



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 15, 2024 – 01:54 AM EST

PDB ID : 2O2Y  
Title : The crystal structure of P. falciparum enoyl acyl carrier protein reductase  
Authors : Muench, S.P.; Prigge, S.T.; McLeod, R.; Rafferty, J.B.; Kirisits, M.J.; Roberts, C.W.; Mui, E.J.; Rice, D.W.  
Deposited on : 2006-11-30  
Resolution : 2.20 Å(reported)

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We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.21  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.004 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

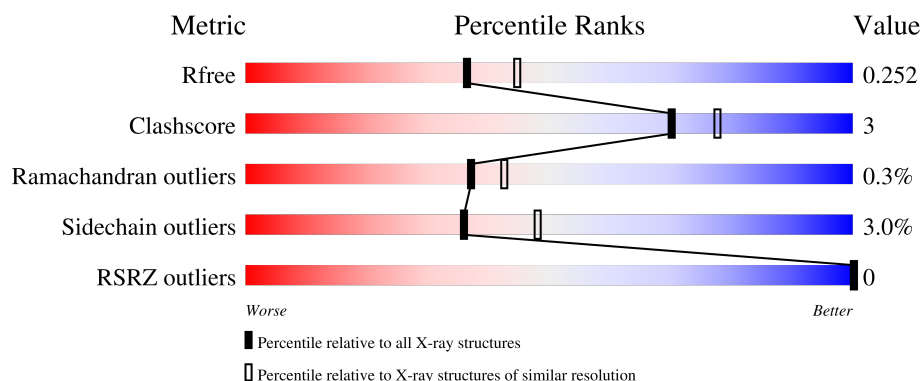
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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  $\geq 3$ , 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	349	 74% 9% 17%
1	B	349	 74% 8% 17%
1	C	349	 75% 8% 16%
1	D	349	 73% 8% 17%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9909 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 Enoyl-acyl carrier reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2288	1460	385	432	11			
1	B	290	Total	C	N	O	S	13	0	0
			2293	1463	385	434	11			
1	C	293	Total	C	N	O	S	18	0	0
			2310	1474	386	440	10			
1	D	288	Total	C	N	O	S	4	0	0
			2270	1451	378	430	11			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

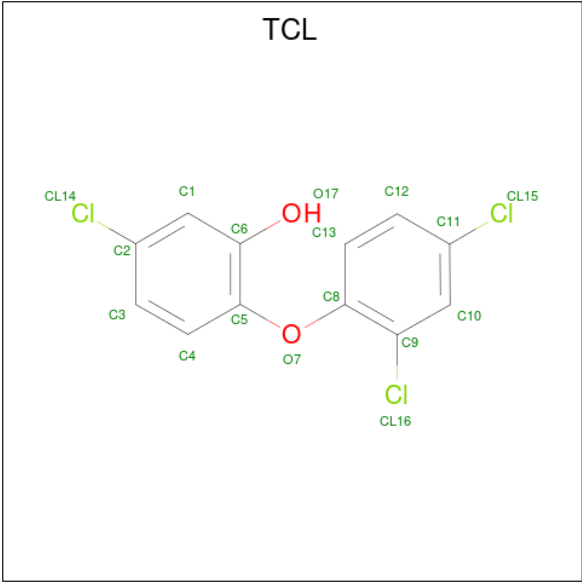
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		
2	D	1	Total	Cl	0	0
			1	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



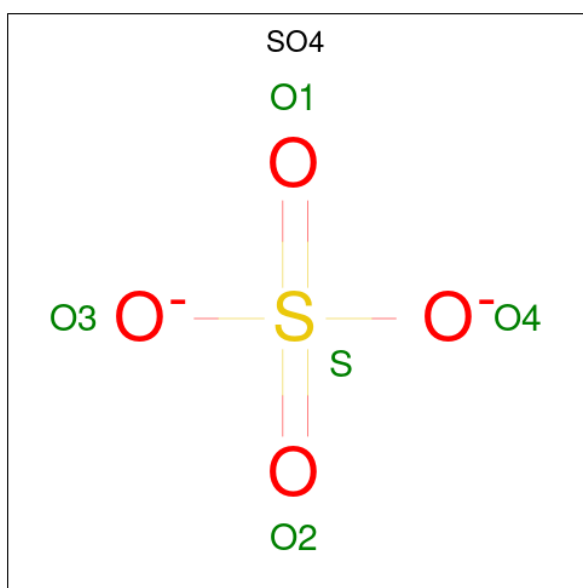
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is TRICLOSAN (three-letter code: TCL) (formula: C<sub>12</sub>H<sub>7</sub>Cl<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	O	0	0
			17	12	3	2		
4	B	1	Total	C	Cl	O	0	0
			17	12	3	2		
4	C	1	Total	C	Cl	O	0	0
			17	12	3	2		
4	D	1	Total	C	Cl	O	0	0
			17	12	3	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	106	Total	O	0	0
			106	106		
6	B	130	Total	O	0	0
			130	130		
6	C	109	Total	O	0	0
			109	109		
6	D	150	Total	O	0	0
			150	150		



- Molecule 1: Enoyl-acyl carrier reductase

GLU	LEU	ALA
	ASN	SER
ASN	ASN	ASN
	THR	ILE
TYR	TYR	TYR
	GLU	LYS
ASN	ASN	ILE
	ASN	LYS
THR	THR	GLU
	GLN	ASN
ASN	ASN	ASN
	LYS	ASN
ASN	ASN	GLU
	ARG	D15
SER	SER	I22
	HIS	S37
ASP	VAL	F45
	HIS	K63
ASN	ILE	K74
	MET	I78
ASN	ASN	P81
	SER	S87
GLY	GLU	E96
	LYS	M106
ASN	ASN	L107
	SER	Q121
ALA	SER	H131
	GLN	Q140
ASN	ASN	K157
	Y288	S161
Y292	Q301	K167
	T306	P192
R318	E319	S200
	P340	K233
D341	ASN	T238
	R345	A239
ASN	GLU	I240
	ASN	Y241
ASN	ASN	P261

Chain B:  74% 8% 17%

ASN	GLU	P231	ALA
		N241	SRN
		LYS	ILE
		LEU	TYR
		ASN	LYS
		ASN	ILE
		THR	LYS
		TYR	GLU
		GLU	GLU
		ASN	ASN
		ASN	LYS
		THR	ASN
		GLN	ASN
		ASN	GLU
		LYS	D15
		ASN	S37
		ASN	K38
		ARG	R39
		ASN	
		SER	I43
		HIS	I44
		HIS	F45
		ASP	
		VAL	K60
		HIS	
		ASN	M68
		ILE	I69
		MET	I70
		ASN	D71
		ASN	K72
		SER	
		GLY	M81
		GLU	
		LYS	N109
		GLU	
		GLU	D114
		LYS	
		LYS	H131
		ASN	S132
		ALA	L133
		SER	A134
		SER	N135
		GLW	A136
		ASN	
		Y283	K149
		T284	
		Y292	F169
		Y296	V170
			M171
			I172
		S313	M173
		L334	S181
			L182
		L339	M198
		R345	
		ASN	T227
		GLU	

