



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:13 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 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

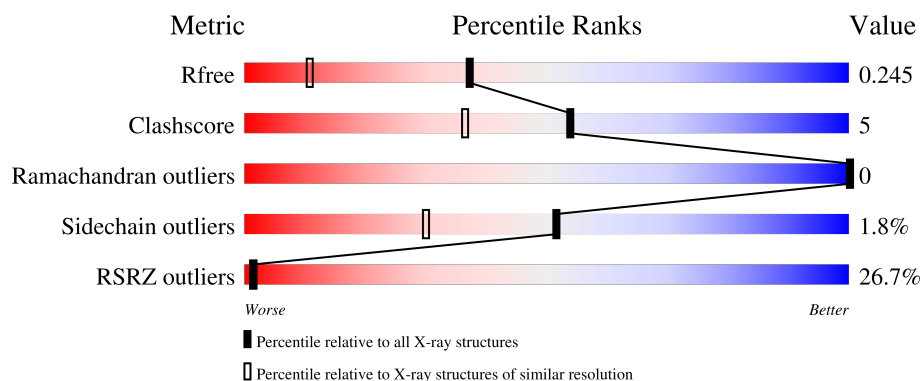
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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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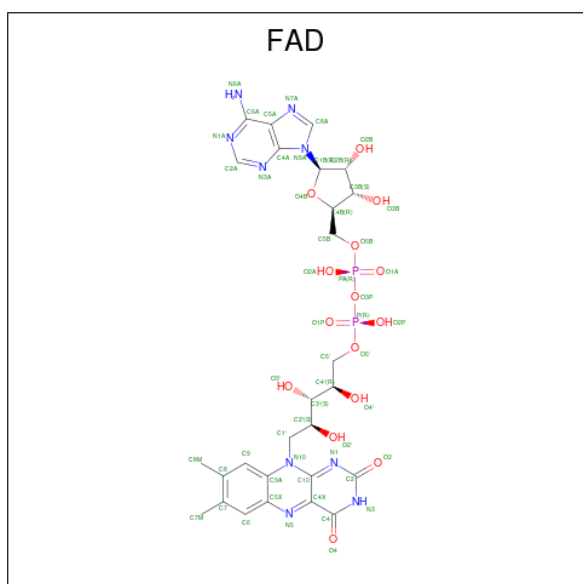
Chain	Residue	Modelled	Actual	Comment	Reference
B	412	HIS	-	expression tag	UNP Q39QF5
C	381	LYS	-	expression tag	UNP Q39QF5
C	382	GLY	-	expression tag	UNP Q39QF5
C	383	GLU	-	expression tag	UNP Q39QF5
C	384	LEU	-	expression tag	UNP Q39QF5
C	385	ASN	-	expression tag	UNP Q39QF5
C	386	SER	-	expression tag	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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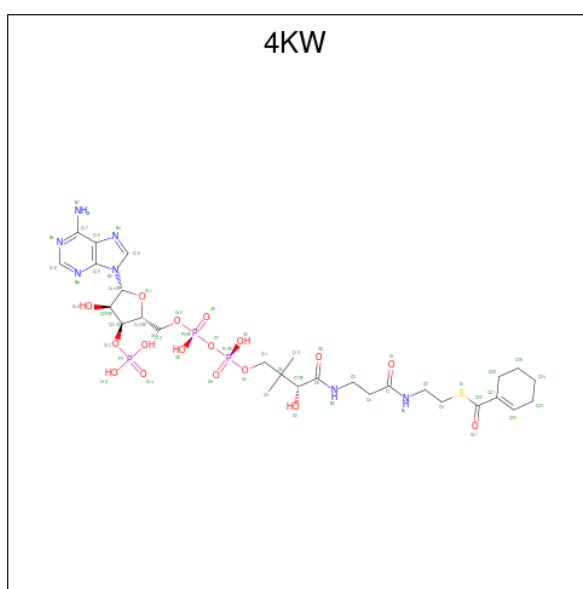
Chain	Residue	Modelled	Actual	Comment	Reference
D	390	GLY	-	expression tag	UNP Q39QF5
D	391	LYS	-	expression tag	UNP Q39QF5
D	392	PRO	-	expression tag	UNP Q39QF5
D	393	ILE	-	expression tag	UNP Q39QF5
D	394	PRO	-	expression tag	UNP Q39QF5
D	395	ASN	-	expression tag	UNP Q39QF5
D	396	PRO	-	expression tag	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: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



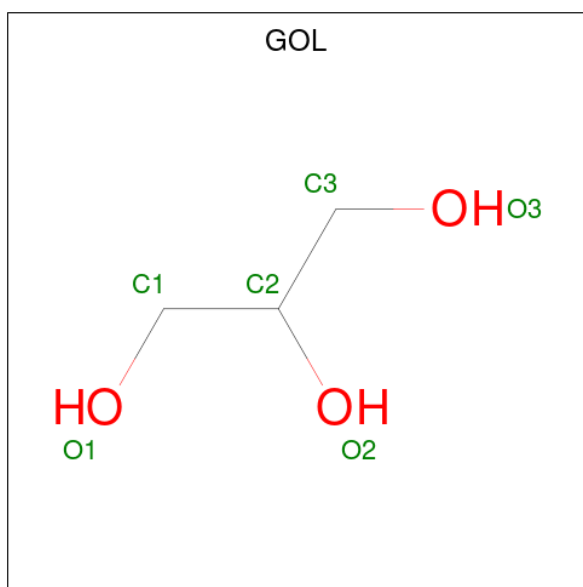
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- 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 56	C 28	N 7	O 17	P 3	S 1	0	0
3	B	1	Total 56	C 28	N 7	O 17	P 3	S 1	0	0
3	C	1	Total 56	C 28	N 7	O 17	P 3	S 1	0	0
3	D	1	Total 56	C 28	N 7	O 17	P 3	S 1	0	0

- 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		

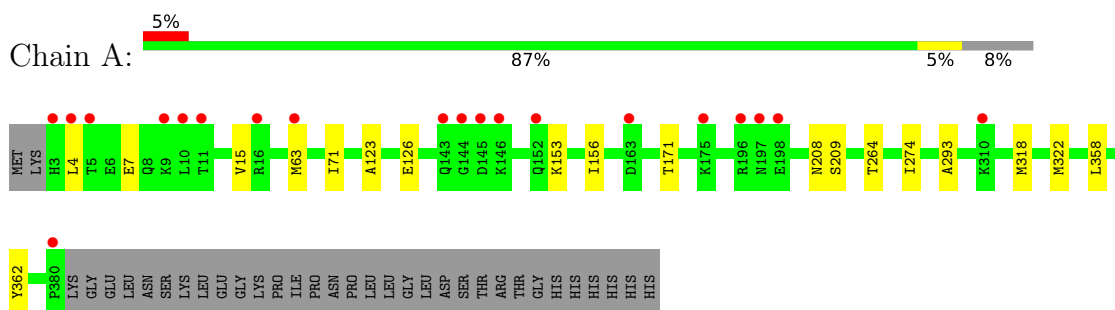
- Molecule 5 is water.

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		

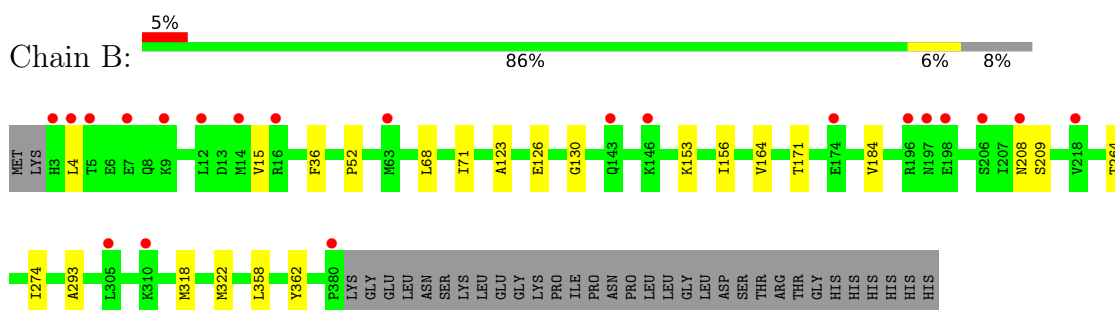
3 Residue-property plots [i](#)

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.

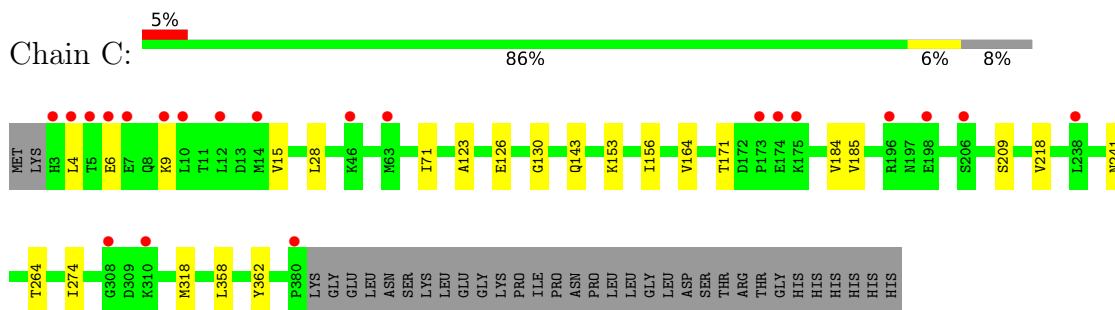
- Molecule 1: Short-chain acyl-CoA dehydrogenase



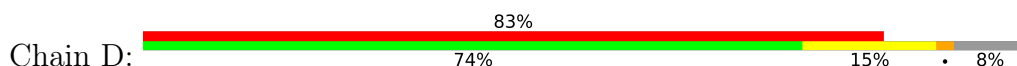
- Molecule 1: Short-chain acyl-CoA dehydrogenase



- Molecule 1: Short-chain acyl-CoA dehydrogenase



- Molecule 1: Short-chain acyl-CoA dehydrogenase



T365	L304	V243	S181	A121	T61
M366	L305	F244	A182	L122	E62
Q367	D306	C245	F183	A123	M63
T368	G307	A246	V184	A124	G64
T369	D308	A247	V185	T125	V65
R370	D309	Q248	E186	E126	L66
M371	K310	A249	K187	P127	T67
V372	K311	V250	G188	A128	L68
T373	A312	G251	T189	A129	A69
G374	V313	I252	P190	G130	L70
R375	L314	A253	G191	S131	T11
A376	Y315	Q254	L192	D132	L72
L377	G316	G255	V193	L133	E73
L378	S317	A256	Y194	L134	E74
F379	M318	L257	G195	A135	L75
P380	A319	D258	R196	M136	G76
LYS	K320	I259	N197	K137	R77
GLY	T321	A260	E198	T138	V78
GLU	M322	V261	S199	R139	C79
LEU	A323	R262	K200	A140	A80
ASN	ASN	A324	M201	L141	R21
SER	D325	H263	G202	R142	E22
LYS	T326	T264	M203	Q143	T23
LEU	A327	R267	R204	G144	L84
GLU	M328	V268	G205	D145	L85
GLY	R329	Q269	S206	K146	L86
LYS	V330	F270	I207	V147	I87
PRO	T331	Q271	N208	V148	A27
ILE	T332	K272	S209	I149	L28
PRO	D333	P273	E210	N150	Q89
ASN	A334	I274	L211	G151	T90
PRO	V335	A275	F212	Q152	D91
LEU	Q336	H276	F213	K153	E92
LEU	V337	L277		C154	M93
GLY	L338	A278	E217	F155	L94
LEU	G339	P279	V218	I156	S34
ASP	G340	V280	P219	I157	L35
SER	Q341	Q281	A220	N158	F36
THR	G342	F282	E221	G159	P37
ARG	Y343	M283	N222	S160	E38
THR	M344	V284	I223	V161	Y39
GLY	K345	A285	I224	A162	A40
HIS	E346	D286	G225	D163	R41
HIS	N347	N287	A226	V164	D42
HIS	G348	A288	E227	I165	L43
HIS	V349	T289	G228	V166	F44
HIS	E350	A290	T229	V167	A45
HIS	R351	V291	G230	V168	K46
HIS	M352	E292	F231	A169	L47
HIS	G353	A293	A232	Y170	R107
	A356	R294	N233	T171	Y108
	K357	R295	L234	D172	L109
	L358	L296	P173	L53	L49
	T359	L297	E174	G114	L50
	Q360	T298	K175	E115	N51
	I361	R299	L238	S116	P52
	Y362	K300	S239	A56	L54
	T363	A301	T240	K178	P55
	G364	A302	N241	G179	A57
		E303	R242	I180	Y58
				T120	L118
					L119
					T120

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

All (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
1	D	196	ARG	CB-CA-C	-6.42	98.53	109.51
1	D	236	GLN	CB-CA-C	6.35	121.64	110.85
1	C	209	SER	N-CA-C	6.06	119.81	110.06
1	D	377	LEU	CA-C-N	-6.02	112.61	122.54
1	D	377	LEU	C-N-CA	-6.02	112.61	122.54
1	B	209	SER	N-CA-C	5.84	119.23	109.95
1	B	171	THR	N-CA-C	-5.80	106.36	113.50
1	A	209	SER	N-CA-C	5.79	119.50	110.17
1	D	171	THR	N-CA-C	-5.73	106.45	113.50
1	A	171	THR	N-CA-C	-5.72	106.46	113.50
1	D	38	GLU	CB-CA-C	5.68	120.23	110.79
1	C	171	THR	N-CA-C	-5.53	106.70	113.50
1	D	209	SER	N-CA-C	5.47	118.98	110.17
1	A	208	ASN	CA-CB-CG	-5.46	107.14	112.60
1	B	36	PHE	N-CA-C	-5.22	103.20	109.83

