



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:09 AM UTC

PDB ID : 7P9X / pdb_00007p9x
Title : Structure of cyclohex-1-ene-1-carboxyl-CoA dehydrogenase complexed with c
yclohex-1-ene-1-carboxyl-CoA
Authors : Ermler, U.; Weidenweber, S.; Boll, M.
Deposited on : 2021-07-28
Resolution : 1.65 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

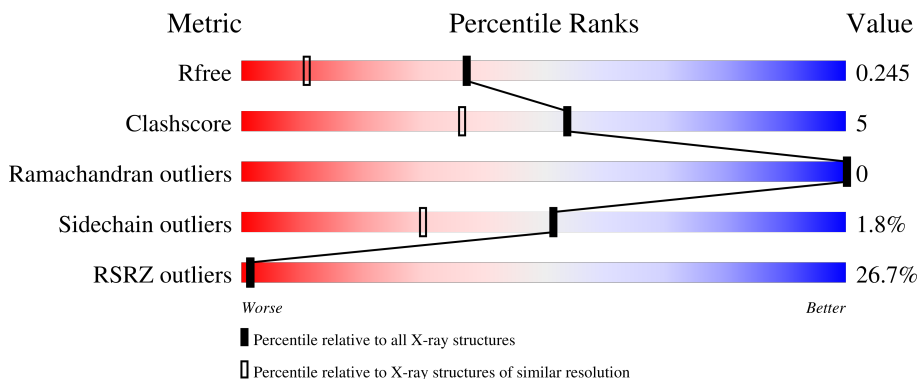
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	412	5% 87% 5% 8%
1	B	412	5% 86% 6% 8%
1	C	412	5% 86% 6% 8%
1	D	412	83% 74% 15% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13151 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 Short-chain acyl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	6	0
			2899	1819	503	556	21			
1	B	378	Total	C	N	O	S	0	5	0
			2889	1814	501	552	22			
1	C	378	Total	C	N	O	S	0	7	0
			2904	1826	502	554	22			
1	D	377	Total	C	N	O	S	0	6	0
			2892	1814	506	551	21			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	381	LYS	-	expression tag	UNP Q39QF5
A	382	GLY	-	expression tag	UNP Q39QF5
A	383	GLU	-	expression tag	UNP Q39QF5
A	384	LEU	-	expression tag	UNP Q39QF5
A	385	ASN	-	expression tag	UNP Q39QF5
A	386	SER	-	expression tag	UNP Q39QF5
A	387	LYS	-	expression tag	UNP Q39QF5
A	388	LEU	-	expression tag	UNP Q39QF5
A	389	GLU	-	expression tag	UNP Q39QF5
A	390	GLY	-	expression tag	UNP Q39QF5
A	391	LYS	-	expression tag	UNP Q39QF5
A	392	PRO	-	expression tag	UNP Q39QF5
A	393	ILE	-	expression tag	UNP Q39QF5
A	394	PRO	-	expression tag	UNP Q39QF5
A	395	ASN	-	expression tag	UNP Q39QF5
A	396	PRO	-	expression tag	UNP Q39QF5
A	397	LEU	-	expression tag	UNP Q39QF5
A	398	LEU	-	expression tag	UNP Q39QF5
A	399	GLY	-	expression tag	UNP Q39QF5
A	400	LEU	-	expression tag	UNP Q39QF5
A	401	ASP	-	expression tag	UNP Q39QF5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	402	SER	-	expression tag	UNP Q39QF5
A	403	THR	-	expression tag	UNP Q39QF5
A	404	ARG	-	expression tag	UNP Q39QF5
A	405	THR	-	expression tag	UNP Q39QF5
A	406	GLY	-	expression tag	UNP Q39QF5
A	407	HIS	-	expression tag	UNP Q39QF5
A	408	HIS	-	expression tag	UNP Q39QF5
A	409	HIS	-	expression tag	UNP Q39QF5
A	410	HIS	-	expression tag	UNP Q39QF5
A	411	HIS	-	expression tag	UNP Q39QF5
A	412	HIS	-	expression tag	UNP Q39QF5
B	381	LYS	-	expression tag	UNP Q39QF5
B	382	GLY	-	expression tag	UNP Q39QF5
B	383	GLU	-	expression tag	UNP Q39QF5
B	384	LEU	-	expression tag	UNP Q39QF5
B	385	ASN	-	expression tag	UNP Q39QF5
B	386	SER	-	expression tag	UNP Q39QF5
B	387	LYS	-	expression tag	UNP Q39QF5
B	388	LEU	-	expression tag	UNP Q39QF5
B	389	GLU	-	expression tag	UNP Q39QF5
B	390	GLY	-	expression tag	UNP Q39QF5
B	391	LYS	-	expression tag	UNP Q39QF5
B	392	PRO	-	expression tag	UNP Q39QF5
B	393	ILE	-	expression tag	UNP Q39QF5
B	394	PRO	-	expression tag	UNP Q39QF5
B	395	ASN	-	expression tag	UNP Q39QF5
B	396	PRO	-	expression tag	UNP Q39QF5
B	397	LEU	-	expression tag	UNP Q39QF5
B	398	LEU	-	expression tag	UNP Q39QF5
B	399	GLY	-	expression tag	UNP Q39QF5
B	400	LEU	-	expression tag	UNP Q39QF5
B	401	ASP	-	expression tag	UNP Q39QF5
B	402	SER	-	expression tag	UNP Q39QF5
B	403	THR	-	expression tag	UNP Q39QF5
B	404	ARG	-	expression tag	UNP Q39QF5
B	405	THR	-	expression tag	UNP Q39QF5
B	406	GLY	-	expression tag	UNP Q39QF5
B	407	HIS	-	expression tag	UNP Q39QF5
B	408	HIS	-	expression tag	UNP Q39QF5
B	409	HIS	-	expression tag	UNP Q39QF5
B	410	HIS	-	expression tag	UNP Q39QF5
B	411	HIS	-	expression tag	UNP Q39QF5

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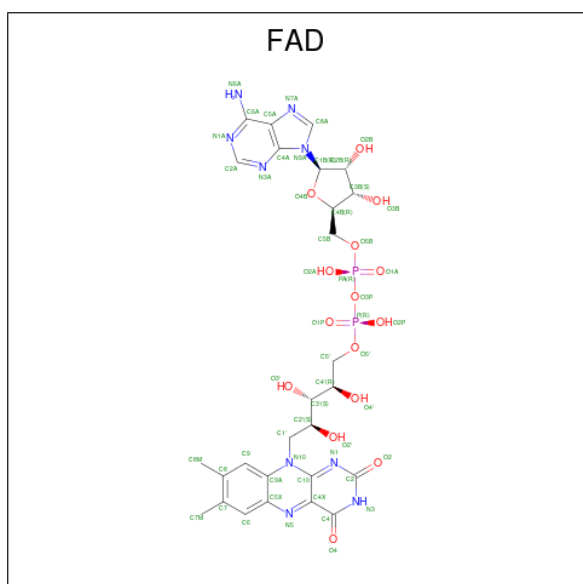
Chain	Residue	Modelled	Actual	Comment	Reference
B	412	HIS	-	expression tag	UNP Q39QF5
C	381	LYS	-	expression tag	UNP Q39QF5
C	382	GLY	-	expression tag	UNP Q39QF5
C	383	GLU	-	expression tag	UNP Q39QF5
C	384	LEU	-	expression tag	UNP Q39QF5
C	385	ASN	-	expression tag	UNP Q39QF5
C	386	SER	-	expression tag	UNP Q39QF5
C	387	LYS	-	expression tag	UNP Q39QF5
C	388	LEU	-	expression tag	UNP Q39QF5
C	389	GLU	-	expression tag	UNP Q39QF5
C	390	GLY	-	expression tag	UNP Q39QF5
C	391	LYS	-	expression tag	UNP Q39QF5
C	392	PRO	-	expression tag	UNP Q39QF5
C	393	ILE	-	expression tag	UNP Q39QF5
C	394	PRO	-	expression tag	UNP Q39QF5
C	395	ASN	-	expression tag	UNP Q39QF5
C	396	PRO	-	expression tag	UNP Q39QF5
C	397	LEU	-	expression tag	UNP Q39QF5
C	398	LEU	-	expression tag	UNP Q39QF5
C	399	GLY	-	expression tag	UNP Q39QF5
C	400	LEU	-	expression tag	UNP Q39QF5
C	401	ASP	-	expression tag	UNP Q39QF5
C	402	SER	-	expression tag	UNP Q39QF5
C	403	THR	-	expression tag	UNP Q39QF5
C	404	ARG	-	expression tag	UNP Q39QF5
C	405	THR	-	expression tag	UNP Q39QF5
C	406	GLY	-	expression tag	UNP Q39QF5
C	407	HIS	-	expression tag	UNP Q39QF5
C	408	HIS	-	expression tag	UNP Q39QF5
C	409	HIS	-	expression tag	UNP Q39QF5
C	410	HIS	-	expression tag	UNP Q39QF5
C	411	HIS	-	expression tag	UNP Q39QF5
C	412	HIS	-	expression tag	UNP Q39QF5
D	381	LYS	-	expression tag	UNP Q39QF5
D	382	GLY	-	expression tag	UNP Q39QF5
D	383	GLU	-	expression tag	UNP Q39QF5
D	384	LEU	-	expression tag	UNP Q39QF5
D	385	ASN	-	expression tag	UNP Q39QF5
D	386	SER	-	expression tag	UNP Q39QF5
D	387	LYS	-	expression tag	UNP Q39QF5
D	388	LEU	-	expression tag	UNP Q39QF5
D	389	GLU	-	expression tag	UNP Q39QF5

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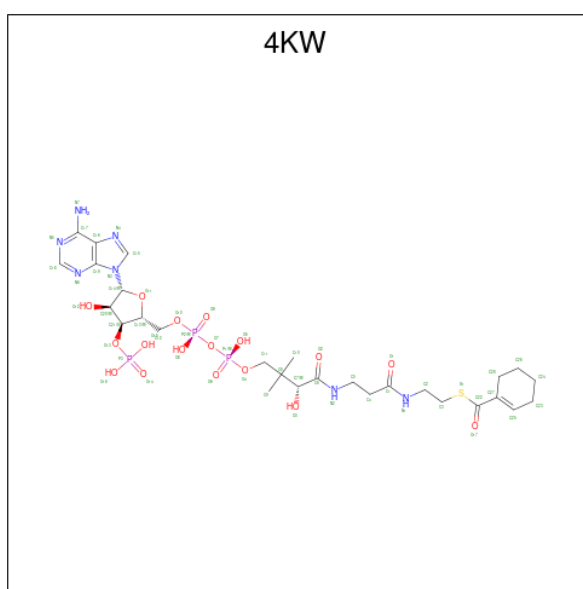
Chain	Residue	Modelled	Actual	Comment	Reference
D	390	GLY	-	expression tag	UNP Q39QF5
D	391	LYS	-	expression tag	UNP Q39QF5
D	392	PRO	-	expression tag	UNP Q39QF5
D	393	ILE	-	expression tag	UNP Q39QF5
D	394	PRO	-	expression tag	UNP Q39QF5
D	395	ASN	-	expression tag	UNP Q39QF5
D	396	PRO	-	expression tag	UNP Q39QF5
D	397	LEU	-	expression tag	UNP Q39QF5
D	398	LEU	-	expression tag	UNP Q39QF5
D	399	GLY	-	expression tag	UNP Q39QF5
D	400	LEU	-	expression tag	UNP Q39QF5
D	401	ASP	-	expression tag	UNP Q39QF5
D	402	SER	-	expression tag	UNP Q39QF5
D	403	THR	-	expression tag	UNP Q39QF5
D	404	ARG	-	expression tag	UNP Q39QF5
D	405	THR	-	expression tag	UNP Q39QF5
D	406	GLY	-	expression tag	UNP Q39QF5
D	407	HIS	-	expression tag	UNP Q39QF5
D	408	HIS	-	expression tag	UNP Q39QF5
D	409	HIS	-	expression tag	UNP Q39QF5
D	410	HIS	-	expression tag	UNP Q39QF5
D	411	HIS	-	expression tag	UNP Q39QF5
D	412	HIS	-	expression tag	UNP Q39QF5

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is 1-monoenoyl-CoA (CCD ID: 4KW) (formula: $C_{28}H_{44}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			56	28	7	17	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			56	28	7	17	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			56	28	7	17	3	1		
3	D	1	Total	C	N	O	P	S	0	0
			56	28	7	17	3	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



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

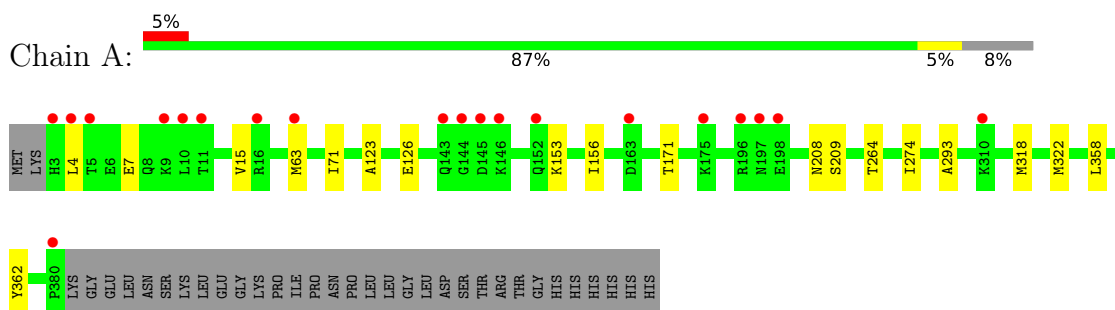
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	307	Total	O	0	0
			307	307		
5	B	328	Total	O	0	1
			329	329		
5	C	336	Total	O	0	0
			336	336		
5	D	117	Total	O	0	0
			117	117		

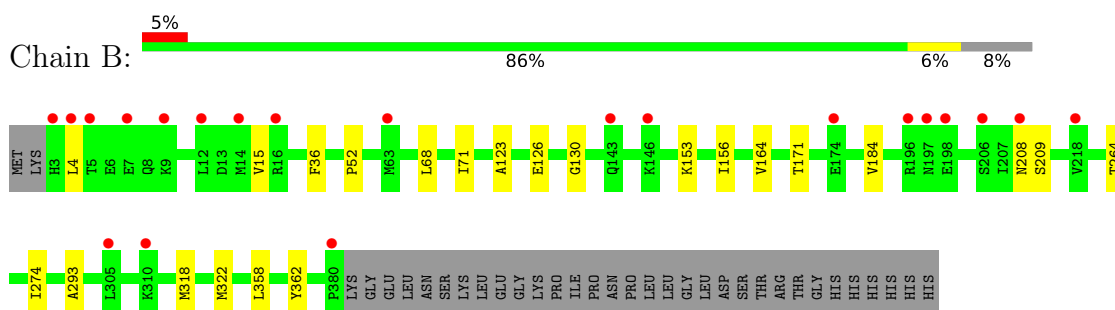
3 Residue-property plots [i](#)

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.

