Full wwPDB X-ray Structure Validation Report (i)

Oct 19, 2020 – 10:09 AM BST

PDB ID	:	6TIA
Title	:	IRAK4 IN COMPLEX WITH inhibitor
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Deposited on	:	2019-11-22
Resolution	:	2.52 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 (i) symbol.

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

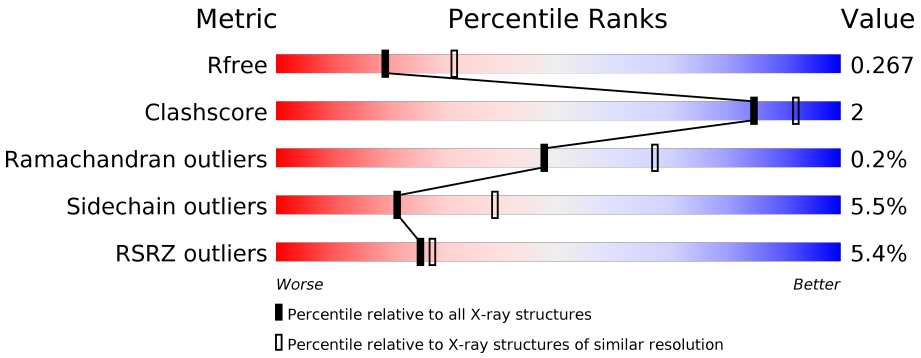
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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}	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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 <=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	308	8%, 84%, 8%, 6%
1	B	308	2%, 83%, 9%, 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ND2	A	505	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5064 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.

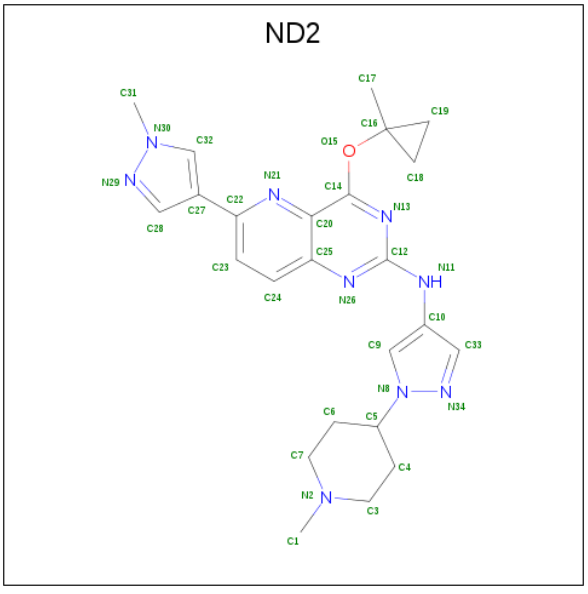
- Molecule 1 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	P	S	0	0	0
			2268	1423	382	447	2	14			
1	B	287	Total	C	N	O	P	S	0	0	0
			2261	1419	381	445	2	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	GLY	-	expression tag	UNP Q9NWZ3
B	153	GLY	-	expression tag	UNP Q9NWZ3

- Molecule 2 is 4-(1-methylcyclopropyl)oxy- {N}-[1-(1-methylpiperidin-4-yl)pyrazol-4-yl]-6 -(1-methylpyrazol-4-yl)pyrido[3,2-d]pyrimidin-2-amine (three-letter code: ND2) (formula: $C_{24}H_{29}N_9O$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			34	24	9	1		
2	A	1	Total	C	N	O	0	0
			34	24	9	1		
2	A	1	Total	C	N	O	0	0
			34	24	9	1		
2	A	1	Total	C	N	O	0	0
			34	24	9	1		
2	A	1	Total	C	N	O	0	0
			34	24	9	1		
2	B	1	Total	C	N	O	0	0
			34	24	9	1		
2	B	1	Total	C	N	O	0	0
			34	24	9	1		
2	B	1	Total	C	N	O	0	0
			34	24	9	1		
2	B	1	Total	C	N	O	0	0
			34	24	9	1		
2	B	1	Total	C	N	O	0	0
			34	24	9	1		

- Molecule 3 is water.

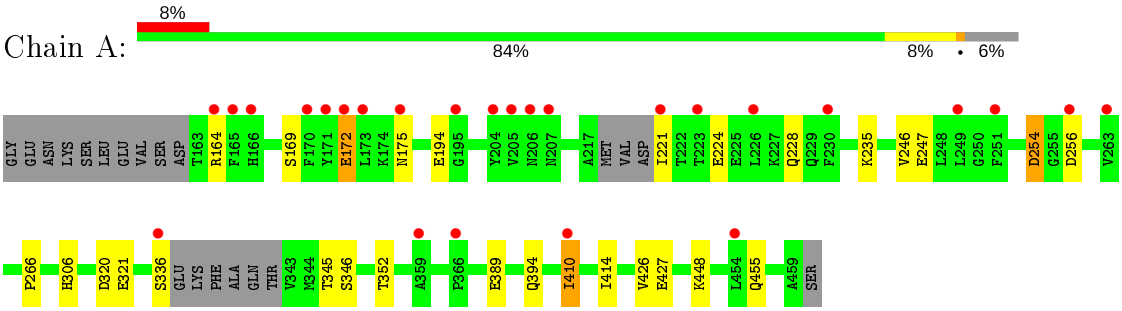
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total	O	0	0
			68	68		
3	B	127	Total	O	0	0
			127	127		

3 Residue-property plots

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

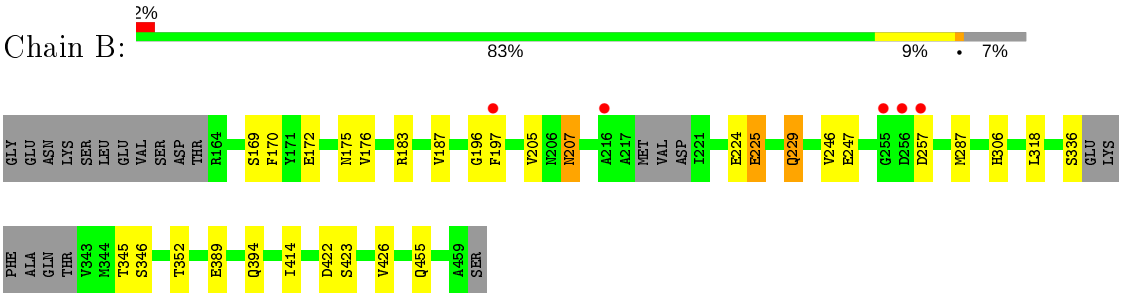
- Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain A:



- Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	90.90Å 140.57Å 56.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.33 – 2.52 76.33 – 2.52	Depositor EDS
% Data completeness (in resolution range)	93.7 (76.33-2.52) 93.7 (76.33-2.52)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.216 , 0.261 0.224 , 0.267	Depositor DCC
R_{free} test set	1164 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	60.8	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 71.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5064	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: TPO, ND2, SEP

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	0/2283	0.68	0/3076
1	B	0.51	0/2276	0.70	0/3066
All	All	0.49	0/4559	0.69	0/6142

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2268	0	2236	7	0
1	B	2261	0	2229	12	0
2	A	170	0	0	1	0
2	B	170	0	0	1	0
3	A	68	0	0	0	0
3	B	127	0	0	1	0
All	All	5064	0	4465	21	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 2.

All (21) 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:A:410:ILE:HG21	1:A:427:GLU:HG2	1.74	0.68
1:B:287:MET:HG2	3:B:713:HOH:O	1.96	0.65
1:B:246:VAL:HG11	1:B:318:LEU:HD12	1.78	0.65
1:A:266:PRO:HD2	1:A:320:ASP:HA	1.86	0.55
1:B:176:VAL:HG11	1:B:205:VAL:HG22	1.91	0.53
1:B:225:GLU:O	1:B:229:GLN:HG2	2.12	0.50
2:A:501:ND2:C33	2:A:501:ND2:N13	2.75	0.49
2:B:503:ND2:C33	2:B:503:ND2:N13	2.75	0.48
1:A:414:ILE:HG12	1:A:426:VAL:HG11	1.96	0.48
1:B:207:ASN:H	1:B:207:ASN:HD22	1.63	0.47
1:B:414:ILE:HG12	1:B:426:VAL:HG11	1.98	0.45
1:A:169:SER:H	1:A:172:GLU:HG2	1.81	0.44
1:B:170:PHE:CE1	1:B:257:ASP:HB3	2.53	0.43
1:B:169:SER:HB3	1:B:172:GLU:HG3	2.02	0.42
1:A:389:GLU:HA	1:A:394:GLN:HE21	1.85	0.41
1:B:196:GLY:HA2	1:B:197:PHE:HA	1.88	0.41
1:B:389:GLU:HA	1:B:394:GLN:HE21	1.86	0.41
1:B:306:HIS:HB3	1:B:336:SER:HB2	2.03	0.41
1:B:183:ARG:HH21	1:B:187:VAL:HG12	1.86	0.41
1:A:410:ILE:O	1:A:414:ILE:HG13	2.20	0.40
1:A:306:HIS:HB3	1:A:336:SER:HB2	2.03	0.40

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	280/308 (91%)	271 (97%)	8 (3%)	1 (0%)	34 53
1	B	279/308 (91%)	264 (95%)	15 (5%)	0	100 100
All	All	559/616 (91%)	535 (96%)	23 (4%)	1 (0%)	47 67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	248/266 (93%)	231 (93%)	17 (7%)	15 28
1	B	247/266 (93%)	237 (96%)	10 (4%)	31 54
All	All	495/532 (93%)	468 (94%)	27 (6%)	21 39

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	ARG
1	A	172	GLU
1	A	175	ASN
1	A	194	GLU
1	A	221	ILE
1	A	224	GLU
1	A	228	GLN
1	A	235	LYS
1	A	246	VAL
1	A	247	GLU
1	A	254	ASP
1	A	256	ASP
1	A	321	GLU
1	A	352	THR
1	A	410	ILE
1	A	448	LYS
1	A	455	GLN
1	B	175	ASN
1	B	207	ASN
1	B	224	GLU
1	B	225	GLU
1	B	229	GLN

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Mol	Chain	Res	Type
1	B	247	GLU
1	B	352	THR
1	B	422	ASP
1	B	423	SER
1	B	455	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	A	293	GLN
1	A	394	GLN
1	B	207	ASN
1	B	293	GLN
1	B	394	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	SEP	B	346	1	8,9,10	0.96	1 (12%)	8,12,14	1.33	1 (12%)
1	TPO	A	345	1	8,10,11	1.37	2 (25%)	10,14,16	1.18	0
1	SEP	A	346	1	8,9,10	0.69	0	8,12,14	1.26	1 (12%)
1	TPO	B	345	1	8,10,11	1.33	2 (25%)	10,14,16	1.02	0

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
1	SEP	B	346	1	-	0/5/8/10	-
1	TPO	A	345	1	-	3/9/11/13	-
1	SEP	A	346	1	-	1/5/8/10	-
1	TPO	B	345	1	-	3/9/11/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	345	TPO	CG2-CB	2.40	1.57	1.51
1	A	345	TPO	CB-CA	2.26	1.58	1.53
1	B	346	SEP	P-O1P	2.10	1.57	1.50
1	A	345	TPO	CG2-CB	2.08	1.56	1.51
1	B	345	TPO	CB-CA	2.08	1.58	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	346	SEP	O3P-P-OG	3.03	114.80	106.73
1	B	346	SEP	OG-P-O1P	2.74	114.15	106.47