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:D:338:LEU:HD22	1:D:347[B]:ASN:HD21	1.44	0.82
1:D:136:MET:HG2	5:D:609:HOH:O	1.82	0.80
1:D:70:LEU:HD23	1:D:299:ARG:CZ	2.13	0.78
1:D:272:LYS:HD2	1:D:276:HIS:CD2	2.19	0.76
1:C:6:GLU:OE1	1:C:9:LYS:NZ	2.14	0.76
1:D:4:LEU:HD21	1:D:9:LYS:HD2	1.67	0.75
1:D:338:LEU:CD2	1:D:347[B]:ASN:HD21	1.99	0.75
1:D:122:LEU:HD13	5:D:601:HOH:O	1.87	0.75
1:D:272:LYS:HD2	1:D:276:HIS:HD2	1.54	0.73
1:D:269:GLN:HB2	1:D:274:ILE:HD11	1.70	0.73
1:D:4:LEU:HD11	1:D:9:LYS:N	2.04	0.72
1:D:138:THR:HG22	1:D:151:GLY:HA3	1.71	0.72
1:A:63:MET:HG2	5:A:765:HOH:O	1.90	0.71
1:D:4:LEU:CD2	1:D:9:LYS:HE2	2.22	0.70
1:D:4:LEU:HD11	1:D:9:LYS:HB2	1.74	0.70
1:D:343:TYR:CB	5:D:616:HOH:O	2.42	0.68
1:D:107:ARG:HD3	1:D:108:TYR:CE2	2.29	0.68
1:D:31:ASP:HB2	1:D:351[B]:ARG:CZ	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:LEU:CD2	1:D:9:LYS:CE	2.72	0.67
1:D:70:LEU:HD23	1:D:299:ARG:NH2	2.10	0.67
1:D:31:ASP:HB2	1:D:351[B]:ARG:NE	2.09	0.67
1:D:4:LEU:HD21	1:D:9:LYS:CE	2.25	0.66
1:B:208:ASN:HD22	2:B:501:FAD:HM72	1.61	0.65
1:D:4:LEU:HD21	1:D:9:LYS:HB2	1.80	0.64
1:D:343:TYR:HB3	5:D:616:HOH:O	1.96	0.62
1:D:180:ILE:HD11	5:D:609:HOH:O	2.01	0.61
1:D:70:LEU:CD2	1:D:299:ARG:CZ	2.79	0.60
1:D:4:LEU:HD11	1:D:9:LYS:CA	2.32	0.58
1:D:371:MET:O	1:D:375:ARG:HG2	2.03	0.58
1:D:36:PHE:HD2	1:D:38:GLU:CD	2.12	0.58
1:D:274:ILE:HG13	1:D:277:LEU:HD12	1.86	0.57
1:D:70:LEU:CD2	1:D:299:ARG:NH1	2.68	0.57
1:D:3:HIS:CD2	1:D:3:HIS:N	2.72	0.57
1:D:276:HIS:CE1	1:D:277:LEU:CD2	2.87	0.57
1:D:107:ARG:NH2	1:D:221:GLU:HG3	2.19	0.56
1:D:66:LEU:HG	1:D:70:LEU:HD11	1.87	0.56
1:D:343:TYR:HB2	5:D:616:HOH:O	2.06	0.55
1:D:286:ASP:HB3	5:D:665:HOH:O	2.06	0.55
1:D:4:LEU:HD21	1:D:9:LYS:CG	2.36	0.55
1:D:347[B]:ASN:ND2	1:D:349:VAL:HG22	2.22	0.54
1:C:358:LEU:HD21	2:C:501:FAD:HM73	1.88	0.54
1:D:4:LEU:HD11	1:D:9:LYS:CB	2.38	0.54
1:D:138:THR:HG21	1:D:153:LYS:HE2	1.88	0.54
1:D:30:LEU:HD12	1:D:35:LEU:HD12	1.88	0.53
1:A:293:ALA:HB1	1:B:293:ALA:HB1	1.90	0.53
1:D:6:GLU:OE1	1:D:9:LYS:HD2	2.10	0.52
1:D:24:ALA:HB2	1:D:78:VAL:CG1	2.40	0.52
1:D:36:PHE:CD2	1:D:38:GLU:CD	2.88	0.52
1:D:274:ILE:HG13	1:D:277:LEU:CD1	2.40	0.52
1:D:276:HIS:CE1	1:D:277:LEU:HG	2.45	0.52
1:D:276:HIS:CE1	1:D:277:LEU:HD21	2.45	0.51
1:D:276:HIS:ND1	1:D:277:LEU:HG	2.25	0.51
1:A:358:LEU:HD21	2:A:501:FAD:HM73	1.92	0.51
1:C:126:GLU:HG2	1:C:153:LYS:HD3	1.93	0.51
1:D:293:ALA:HB2	5:D:610:HOH:O	2.09	0.51
1:D:338:LEU:CD2	1:D:347[B]:ASN:ND2	2.72	0.51
1:D:24:ALA:HB2	1:D:78:VAL:HG11	1.92	0.51
1:D:39:TYR:OH	1:D:43:LEU:HD22	2.11	0.50
1:D:351[B]:ARG:CZ	5:D:640:HOH:O	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:VAL:HG22	1:C:218:VAL:HG11	1.95	0.49
1:D:36:PHE:HD2	1:D:38:GLU:CG	2.25	0.49
1:D:126:GLU:HG2	1:D:153:LYS:HD3	1.93	0.49
1:D:4:LEU:HD21	1:D:9:LYS:HE2	1.90	0.49
1:B:126:GLU:HG2	1:B:153:LYS:HD3	1.95	0.49
1:D:4:LEU:HD21	1:D:9:LYS:CB	2.43	0.49
1:D:36:PHE:HD2	1:D:38:GLU:HG2	1.77	0.48
1:D:66:LEU:O	1:D:70:LEU:HD12	2.13	0.48
1:B:358:LEU:HD21	2:B:501:FAD:HM73	1.95	0.48
1:A:126:GLU:HG2	1:A:153:LYS:HD3	1.94	0.47
1:D:342:GLY:HA2	1:D:347[B]:ASN:ND2	2.29	0.47
1:D:107:ARG:CD	1:D:108:TYR:CE2	2.98	0.47
1:A:123:ALA:HB1	1:A:153:LYS:HG3	1.97	0.46
1:D:269:GLN:CB	1:D:274:ILE:HD12	2.35	0.46
1:C:143:GLN:HG2	5:C:724:HOH:O	2.16	0.45
1:A:123:ALA:HA	1:A:156:ILE:HD12	1.99	0.45
1:D:123:ALA:HB1	1:D:153:LYS:HG3	1.98	0.45
1:D:123:ALA:HA	1:D:156:ILE:HD12	1.98	0.45
1:D:185:VAL:HG22	1:D:218:VAL:HG11	1.99	0.45
1:C:164:VAL:HG13	1:C:184:VAL:HG13	1.99	0.44
1:D:15:VAL:HG21	1:D:71:ILE:HG12	1.98	0.44
1:D:269:GLN:CB	1:D:274:ILE:CD1	2.82	0.44
1:D:164:VAL:HG13	1:D:184:VAL:HG13	2.00	0.44
1:D:52:PRO:HG2	1:D:68:LEU:HD13	2.00	0.44
1:D:300:LYS:O	1:D:303:GLU:HG2	2.18	0.44
1:C:123:ALA:HA	1:C:156:ILE:HD12	2.00	0.43
1:B:15:VAL:HG21	1:B:71:ILE:HG12	2.00	0.43
1:C:15:VAL:HG21	1:C:71:ILE:HG12	2.00	0.43
1:D:12:LEU:O	1:D:16:ARG:HG3	2.19	0.43
1:A:264:THR:HA	1:A:274:ILE:HG13	2.01	0.43
1:B:52:PRO:HG2	1:B:68:LEU:HD13	2.01	0.42
1:C:264:THR:HA	1:C:274:ILE:HG13	2.01	0.42
1:D:257:LEU:CD2	4:D:504:GOL:H11	2.49	0.42
1:D:3:HIS:HB2	1:D:4:LEU:H	1.43	0.42
1:D:4:LEU:CD2	1:D:9:LYS:HD2	2.41	0.42
1:D:39:TYR:CZ	1:D:43:LEU:HD22	2.53	0.42
1:D:22:GLU:HG3	1:D:39:TYR:OH	2.20	0.42
1:B:123:ALA:HA	1:B:156:ILE:HD12	2.01	0.42
1:C:123:ALA:HB1	1:C:153:LYS:HG3	2.02	0.42
1:B:123:ALA:HB1	1:B:153:LYS:HG3	2.02	0.42
1:D:22:GLU:CG	1:D:39:TYR:OH	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:VAL:HG21	1:A:71:ILE:HG12	2.02	0.42
1:D:372:VAL:HG21	5:D:622:HOH:O	2.20	0.42
1:D:272:LYS:HB2	1:D:276:HIS:CD2	2.55	0.42
1:D:17:ASP:OD1	1:D:21:ARG:HD2	2.20	0.41
1:A:322[A]:MET:HE1	1:B:322[A]:MET:HE1	2.03	0.41
1:D:264:THR:HA	1:D:274:ILE:HG22	2.02	0.41
1:D:29:GLU:HG3	1:D:29:GLU:H	1.71	0.41
1:B:130:GLY:HA3	2:B:501:FAD:O2P	2.21	0.40
1:B:264:THR:HA	1:B:274:ILE:HG13	2.03	0.40
1:C:130:GLY:HA3	2:C:501:FAD:O2P	2.21	0.40
1:D:244:PHE:CE2	5:D:602:HOH:O	2.74	0.40
1:D:338:LEU:HD23	1:D:347[B]:ASN:ND2	2.36	0.40
1:B:164:VAL:HG13	1:B:184:VAL:HG13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 ⓘ

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

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	7	GLU
1	A	362	TYR
1	B	4	LEU
1	B	362	TYR
1	C	4[A]	LEU
1	C	4[B]	LEU
1	C	28[A]	LEU
1	C	28[B]	LEU
1	C	362	TYR
1	D	3	HIS
1	D	7	GLU
1	D	29	GLU
1	D	35	LEU
1	D	70	LEU
1	D	236	GLN
1	D	274	ILE
1	D	276	HIS
1	D	303	GLU
1	D	310	LYS
1	D	311	LYS
1	D	322	MET
1	D	362	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	HIS
1	A	281	GLN
1	A	367	GLN
1	B	269	GLN
1	B	281	GLN
1	C	263	HIS
1	C	269	GLN
1	C	367	GLN
1	D	3	HIS
1	D	152	GLN
1	D	222	ASN
1	D	236	GLN
1	D	276	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
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

All (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
2	B	501	FAD	C4X-N5	8.71	1.49	1.30
2	C	501	FAD	C4X-N5	8.71	1.49	1.30
2	A	501	FAD	C4X-N5	8.57	1.49	1.30
3	A	502	4KW	P1-O7	5.76	1.65	1.59
3	B	502	4KW	O17-C22	5.33	1.34	1.22
3	D	502	4KW	P1-O7	5.24	1.65	1.59
3	C	502	4KW	O3-C7	5.24	1.51	1.42
3	A	502	4KW	O17-C22	5.21	1.33	1.22
3	B	502	4KW	O3-C7	5.09	1.51	1.42
2	B	501	FAD	C5A-C4A	5.03	1.48	1.39
2	D	501	FAD	C5A-C4A	4.98	1.48	1.39
3	D	502	4KW	O17-C22	4.91	1.33	1.22
3	C	502	4KW	O17-C22	4.82	1.33	1.22
2	C	501	FAD	C5A-C4A	4.81	1.47	1.39
3	D	502	4KW	O3-C7	4.80	1.50	1.42
2	B	501	FAD	O2'-C2'	-4.60	1.33	1.43
3	A	502	4KW	O3-C7	4.58	1.50	1.42
2	C	501	FAD	O2'-C2'	-4.56	1.33	1.43
2	A	501	FAD	C5A-C4A	4.56	1.47	1.39
2	A	501	FAD	O2'-C2'	-4.46	1.34	1.43
2	D	501	FAD	O2'-C2'	-4.44	1.34	1.43
3	B	502	4KW	P1-O7	4.41	1.64	1.59
2	C	501	FAD	C5X-N5	4.39	1.47	1.39
2	B	501	FAD	C5X-N5	4.39	1.47	1.39
3	C	502	4KW	C17-N7	4.31	1.45	1.34
2	A	501	FAD	C5X-N5	4.25	1.47	1.39
3	C	502	4KW	P1-O7	4.11	1.63	1.59
3	D	502	4KW	C17-N7	3.80	1.43	1.34
2	D	501	FAD	O3'-C3'	-3.63	1.34	1.43
3	B	502	4KW	C17-N7	3.61	1.43	1.34
2	A	501	FAD	O3'-C3'	-3.56	1.34	1.43
2	B	501	FAD	O3'-C3'	-3.50	1.34	1.43
2	C	501	FAD	O3'-C3'	-3.45	1.34	1.43
2	D	501	FAD	C10-N1	3.44	1.40	1.33
3	C	502	4KW	C11-C8	3.33	1.58	1.52
3	A	502	4KW	C17-N7	3.27	1.42	1.34
3	D	502	4KW	C6-N2	3.23	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	4KW	C15-N4	3.20	1.37	1.31
3	A	502	4KW	C15-N4	3.17	1.37	1.31
2	C	501	FAD	C10-N1	3.15	1.39	1.33
3	C	502	4KW	C15-N4	3.15	1.37	1.31
3	B	502	4KW	C15-N4	3.14	1.37	1.31
3	A	502	4KW	C11-C8	3.09	1.57	1.52
3	A	502	4KW	C6-N2	3.08	1.40	1.33
3	D	502	4KW	C11-C8	3.05	1.57	1.52
2	D	501	FAD	C5X-N5	3.03	1.45	1.39
3	B	502	4KW	C1-N1	3.02	1.40	1.33
2	A	501	FAD	C10-N1	3.00	1.39	1.33
2	B	501	FAD	C10-N1	2.98	1.39	1.33
3	B	502	4KW	C11-C8	2.88	1.57	1.52
3	C	502	4KW	C6-N2	2.87	1.40	1.33
3	C	502	4KW	C1-N1	2.86	1.40	1.33
3	D	502	4KW	C1-N1	2.78	1.40	1.33
3	A	502	4KW	C1-N1	2.76	1.39	1.33
3	A	502	4KW	C2-N1	2.75	1.52	1.46
2	A	501	FAD	C10-N10	2.73	1.43	1.37
3	D	502	4KW	C2-N1	2.67	1.52	1.46
3	B	502	4KW	C6-N2	2.63	1.39	1.33
2	D	501	FAD	C5A-C6A	2.62	1.48	1.41
2	A	501	FAD	P-O3P	2.56	1.62	1.59
3	C	502	4KW	O1-C1	2.52	1.28	1.23
2	D	501	FAD	C10-N10	2.49	1.42	1.37
3	A	502	4KW	C10-C8	2.42	1.58	1.53
2	B	501	FAD	C10-N10	2.40	1.42	1.37
2	A	501	FAD	C5A-C6A	2.39	1.47	1.41
2	C	501	FAD	C10-N10	2.38	1.42	1.37
2	B	501	FAD	C5A-C6A	2.31	1.47	1.41
3	A	502	4KW	P2-O7	2.31	1.62	1.59
3	B	502	4KW	C10-C8	2.31	1.58	1.53
3	B	502	4KW	O1-C1	2.29	1.27	1.23
2	B	501	FAD	C9-C9A	2.26	1.43	1.39
3	D	502	4KW	O1-C1	2.26	1.27	1.23
3	A	502	4KW	C20-C21	-2.25	1.48	1.53
3	B	502	4KW	P2-O7	2.22	1.61	1.59
2	D	501	FAD	C7M-C7	2.22	1.55	1.51
2	B	501	FAD	C5A-N7A	-2.20	1.35	1.39
2	C	501	FAD	C5A-C6A	2.20	1.47	1.41
2	B	501	FAD	C8A-N7A	2.18	1.35	1.31
3	D	502	4KW	P2-O7	2.18	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FAD	C9-C9A	2.18	1.43	1.39
2	D	501	FAD	PA-O3P	2.17	1.61	1.59
3	D	502	4KW	C10-C8	2.17	1.58	1.53
2	D	501	FAD	C9-C8	2.17	1.42	1.39
3	C	502	4KW	C16-C19	2.14	1.42	1.39
2	D	501	FAD	C9-C9A	2.14	1.43	1.39
3	B	502	4KW	C2-N1	2.14	1.51	1.46
3	C	502	4KW	C2-N1	2.13	1.51	1.46
2	C	501	FAD	C9-C9A	2.13	1.43	1.39
3	C	502	4KW	C5-N2	2.11	1.50	1.46
2	C	501	FAD	P-O3P	2.11	1.61	1.59
2	A	501	FAD	C5A-N7A	-2.10	1.35	1.39
2	C	501	FAD	C5A-N7A	-2.05	1.35	1.39
2	D	501	FAD	C5A-N7A	-2.02	1.35	1.39
2	A	501	FAD	C4A-N9A	-2.01	1.33	1.37
3	B	502	4KW	C16-C19	2.01	1.42	1.39
3	C	502	4KW	C10-C8	2.01	1.57	1.53
3	B	502	4KW	C20-C21	-2.01	1.48	1.53
3	D	502	4KW	C20-C21	-2.00	1.48	1.53