Chain C:  75% 8% • 16%

GLU	ASN	ASN	THR	TYL	GLY	ASN	ASN	THR	ASN	ASN	GLN	ASN	LYS	ASN	MH3	EI4	R39	K42	W48	P49	P50	M53	N66	D67	M68	I69	K72	K75	M76	M77	A86	K102	M117	M135	A136	D142	R148	V170	M198	Y214	A237	M241	LYS	LEU							
	ASN	ASN	THR	TYL	GLY	ASN	ASN	THR	ASN	ASN	GLN	ASN	LYS	ASN	ASN	ARG	ASN	SER	HIS	ASP	VAL	HIS	ASN	ILE	MET	ASN	ASN	GLY	GLU	LYS	LYS	ASN	SER	ALA	SER	GLN	ASN	Y283	L286	Y292	R300	G301	K302	G333	L336	K337	F338	L339	R345	K346	GLU



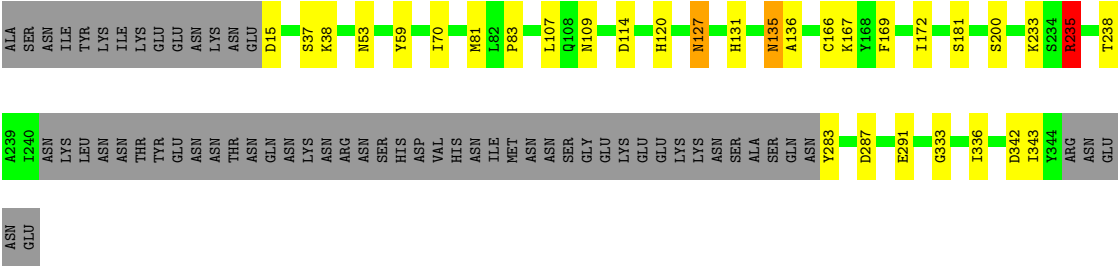
Chain D: 

73%

8%

•

17%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.18Å 82.37Å 94.82Å 90.00° 90.77° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 30.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.7 (30.00-2.20) 97.7 (30.00-2.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.86 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.200 , 0.246 0.208 , 0.252	Depositor DCC
$R_{free}$ test set	3374 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.5	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 19.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9909	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, TCL, CL, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.48	0/2331	0.61	0/3147
1	B	0.61	3/2336 (0.1%)	0.77	6/3154 (0.2%)
1	C	0.61	5/2353 (0.2%)	0.79	8/3178 (0.3%)
1	D	0.58	1/2313 (0.0%)	0.70	3/3124 (0.1%)
All	All	0.57	9/9333 (0.1%)	0.72	17/12603 (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	B	0	1
1	C	0	2
All	All	0	3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	60	LYS	CA-CB	-14.15	1.22	1.53
1	C	117	ASN	CG-OD1	-11.33	0.99	1.24
1	D	166	CYS	CB-SG	-10.70	1.64	1.82
1	C	42	LYS	CG-CD	-8.06	1.25	1.52
1	C	86	ALA	CA-CB	6.71	1.66	1.52

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	68	MET	CG-SD-CE	20.00	132.19	100.20
1	D	81	MET	CG-SD-CE	15.30	124.68	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	MET	CG-SD-CE	13.58	121.92	100.20
1	B	198	MET	CG-SD-CE	12.95	120.92	100.20
1	C	53	ASN	OD1-CG-ND2	-10.96	96.68	121.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	133	LEU	Mainchain
1	C	117	ASN	Sidechain
1	C	53	ASN	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2288	0	2286	20	0
1	B	2293	0	2291	17	0
1	C	2310	0	2295	15	0
1	D	2270	0	2263	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	44	0	26	0	0
3	B	44	0	26	1	0
3	C	44	0	26	0	0
3	D	44	0	26	0	0
4	A	17	0	6	0	0
4	B	17	0	6	0	0
4	C	17	0	6	0	0
4	D	17	0	6	0	0
5	D	5	0	0	1	0
6	A	106	0	0	2	0
6	B	130	0	0	1	0
6	C	109	0	0	3	0
6	D	150	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9909	0	9263	61	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 3.

The worst 5 of 61 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:59:TYR:O	5:D:713:SO4:O4	2.04	0.75
1:B:339:LEU:HD22	1:C:292:TYR:CE1	2.23	0.73
1:B:292:TYR:CD1	1:C:339:LEU:HD22	2.31	0.65
1:A:319:GLU:OE1	1:C:39:ARG:NH2	2.30	0.65
1:D:283:TYR:CE2	1:D:291:GLU:OE1	2.51	0.64

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	286/349 (82%)	272 (95%)	13 (4%)	1 (0%)	37	42
1	B	286/349 (82%)	276 (96%)	9 (3%)	1 (0%)	37	42
1	C	289/349 (83%)	277 (96%)	10 (4%)	2 (1%)	19	19
1	D	284/349 (81%)	274 (96%)	10 (4%)	0	100	100
All	All	1145/1396 (82%)	1099 (96%)	42 (4%)	4 (0%)	37	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	72	LYS

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Mol	Chain	Res	Type
1	C	14	GLU
1	B	72	LYS
1	A	240	ILE

### 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	248/307 (81%)	240 (97%)	8 (3%)	34	45
1	B	249/307 (81%)	243 (98%)	6 (2%)	44	57
1	C	249/307 (81%)	240 (96%)	9 (4%)	30	40
1	D	246/307 (80%)	239 (97%)	7 (3%)	38	51
All	All	992/1228 (81%)	962 (97%)	30 (3%)	36	48

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	75	LYS
1	D	200	SER
1	C	135	ASN
1	D	342	ASP
1	D	53	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	140	GLN
1	D	58	ASN
1	D	53	ASN
1	D	61	ASN
1	B	117	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	NAD	B	1450	-	42,48,48	1.79	5 (11%)	50,73,73	1.40	3 (6%)
5	SO4	D	713	-	4,4,4	0.44	0	6,6,6	0.42	0
3	NAD	D	550	-	42,48,48	1.65	4 (9%)	50,73,73	1.87	9 (18%)
4	TCL	B	706	-	18,18,18	1.67	2 (11%)	25,25,25	1.16	2 (8%)
4	TCL	C	708	-	18,18,18	1.85	4 (22%)	25,25,25	1.14	1 (4%)
3	NAD	C	750	-	42,48,48	1.70	3 (7%)	50,73,73	1.48	5 (10%)
4	TCL	D	707	-	18,18,18	1.87	2 (11%)	25,25,25	1.01	1 (4%)
3	NAD	A	650	-	42,48,48	1.79	4 (9%)	50,73,73	1.46	3 (6%)
4	TCL	A	705	-	18,18,18	1.77	2 (11%)	25,25,25	1.01	1 (4%)