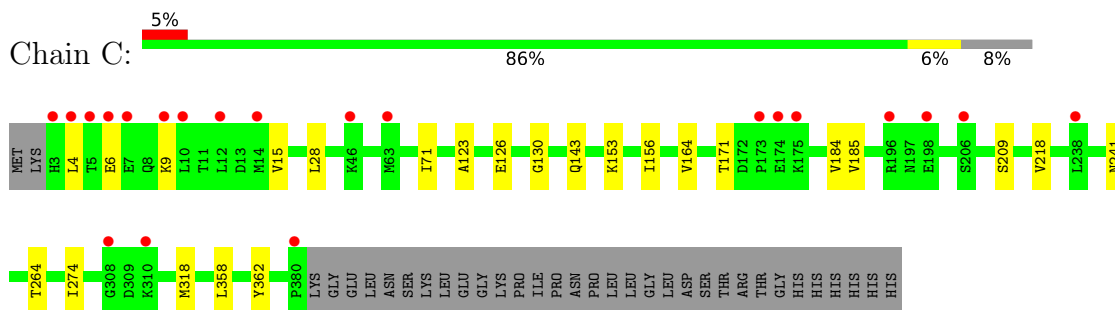
- Molecule 1: Short-chain acyl-CoA dehydrogenase



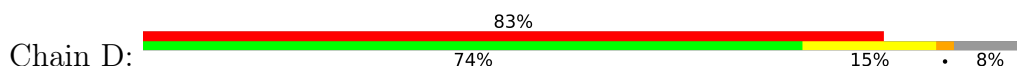
- Molecule 1: Short-chain acyl-CoA dehydrogenase



- Molecule 1: Short-chain acyl-CoA dehydrogenase



- Molecule 1: Short-chain acyl-CoA dehydrogenase



T365	L304	V243	S181	A121	T61	MET
N366	L305	F244	A182	L122	E62	LYS
Q367	D306	C245	F183	A123	M63	H3
I368	D307	A246	V184	A124	G64	L4
T369	G308	A247	V185	T125	V65	T5
R370	D309	Q248	E186	E126	L66	E6
M371	K310	A249	K187	F127	T67	E7
V372	K311	V250	G188	A128	L68	Q8
T373	A312	G251	T189	A129	A69	K9
G374	V313	I252	F190	G130	L70	L10
R375	L314	A253	G191	S131	I71	T11
A376	Y315	Q254	L192	D132	L72	L12
L377	G316	G255	V193	L133	E73	D13
L378	S317	A256	Y194	L134	E74	M14
F379	M318	L257	G195	M136	L75	V15
P380	A319	D258	R196	A137	G76	R16
LYS	K320	I259	N197	K137	R77	D17
GLY	K321	A260	E198	T138	V78	Y18
GLU	M322	V261	S199	R139	C79	A19
LEU	A323	R262	K200	A140	A80	T20
ASN	S324	H263	M201	V141	S81	R21
SER	D325	T264	G202	R142	T82	E22
LYS	T326		M203	Q143	A83	I23
LEU	A327		R204	G144	L84	A24
GLU	M328	R267	G205	D145	L85	P25
GLY	R329	Q269	S206	K146	L86	R26
LYS	V330	F270	I207	Y147	I87	A27
PRO	T331	G271	M208	V148	A88	L28
ILE	T332	K272	S209	N150	Q89	E29
PRO	D333	P273	E210	G151	T90	L30
ASN	A334	I274	L211	Q152	D91	D31
PRO	V335	A275	F212	K153	G92	E32
LEU	Q336	H276	F213	L154	M93	LYS
LEU	V337	L277	E217	C155	L94	S34
GLY	L338	A278	V218	F155	P95	L35
LEU	G339	P279	P219	I156	I96	F36
ASP	G340	V280	A220	T157	I97	P37
SER	S341	Q281	E221	M158	H98	E38
THR	G342	F282	N222	G159	G99	Y39
ARG	Y343	M283	I223	S160	G100	A40
THR	M344	V284	I224	V161	S101	R41
GLY	K345	A285	I224	A162	P102	D42
HIS	E346	D286	Q225	D163	E103	L43
HIS	N347	M287	A226	V164	L104	F44
HIS	G348	A288	E227	I165	K105	A45
HIS	V349	T289	G228	V166	E106	K46
HIS	E350	A290	T229	V167	R107	L47
HIS	R351	V291	G230	Y168	Y108	G48
HIS	M352	E292	F231	A169	L109	L49
	M353	A293	A232	Y170	R110	L50
		S294	N233	T171	R111	N51
		R295	I234	D172	F112	P52
		L296	M235	P173	A113	L53
		L297	Q236	E174	G114	L54
		T298	T237	K175	E115	P55
		R299	L238	G176	S116	A56
		K300	T239	S177	T117	A57
		A301	T240	K178	L118	Y58
		A302	N241	G179	L119	G59
		E303	R242	I180	T120	G60

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	172.91Å 333.85Å 76.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.25 – 1.65 48.25 – 1.65	Depositor EDS
% Data completeness (in resolution range)	93.0 (48.25-1.65) 93.0 (48.25-1.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 1.65Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.222 , 0.236 0.232 , 0.245	Depositor DCC
R_{free} test set	12200 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13151	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 62.54 % 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 1.1094e-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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, GOL, 4KW

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	0.78	1/2937 (0.0%)	1.04	3/3967 (0.1%)
1	B	0.79	1/2927 (0.0%)	1.02	3/3953 (0.1%)
1	C	0.80	1/2942 (0.0%)	1.05	3/3973 (0.1%)
1	D	0.83	2/2929 (0.1%)	1.20	11/3954 (0.3%)
All	All	0.80	5/11735 (0.0%)	1.08	20/15847 (0.1%)

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	D	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	318	MET	SD-CE	-10.14	1.54	1.79
1	C	318	MET	SD-CE	-9.62	1.55	1.79
1	A	318	MET	SD-CE	-9.09	1.56	1.79
1	D	35	LEU	CB-CG	-6.17	1.41	1.53
1	D	35	LEU	CA-C	-5.08	1.46	1.52

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	241	ASN	CA-CB-CG	11.60	124.20	112.60
1	D	6	GLU	CB-CA-C	9.34	128.53	109.95
1	D	303	GLU	CB-CG-CD	7.58	125.49	112.60
1	D	34	SER	CA-C-N	-6.58	111.75	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	34	SER	C-N-CA	-6.58	111.75	122.81

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	196	ARG	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2899	0	2947	9	0
1	B	2889	0	2943	13	0
1	C	2904	0	2964	11	0
1	D	2892	0	2946	87	0
2	A	53	0	27	1	0
2	B	53	0	27	3	0
2	C	53	0	27	2	0
2	D	53	0	27	0	0
3	A	56	0	0	0	0
3	B	56	0	0	0	0
3	C	56	0	0	0	0
3	D	56	0	0	0	0
4	A	6	0	8	0	0
4	B	12	0	16	0	0
4	C	12	0	16	0	0
4	D	12	0	16	1	0
5	A	307	0	0	1	0
5	B	329	0	0	1	0
5	C	336	0	0	1	0
5	D	117	0	0	12	0
All	All	13151	0	11964	118	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 118 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:D:269:GLN:HB2	1:D:274:ILE:CD1	1.93	0.99
1:D:269:GLN:HB2	1:D:274:ILE:HD12	1.49	0.92
1:D:4:LEU:HD21	1:D:9:LYS:CD	2.03	0.89
1:B:208:ASN:HB2	5:B:605[B]:HOH:O	1.75	0.86
1:D:29:GLU:HG3	5:D:619:HOH:O	1.77	0.83

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	382/412 (93%)	377 (99%)	5 (1%)	0	100	100
1	B	381/412 (92%)	376 (99%)	5 (1%)	0	100	100
1	C	383/412 (93%)	378 (99%)	5 (1%)	0	100	100
1	D	379/412 (92%)	374 (99%)	5 (1%)	0	100	100
All	All	1525/1648 (92%)	1505 (99%)	20 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	304/328 (93%)	301 (99%)	3 (1%)	68	52
1	B	303/328 (92%)	301 (99%)	2 (1%)	76	64
1	C	305/328 (93%)	300 (98%)	5 (2%)	55	34
1	D	303/328 (92%)	290 (96%)	13 (4%)	26	6
All	All	1215/1312 (93%)	1192 (98%)	23 (2%)	51	28

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	70	LEU
1	D	276	HIS
1	D	274	ILE
1	D	303	GLU
1	C	4[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	367	GLN
1	D	3	HIS
1	D	276	HIS
1	D	222	ASN
1	D	236	GLN

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

15 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
4	GOL	A	503	-	5,5,5	0.09	0	5,5,5	0.81	0
4	GOL	D	504	-	5,5,5	0.29	0	5,5,5	0.41	0
3	4KW	A	502	-	55,59,59	1.85	12 (21%)	77,87,87	2.07	25 (32%)
4	GOL	B	504	-	5,5,5	0.14	0	5,5,5	0.29	0
4	GOL	C	503	-	5,5,5	0.17	0	5,5,5	0.21	0
2	FAD	D	501	-	58,58,58	2.39	14 (24%)	85,89,89	2.20	29 (34%)
3	4KW	D	502	-	55,59,59	1.84	13 (23%)	77,87,87	2.09	23 (29%)
2	FAD	B	501	-	58,58,58	2.32	12 (20%)	85,89,89	2.23	29 (34%)
4	GOL	C	504	-	5,5,5	0.13	0	5,5,5	0.19	0
2	FAD	A	501	-	58,58,58	2.31	13 (22%)	85,89,89	2.26	28 (32%)
3	4KW	C	502	-	55,59,59	1.81	13 (23%)	77,87,87	2.08	25 (32%)
4	GOL	D	503	-	5,5,5	0.23	0	5,5,5	0.58	0
4	GOL	B	503	-	5,5,5	0.20	0	5,5,5	0.38	0
2	FAD	C	501	-	58,58,58	2.33	12 (20%)	85,89,89	2.19	28 (32%)
3	4KW	B	502	-	55,59,59	1.80	14 (25%)	77,87,87	2.08	22 (28%)

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	GOL	A	503	-	-	3/4/4/4	-
4	GOL	D	504	-	-	0/4/4/4	-
3	4KW	A	502	-	-	6/53/79/79	0/4/4/4
4	GOL	B	504	-	-	2/4/4/4	-
4	GOL	C	503	-	-	0/4/4/4	-
2	FAD	D	501	-	-	6/34/50/50	0/6/6/6
3	4KW	D	502	-	-	6/53/79/79	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	501	-	-	6/34/50/50	0/6/6/6
4	GOL	C	504	-	-	1/4/4/4	-
2	FAD	A	501	-	-	6/34/50/50	0/6/6/6
3	4KW	C	502	-	-	5/53/79/79	0/4/4/4
4	GOL	D	503	-	-	2/4/4/4	-
4	GOL	B	503	-	-	0/4/4/4	-
2	FAD	C	501	-	-	6/34/50/50	0/6/6/6
3	4KW	B	502	-	-	6/53/79/79	0/4/4/4

The worst 5 of 103 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FAD	C2'-C3'	-9.57	1.36	1.53
2	C	501	FAD	C2'-C3'	-9.38	1.37	1.53
2	A	501	FAD	C2'-C3'	-9.29	1.37	1.53
2	D	501	FAD	C4X-N5	9.08	1.50	1.30
2	B	501	FAD	C2'-C3'	-9.08	1.37	1.53

The worst 5 of 209 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	C9A-C5X-N5	-8.58	113.35	122.45
2	B	501	FAD	C9A-C5X-N5	-7.90	114.08	122.45
2	C	501	FAD	C9A-C5X-N5	-7.68	114.30	122.45
3	D	502	4KW	C3-S1-C22	7.18	108.31	99.85
3	C	502	4KW	C3-S1-C22	7.11	108.23	99.85