All (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
2	D	501	FAD	C9A-C5X-N5	-7.10	114.92	122.45
3	B	502	4KW	C3-S1-C22	7.03	108.14	99.85
3	A	502	4KW	C3-S1-C22	6.56	107.58	99.85
3	A	502	4KW	C16-C19-N6	-5.52	119.11	126.72
3	D	502	4KW	C16-C19-N6	-5.30	119.42	126.72
3	C	502	4KW	C16-C19-N6	-5.29	119.43	126.72
3	B	502	4KW	C16-C19-N6	-5.29	119.44	126.72
2	C	501	FAD	C5A-C4A-N3A	-5.13	119.65	126.72
2	D	501	FAD	C5A-C4A-N3A	-5.11	119.68	126.72
2	A	501	FAD	C5A-C4A-N3A	-5.10	119.69	126.72
2	D	501	FAD	N3A-C4A-N9A	4.98	135.64	127.17
2	B	501	FAD	C5A-C4A-N3A	-4.97	119.87	126.72
2	D	501	FAD	C10-C4X-N5	-4.96	114.69	124.81
2	C	501	FAD	N3A-C4A-N9A	4.90	135.50	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	N3A-C4A-N9A	4.85	135.42	127.17
2	A	501	FAD	C10-C4X-N5	-4.80	115.02	124.81
2	B	501	FAD	N3A-C4A-N9A	4.79	135.31	127.17
2	C	501	FAD	O3'-C3'-C2'	4.76	119.75	108.93
2	C	501	FAD	C10-C4X-N5	-4.66	115.30	124.81
2	B	501	FAD	C10-C4X-N5	-4.63	115.36	124.81
2	A	501	FAD	O3'-C3'-C2'	4.55	119.28	108.93
2	D	501	FAD	O3'-C3'-C2'	4.53	119.23	108.93
2	B	501	FAD	C6-C5X-N5	-4.46	111.04	118.44
2	B	501	FAD	O3'-C3'-C2'	4.37	118.85	108.93
2	D	501	FAD	O2'-C2'-C3'	4.35	119.43	109.25
3	C	502	4KW	N6-C18-N5	-4.27	122.12	128.58
2	B	501	FAD	N3A-C2A-N1A	-4.25	122.15	128.58
2	C	501	FAD	O2'-C2'-C3'	4.23	119.15	109.25
3	A	502	4KW	N3-C15-N4	-4.17	108.02	113.94
2	A	501	FAD	O2'-C2'-C3'	4.16	118.98	109.25
3	B	502	4KW	N6-C18-N5	-4.15	122.30	128.58
2	A	501	FAD	C4'-C3'-C2'	4.14	120.46	113.57
2	C	501	FAD	C6-C5X-N5	-4.12	111.60	118.44
2	B	501	FAD	C4A-N9A-C8A	4.10	110.04	105.74
2	D	501	FAD	C4'-C3'-C2'	4.07	120.34	113.57
3	D	502	4KW	N3-C15-N4	-4.06	108.18	113.94
2	A	501	FAD	C6-C5X-N5	-4.04	111.74	118.44
2	A	501	FAD	N3A-C2A-N1A	-4.04	122.47	128.58
2	B	501	FAD	O2'-C2'-C3'	4.01	118.63	109.25
2	A	501	FAD	C4A-N9A-C8A	4.00	109.93	105.74
2	C	501	FAD	C4'-C3'-C2'	3.97	120.18	113.57
2	D	501	FAD	C4A-N9A-C8A	3.97	109.91	105.74
2	C	501	FAD	C4A-N9A-C8A	3.96	109.90	105.74
3	B	502	4KW	N3-C15-N4	-3.96	108.32	113.94
2	B	501	FAD	C4'-C3'-C2'	3.94	120.13	113.57
2	D	501	FAD	N3A-C2A-N1A	-3.94	122.62	128.58
3	D	502	4KW	N6-C18-N5	-3.91	122.66	128.58
3	A	502	4KW	N6-C19-N3	3.91	133.82	127.17
2	A	501	FAD	C9A-N10-C10	-3.82	114.93	120.75
3	D	502	4KW	C19-N3-C15	3.81	109.73	105.74
3	B	502	4KW	C19-C16-N4	-3.79	106.24	110.58
2	C	501	FAD	N3A-C2A-N1A	-3.78	122.85	128.58
3	D	502	4KW	N6-C19-N3	3.76	133.56	127.17
3	D	502	4KW	C19-C16-N4	-3.74	106.30	110.58
3	C	502	4KW	C3-C2-N1	-3.74	104.61	112.41
3	A	502	4KW	C19-N3-C15	3.72	109.65	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	4KW	N6-C19-N3	3.69	133.44	127.17
3	B	502	4KW	N6-C19-N3	3.67	133.41	127.17
3	A	502	4KW	C3-C2-N1	-3.63	104.83	112.41
3	A	502	4KW	C19-C16-N4	-3.62	106.44	110.58
3	B	502	4KW	C18-N6-C19	3.56	120.52	111.83
3	C	502	4KW	C18-N6-C19	3.55	120.51	111.83
3	A	502	4KW	N6-C18-N5	-3.55	123.21	128.58
3	B	502	4KW	C19-N3-C15	3.54	109.45	105.74
2	A	501	FAD	C2A-N3A-C4A	3.51	120.40	111.83
2	D	501	FAD	C8M-C8-C9	-3.50	113.40	119.57
3	A	502	4KW	O2-C6-C7	-3.49	111.16	120.89
2	D	501	FAD	C9A-N10-C10	-3.48	115.44	120.75
2	D	501	FAD	C2A-N3A-C4A	3.48	120.33	111.83
3	C	502	4KW	C19-C16-N4	-3.47	106.61	110.58
3	B	502	4KW	O2-C6-N2	3.46	130.31	122.98
2	B	501	FAD	C9A-N10-C10	-3.46	115.47	120.75
3	B	502	4KW	O2-C6-C7	-3.45	111.26	120.89
3	A	502	4KW	C18-N6-C19	3.44	120.23	111.83
2	B	501	FAD	C2A-N3A-C4A	3.44	120.23	111.83
3	D	502	4KW	C3-C2-N1	-3.43	105.25	112.41
3	B	502	4KW	C3-C2-N1	-3.43	105.26	112.41
3	A	502	4KW	C16-N4-C15	3.42	108.82	103.45
3	D	502	4KW	O2-C6-C7	-3.42	111.36	120.89
3	B	502	4KW	C16-N4-C15	3.41	108.81	103.45
3	D	502	4KW	C16-N4-C15	3.38	108.76	103.45
3	D	502	4KW	C18-N6-C19	3.38	120.08	111.83
2	C	501	FAD	C2A-N3A-C4A	3.38	120.08	111.83
2	B	501	FAD	C8M-C8-C9	-3.36	113.66	119.57
2	C	501	FAD	C9A-N10-C10	-3.34	115.66	120.75
2	B	501	FAD	O3'-C3'-C4'	3.34	116.51	108.93
3	C	502	4KW	C9-C8-C11	3.31	113.69	108.22
3	C	502	4KW	N3-C15-N4	-3.30	109.25	113.94
2	D	501	FAD	O3'-C3'-C4'	3.28	116.37	108.93
3	C	502	4KW	O2-C6-C7	-3.25	111.82	120.89
3	A	502	4KW	O2-C6-N2	3.24	129.84	122.98
2	B	501	FAD	C4X-C10-N1	-3.22	116.69	124.59
2	C	501	FAD	O3'-C3'-C4'	3.19	116.17	108.93
3	C	502	4KW	C24-C23-C25	3.18	119.08	112.27
3	D	502	4KW	C9-C8-C11	3.15	113.43	108.22
2	A	501	FAD	O3'-C3'-C4'	3.15	116.08	108.93
3	D	502	4KW	O2-C6-N2	3.15	129.64	122.98
2	D	501	FAD	C4X-C10-N1	-3.14	116.89	124.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	4KW	C24-C23-C25	3.10	118.92	112.27
2	A	501	FAD	C8M-C8-C9	-3.09	114.13	119.57
3	B	502	4KW	C24-C23-C25	3.08	118.88	112.27
2	A	501	FAD	C4X-C10-N1	-3.08	117.04	124.59
2	A	501	FAD	C1'-C2'-C3'	3.04	117.89	109.66
3	A	502	4KW	C24-C23-C25	3.03	118.77	112.27
3	C	502	4KW	C19-N3-C15	3.03	108.92	105.74
3	C	502	4KW	O4-C11-C8	-3.02	105.69	110.55
3	C	502	4KW	O2-C6-N2	2.98	129.29	122.98
3	B	502	4KW	C10-C8-C11	2.97	113.13	108.22
2	C	501	FAD	C8M-C8-C9	-2.95	114.38	119.57
3	D	502	4KW	C10-C8-C11	2.94	113.08	108.22
3	C	502	4KW	O5-P1-O7	-2.94	99.33	107.27
3	C	502	4KW	C16-N4-C15	2.93	108.06	103.45
2	D	501	FAD	C1'-C2'-C3'	2.92	117.57	109.66
2	B	501	FAD	C2A-N1A-C6A	2.91	123.51	118.73
2	B	501	FAD	C1'-C2'-C3'	2.91	117.54	109.66
2	C	501	FAD	C4X-C10-N1	-2.90	117.48	124.59
2	C	501	FAD	C1'-C2'-C3'	2.88	117.47	109.66
3	A	502	4KW	O4-C11-C8	-2.87	105.94	110.55
3	A	502	4KW	C9-C8-C11	2.84	112.90	108.22
3	B	502	4KW	O4-C11-C8	-2.77	106.09	110.55
3	B	502	4KW	O5-P1-O7	-2.73	99.89	107.27
3	D	502	4KW	O5-P1-O7	-2.71	99.94	107.27
3	A	502	4KW	O5-P1-O7	-2.68	100.03	107.27
2	D	501	FAD	C6-C5X-N5	-2.66	114.03	118.44
2	C	501	FAD	C6-C5X-C9A	-2.66	115.40	119.05
2	B	501	FAD	N9A-C8A-N7A	-2.64	110.18	113.94
2	A	501	FAD	C4A-C5A-N7A	-2.63	107.57	110.58
2	D	501	FAD	O4-C4-C4X	-2.60	119.68	126.53
2	A	501	FAD	C2A-N1A-C6A	2.57	122.95	118.73
2	B	501	FAD	C6-C5X-C9A	-2.56	115.53	119.05
3	D	502	4KW	O4-C11-C8	-2.55	106.44	110.55
3	B	502	4KW	O8-P2-O7	2.55	114.17	107.27
3	C	502	4KW	C23-C25-C27	-2.55	115.94	123.14
2	C	501	FAD	O2A-PA-O1A	2.54	124.28	112.44
2	B	501	FAD	C4A-C5A-N7A	-2.52	107.70	110.58
2	A	501	FAD	C5A-N7A-C8A	2.49	107.36	103.45
2	D	501	FAD	N9A-C8A-N7A	-2.49	110.41	113.94
3	A	502	4KW	C26-C28-C27	2.49	117.21	112.14
2	B	501	FAD	C5A-N7A-C8A	2.48	107.35	103.45
3	A	502	4KW	C10-C8-C11	2.48	112.32	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	N9A-C8A-N7A	-2.47	110.43	113.94
3	B	502	4KW	C2-N1-C1	-2.47	118.23	122.82
2	A	501	FAD	C4X-C10-N10	2.46	120.00	116.48
3	A	502	4KW	C2-N1-C1	-2.45	118.26	122.82
2	D	501	FAD	C9-C9A-N10	-2.44	118.58	121.85
3	C	502	4KW	C10-C8-C11	2.43	112.24	108.22
2	A	501	FAD	C6-C5X-C9A	-2.43	115.71	119.05
2	C	501	FAD	N9A-C8A-N7A	-2.43	110.49	113.94
2	D	501	FAD	C5A-N7A-C8A	2.42	107.25	103.45
3	C	502	4KW	O8-P2-O7	2.39	113.75	107.27
2	D	501	FAD	C2A-N1A-C6A	2.38	122.65	118.73
2	B	501	FAD	C10-N1-C2	2.38	122.00	116.85
3	C	502	4KW	C2-N1-C1	-2.38	118.39	122.82
3	C	502	4KW	C9-C8-C7	2.37	112.81	108.77
3	A	502	4KW	O8-P2-O7	2.37	113.68	107.27
2	B	501	FAD	C8M-C8-C7	2.37	125.60	120.76
2	D	501	FAD	C4A-C5A-N7A	-2.36	107.88	110.58
2	C	501	FAD	C2A-N1A-C6A	2.36	122.60	118.73
3	B	502	4KW	C26-C24-C23	-2.35	100.37	113.13
3	D	502	4KW	O5-P1-O4	2.35	118.22	107.57
2	C	501	FAD	C5A-N7A-C8A	2.34	107.13	103.45
2	C	501	FAD	C4A-C5A-N7A	-2.34	107.91	110.58
3	C	502	4KW	C26-C24-C23	-2.33	100.49	113.13
2	B	501	FAD	O4-C4-C4X	-2.31	120.42	126.53
3	D	502	4KW	O8-P2-O7	2.31	113.52	107.27
3	D	502	4KW	C26-C28-C27	2.28	116.79	112.14
2	D	501	FAD	C4-N3-C2	-2.27	121.60	125.64
2	C	501	FAD	C4X-C10-N10	2.27	119.73	116.48
3	D	502	4KW	C23-C25-C27	-2.27	116.73	123.14
2	A	501	FAD	O4-C4-C4X	-2.26	120.57	126.53
2	A	501	FAD	C9-C9A-N10	-2.24	118.83	121.85
3	B	502	4KW	C23-C25-C27	-2.24	116.83	123.14
3	A	502	4KW	C23-C25-C27	-2.22	116.86	123.14
2	C	501	FAD	O4-C4-C4X	-2.22	120.67	126.53
2	D	501	FAD	C4X-C10-N10	2.22	119.66	116.48
2	A	501	FAD	C10-N1-C2	2.22	121.65	116.85
3	A	502	4KW	O10-P2-O9	2.21	117.69	108.94
2	B	501	FAD	C4-N3-C2	-2.21	121.72	125.64
2	B	501	FAD	C4X-C10-N10	2.18	119.60	116.48
3	D	502	4KW	C26-C24-C23	-2.17	101.36	113.13
2	C	501	FAD	C8M-C8-C7	2.17	125.19	120.76
3	A	502	4KW	C26-C24-C23	-2.15	101.46	113.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	FAD	C10-N1-C2	2.15	121.50	116.85
2	C	501	FAD	C10-N1-C2	2.15	121.50	116.85
3	D	502	4KW	C2-N1-C1	-2.12	118.87	122.82
2	A	501	FAD	O2A-PA-O1A	2.12	122.31	112.44
3	C	502	4KW	C26-C28-C27	2.11	116.45	112.14
2	B	501	FAD	N6A-C6A-N1A	2.11	123.08	118.38
3	A	502	4KW	O5-P1-O4	2.10	117.07	107.57
2	B	501	FAD	C4X-C4-N3	2.09	118.57	113.25
2	A	501	FAD	C5X-N5-C4X	2.09	121.46	118.09
2	C	501	FAD	C9-C9A-N10	-2.08	119.06	121.85
3	C	502	4KW	O5-P1-O4	2.06	116.90	107.57
2	A	501	FAD	C4-N3-C2	-2.06	121.99	125.64
2	D	501	FAD	N6A-C6A-N1A	2.05	122.94	118.38
2	D	501	FAD	C4X-C4-N3	2.03	118.42	113.25
3	C	502	4KW	C4-C5-N2	-2.03	107.68	112.00
3	A	502	4KW	P3-O13-C21	-2.02	118.03	123.43
3	B	502	4KW	C9-C8-C11	2.02	111.56	108.22
3	B	502	4KW	P3-O13-C21	-2.02	118.03	123.43
2	B	501	FAD	C9-C9A-N10	-2.02	119.14	121.85
2	C	501	FAD	N6A-C6A-N1A	2.02	122.88	118.38
2	D	501	FAD	O2A-PA-O1A	2.01	121.81	112.44
2	D	501	FAD	C8M-C8-C7	2.00	124.85	120.76

There are no chirality outliers.

All (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'
2	B	501	FAD	C2'-C1'-N10-C10
2	B	501	FAD	N10-C1'-C2'-C3'
2	B	501	FAD	C1'-C2'-C3'-C4'
2	B	501	FAD	O2'-C2'-C3'-C4'
2	B	501	FAD	O3'-C3'-C4'-C5'
2	C	501	FAD	C2'-C1'-N10-C10
2	C	501	FAD	N10-C1'-C2'-C3'
2	C	501	FAD	C1'-C2'-C3'-C4'
2	C	501	FAD	O2'-C2'-C3'-C4'
2	C	501	FAD	O3'-C3'-C4'-C5'

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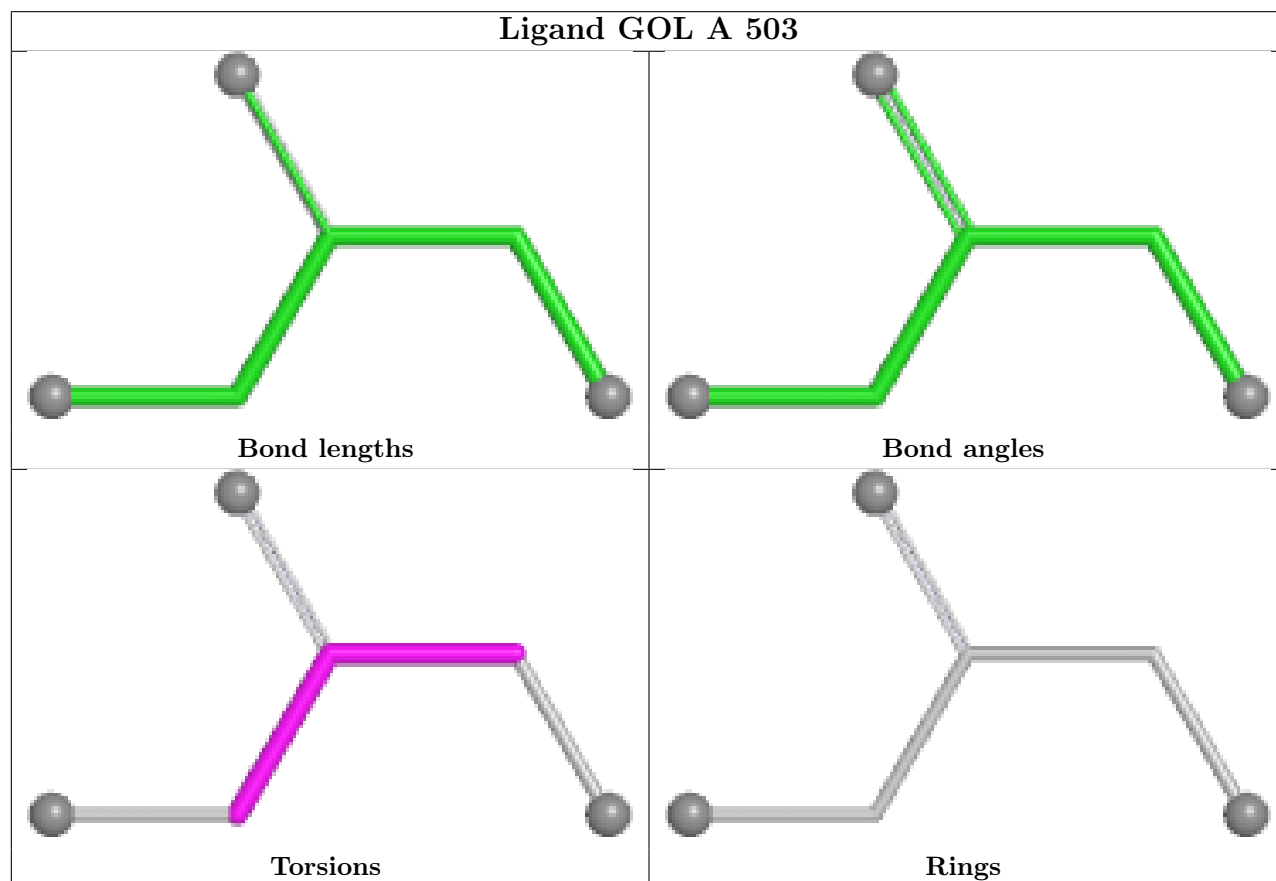
Mol	Chain	Res	Type	Atoms
2	D	501	FAD	C2'-C1'-N10-C10
2	D	501	FAD	N10-C1'-C2'-C3'
2	D	501	FAD	C1'-C2'-C3'-C4'
2	D	501	FAD	O2'-C2'-C3'-C4'
2	D	501	FAD	O3'-C3'-C4'-C5'
3	A	502	4KW	C1-C4-C5-N2
3	A	502	4KW	C27-C22-S1-C3
3	A	502	4KW	O17-C22-C27-C28
3	B	502	4KW	C1-C4-C5-N2
3	B	502	4KW	C27-C22-S1-C3
3	B	502	4KW	O17-C22-C27-C28
3	C	502	4KW	C1-C4-C5-N2
3	C	502	4KW	C27-C22-S1-C3
3	C	502	4KW	O17-C22-C27-C28
3	D	502	4KW	C1-C4-C5-N2
3	D	502	4KW	C27-C22-S1-C3
3	D	502	4KW	O17-C22-C27-C28
4	A	503	GOL	O1-C1-C2-C3
4	B	504	GOL	O1-C1-C2-O2
4	B	504	GOL	O1-C1-C2-C3
2	A	501	FAD	O3'-C3'-C4'-O4'
2	B	501	FAD	O3'-C3'-C4'-O4'
2	C	501	FAD	O3'-C3'-C4'-O4'
2	D	501	FAD	O3'-C3'-C4'-O4'
4	D	503	GOL	O1-C1-C2-C3
4	A	503	GOL	O1-C1-C2-O2
4	D	503	GOL	O1-C1-C2-O2
3	C	502	4KW	O17-C22-C27-C25
3	D	502	4KW	O17-C22-C27-C25
3	D	502	4KW	N2-C6-C7-O3
4	A	503	GOL	O2-C2-C3-O3
3	A	502	4KW	O17-C22-C27-C25
3	B	502	4KW	O17-C22-C27-C25
4	C	504	GOL	O1-C1-C2-C3
3	A	502	4KW	P1-O7-P2-O8
3	C	502	4KW	P1-O7-P2-O8
3	B	502	4KW	P1-O7-P2-O8
3	D	502	4KW	P1-O7-P2-O8
3	A	502	4KW	N2-C6-C7-O3
3	B	502	4KW	N2-C6-C7-O3