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	A	345	TPO	O-C-CA-CB
1	A	345	TPO	CB-OG1-P-O1P
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	O-C-CA-CB
1	A	346	SEP	CB-OG-P-O1P
1	B	345	TPO	CB-OG1-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ND2	A	501	-	33,39,39	1.38	3 (9%)	39,58,58	2.55	16 (41%)
2	ND2	A	504	-	33,39,39	1.45	3 (9%)	39,58,58	2.35	15 (38%)
2	ND2	A	505	-	33,39,39	1.53	3 (9%)	39,58,58	2.78	15 (38%)
2	ND2	B	503	-	33,39,39	1.56	4 (12%)	39,58,58	2.78	17 (43%)
2	ND2	B	504	-	33,39,39	1.53	3 (9%)	39,58,58	2.16	10 (25%)
2	ND2	B	501	-	33,39,39	1.62	4 (12%)	39,58,58	2.79	17 (43%)
2	ND2	A	503	-	33,39,39	1.56	4 (12%)	39,58,58	2.64	14 (35%)
2	ND2	B	505	-	33,39,39	1.36	3 (9%)	39,58,58	3.15	17 (43%)
2	ND2	B	502	-	33,39,39	1.44	3 (9%)	39,58,58	2.40	16 (41%)
2	ND2	A	502	-	33,39,39	1.41	3 (9%)	39,58,58	2.24	14 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ND2	A	501	-	-	2/7/31/31	0/6/6/6
2	ND2	A	504	-	-	0/7/31/31	0/6/6/6
2	ND2	A	505	-	-	3/7/31/31	0/6/6/6
2	ND2	B	503	-	-	0/7/31/31	0/6/6/6
2	ND2	B	504	-	-	4/7/31/31	0/6/6/6
2	ND2	B	501	-	-	0/7/31/31	0/6/6/6
2	ND2	A	503	-	-	3/7/31/31	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ND2	B	505	-	-	1/7/31/31	0/6/6/6
2	ND2	B	502	-	-	1/7/31/31	0/6/6/6
2	ND2	A	502	-	-	1/7/31/31	0/6/6/6

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	ND2	C18-C16	5.03	1.54	1.49
2	B	501	ND2	C19-C16	5.02	1.54	1.49
2	A	503	ND2	C18-C16	4.86	1.54	1.49
2	B	504	ND2	C18-C16	4.79	1.54	1.49
2	B	503	ND2	C19-C16	4.66	1.54	1.49
2	A	505	ND2	C19-C16	4.62	1.54	1.49
2	A	502	ND2	C18-C16	4.49	1.53	1.49
2	A	505	ND2	C18-C16	4.47	1.53	1.49
2	B	502	ND2	C19-C16	4.46	1.53	1.49
2	B	502	ND2	C18-C16	4.43	1.53	1.49
2	B	503	ND2	C18-C16	4.40	1.53	1.49
2	B	504	ND2	C19-C16	4.38	1.53	1.49
2	A	504	ND2	C19-C16	4.35	1.53	1.49
2	B	505	ND2	C19-C16	4.35	1.53	1.49
2	A	503	ND2	C19-C16	4.27	1.53	1.49
2	A	502	ND2	C19-C16	4.10	1.53	1.49
2	A	504	ND2	C18-C16	4.05	1.53	1.49
2	A	501	ND2	C19-C16	3.80	1.53	1.49
2	A	501	ND2	C18-C16	3.73	1.53	1.49
2	B	505	ND2	C18-C16	3.34	1.52	1.49
2	B	501	ND2	C9-N8	2.78	1.38	1.35
2	B	504	ND2	C33-C10	2.75	1.41	1.38
2	A	501	ND2	C33-C10	2.70	1.41	1.38
2	B	503	ND2	C9-N8	2.62	1.38	1.35
2	A	503	ND2	C33-C10	2.55	1.41	1.38
2	A	504	ND2	C33-C10	2.54	1.41	1.38
2	B	503	ND2	C12-N11	2.54	1.41	1.36
2	A	502	ND2	C33-C10	2.46	1.41	1.38
2	A	505	ND2	C33-C10	2.40	1.40	1.38
2	B	505	ND2	C33-C10	2.38	1.40	1.38
2	A	503	ND2	C12-N11	2.29	1.41	1.36
2	B	502	ND2	C33-C10	2.16	1.40	1.38
2	B	501	ND2	C7-N2	2.05	1.50	1.46

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	505	ND2	C16-O15-C14	9.21	132.59	123.25
2	B	505	ND2	C7-C6-C5	7.90	116.62	110.44
2	A	503	ND2	C22-N21-C20	7.01	123.64	118.26
2	B	505	ND2	C16-O15-C14	6.87	130.22	123.25
2	B	503	ND2	C9-N8-C5	6.73	131.44	125.48
2	B	505	ND2	C3-C4-C5	6.28	115.35	110.44
2	B	505	ND2	C22-N21-C20	6.25	123.06	118.26
2	B	501	ND2	C9-N8-C5	5.95	130.75	125.48
2	B	501	ND2	C7-C6-C5	5.86	115.03	110.44
2	A	503	ND2	C31-N30-N29	5.65	127.15	120.50
2	A	505	ND2	C22-N21-C20	5.48	122.47	118.26
2	A	501	ND2	C12-N13-C14	5.27	124.48	115.18
2	B	501	ND2	C12-N13-C14	5.24	124.42	115.18
2	A	503	ND2	C12-N13-C14	5.20	124.35	115.18
2	B	503	ND2	C22-N21-C20	5.18	122.23	118.26
2	A	501	ND2	C3-C4-C5	-5.17	106.40	110.44
2	B	503	ND2	C31-N30-N29	5.10	126.50	120.50
2	B	505	ND2	C31-N30-N29	5.05	126.44	120.50
2	A	505	ND2	C31-N30-N29	4.99	126.37	120.50
2	B	504	ND2	C31-N30-N29	4.94	126.31	120.50
2	B	505	ND2	C12-N13-C14	4.90	123.83	115.18
2	B	502	ND2	C31-N30-N29	4.87	126.22	120.50
2	B	503	ND2	C12-N13-C14	4.85	123.74	115.18
2	A	505	ND2	C12-N13-C14	4.78	123.62	115.18
2	B	502	ND2	C22-N21-C20	4.71	121.88	118.26
2	B	505	ND2	C28-N29-N30	4.64	109.06	104.23
2	A	503	ND2	C32-N30-N29	-4.62	107.53	111.56
2	A	504	ND2	C7-C6-C5	4.62	114.05	110.44
2	A	503	ND2	C28-N29-N30	4.62	109.04	104.23
2	A	501	ND2	C9-N8-C5	4.61	129.56	125.48
2	A	504	ND2	C22-N21-C20	4.59	121.78	118.26
2	B	501	ND2	C22-N21-C20	4.57	121.76	118.26
2	A	502	ND2	C28-N29-N30	4.55	108.97	104.23
2	A	505	ND2	C28-N29-N30	4.55	108.96	104.23
2	B	505	ND2	C32-N30-N29	-4.53	107.61	111.56
2	A	504	ND2	C12-N13-C14	4.48	123.09	115.18
2	B	504	ND2	C28-N29-N30	4.48	108.89	104.23
2	A	502	ND2	C12-N13-C14	4.42	122.98	115.18
2	B	503	ND2	C32-N30-N29	-4.42	107.71	111.56
2	A	502	ND2	C32-N30-N29	-4.41	107.72	111.56
2	B	504	ND2	C32-N30-N29	-4.38	107.74	111.56
2	A	502	ND2	C31-N30-N29	4.38	125.65	120.50
2	B	503	ND2	C28-N29-N30	4.36	108.77	104.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	504	ND2	C31-N30-N29	4.35	125.62	120.50
2	B	504	ND2	C12-N13-C14	4.34	122.84	115.18
2	A	501	ND2	C28-N29-N30	4.34	108.75	104.23
2	B	503	ND2	O15-C14-N13	4.33	126.12	118.86
2	B	501	ND2	C6-C7-N2	4.31	117.01	111.22
2	B	501	ND2	N26-C12-N13	-4.31	119.41	126.23
2	B	502	ND2	C9-N8-C5	4.28	129.27	125.48
2	A	501	ND2	C22-N21-C20	4.27	121.54	118.26
2	B	504	ND2	C22-N21-C20	4.26	121.53	118.26
2	A	505	ND2	C32-N30-N29	-4.24	107.87	111.56
2	B	501	ND2	C7-N2-C3	4.23	115.44	109.52
2	B	502	ND2	C12-N13-C14	4.20	122.59	115.18
2	B	503	ND2	C16-O15-C14	4.18	127.49	123.25
2	A	501	ND2	C32-N30-N29	-4.17	107.93	111.56
2	A	503	ND2	C16-O15-C14	4.15	127.46	123.25
2	B	502	ND2	C16-O15-C14	4.08	127.39	123.25
2	A	504	ND2	C3-C4-C5	4.06	113.62	110.44
2	A	504	ND2	C28-N29-N30	3.97	108.37	104.23
2	A	501	ND2	C31-N30-N29	3.93	125.12	120.50
2	B	502	ND2	C28-N29-N30	3.93	108.32	104.23
2	B	501	ND2	C12-N26-C25	3.89	121.94	115.60
2	A	502	ND2	C22-N21-C20	3.87	121.23	118.26
2	A	504	ND2	C32-N30-N29	-3.81	108.24	111.56
2	A	502	ND2	C7-N2-C3	3.80	114.84	109.52
2	B	501	ND2	C16-O15-C14	-3.80	119.39	123.25
2	B	505	ND2	C6-C5-C4	3.74	117.31	110.16
2	A	503	ND2	C20-C14-N13	-3.70	116.21	123.26
2	B	503	ND2	N26-C12-N13	-3.63	120.49	126.23
2	B	501	ND2	C31-N30-N29	3.60	124.74	120.50
2	A	501	ND2	N26-C12-N13	-3.60	120.54	126.23
2	B	502	ND2	C32-N30-N29	-3.55	108.47	111.56
2	B	501	ND2	C32-N30-N29	-3.54	108.47	111.56
2	A	505	ND2	C12-N26-C25	3.52	121.34	115.60
2	A	503	ND2	N26-C12-N13	-3.48	120.72	126.23
2	A	501	ND2	C7-N2-C3	3.46	114.36	109.52
2	B	501	ND2	C28-N29-N30	3.43	107.81	104.23
2	A	505	ND2	N26-C12-N13	-3.43	120.80	126.23
2	A	501	ND2	C7-C6-C5	-3.42	107.76	110.44
2	B	502	ND2	C9-C10-C33	3.40	107.60	106.02
2	A	505	ND2	C17-C16-C19	-3.38	113.08	119.99
2	B	503	ND2	C20-C14-N13	-3.34	116.90	123.26
2	A	505	ND2	C20-C14-N13	-3.33	116.92	123.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	505	ND2	C12-N26-C25	3.32	121.01	115.60
2	A	504	ND2	C12-N26-C25	3.30	120.97	115.60
2	B	504	ND2	C12-N26-C25	3.23	120.86	115.60
2	B	505	ND2	C20-C14-N13	-3.23	117.11	123.26
2	B	504	ND2	N26-C12-N13	-3.23	121.13	126.23
2	B	504	ND2	C7-N2-C3	3.22	114.03	109.52
2	B	503	ND2	C12-N26-C25	3.22	120.85	115.60
2	B	502	ND2	C7-N2-C3	3.20	114.00	109.52
2	B	505	ND2	N26-C12-N13	-3.16	121.22	126.23
2	A	503	ND2	C3-C4-C5	3.16	112.91	110.44
2	A	503	ND2	C12-N26-C25	3.15	120.73	115.60
2	A	504	ND2	N26-C12-N13	-3.14	121.26	126.23
2	B	502	ND2	C12-N26-C25	3.13	120.71	115.60
2	A	504	ND2	C20-C14-N13	-3.11	117.35	123.26
2	B	502	ND2	C20-C14-N13	-3.10	117.36	123.26
2	B	502	ND2	O15-C14-N13	3.09	124.05	118.86
2	A	502	ND2	N26-C12-N13	-3.09	121.34	126.23
2	A	502	ND2	C12-N26-C25	3.08	120.62	115.60
2	A	501	ND2	C20-C14-N13	-3.07	117.41	123.26
2	A	502	ND2	C9-N8-C5	3.06	128.19	125.48
2	B	504	ND2	C24-C25-N26	3.06	123.36	118.69
2	A	502	ND2	C16-O15-C14	-3.04	120.16	123.25
2	A	501	ND2	C12-N26-C25	3.03	120.54	115.60
2	B	503	ND2	C24-C25-N26	3.03	123.31	118.69
2	A	504	ND2	O15-C14-N13	3.02	123.93	118.86
2	B	501	ND2	C3-C4-C5	-3.00	108.09	110.44
2	B	503	ND2	C7-C6-C5	2.99	112.78	110.44
2	B	501	ND2	C24-C25-N26	2.92	123.15	118.69
2	B	505	ND2	C6-C7-N2	2.91	115.12	111.22
2	B	505	ND2	C25-C20-N21	-2.88	118.20	121.31
2	A	503	ND2	C24-C25-N26	2.76	122.91	118.69
2	B	501	ND2	C20-C14-N13	-2.76	118.01	123.26
2	A	505	ND2	C25-C20-N21	-2.73	118.36	121.31
2	B	505	ND2	O15-C14-N13	-2.70	114.34	118.86
2	B	504	ND2	C20-C14-N13	-2.69	118.14	123.26
2	B	503	ND2	C17-C16-C18	-2.60	114.68	119.99
2	B	502	ND2	N26-C12-N13	-2.59	122.13	126.23
2	A	502	ND2	C20-C14-N13	-2.57	118.37	123.26
2	A	501	ND2	C9-C10-C33	2.50	107.18	106.02
2	B	503	ND2	C6-C5-C4	2.46	114.86	110.16
2	B	503	ND2	C7-N2-C3	2.46	112.96	109.52
2	A	503	ND2	C17-C16-C19	-2.42	115.05	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	504	ND2	C24-C25-N26	2.34	122.26	118.69
2	B	502	ND2	C24-C25-N26	2.30	122.21	118.69
2	A	501	ND2	C4-C3-N2	-2.29	108.16	111.22
2	A	501	ND2	C24-C25-N26	2.29	122.18	118.69
2	B	501	ND2	C18-C16-C19	-2.28	59.29	61.21
2	A	502	ND2	C27-C22-N21	2.24	120.20	117.09
2	A	505	ND2	C7-N2-C3	2.24	112.66	109.52
2	B	503	ND2	C3-C4-C5	2.17	112.14	110.44
2	A	503	ND2	C9-N8-C5	2.17	127.40	125.48
2	A	504	ND2	C17-C16-C19	-2.16	115.57	119.99
2	A	502	ND2	C24-C25-N26	2.14	121.95	118.69
2	A	505	ND2	N11-C12-N13	2.13	124.14	116.92
2	B	505	ND2	C17-C16-C18	-2.12	115.65	119.99
2	A	501	ND2	C10-N11-C12	-2.12	123.09	129.23
2	A	504	ND2	C9-C10-C33	2.12	107.00	106.02
2	A	503	ND2	C7-N2-C3	2.09	112.45	109.52
2	B	502	ND2	C17-C16-C18	-2.09	115.72	119.99
2	B	505	ND2	C9-C10-C33	2.08	106.98	106.02
2	A	505	ND2	C18-C16-C19	-2.07	59.46	61.21
2	A	504	ND2	C6-C5-C4	2.06	114.10	110.16
2	A	502	ND2	C9-C10-C33	2.05	106.97	106.02
2	B	501	ND2	C1-N2-C3	-2.02	107.64	110.66
2	A	505	ND2	C9-C10-C33	2.01	106.95	106.02
2	B	502	ND2	C18-C16-C19	-2.01	59.51	61.21

