:B:46:LEU:HD11	1:B:99:LEU:HB2	2.01	0.42
1:E:79:SER:HB2	1:F:79:SER:HG	1.84	0.42
1:F:46:LEU:HD12	1:F:46:LEU:O	2.19	0.42
1:C:101:GLY:O	1:C:104:ALA:HB3	2.19	0.42
1:C:409:GLN:NE2	2:C:2009:SO4:O1	2.52	0.42
1:F:412:THR:OG1	1:F:414:ARG:HB2	2.19	0.42
1:C:119:GLY:HA2	1:C:129:ALA:HA	2.01	0.42
1:E:228:ARG:HG3	1:E:228:ARG:HH11	1.84	0.42
1:G:312:ILE:HA	1:G:313:PRO:HD2	1.89	0.42
1:G:414:ARG:HA	1:G:441:SER:HA	2.01	0.42
1:A:231:GLN:HA	1:A:235:PHE:O	2.20	0.42
1:B:249:LYS:HB2	1:B:251:ASP:OD1	2.20	0.42
1:F:402:GLY:HA3	1:F:421:LEU:O	2.20	0.42
1:C:123:GLY:C	1:C:125:ASN:H	2.28	0.42
1:H:136:THR:HG22	1:H:137:GLN:N	2.35	0.42
1:H:443:GLU:O	1:H:444:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ASP:C	1:A:135:GLY:H	2.27	0.41
1:C:336:ILE:O	1:C:340:GLU:HG3	2.19	0.41
1:D:282:PRO:HG2	1:D:301:ARG:HG3	2.01	0.41
1:G:396:THR:HG22	1:H:55:ALA:HB2	2.02	0.41
1:H:54:LYS:CA	1:H:54:LYS:HE3	2.50	0.41
1:E:308:PHE:CZ	1:E:334:GLU:HG2	2.55	0.41
1:F:46:LEU:HD11	1:F:99:LEU:HB2	2.01	0.41
1:F:259:GLU:HB2	1:F:264:GLY:O	2.19	0.41
1:H:7:ALA:HB2	1:H:33:VAL:HG23	2.01	0.41
1:H:136:THR:CG2	1:H:137:GLN:N	2.83	0.41
1:H:428:MET:HE3	1:H:428:MET:HB2	1.88	0.41
1:A:372:GLU:CD	1:A:372:GLU:H	2.28	0.41
1:C:231:GLN:HA	1:C:235:PHE:O	2.20	0.41
1:F:312:ILE:HA	1:F:313:PRO:HD3	1.73	0.41
1:H:46:LEU:HA	1:H:51:ILE:HG12	2.02	0.41
1:H:265:LYS:O	1:H:267:GLU:HG3	2.19	0.41
1:H:444:ASP:O	1:H:448:VAL:HG23	2.20	0.41
1:B:24:LYS:O	1:B:28:LEU:HD13	2.20	0.41
1:C:290:GLU:CD	1:C:290:GLU:H	2.28	0.41
1:A:396:THR:CG2	1:B:55:ALA:HB2	2.51	0.41
1:B:330:LYS:O	1:B:334:GLU:HG3	2.21	0.41
1:D:84:ASN:ND2	1:D:87:LYS:HB2	2.35	0.41
1:E:304:VAL:HB	1:E:308:PHE:HA	2.02	0.41
1:F:452:HIS:HA	1:F:453:PRO:HA	1.80	0.41
1:G:412:THR:O	1:G:413:ASP:CB	2.68	0.41
1:C:282:PRO:CG	1:C:301:ARG:HG2	2.50	0.41
1:D:35:ILE:HD11	1:D:139:ILE:CD1	2.50	0.41
1:D:259:GLU:HB2	1:D:264:GLY:O	2.20	0.41
1:C:420:ILE:HD13	1:C:428:MET:HB3	2.02	0.41
1:D:209:PHE:HD1	1:D:242:LYS:HB3	1.86	0.41
1:D:312:ILE:HA	1:D:313:PRO:HD2	1.68	0.41
1:H:410:LYS:HB2	1:H:410:LYS:HE2	1.84	0.41
1:G:20:VAL:CG1	1:G:336:ILE:HG13	2.51	0.41
1:G:146:ILE:O	1:G:317:ALA:HA	2.20	0.41
1:A:39:GLU:HG3	5:A:2096:HOH:O	2.20	0.41
1:B:322:VAL:HG12	1:B:323:ALA:N	2.35	0.41
1:C:161:ASP:OD1	1:C:163:ASP:HB3	2.21	0.41
1:C:226:PHE:CZ	1:C:230:LEU:HD11	2.55	0.41
1:D:12:ILE:HD13	1:D:287:LEU:HD11	2.02	0.41
1:D:121:ILE:CG2	1:D:292:LEU:HD11	2.48	0.41
1:E:85:LEU:HD12	1:E:85:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:161:ASP:OD1	1:E:163:ASP:HB3	2.21	0.41
1:F:445:ILE:HG21	1:F:463:ASN:ND2	2.36	0.41
1:G:174:LEU:HD12	1:G:197:TRP:CE2	2.56	0.41
1:B:83:LEU:HD22	1:B:200:LEU:HD22	2.03	0.41
1:D:358:ILE:HD12	1:D:364:VAL:HB	2.03	0.41
1:F:188:VAL:HG23	1:F:189:ILE:N	2.36	0.41
1:G:80:GLU:HB2	1:G:82:ARG:CZ	2.50	0.41
1:A:178:PRO:HG3	1:A:181:MET:HE2	2.01	0.40
1:E:46:LEU:HD11	1:E:99:LEU:HB2	2.02	0.40
1:E:58:ASN:ND2	5:E:2085:HOH:O	2.55	0.40
1:G:282:PRO:HB3	1:G:321:VAL:HA	2.02	0.40
1:A:180:LYS:HD3	1:A:270:THR:O	2.20	0.40
1:A:182:VAL:HG11	1:A:256:VAL:HG21	2.03	0.40
1:B:308:PHE:O	1:B:316:TYR:HB3	2.21	0.40
1:C:188:VAL:HG13	1:C:358:ILE:HG12	2.03	0.40
1:E:16:PRO:HD2	3:E:480:FAD:O5'	2.21	0.40
1:F:414:ARG:CG	1:F:414:ARG:NH1	2.85	0.40
1:A:6:ASP:HA	1:A:140:ASP:O	2.22	0.40
1:B:150:SER:CB	1:B:281:ARG:O	2.70	0.40
1:E:340:GLU:CD	1:F:447:ARG:HH22	2.29	0.40
1:G:50:CYS:O	1:G:54:LYS:HD2	2.20	0.40
1:G:222:ILE:HG23	1:G:421:LEU:HB2	2.04	0.40
1:A:146:ILE:O	1:A:317:ALA:HA	2.22	0.40
1:C:179:GLU:HB3	1:C:272:ASP:OD2	2.21	0.40
1:C:396:THR:HG23	1:D:55:ALA:HB2	2.04	0.40
1:D:210:LEU:HB3	2:D:2016:SO4:O4	2.21	0.40
1:F:409:GLN:HG3	1:F:412:THR:H	1.87	0.40
1:G:216:VAL:O	1:G:216:VAL:HG13	2.21	0.40
1:H:436:LEU:HD12	1:H:436:LEU:HA	1.82	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:2166:HOH:O	5:H:2166:HOH:O[2_675]	2.00	0.20

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	471/474 (99%)	447 (95%)	21 (4%)	3 (1%)	21	36
1	B	469/474 (99%)	444 (95%)	23 (5%)	2 (0%)	30	47
1	C	469/474 (99%)	441 (94%)	26 (6%)	2 (0%)	30	47
1	D	473/474 (100%)	448 (95%)	24 (5%)	1 (0%)	43	62
1	E	470/474 (99%)	448 (95%)	19 (4%)	3 (1%)	21	36
1	F	470/474 (99%)	453 (96%)	17 (4%)	0	100	100
1	G	471/474 (99%)	451 (96%)	19 (4%)	1 (0%)	43	62
1	H	469/474 (99%)	448 (96%)	21 (4%)	0	100	100
All	All	3762/3792 (99%)	3580 (95%)	170 (4%)	12 (0%)	36	53

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	SER
1	G	79	SER
1	A	266	ALA
1	E	131	LYS
1	B	131	LYS
1	B	360	THR
1	C	360	THR
1	C	133	ASP
1	D	259	GLU
1	E	313	PRO
1	E	263	GLY
1	A	313	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	373/373 (100%)	355 (95%)	18 (5%)	23	43
1	B	371/373 (100%)	362 (98%)	9 (2%)	43	69
1	C	371/373 (100%)	358 (96%)	13 (4%)	32	56
1	D	374/373 (100%)	359 (96%)	15 (4%)	28	51
1	E	372/373 (100%)	359 (96%)	13 (4%)	32	56
1	F	372/373 (100%)	360 (97%)	12 (3%)	34	60
1	G	373/373 (100%)	361 (97%)	12 (3%)	34	60
1	H	371/373 (100%)	363 (98%)	8 (2%)	45	71
All	All	2977/2984 (100%)	2877 (97%)	100 (3%)	32	57

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	TYR
1	A	50	CYS
1	A	54	LYS
1	A	88	MET
1	A	124	LYS
1	A	174	LEU
1	A	179	GLU
1	A	213	VAL
1	A	242	LYS
1	A	247	THR
1	A	249	LYS
1	A	251	ASP
1	A	265	LYS
1	A	276	VAL
1	A	277	CYS
1	A	376	GLU
1	A	438	TYR
1	A	472	ILE
1	B	19	TYR
1	B	28	LEU
1	B	32	THR
1	B	50	CYS
1	B	54	LYS

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Mol	Chain	Res	Type
1	B	228	ARG
1	B	277	CYS
1	B	387	PRO
1	B	436	LEU
1	C	19	TYR
1	C	46	LEU
1	C	50	CYS
1	C	54	LYS
1	C	78	MET
1	C	87	LYS
1	C	174	LEU
1	C	224	LYS
1	C	277	CYS
1	C	306	THR
1	C	321	VAL
1	C	354	VAL
1	C	436	LEU
1	D	19	TYR
1	D	39	GLU
1	D	46	LEU
1	D	50	CYS
1	D	54	LYS
1	D	79	SER
1	D	82	ARG
1	D	124	LYS
1	D	285	LYS
1	D	290	GLU
1	D	321	VAL
1	D	329	HIS
1	D	376	GLU
1	D	379	ILE
1	D	438	TYR
1	E	6	ASP
1	E	19	TYR
1	E	39	GLU
1	E	50	CYS
1	E	54	LYS
1	E	164	THR
1	E	231	GLN
1	E	250	SER
1	E	259	GLU
1	E	277	CYS

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Mol	Chain	Res	Type
1	E	339	VAL
1	E	436	LEU
1	E	472	ILE
1	F	19	TYR
1	F	50	CYS
1	F	54	LYS
1	F	224	LYS
1	F	232	LYS
1	F	273	VAL
1	F	277	CYS
1	F	318	ILE
1	F	376	GLU
1	F	409	GLN
1	F	414	ARG
1	F	467	SER
1	G	3	GLN
1	G	19	TYR
1	G	50	CYS
1	G	54	LYS
1	G	80	GLU
1	G	136	THR
1	G	152	VAL
1	G	213	VAL
1	G	238	LYS
1	G	277	CYS
1	G	318	ILE
1	G	431	GLU
1	H	19	TYR
1	H	50	CYS
1	H	54	LYS
1	H	78	MET
1	H	224	LYS
1	H	277	CYS
1	H	380	GLU
1	H	436	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	143	ASN
1	A	227	GLN

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Mol	Chain	Res	Type
1	A	231	GLN
1	A	240	ASN
1	B	47	ASN
1	B	58	ASN
1	B	61	HIS
1	B	143	ASN
1	B	240	ASN
1	B	348	HIS
1	B	409	GLN
1	B	430	ASN
1	C	47	ASN
1	C	58	ASN
1	C	125	ASN
1	C	227	GLN
1	C	231	GLN
1	C	348	HIS
1	C	409	GLN
1	D	61	HIS
1	D	64	HIS
1	D	109	GLN
1	D	116	ASN
1	D	225	ASN
1	D	227	GLN
1	D	231	GLN
1	E	27	GLN
1	E	58	ASN
1	E	67	HIS
1	E	109	GLN
1	E	110	ASN
1	E	137	GLN
1	E	227	GLN
1	E	231	GLN
1	E	286	ASN
1	E	409	GLN
1	F	110	ASN
1	F	125	ASN
1	F	198	GLN
1	F	227	GLN
1	F	231	GLN
1	F	352	ASN
1	G	3	GLN
1	G	126	GLN

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Mol	Chain	Res	Type
1	G	137	GLN
1	G	227	GLN
1	G	231	GLN
1	G	361	HIS
1	H	58	ASN
1	H	61	HIS
1	H	114	HIS
1	H	116	ASN
1	H	143	ASN
1	H	225	ASN
1	H	240	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 ⓘ

52 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	SO4	A	2000	-	4,4,4	0.70	0	6,6,6	0.05	0
2	SO4	E	2020	-	4,4,4	0.70	0	6,6,6	0.09	0
2	SO4	C	2008	-	4,4,4	0.69	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	H	2031	-	4,4,4	0.70	0	6,6,6	0.07	0
2	SO4	E	2019	-	4,4,4	0.69	0	6,6,6	0.10	0
3	FAD	D	480	-	58,58,58	1.34	7 (12%)	85,89,89	1.11	7 (8%)
2	SO4	G	2026	-	4,4,4	0.69	0	6,6,6	0.10	0
4	NAD	D	481	-	46,48,48	1.33	7 (15%)	64,73,73	1.54	11 (17%)
2	SO4	H	2033	-	4,4,4	0.70	0	6,6,6	0.09	0
3	FAD	H	480	-	58,58,58	1.35	7 (12%)	85,89,89	1.13	9 (10%)
2	SO4	E	2017	-	4,4,4	0.69	0	6,6,6	0.10	0
4	NAD	B	481	-	28,29,48	1.31	3 (10%)	43,45,73	1.82	11 (25%)
2	SO4	D	2015	-	4,4,4	0.70	0	6,6,6	0.10	0
4	NAD	E	481	-	28,29,48	1.32	3 (10%)	43,45,73	1.81	10 (23%)
2	SO4	C	2009	-	4,4,4	0.69	0	6,6,6	0.09	0
2	SO4	E	2018	-	4,4,4	0.70	0	6,6,6	0.08	0
2	SO4	F	2023	-	4,4,4	0.70	0	6,6,6	0.08	0
2	SO4	G	2028	-	4,4,4	0.70	0	6,6,6	0.08	0
3	FAD	G	480	-	58,58,58	1.47	7 (12%)	85,89,89	1.09	5 (5%)
2	SO4	A	2002	-	4,4,4	0.70	0	6,6,6	0.08	0
2	SO4	G	2027	-	4,4,4	0.70	0	6,6,6	0.07	0
2	SO4	B	2006	-	4,4,4	0.70	0	6,6,6	0.09	0
4	NAD	C	481	-	28,29,48	1.35	5 (17%)	43,45,73	1.81	10 (23%)
2	SO4	A	2003	-	4,4,4	0.71	0	6,6,6	0.09	0
4	NAD	F	481	-	28,29,48	1.36	5 (17%)	43,45,73	1.75	9 (20%)
2	SO4	D	2014	-	4,4,4	0.70	0	6,6,6	0.09	0
2	SO4	C	2010	-	4,4,4	0.69	0	6,6,6	0.10	0
2	SO4	F	2022	-	4,4,4	0.69	0	6,6,6	0.10	0
2	SO4	G	2030	-	4,4,4	0.71	0	6,6,6	0.09	0
2	SO4	H	2034	-	4,4,4	0.69	0	6,6,6	0.08	0
2	SO4	D	2013	-	4,4,4	0.69	0	6,6,6	0.10	0
4	NAD	G	481	-	28,29,48	1.33	4 (14%)	43,45,73	1.76	9 (20%)
2	SO4	F	2024	-	4,4,4	0.69	0	6,6,6	0.07	0
2	SO4	H	2035	-	4,4,4	0.70	0	6,6,6	0.08	0
4	NAD	H	481	-	28,29,48	1.32	3 (10%)	43,45,73	1.82	10 (23%)
3	FAD	E	480	-	58,58,58	1.36	9 (15%)	85,89,89	1.07	6 (7%)
3	FAD	A	480	-	58,58,58	1.38	7 (12%)	85,89,89	1.04	6 (7%)
2	SO4	G	2029	-	4,4,4	0.69	0	6,6,6	0.07	0
2	SO4	B	2004	-	4,4,4	0.69	0	6,6,6	0.10	0
4	NAD	A	481	-	46,48,48	1.31	7 (15%)	64,73,73	1.59	12 (18%)
2	SO4	D	2016	-	4,4,4	0.71	0	6,6,6	0.09	0
2	SO4	H	2032	-	4,4,4	0.69	0	6,6,6	0.07	0
3	FAD	B	480	-	58,58,58	1.44	9 (15%)	85,89,89	1.08	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	2001	-	4,4,4	0.70	0	6,6,6	0.06	0
2	SO4	B	2007	-	4,4,4	0.70	0	6,6,6	0.08	0
2	SO4	C	2011	-	4,4,4	0.70	0	6,6,6	0.05	0
2	SO4	F	2025	-	4,4,4	0.70	0	6,6,6	0.07	0
3	FAD	C	480	-	58,58,58	1.51	10 (17%)	85,89,89	1.06	7 (8%)
2	SO4	B	2005	-	4,4,4	0.70	0	6,6,6	0.09	0
2	SO4	E	2021	-	4,4,4	0.70	0	6,6,6	0.10	0
2	SO4	D	2012	-	4,4,4	0.69	0	6,6,6	0.08	0
3	FAD	F	480	-	58,58,58	1.40	7 (12%)	85,89,89	1.10	6 (7%)