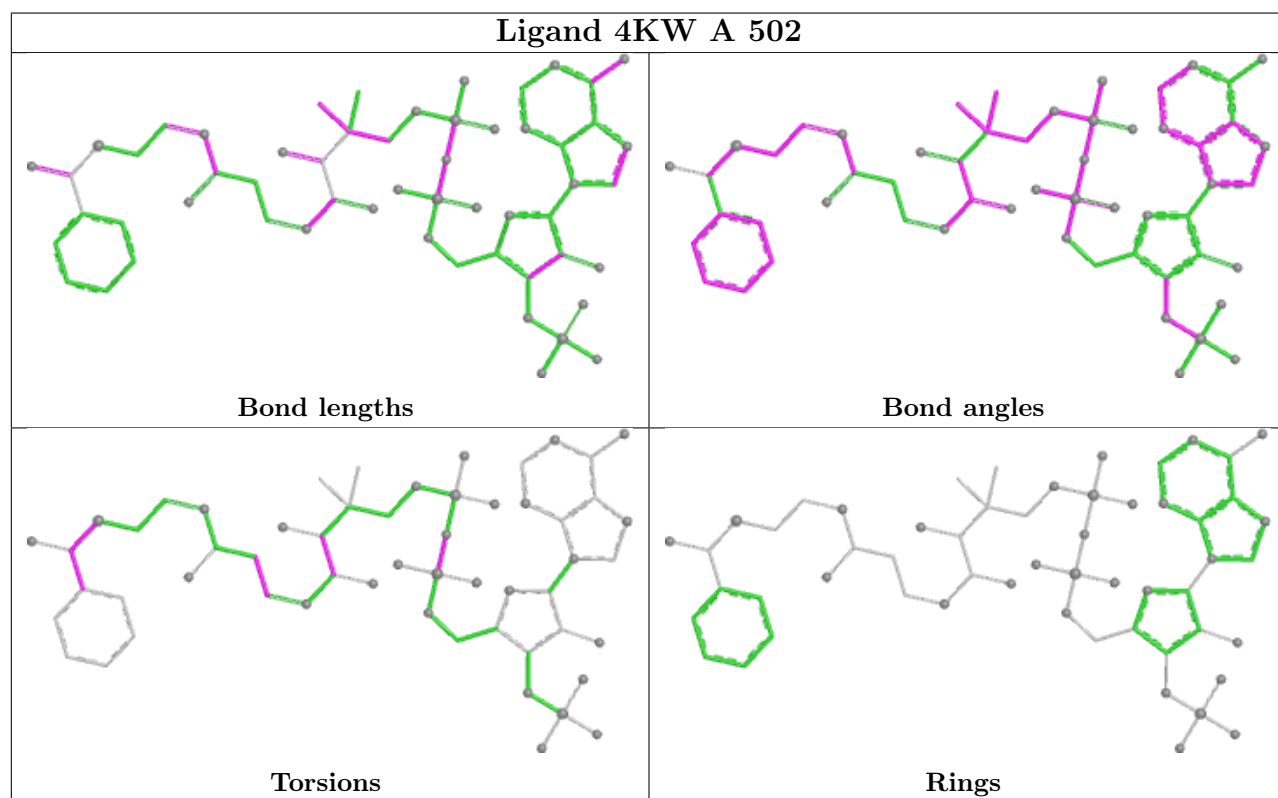
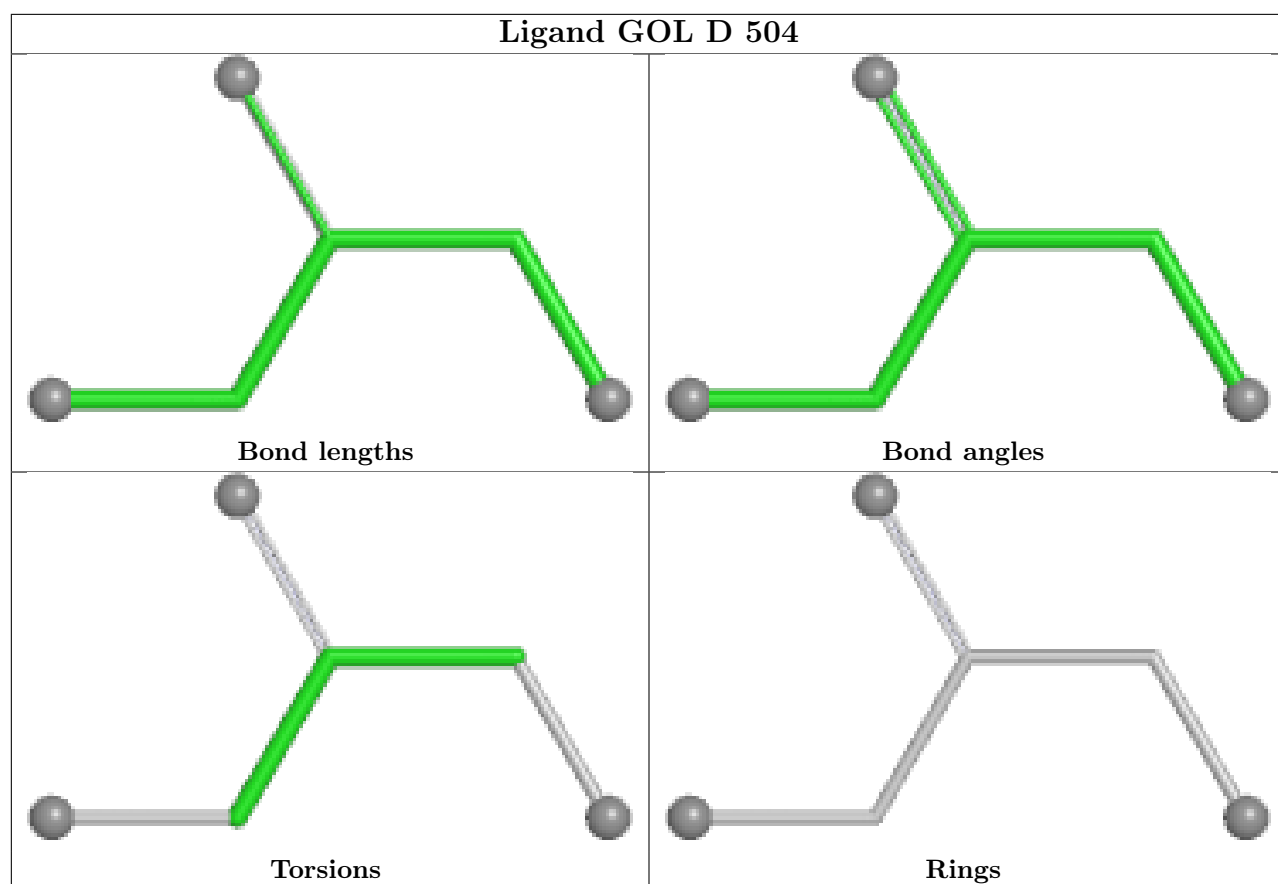
There are no ring outliers.

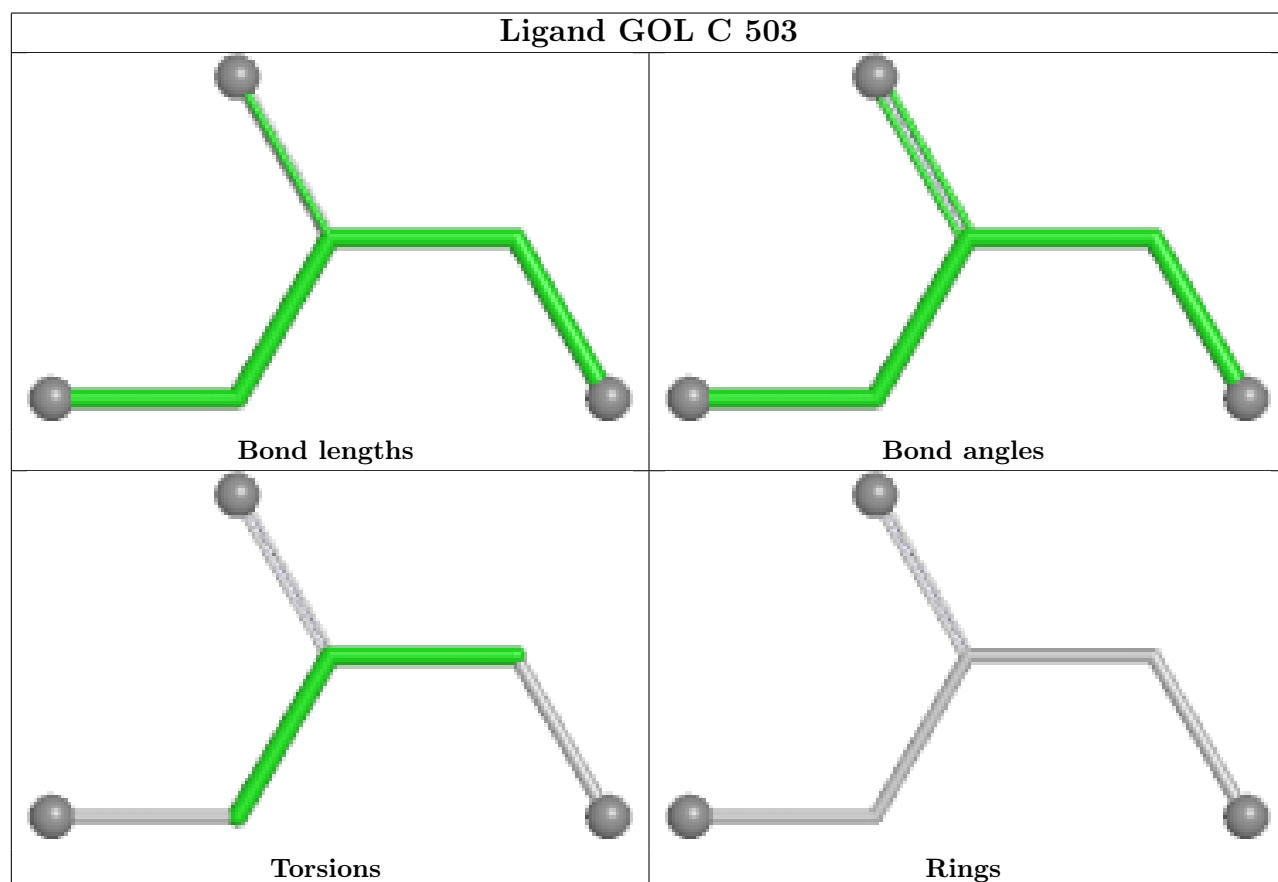
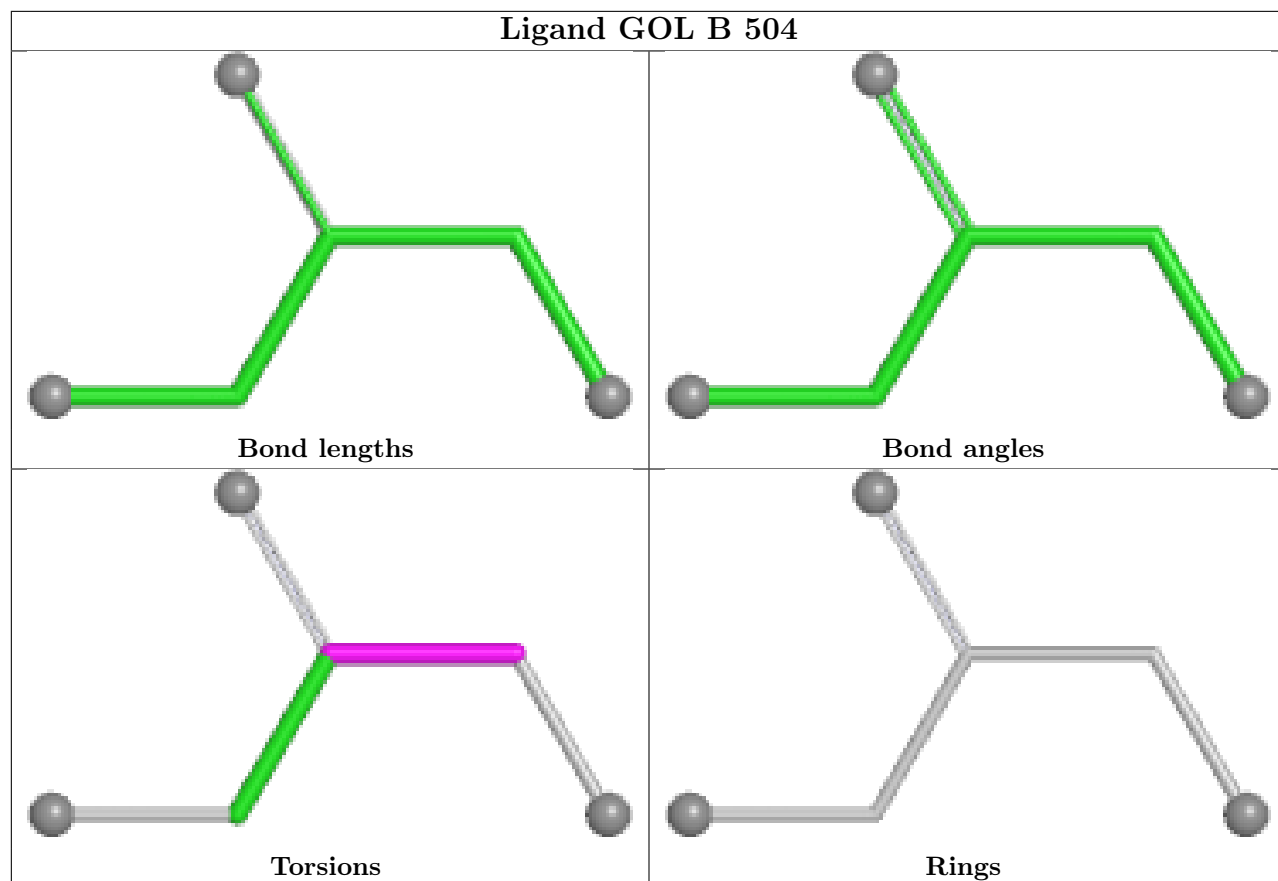
4 monomers are involved in 7 short contacts:

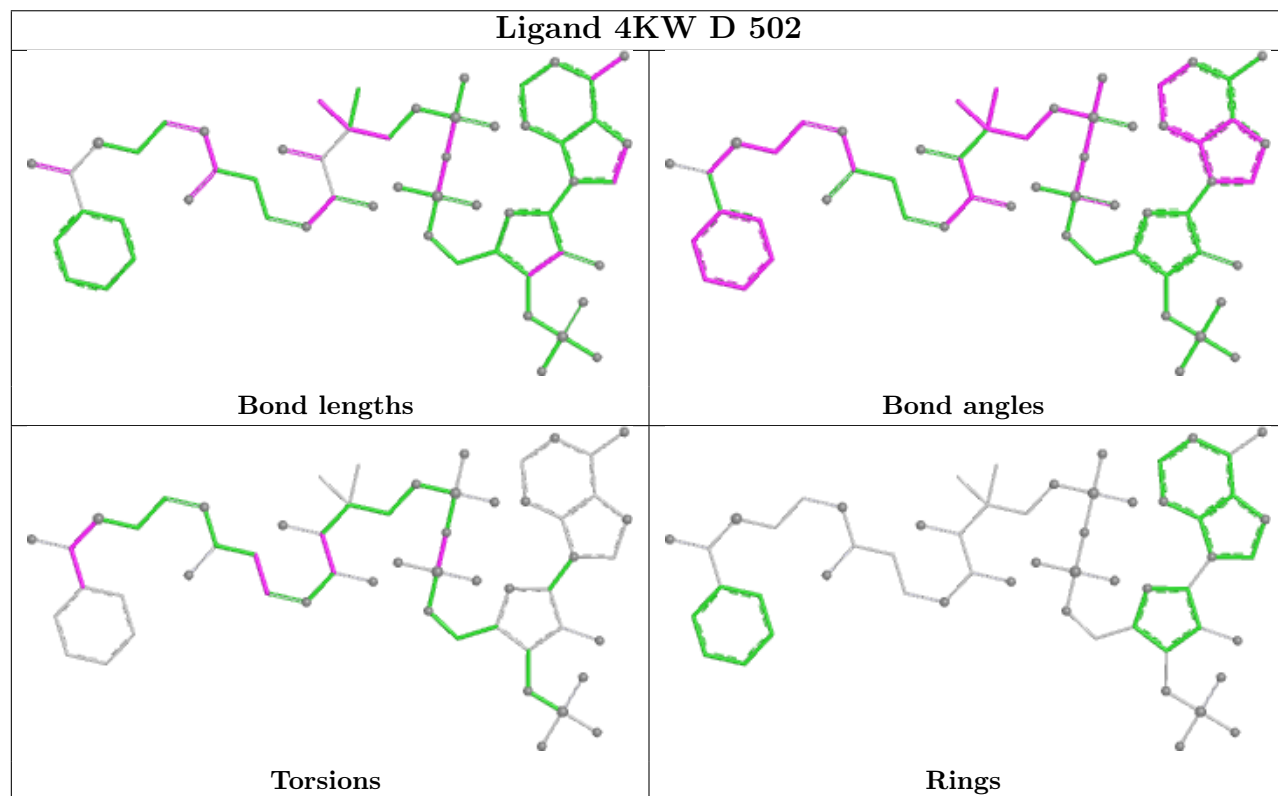
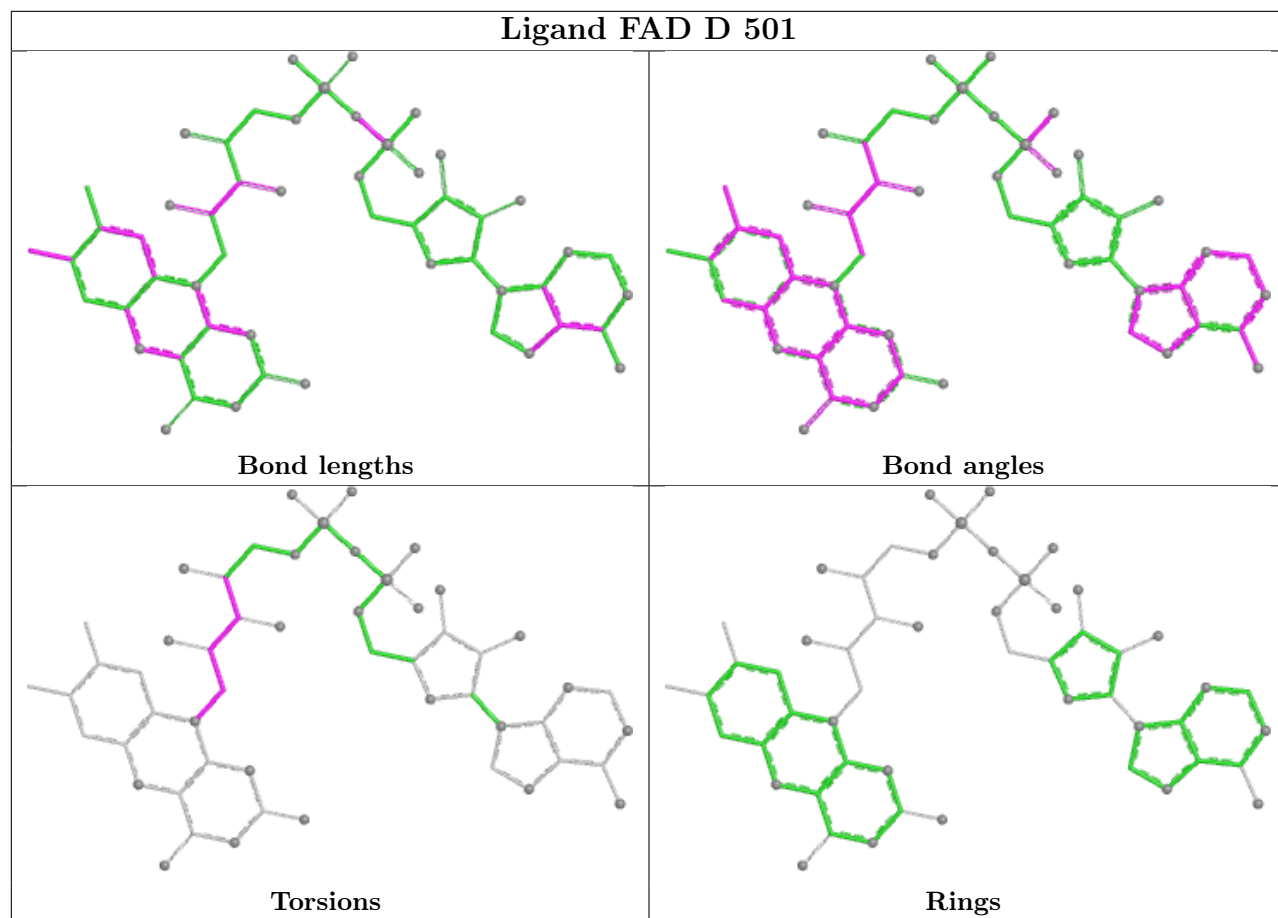
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	504	GOL	1	0
2	B	501	FAD	3	0
2	A	501	FAD	1	0
2	C	501	FAD	2	0

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.