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	504	ND2	N13-C14-O15-C16
2	B	504	ND2	C18-C16-O15-C14
2	A	503	ND2	N13-C14-O15-C16
2	A	503	ND2	C18-C16-O15-C14
2	B	502	ND2	C19-C16-O15-C14
2	A	502	ND2	N13-C14-O15-C16
2	A	501	ND2	C19-C16-O15-C14
2	A	501	ND2	C18-C16-O15-C14
2	A	505	ND2	C19-C16-O15-C14
2	A	505	ND2	C18-C16-O15-C14
2	B	504	ND2	C19-C16-O15-C14
2	A	503	ND2	C19-C16-O15-C14
2	A	505	ND2	N13-C14-O15-C16

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Mol	Chain	Res	Type	Atoms
2	B	505	ND2	N13-C14-O15-C16
2	B	504	ND2	N13-C12-N11-C10

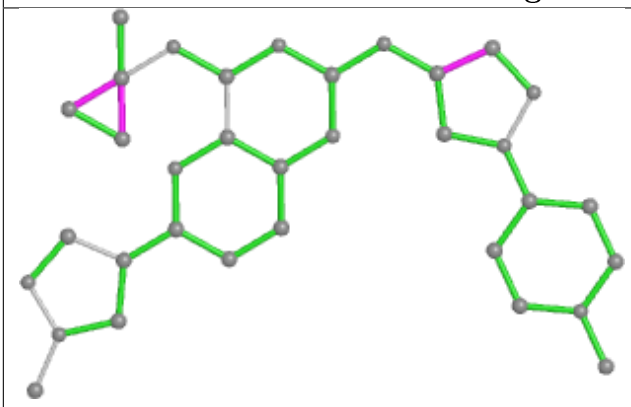
There are no ring outliers.

2 monomers are involved in 2 short contacts:

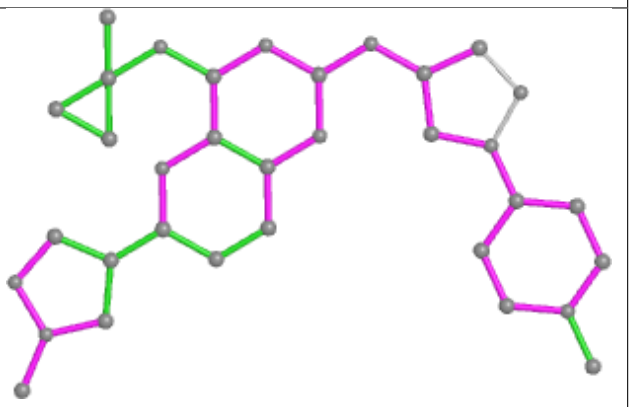
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	ND2	1	0
2	B	503	ND2	1	0

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 then 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.

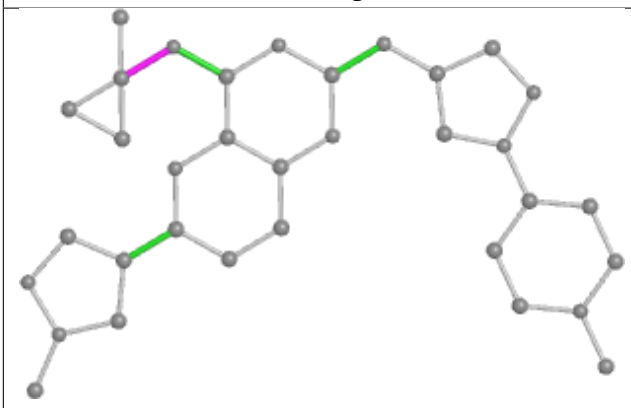
Ligand ND2 A 501



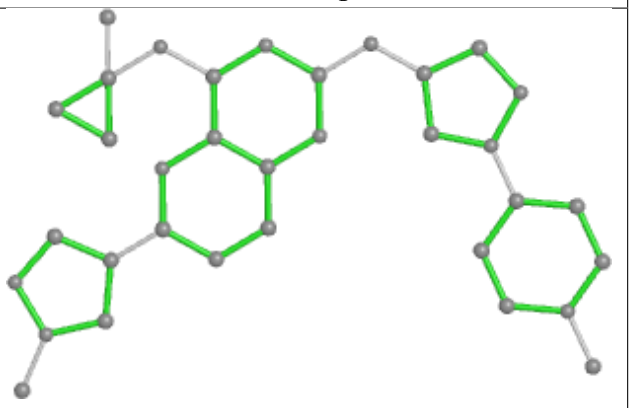
Bond lengths



Bond angles

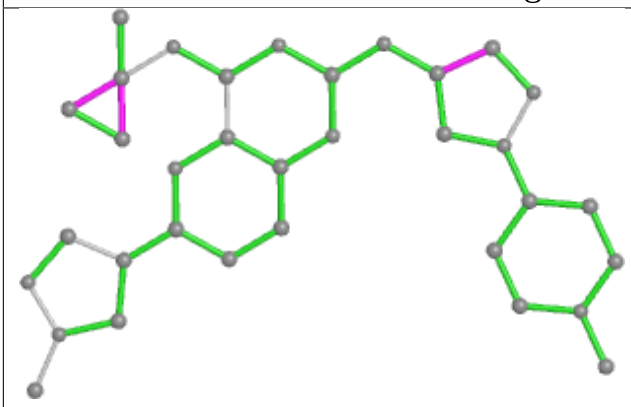


Torsions

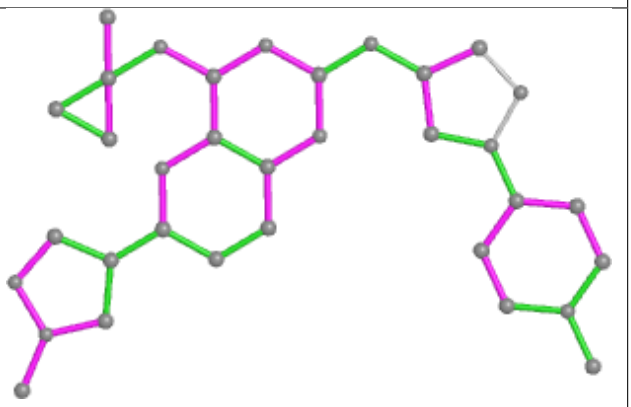


Rings

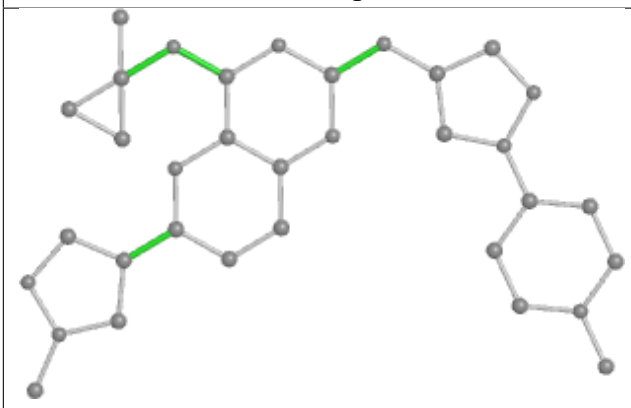
Ligand ND2 A 504



Bond lengths



Bond angles



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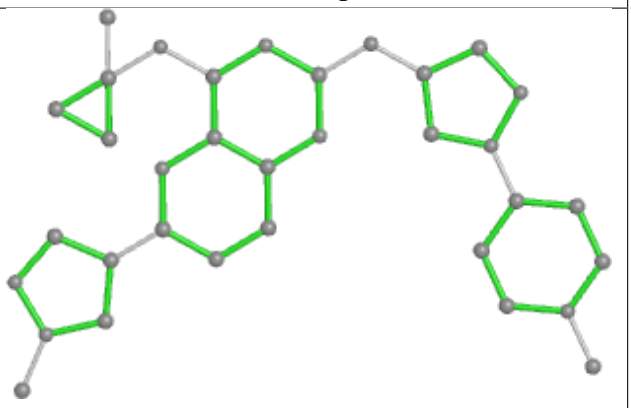
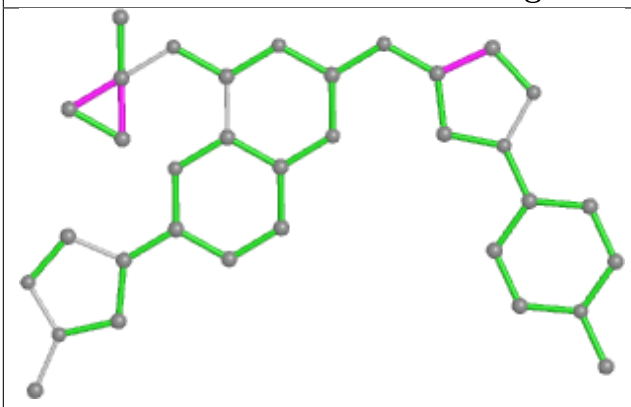
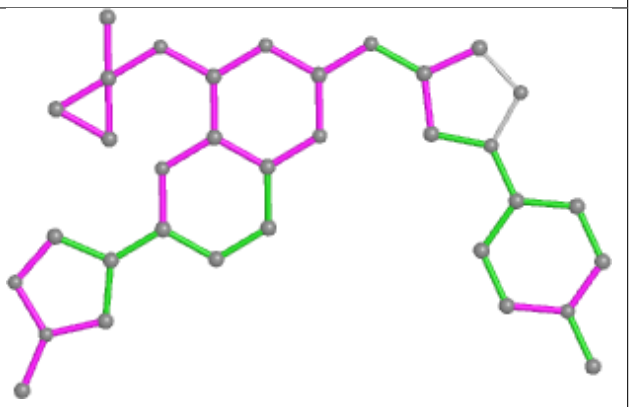