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
4	NAD	A	481	-	-	4/30/62/62	0/5/5/5
3	FAD	B	480	-	-	4/34/50/50	0/6/6/6
3	FAD	D	480	-	-	4/34/50/50	0/6/6/6
4	NAD	E	481	-	-	3/16/32/62	0/3/3/5
4	NAD	G	481	-	-	0/16/32/62	0/3/3/5
3	FAD	G	480	-	-	4/34/50/50	0/6/6/6
4	NAD	D	481	-	-	5/30/62/62	0/5/5/5
3	FAD	C	480	-	-	3/34/50/50	0/6/6/6
3	FAD	H	480	-	-	4/34/50/50	0/6/6/6
4	NAD	C	481	-	-	4/16/32/62	0/3/3/5
4	NAD	F	481	-	-	4/16/32/62	0/3/3/5
4	NAD	H	481	-	-	0/16/32/62	0/3/3/5
4	NAD	B	481	-	-	0/16/32/62	0/3/3/5
3	FAD	E	480	-	-	4/34/50/50	0/6/6/6
3	FAD	A	480	-	-	4/34/50/50	0/6/6/6
3	FAD	F	480	-	-	4/34/50/50	0/6/6/6

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	481	NAD	C2N-N1N	5.15	1.40	1.35
4	A	481	NAD	C2N-N1N	5.13	1.40	1.35
3	B	480	FAD	C4X-N5	4.75	1.41	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	480	FAD	C4X-N5	4.73	1.41	1.30
3	A	480	FAD	PA-O3P	4.63	1.64	1.59
3	D	480	FAD	C4X-N5	4.28	1.40	1.30
3	H	480	FAD	C4X-N5	4.27	1.40	1.30
3	E	480	FAD	C4X-N5	4.15	1.39	1.30
3	G	480	FAD	PA-O3P	4.08	1.63	1.59
3	G	480	FAD	C4X-N5	4.06	1.39	1.30
3	A	480	FAD	C4X-N5	4.05	1.39	1.30
3	D	480	FAD	PA-O3P	4.05	1.63	1.59
3	H	480	FAD	PA-O3P	3.98	1.63	1.59
4	F	481	NAD	PN-O1N	3.72	1.62	1.50
4	C	481	NAD	PN-O1N	3.72	1.62	1.50
3	C	480	FAD	C10-N1	3.65	1.40	1.33
3	F	480	FAD	C4X-N5	3.63	1.38	1.30
4	G	481	NAD	PN-O1N	3.62	1.61	1.50
4	H	481	NAD	PN-O1N	3.58	1.61	1.50
4	B	481	NAD	PN-O1N	3.56	1.61	1.50
4	E	481	NAD	PN-O1N	3.55	1.61	1.50
3	B	480	FAD	C10-N1	3.37	1.40	1.33
3	C	480	FAD	PA-O3P	3.27	1.63	1.59
3	B	480	FAD	PA-O3P	3.27	1.63	1.59
3	F	480	FAD	O2-C2	-3.23	1.18	1.24
3	G	480	FAD	C5B-C4B	3.20	1.61	1.51
3	G	480	FAD	C9A-C5X	3.16	1.46	1.41
4	D	481	NAD	C5A-N7A	-3.15	1.33	1.39
4	A	481	NAD	C5A-N7A	-3.15	1.33	1.39
4	E	481	NAD	C5A-N7A	-3.14	1.33	1.39
4	F	481	NAD	C5A-N7A	-3.12	1.33	1.39
4	G	481	NAD	C5A-N7A	-3.11	1.33	1.39
3	F	480	FAD	C10-N1	3.09	1.39	1.33
4	C	481	NAD	C5A-N7A	-3.09	1.33	1.39
4	B	481	NAD	C5A-N7A	-3.08	1.33	1.39
3	B	480	FAD	C9A-C5X	3.08	1.46	1.41
4	H	481	NAD	C5A-N7A	-3.05	1.33	1.39
3	F	480	FAD	C9A-C5X	3.01	1.46	1.41
3	E	480	FAD	C10-N1	2.98	1.39	1.33
3	G	480	FAD	C10-N1	2.96	1.39	1.33
3	F	480	FAD	PA-O3P	2.90	1.62	1.59
3	C	480	FAD	C9A-C5X	2.89	1.45	1.41
3	G	480	FAD	C6-C7	2.85	1.43	1.39
3	A	480	FAD	C9A-C5X	2.72	1.45	1.41
3	F	480	FAD	C5B-C4B	2.69	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	481	NAD	O4D-C1D	2.69	1.44	1.40
3	C	480	FAD	C9-C8	2.69	1.43	1.39
3	C	480	FAD	C10-N10	2.66	1.43	1.37
3	B	480	FAD	C2A-N1A	2.58	1.38	1.33
3	H	480	FAD	C9A-C5X	2.55	1.45	1.41
3	C	480	FAD	C9-C9A	2.54	1.43	1.39
3	H	480	FAD	C5B-C4B	2.52	1.59	1.51
3	D	480	FAD	C9A-C5X	2.49	1.45	1.41
3	E	480	FAD	C6-C7	2.47	1.43	1.39
3	E	480	FAD	C2A-N1A	2.46	1.38	1.33
3	G	480	FAD	C2A-N1A	2.42	1.38	1.33
3	B	480	FAD	C5B-C4B	2.40	1.58	1.51
3	H	480	FAD	C2A-N1A	2.39	1.38	1.33
3	D	480	FAD	C5B-C4B	2.38	1.58	1.51
3	C	480	FAD	C2A-N1A	2.38	1.38	1.33
4	A	481	NAD	C6N-N1N	2.37	1.40	1.35
3	H	480	FAD	O2-C2	-2.37	1.19	1.24
4	D	481	NAD	C6N-N1N	2.36	1.40	1.35
4	G	481	NAD	C8A-N9A	-2.36	1.33	1.37
4	A	481	NAD	O4D-C1D	2.36	1.44	1.40
4	C	481	NAD	C8A-N9A	-2.33	1.33	1.37
4	F	481	NAD	C8A-N9A	-2.32	1.33	1.37
4	E	481	NAD	C8A-N9A	-2.31	1.33	1.37
3	C	480	FAD	C9A-N10	2.30	1.45	1.41
3	D	480	FAD	O2-C2	-2.30	1.19	1.24
4	C	481	NAD	PN-O5D	-2.29	1.46	1.54
4	B	481	NAD	C8A-N9A	-2.29	1.33	1.37
4	D	481	NAD	C8A-N9A	-2.28	1.33	1.37
4	A	481	NAD	C8A-N9A	-2.27	1.33	1.37
4	H	481	NAD	C8A-N9A	-2.27	1.33	1.37
4	F	481	NAD	PN-O5D	-2.19	1.46	1.54
3	B	480	FAD	C10-N10	2.19	1.42	1.37
3	E	480	FAD	C10-N10	2.18	1.42	1.37
3	E	480	FAD	C9A-C5X	2.16	1.44	1.41
3	D	480	FAD	C2A-N1A	2.15	1.37	1.33
4	A	481	NAD	C3N-C7N	2.15	1.53	1.50
3	A	480	FAD	C2A-N1A	2.14	1.37	1.33
3	B	480	FAD	C8-C7	2.13	1.46	1.40
4	D	481	NAD	C4A-N9A	-2.12	1.33	1.37
3	A	480	FAD	C10-N1	2.12	1.37	1.33
3	D	480	FAD	PA-O5B	-2.11	1.51	1.59
3	F	480	FAD	C2A-N1A	2.11	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	480	FAD	C10-N1	2.10	1.37	1.33
4	F	481	NAD	C4A-N9A	-2.07	1.33	1.37
3	C	480	FAD	C6-C7	2.07	1.42	1.39
4	G	481	NAD	C4A-N9A	-2.06	1.33	1.37
3	A	480	FAD	C5B-C4B	2.06	1.57	1.51
4	A	481	NAD	C4A-N9A	-2.06	1.33	1.37
3	E	480	FAD	O2-C2	-2.05	1.20	1.24
3	B	480	FAD	O2-C2	-2.04	1.20	1.24
3	E	480	FAD	C9-C9A	2.04	1.42	1.39
3	A	480	FAD	C8-C7	2.03	1.45	1.40
4	C	481	NAD	C4A-N9A	-2.03	1.33	1.37
3	E	480	FAD	PA-O5B	-2.02	1.51	1.59
4	D	481	NAD	C3N-C7N	2.01	1.53	1.50

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	481	NAD	C5A-C4A-N3A	-5.40	119.29	126.72
4	C	481	NAD	C5A-C4A-N3A	-5.31	119.41	126.72
4	H	481	NAD	C5A-C4A-N3A	-5.30	119.42	126.72
4	B	481	NAD	C5A-C4A-N3A	-5.25	119.49	126.72
4	A	481	NAD	N3A-C2A-N1A	-5.12	120.84	128.58
4	D	481	NAD	N3A-C2A-N1A	-5.11	120.84	128.58
4	F	481	NAD	N3A-C2A-N1A	-5.03	120.97	128.58
4	F	481	NAD	C5A-C4A-N3A	-4.96	119.89	126.72
4	G	481	NAD	C5A-C4A-N3A	-4.94	119.91	126.72
4	G	481	NAD	N3A-C2A-N1A	-4.92	121.14	128.58
4	A	481	NAD	C5A-C4A-N3A	-4.90	119.97	126.72
4	H	481	NAD	N3A-C2A-N1A	-4.88	121.20	128.58
4	C	481	NAD	N3A-C2A-N1A	-4.87	121.21	128.58
4	B	481	NAD	N3A-C2A-N1A	-4.86	121.23	128.58
4	D	481	NAD	C5A-C4A-N3A	-4.73	120.20	126.72
4	E	481	NAD	N3A-C2A-N1A	-4.66	121.53	128.58
4	A	481	NAD	C4D-O4D-C1D	-3.78	106.46	109.92
4	H	481	NAD	C2A-N3A-C4A	3.74	120.96	111.83
4	C	481	NAD	C2A-N3A-C4A	3.72	120.91	111.83
4	B	481	NAD	C2A-N3A-C4A	3.69	120.85	111.83
4	E	481	NAD	N3A-C4A-N9A	3.69	133.45	127.17
4	B	481	NAD	N3A-C4A-N9A	3.67	133.42	127.17
4	A	481	NAD	C2A-N3A-C4A	3.66	120.77	111.83
4	E	481	NAD	C2A-N3A-C4A	3.65	120.74	111.83
4	H	481	NAD	N3A-C4A-N9A	3.63	133.35	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	481	NAD	C2A-N3A-C4A	3.63	120.70	111.83
4	C	481	NAD	N3A-C4A-N9A	3.63	133.34	127.17
4	D	481	NAD	C2A-N3A-C4A	3.59	120.61	111.83
4	G	481	NAD	C2A-N3A-C4A	3.59	120.59	111.83
4	D	481	NAD	N3A-C4A-N9A	3.58	133.25	127.17
4	A	481	NAD	N3A-C4A-N9A	3.58	133.25	127.17
4	F	481	NAD	N3A-C4A-N9A	3.50	133.13	127.17
4	G	481	NAD	N3A-C4A-N9A	3.49	133.10	127.17
3	D	480	FAD	O4B-C1B-C2B	-3.13	99.91	106.62
4	D	481	NAD	N9A-C8A-N7A	-3.07	109.59	113.94
4	B	481	NAD	N9A-C8A-N7A	-2.95	109.75	113.94
4	A	481	NAD	N9A-C8A-N7A	-2.93	109.78	113.94
4	G	481	NAD	N9A-C8A-N7A	-2.91	109.81	113.94
4	E	481	NAD	O4B-C1B-C2B	-2.89	100.44	106.62
4	D	481	NAD	C4B-O4B-C1B	-2.87	103.12	109.47
4	C	481	NAD	N9A-C8A-N7A	-2.87	109.87	113.94
4	H	481	NAD	N9A-C8A-N7A	-2.87	109.87	113.94
4	A	481	NAD	C4B-O4B-C1B	-2.84	103.19	109.47
4	C	481	NAD	C4A-C5A-N7A	-2.83	107.34	110.58
4	H	481	NAD	C4A-C5A-N7A	-2.81	107.36	110.58
3	A	480	FAD	O4B-C1B-C2B	-2.81	100.61	106.62
3	B	480	FAD	C9A-C5X-N5	-2.81	119.47	122.45
4	B	481	NAD	C4B-O4B-C1B	-2.81	103.27	109.47
4	E	481	NAD	C4A-C5A-N7A	-2.79	107.39	110.58
4	F	481	NAD	N9A-C8A-N7A	-2.77	110.00	113.94
4	B	481	NAD	C5A-N7A-C8A	2.76	107.79	103.45
4	B	481	NAD	C4A-C5A-N7A	-2.75	107.44	110.58
4	H	481	NAD	C5A-N7A-C8A	2.73	107.74	103.45
4	C	481	NAD	C5A-N7A-C8A	2.72	107.72	103.45
4	E	481	NAD	N9A-C8A-N7A	-2.72	110.08	113.94
3	C	480	FAD	C9A-C5X-N5	-2.72	119.57	122.45
3	E	480	FAD	C9A-C5X-N5	-2.71	119.57	122.45
4	C	481	NAD	O4B-C1B-C2B	-2.70	100.83	106.62
4	E	481	NAD	C5A-N7A-C8A	2.67	107.65	103.45
4	G	481	NAD	C5A-N7A-C8A	2.67	107.65	103.45
3	G	480	FAD	C9A-C5X-N5	-2.67	119.62	122.45
3	C	480	FAD	O4B-C1B-C2B	-2.67	100.91	106.62
4	G	481	NAD	C4A-C5A-N7A	-2.65	107.55	110.58
4	E	481	NAD	O5D-PN-O3	2.64	113.47	104.64
3	F	480	FAD	C9A-C5X-N5	-2.61	119.68	122.45
4	A	481	NAD	C5A-N7A-C8A	2.60	107.53	103.45
4	D	481	NAD	C5A-N7A-C8A	2.59	107.52	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	481	NAD	C4A-C5A-N7A	-2.57	107.64	110.58
4	F	481	NAD	C5A-N7A-C8A	2.57	107.49	103.45
4	D	481	NAD	C4A-N9A-C8A	2.55	108.41	105.74
4	C	481	NAD	O5D-PN-O3	2.51	113.04	104.64
3	F	480	FAD	N3A-C2A-N1A	-2.49	124.82	128.58
4	G	481	NAD	O5D-PN-O3	2.48	112.95	104.64
4	H	481	NAD	O5D-PN-O3	2.48	112.95	104.64
3	E	480	FAD	O4B-C1B-C2B	-2.48	101.32	106.62
3	H	480	FAD	C4-C4X-N5	2.47	121.61	118.21
4	H	481	NAD	O4B-C1B-C2B	-2.47	101.34	106.62
4	B	481	NAD	O5D-PN-O3	2.45	112.84	104.64
3	G	480	FAD	O4B-C1B-C2B	-2.42	101.43	106.62
4	A	481	NAD	C4A-C5A-N7A	-2.42	107.81	110.58
3	B	480	FAD	C4-C4X-N5	2.41	121.53	118.21
3	D	480	FAD	C4-C4X-N5	2.39	121.51	118.21
3	D	480	FAD	C4X-C10-N10	2.39	119.90	116.48
3	B	480	FAD	O4B-C1B-C2B	-2.37	101.54	106.62
3	E	480	FAD	C4-C4X-N5	2.37	121.48	118.21
3	F	480	FAD	C2B-C1B-N9A	2.36	119.16	113.30
3	H	480	FAD	O4B-C1B-C2B	-2.34	101.61	106.62
4	H	481	NAD	C4B-O4B-C1B	-2.33	104.31	109.47
3	C	480	FAD	C4-C4X-N5	2.32	121.42	118.21
4	D	481	NAD	C4A-C5A-N7A	-2.32	107.93	110.58
4	F	481	NAD	O5D-PN-O3	2.31	112.38	104.64
3	H	480	FAD	N3A-C2A-N1A	-2.30	125.11	128.58
3	H	480	FAD	C9A-C5X-N5	-2.29	120.02	122.45
4	A	481	NAD	C4A-N9A-C8A	2.25	108.10	105.74
3	F	480	FAD	O4B-C1B-C2B	-2.24	101.82	106.62
4	A	481	NAD	O4B-C1B-C2B	-2.24	101.83	106.62
3	H	480	FAD	O3P-PA-O1A	-2.22	104.01	110.70
3	G	480	FAD	N3A-C2A-N1A	-2.22	125.22	128.58
3	D	480	FAD	C9A-C5X-N5	-2.22	120.10	122.45
3	G	480	FAD	O3P-PA-O1A	-2.21	104.07	110.70
4	C	481	NAD	C4B-O4B-C1B	-2.20	104.61	109.47
4	D	481	NAD	O4B-C1B-C2B	-2.20	101.91	106.62
3	F	480	FAD	O3P-PA-O1A	-2.19	104.11	110.70
4	G	481	NAD	C4A-N9A-C8A	2.19	108.03	105.74
3	C	480	FAD	O3P-PA-O1A	-2.19	104.13	110.70
3	E	480	FAD	C5X-N5-C4X	2.18	121.62	118.09
3	B	480	FAD	O3P-PA-O1A	-2.18	104.16	110.70
3	E	480	FAD	O3P-PA-O1A	-2.17	104.17	110.70
3	A	480	FAD	C9A-C5X-N5	-2.17	120.16	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	480	FAD	O3P-PA-O1A	-2.16	104.21	110.70
3	A	480	FAD	C4X-C10-N10	2.16	119.57	116.48
3	C	480	FAD	C5X-N5-C4X	2.15	121.57	118.09
3	G	480	FAD	O3'-C3'-C4'	-2.14	104.07	108.93
3	A	480	FAD	C4-C4X-N5	2.12	121.14	118.21
3	D	480	FAD	C10-C4X-N5	-2.12	120.49	124.81
3	A	480	FAD	O3P-PA-O1A	-2.11	104.34	110.70
4	D	481	NAD	C3N-C7N-N7N	-2.11	115.13	117.74
3	B	480	FAD	N3A-C2A-N1A	-2.11	125.38	128.58
4	E	481	NAD	C4B-O4B-C1B	-2.11	104.81	109.47
4	B	481	NAD	O4B-C1B-C2B	-2.09	102.14	106.62
4	B	481	NAD	C4A-N9A-C8A	2.09	107.93	105.74
3	C	480	FAD	C10-C4X-N5	-2.08	120.56	124.81
3	H	480	FAD	O4'-C4'-C3'	2.08	114.11	109.25
3	H	480	FAD	C4X-C10-N10	2.07	119.45	116.48
4	F	481	NAD	C4A-N9A-C8A	2.05	107.89	105.74
3	E	480	FAD	C10-C4X-N5	-2.04	120.64	124.81
3	H	480	FAD	C10-C4X-N5	-2.03	120.65	124.81
3	B	480	FAD	C4X-C10-N10	2.03	119.39	116.48
3	F	480	FAD	O4'-C4'-C3'	2.03	114.00	109.25
3	A	480	FAD	C10-C4X-N5	-2.03	120.66	124.81
4	A	481	NAD	C6N-N1N-C2N	-2.03	120.15	121.88
3	C	480	FAD	N3A-C2A-N1A	-2.02	125.52	128.58
3	H	480	FAD	O3'-C3'-C4'	-2.02	104.35	108.93
3	D	480	FAD	C2B-C1B-N9A	2.01	118.31	113.30