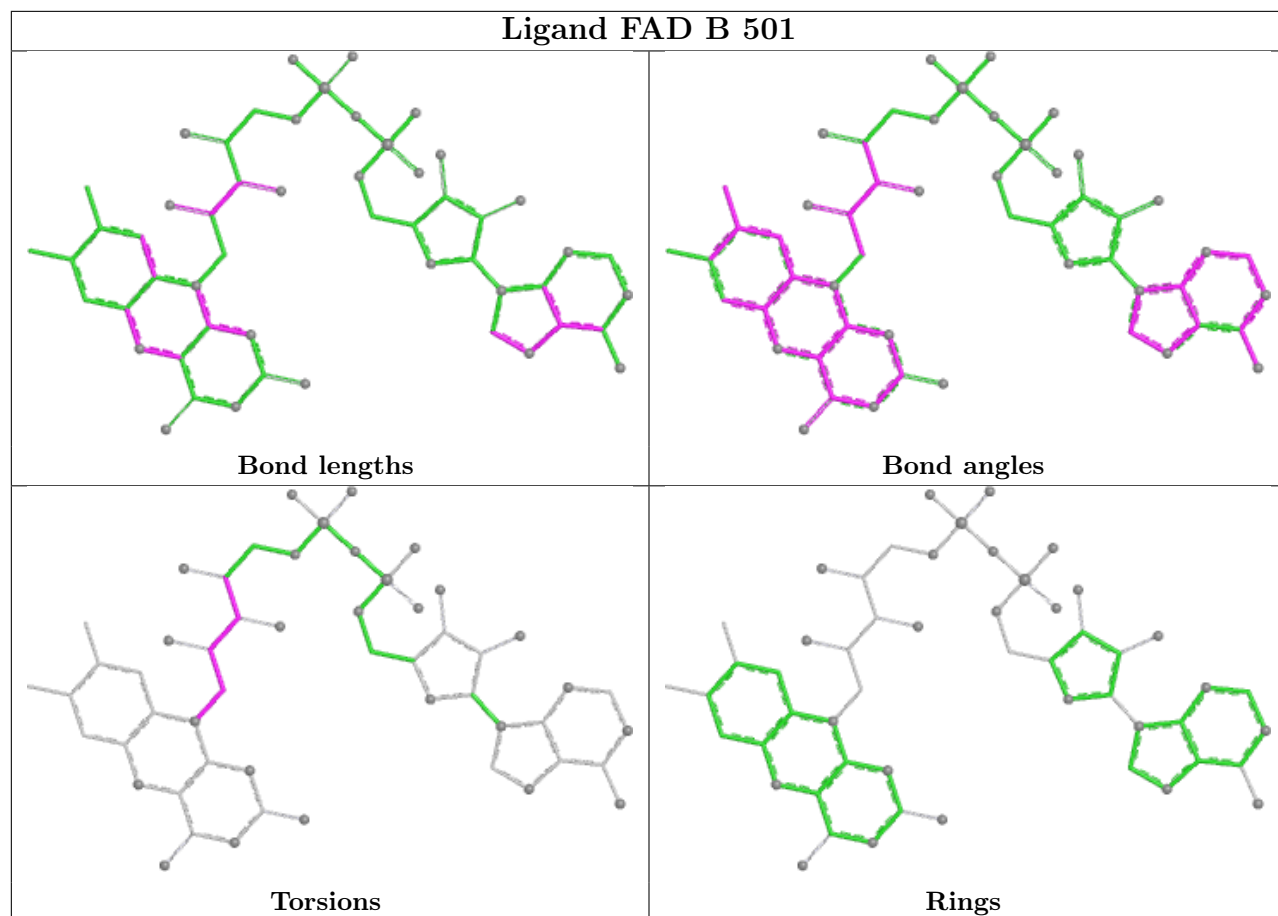




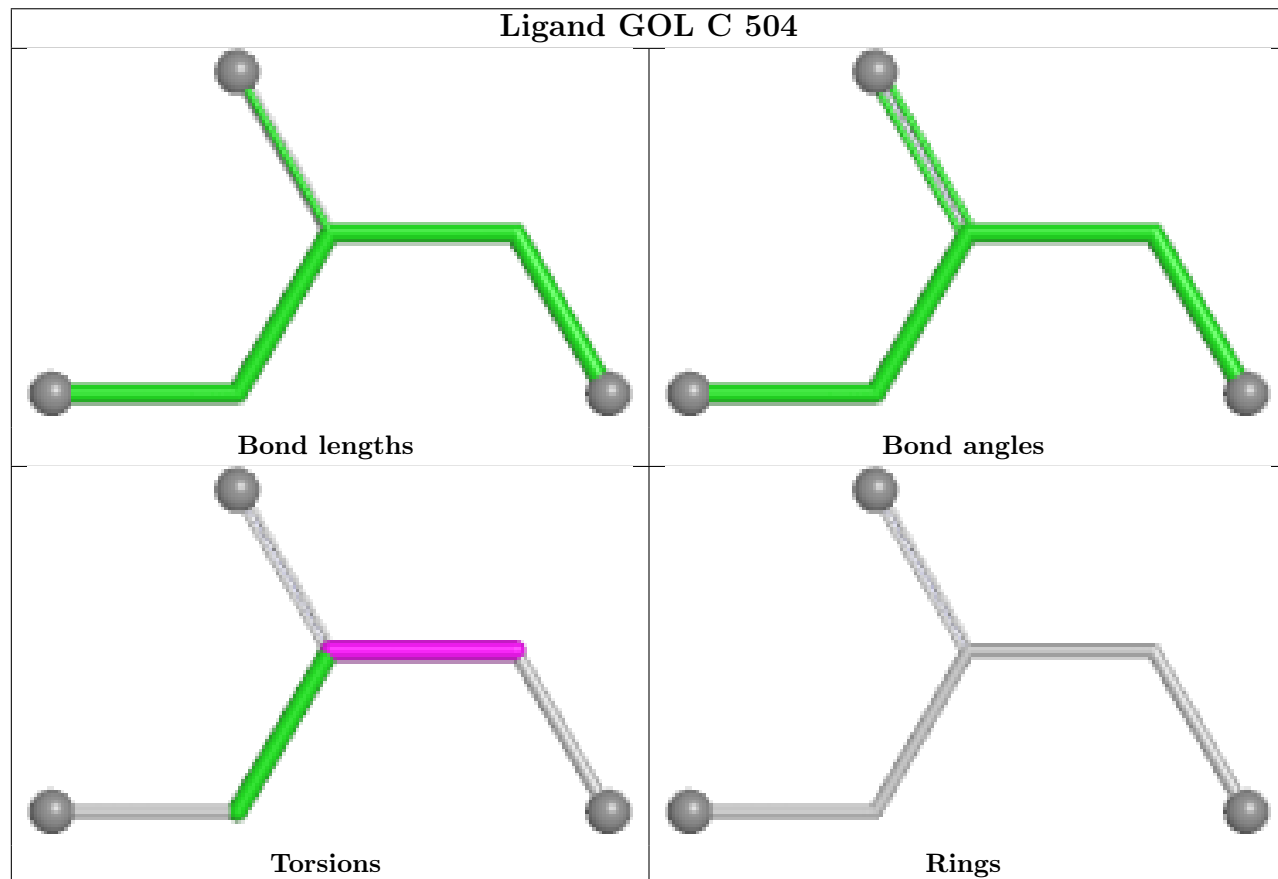




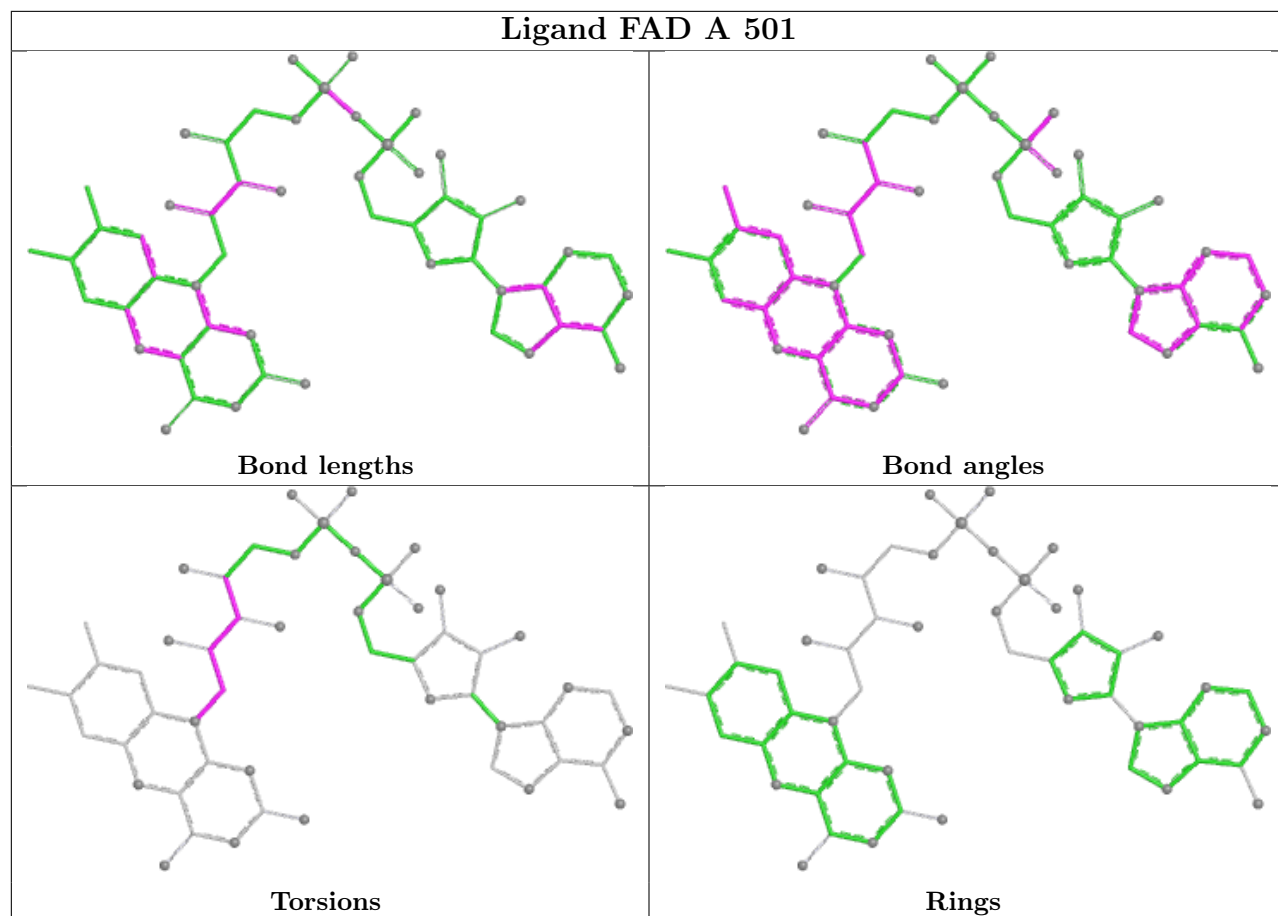
Ligand FAD B 501



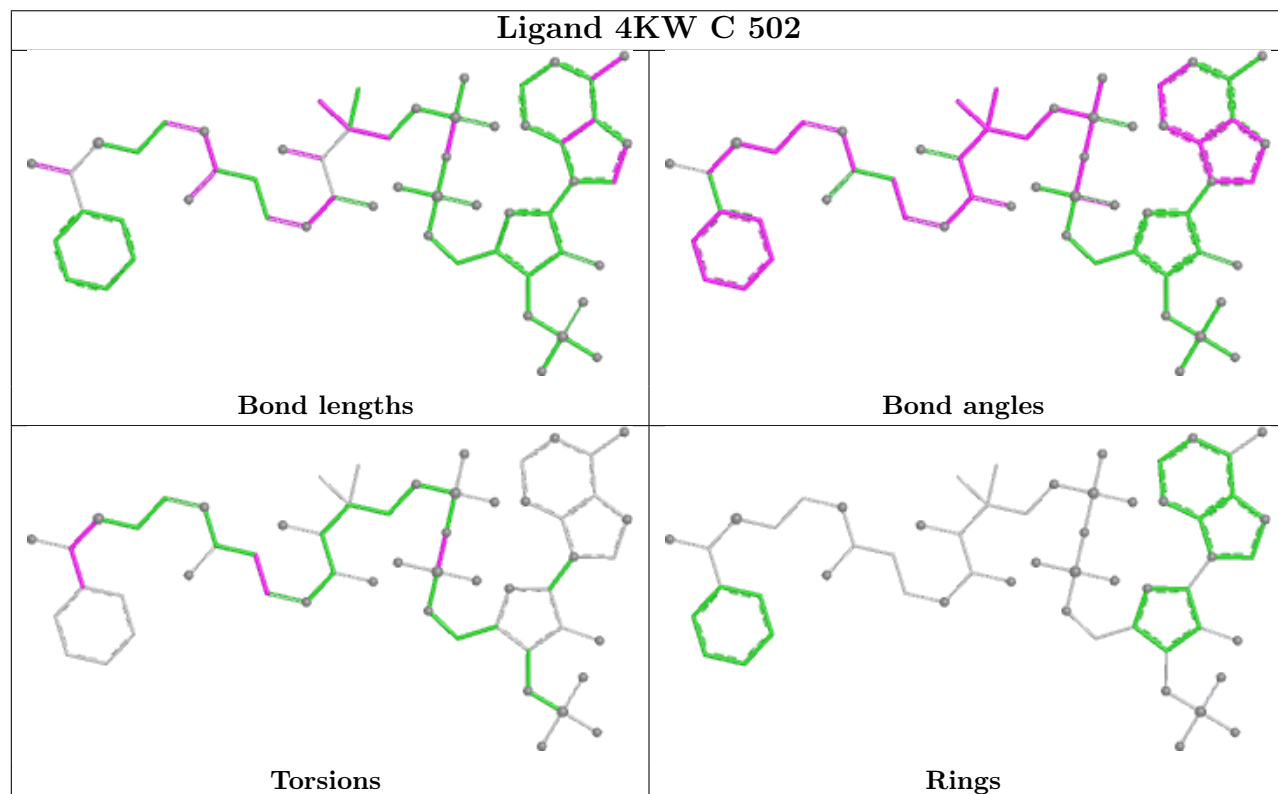
Ligand GOL C 504

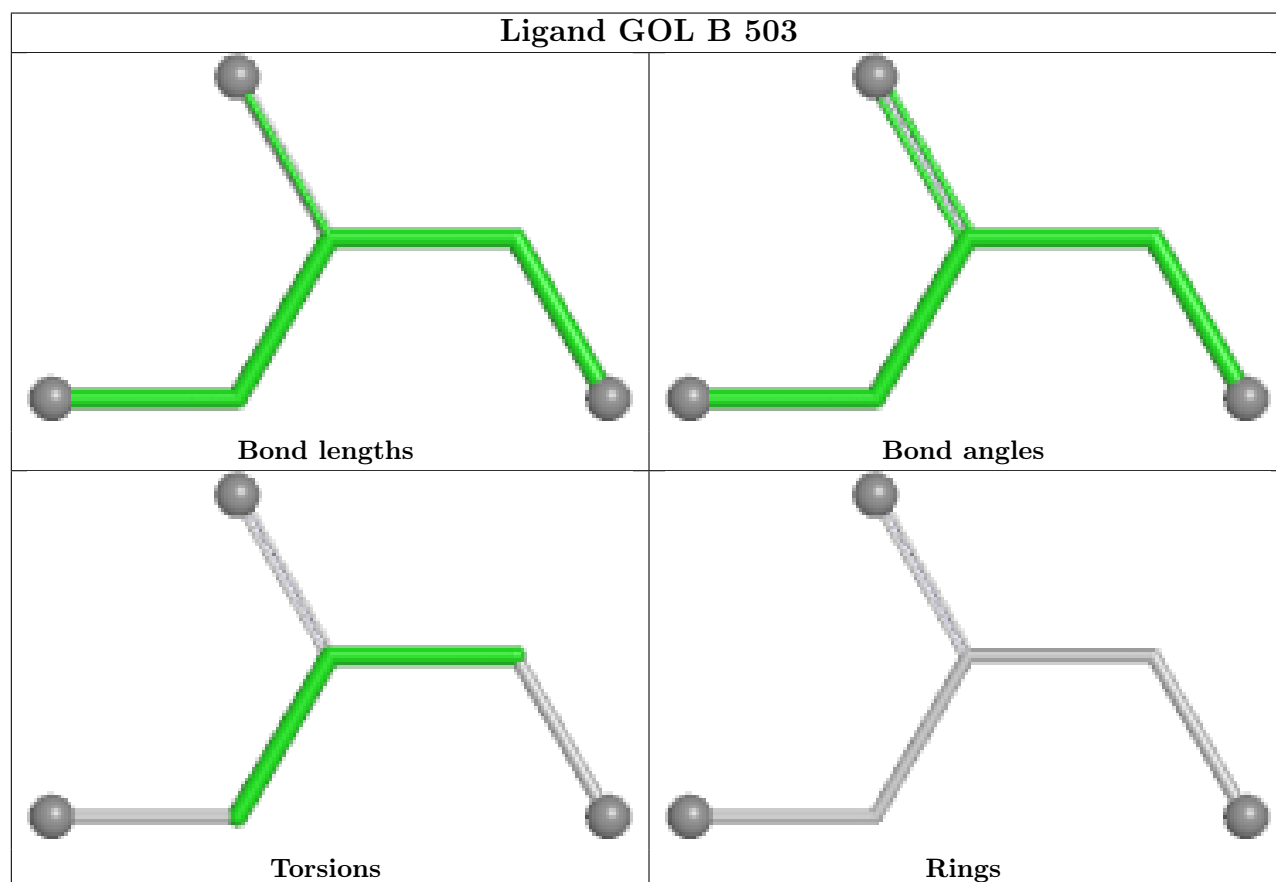
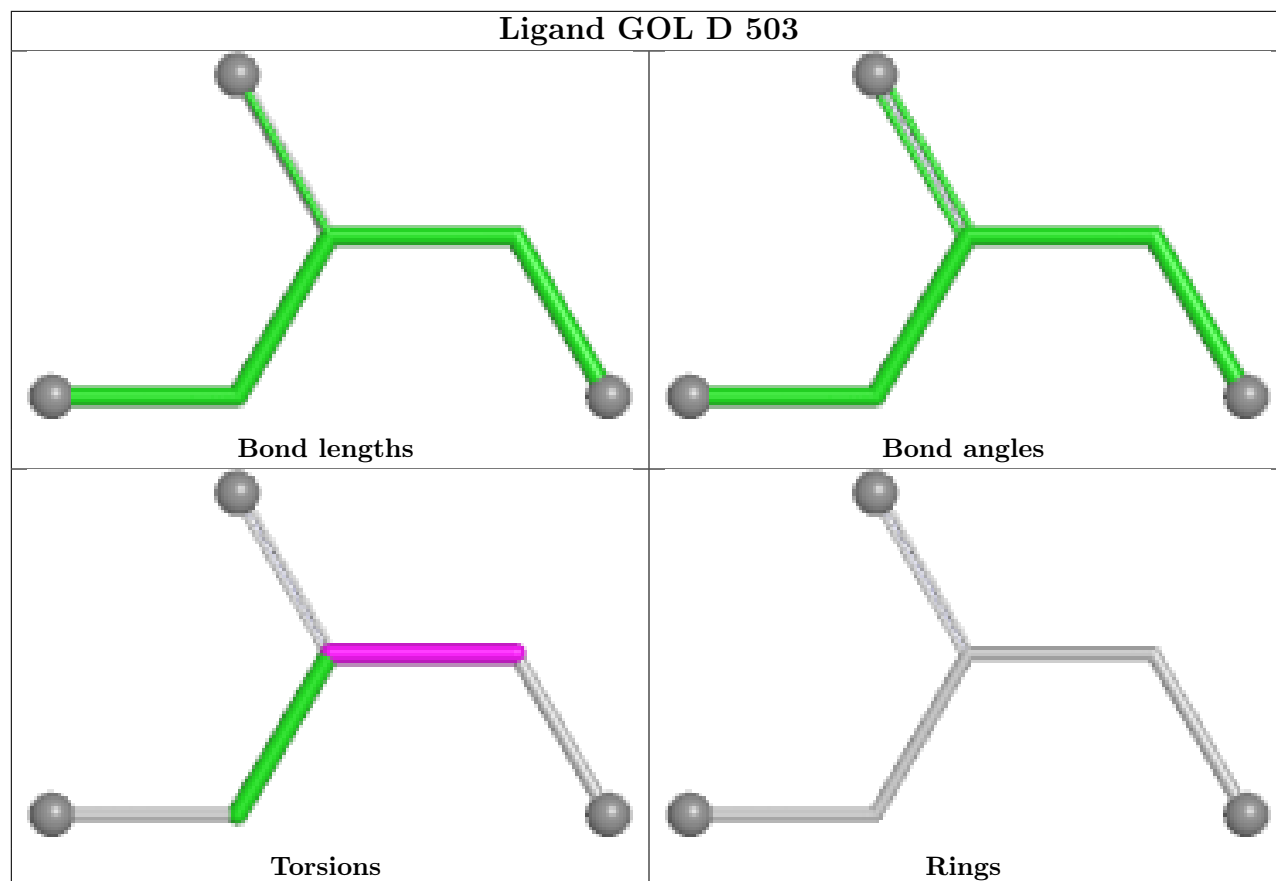


Ligand FAD A 501

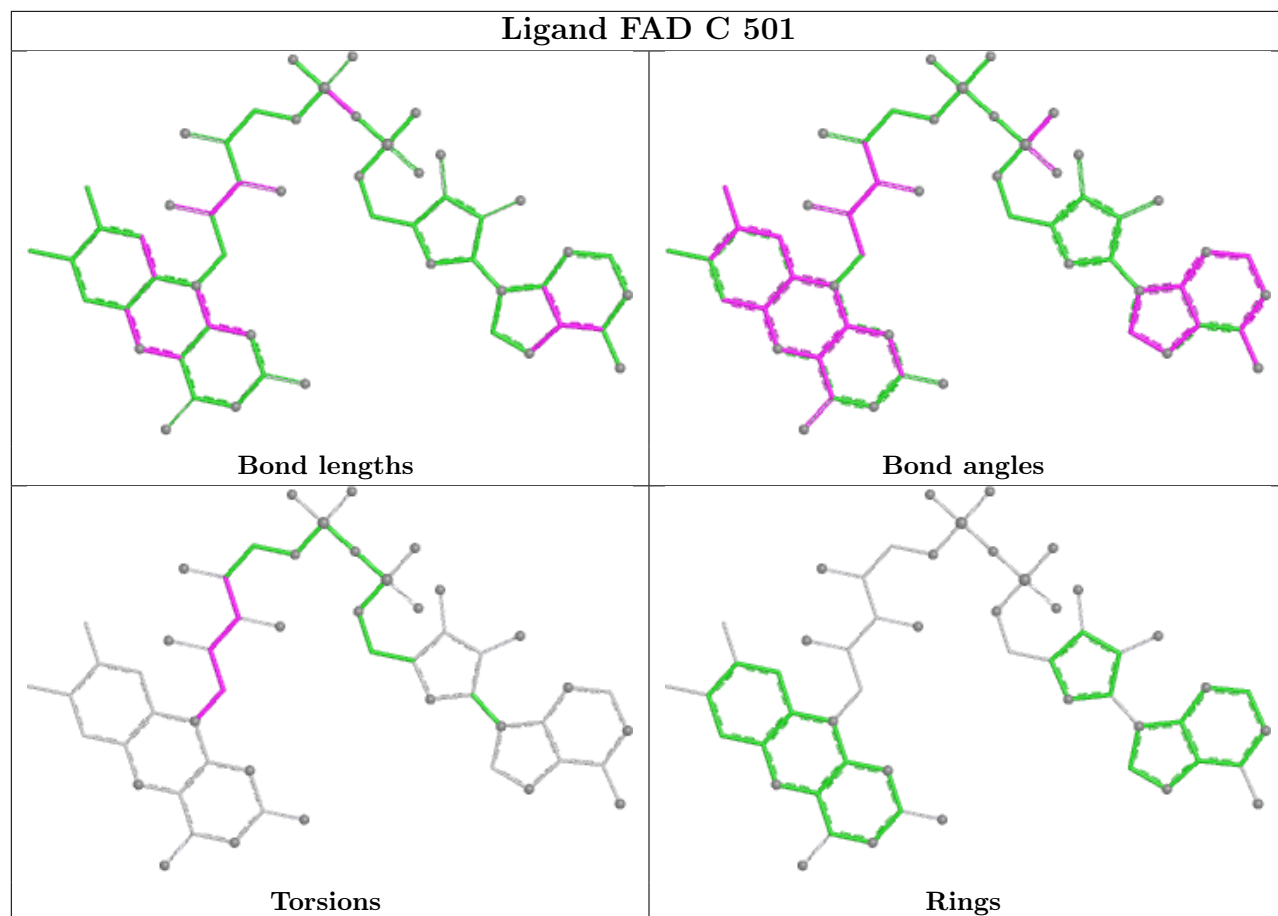


Ligand 4KW C 502

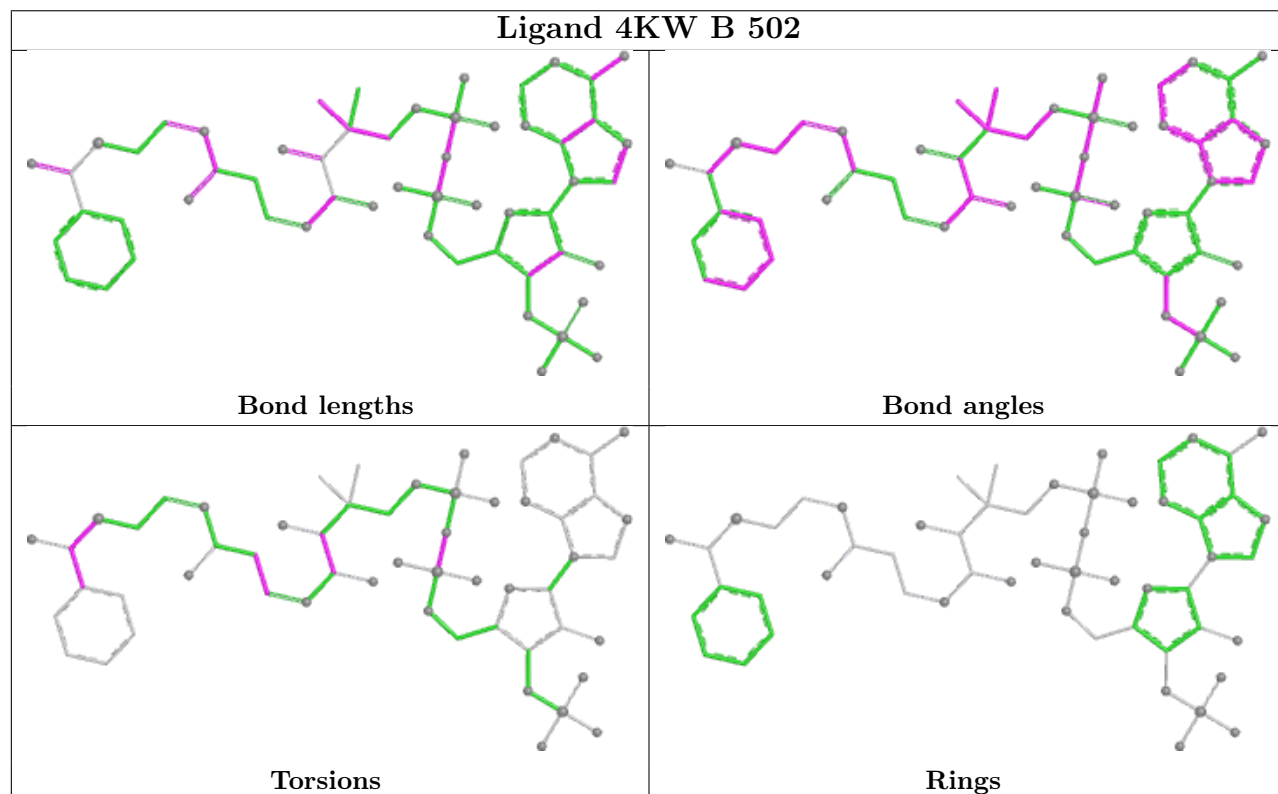




Ligand FAD C 501



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

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	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%)

All (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
1	D	378	LEU	8.4
1	D	23	ILE	8.3
1	D	4	LEU	8.1
1	D	94	LEU	7.9
1	D	18	VAL	7.8
1	D	234	LEU	7.8
1	D	218	VAL	7.6
1	D	56	ALA	7.5
1	D	35	LEU	7.4
1	D	311	LYS	7.3