Rings

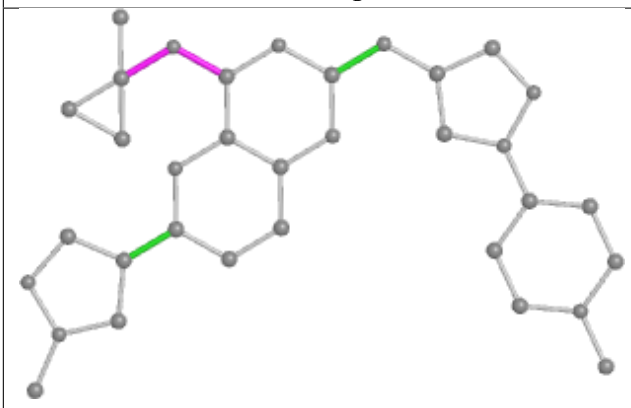
Ligand ND2 A 505



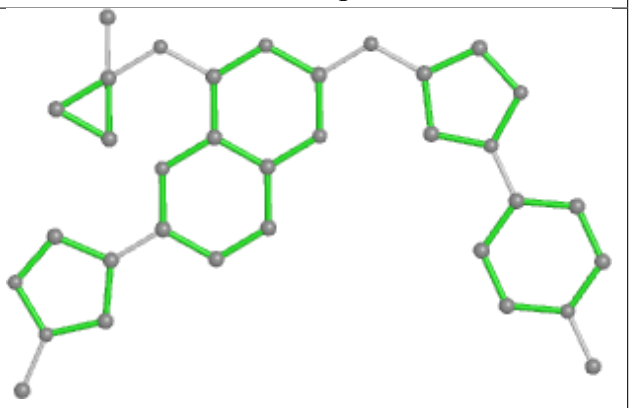
Bond lengths



Bond angles

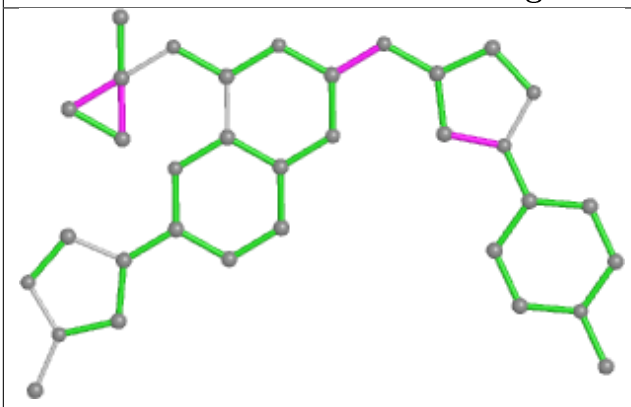


Torsions

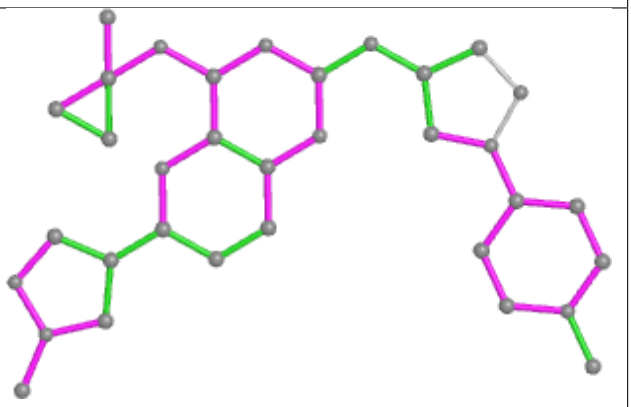


Rings

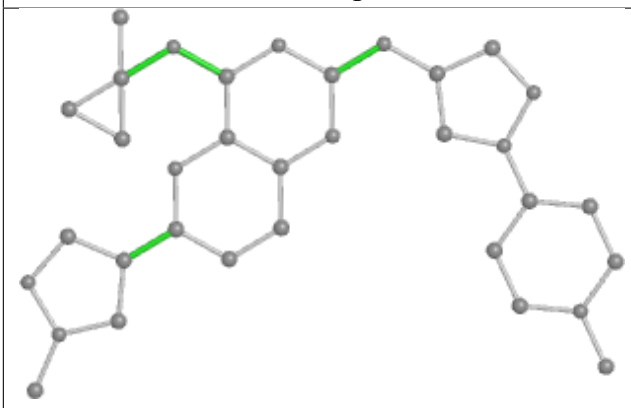
Ligand ND2 B 503



Bond lengths



Bond angles



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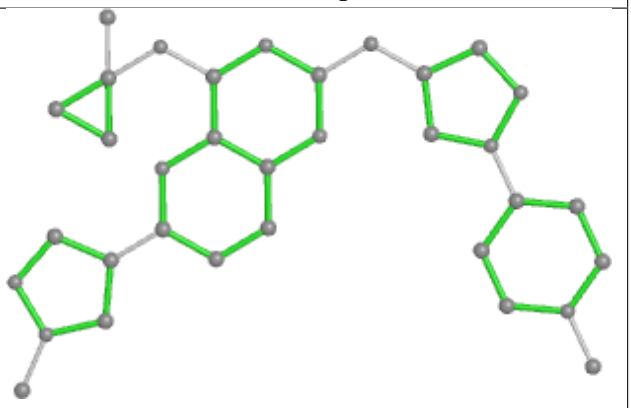
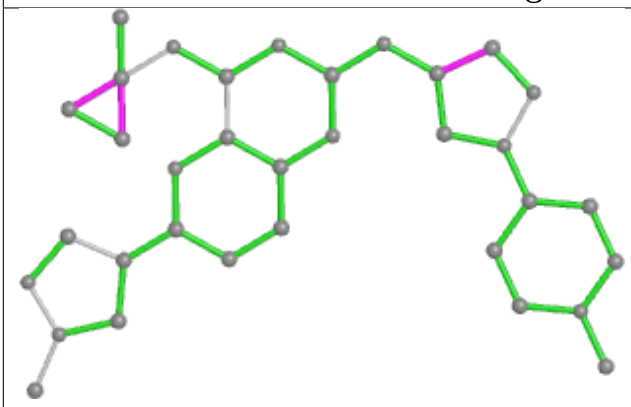
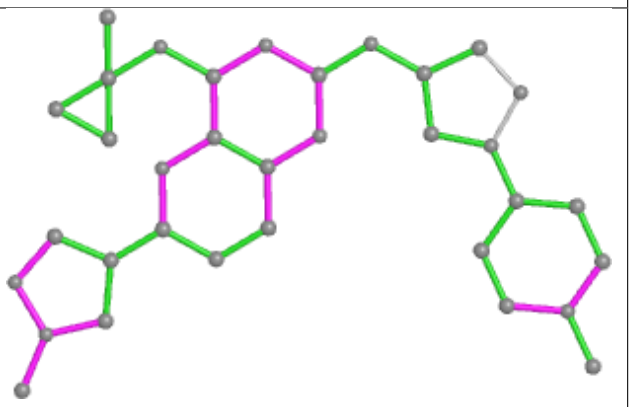