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

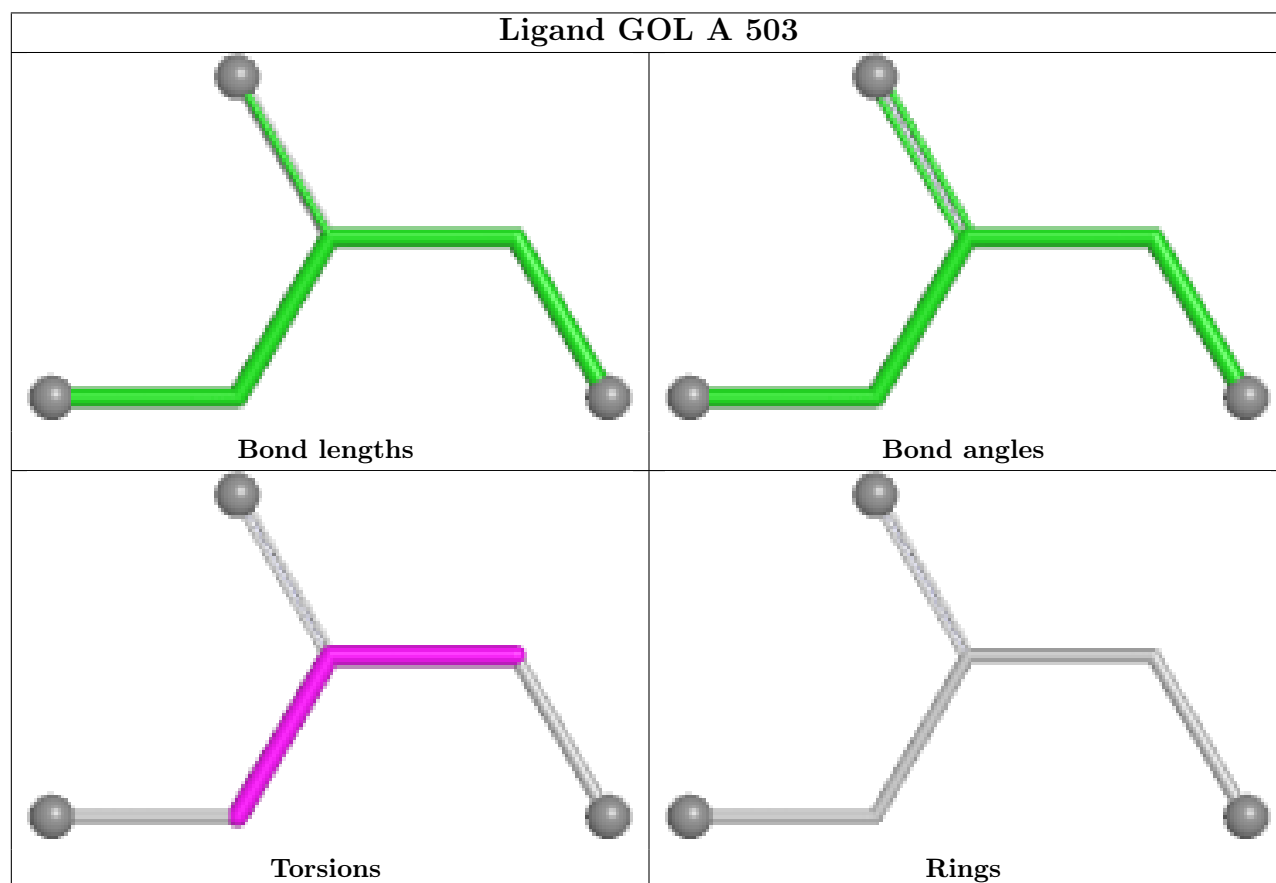
Mol	Chain	Res	Type	Atoms
2	A	501	FAD	C2'-C1'-N10-C10
2	A	501	FAD	N10-C1'-C2'-C3'
2	A	501	FAD	C1'-C2'-C3'-C4'
2	A	501	FAD	O2'-C2'-C3'-C4'
2	A	501	FAD	O3'-C3'-C4'-C5'

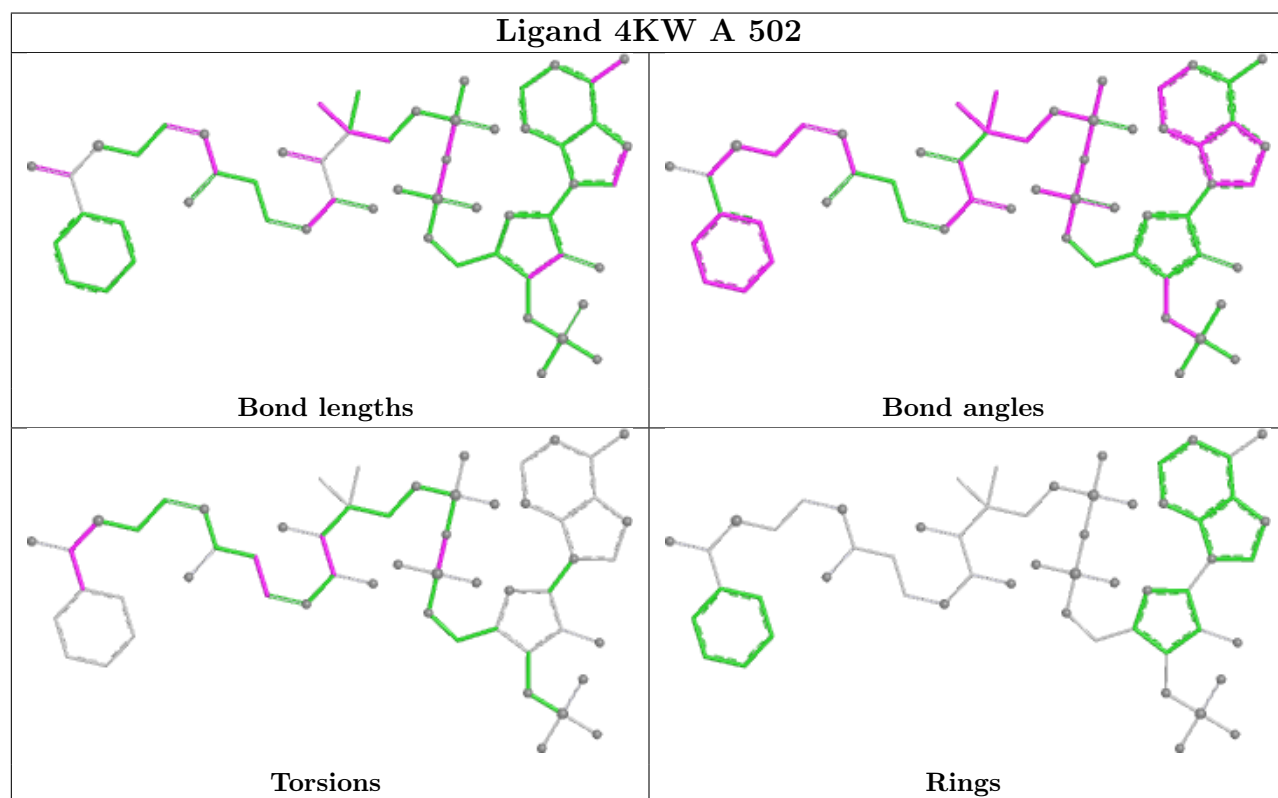
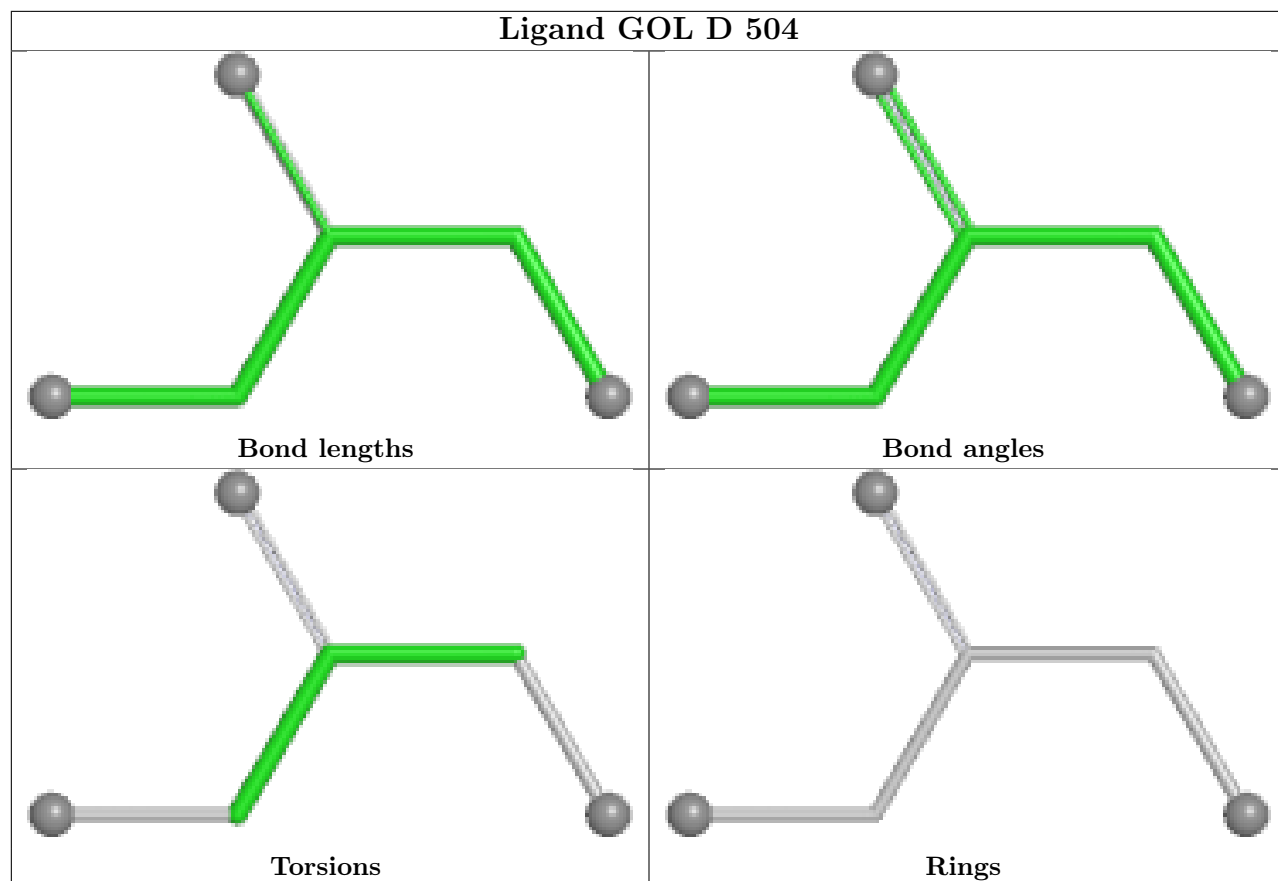
There are no ring outliers.

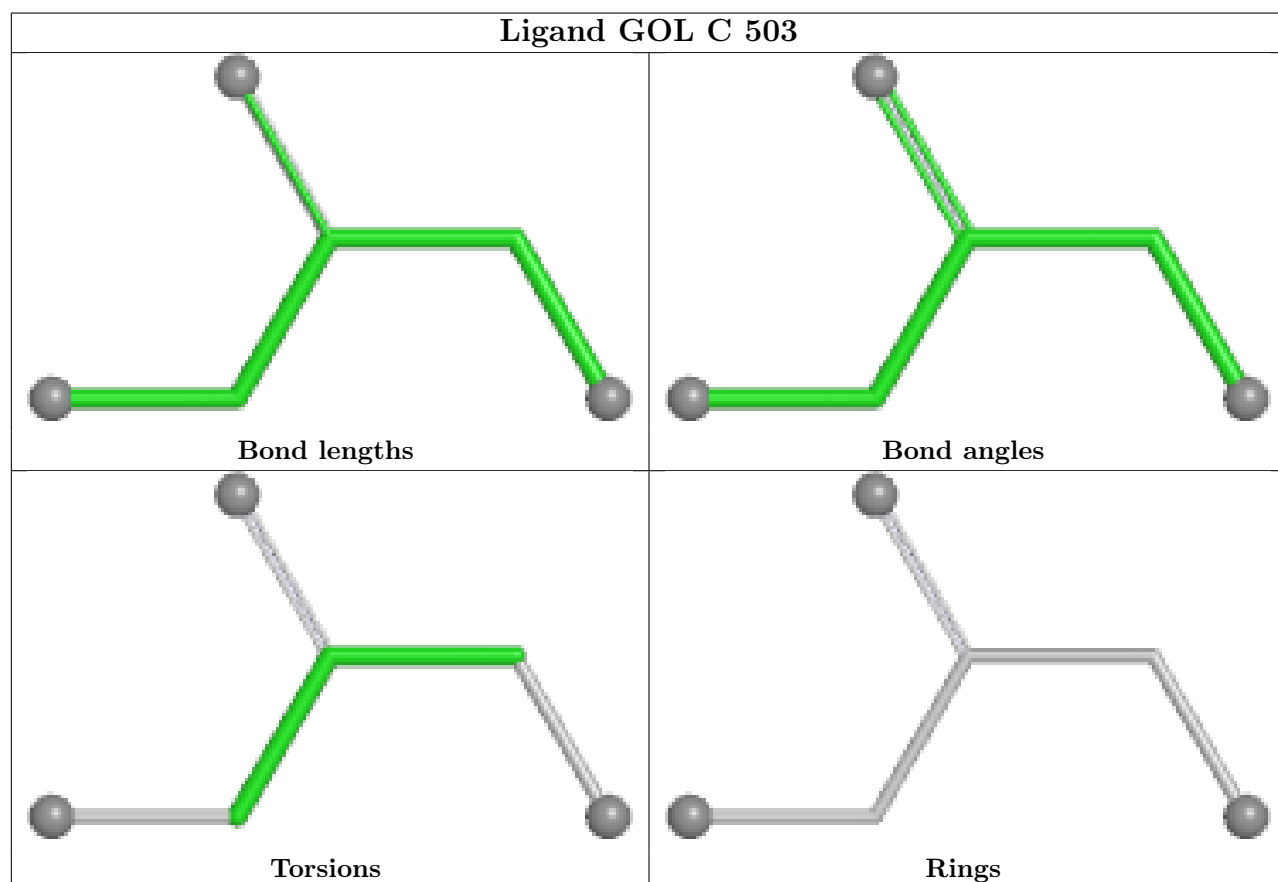
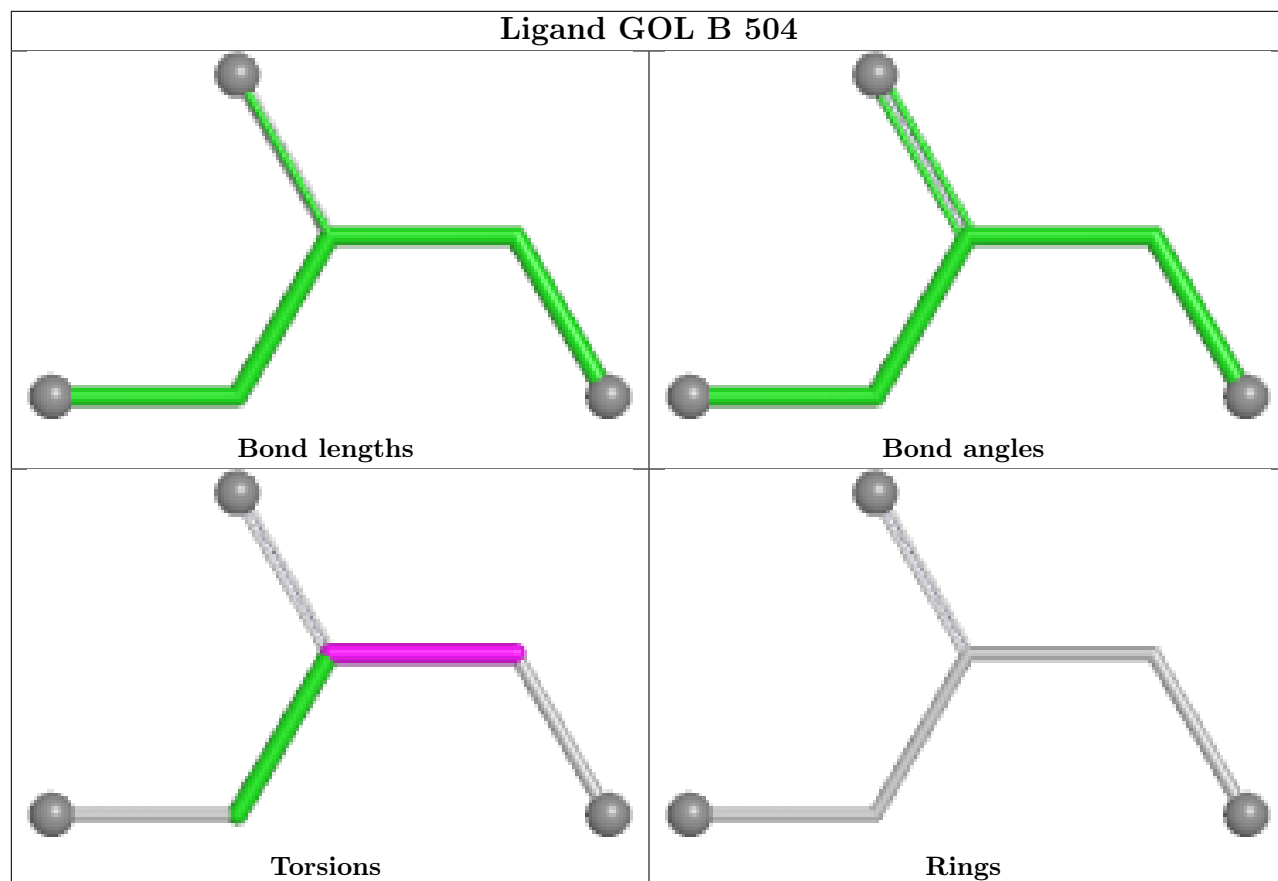
4 monomers are involved in 7 short contacts:

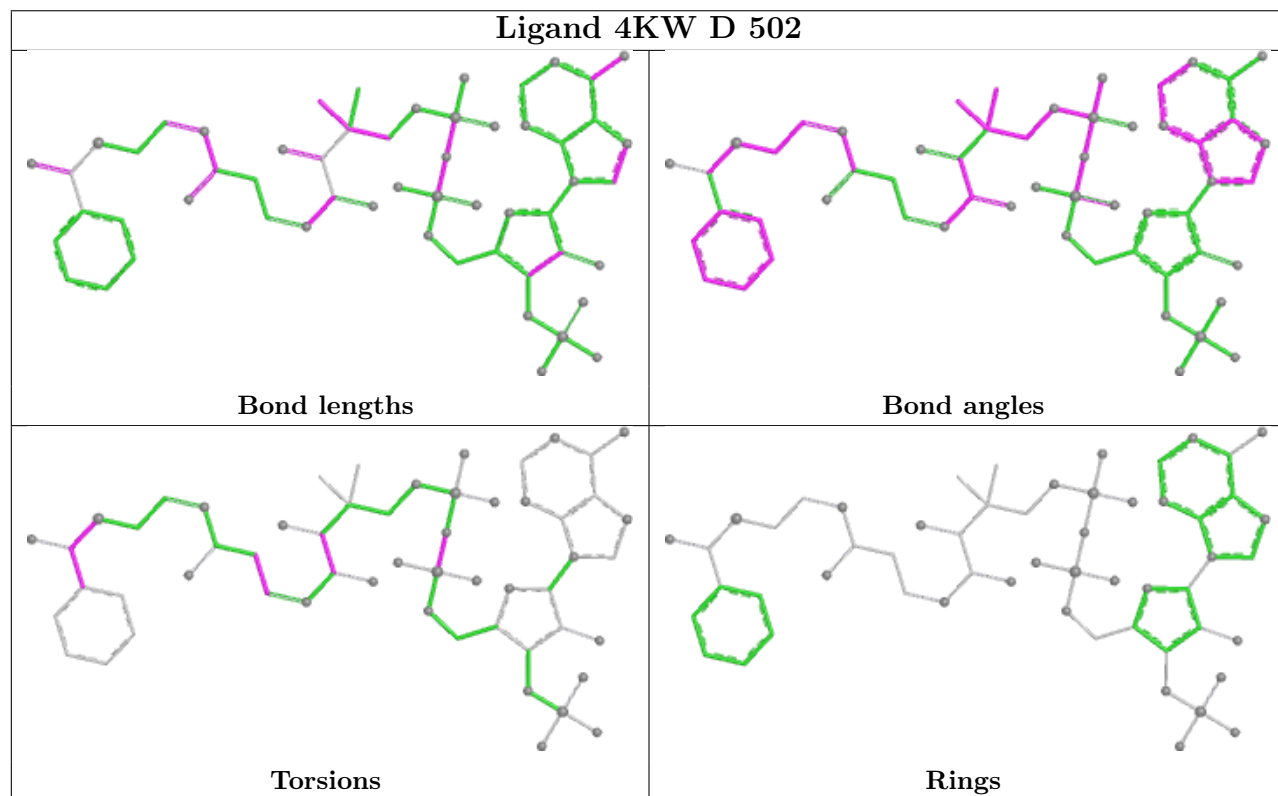
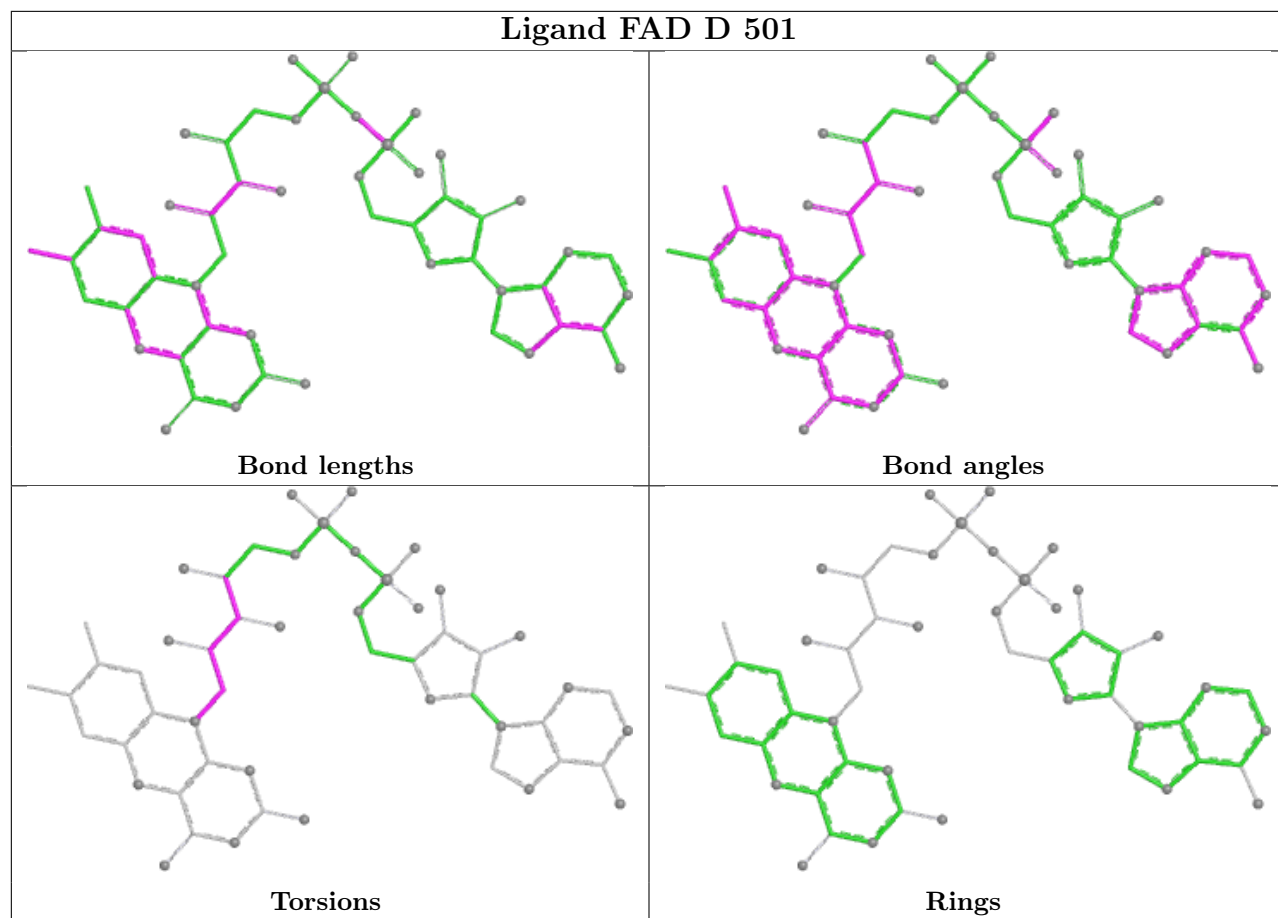
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	504	GOL	1	0
2	B	501	FAD	3	0
2	A	501	FAD	1	0
2	C	501	FAD	2	0

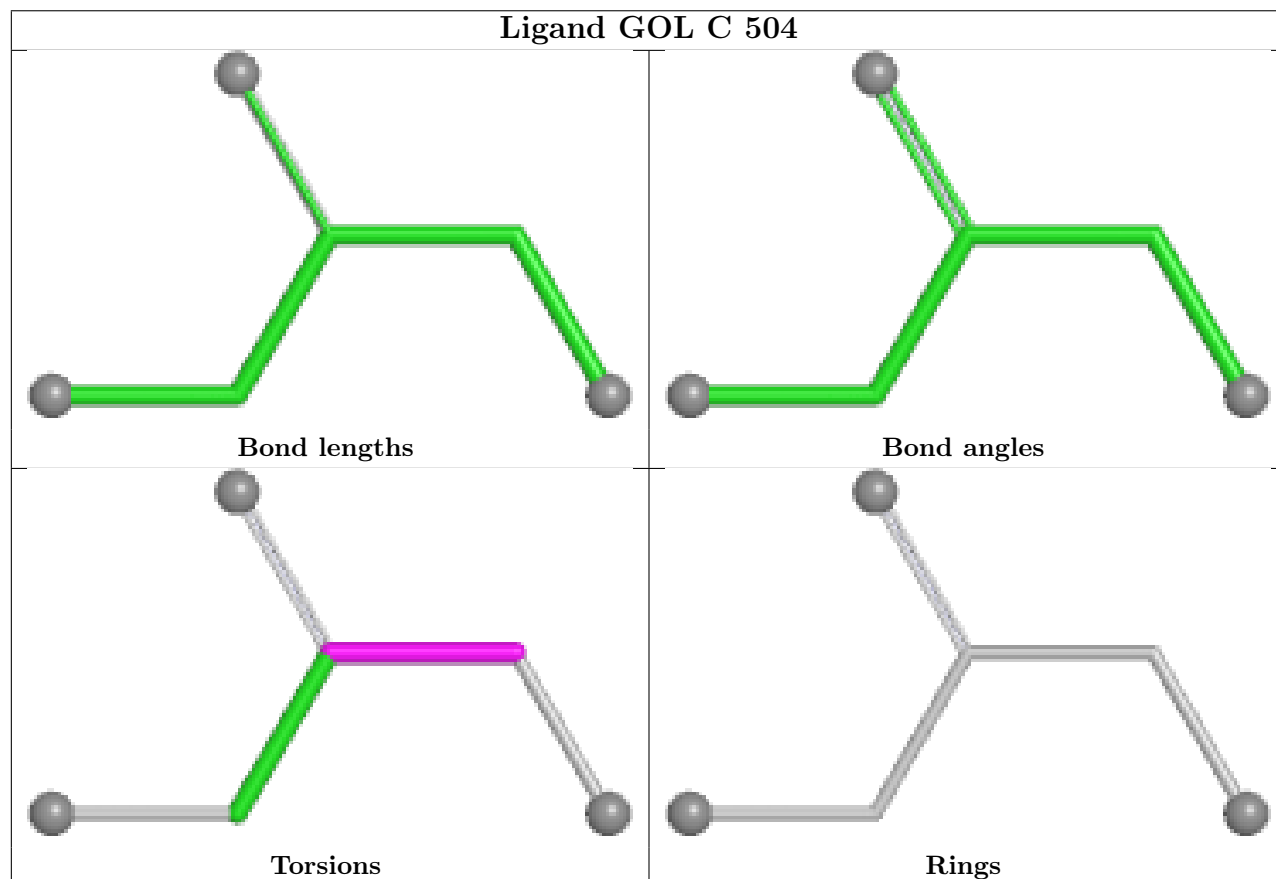
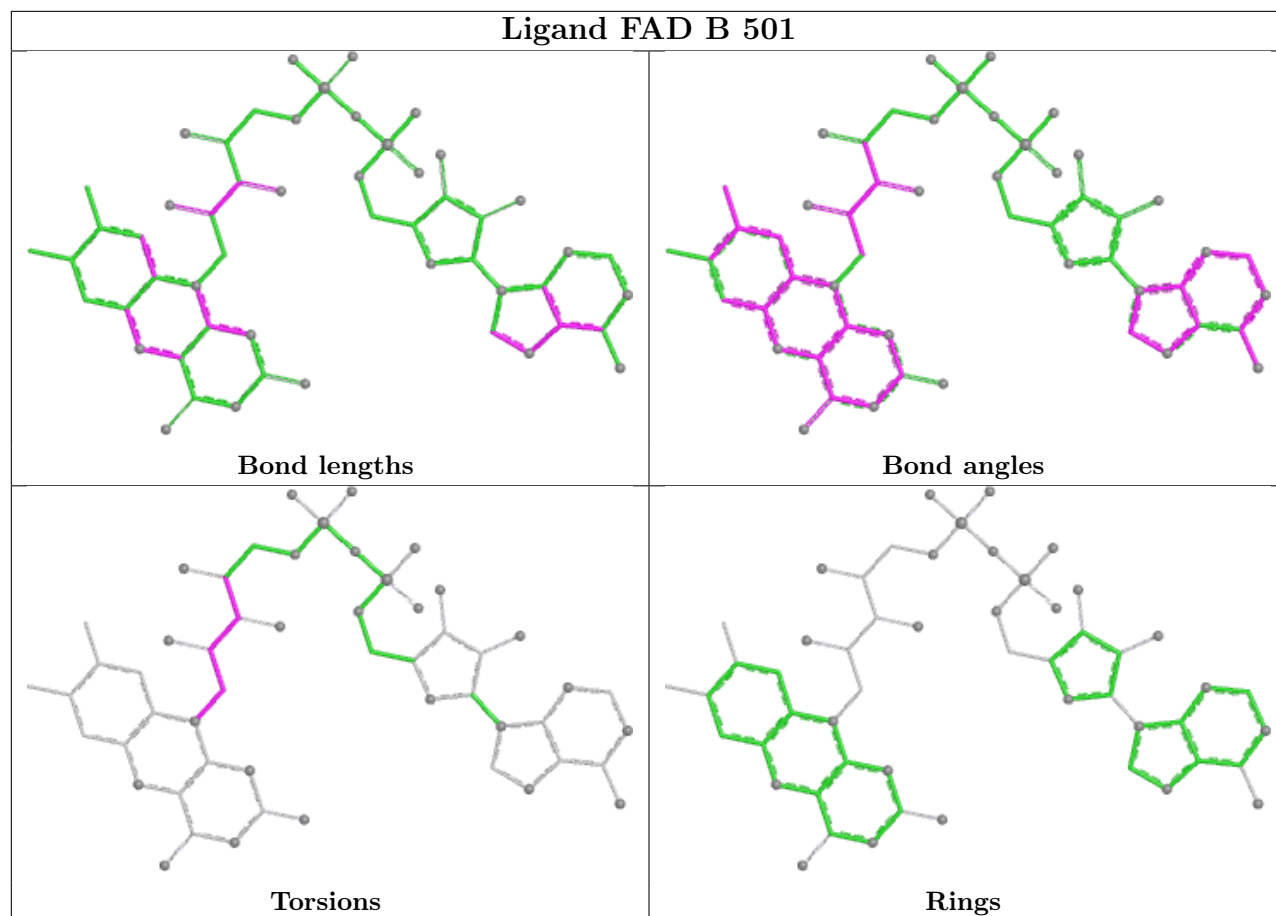
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