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	481	NAD	C5B-O5B-PA-O1A
4	C	481	NAD	C5B-O5B-PA-O1A
4	E	481	NAD	C5B-O5B-PA-O2A
4	E	481	NAD	C5B-O5B-PA-O3
4	F	481	NAD	C5B-O5B-PA-O1A
4	F	481	NAD	C5B-O5B-PA-O3
3	C	480	FAD	O4B-C4B-C5B-O5B
3	D	480	FAD	O4B-C4B-C5B-O5B
3	E	480	FAD	O4B-C4B-C5B-O5B
3	F	480	FAD	O4B-C4B-C5B-O5B
3	G	480	FAD	O4B-C4B-C5B-O5B
3	A	480	FAD	O4B-C4B-C5B-O5B

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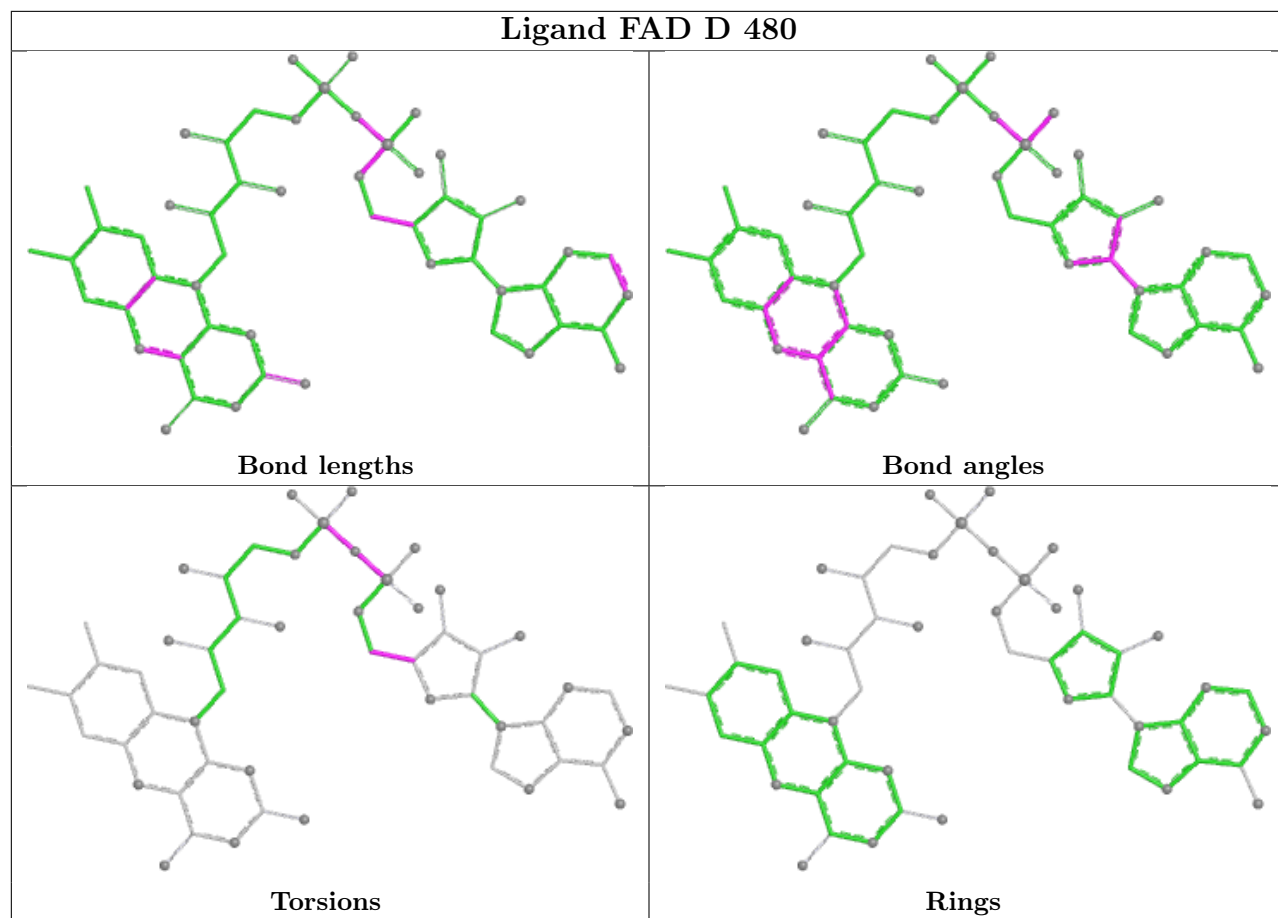
Mol	Chain	Res	Type	Atoms
3	B	480	FAD	O4B-C4B-C5B-O5B
3	B	480	FAD	C3B-C4B-C5B-O5B
3	C	480	FAD	C3B-C4B-C5B-O5B
3	F	480	FAD	C3B-C4B-C5B-O5B
3	D	480	FAD	C3B-C4B-C5B-O5B
3	E	480	FAD	C3B-C4B-C5B-O5B
3	G	480	FAD	C3B-C4B-C5B-O5B
4	D	481	NAD	PA-O3-PN-O1N
3	H	480	FAD	O4B-C4B-C5B-O5B
3	A	480	FAD	PA-O3P-P-O5'
3	B	480	FAD	PA-O3P-P-O5'
3	D	480	FAD	PA-O3P-P-O5'
3	F	480	FAD	PA-O3P-P-O5'
3	G	480	FAD	PA-O3P-P-O5'
3	A	480	FAD	C3B-C4B-C5B-O5B
3	A	480	FAD	P-O3P-PA-O1A
3	B	480	FAD	P-O3P-PA-O1A
3	C	480	FAD	P-O3P-PA-O1A
3	D	480	FAD	P-O3P-PA-O1A
3	E	480	FAD	P-O3P-PA-O1A
3	F	480	FAD	P-O3P-PA-O1A
3	G	480	FAD	P-O3P-PA-O1A
3	H	480	FAD	P-O3P-PA-O1A
4	D	481	NAD	PN-O3-PA-O1A
4	A	481	NAD	C5B-O5B-PA-O2A
4	A	481	NAD	C5B-O5B-PA-O3
4	C	481	NAD	C5B-O5B-PA-O2A
4	C	481	NAD	C5B-O5B-PA-O3
4	F	481	NAD	C5B-O5B-PA-O2A
4	D	481	NAD	PA-O3-PN-O2N
4	F	481	NAD	PN-O3-PA-O2A
3	H	480	FAD	C3B-C4B-C5B-O5B
4	D	481	NAD	PN-O3-PA-O2A
3	H	480	FAD	P-O3P-PA-O2A
4	E	481	NAD	O4B-C4B-C5B-O5B
4	D	481	NAD	O4B-C4B-C5B-O5B
3	E	480	FAD	P-O3P-PA-O2A
4	A	481	NAD	O4B-C4B-C5B-O5B
4	C	481	NAD	O4B-C4B-C5B-O5B

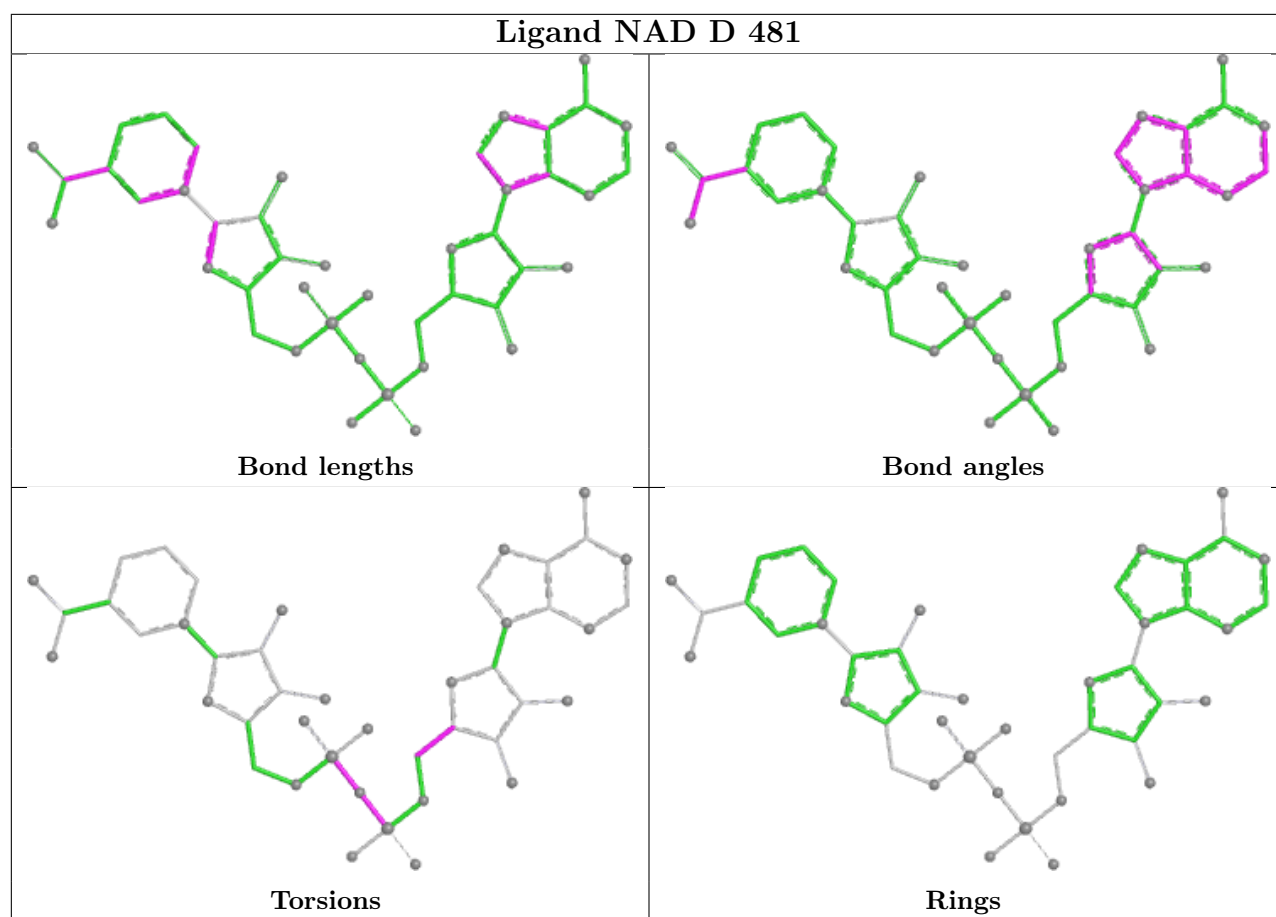
There are no ring outliers.