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
3	NAD	B	1450	-	-	12/26/62/62	0/5/5/5
3	NAD	D	550	-	-	7/26/62/62	0/5/5/5
4	TCL	B	706	-	-	0/4/4/4	0/2/2/2
4	TCL	C	708	-	-	0/4/4/4	0/2/2/2
3	NAD	C	750	-	-	5/26/62/62	0/5/5/5
4	TCL	D	707	-	-	0/4/4/4	0/2/2/2
3	NAD	A	650	-	-	4/26/62/62	0/5/5/5
4	TCL	A	705	-	-	0/4/4/4	0/2/2/2

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	650	NAD	O7N-C7N	8.96	1.40	1.24
3	B	1450	NAD	O7N-C7N	8.58	1.40	1.24
3	C	750	NAD	O7N-C7N	8.16	1.39	1.24
3	D	550	NAD	O7N-C7N	8.08	1.39	1.24
4	D	707	TCL	C6-C5	4.87	1.48	1.40

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	750	NAD	N3A-C2A-N1A	-7.01	119.16	128.67
3	A	650	NAD	N3A-C2A-N1A	-6.91	119.29	128.67
3	D	550	NAD	N3A-C2A-N1A	-6.56	119.77	128.67
3	B	1450	NAD	N3A-C2A-N1A	-6.16	120.32	128.67
3	D	550	NAD	C4B-O4B-C1B	-5.10	105.25	109.92

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

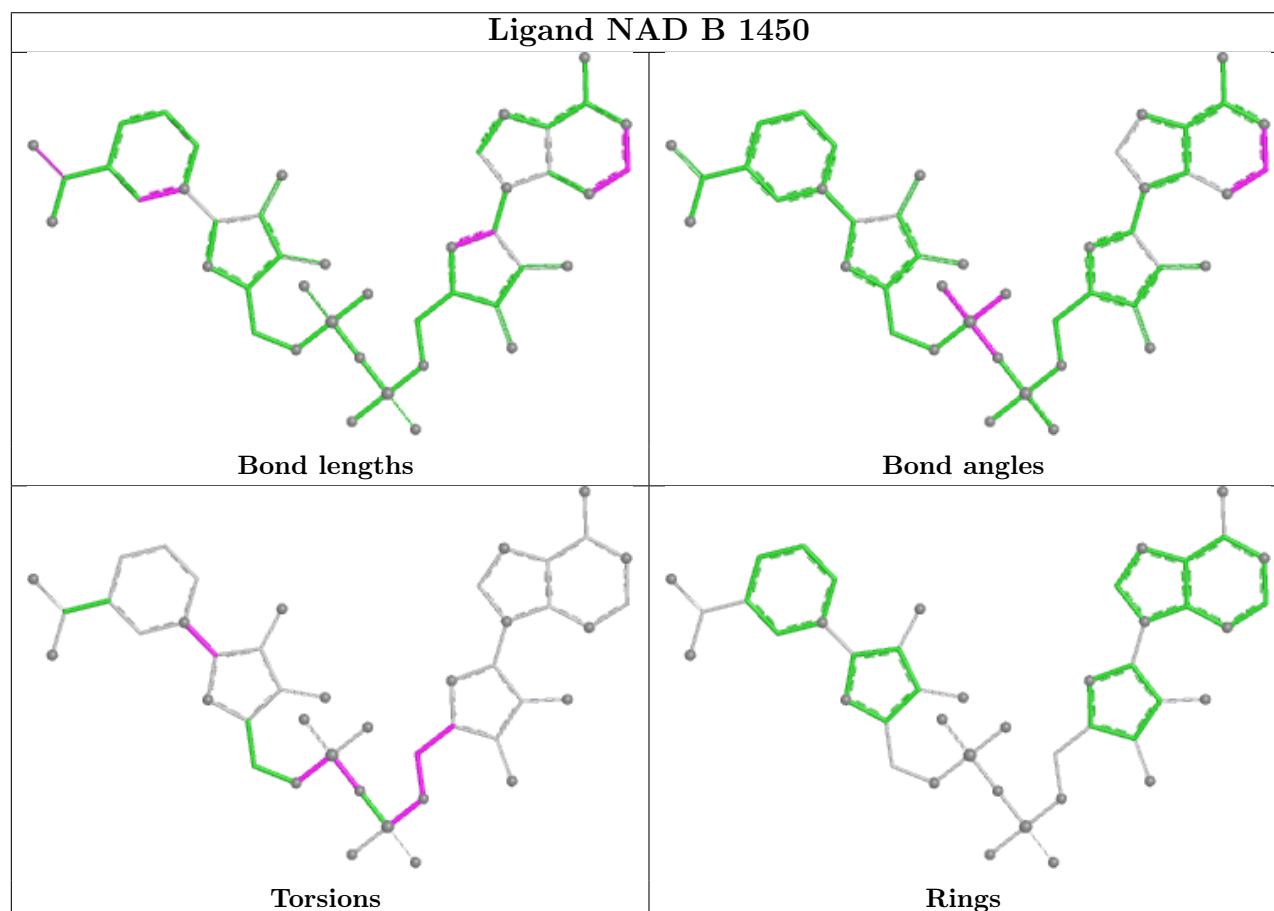
Mol	Chain	Res	Type	Atoms
3	A	650	NAD	C5D-O5D-PN-O3
3	A	650	NAD	C5D-O5D-PN-O1N
3	B	1450	NAD	C5B-O5B-PA-O2A
3	B	1450	NAD	C5B-O5B-PA-O3
3	B	1450	NAD	C5D-O5D-PN-O3