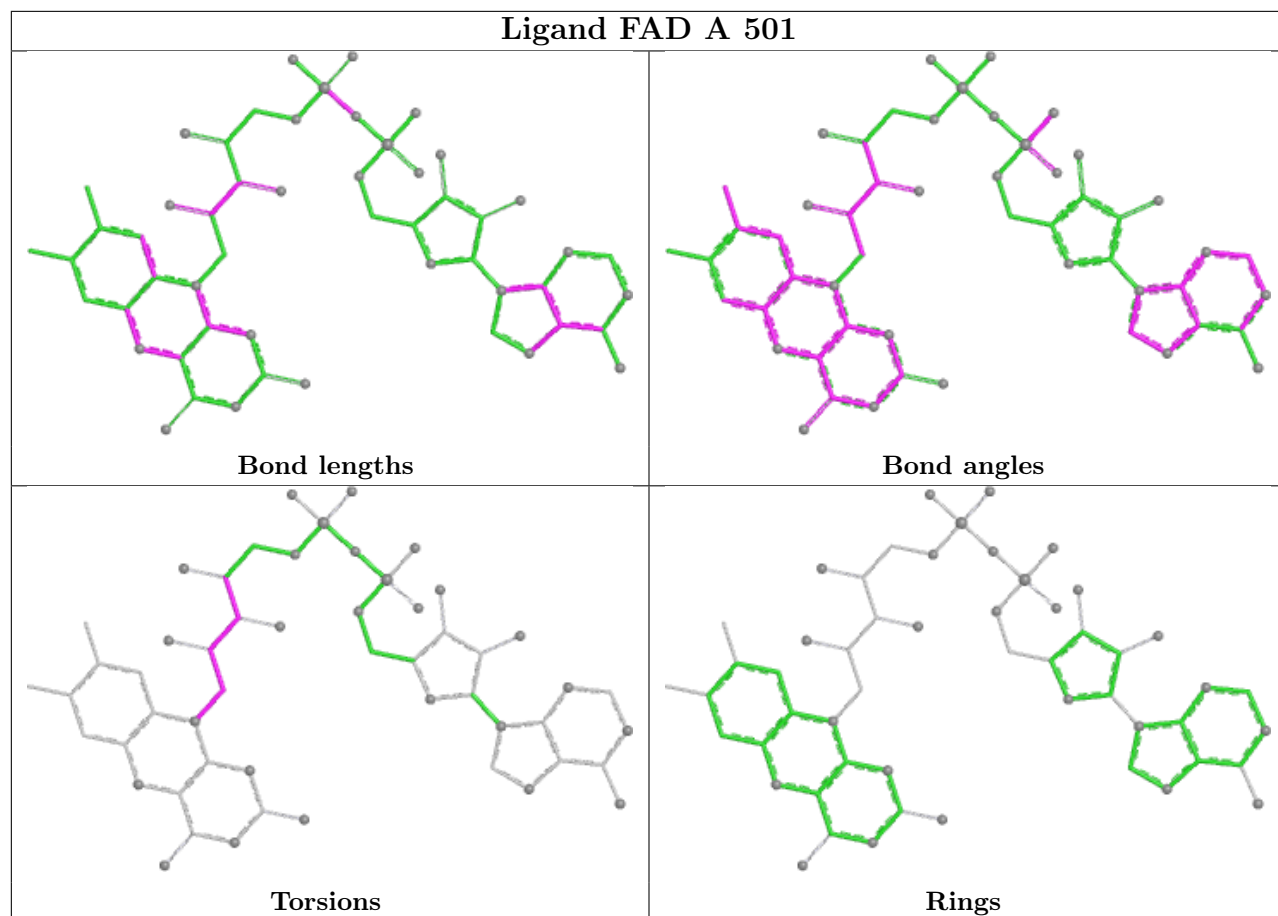




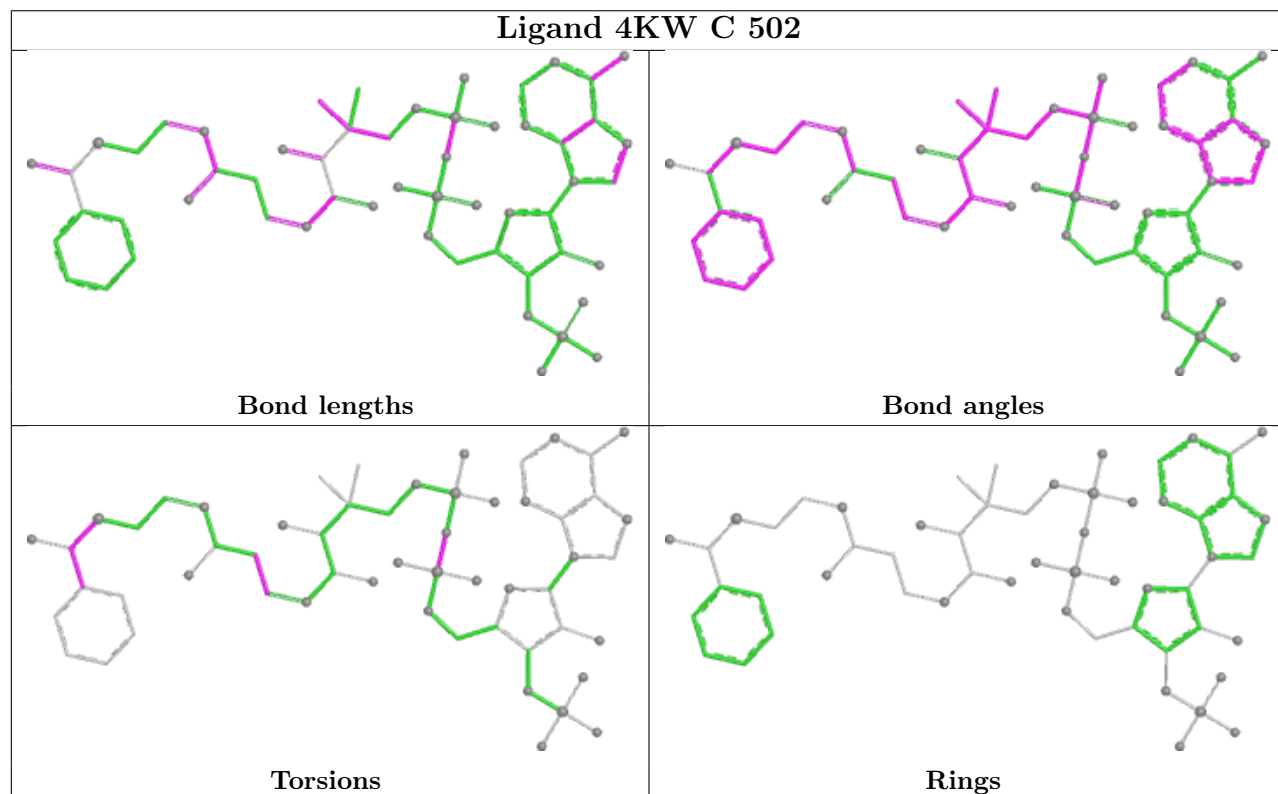


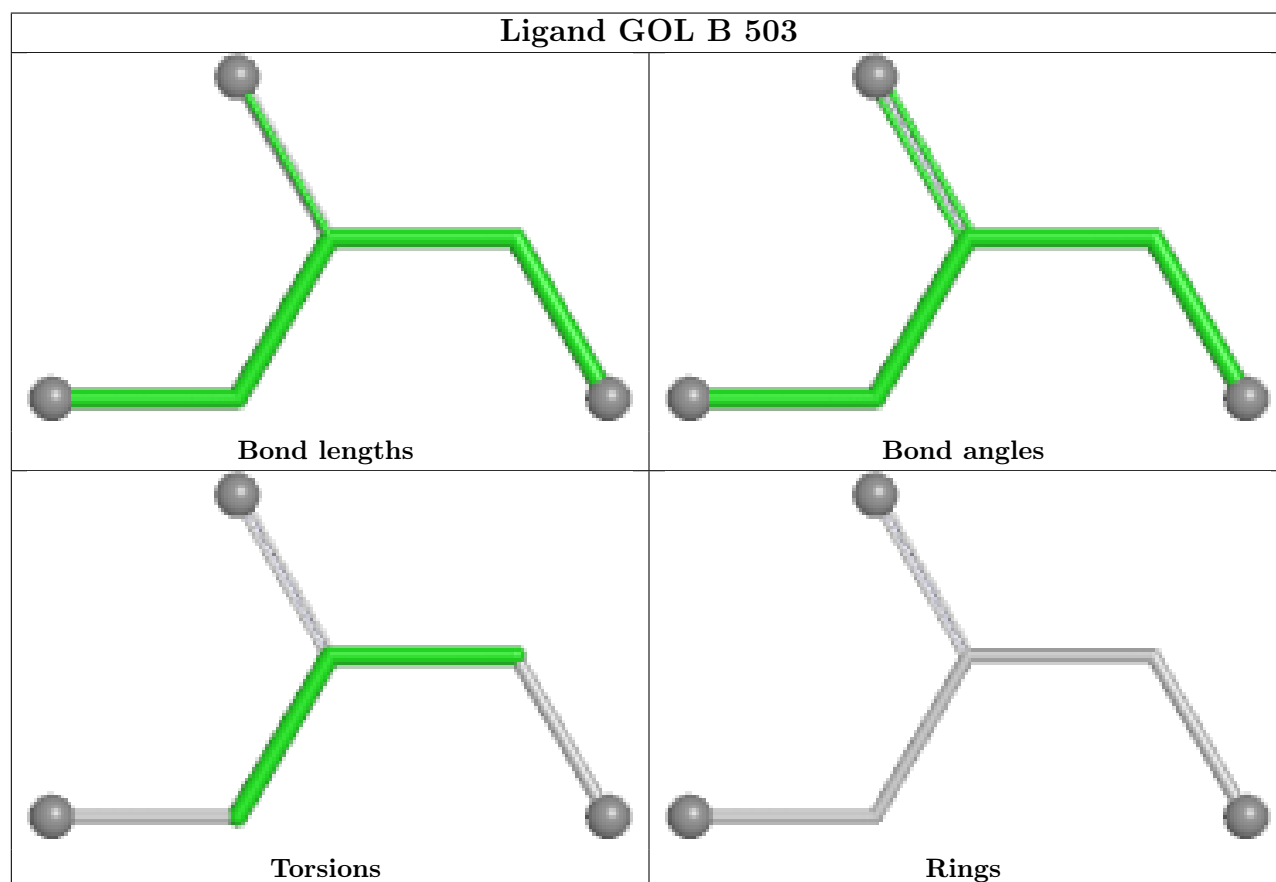
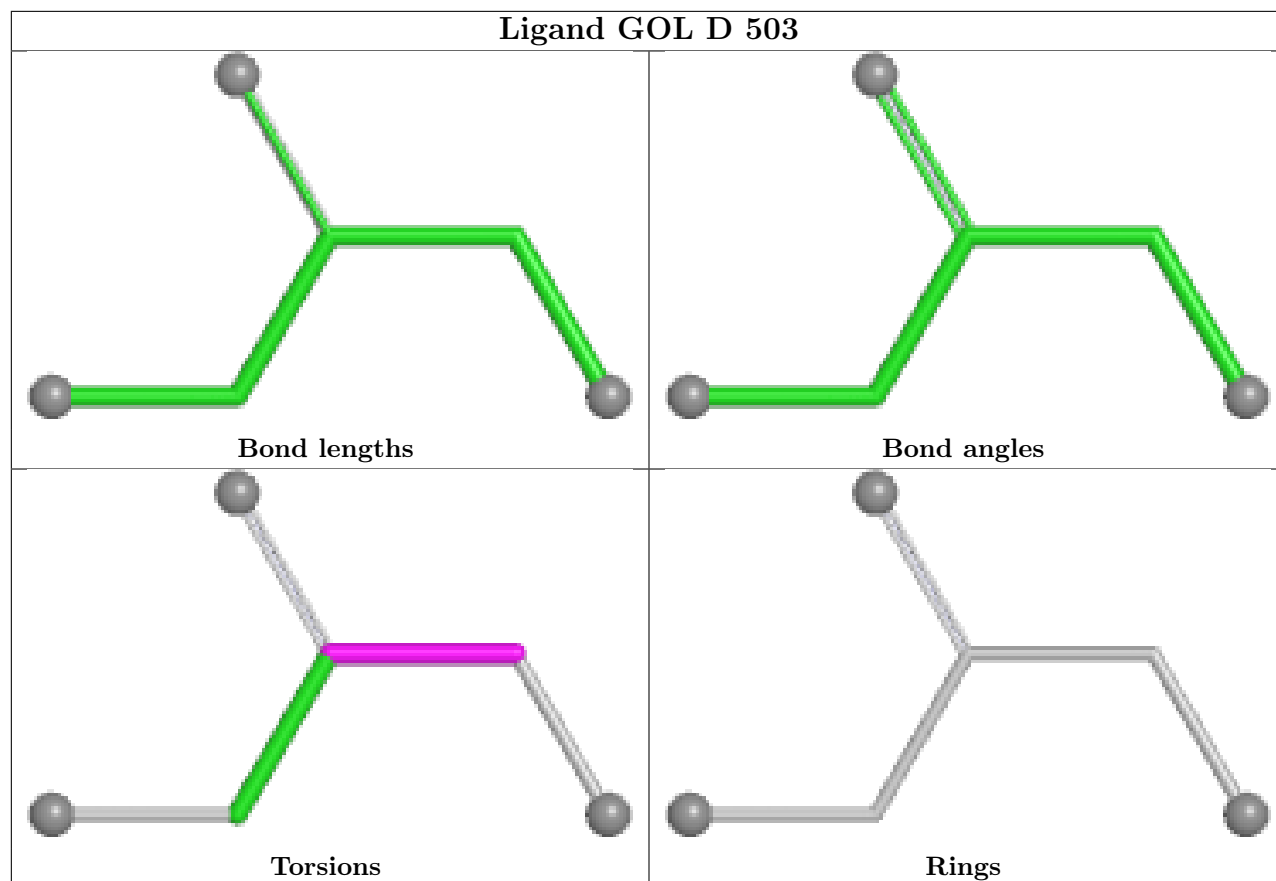