20 monomers are involved in 40 short contacts:

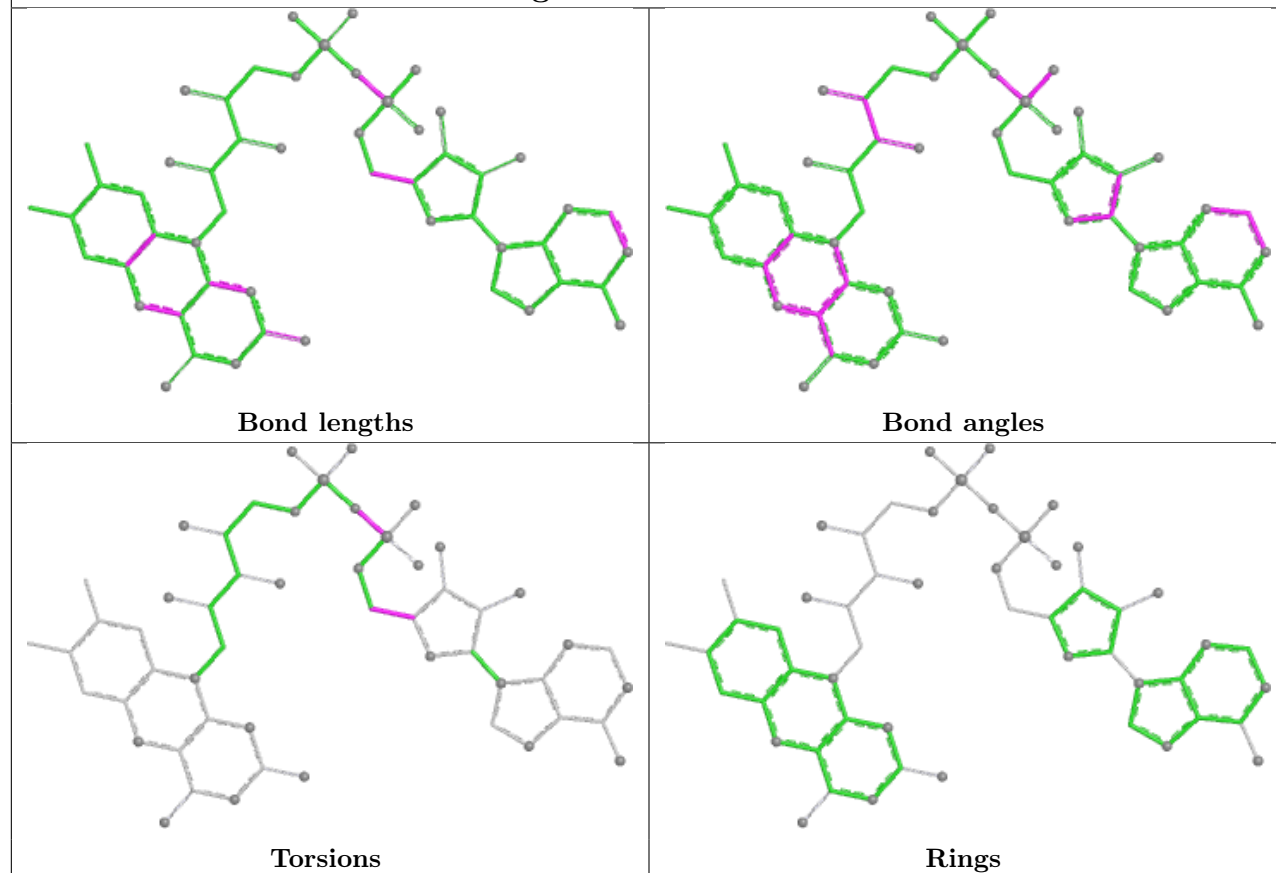
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	480	FAD	3	0
4	D	481	NAD	2	0
3	H	480	FAD	2	0
2	C	2009	SO4	1	0
3	G	480	FAD	3	0
2	A	2003	SO4	3	0
4	F	481	NAD	2	0
2	D	2014	SO4	2	0
2	G	2030	SO4	1	0
2	F	2024	SO4	1	0
4	H	481	NAD	1	0
3	E	480	FAD	3	0
3	A	480	FAD	2	0
2	B	2004	SO4	1	0
2	D	2016	SO4	2	0
3	B	480	FAD	4	0
2	B	2007	SO4	2	0
3	C	480	FAD	2	0
2	E	2021	SO4	1	0
3	F	480	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.

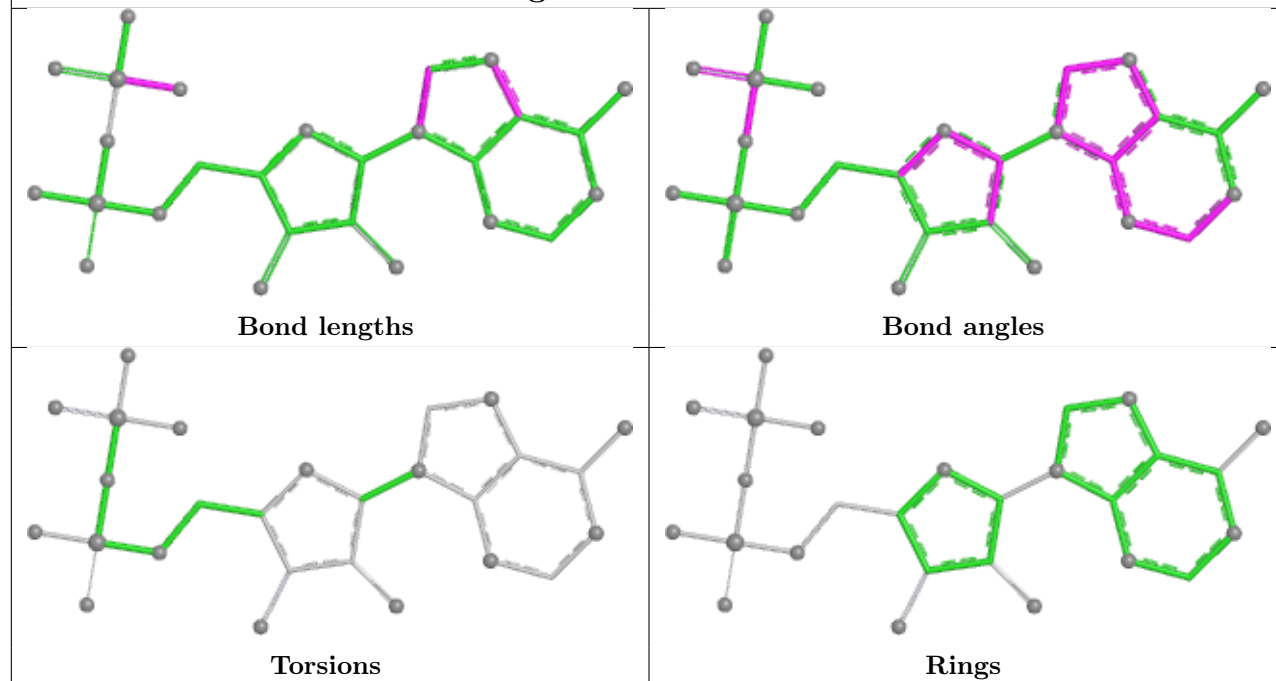


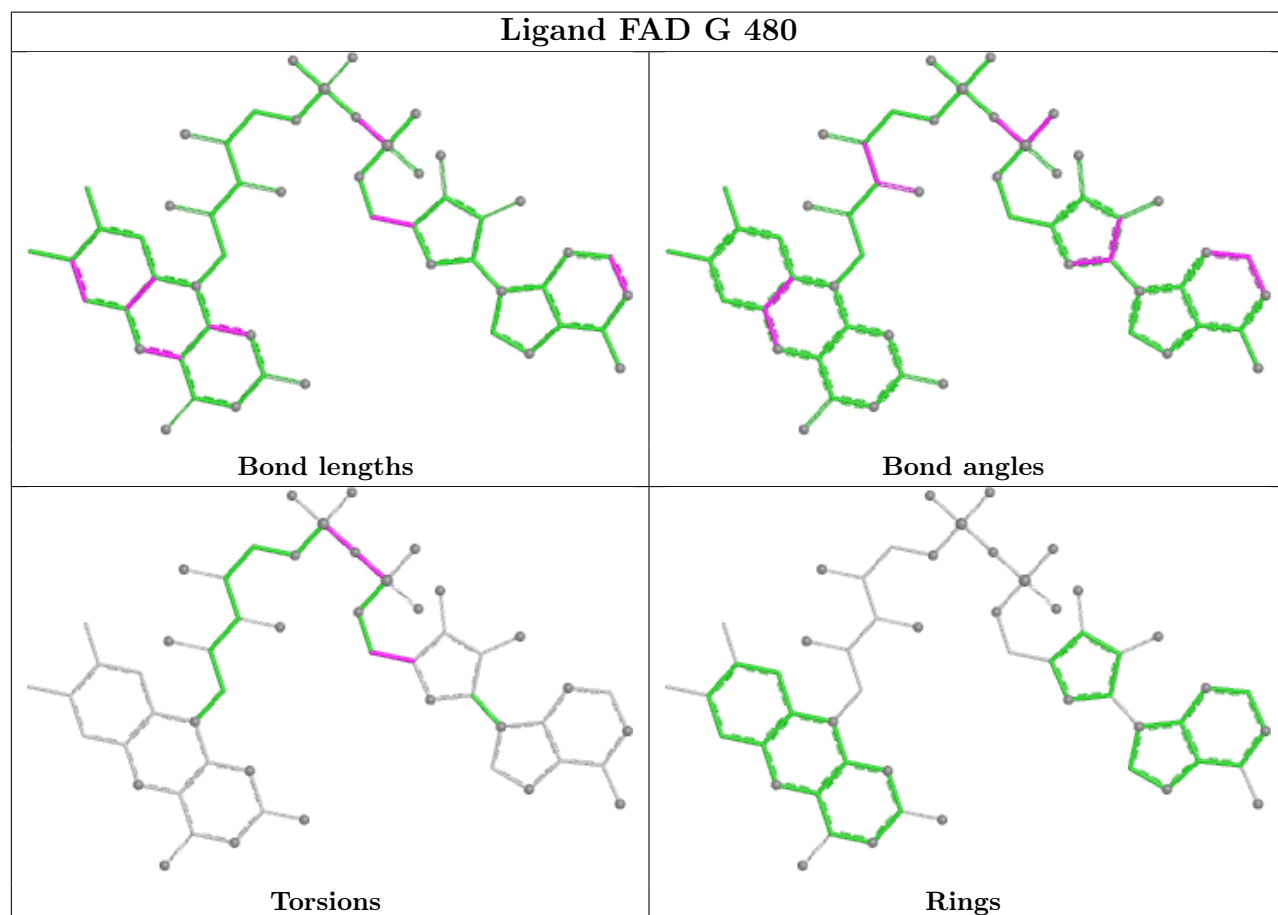
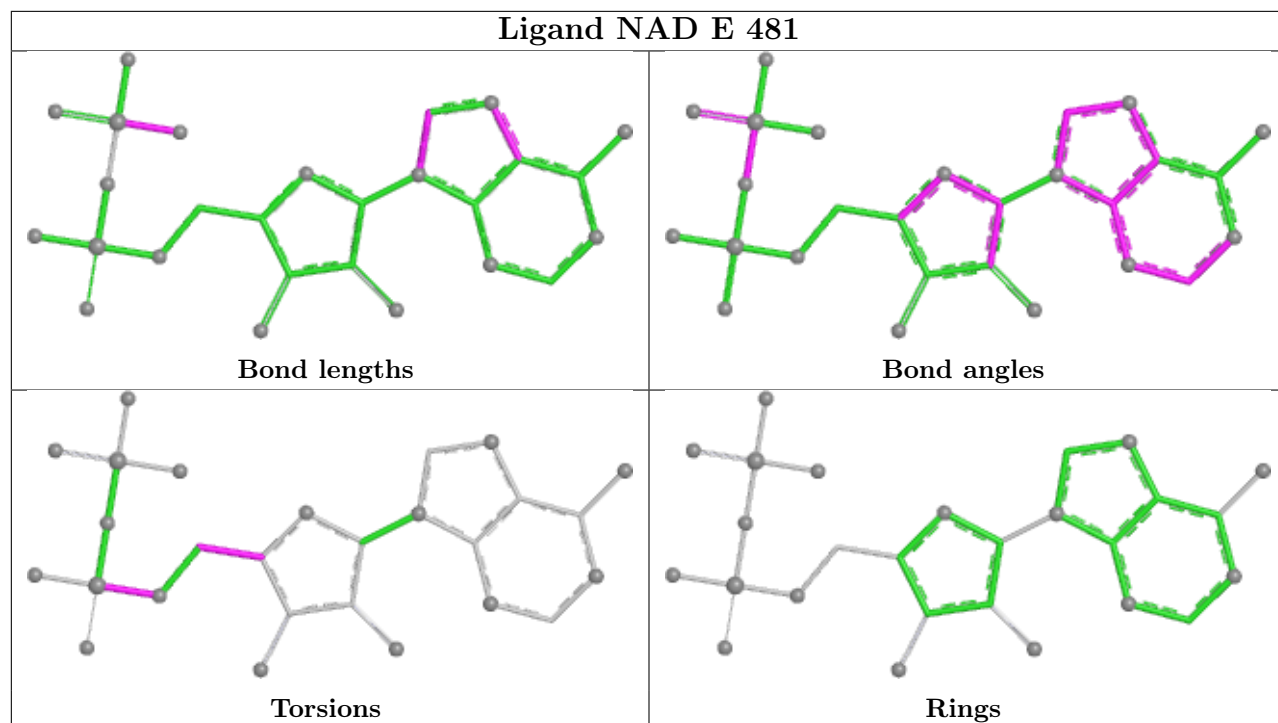


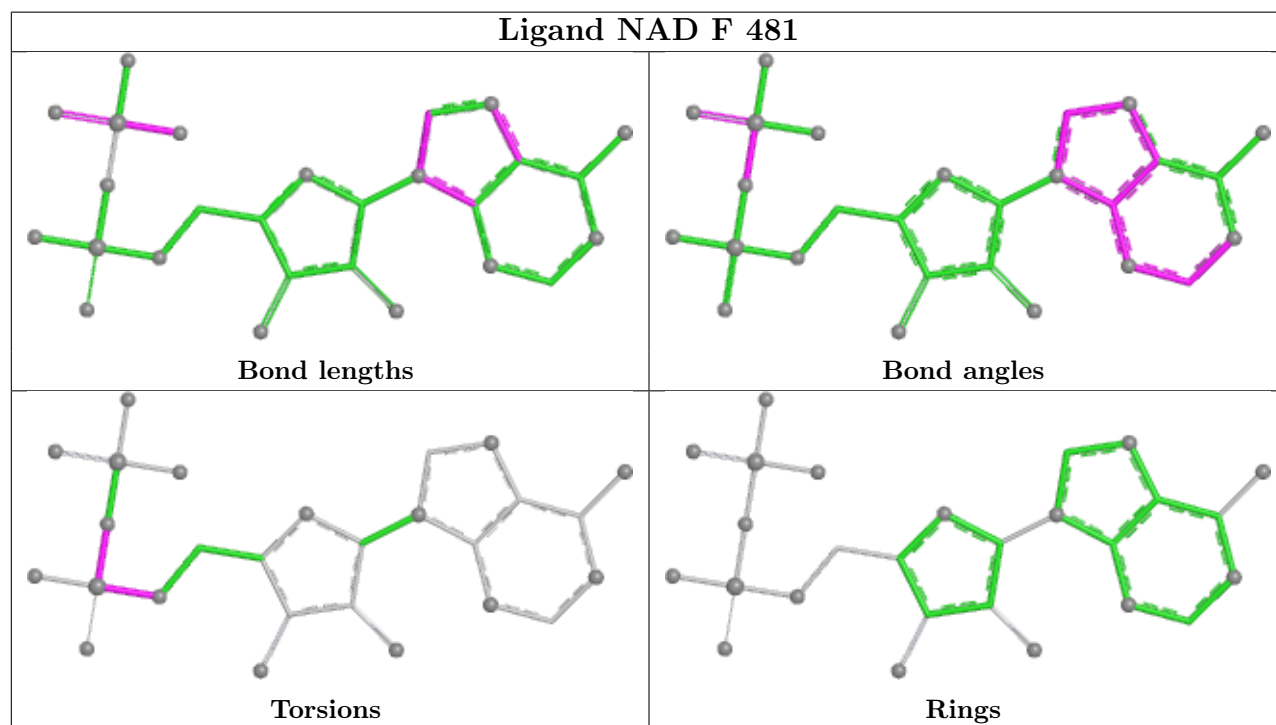
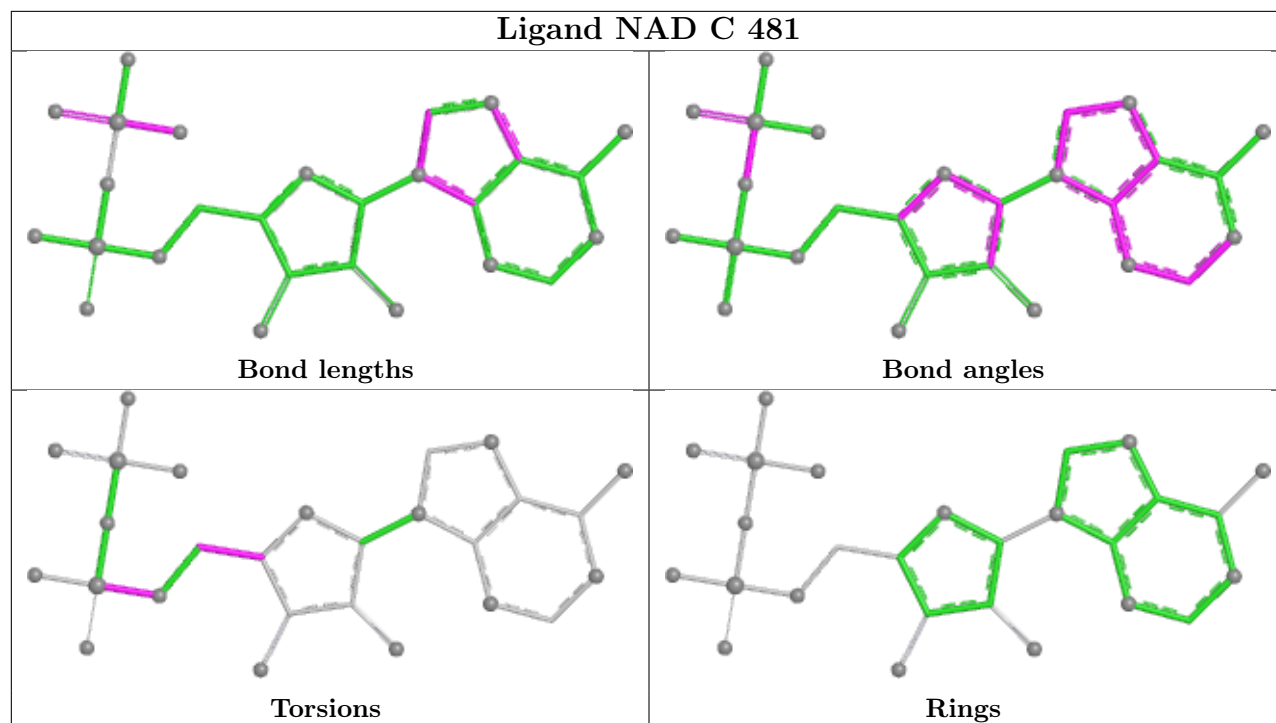
Ligand FAD H 480