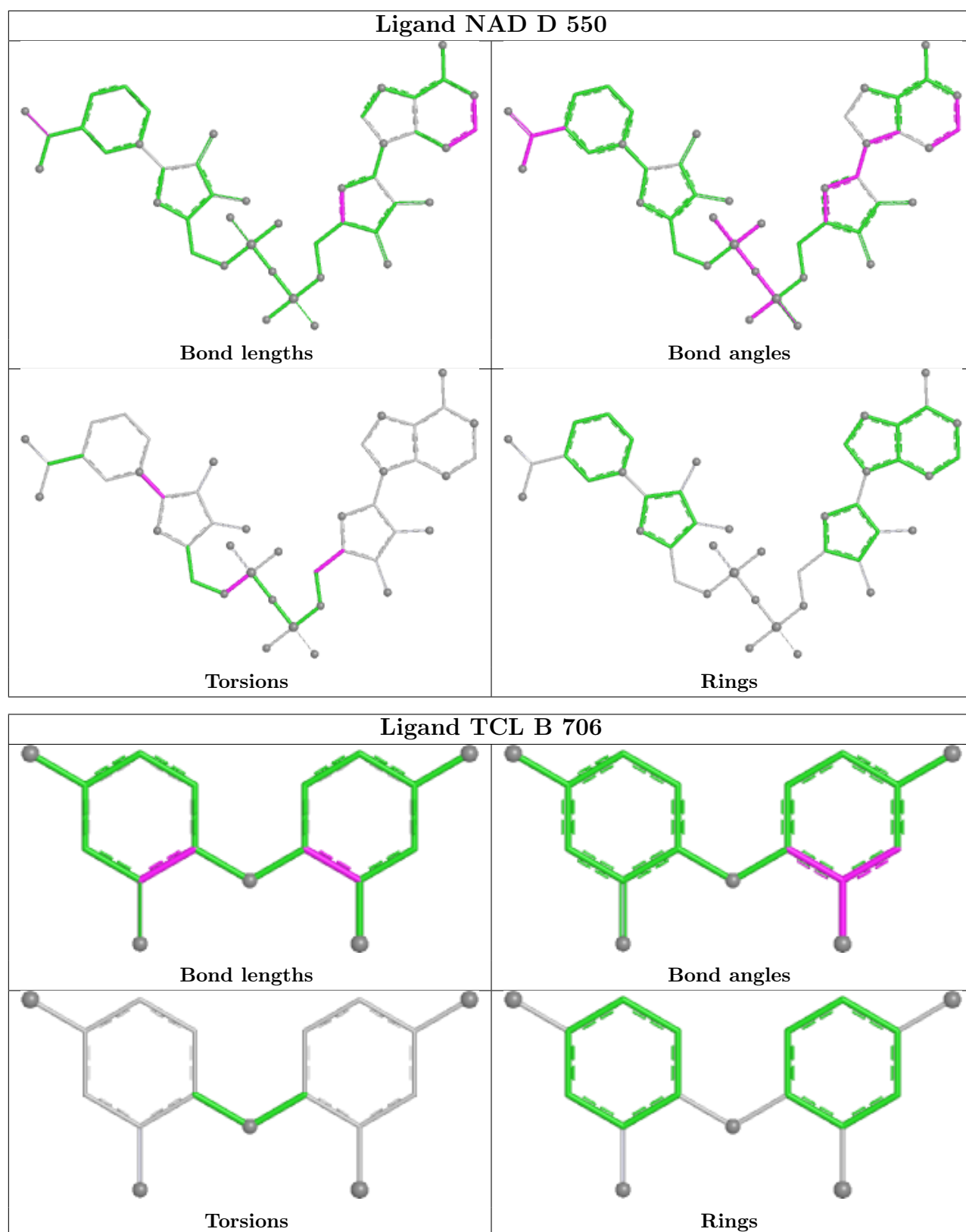
There are no ring outliers.

2 monomers are involved in 2 short contacts:

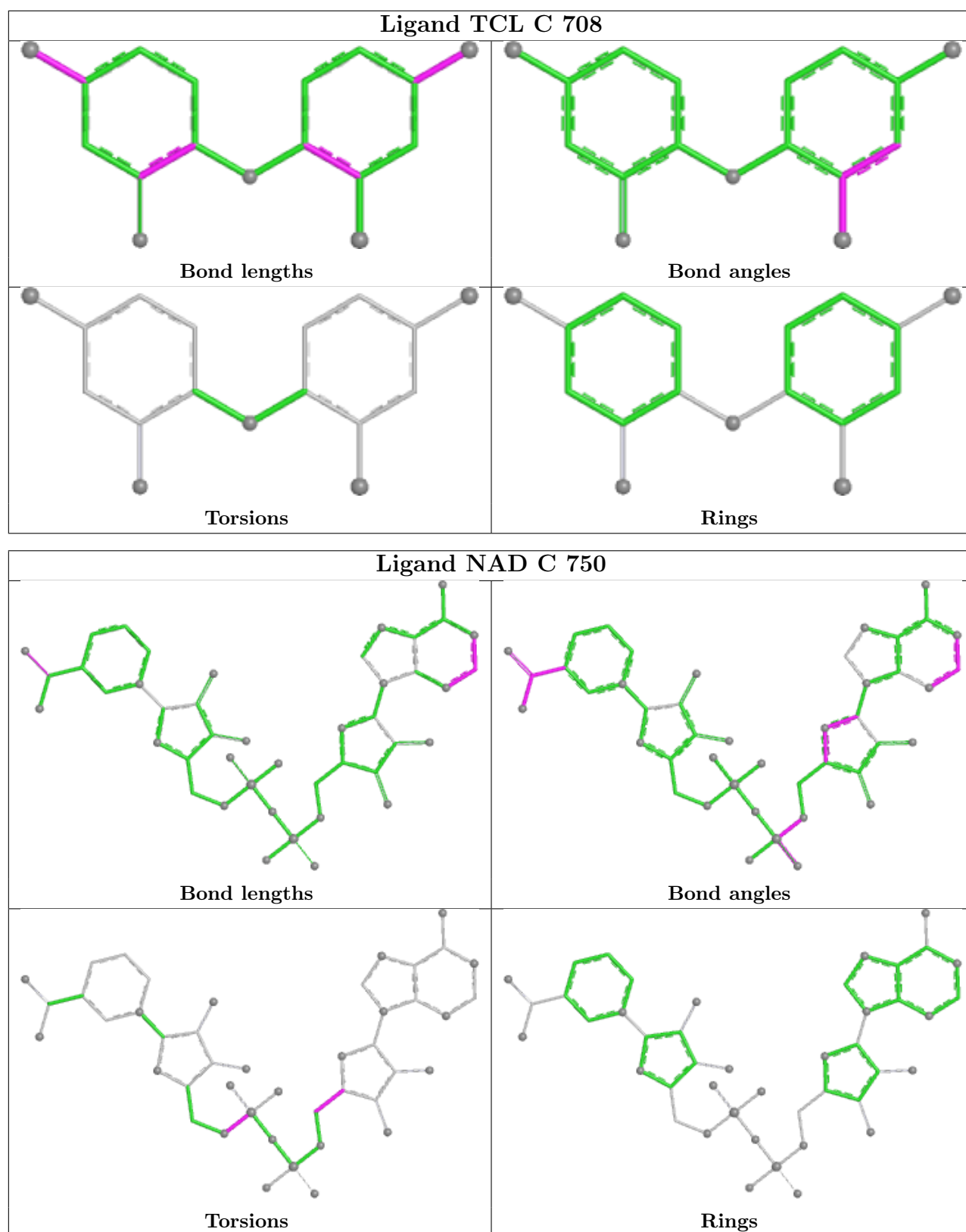
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1450	NAD	1	0
5	D	713	SO4	1	0