1	D	197[A]	ASN	7.2
1	D	169	ALA	7.2
1	D	3	HIS	7.2
1	D	63[A]	MET	7.1
1	D	297	LEU	7.1
1	D	14	MET	7.0

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Mol	Chain	Res	Type	RSRZ
1	D	71	ILE	7.0
1	D	65	VAL	6.9
1	D	232	ALA	6.9
1	D	185	VAL	6.9
1	D	365	THR	6.9
1	D	249	ALA	6.8
1	D	223	ILE	6.8
1	D	372	VAL	6.7
1	D	109	LEU	6.6
1	D	380	PRO	6.6
1	D	377	LEU	6.6
1	D	231	PHE	6.5
1	D	10	LEU	6.5
1	D	67	THR	6.5
1	D	313	VAL	6.5
1	D	85	LEU	6.4
1	D	317	SER	6.4
1	D	261	VAL	6.3
1	D	19	ALA	6.2
1	D	49	LEU	6.2
1	D	86	LEU	6.2
1	D	284	VAL	6.2
1	D	280	VAL	6.1
1	D	149	ILE	6.1
1	D	9	LYS	6.1
1	D	314	LEU	6.0
1	D	97	ILE	6.0
1	D	20	THR	5.9
1	D	335	VAL	5.9
1	D	224	ILE	5.9
1	D	68	LEU	5.9
1	D	98	HIS	5.8
1	D	256	ALA	5.8
1	D	53	LEU	5.7
1	D	239	SER	5.7
1	D	270	PHE	5.7
1	D	379	PHE	5.7
1	D	274	ILE	5.7
1	D	361	ILE	5.7
1	D	135	ALA	5.7
1	D	211	LEU	5.6
1	D	240	THR	5.6