Rings

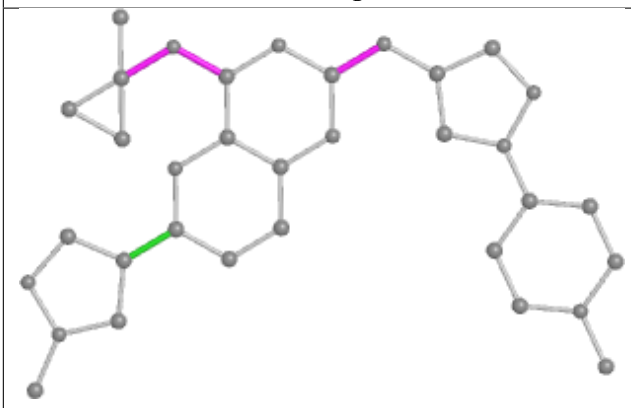
Ligand ND2 B 504



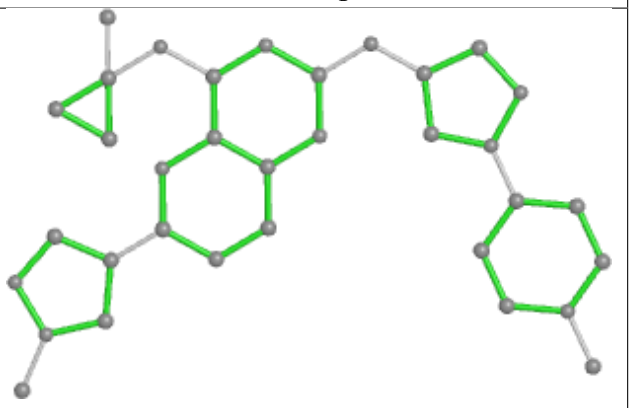
Bond lengths



Bond angles

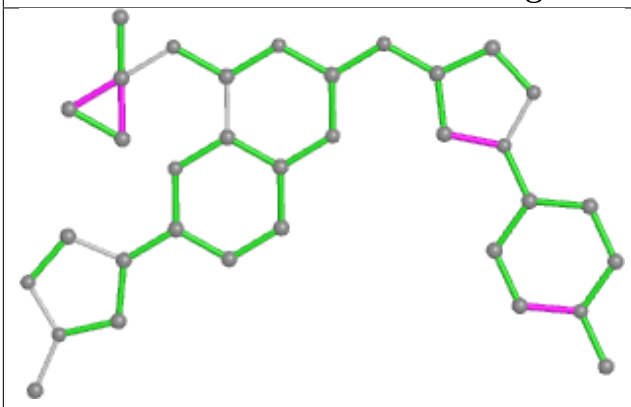


Torsions

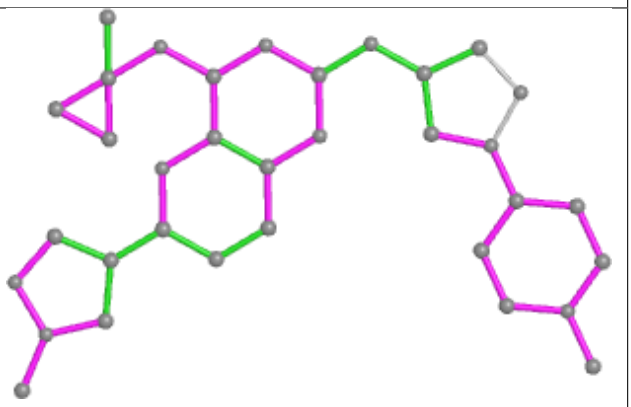


Rings

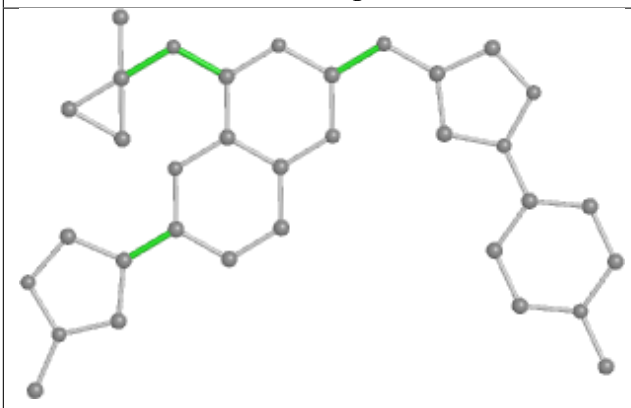
Ligand ND2 B 501



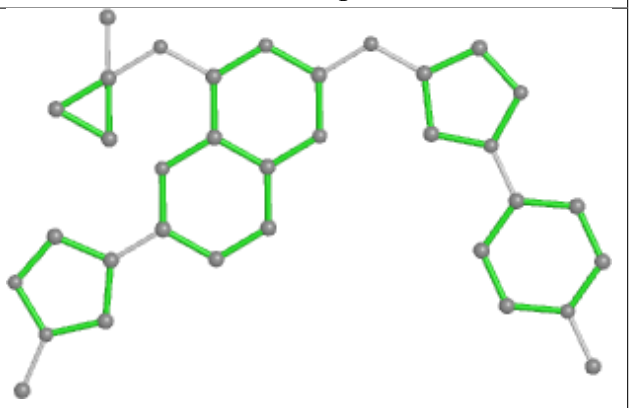
Bond lengths



Bond angles

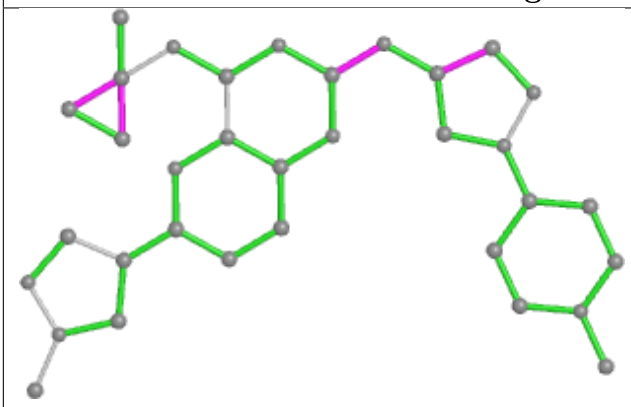


Torsions

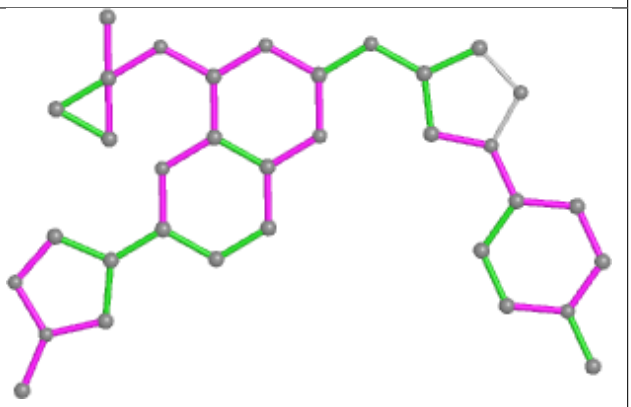


Rings

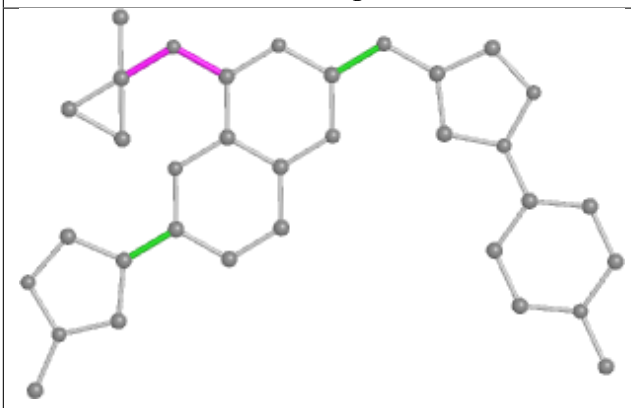
Ligand ND2 A 503



Bond lengths



Bond angles



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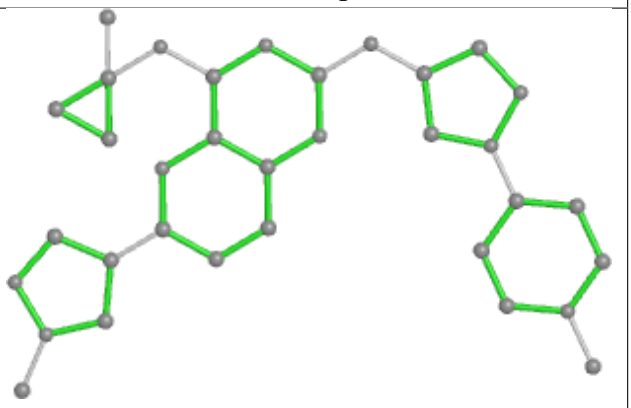
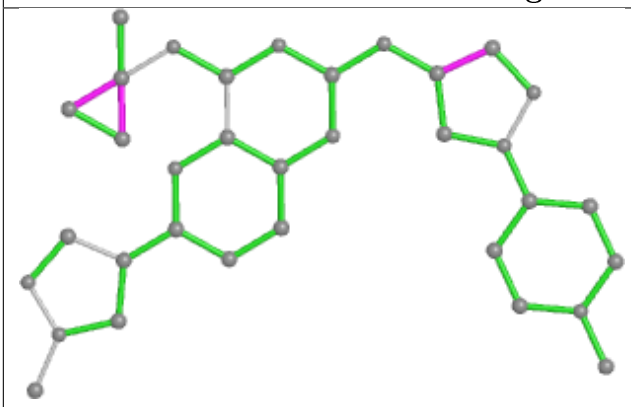
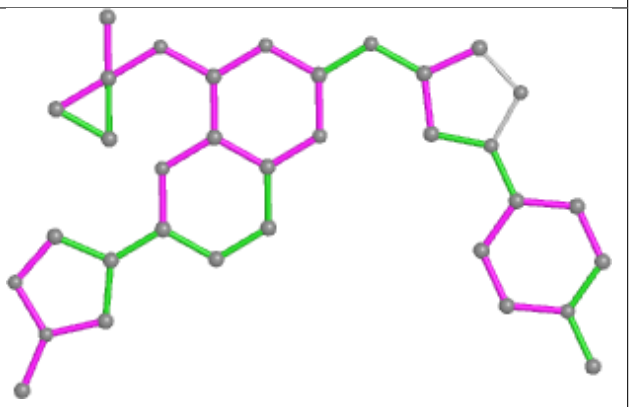