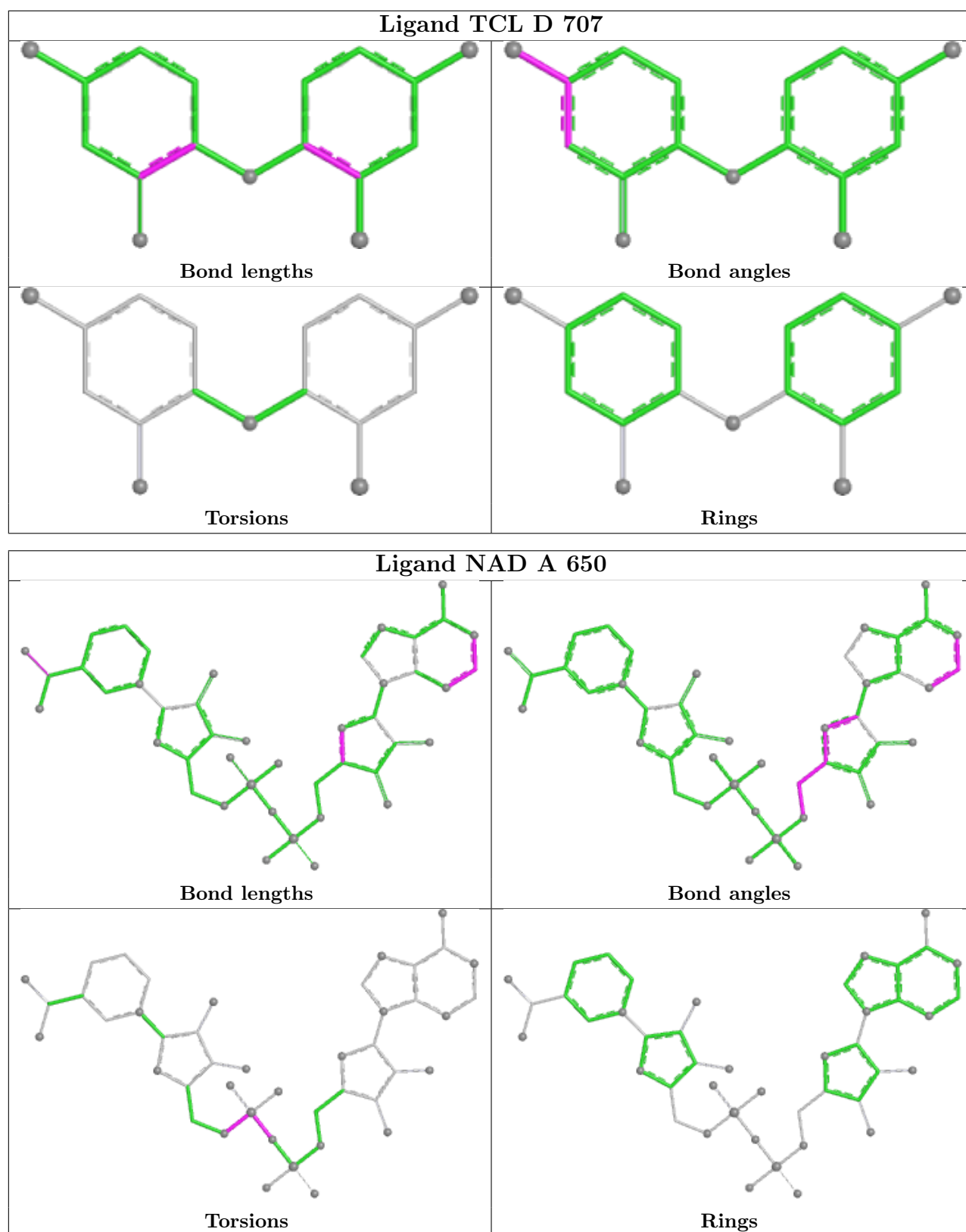
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