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Mol	Chain	Res	Type	RSRZ
1	D	55	PRO	5.6
1	D	50	LEU	5.6
1	D	315	TYR	5.6
1	D	243	VAL	5.5
1	D	291	VAL	5.5
1	D	282	PHE	5.5
1	D	99	GLY	5.5
1	D	296	LEU	5.5
1	D	273	PRO	5.5
1	D	299	ARG	5.5
1	B	208	ASN	5.5
1	D	37	PRO	5.5
1	D	225	GLY	5.4
1	D	28	LEU	5.4
1	D	52	PRO	5.4
1	D	134	LEU	5.4
1	D	245	CYS	5.3
1	D	133	LEU	5.3
1	D	168	TYR	5.3
1	D	178	LYS	5.3
1	D	45	ALA	5.3
1	D	302	ALA	5.3
1	D	72	LEU	5.3
1	D	123	ALA	5.3
1	D	66	LEU	5.3
1	D	247	ALA	5.3
1	D	47	LEU	5.2
1	D	75	LEU	5.2
1	D	241	ASN	5.2
1	D	58	TYR	5.2
1	D	362	TYR	5.2
1	D	283	MET	5.2
1	D	164	VAL	5.2
1	D	54	LEU	5.2
1	D	301	ALA	5.2
1	D	16	ARG	5.2
1	D	105	LYS	5.2
1	D	175	LYS	5.2
1	D	8	GLN	5.2
1	D	277	LEU	5.1
1	D	183	PHE	5.1
1	D	327	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
1	D	39	TYR	5.1
1	D	226	ALA	5.0
1	D	276	HIS	5.0
1	D	310	LYS	5.0
1	D	27	ALA	5.0
1	D	57	ALA	5.0
1	D	272	LYS	4.9
1	D	6	GLU	4.9
1	D	87	ILE	4.9
1	D	180	ILE	4.9
1	D	40	ALA	4.9
1	D	371	MET	4.9
1	D	192	LEU	4.8
1	D	294	SER	4.8
1	D	176	GLY	4.8
1	D	125	THR	4.8
1	D	264	THR	4.8
1	D	244	PHE	4.8
1	D	24	ALA	4.8
1	D	141	VAL	4.7
1	D	373	THR	4.7
1	D	368	ILE	4.6
1	D	351[A]	ARG	4.6
1	D	29	GLU	4.6
1	D	236	GLN	4.6
1	D	70	LEU	4.6
1	D	329[A]	ARG	4.6
1	D	96	ILE	4.6
1	D	179	GLY	4.6
1	D	347[A]	ASN	4.6
1	D	44	PHE	4.6
1	D	156	ILE	4.6
1	D	250	VAL	4.5
1	D	349	VAL	4.5
1	D	323	ALA	4.5
1	D	298	THR	4.5
1	D	319	ALA	4.5
1	D	203	MET	4.5
1	D	43	LEU	4.5
1	D	124	ALA	4.5
1	D	13	ASP	4.5
1	D	289	THR	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	330	VAL	4.4
1	D	146	LYS	4.4
1	D	129	ALA	4.4
1	D	279	PRO	4.4
1	D	260	ALA	4.4
1	C	7	GLU	4.4
1	D	285	ALA	4.4
1	D	108	TYR	4.3
1	C	3	HIS	4.3
1	D	30	LEU	4.3
1	D	38	GLU	4.3
1	D	198	GLU	4.3
1	D	287	MET	4.3
1	D	83	ALA	4.3
1	D	69	ALA	4.2
1	B	12	LEU	4.2
1	D	84	LEU	4.2
1	D	7	GLU	4.2
1	D	229	THR	4.2
1	D	81	SER	4.2
1	D	147	TYR	4.2
1	D	181	SER	4.1
1	D	59	GLY	4.1
1	D	138	THR	4.1
1	D	131	SER	4.1
1	D	5	THR	4.1
1	D	61	THR	4.1
1	D	167	VAL	4.1
1	D	80	ALA	4.1
1	B	3	HIS	4.1
1	D	122	LEU	4.1
1	D	304	LEU	4.1
1	D	281	GLN	4.1
1	D	369	THR	4.1
1	D	259	ILE	4.1
1	D	275	ALA	4.0
1	D	95	PRO	4.0
1	B	4	LEU	4.0
1	D	213	PHE	4.0
1	D	305	LEU	4.0
1	D	62	GLU	4.0
1	B	310	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	310	LYS	4.0
1	D	157	THR	4.0
1	D	237	THR	4.0
1	C	4[A]	LEU	4.0
1	D	48	GLY	3.9
1	D	220	ALA	3.9
1	D	193	VAL	3.9
1	D	93	MET	3.9
1	D	189	THR	3.9
1	D	119	LEU	3.9
1	D	253	ALA	3.9
1	D	36	PHE	3.9
1	D	165	ILE	3.9
1	D	252	ILE	3.9
1	B	198	GLU	3.9
1	D	76	GLY	3.9
1	D	140	ALA	3.9
1	D	190	PRO	3.9
1	D	320	LYS	3.9
1	D	25	PRO	3.8
1	D	363	THR	3.8
1	D	233	ASN	3.8
1	D	309	ASP	3.8
1	D	212	PHE	3.8
1	C	10	LEU	3.8
1	D	246	ALA	3.8
1	D	359	THR	3.7
1	A	3	HIS	3.7
1	D	271	GLY	3.7
1	D	90	THR	3.7
1	D	92	GLY	3.7
1	D	130	GLY	3.7
1	D	51	ASN	3.7
1	C	46	LYS	3.7
1	D	312	ALA	3.7
1	D	251	GLY	3.7
1	D	307	ASP	3.6
1	D	100	GLY	3.6
1	D	228	GLY	3.6
1	D	364	GLY	3.6
1	D	127	PRO	3.6
1	D	121	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	230	GLY	3.6
1	D	375	ARG	3.6
1	D	343	TYR	3.6
1	D	74	GLU	3.6
1	D	219	PRO	3.6
1	D	112	PHE	3.6
1	D	200	LYS	3.6
1	D	32	GLU	3.6
1	A	196	ARG	3.5
1	D	205	GLY	3.5
1	C	6	GLU	3.5
1	D	166	VAL	3.5
1	D	268	VAL	3.5
1	D	144	GLY	3.5
1	D	60	GLY	3.5
1	D	155	PHE	3.5
1	D	206	SER	3.5
1	D	308	GLY	3.5
1	D	316	GLY	3.5
1	D	293	ALA	3.4
1	D	77	ARG	3.4
1	D	139	ARG	3.4
1	D	235	MET	3.4
1	A	198	GLU	3.4
1	D	110	ARG	3.4
1	D	337	VAL	3.4
1	D	367	GLN	3.4
1	D	207	ILE	3.4
1	D	82	THR	3.4
1	D	209	SER	3.4
1	D	290	ALA	3.3
1	D	356	ALA	3.3
1	D	338	LEU	3.3
1	D	102	PRO	3.3
1	D	22	GLU	3.3
1	D	170	TYR	3.3
1	D	339	GLY	3.3
1	D	278	ALA	3.3
1	D	114	GLY	3.2
1	D	255	GLY	3.2
1	D	88	ALA	3.2
1	D	199[A]	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	146	LYS	3.2
1	D	202	GLY	3.2
1	D	288	ALA	3.2
1	D	117	THR	3.2
1	D	173	PRO	3.1
1	B	196	ARG	3.1
1	D	104	LEU	3.1
1	D	113	ALA	3.1
1	D	376	ALA	3.1
1	D	358	LEU	3.1
1	A	175	LYS	3.1
1	D	321	THR	3.1
1	B	63[A]	MET	3.1
1	B	7	GLU	3.1
1	D	159	GLY	3.0
1	D	153	LYS	3.0
1	D	21	ARG	3.0
1	D	257	LEU	3.0
1	D	334	ALA	3.0
1	A	5	THR	3.0
1	A	4	LEU	3.0
1	D	177	SER	3.0
1	D	137	LYS	3.0
1	D	194	TYR	3.0
1	D	118	LEU	3.0
1	D	184	VAL	2.9
1	D	328	MET	2.9
1	D	187	LYS	2.9
1	B	197[A]	ASN	2.9
1	D	341	SER	2.9
1	D	120	THR	2.9
1	D	128	ALA	2.9
1	A	197[A]	ASN	2.9
1	D	306	ASP	2.9
1	C	63[A]	MET	2.9
1	D	322	MET	2.8
1	D	101	SER	2.8
1	D	152	GLN	2.8
1	A	63	MET	2.8
1	D	46	LYS	2.8
1	D	374	GLY	2.8
1	D	158	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	174	GLU	2.8
1	D	227	GLU	2.8
1	D	292	GLU	2.8
1	A	9	LYS	2.8
1	A	310	LYS	2.7
1	D	111	ARG	2.7
1	D	332	THR	2.7
1	A	163	ASP	2.7
1	D	204	ARG	2.7
1	D	263	HIS	2.7
1	D	286	ASP	2.7
1	D	196	ARG	2.6
1	D	64	GLY	2.6
1	A	10	LEU	2.6
1	B	14	MET	2.6
1	D	353	MET	2.6
1	A	380	PRO	2.6
1	C	174	GLU	2.6
1	D	73	GLU	2.6
1	D	344	MET	2.6
1	B	5	THR	2.6
1	D	303	GLU	2.6
1	D	336	GLN	2.6
1	B	218	VAL	2.6
1	A	146	LYS	2.6
1	D	345	LYS	2.6
1	D	208	ASN	2.6
1	D	26	ARG	2.5
1	D	295	ARG	2.5
1	D	17	ASP	2.5
1	D	171	THR	2.5
1	D	148	VAL	2.5
1	C	175	LYS	2.5
1	A	152[A]	GLN	2.5
1	D	300	LYS	2.5
1	D	370	ARG	2.5
1	D	42	ASP	2.4
1	D	142	ARG	2.4
1	A	11	THR	2.4
1	D	31	ASP	2.4
1	D	132	ASP	2.4
1	D	163	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	79	CYS	2.4
1	A	143	GLN	2.4
1	D	145	ASP	2.4
1	B	305	LEU	2.4
1	B	174	GLU	2.4
1	D	186	GLU	2.4
1	B	206	SER	2.3
1	D	116	SER	2.3
1	D	318	MET	2.3
1	B	380	PRO	2.3
1	D	136	MET	2.3
1	C	12	LEU	2.3
1	D	248	GLN	2.3
1	D	222	ASN	2.3
1	C	5	THR	2.3
1	D	357	LYS	2.2
1	D	348	GLY	2.2
1	D	242	ARG	2.2
1	C	238	LEU	2.2
1	C	196	ARG	2.2
1	B	9	LYS	2.2
1	D	324	SER	2.2
1	D	91	ASP	2.2
1	C	173	PRO	2.2
1	D	34	SER	2.2
1	D	89	GLN	2.1
1	D	360	GLN	2.1
1	D	366	ASN	2.1
1	C	380	PRO	2.1
1	B	16	ARG	2.1
1	A	144	GLY	2.1
1	B	143	GLN	2.1
1	C	206	SER	2.1
1	D	210	GLU	2.1
1	D	326	THR	2.1
1	D	267	ARG	2.1
1	D	191	GLY	2.0
1	D	217	GLU	2.0
1	A	16	ARG	2.0
1	D	161	VAL	2.0
1	C	9	LYS	2.0
1	C	198	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	14	MET	2.0
1	C	308	GLY	2.0
1	D	269	GLN	2.0
1	D	262	ARG	2.0
1	A	145	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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.

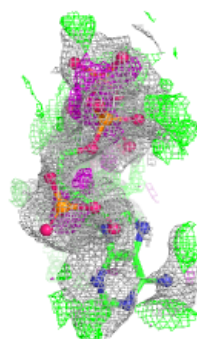
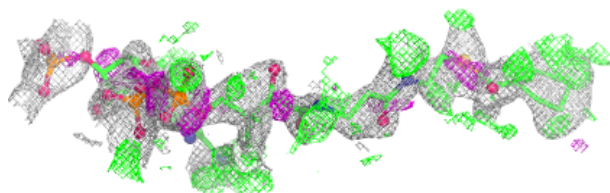
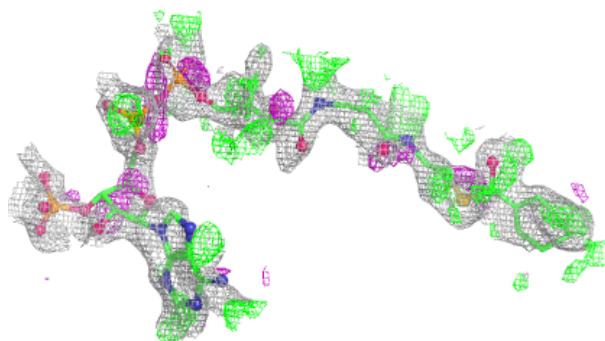
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	4KW	D	502	56/56	0.59	0.25	39,55,86,86	0
2	FAD	D	501	53/53	0.76	0.17	31,35,39,41	0
4	GOL	D	504	6/6	0.77	0.24	45,47,50,51	0
4	GOL	D	503	6/6	0.80	0.52	78,83,83,85	6
4	GOL	C	504	6/6	0.83	0.18	40,44,46,48	0
4	GOL	B	504	6/6	0.90	0.14	31,38,41,42	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.

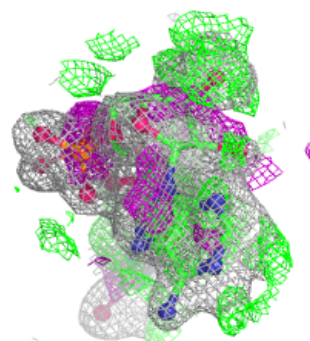
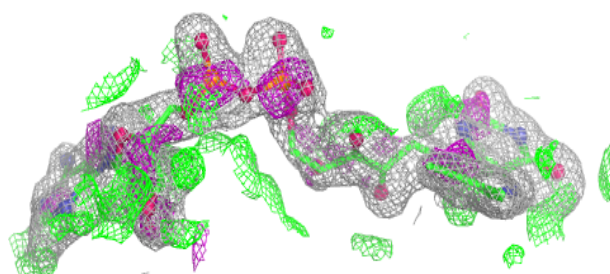
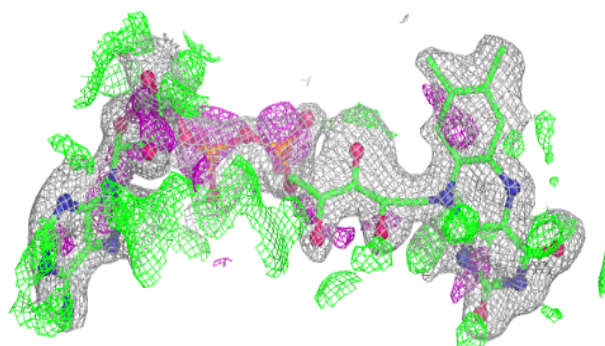
Electron density around 4KW D 502:

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



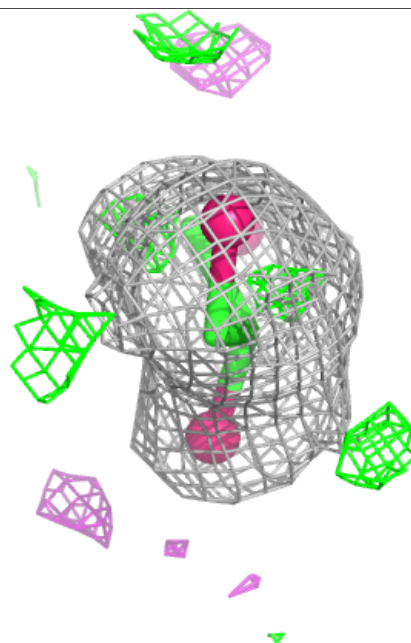
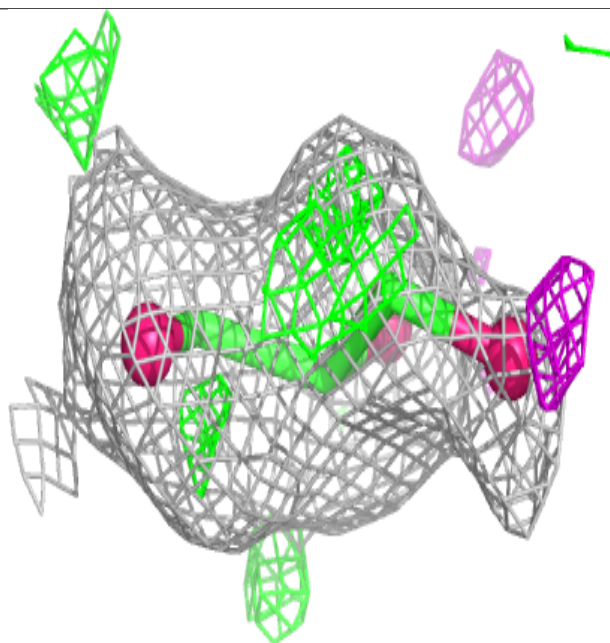
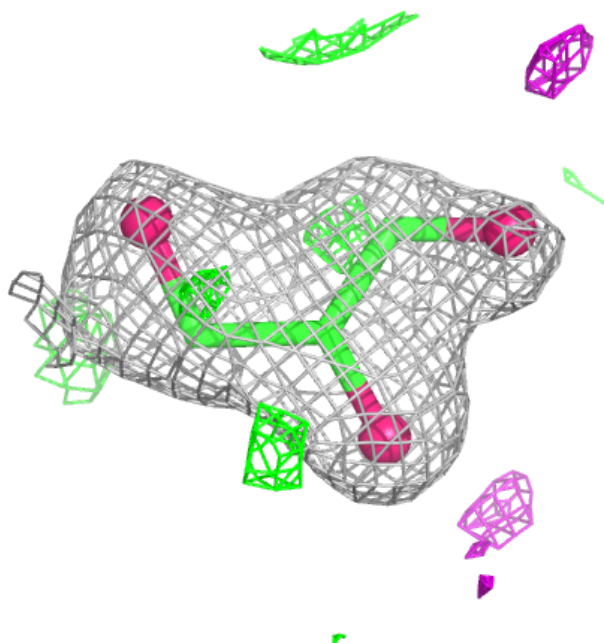
Electron density around FAD D 501:

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



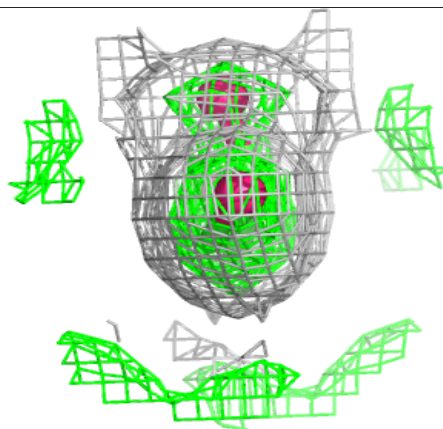
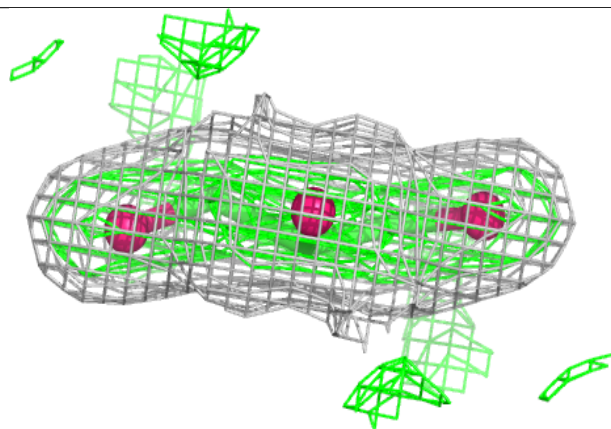
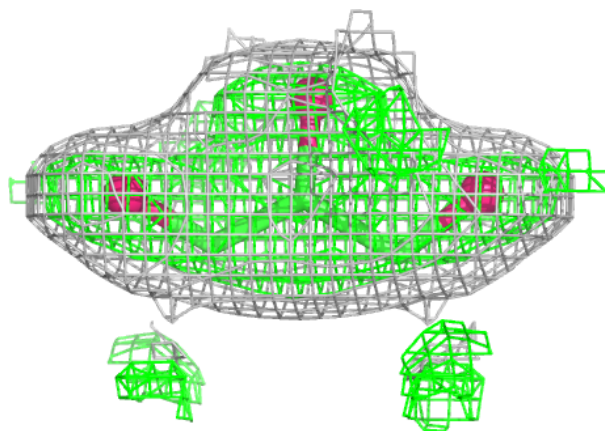
Electron density around GOL D 504:

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



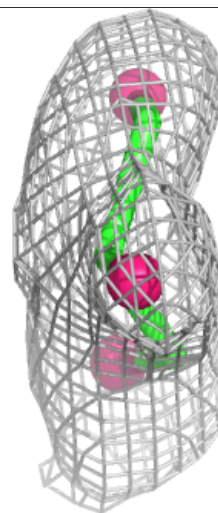
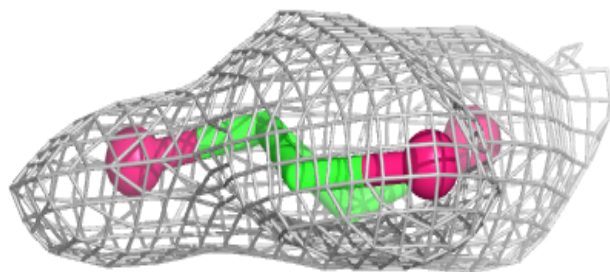
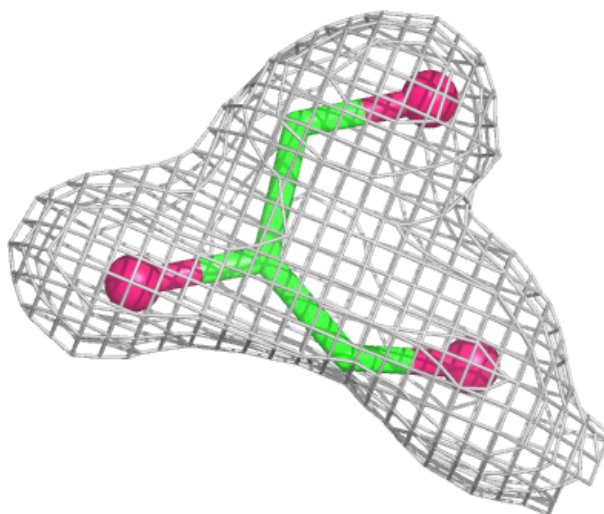
Electron density around GOL D 503:

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



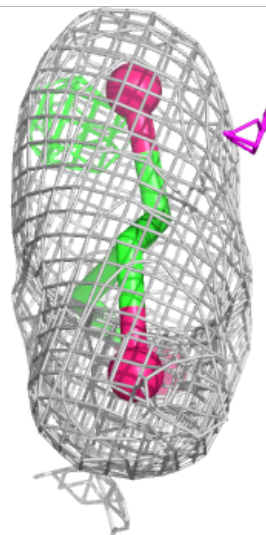
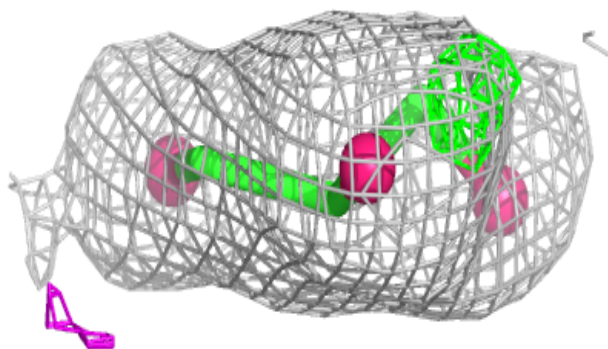
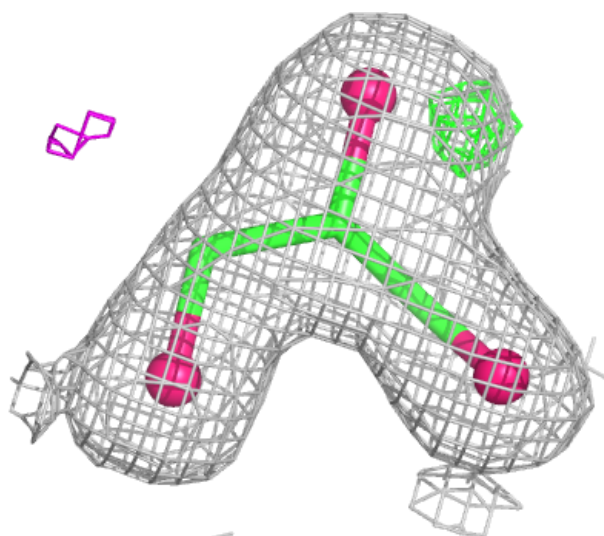
Electron density around GOL C 504:

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



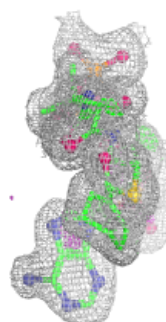
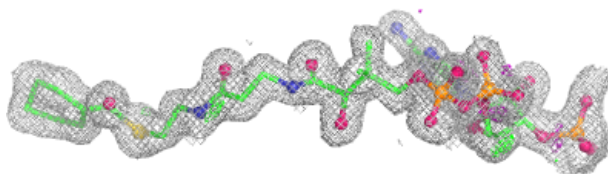
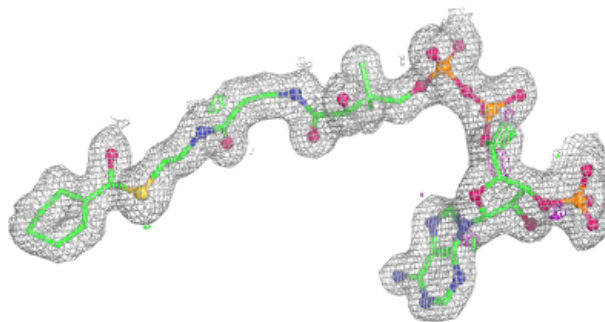
Electron density around GOL B 504:

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

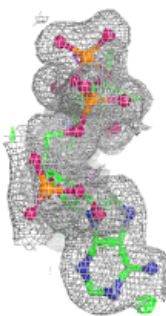
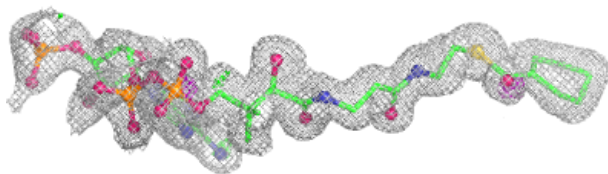
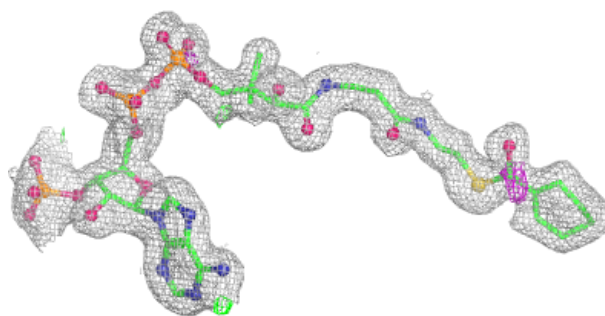


Electron density around 4KW C 502:

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

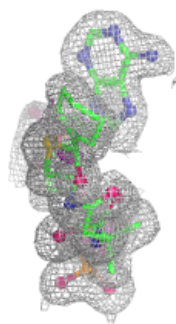
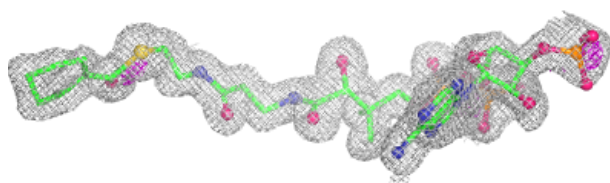
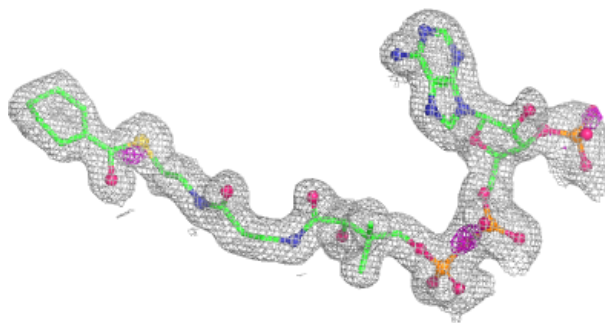
**Electron density around 4KW B 502:**

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

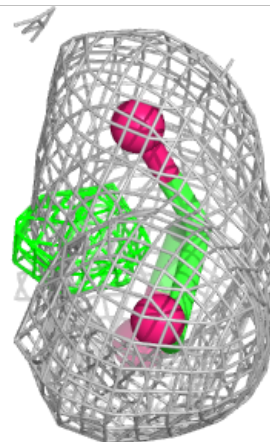
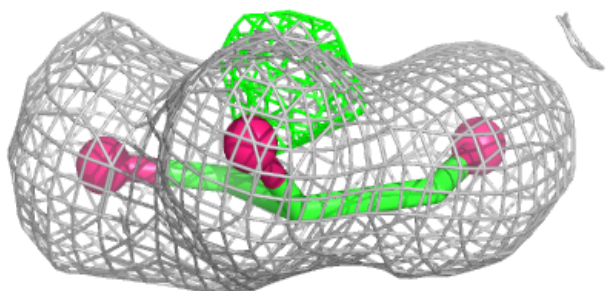
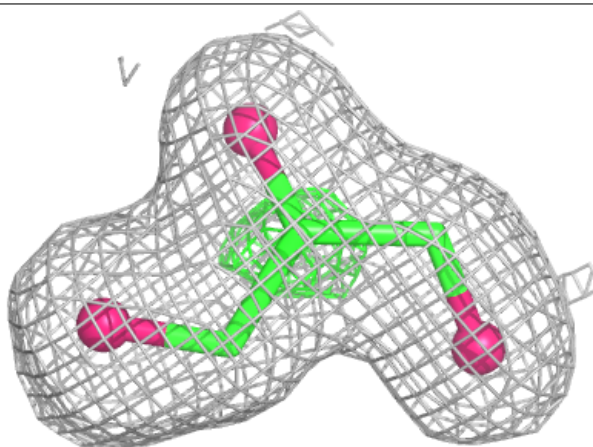


Electron density around 4KW A 502:

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

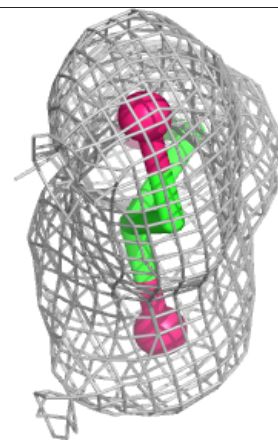
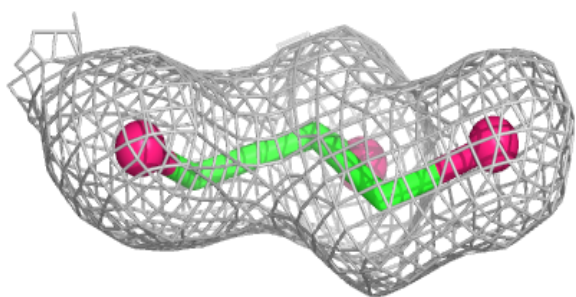
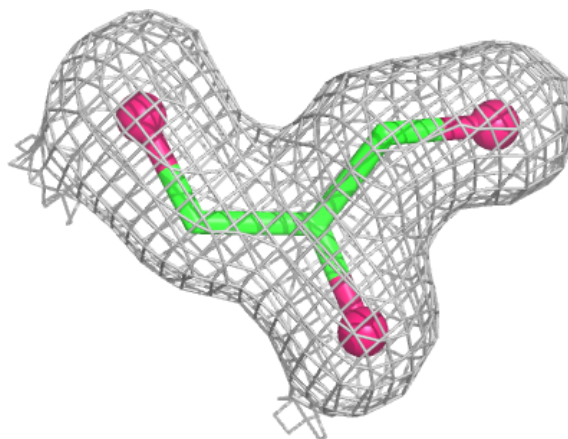
**Electron density around GOL A 503:**

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



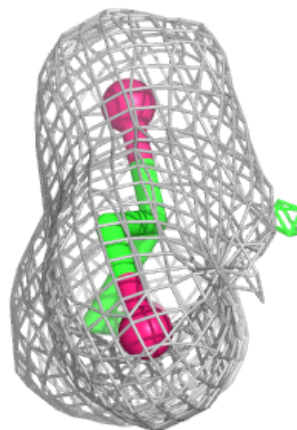
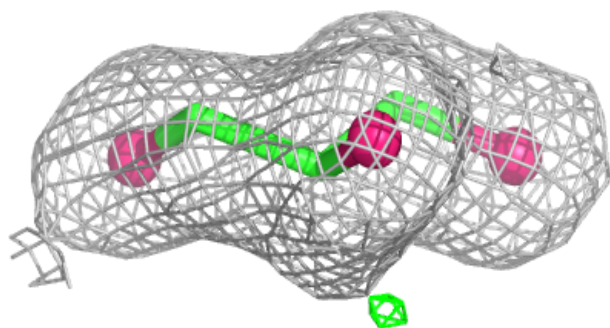
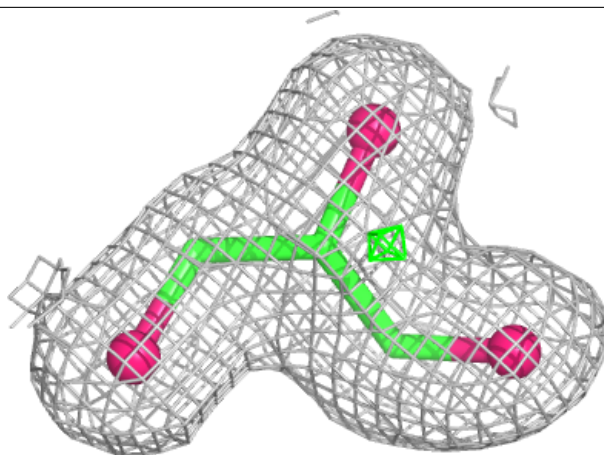
Electron density around GOL C 503:

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

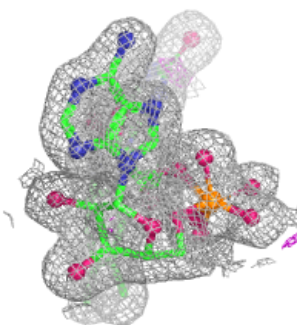
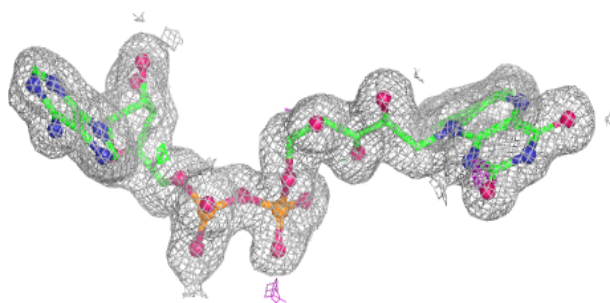
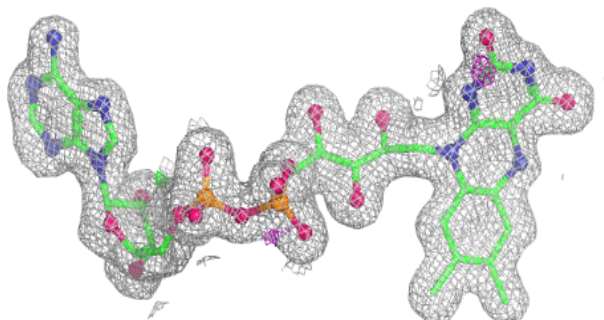


Electron density around GOL B 503:

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

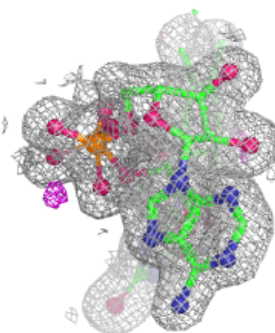
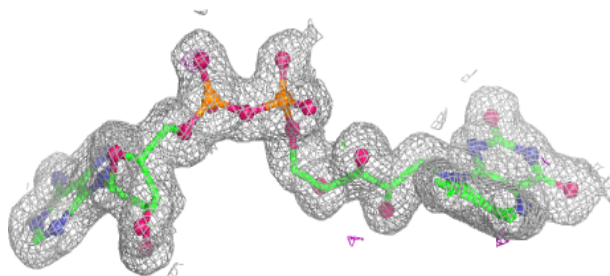
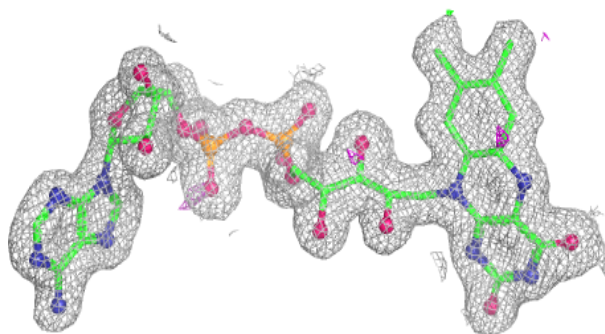
**Electron density around FAD A 501:**

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

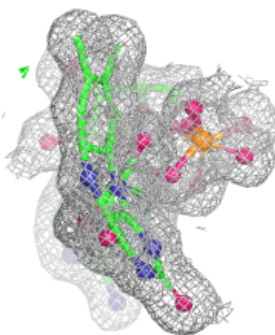
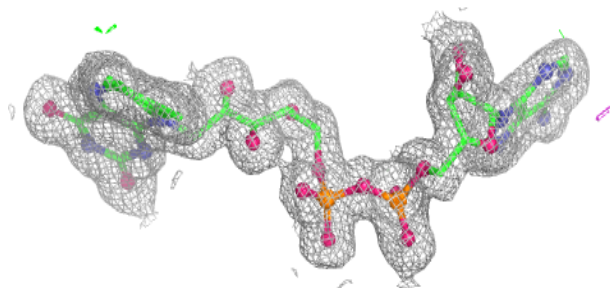
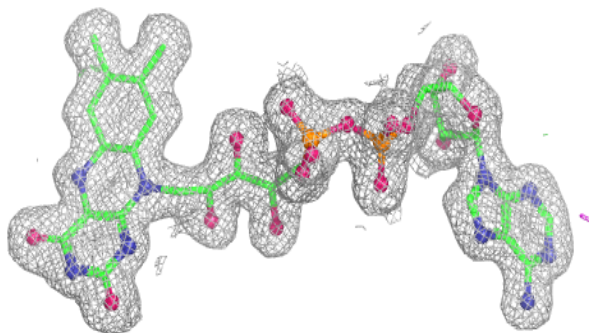


Electron density around FAD B 501:

$2mF_o-DF_c$ (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.