Rings

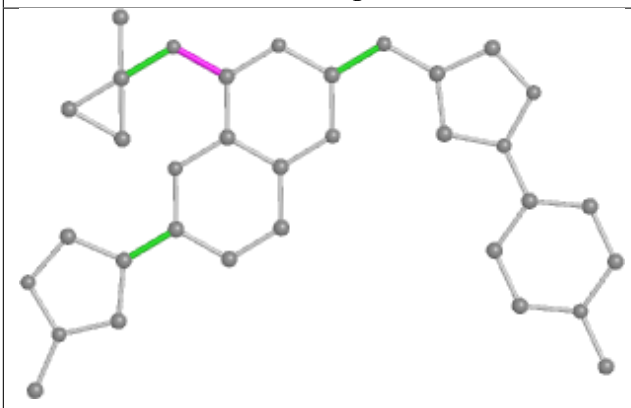
Ligand ND2 B 505



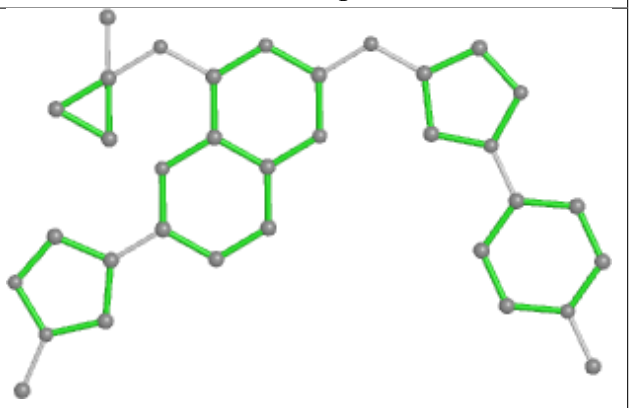
Bond lengths



Bond angles

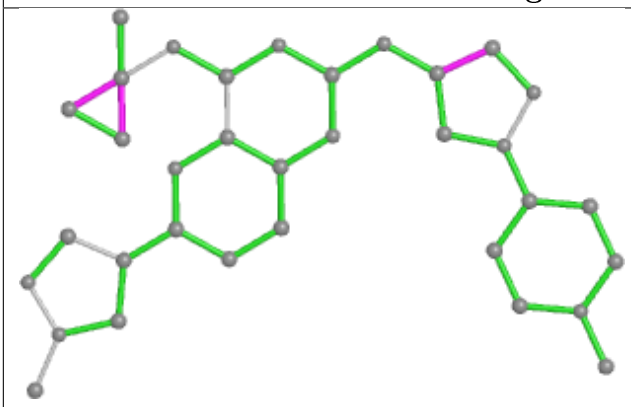


Torsions

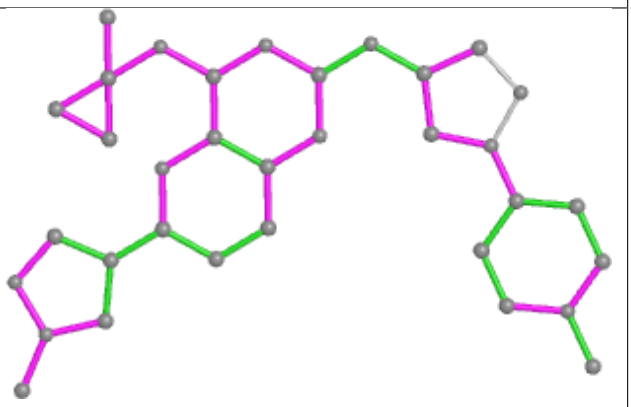


Rings

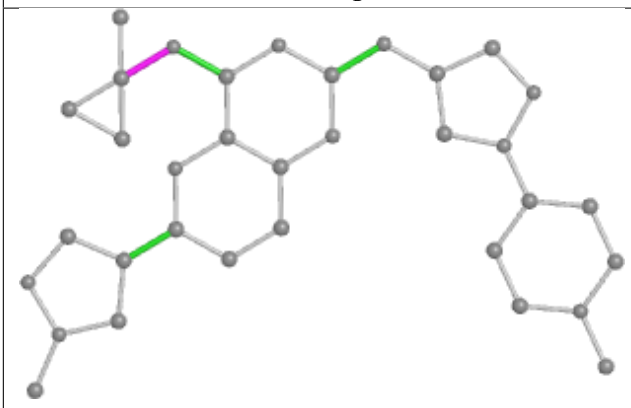
Ligand ND2 B 502



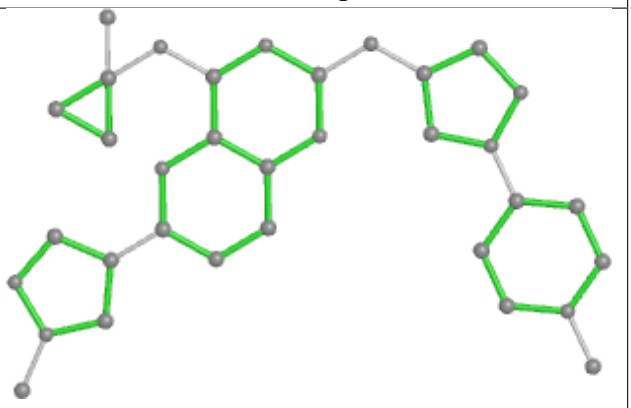
Bond lengths



Bond angles

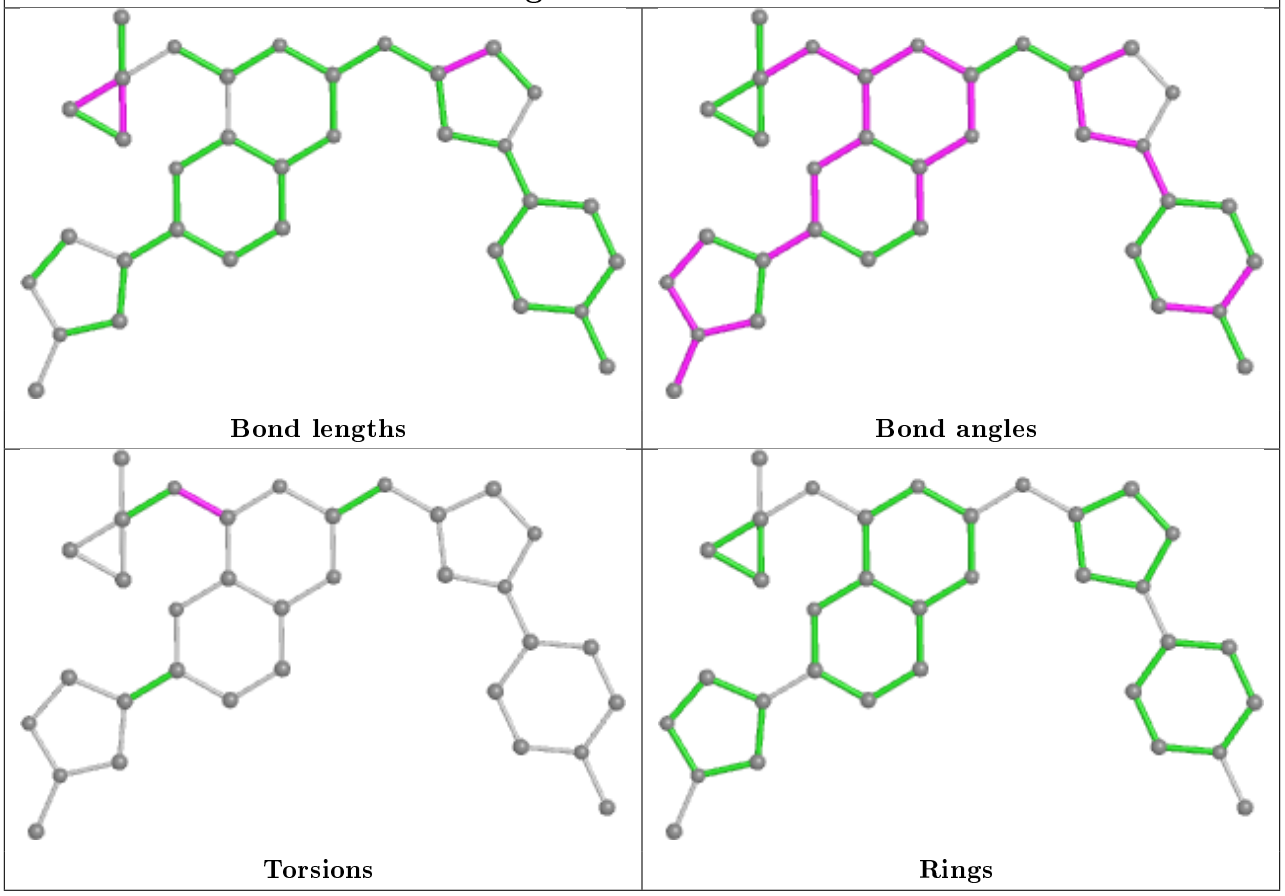


Torsions



Rings

Ligand ND2 A 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, 95^{th} 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	286/308 (92%)	0.70	26 (9%) 9 9	47, 78, 124, 144	0
1	B	285/308 (92%)	0.38	5 (1%) 68 71	36, 61, 97, 119	0
All	All	571/616 (92%)	0.54	31 (5%) 25 28	36, 70, 115, 144	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	GLY	6.0
1	A	171	TYR	5.9
1	A	336	SER	5.6
1	A	256	ASP	4.7
1	A	410	ILE	4.6
1	A	205	VAL	4.4
1	A	204	TYR	4.2
1	B	216	ALA	4.2
1	B	197	PHE	4.1
1	A	172	GLU	4.0
1	B	256	ASP	3.9
1	B	255	GLY	3.4
1	A	206	ASN	3.2
1	A	359	ALA	3.2
1	A	207	ASN	3.0
1	A	226	LEU	3.0
1	A	454	LEU	2.9
1	A	175	ASN	2.8
1	A	230	PHE	2.8
1	A	221	ILE	2.7
1	A	165	PHE	2.7
1	A	164	ARG	2.5
1	A	251	PHE	2.4
1	A	173	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	166	HIS	2.3
1	A	170	PHE	2.3
1	A	263	VAL	2.2
1	B	257	ASP	2.2
1	A	223	THR	2.2
1	A	249	LEU	2.2
1	A	366	PRO	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	SEP	B	346	10/11	0.83	0.14	87,93,102,102	0
1	SEP	A	346	10/11	0.86	0.14	94,100,108,108	0
1	TPO	A	345	11/12	0.91	0.16	86,92,95,96	0
1	TPO	B	345	11/12	0.95	0.16	79,83,86,86	0

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ND2	A	505	34/34	0.69	0.44	118,123,131,132	0
2	ND2	A	503	34/34	0.70	0.32	112,118,128,128	0
2	ND2	B	503	34/34	0.71	0.37	102,105,110,111	0
2	ND2	A	504	34/34	0.73	0.34	120,123,145,145	0
2	ND2	B	505	34/34	0.76	0.33	105,111,122,122	0
2	ND2	B	504	34/34	0.77	0.40	105,110,123,123	0
2	ND2	A	502	34/34	0.78	0.39	102,107,116,116	0

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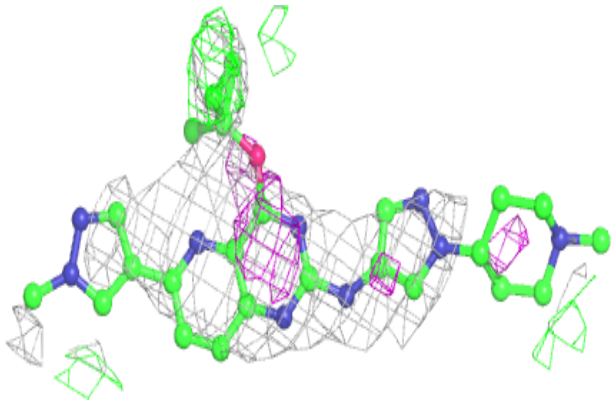
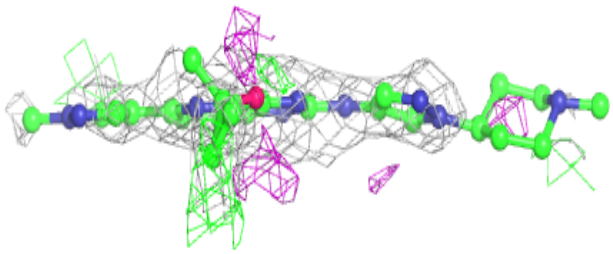
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ND2	B	502	34/34	0.86	0.22	84,92,97,98	0
2	ND2	A	501	34/34	0.92	0.18	64,72,76,77	0
2	ND2	B	501	34/34	0.96	0.18	37,44,65,65	0

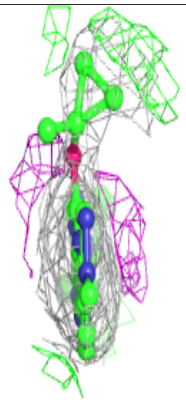
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ND2 A 505:

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

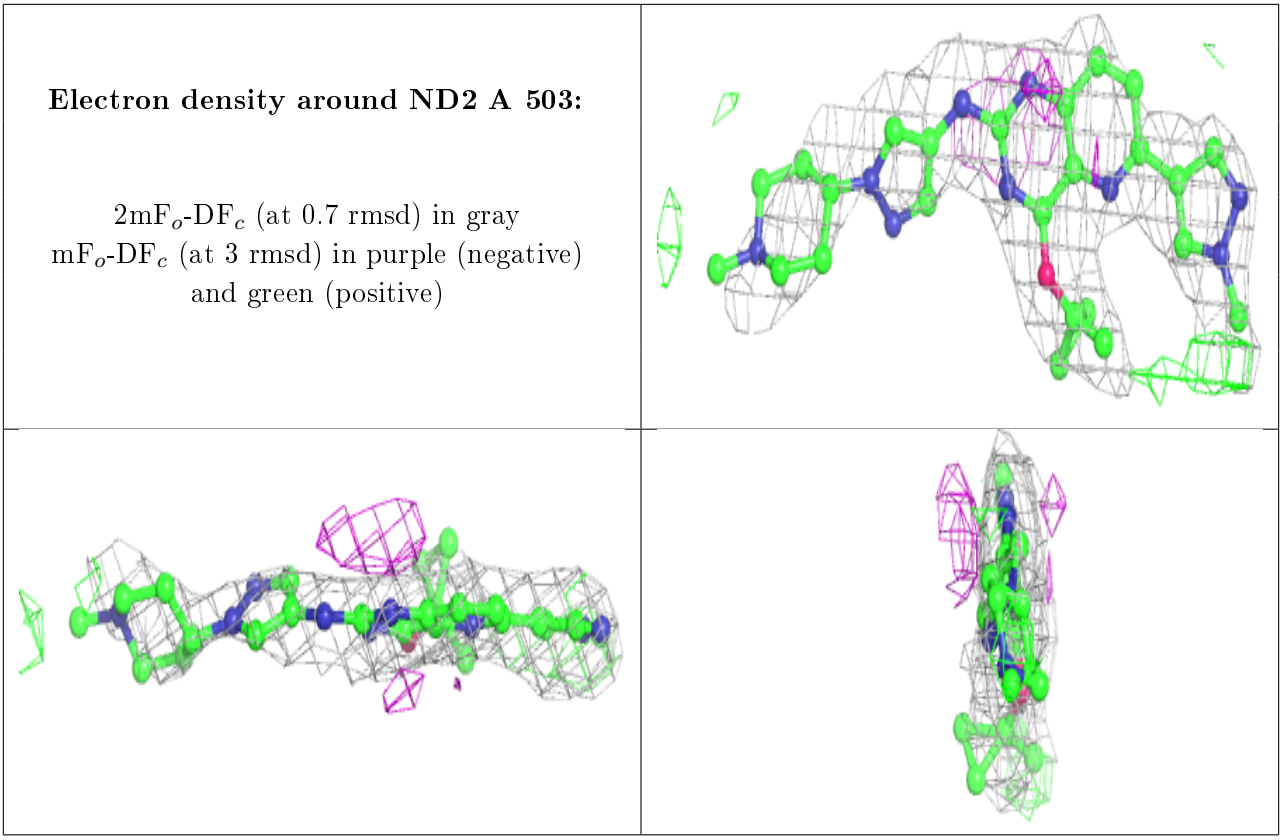






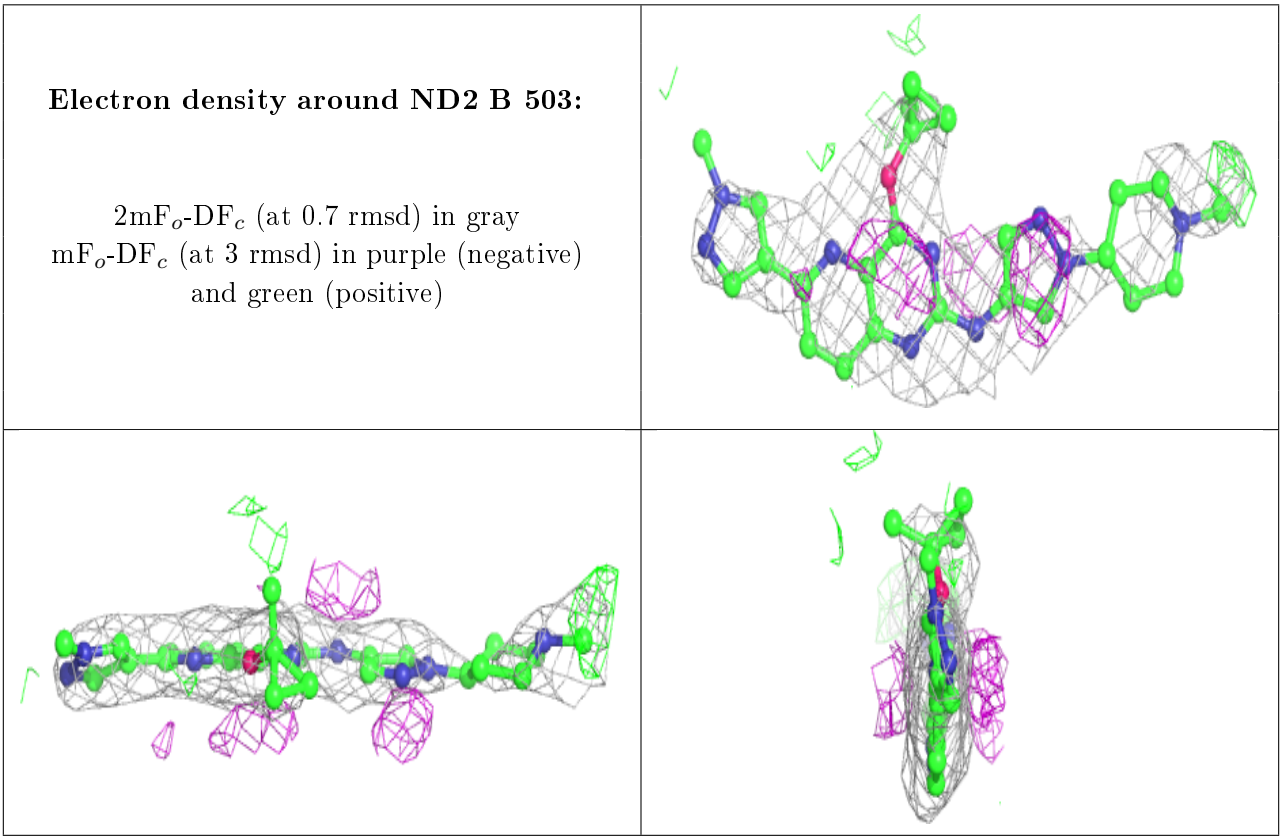
Electron density around ND2 A 503:

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



Electron density around ND2 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 ND2 A 504:

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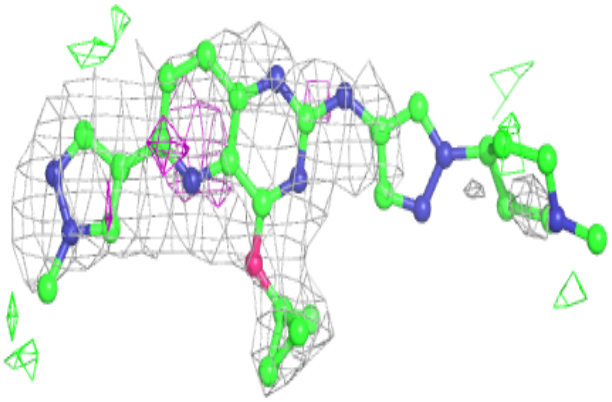
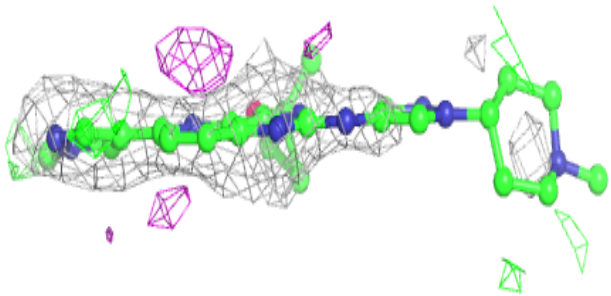
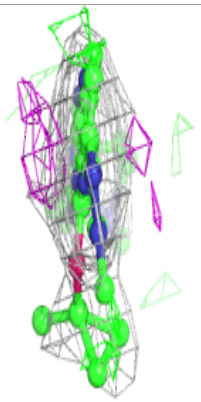
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







Electron density around ND2 B 505:

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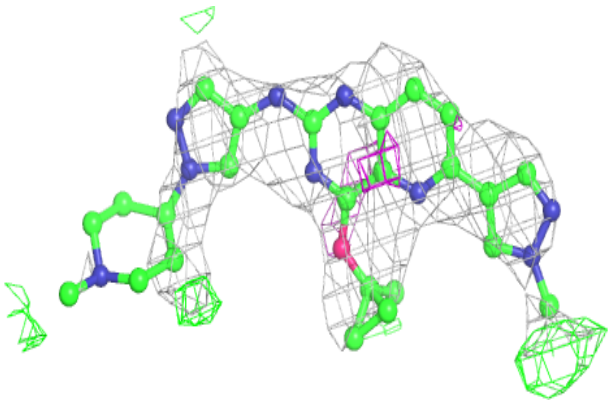
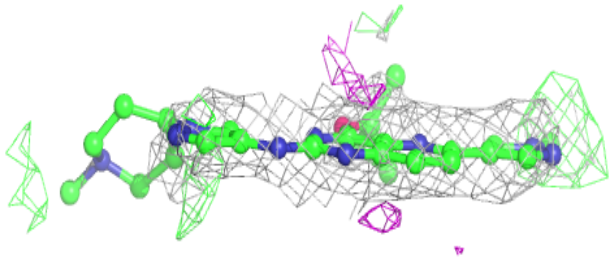
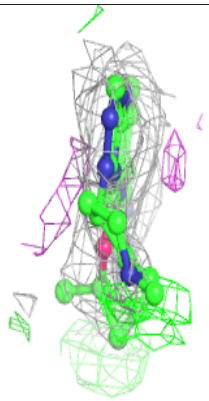
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

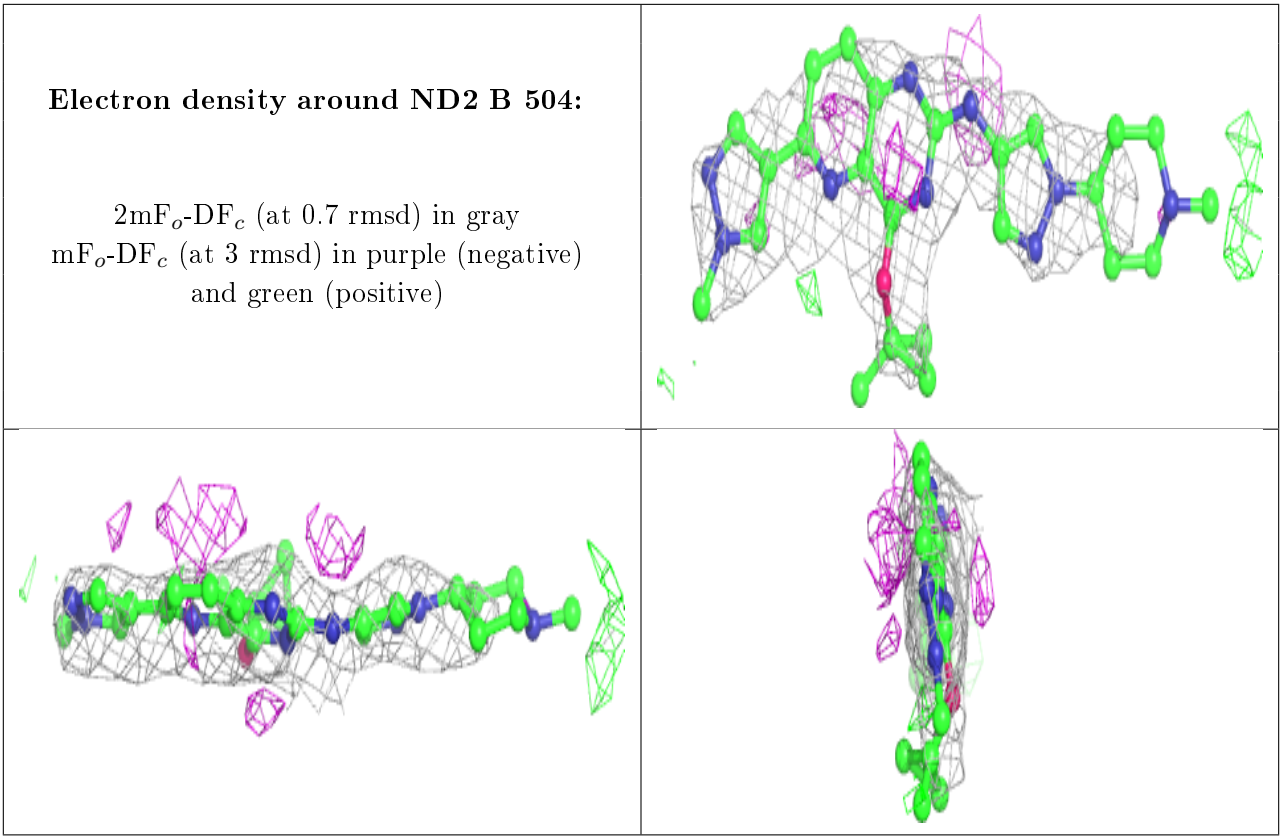






Electron density around ND2 B 504:

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



Electron density around ND2 A 502:

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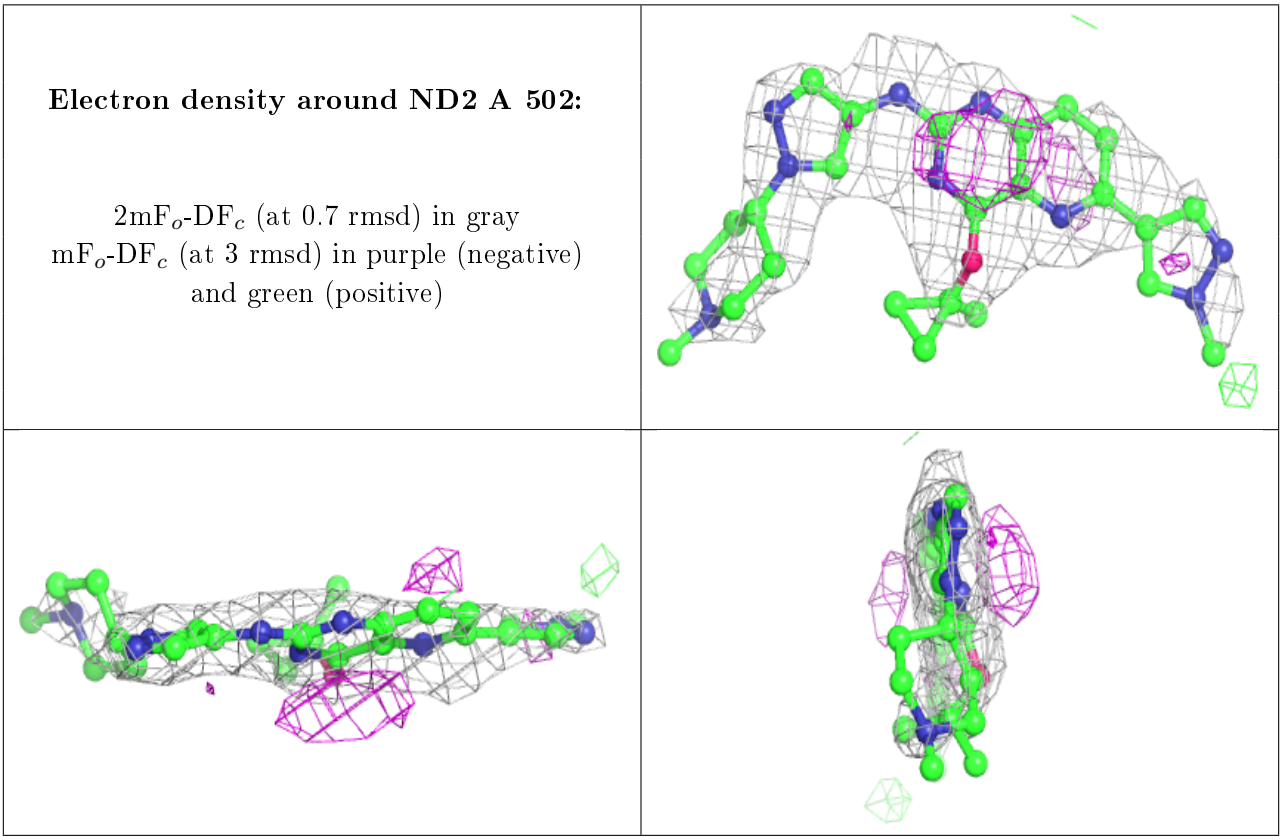
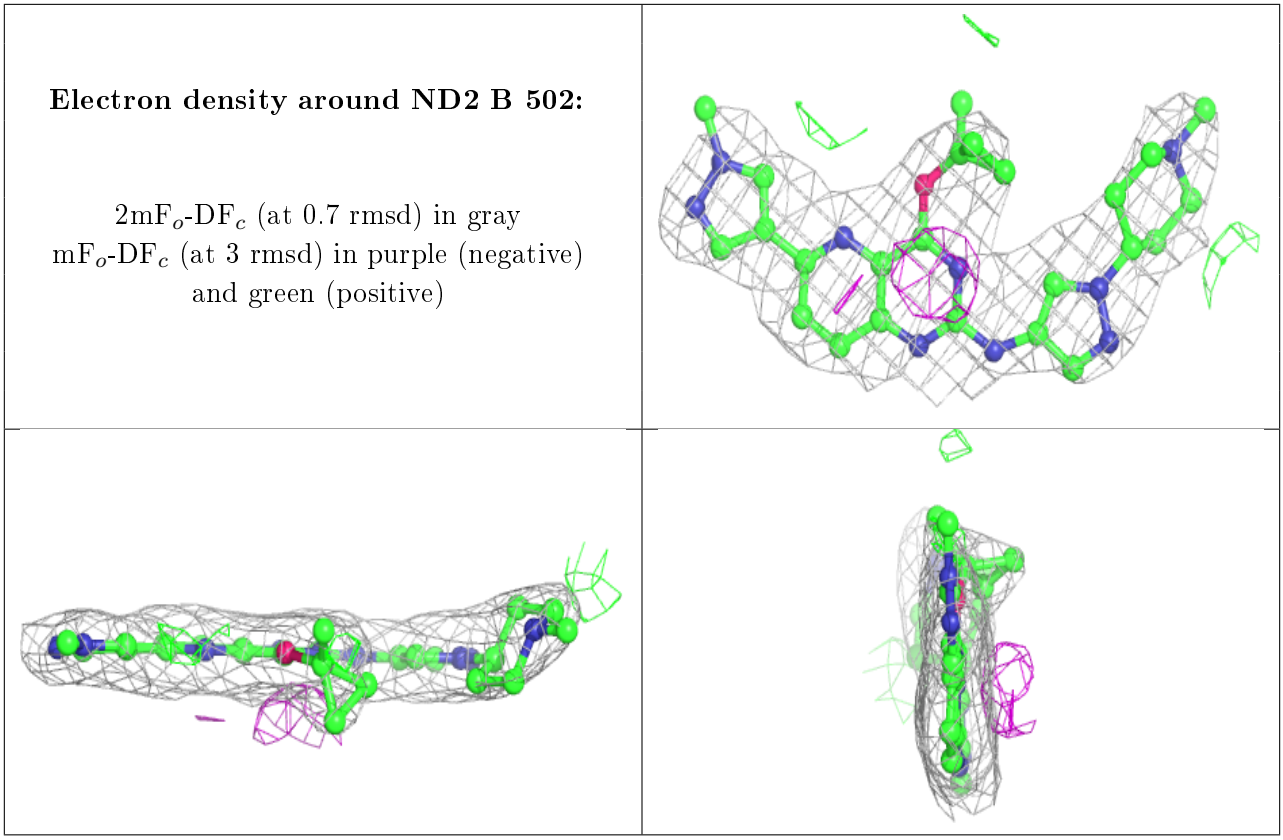
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ND2 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 ND2 A 501:

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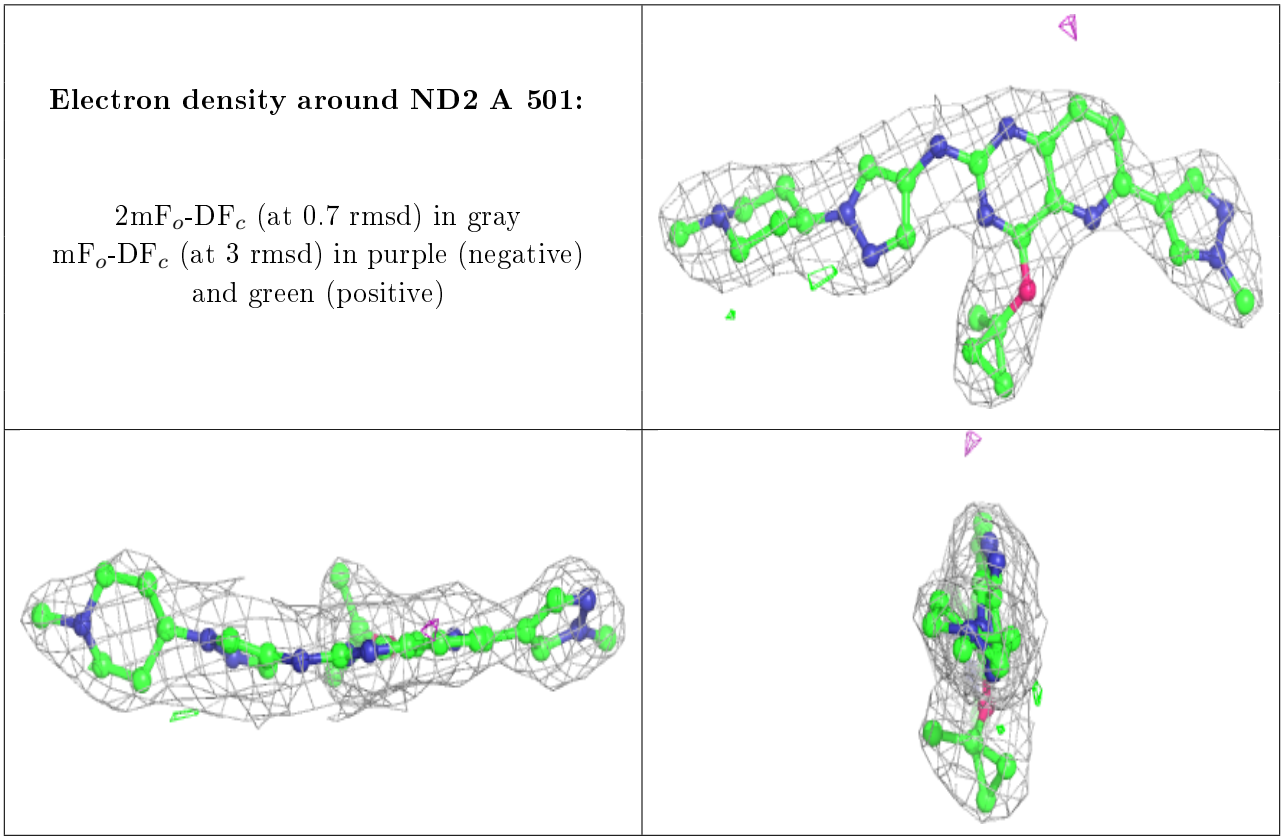
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ND2 B 501:

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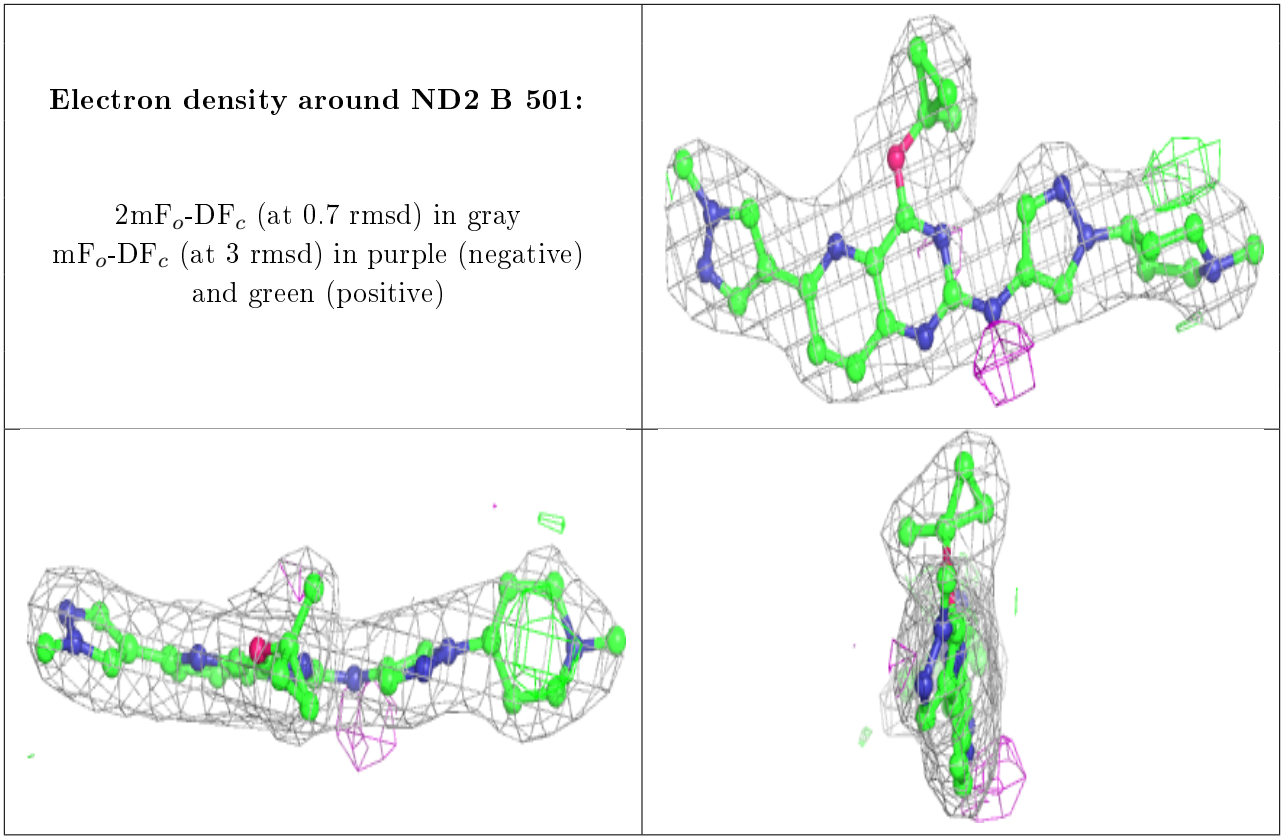
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.