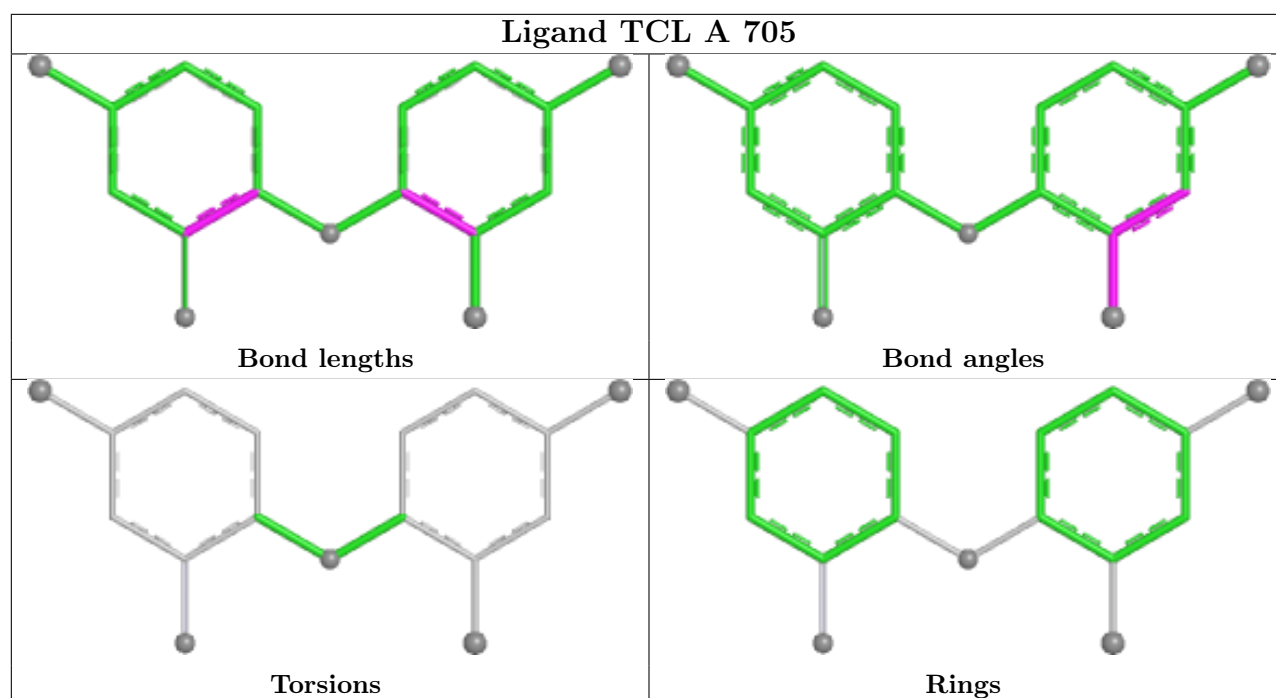












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	290/349 (83%)	-1.56	0 100 100	17, 20, 25, 30	0
1	B	290/349 (83%)	-1.61	0 100 100	13, 20, 25, 32	11 (3%)
1	C	293/349 (83%)	-1.60	0 100 100	15, 20, 26, 33	15 (5%)
1	D	288/349 (82%)	-1.65	0 100 100	17, 20, 25, 30	4 (1%)
All	All	1161/1396 (83%)	-1.61	0 100 100	13, 20, 25, 33	30 (2%)

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

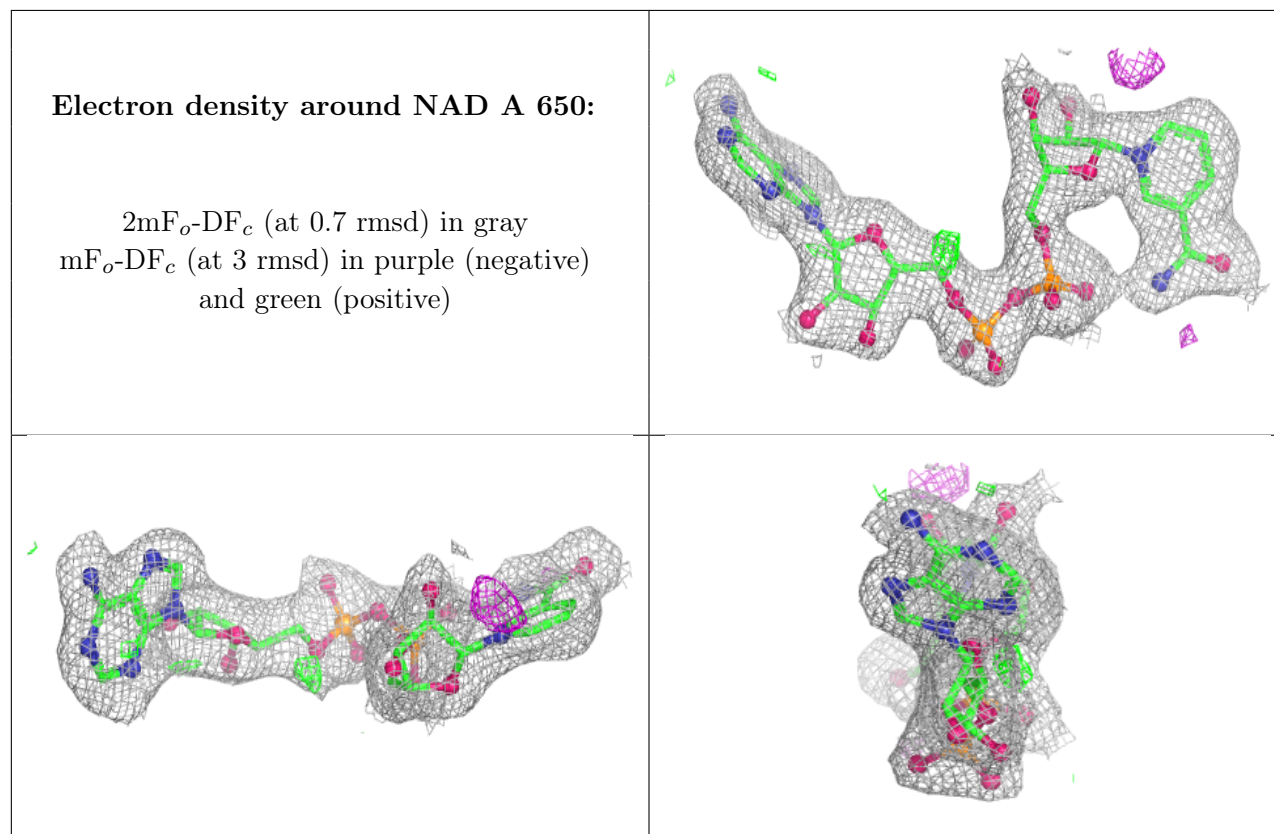
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	SO4	D	713	5/5	0.97	0.06	46,47,48,49	0
2	CL	C	712	1/1	0.99	0.02	23,23,23,23	0
3	NAD	A	650	44/44	0.99	0.03	20,21,24,24	0
3	NAD	B	1450	44/44	0.99	0.02	18,22,25,26	0

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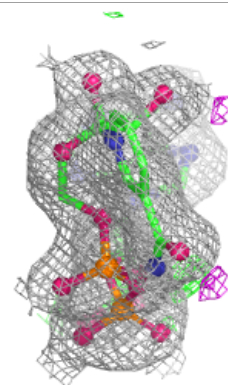
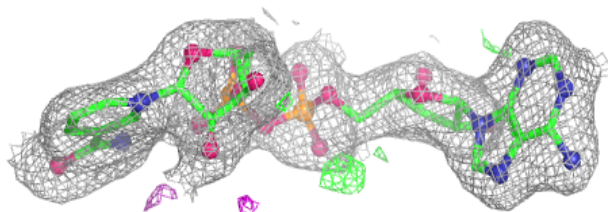
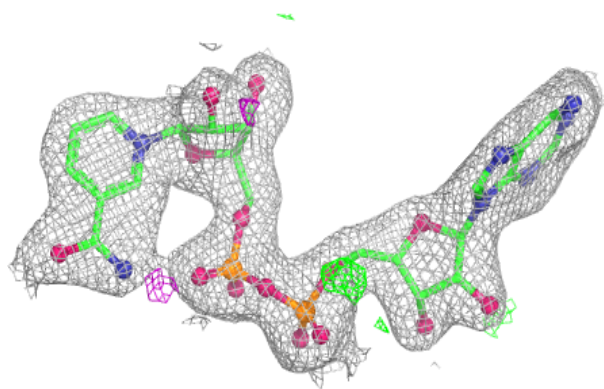
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	B	711	1/1	0.99	0.03	22,22,22,22	0
2	CL	D	709	1/1	1.00	0.02	16,16,16,16	0
3	NAD	C	750	44/44	1.00	0.02	17,21,24,26	0
3	NAD	D	550	44/44	1.00	0.02	20,22,25,28	0
4	TCL	A	705	17/17	1.00	0.02	21,22,22,24	0
4	TCL	B	706	17/17	1.00	0.02	22,23,24,25	0
4	TCL	C	708	17/17	1.00	0.03	21,22,23,23	0
4	TCL	D	707	17/17	1.00	0.02	21,23,26,27	0
2	CL	A	710	1/1	1.00	0.01	14,14,14,14	0