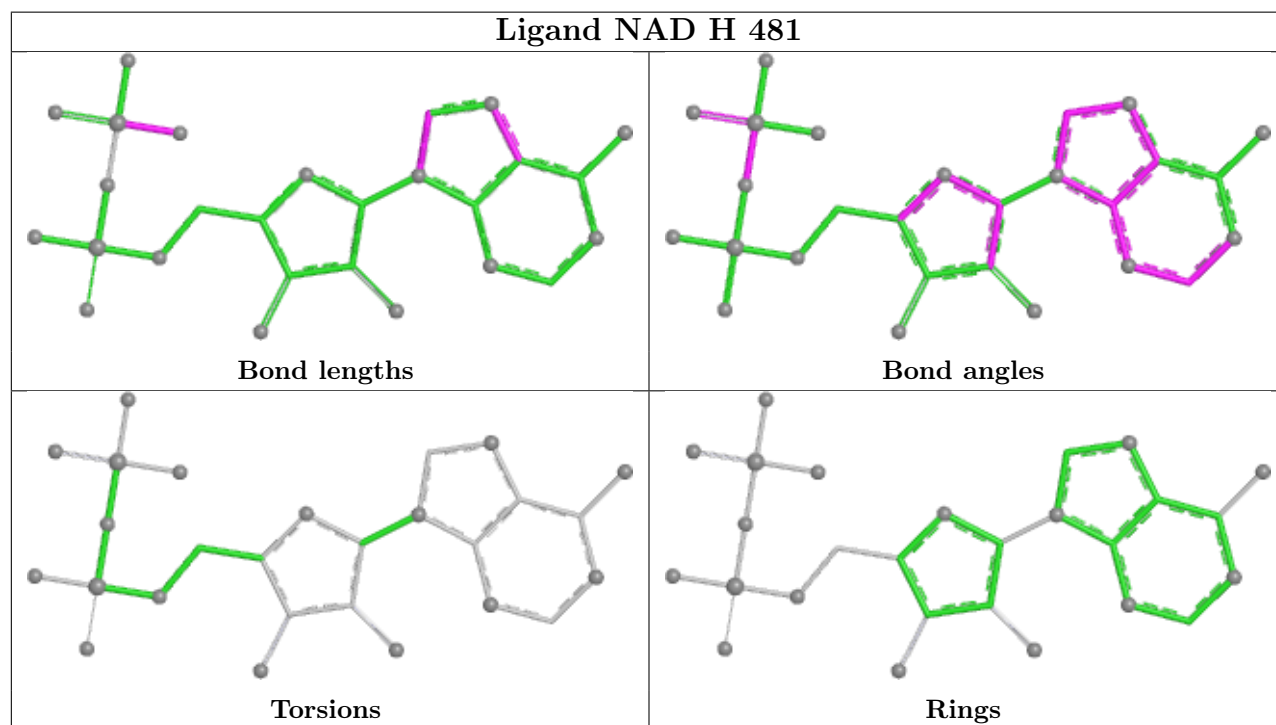
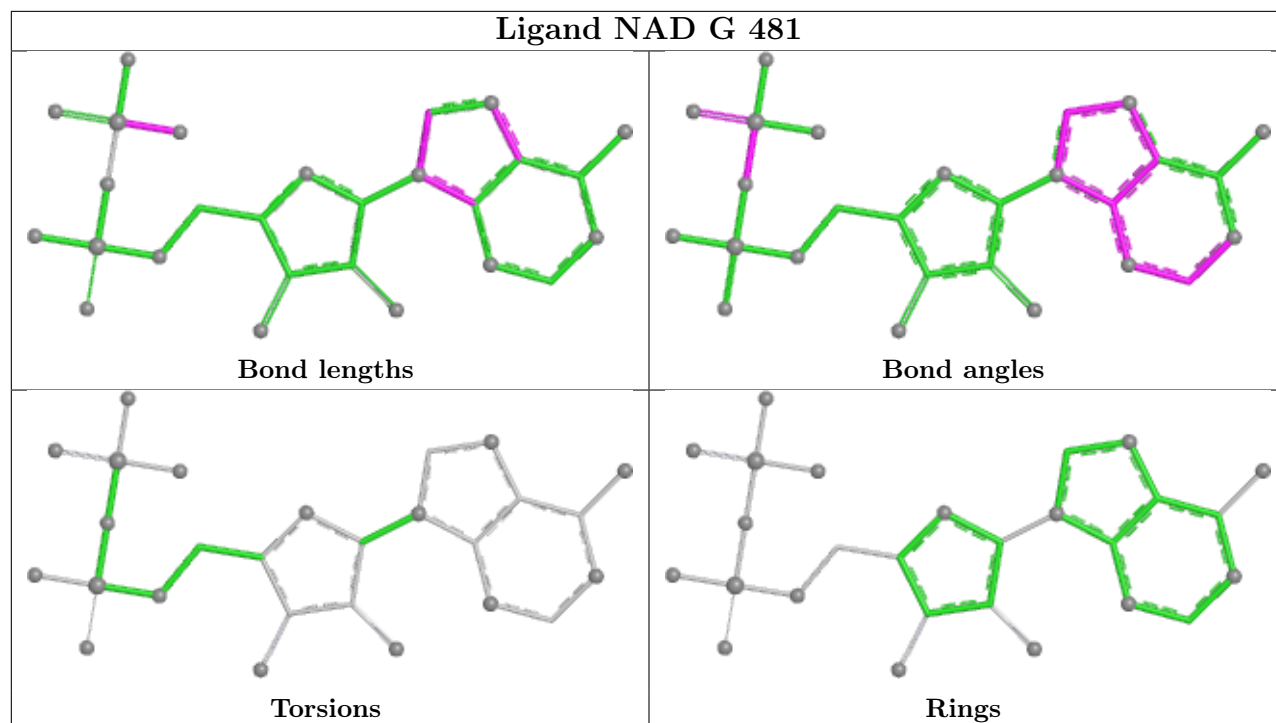