Ligand FAD A 501

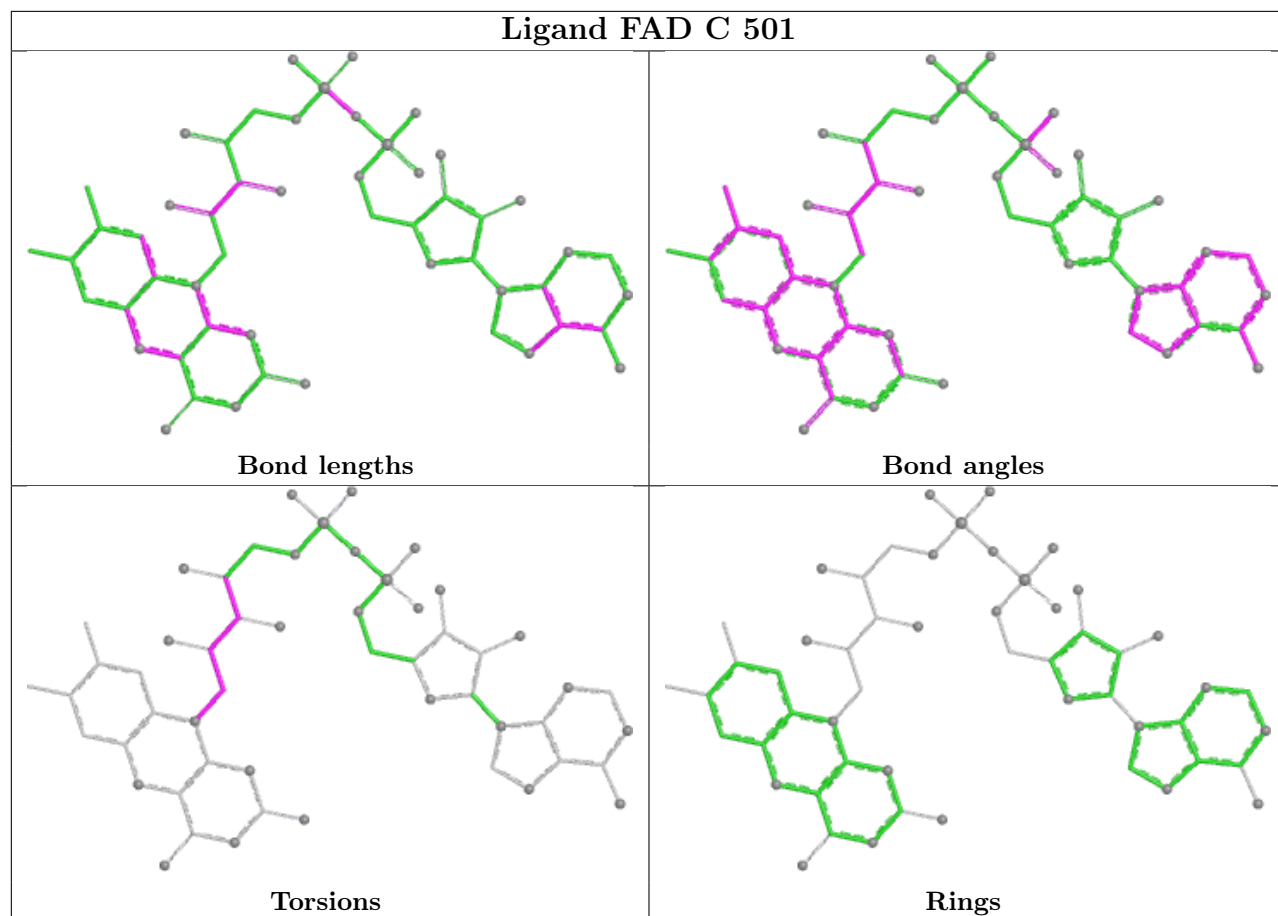


Ligand 4KW C 502

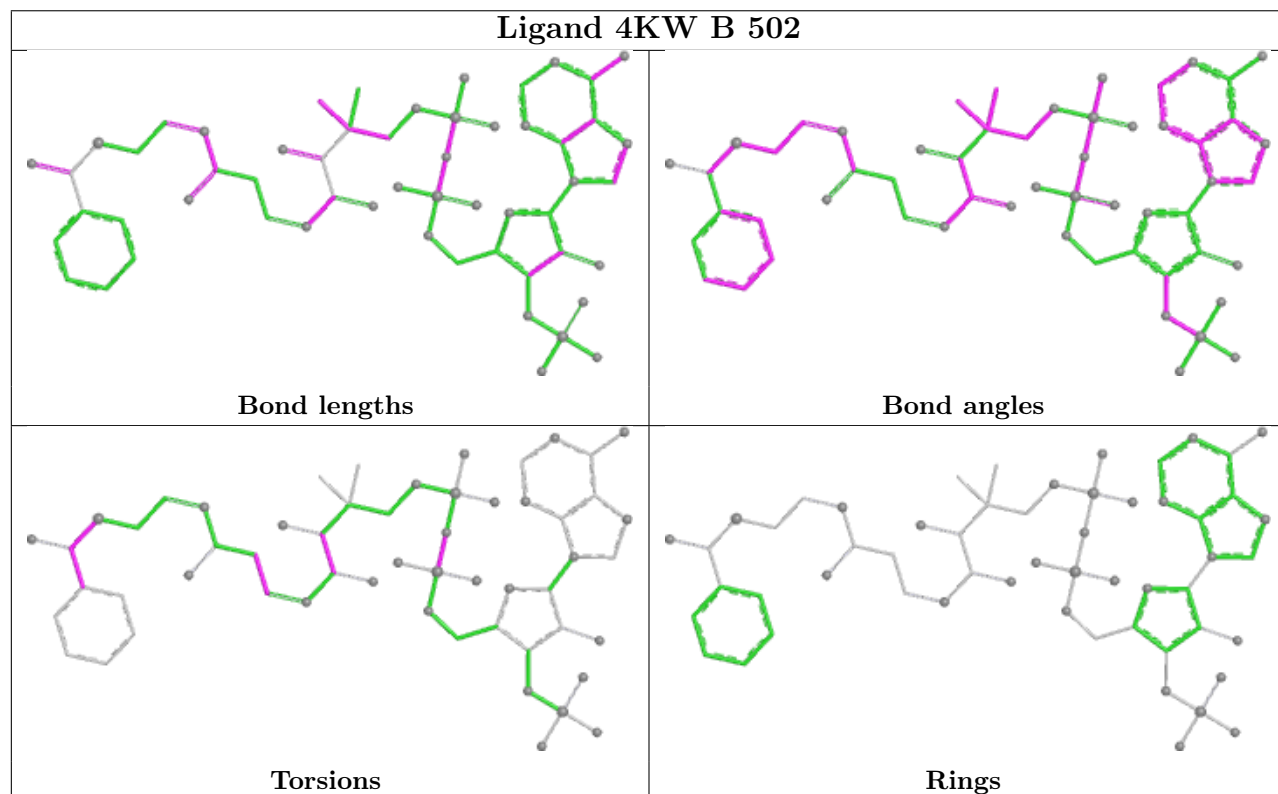




Ligand FAD C 501



Ligand 4KW B 502



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	378/412 (91%)	0.31	20 (5%) 32 36	7, 23, 43, 70	6 (1%)
1	B	378/412 (91%)	0.28	21 (5%) 30 34	6, 21, 39, 65	5 (1%)
1	C	378/412 (91%)	0.30	21 (5%) 30 34	7, 22, 39, 65	7 (1%)
1	D	377/412 (91%)	4.10	342 (90%) 0 0	12, 39, 63, 105	6 (1%)
All	All	1511/1648 (91%)	1.25	404 (26%) 1 1	6, 25, 53, 105	24 (1%)

The worst 5 of 404 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	238	LEU	11.4
1	D	11	THR	10.0
1	D	15	VAL	10.0
1	D	12	LEU	9.8
1	D	78	VAL	9.2

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](#)

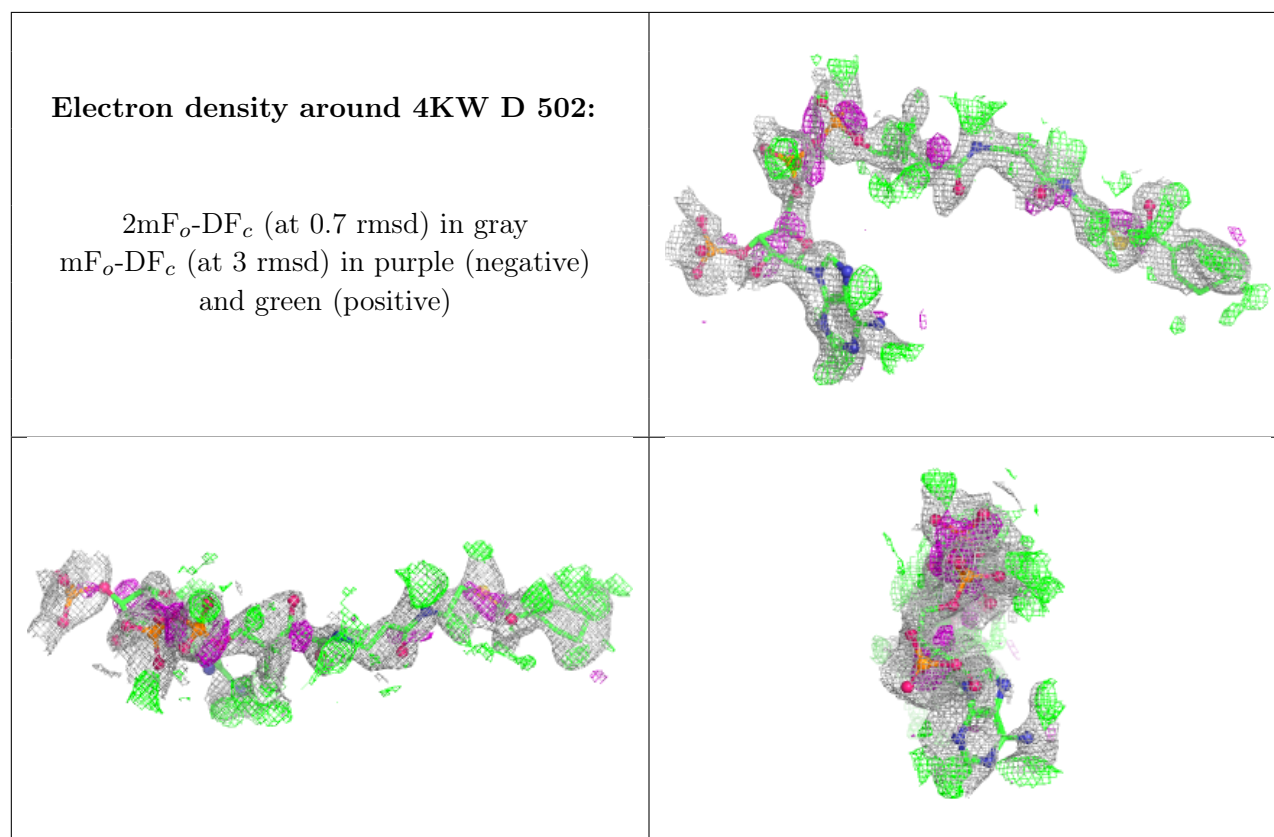
There are no oligosaccharides in this entry.