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

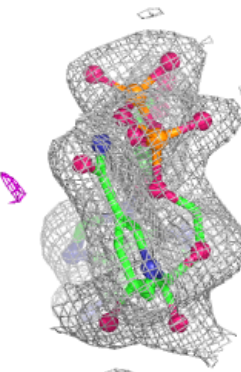
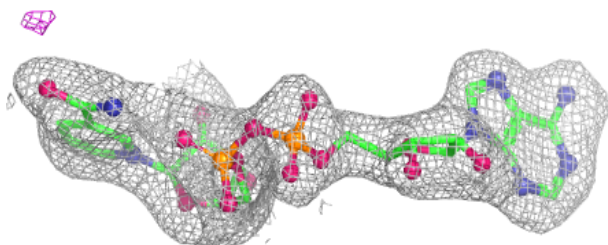
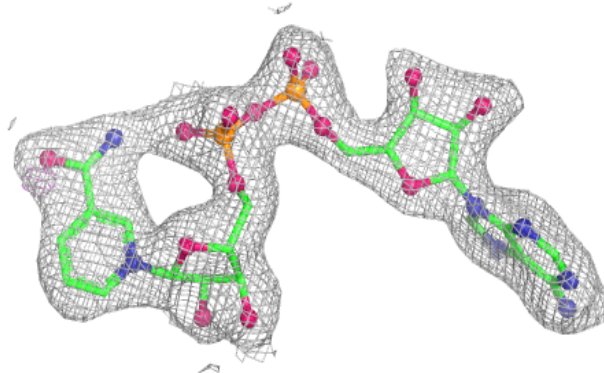


**Electron density around NAD B 1450:**

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

**Electron density around NAD C 750:**

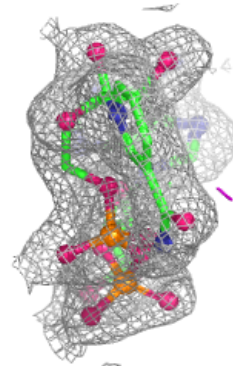
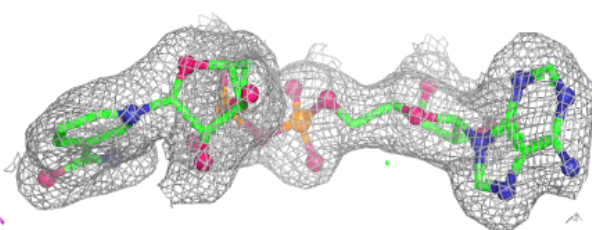
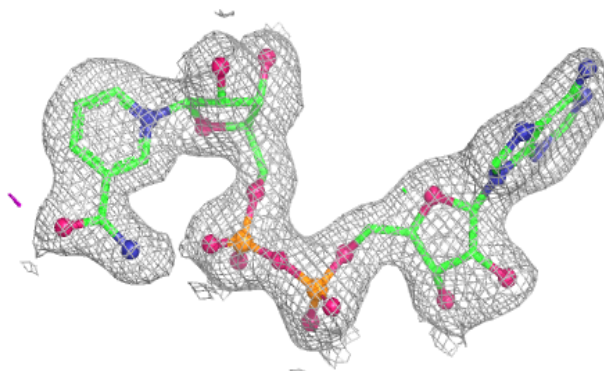
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



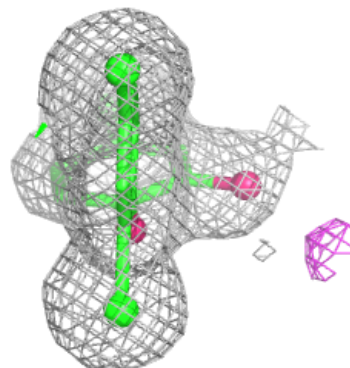
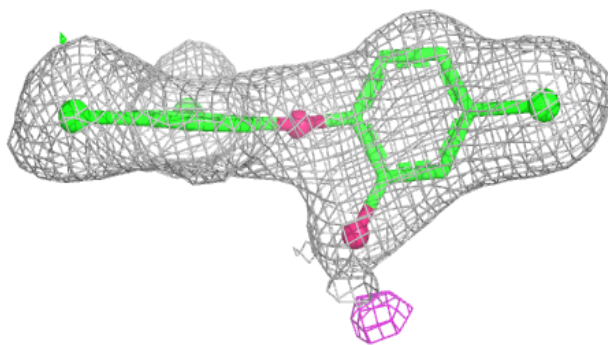
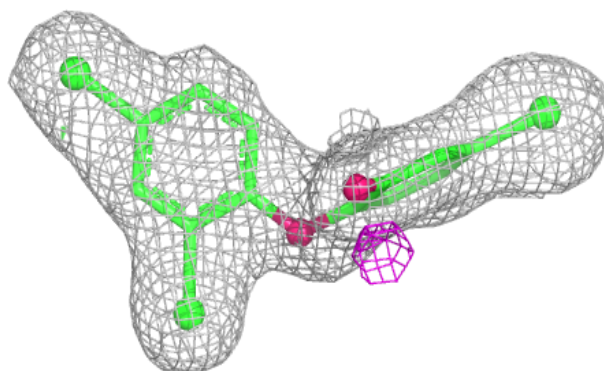