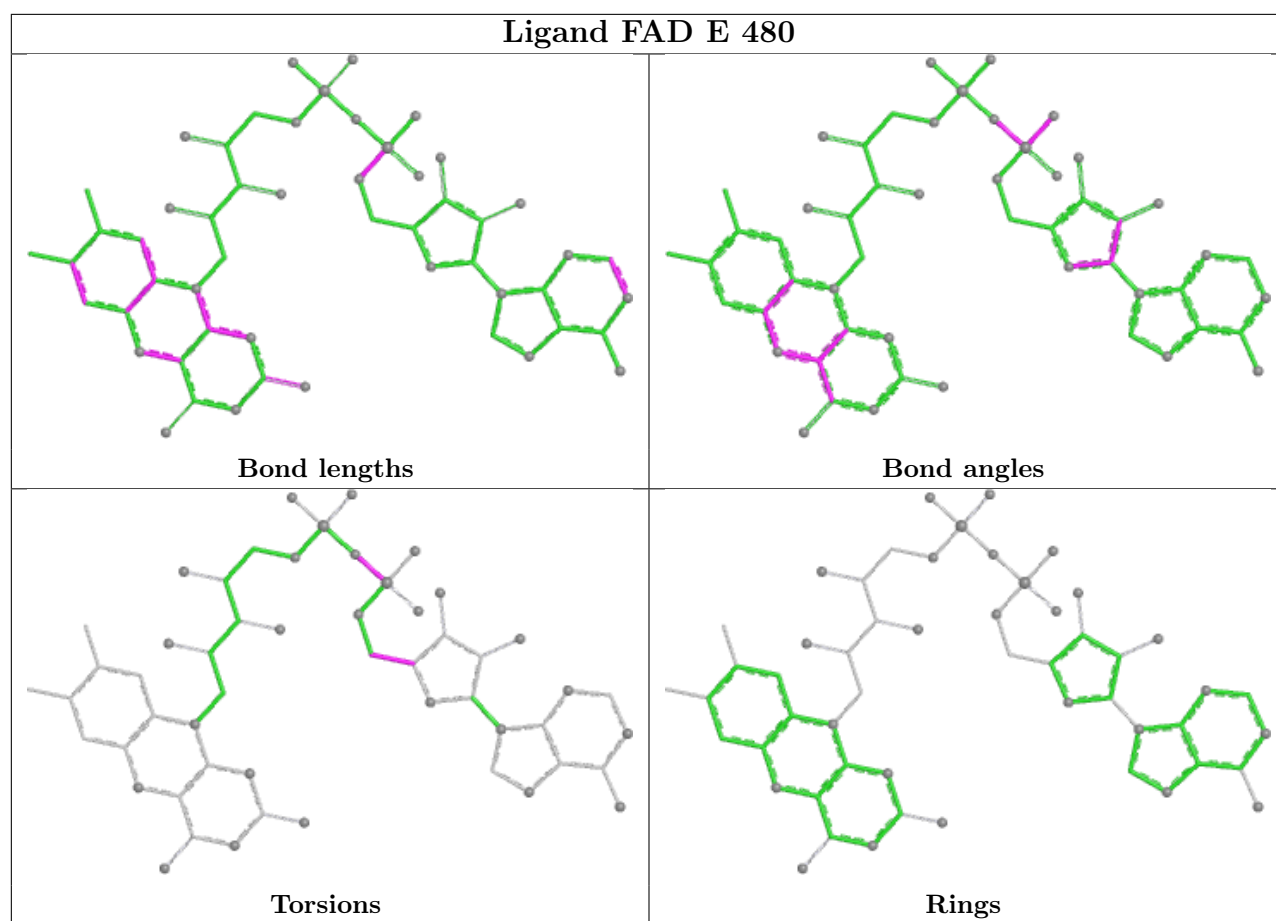
Ligand NAD B 481



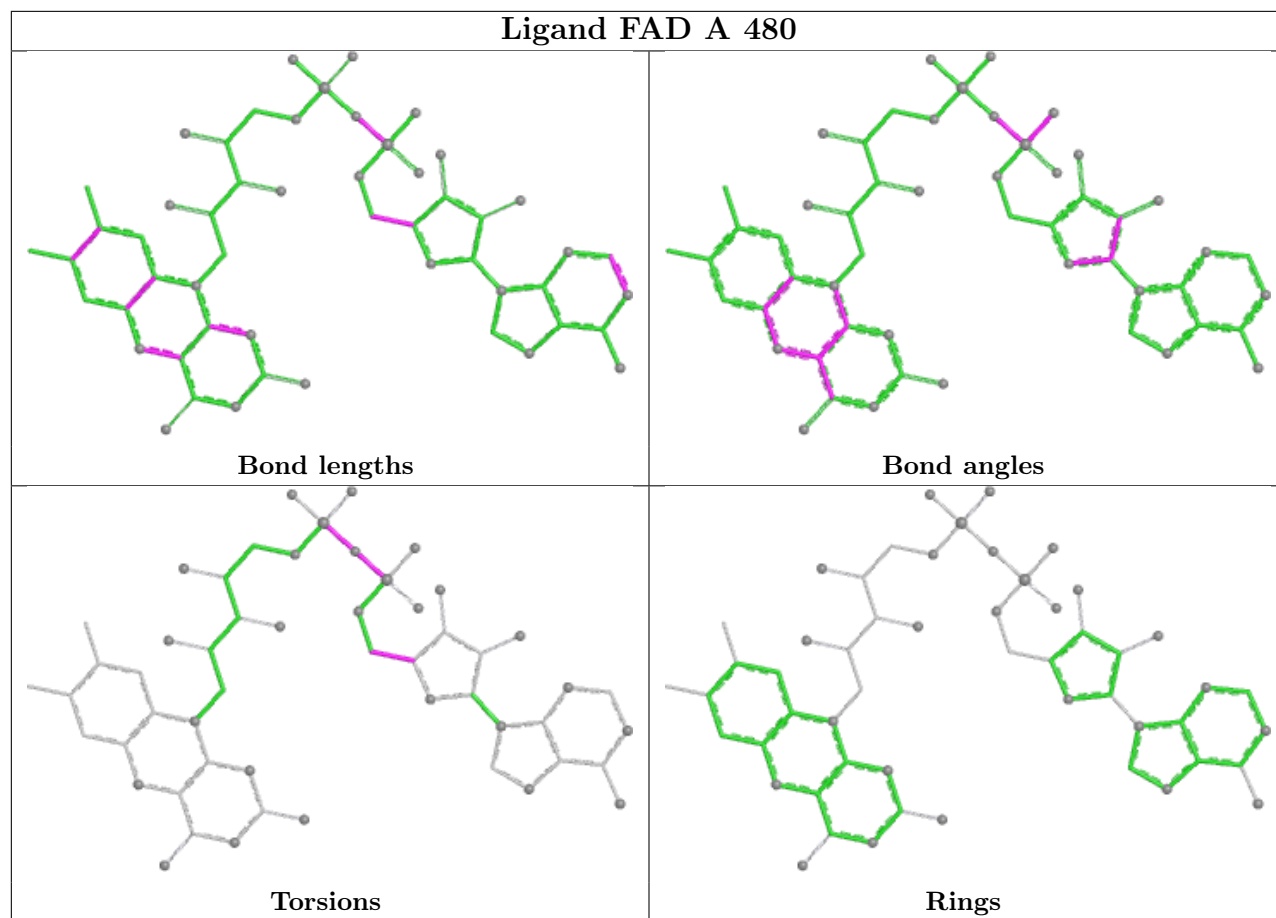


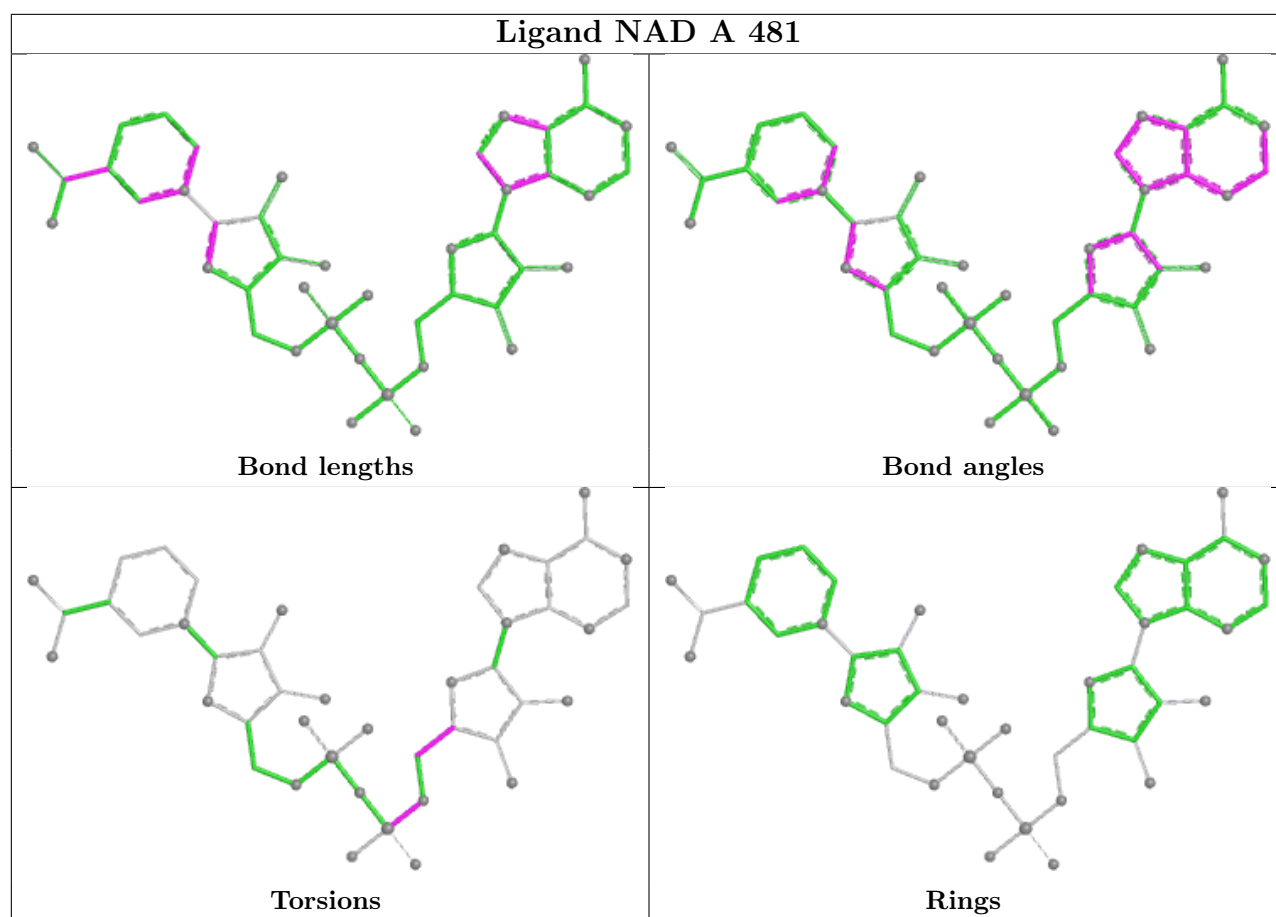


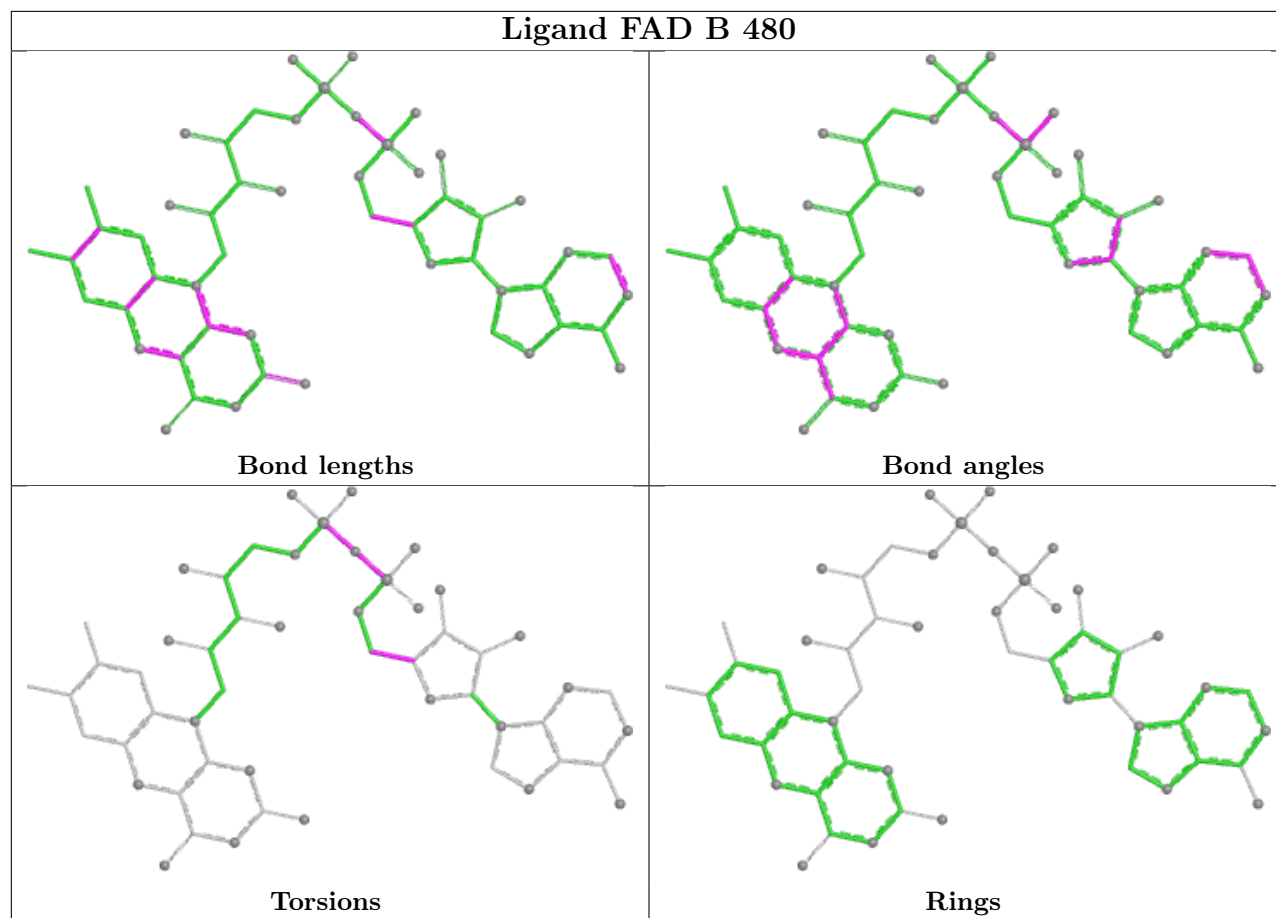


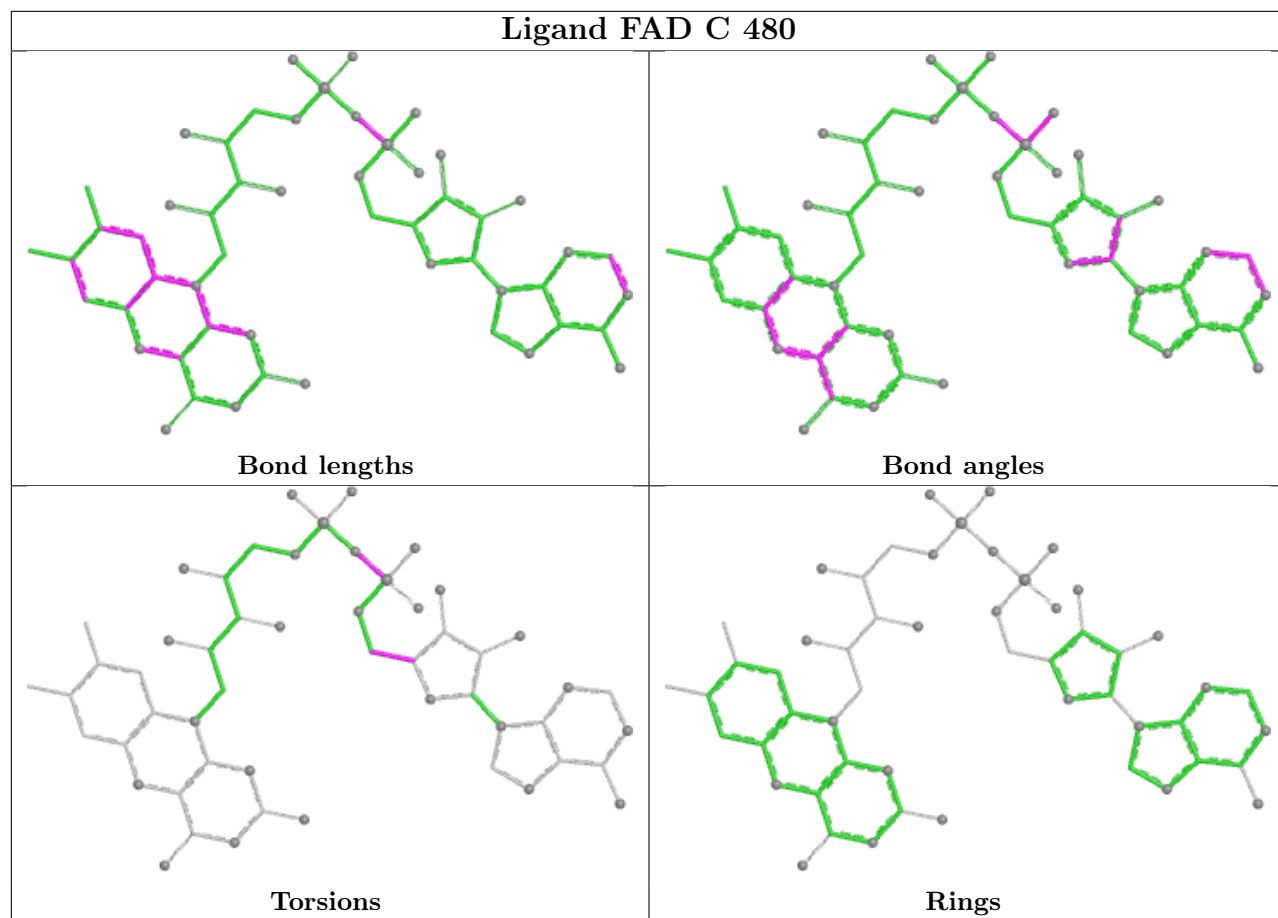


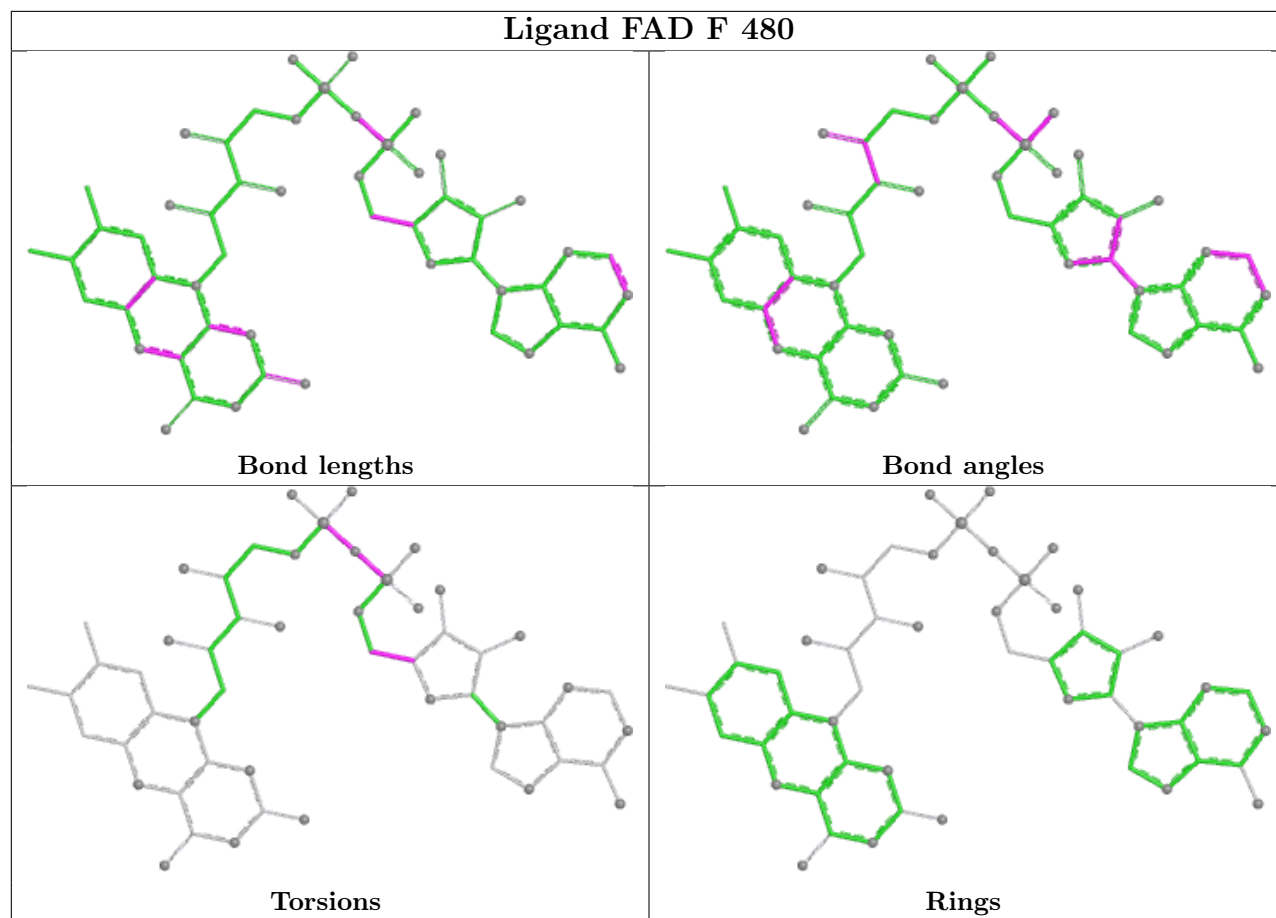
Ligand FAD A 480











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	472/474 (99%)	-0.03	9 (1%) 66 63	18, 36, 60, 82	1 (0%)
1	B	471/474 (99%)	0.08	8 (1%) 69 66	18, 40, 70, 84	0
1	C	471/474 (99%)	0.07	6 (1%) 75 72	18, 41, 69, 83	1 (0%)
1	D	474/474 (100%)	-0.02	7 (1%) 72 69	17, 37, 60, 84	1 (0%)
1	E	472/474 (99%)	-0.02	8 (1%) 69 66	17, 35, 64, 85	0
1	F	471/474 (99%)	-0.31	3 (0%) 85 84	17, 29, 47, 68	2 (0%)
1	G	472/474 (99%)	-0.31	3 (0%) 85 84	17, 29, 46, 64	1 (0%)
1	H	471/474 (99%)	-0.16	3 (0%) 85 84	15, 34, 56, 69	0
All	All	3774/3792 (99%)	-0.09	47 (1%) 76 74	15, 35, 62, 85	6 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	4	PRO	4.4
1	B	4	PRO	4.2
1	C	4	PRO	4.1
1	D	1	ALA	3.6
1	G	250	SER	3.3
1	D	3	GLN	3.1
1	B	346	ALA	3.0
1	B	5	ILE	2.9
1	E	132	ALA	2.9
1	E	348	HIS	2.9
1	B	292	LEU	2.9
1	D	266	ALA	2.8
1	A	249	LYS	2.8
1	F	4	PRO	2.7
1	A	105[A]	HIS	2.7
1	C	134	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	33	VAL	2.6
1	G	105[A]	HIS	2.6
1	E	131	LYS	2.6
1	E	124	LYS	2.5
1	A	263	GLY	2.5
1	C	139	ILE	2.5
1	A	252	GLY	2.5
1	A	254	ILE	2.4
1	B	348	HIS	2.4
1	E	79	SER	2.4
1	H	79	SER	2.4
1	A	266	ALA	2.3
1	H	348	HIS	2.3
1	G	80	GLU	2.3
1	E	5	ILE	2.3
1	D	5	ILE	2.3
1	A	247	THR	2.2
1	A	264	GLY	2.2
1	D	250	SER	2.2
1	E	4	PRO	2.2
1	C	349	ILE	2.2
1	A	250	SER	2.2
1	B	134	GLY	2.2
1	F	124	LYS	2.1
1	C	291	GLU	2.1
1	D	82	ARG	2.1
1	D	379	ILE	2.1
1	F	105[A]	HIS	2.1
1	B	132	ALA	2.0
1	E	3	GLN	2.0
1	C	317	ALA	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
2	SO4	E	2018	5/5	0.50	0.18	120,120,120,120	0
2	SO4	H	2032	5/5	0.58	0.19	120,120,121,121	0
2	SO4	D	2014	5/5	0.60	0.19	148,148,148,148	0
2	SO4	G	2029	5/5	0.68	0.16	119,119,119,120	0
2	SO4	F	2025	5/5	0.73	0.18	107,108,109,109	0
2	SO4	G	2028	5/5	0.76	0.18	127,127,128,128	0
2	SO4	G	2027	5/5	0.77	0.17	80,80,81,81	0
2	SO4	D	2013	5/5	0.77	0.15	87,88,88,88	0
2	SO4	F	2024	5/5	0.77	0.18	121,121,121,121	0
2	SO4	A	2001	5/5	0.77	0.14	82,83,83,83	0
2	SO4	D	2016	5/5	0.80	0.19	83,83,84,84	0
2	SO4	A	2002	5/5	0.80	0.17	123,124,124,124	0
2	SO4	H	2034	5/5	0.80	0.14	80,80,81,81	0
2	SO4	G	2030	5/5	0.82	0.22	79,79,80,80	0
2	SO4	E	2020	5/5	0.82	0.12	90,90,91,91	0
2	SO4	B	2006	5/5	0.82	0.12	104,104,104,104	0
2	SO4	C	2009	5/5	0.83	0.18	91,91,91,91	0
2	SO4	A	2003	5/5	0.83	0.20	87,87,87,88	0
2	SO4	D	2015	5/5	0.85	0.15	115,115,115,115	0
4	NAD	C	481	27/44	0.85	0.15	70,73,87,87	0
4	NAD	F	481	27/44	0.85	0.15	50,57,80,81	0
4	NAD	A	481	44/44	0.86	0.16	52,64,86,88	0
2	SO4	B	2005	5/5	0.87	0.16	88,88,89,89	0