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.

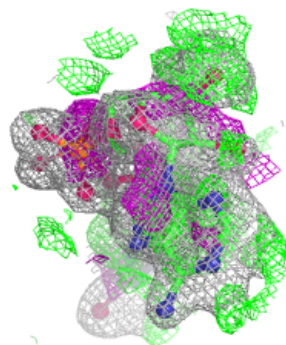
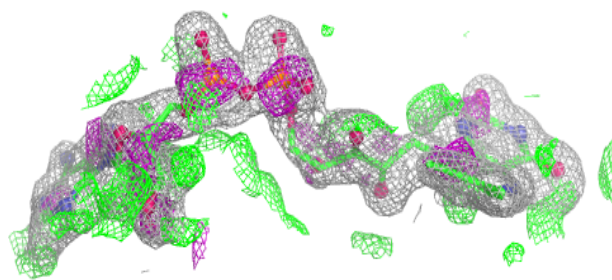
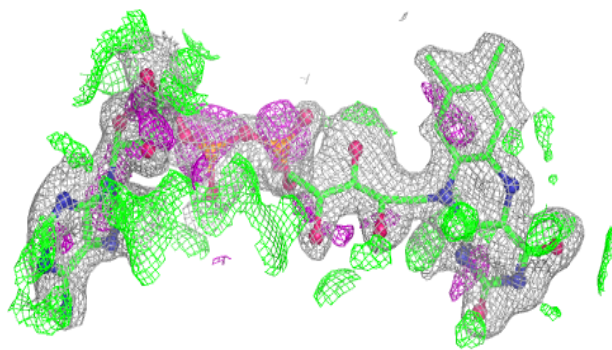
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	4KW	D	502	56/56	0.59	0.25	39,55,86,86	0
2	FAD	D	501	53/53	0.76	0.17	31,35,39,41	0
4	GOL	D	504	6/6	0.77	0.24	45,47,50,51	0
4	GOL	D	503	6/6	0.80	0.52	78,83,83,85	6
4	GOL	C	504	6/6	0.83	0.18	40,44,46,48	0
4	GOL	B	504	6/6	0.90	0.14	31,38,41,42	0
3	4KW	C	502	56/56	0.93	0.10	18,31,55,58	0
3	4KW	B	502	56/56	0.93	0.10	20,28,60,61	0
3	4KW	A	502	56/56	0.94	0.10	19,28,56,58	0
4	GOL	A	503	6/6	0.94	0.10	21,28,29,30	0
4	GOL	C	503	6/6	0.95	0.08	20,22,24,25	0
4	GOL	B	503	6/6	0.95	0.07	22,22,23,25	0
2	FAD	A	501	53/53	0.96	0.07	15,20,23,24	0
2	FAD	B	501	53/53	0.97	0.07	17,20,23,24	0
2	FAD	C	501	53/53	0.97	0.06	14,18,20,23	0

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



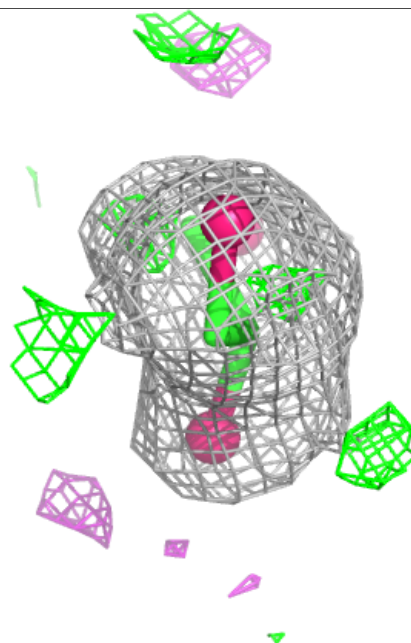
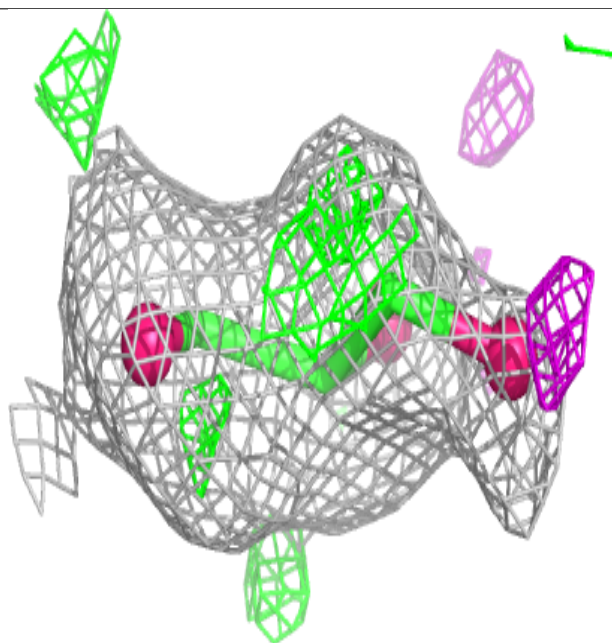
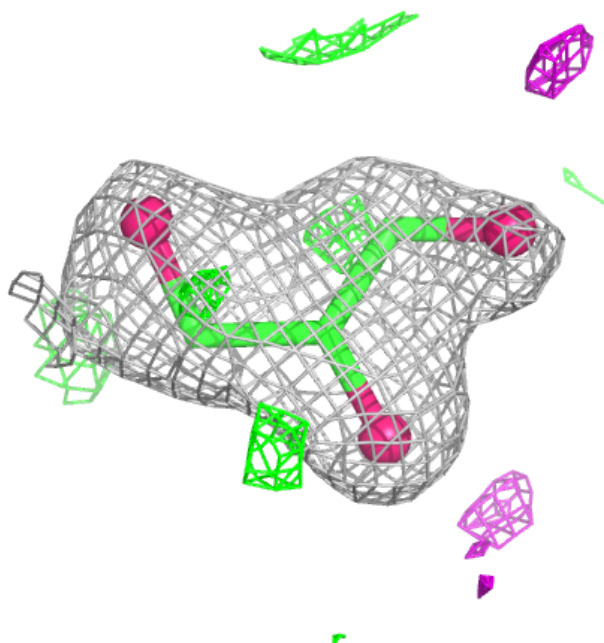
Electron density around FAD D 501:

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



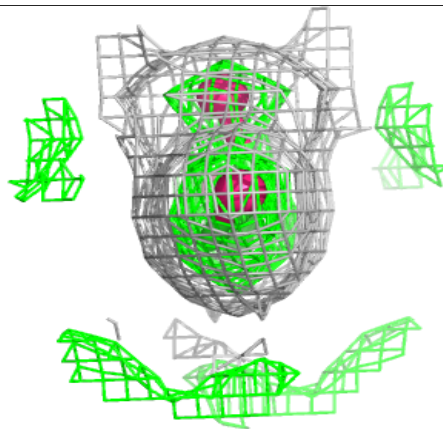
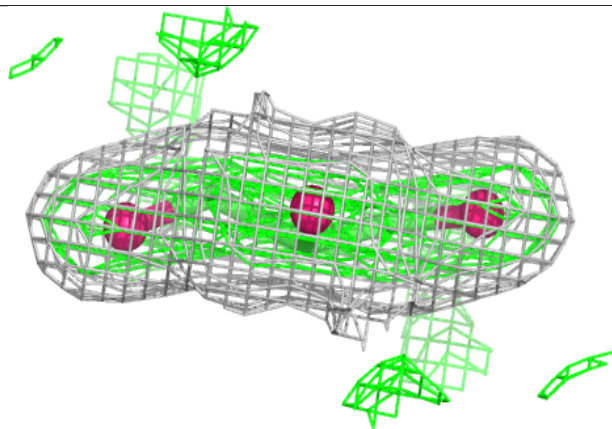
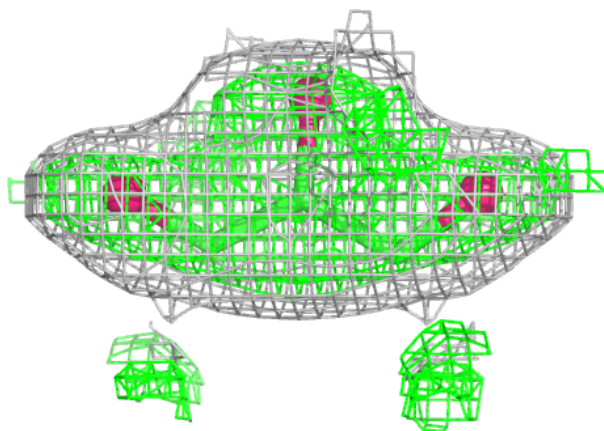
Electron density around GOL D 504:

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



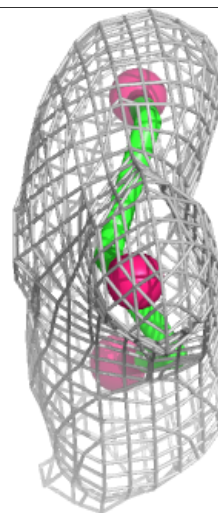
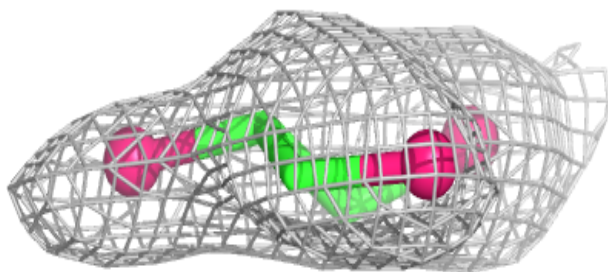
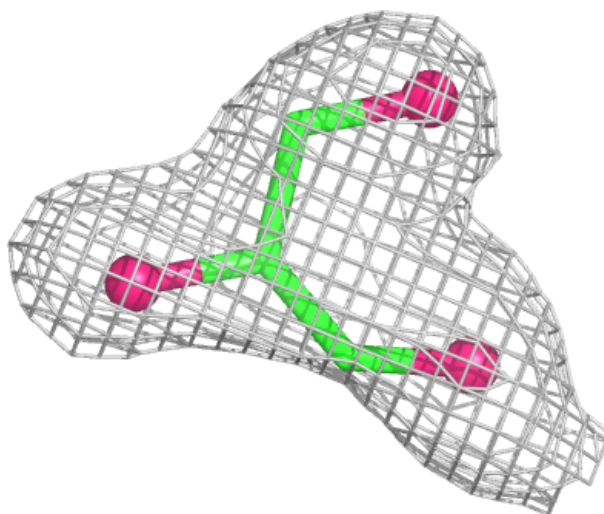
Electron density around GOL D 503:

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



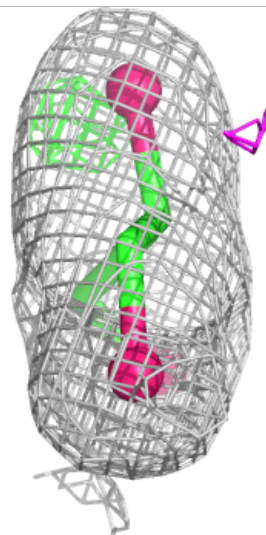
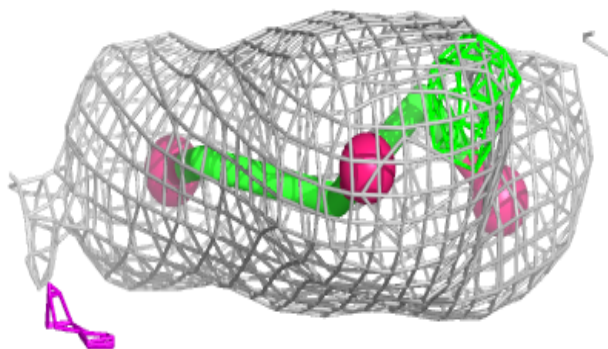
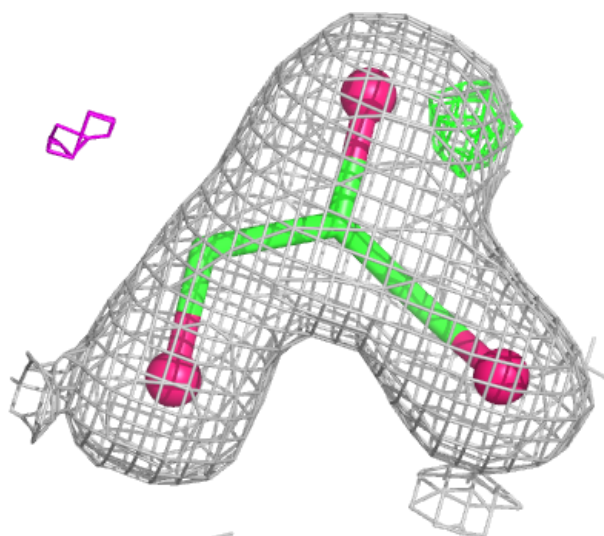
Electron density around GOL C 504:

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



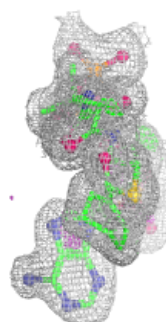
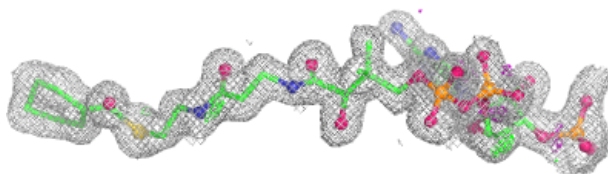
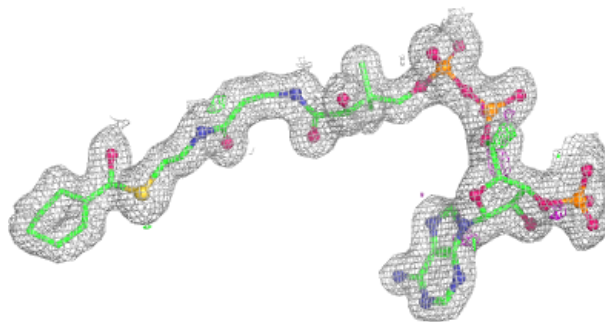
Electron density around GOL B 504:

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

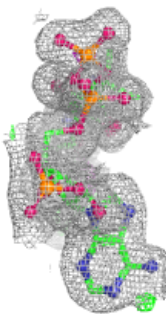
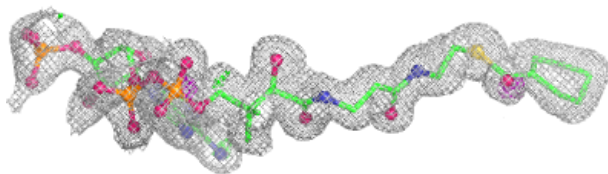
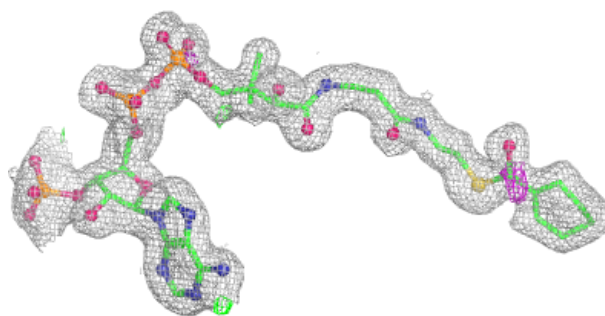


Electron density around 4KW C 502:

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

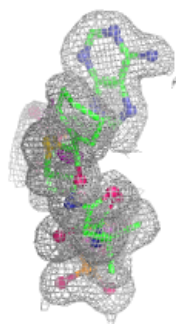
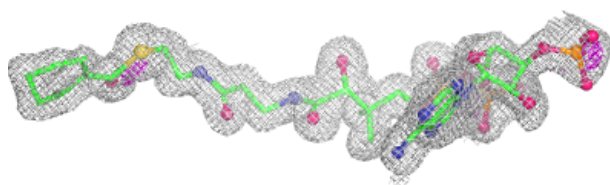
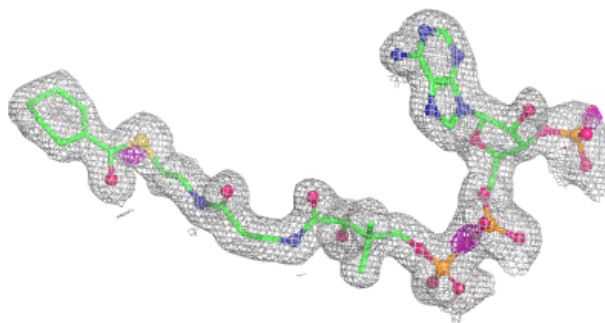
**Electron density around 4KW B 502:**

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

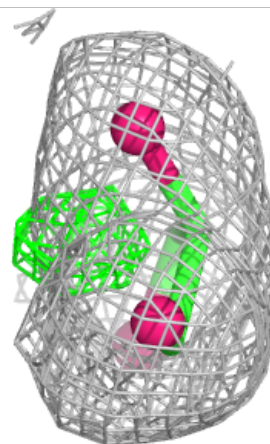
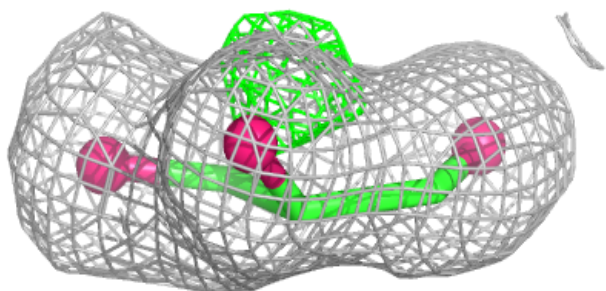
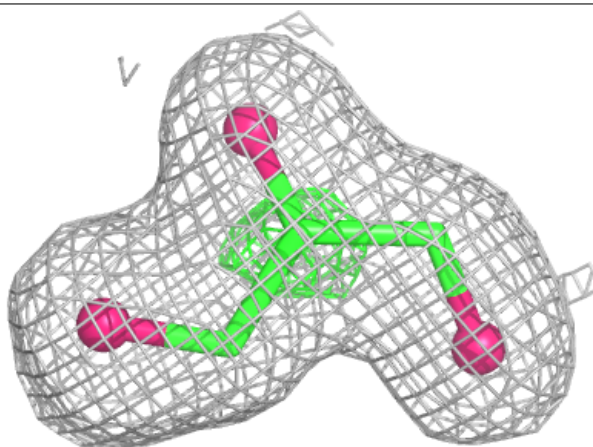


Electron density around 4KW A 502:

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

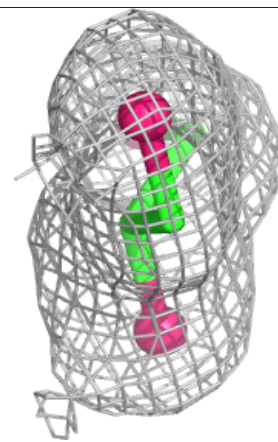
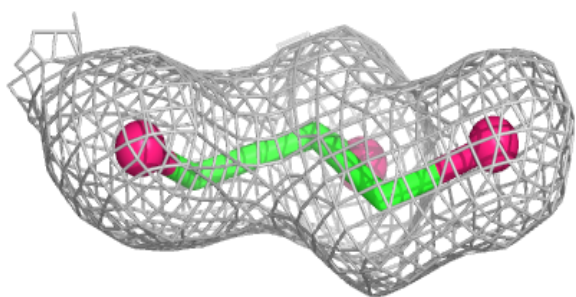
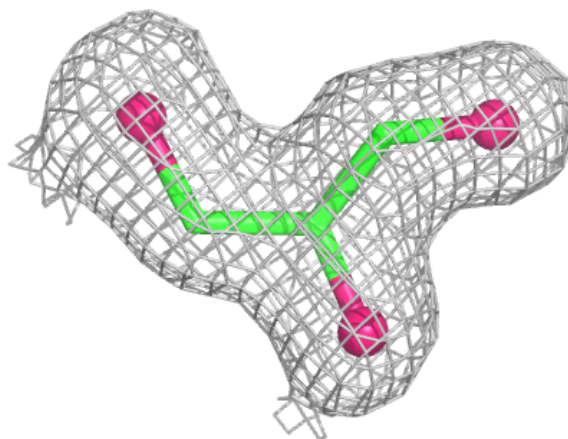
**Electron density around GOL A 503:**

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



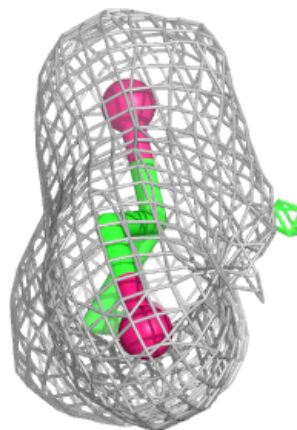
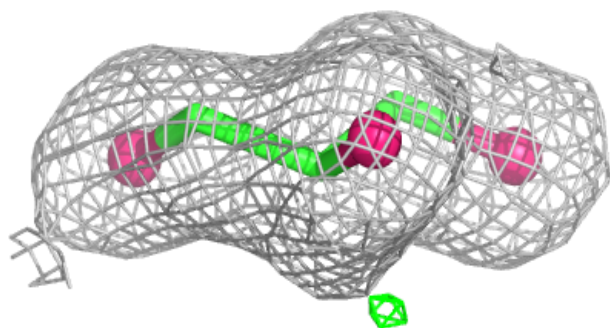
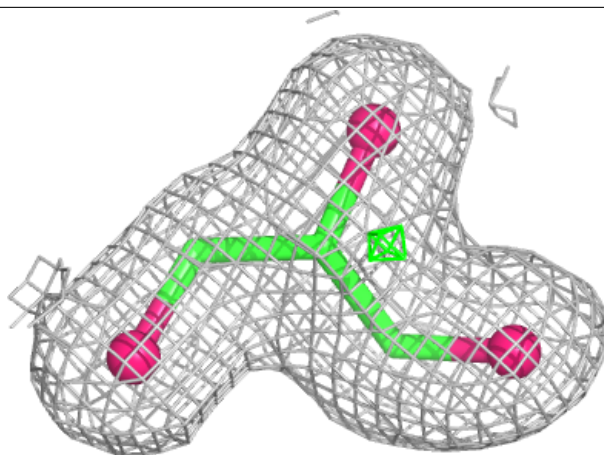
Electron density around GOL C 503:

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

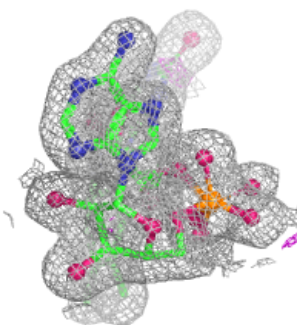
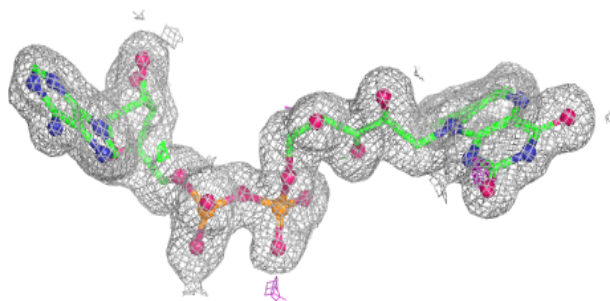
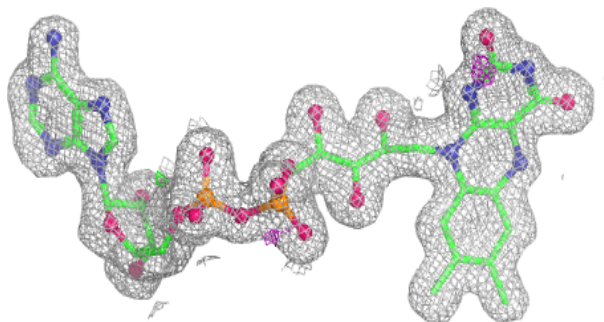


Electron density around GOL B 503:

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

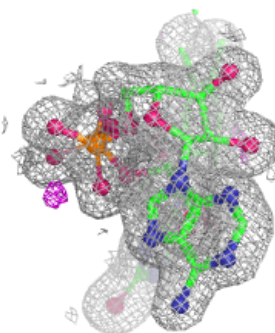
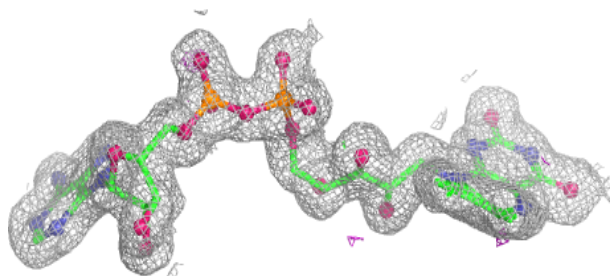
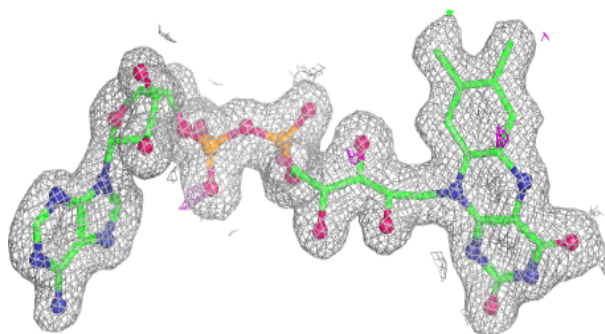
**Electron density around FAD A 501:**

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

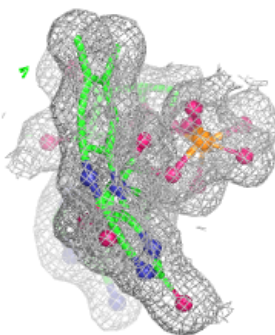
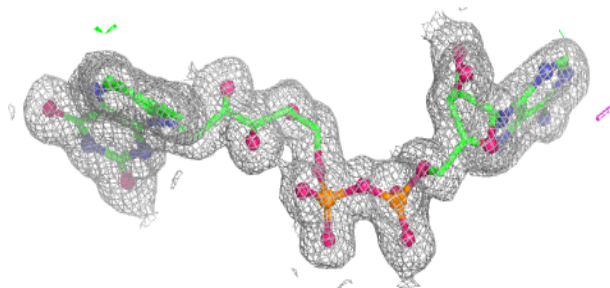
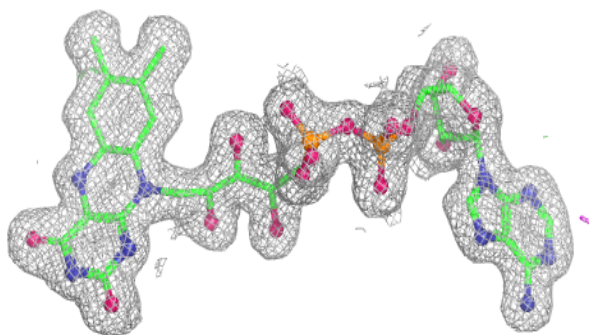


Electron density around FAD B 501:

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

**Electron density around FAD C 501:**

$2mF_o-DF_c$ (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.