**Electron density around NAD D 550:**

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

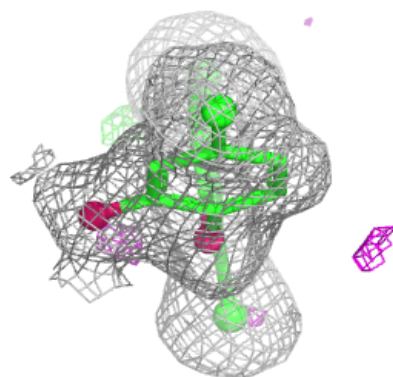
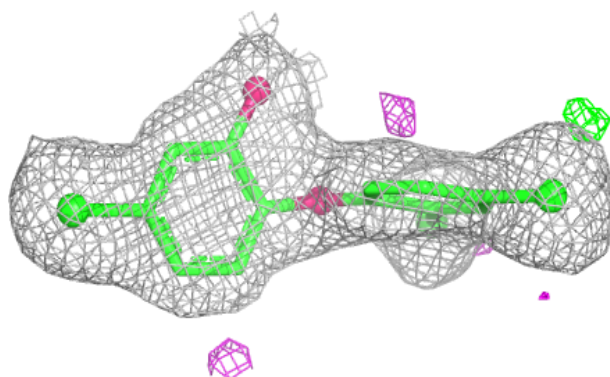
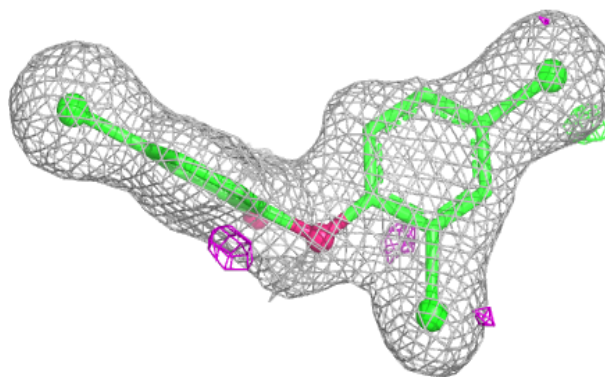
**Electron density around TCL A 705:**

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

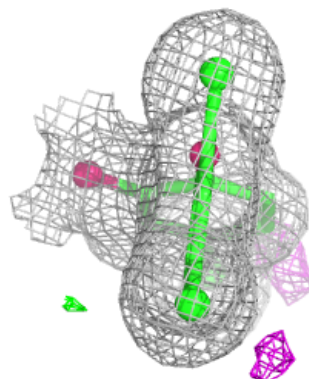
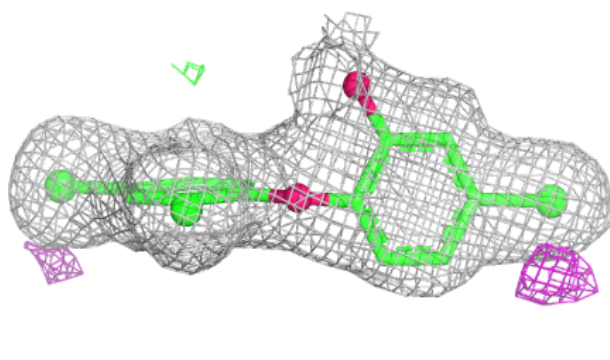
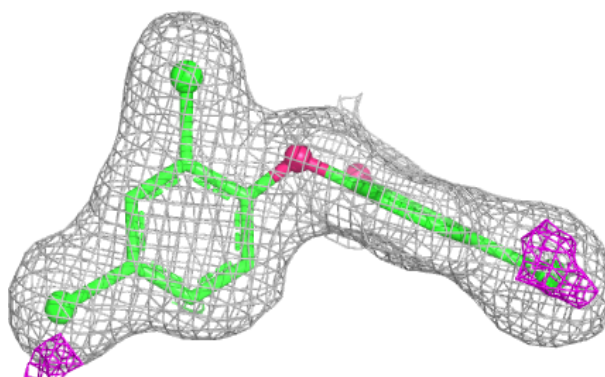


**Electron density around TCL B 706:**

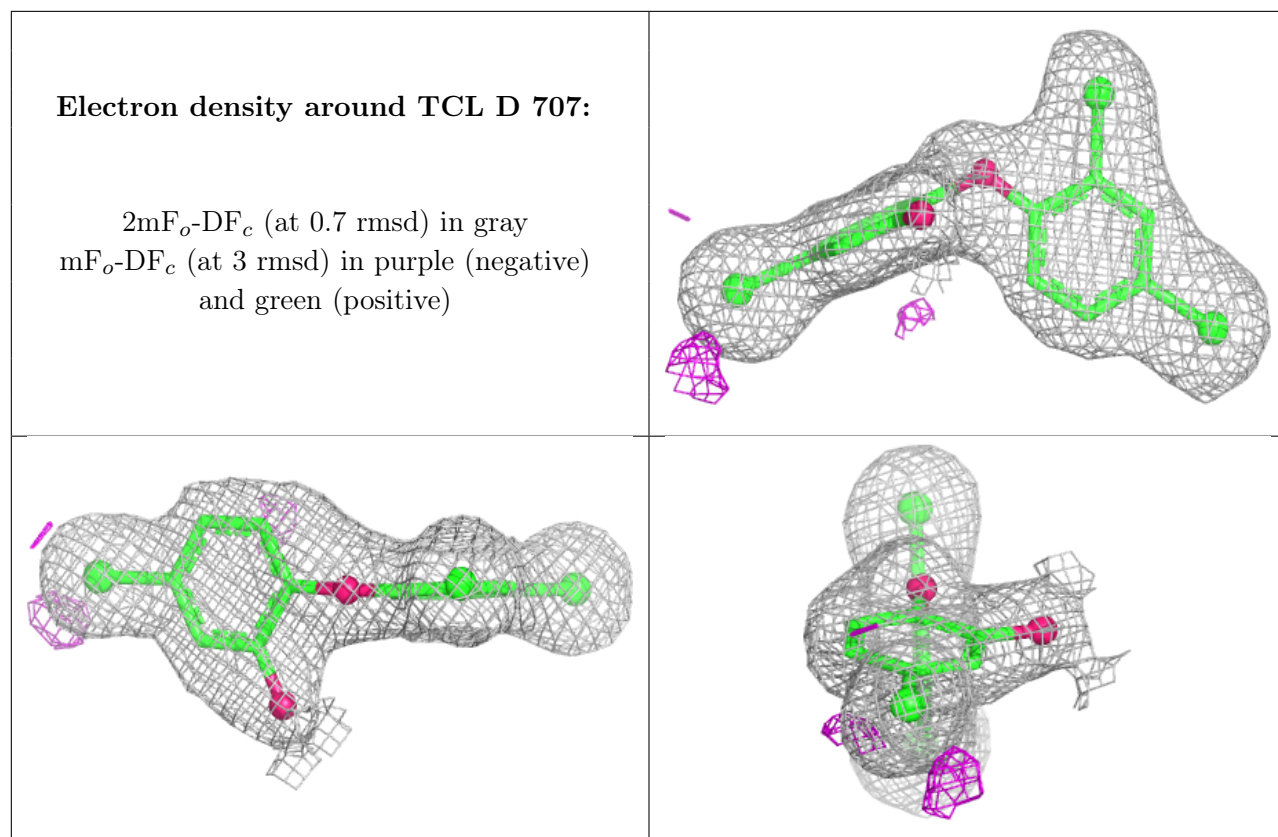
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around TCL C 708:**

$2mF_o-DF_c$  (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.