2	SO4	C	2010	5/5	0.87	0.11	103,103,103,103	0
2	SO4	H	2035	5/5	0.87	0.24	78,78,78,78	0
2	SO4	E	2021	5/5	0.87	0.18	79,79,79,80	0
2	SO4	F	2023	5/5	0.87	0.13	76,76,77,77	0
2	SO4	B	2007	5/5	0.87	0.20	78,78,79,79	0
4	NAD	B	481	27/44	0.89	0.12	63,66,81,82	0
2	SO4	C	2011	5/5	0.89	0.14	82,83,83,84	0
2	SO4	G	2026	5/5	0.89	0.12	62,63,64,66	0
4	NAD	E	481	27/44	0.90	0.12	58,64,71,72	0
2	SO4	H	2033	5/5	0.90	0.14	81,81,82,83	0
4	NAD	G	481	27/44	0.90	0.10	31,37,63,64	0
4	NAD	H	481	27/44	0.90	0.10	51,55,69,69	0
2	SO4	E	2019	5/5	0.91	0.13	78,79,80,80	0
2	SO4	D	2012	5/5	0.91	0.10	71,71,72,72	0

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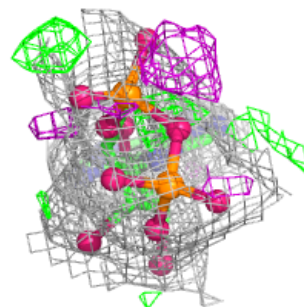
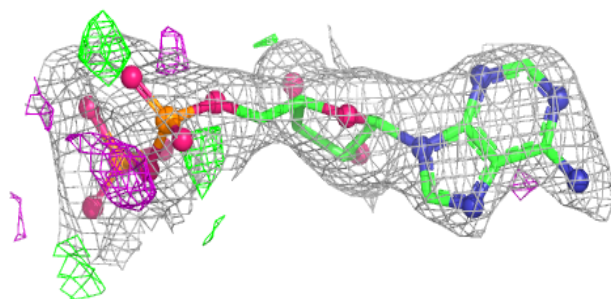
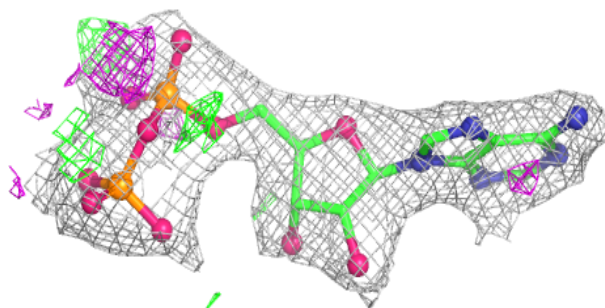
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAD	D	481	44/44	0.92	0.11	55,59,64,64	0
2	SO4	A	2000	5/5	0.93	0.08	67,68,69,69	0
2	SO4	F	2022	5/5	0.93	0.11	62,62,64,66	0
2	SO4	H	2031	5/5	0.94	0.11	57,58,59,60	0
3	FAD	B	480	53/53	0.94	0.09	32,37,45,46	0
2	SO4	C	2008	5/5	0.95	0.09	64,65,66,66	0
3	FAD	C	480	53/53	0.95	0.08	27,37,51,52	0
3	FAD	E	480	53/53	0.96	0.08	26,32,44,44	0
3	FAD	H	480	53/53	0.96	0.08	24,31,43,44	0
2	SO4	B	2004	5/5	0.96	0.09	64,64,65,66	0
3	FAD	A	480	53/53	0.96	0.09	22,30,34,36	0
3	FAD	D	480	53/53	0.96	0.07	21,29,33,35	0
2	SO4	E	2017	5/5	0.97	0.07	56,56,57,59	0
3	FAD	F	480	53/53	0.97	0.07	19,22,28,31	0
3	FAD	G	480	53/53	0.97	0.07	18,23,28,31	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.

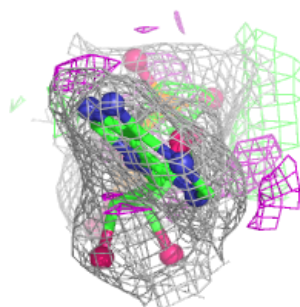
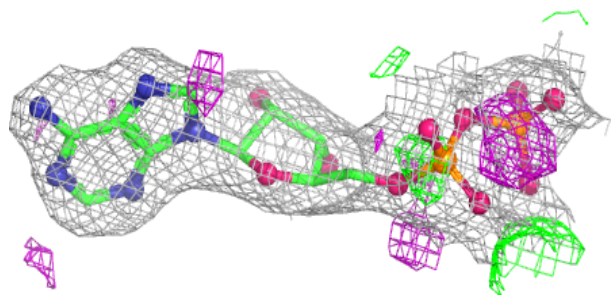
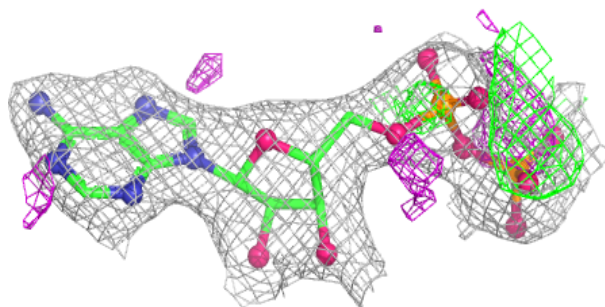
Electron density around NAD C 481:

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



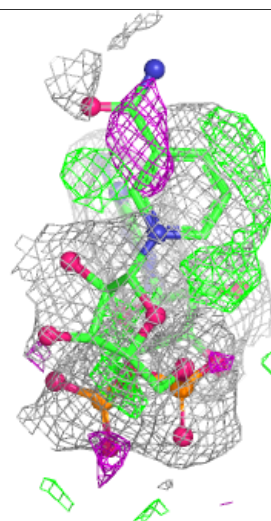
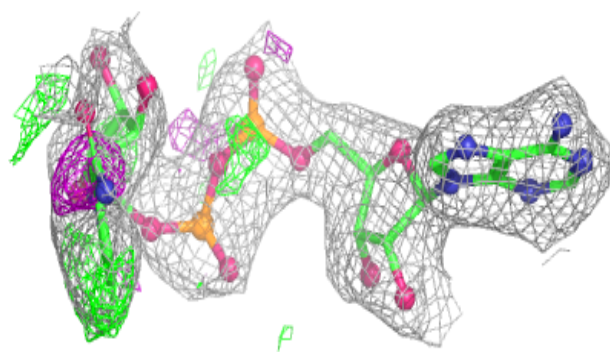
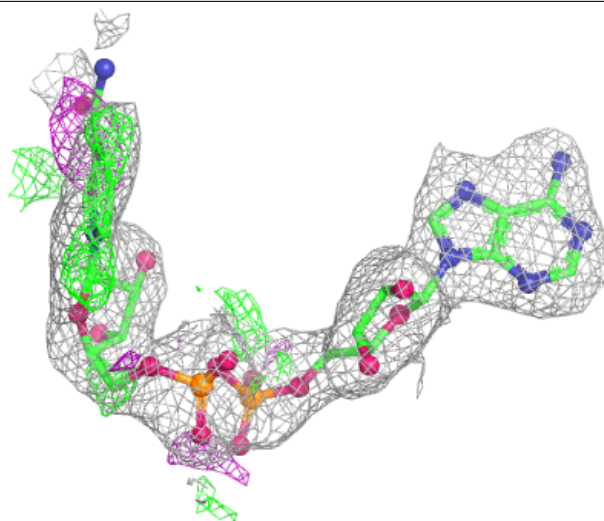
Electron density around NAD F 481:

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and green (positive)



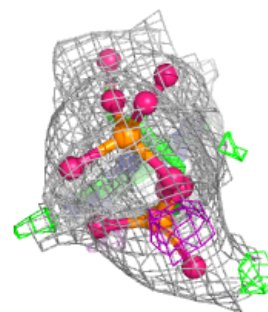
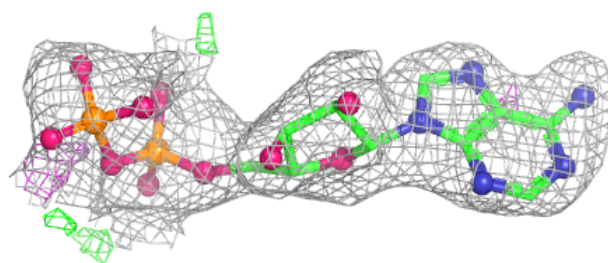
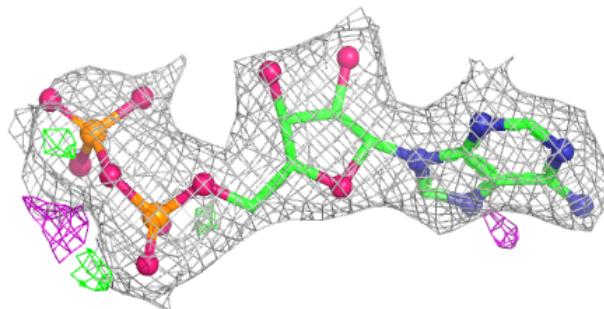
Electron density around NAD A 481:

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

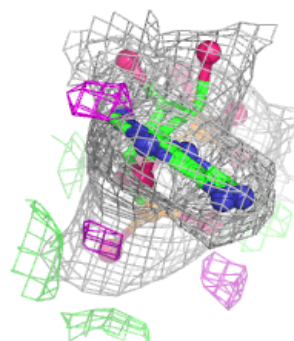
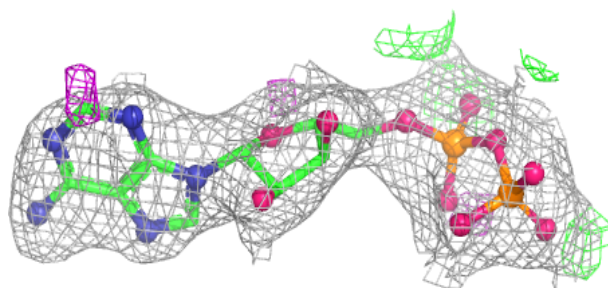
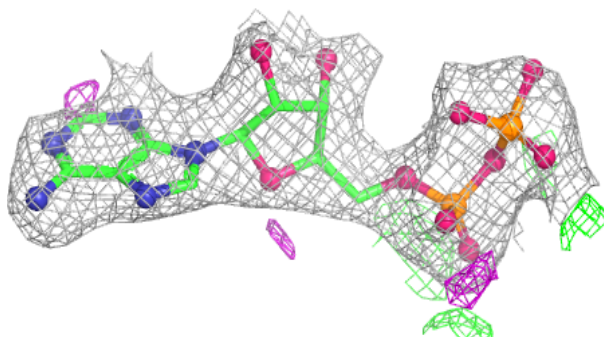


Electron density around NAD B 481:

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

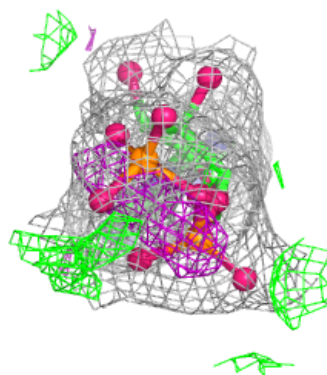
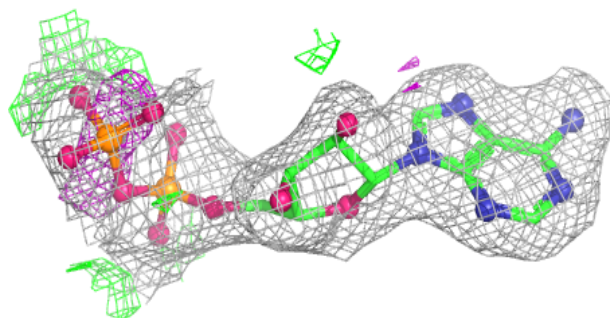
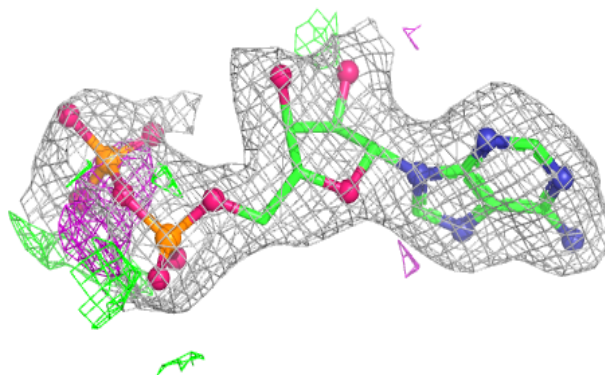
**Electron density around NAD E 481:**

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

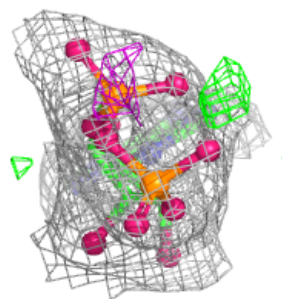
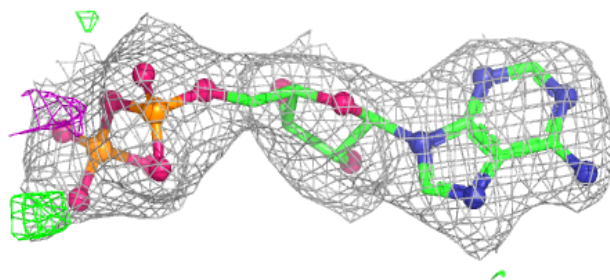


Electron density around NAD G 481:

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

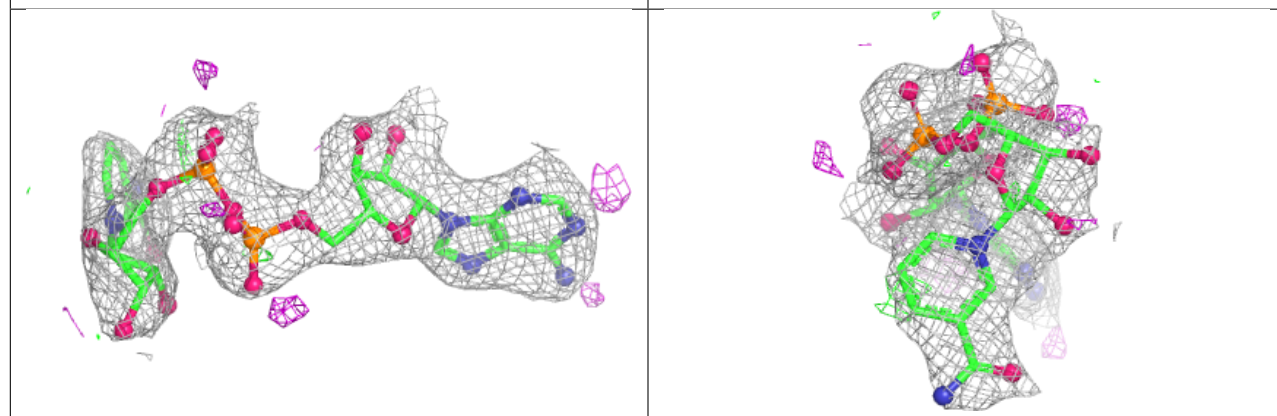
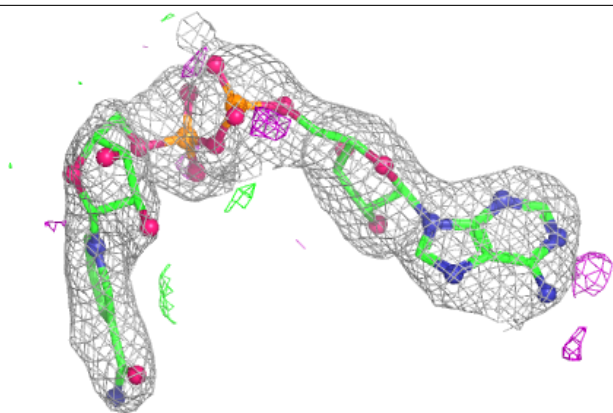
**Electron density around NAD H 481:**

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

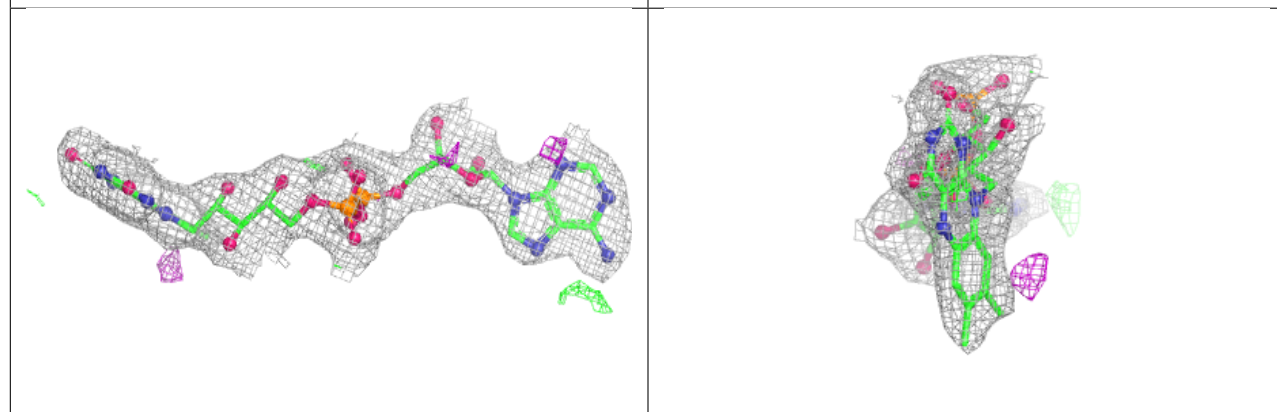
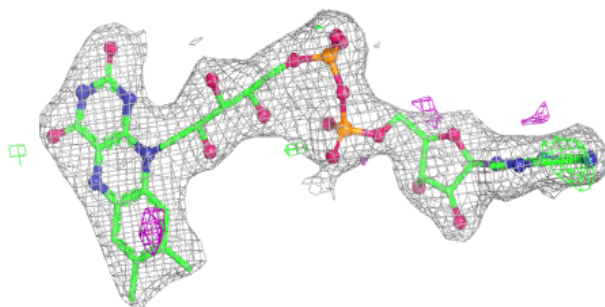


Electron density around NAD D 481:

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

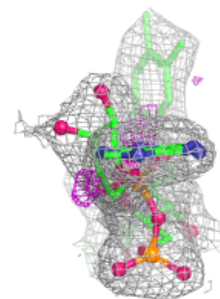
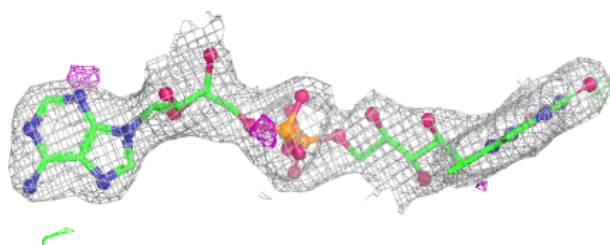
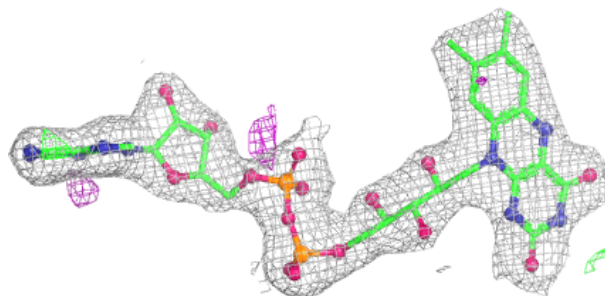
**Electron density around FAD B 480:**

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

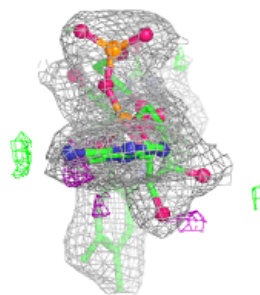
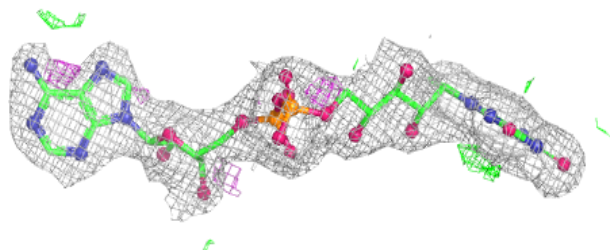
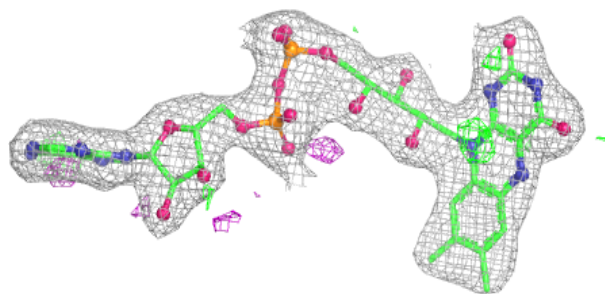


Electron density around FAD C 480:

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

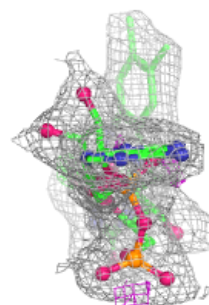
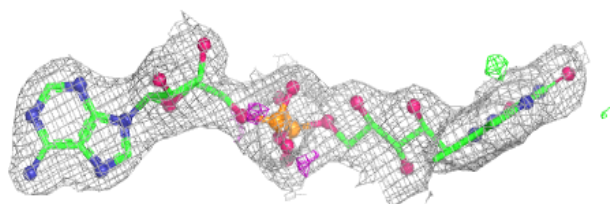
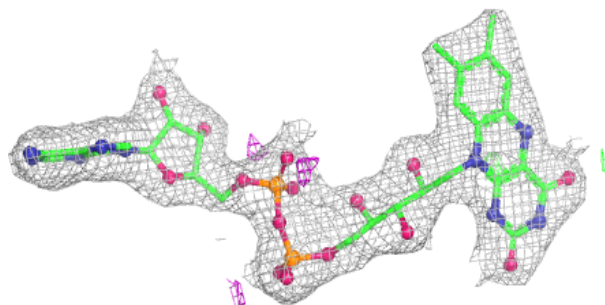
**Electron density around FAD E 480:**

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

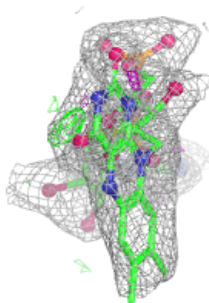
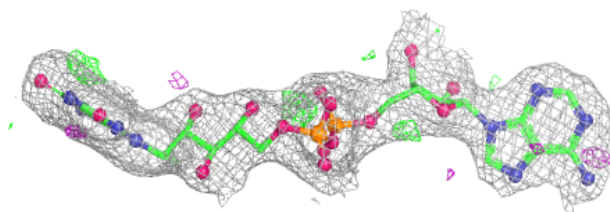
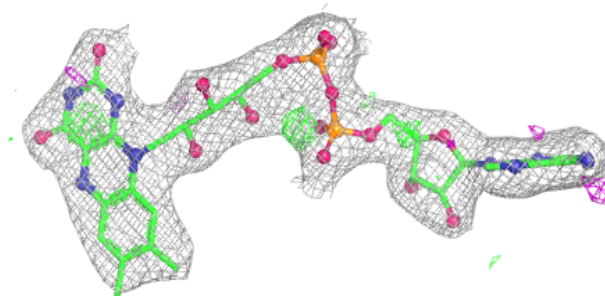


Electron density around FAD H 480:

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

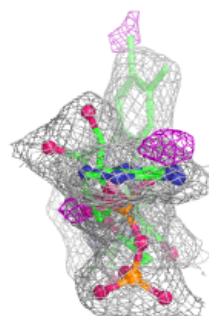
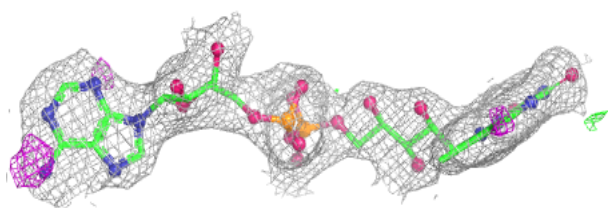
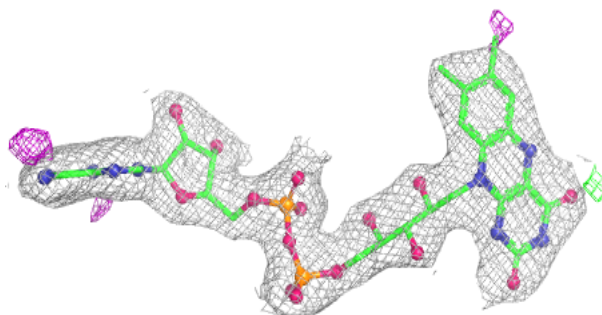
**Electron density around FAD A 480:**

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

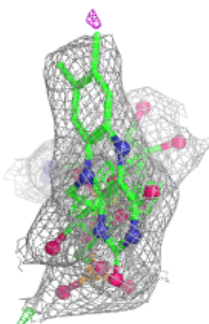
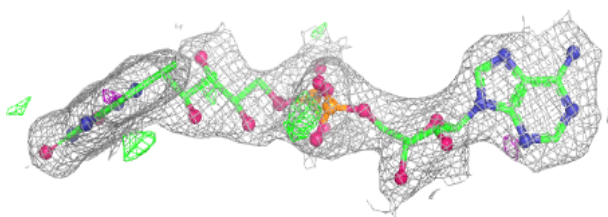
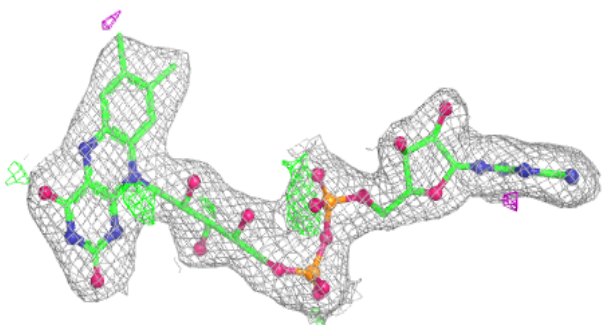


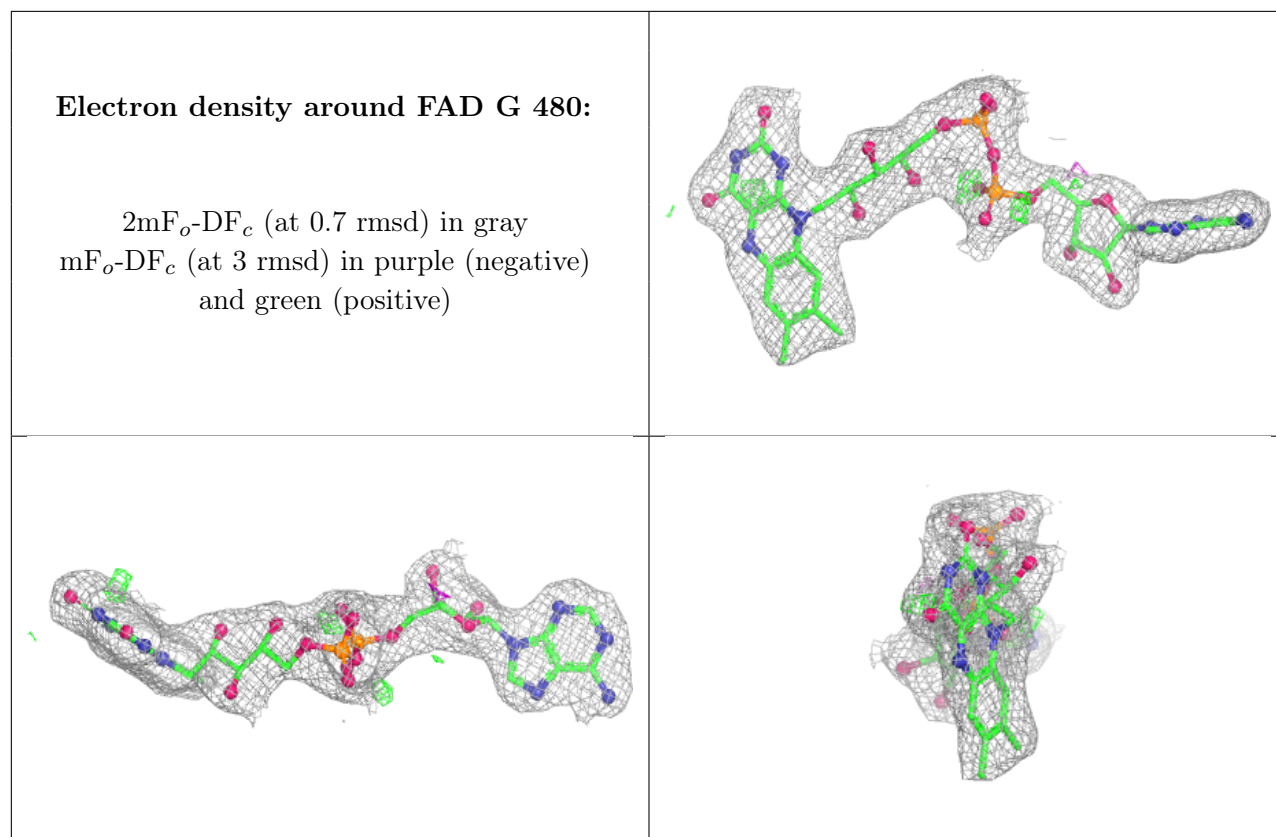
Electron density around FAD D 480:

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

**Electron density around FAD F 480:**

$2mF_o-DF_c$ (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.